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**Electronic Supplementary Information (ESI)**

# Role of Mutations in a Chemoenzymatic Enantiodivergent C($sp^3$)−H Insertion: Exploring the Mechanism and Origin of Stereoselectivity

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## 1. Computational Details

### 1.1. Quantum Mechanical (Density Functional Theory) calculations

All calculations were carried out with the DFT method implemented in the Gaussian16 program.[1] The (U)B3LYP functional along with SDD basis set with an effective core potential (ECP) for Fe and standard split valence Pople's basis set 6-31G** for all other atoms were used for gas-phase geometry optimizations.[2–7] (U)B3LYP with broken symmetry approach was used for open shell singlet (OSS) calculations.[8] The guess = (mix, read) keyword was used on a previously calculated triplet wavefunction to obtain an OSS orbital guess, followed by a full geometry optimization of the system from this guess. Various benchmark studies by Shaik demonstrated using (U)B327LYP functional for studying iron porphyrin carbenes. (U)B3LYP has also been extensively proven to perform accurately in the computational modeling of iron-oxo chemistry.[9,10] Harmonic analyses were performed at the same level of theory to verify all the stationary points as minima or first-order saddle points, as well as to obtain the thermodynamic contributions to energy, enthalpy, and free energy at 1atm and 298.15K.[11] Further, intrinsic reaction coordinate (IRC) calculations were carried out to ascertain the correctness of the TS.[12–15] For all stationary points, single-point calculations were performed to refine the energies further using a higher basis set, 6-311++G** along with the D3 version of Grimme's dispersion correction.[16] Single-point calculations also included the solvent effect to study the non-polar protein environment's effect. To include the effect of the reaction medium, single-point calculations also included the solvent effect using the polarization continuum model (PCM) with

diethyl ether (ε = 4.3) as solvent[17,18] was used employing the self-consistent reaction field (SCRF) method to have an estimation of the dielectric permittivity in the enzyme active site. The use of a dielectric constant ε=4.3 has been proven to be a good and general model to account for electronic polarization and small backbone fluctuations in enzyme active sites.[19,20] The zero-point energy (ZPE), thermal and entropic corrections obtained at 298.15K and 1atm pressure calculated in the gas phase at (U)B3LYP/6-31G**,SDD (Fe) level of theory were added to the "bottom-of-the-well" energies obtained from single point calculations at the $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3/6-311++G**,SDD (Fe) level of theory. The free energies reported in the text are at the $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3/6-311++G**,SDD(Fe)//(U)B3LYP/6-31G**,SDD(Fe) unless mentioned otherwise. Optimized DFT structures are illustrated with CYLView.[21]

**1.2. Benchmark Results**

To ensure that the performance of B3LYP is relatively reliable in the present system, we performed benchmark calculations of various DFT methods. Using the (U)B3LYP optimized structures, single-point energy calculations were performed using several hybrid functionals using the same basis sets (SDD for Fe and 6-311++G** for all other atoms). The hybrid functionals used in our benchmark calculations were (U)B3LYP-D3(BJ), (U)MN15, (U)TPSSh, (U)M06, and (U)PBEPBE. Single-point energy calculations were also performed using the standalone pure functional – (U)M06-L. The relative free energy values for the key stationary points using different methods are summarized in Table S1. The activation-free energies calculated using other methods were found to be roughly similar.

**Table S1** Relative free energies (ΔG) (single-point energies) at different DFT methods with optimized geometries at the (U)B3LYP/6-31G**,SDD(Fe) level (**B1**) for the truncated model system

| | ***Spin state*** | **A+S1** | **B'** | **B** | **TS(B-C)** | **C** | **TS(C-D)** | **D** | **TS(D-P)** |
|---|---|---|---|---|---|---|---|---|---|
| **PCM$_{(\varepsilon=4.3)}$/B3LYP-D3,6-311++G**, SDD(Fe)//B1** | *CSS* | 24.7 | 20.8 | - | 41.9 | 7.3 | 24.3 | - | - |
| | *OSS* | 20.8 | 16.6 | 24.3 | 27.9 | -2.8 | 15.3 | 1.1 | 14.2 |
| | *Triplet* | 16.5 | 12.5 | 23.7 | 27.0 | -1.4 | 17.2 | -2.9 | 7.8 |
| | *Quintet* | 0.0 | 10.4 | - | 38.3 | 7.3 | 23.7 | 3.4 | 5.2 |
| **PCM$_{(\varepsilon=4.3)}$/B3LYP-D3(BJ),6-311++G**, SDD(Fe)//B1** | *CSS* | 23.8 | 20.5 | - | 41.3 | 7.6 | 25.0 | - | - |
| | *OSS* | 20.0 | 20.0 | 23.9 | 50.8 | 11.3 | 16.1 | 2.6 | 14.6 |
| | *Triplet* | 15.5 | 11.7 | 23.2 | 26.8 | -0.8 | 18.1 | -1.5 | 7.2 |
| | *Quintet* | 0.0 | 6.1 | - | 28.6 | 8.3 | 25.2 | 5.3 | 5.7 |
| **PCM$_{(\varepsilon=4.3)}$/MN15,6-311++G**, SDD(Fe)//B1** | *CSS* | 42.0 | 39.9 | - | 56.4 | 24.3 | 43.3 | - | - |
| | *OSS* | 42.8 | -[a] | 27.4 | -[a] | 30.2 | 33.2 | 16.0 | 31.0 |
| | *Triplet* | 26.2 | 14.8 | 34.8 | 41.7 | 14.7 | 35.4 | 12.2 | 15.1 |
| | *Quintet* | 0.0 | 9.5 | - | 42.6 | 11.3 | 30.8 | 15.6 | 33.3 |
| **PCM$_{(\varepsilon=4.3)}$/TPSSh,6-311++G**, SDD(Fe)//B1** | *CSS* | 26.1 | 30.8 | - | 51.3 | 14.8 | 50.3 | - | - |
| | *OSS* | 21.2 | 30.4 | -[a] | -[a] | -[a] | 41.4 | 19.3 | 36.8 |
| | *Triplet* | 15.1 | 18.9 | 35.7 | 37.8 | 8.2 | 43.3 | 18.7 | 31.3 |
| | *Quintet* | 0.0 | 12.0 | - | 51.0 | 16.4 | 48.7 | 23.6 | 25.1 |
| | *CSS* | 47.9 | 47.0 | - | 61.3 | 31.7 | | - | - |
| | *OSS* | 47.4 | 47.2 | 48.1 | -[a] | -[a] | -[a] | 28.9 | 48.5 |

| | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|
| **PCM$_{(\varepsilon=4.3)}$/M06,6-311++G**, SDD(Fe)//B1** | *Triplet* | 22.7 | -[a] | 47.8 | 50.4 | 23.4 | 46.6 | 24.6 | 25.8 |
| | *Quintet* | 0.0 | 8.5 | - | 44.3 | 12.8 | 21.5 | 12.7 | 15.5 |
| **PCM$_{(\varepsilon=4.3)}$/PBEPBE,6-311++G**, SDD(Fe)//B1** | *CSS* | 8.7 | 12.4 | - | 30.2 | -4.5 | 25.2 | - | - |
| | *OSS* | 7.5 | -[a] | 24.4 | 26.4 | -2.3 | 23.5 | 8.1 | 19.5 |
| | *Triplet* | 2.3 | 5.0 | 23.9 | 25.2 | -3.9 | 27.5 | 6.8 | 16.9 |
| | *Quintet* | 0.0 | 10.5 | - | 42.8 | 9.1 | 37.8 | 18.9 | 23.3 |
| **PCM$_{(\varepsilon=4.3)}$/M06-L,6-311++G**, SDD(Fe)//B1** | *CSS* | 16.1 | 16.0 | - | 28.1 | -2.2 | 16.4 | - | - |
| | *OSS* | 16.6 | -[a] | 20.9 | 23.4 | -[a] | 15.3 | 2.2 | 14.0 |
| | *Triplet* | 8.8 | 7.6 | 20.5 | 22.3 | -5.0 | 19.0 | -1.9 | 7.7 |
| | *Quintet* | 0.0 | 0.0 | - | 33.7 | 1.5 | 20.4 | 4.6 | 11.0 |

-[a] We are unfortunate to get the single-point energies as they converged to CSS.
Relative free energies are given in kcal/mol.

In addition to the single-point energy calculations, geometry optimizations were carried out at the dispersion-corrected (U)B3LYP-D3(BJ) functional using SDD pseudopotential on Fe and 6-31G** for all other atoms. The energies were refined by carrying out single-point energy calculations by employing diethylether as a solvent, using the PCM solvation model, and at a higher basis set – 6-311++G** for all other atoms except Fe, for which SDD was used. The "guess=mix" keyword was used for optimizing open-shell singlet structures, and the stability of the wavefunctions was checked using the keyword "stable". Geometry optimizations were also performed using the (U)ωB97XD functional and the same basis sets for the lowest energy pathway. A comparison of the energetics of the truncated model system using different DFT methods is summarized in Table S2. The ground state electronic structure of the metallocarbene intermediate **C** and the enantiodetermining HAT TS (**TS(C-D)**) using different DFT methods are précised in

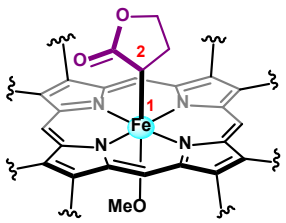
Tables S3 and S4, respectively, with a comparison of spin state energetics, Mulliken spin densities, and geometric parameters.

**Table S2** Relative free energies (ΔG) of the truncated model system at (i) $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3(B)),6-311++G**, SDD(Fe)//(U)B3LYP-D3(B)),6-31G**, SDD(Fe) (**B2'//B2**), (ii) $PCM_{(\varepsilon=4.3)}$/(U)ωB97XD, 6-311++G**,SDD(Fe)//(U)ωB97XD,6-31G**, SDD(Fe) (**B3'//B3**). For the **B3'//B3** level of theory, only the lowest-energy pathway was checked

| | ***Spin state*** | **A+S1** | **B'** | **B** | **TS(B-C)** | **C** | **TS(C-D)** | **D** | **TS(D-P)** |
|---|---|---|---|---|---|---|---|---|---|
| **B2'//B2** | *CSS* | 23.8 | 22.6 | - | 41.8 | 7.4 | 24.3 | - | - |
| | *OSS* | 22.9 | 21.9 | 25.9 | 27.1 | -2.2 | 15.0 | | -[n.d.] |
| | *Triplet* | 15.5 | 12.5 | 25.3 | 26.9 | -0.8 | 16.8 | -2.7 | 9.6 |
| | *Quintet* | 0.0 | -4.1 | - | 37.1 | 8.4 | 24.0 | 3.9 | -[a] |
| **B3'//B3** | *CSS* | -[n.d.] | -[n.d.] | - | -[n.d.] | -[n.d.] | 28.7 | - | - |
| | *OSS* | -[n.d.] | -[n.d.] | -[n.d.] | -[n.d.] | 31.9 | 28.1[b] | -[n.d.] | -[n.d.] |
| | *Triplet* | -[n.d.] | -[n.d.] | 27.9 | 47.3 | 2.0 | 19.6 | 0.1 | -[a] |
| | *Quintet* | 0.0 | 23.2 | - | -[n.d.] | 31.9 | -[n.d.] | -[n.d.] | -[n.d.] |

-[a] We are unfortunate to get the TS. -[b]Several attempts to optimize TS(C-D) always converged to concerted hydride transfer **TS(C-P)**. -[n.d.] The high-energy stationary points were not determined. Relative free energies are given in kcal/mol.

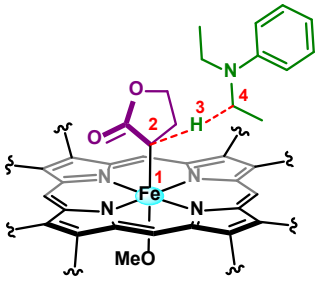
**Table S3** Spin state energetics, key geometric parameters, and Mulliken spin densities of the metallocarbene intermediate **C** at different DFT optimization levels[a]




| | *Spin state* | Singlet-triplet gap ($DE_{ST}$) | Geometric parameters Fe1-C2 | Spin densities Fe1 | Spin densities C2 |
|---|---|---|---|---|---|
| **B1'//B1** | *OSS* | 2.3 | 1.97 | 0.976 | -0.831 |
| | *Triplet* | | 2.00 | 0.993 | 0.719 |
| **B2'//B2** | *OSS* | 2.3 | 1.81 | -0.002 | 0.002 |
| | *Triplet* | | 1.97 | 0.998 | 0.720 |
| **B3'//B3** | *OSS* | -30.1 | 2.00 | 0.989 | 0.741 |
| | *Triplet* | | 1.99 | 0.942 | 0.785 |
| **B4'//B4**[a] | *OSS* | 2.2 | 1.94 | 1.079 | -0.858 |
| | *Triplet* | | 1.95 | 1.177 | 0.623 |

[a]**B1'//B1**: $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3,6-311++G**, SDD(Fe)//(U)B3LYP,6-31G**, SDD(Fe); **B2'//B2**: $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3(B)),6-311++G**, SDD(Fe)//(U)B3LYP-D3(B)),6-31G**, SDD(Fe); **B3'//B3**: $PCM_{(\varepsilon=4.3)}$/(U)ωB97XD, 6-311++G**,SDD(Fe)//(U)ωB97XD,6-31G**, SDD(Fe); **B4'//B4**: $PCM_{(\varepsilon=4.3)}$/(U)M06, 6-311++G**, SDD(Fe)//(U)M06,6-31G**, SDD(Fe). Relative energies are given in kcal/mol.

**Table S4** Spin state energetics, key geometric parameters, and Mulliken spin densities of the enantiodetermining HAT TS **TS(C-D)** at different DFT optimization levels[a]




| Method | *Spin state* | Singlet-triplet gap | Geometric parameters | | | Spin densities | | |
|---|---|---|---|---|---|---|---|---|
| | | ($DE_{ST}$) | Fe1-C2 | C2-H3 | H3-C4 | Fe1 | C2 | C4 |
| **B1'//B1** | *OSS* | 3.0 | 2.10 | 1.36 | 1.40 | 1.000 | -0.512 | -0.312 |
| | *Triplet* | | 2.16 | 1.39 | 1.38 | 0.969 | 0.445 | 0.333 |
| **B2'//B2** | *OSS* | 3.0 | 2.05 | 1.36 | 1.38 | -0.972 | 0.384 | 0.414 |
| | *Triplet* | | 2.11 | 1.39 | 1.37 | 0.975 | 0.441 | 0.335 |
| **B3'//B3** | *OSS* | -7.8 | 2.06 | 1.25 | 1.36 | -[na] | -[na] | -[na] |
| | *Triplet* | | 2.10 | 1.37 | 1.36 | 1.142 | 0.478 | 0.444 |
| **B4'//B4**[a] | *OSS* | 2.1 | 2.05 | 1.35 | 1.40 | 1.155 | -0.523 | -0.436 |
| | *Triplet* | | 2.08 | 1.38 | 1.39 | 1.090 | 0.422 | 0.334 |

[a]**B1'//B1**: $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3,6-311++G**, SDD(Fe)//(U)B3LYP,6-31G**, SDD(Fe); **B2'//B2**: $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3(B)),6-311++G**, SDD(Fe)//(U)B3LYP-D3(B)),6-31G**, SDD(Fe); **B3'//B3**: $PCM_{(\varepsilon=4.3)}$/(U)ωB97XD, 6-311++G**,SDD(Fe)//(U)ωB97XD,6-31G**, SDD(Fe); **B4'//B4**: $PCM_{(\varepsilon=4.3)}$/(U)M06, 6-311++G**, SDD(Fe)//(U)M06,6-31G**, SDD(Fe). Relative energies are given in kcal/mol.

**Table S5** Relative free energies (ΔG) for the C–H insertion step at different spin states using different DFT levels[a]

| | B1'//B1 | B2'//B2 | B3'//B3 |
|---|---|---|---|
| **$^{3}$D** | 0.0 | **0.0** | **0.0** |
| **$^{6}$TS(D-E)** | 0.4 | 2.1 | -2.7 |
| **$^{4}$TS(D-E)** | 4.5 | 4.0 | -[n.d.] |
| **$^{2}$TS(D-E)** | _[b] | _[b] | _[b] |
| **$^{3}$E** | 2.2 | 3.4 | 0.5 |
| **$^{OSS}$E** | -[c] | -[c] | -[c] |
| **$^{3}$TS(E-P)** | 36.9 | 38.7 | 3.8 |
| **$^{OSS}$TS(E-P)** | -[a] | -[a] | -[a] |

[a]**B1'//B1**: PCM$_{(\varepsilon=4.3)}$/(U)B3LYP-D3,6-311++G**, SDD(Fe)//(U)B3LYP,6-31G**, SDD(Fe); **B2'//B2**: PCM$_{(\varepsilon=4.3)}$/(U)B3LYP-D3(B)),6-311++G**, SDD(Fe)//(U)B3LYP-D3(B)),6-31G**, SDD(Fe); **B3'//B3**: PCM$_{(\varepsilon=4.3)}$/(U)ωB97XD, 6-311++G**,SDD(Fe)//(U)ωB97XD,6-31G**, SDD(Fe); **B4'//B4**: PCM$_{(\varepsilon=4.3)}$/(U)M06, 6-311++G**, SDD(Fe)//(U)M06,6-31G**, SDD(Fe).
[b]We are unfortunate to get the TS. [c]Various methods to optimize the intermediate always resulted in P. Relative energies and free energies are given in kcal/mol.

### 1.3. Molecular Dynamics (MD) simulations

Molecular Dynamics simulations were performed using the GPU code (*pmemd*) of the Amber18 package.[22] Parameters for the heme unit were generated within the antechamber and MCPB.py[23] modules in the Amber18 package and the general AMBER forcefield (*gaff*)[24] with partial charges set to fit the electrostatic potential generated at the B3LYP/6-31G** level by the RESP model.[25] The charges were calculated according to the Merz–Singh–Kollman scheme[26,27] using the Gaussian 16 package. Protonation states of the enzyme residues were determined using the H++ server.[28] Each protein was immersed in a pre-equilibrated truncated cuboid box with a 10 Å buffer of TIP3P[29] water molecules using the *leap* module. The systems were neutralized by adding explicit counter ions (Na+ and Cl−). The Amber ff14SB force field[30] was subsequently used in all the MD simulations. After the initial equilibration, a 100ns MD simulation was performed

using an isothermal-isobaric ensemble *(NPT)*. A minimization run was performed for 500,000 cycles. The systems were gently heated from 0 to 300 K for 100ps each step under constant-volume and periodic-boundary conditions. Langevin thermostat was used for temperature control. Water molecules were treated with the SHAKE algorithm. Long-range electrostatic effects were modeled using the particle mesh-Ewald method.[31] An 8Å cut-off was applied to Lennard–Jones and electrostatic interactions. Production trajectories were then run for an additional 100ns under the same simulation conditions. Trajectories were processed and analyzed using the *cpptraj* module from AmberTools utilities. The highly available and related PDB structure (P411-**E10** enzyme variant) was used as the initiation point to prepare two variants, P411-**L9** and P411-**L10,** which Arnold and coworkers have hitherto reported. Seven amino acids, namely: A87, A264, E267, A332, T327, V328, and Q437, were mutated using the mutagenesis tool from Chimera.[32] Classical MD simulations were then performed on the mutated enzyme along with the two key mutants, **L9** (V328L) and **L10** (V328R). A total of five independent replicas of 100 ns each were carried out, starting from different starting velocities, accumulating a total of 500 ns for each **L9** and **L10**. The conformations visited by the enzymes during all this simulation time were clustered based on the protein backbone RMSD. From the RMSD plots we do not see any significant changes in the conformation and structure (Fig. S1).

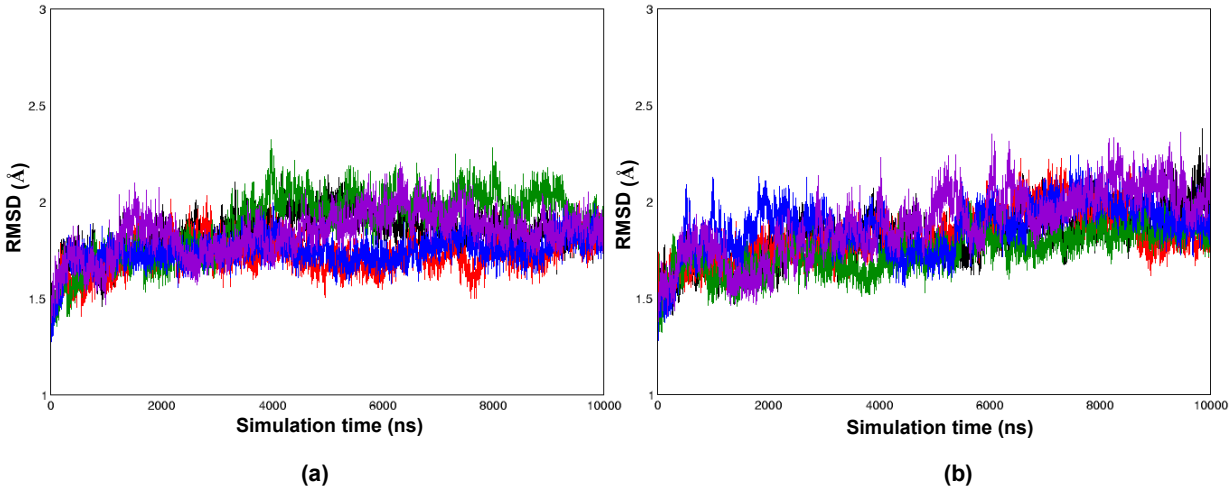



**Fig. S1** Replicas of 100 ns MD simulation trajectories of **L9** (a) and **L10** (b).

### 1.4. Quantum Mechanical (QM) Cluster calculations

QM cluster approaches are being widely used to study metalloenzyme-catalyzed reactions. In the QM cluster, a small but well-chosen part (the active site surrounding regions) is cut out to explore the properties and reaction mechanisms. The steric influence the enzyme imposes on the active site is modeled by a "coordinate locking scheme", i.e., the C(α) atoms of selected residues are frozen at their crystallographic positions. The residues are typically truncated at C(α), and the truncated bonds are saturated by hydrogens. In our study, this resulted in a few imaginary frequencies below -70cm$^{-1,}$ which does not affect the ZPE. It should be noted that we only add the ZPE and thermal corrections to the electronic energy for the QM cluster approach since entropy calculations with frozen atoms are unreliable. The resulting low-energy stationary points were evaluated by DFT. The (U)B3LYP functional along with SDD basis set with an ECP for Fe and 6-31G** for all other atoms. The total electronic energies reported in the text are at the PCM$_{(\varepsilon=4.3)}$/(U)B3LYP-D3/6-311++G**,SDD(Fe)//(U)B3LYP/6-31G**,SDD(Fe) unless mentioned otherwise. Optimized DFT structures are illustrated with CYLView software.

### 1.5. Geometry, Frequency, Noncovalent, extended Tight Binding (GFN-xTB)

We performed the initial conformational screening and optimizations using the GFN-xTB tight binding approach.[33] Gaussian supports the "external" keyword, which invokes third-part computational code to yield energy and its derivatives needed by Gaussian. The package “xtb.sh” was invoked by Gaussian16 to perform the optimizations and frequency.[34] The script “xtb.sh” invokes two executable files "extderi" and "genxyz".

## 2. Interconversion between (*1R*) and (*1S*) radicals

A PES (potential energy scan) was performed by rotating about the dihedral defined by $N_1$-$Fe_2$-$C_3$-$C_4$ ( Fig. S2). This PES describes the interconversion between (*1R*) and (*1S*) radicals with the interconversion barrier represented by the maxima along the PES (6.7 kcal/mol).

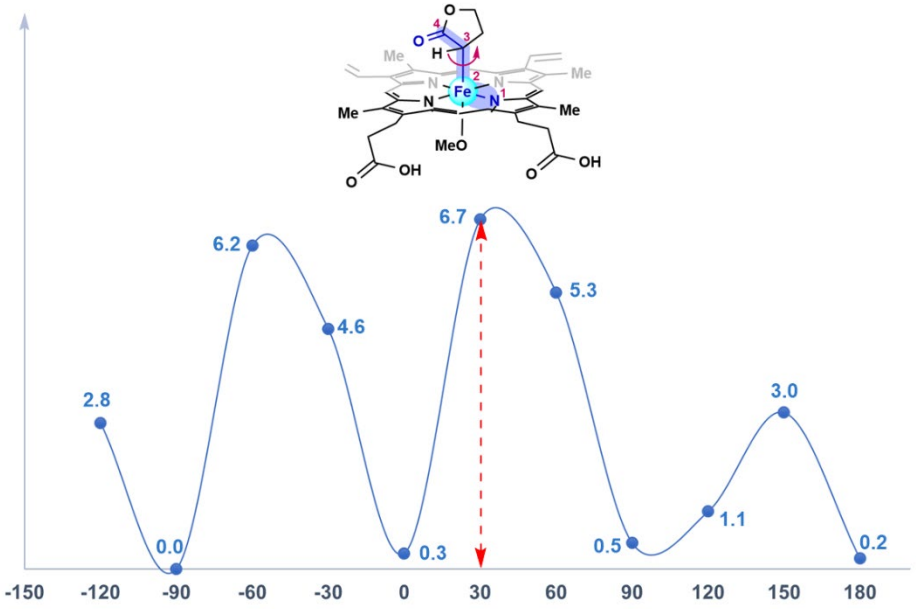


**Fig. S2** PES scan along the $N_1$-$Fe_2$-$C_3$-$C_4$ dihedral in the lowest-energy triplet state. The vertical axis corresponds to relative free energies in kcal/mol, and the horizontal axis defines the dihedral angles in degrees.

### 3. Modeling QM Cluster 1

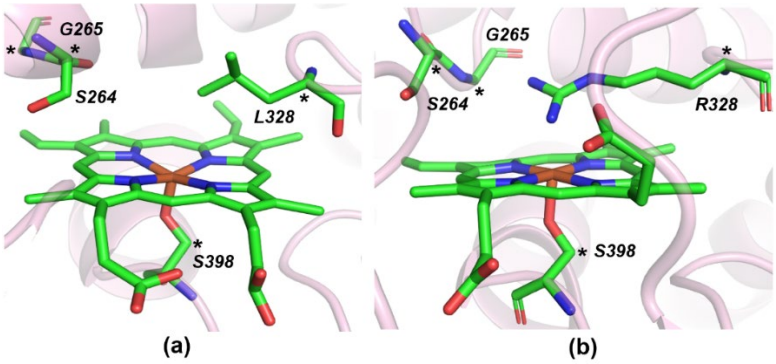
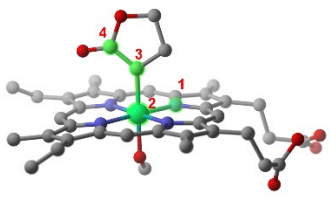



**Fig. S3** Residues chosen for modeling QM cluster-1 for (a) **L9** and (b) **L10** (the asterisks denote the C(α) atoms fixed during the subsequent optimizations). The H atoms are not shown for clarity.

### 3.1. Conformational Sampling using GFN-xTB

Sampling on $\mathbf{C^{L9}}$ (Table S5) reveals that the low-energy conformations allow H-bonding interaction between the ester group of LAC and the side chain of S264.

**Table S6** Conformational sampling of $\mathbf{C^{L9}}$ and $\mathbf{C^{L10}}$ performed by rotating about the highlighted dihedral. The dihedral angles are in degrees, and energies are in kcal/mol[a]



| Conformation | Initial | $C^{L9}$ | | $C^{L10}$ | |
|---|---|---|---|---|---|
| | | Optimized | ΔE | Optimized | ΔE |
| | 1-2-3-4 | 1-2-3-4 | | 1-2-3-4 | |
| **Conf1** | -180 | **-148.6** | **0.5** | 137.1 | 22.6 |
| **Conf2** | -135 | -144.0 | 2.1 | 142.2 | 24.3 |
| **Conf3** | -90 | **-144.7** | **0.0** | **-84.9** | **0.0** |
| **Conf4** | -45 | **-132.6** | **1.4** | **-84.9** | **0.0** |
| **Conf5** | 0 | **-142.5** | **0.2** | -54.7 | 3.2 |
| **Conf6** | 45 | 57.5 | 9.5 | -49.6 | 8.3 |
| **Conf7** | 90 | 68.2 | 9.2 | -50.8 | 7.7 |
| **Conf8** | 135 | -158.0 | 3.1 | -26.9 | 11.9 |
| **Conf9** | 180 | **-148.5** | **0.5** | 137.1 | 22.6 |

[a]other residues are not shown for clarity. The lowest energy conformations (within 2kcal/mol) are shown in bold.

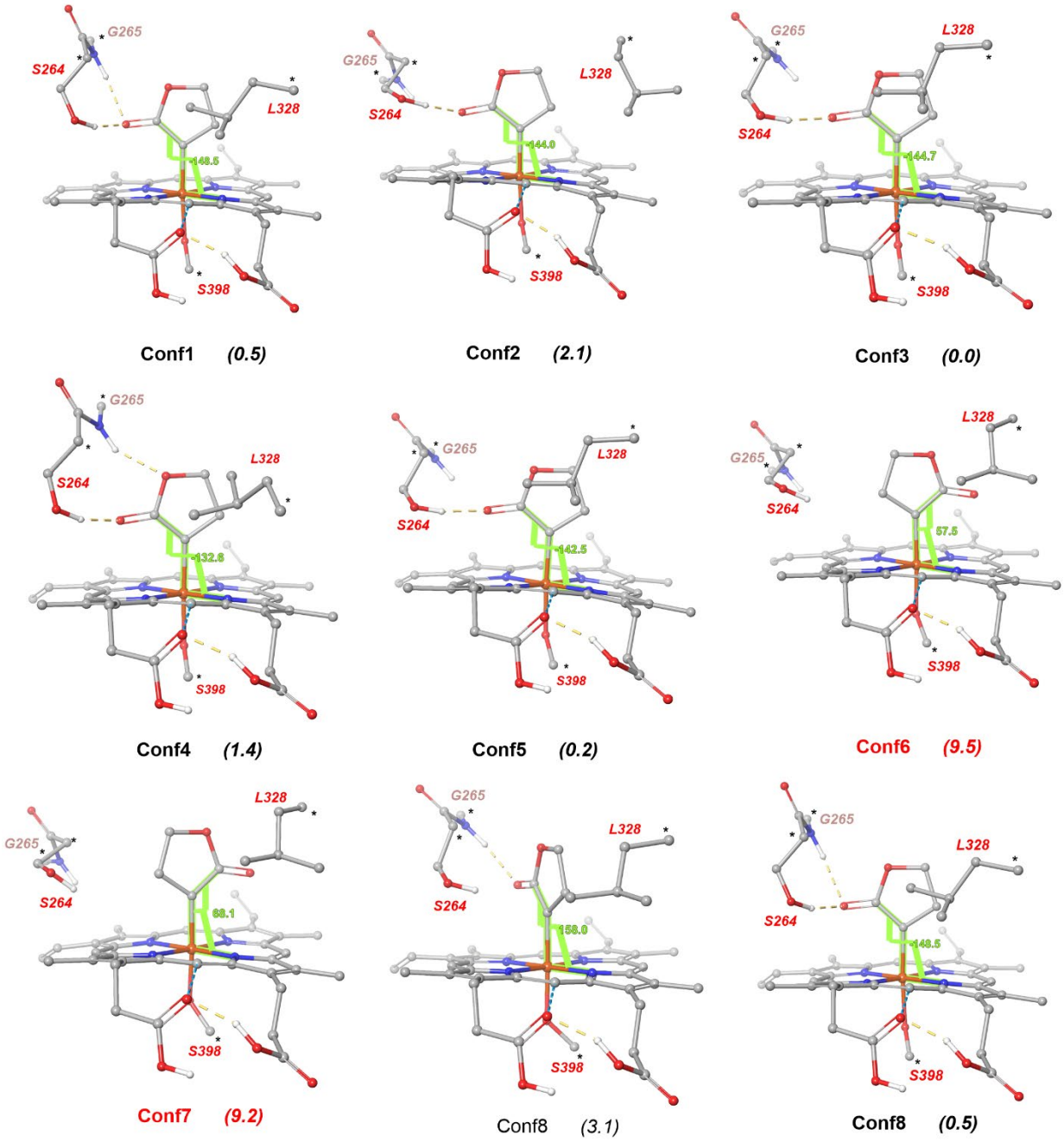



**Fig. S4** Conformational sampling of $\mathbf{C^{L9}}$ performed by rotating about the highlighted dihedral. The low-energy conformations (within 2 kcal/mol) are shown in bold, and the high-energy ones in red. The H-bonding interactions have been demonstrated with dashed orange lines. The energies are given in kcal/mol and dihedrals in degrees. The non-polar H atoms are not shown for clarity.

An overlay of all nine conformations of $\mathbf{C}^{\mathbf{L9}}$ reveals that the active site almost always reshapes itself to allow for H-bond to form between the LAC and the side chain of S264 ( Fig. S5).

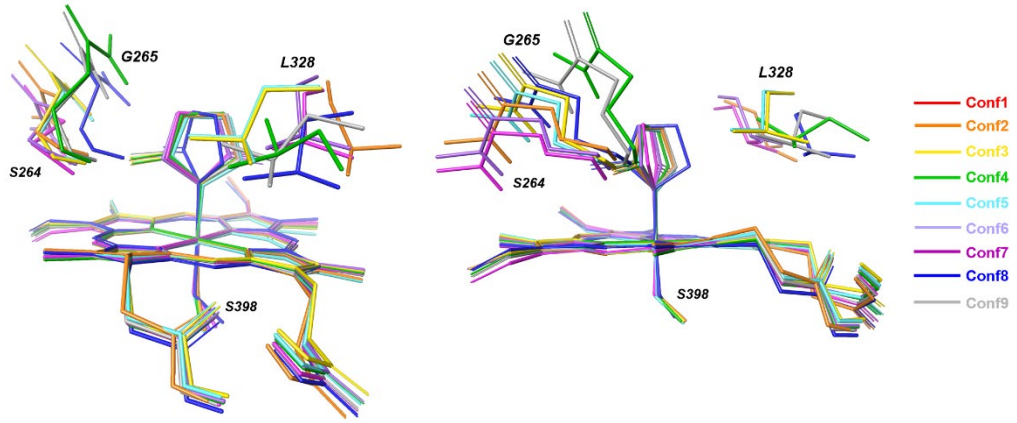



**Fig. S5** Overlayed images of the nine conformations of $\mathbf{C}^{\mathbf{L9}}$ obtained by performing a dihedral scan using xtb. The first panel corresponds to the front view (propionate groups facing the reader), and the next corresponds to the side view. The non-polar H atoms are omitted for clarity.

On the contrary, sampling on $\mathbf{C}^{\mathbf{L10}}$ reveals that the lowest energy conformations correspond to one which exhibits an extensive H-bond network between the ester group of LAC and both S264 and R328 residues, the latter of which forms an H-bond with the propionate group of heme ( Fig. S6).

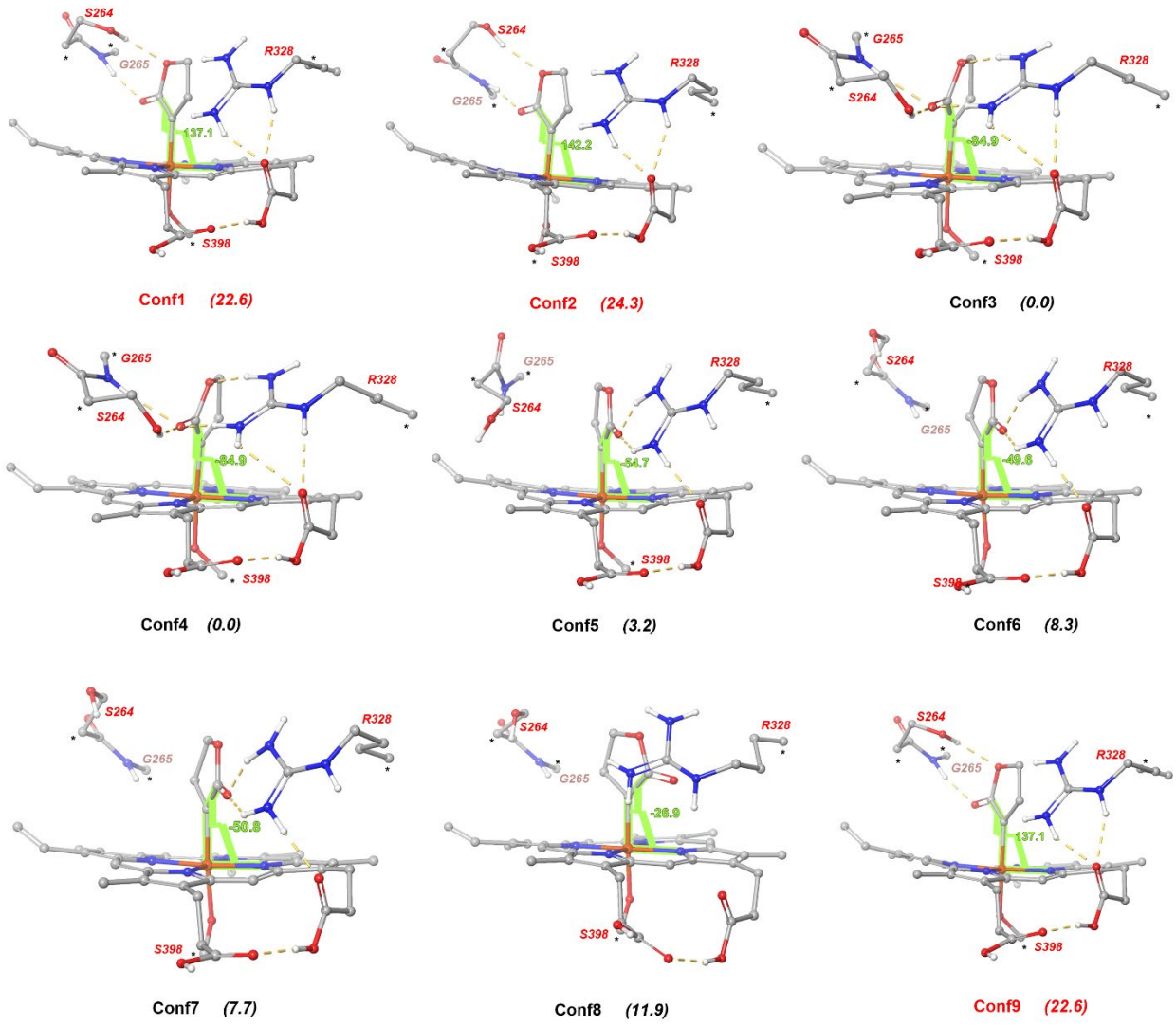



**Fig. S6** Conformational sampling of $\mathbf{C}^{\mathbf{L10}}$ performed by rotating about the highlighted dihedral. The low-energy conformations (within 2 kcal/mol) are shown in bold, and the high-energy ones are shown in red. The H-bonding interactions have been demonstrated with dashed orange lines. The high energy conformations correspond to one where LAC establishes H-bonds with S264. The energies are given in kcal/mol and dihedrals in degrees. The non-polar H atoms are not shown for clarity.

An overlay of all nine conformations of $\mathbf{C}^{\mathbf{L10}}$ shows different orientations explored by LAC ( Fig. S7).

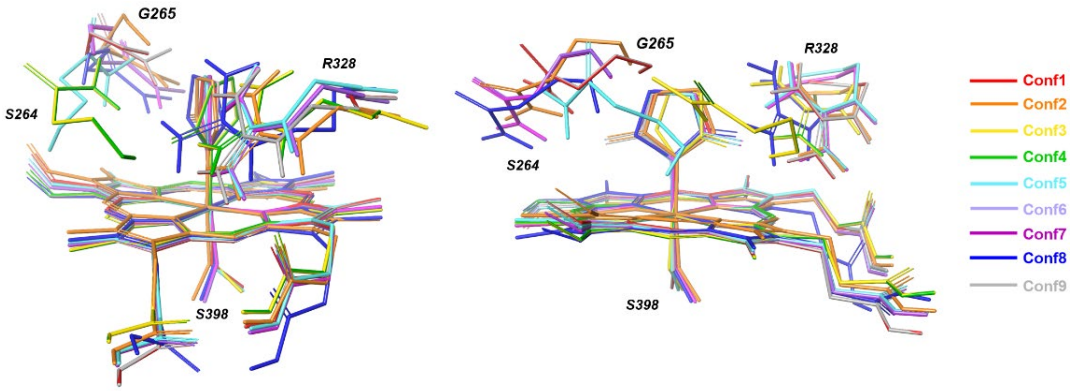



**Fig. S7** Overlayed images of the nine conformations of $\mathbf{C^{L10}}$ obtained by performing a dihedral scan using xTB. The first panel corresponds to the front view (propionate groups facing the reader), and the next corresponds to the side view. The non-polar H atoms are omitted for clarity.

**Table S7** Total Electronic energies (a.u.) at the GFN-xTB level for a conformational sampling of carbene intermediate in **L9** and **L10** for QM cluster 1

| | **L9** | **L10** |
|---|---|---|
| **Conf1** | -187.064403 | -196.525081 |
| **Conf2** | -187.061744 | -196.522474 |
| **Conf3** | -187.065149 | -196.561124 |
| **Conf4** | -187.062917 | -196.561123 |
| **Conf5** | -187.062917 | -196.555995 |
| **Conf6** | -187.050034 | -196.547866 |
| **Conf7** | -187.050562 | -196.548802 |
| **Conf8** | -187.060195 | -196.542215 |
| **Conf9** | -187.064403 | -196.525087 |

### 3.2. Demonstration of $S_2$ binding mode in L9 and L10

Consider the porphyrin ring in the XZ plane (red) with the lactone ring lying in the YZ plane (blue) (main text Fig. 5). Now, considering only the regions defined by the positive Y axis (the top face of the XZ plane); we look at the four octants intersected by the XY and YZ planes. For convenience, we have adopted the nomenclature in the text described in Fig. 5(b) (main text).

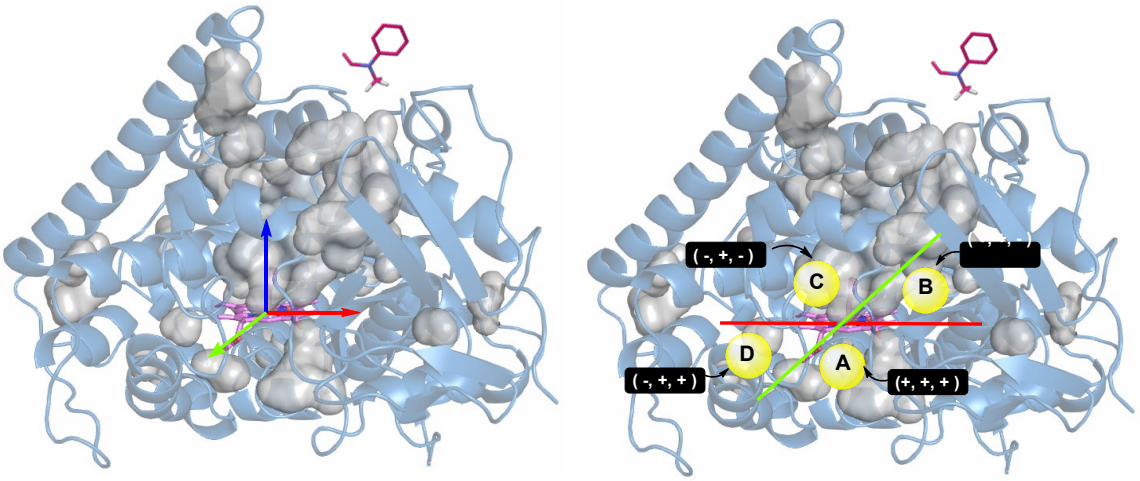



**Fig. S8** Understanding substrate (**$S_2$**) binding. (a) wild-type protein reveals a much larger but ill-defined cavity (blue surface). The four possible modes of **$S_2$** binding are illustrated. **$S_2$** has been shown in salmon pink.

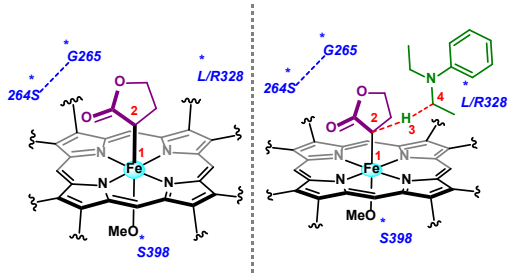
**Table S8** Total Electronic energies (a.u.) at the $PCM_{(diethylether)}$/(U)B3LYP-D3/6-311++G**,SDD(Fe)//(U)B3LYP/6-31G**,SDD(Fe) level for the HAT step in **L9** and **L10** for QM cluster 1

| | **L9** | **L10** |
|---|---|---|
| $\left[{}^{3}\mathbf{TS(C\text{-}D)}^{A}_{(1R)}\right]$ | -3384.776651 | -3550.15943 |

| | | |
|---|---|---|
| $\left[ {}^{3}\mathbf{D}^{A}_{(1R)} \right]$ | -3384.797964 | -3550.18482 |
| $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{A}_{(1S)} \right]$ | -3384.787804 | -3550.159768 |
| $\left[ {}^{3}\mathbf{D}^{A}_{(1S)} \right]$ | -3384.806028 | -3550.188159 |
| $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{C}_{(1R)} \right]$ | -3384.787173 | -3550.150412 |
| $\left[ {}^{3}\mathbf{D}^{C}_{(1R)} \right]$ | -3384.805909 | -3550.18484 |
| $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{C}_{(1S)} \right]$ | -3384.777874 | -3550.157427 |
| $\left[ {}^{3}\mathbf{D}^{C}_{(1S)} \right]$ | -3384.796658 | -3550.182888 |

It should be noted that we have not employed QM cluster 1 for a quantification of stereopreference. It has been used as a model to delve into the conformational flexibility of intermediate **C** and to appreciate the origin of enantioinduction. We shall review the origin of stereopreference implementing a more extensive and "better" QM cluster.

**Table S9** Spin state energetics and Mulliken spin densities of **TS(C-D)** at the $PCM_{(\varepsilon=4.3)}$/(U)B3LYP-D3/6-311++G**,SDD(Fe)//(U)B3LYP/6-31G**,SDD(Fe) level in **L9** for QM cluster 1




| | $DE_{ST}$ | Spin densities of triplet | | Spin densities of OSS | |
|---|---|---|---|---|---|
| | | Fe1 | C2/C4 | Fe1 | C2/C4 |
| $C^{L9}$ | -10.6 | 1.000 | 0.690 | 0.055 | -0.013 |
| $\left[ TS(C\text{-}D)^{A}_{(1R)} \right]^{L9}$ | -9.3 | 0.995 | 0.418 | 1.006 | -0.412 |
| $\left[ TS(C\text{-}D)^{A}_{(1R)} \right]^{L9}$ | -4.1 | 0.996 | 0.001 | 0.007 | -0.001 |

We see that the relative difference between the (*1S*) and (*1R*) selective TSS, $\mathbf{DE_{(R)\text{-}(S)}}$ ($\mathbf{DE}_{(1S)}$ - $\mathbf{DE}_{(1R)}$) is -12.2 kcal/mol compared to -7.0 kcal/mol with respect to triplet. Our results reveal that the C–H insertion occurs through a triplet HAT surface when considering the enzymatic environment. These results also prompted us to conduct subsequent studies using QM clusters in the triplet spin state. We also see that the spin state of the system does not play a role in dictating the stereochemical outcomes of these reactions, as expected intuitively, as steric, and electronic factors primarily govern the latter.

## 4. Modeling QM Cluster 2

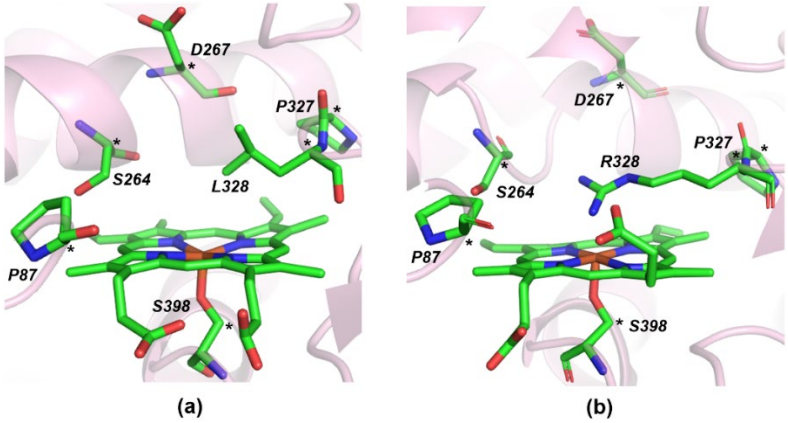



**Fig. S9** Residues chosen for modeling QM cluster-2 for (a) **L9** and (b) **L10** (the asterisks denote the C(α) atoms fixed during the subsequent optimizations). The H atoms are not shown for clarity.

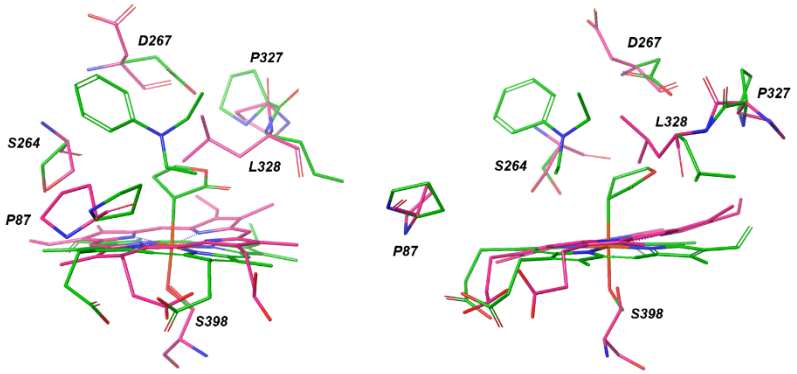
From the preliminary insights obtained using QM cluster 1, we sought to investigate the origin of enantioselectivity in the HAT step. To this end, the high energy HAT TSs, wherein $\mathbf{S_2}$ approaches from face C, were not looked at. We, however, looked at $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{C}}_{(R)} \right]^{\mathbf{L9}}$ which was found to be only 0.4 kcal/mol higher in energy than the lowest HAT TS, $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(S)} \right]^{\mathbf{L9}}$.

**Table S10** Total Electronic energies (a.u.) at the PCM$_{(\text{diethylether})}$/(U)B3LYP-D3/6-311++G**,SDD(Fe)//(U)B3LYP/6-31G**,SDD(Fe) level for the HAT step in **L9**, **L10** and **S264A** mutant for QM Cluster 2

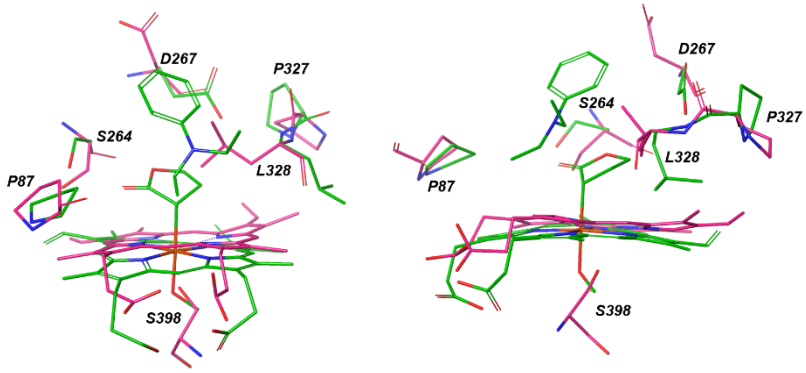
| | **L9** | **L10** | **S264A** |
|---|---|---|---|
| $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{A}_{(R)} \right]$ | -4036.00091604 | -4201.36251779 | -4127.75655202 |
| $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{A}_{(S)} \right]$ | -4036.01115241 | -4201.3566655 | -4127.74604452 |

| | | | |
|---|---|---|---|
| $\left[ {}^{3}\mathrm{TS(C\text{-}D)}^{C}_{(R)} \right]$ | -4036.011152 | -[a] | - |
| $\left[ {}^{3}\mathrm{TS(C\text{-}D)}^{C}_{(S)} \right]$ | -[a] | -[a] | - |

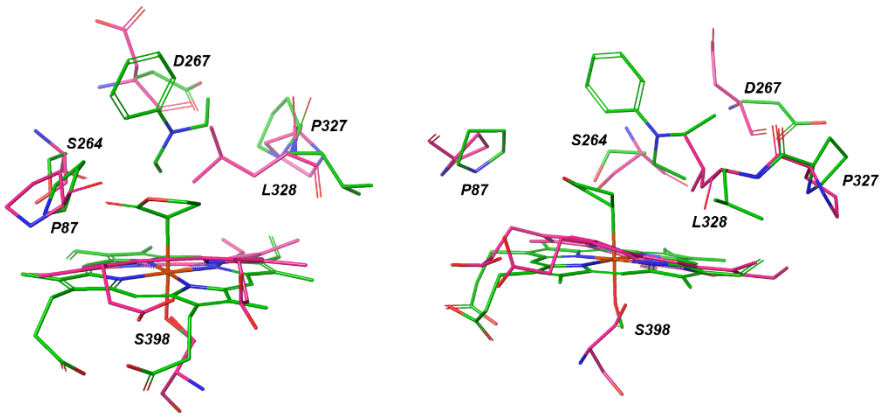
[a]We did not locate this TS (based on preliminary information obtained from QM cluster 1).



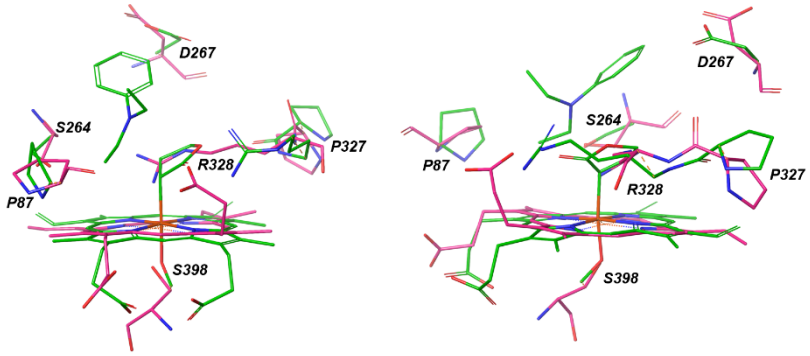

$\left[ {}^{3}\mathrm{TS(C\text{-}D)}^{A}_{(R)} \right]^{L9}$



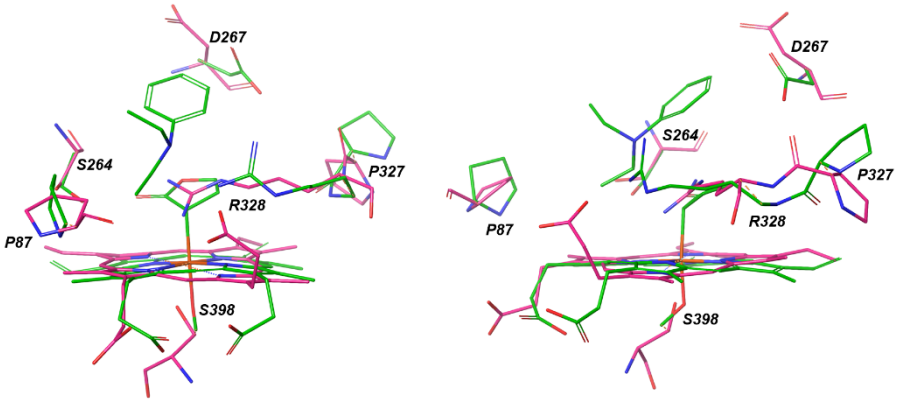

$\left[ {}^{3}\mathrm{TS(C\text{-}D)}^{A}_{(S)} \right]^{L9}$




$$\left[ {}^{3}\mathrm{TS(C\text{-}D)}^{\mathrm{C}}_{(R)} \right]^{\mathrm{L9}}$$




$$\left[ {}^{3}\mathrm{TS(C\text{-}D)}^{\mathrm{A}}_{(R)} \right]^{\mathrm{L10}}$$




$$\left[ {}^{3}\mathrm{TS(C\text{-}D)}^{\mathrm{A}}_{(S)} \right]^{\mathrm{L10}}$$

**Fig. S10** Overlayed images of HAT TSs $^{3}$**TS(C-D)** (in green) with the final MD structures of **L9**/**L10** (in pink). The C(α) atoms of the protein (MD structure) have been superimposed on the C atoms that were frozen during optimization in the QM Cluster 2 calculations. The left panel corresponds to the front view (propionate groups facing the reader), and the right panel corresponds to the side view. The H atoms are omitted for clarity.

Structures corresponding to $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{C}}_{(R)} \right]^{\mathbf{L9}}$ shows the maximum deviation from the MD structure (clear from the distortion of the porphyrin core). This unambiguously suggests that the porphyrin ring undergoes substantial distortion if the substrate $\mathbf{S_2}$ approaches from face **C**. This was also intuitively clear from the cavity surface diagrams (main text Fig. 5), which shows that the protein has indeed evolved to accommodate substrate binding from a particular face only (face **A** in this case). Thus, QM cluster 2 correctly captures the steric and electronic effects presented by key active site residues, thus, rationalizing the enantiodivergence obtained. Overall, results of both QM clusters 1 and 2 explicitly show that substrate ($\mathbf{S_2}$) approach occurs from face **A** and preferential substrate ($\mathbf{S_1}$) binding by H-bonding during HAT TS leads to enantiodifferentiation.

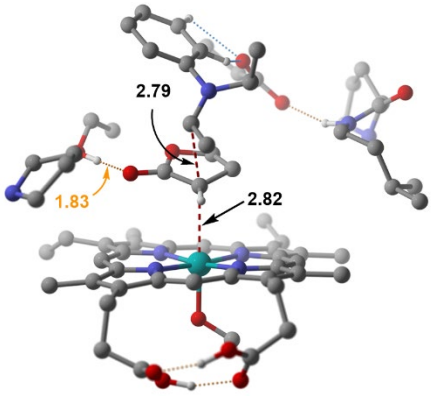



**Fig. S11** Optimized geometries of the radical rebound TS; $\left[ {}^{3}\mathbf{TS(D\text{-}P)}^{\mathbf{A}}_{(1S,2R)} \right]^{\mathbf{L9}}$. Distances are in Å. Numbers in orange refer to the H-bond distances. The H atoms (except the ones taking part in H-bonding) are omitted for clarity.

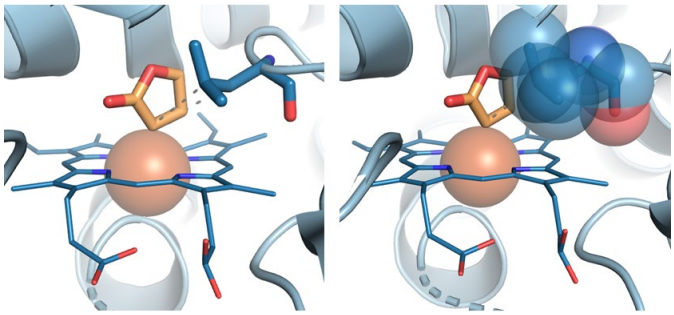



**Fig. S12** Lactone carbene intermediate in **L9** shows the hydrophobic interactions between its hydrophobic face and the mutated residue, L328- shown as sticks in (a) and spheres in (b). Image generated with PLIP (Protein-Ligand Interaction Profiler) Web Server.[35]

**Table S11** Single-point energies of the HAT TSs for **L9** and **L10** at different levels of theories

| | $DE_{(S-R)} = E_{(IR)} - E_{(IS)}$ | |
|---|---|---|
| | **L9** | **L10** |
| **$PCM_{(\varepsilon=4.3)}$/B3LYP-D3,6-311++G**, SDD(Fe)//B3LYP,6-31G**,SDD(Fe)** | -6.4 | 3.6 |
| **$PCM_{(\varepsilon=4.3)}$/B3LYP-D3(bj),6-311++G**, SDD(Fe)//B3LYP,6-31G**,SDD(Fe)** | -6.4 | 4.0 |
| **$PCM_{(\varepsilon=4.3)}$/m06,6-311++G**, SDD(Fe)//B3LYP,6-31G**,SDD(Fe)** | -0.5 | 3.6 |
| **$PCM_{(\varepsilon=4.3)}$/ωB97XD,6-311++G**, SDD(Fe)//B3LYP,6-31G**,SDD(Fe)** | -3.0 | 10.1 |

## 5. Analysis of non-covalent interactions

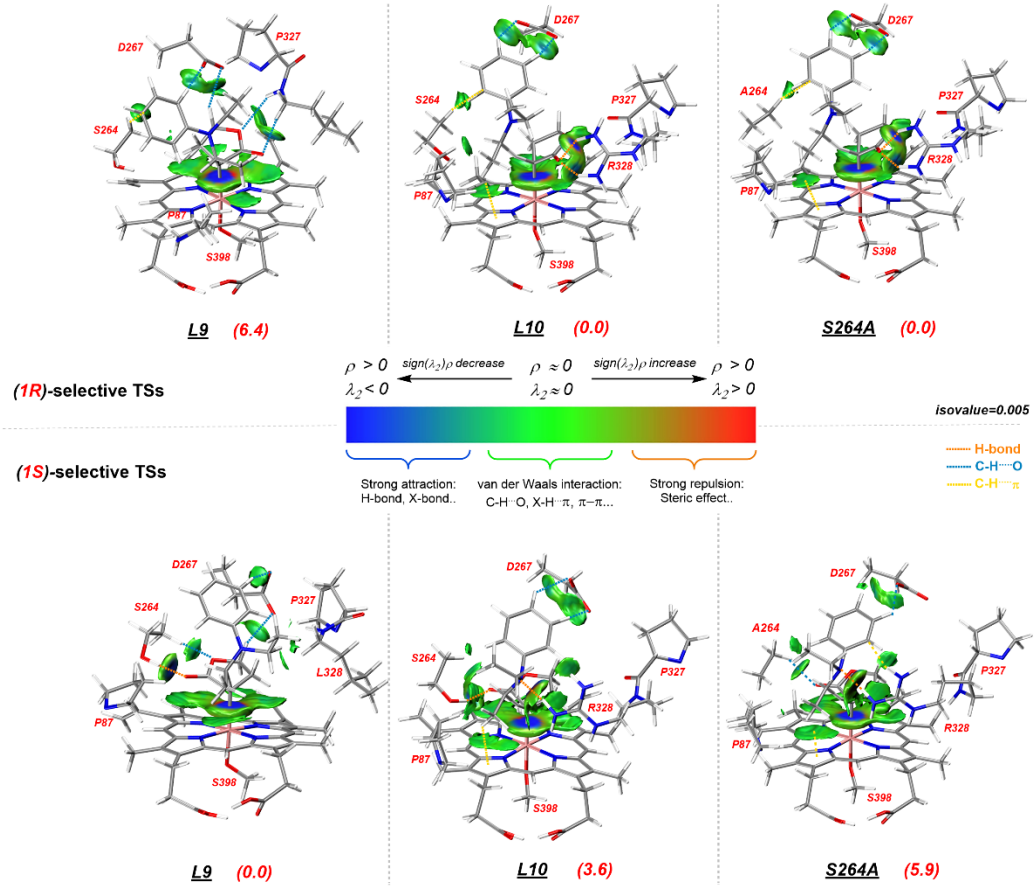



**Fig. S13** The independent gradient model analysis for $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(R)} \right]^{\mathbf{m}}$ (top panel) **a**nd $\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(S)} \right]^{\mathbf{m}}$ (bottom panel) for – **L9** (column 1), **L10** (column 2) and **S264A** mutant (column 3). The numbers in brackets indicate the relative total thermal energies in kcal/mol. Common interpretation of the coloring method of mapped function $sign(\lambda_2)\rho$ in IGMH maps has been shown in the middle.

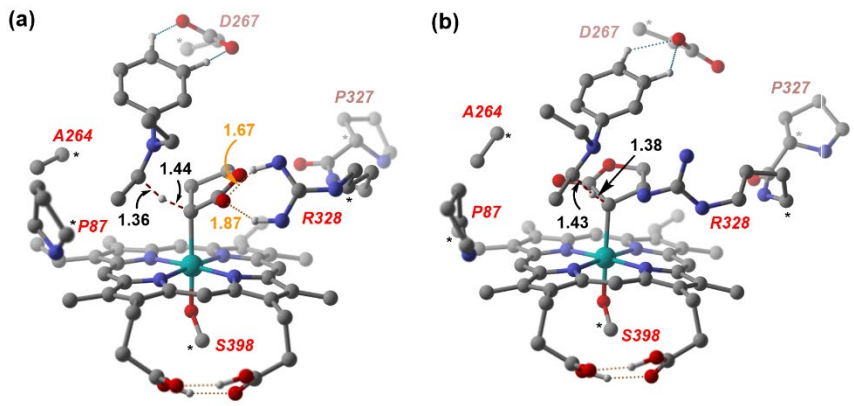



**Fig. S14.** Optimized structures of the diastereomeric HAT TSs of **S264A** mutant with an approach of $S_2$ from face **A**. Distances are in Å. Energies are given in kcal/mol. Numbers in orange refer to the H-bond distances. The H atoms (except the ones taking part in H-bonding) are omitted for clarity.

## 6. Cartesian coordinates and electronic energies of optimized geometries

### (U)B3LYP optimizations

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**$S_1$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-414.7257256

Zero-point correction= 0.084935 (Hartree/Particle)

Thermal correction to Energy= 0.091736

Thermal correction to Enthalpy= 0.092680

Thermal correction to Gibbs Free Energy= 0.053345

Sum of electronic and zero-point Energies= -414.640791

Sum of electronic and thermal Energies= -414.633990

Sum of electronic and thermal Enthalpies= -414.633046

Sum of electronic and thermal Free Energies= -414.672381

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 1.717955 | -0.327299 | 0.022197 |
| N | 2.858625 | -0.323774 | 0.051754 |
| C | 0.419891 | -0.317779 | 0.006406 |
| C | -0.480706 | -1.512781 | -0.137813 |
| C | -1.844189 | -0.830392 | 0.142504 |
| H | -0.277379 | -2.314743 | 0.578263 |
| H | -0.443695 | -1.941113 | -1.147359 |
| H | -2.166932 | -1.001501 | 1.175040 |
| H | -2.631794 | -1.163188 | -0.536197 |
| C | -0.342541 | 0.936707 | -0.015606 |
| O | 0.040905 | 2.079561 | -0.023434 |
| O | -1.669778 | 0.585880 | -0.046610 |

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**$S_2$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-444.8575228

Zero-point correction= 0.231103 (Hartree/Particle)

Thermal correction to Energy= 0.242189

Thermal correction to Enthalpy= 0.243133

Thermal correction to Gibbs Free Energy= 0.193937

Sum of electronic and zero-point Energies= -444.626420

Sum of electronic and thermal Energies= -444.615334

Sum of electronic and thermal Enthalpies= -444.614390

Sum of electronic and thermal Free Energies= -444.663586

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 2.459336 | -1.196595 | -0.103556 |
| C | 1.084281 | -1.206135 | 0.117276 |
| C | 0.354773 | 0.000072 | 0.248474 |
| C | 1.084199 | 1.206259 | 0.117085 |
| C | 2.459290 | 1.196743 | -0.103753 |
| C | 3.167497 | 0.000098 | -0.214905 |
| H | 2.979464 | -2.146908 | -0.193454 |
| H | 0.581389 | -2.162500 | 0.186642 |

| | | | |
|---|---|---|---|
| H | 0.581313 | 2.162638 | 0.186264 |
| H | 2.979336 | 2.147086 | -0.193799 |
| H | 4.238272 | 0.000092 | -0.391926 |
| N | -1.013099 | -0.000010 | 0.514442 |
| C | -1.759420 | -1.250627 | 0.600638 |
| H | -2.670600 | -1.047296 | 1.173019 |
| H | -1.186867 | -1.969802 | 1.198598 |
| C | -1.759564 | 1.250499 | 0.600728 |
| H | -2.670629 | 1.047070 | 1.173262 |
| H | -1.186980 | 1.969730 | 1.198588 |
| C | -2.139241 | 1.881857 | -0.747936 |
| H | -1.253110 | 2.074032 | -1.359191 |
| H | -2.803581 | 1.225347 | -1.317771 |
| H | -2.658051 | 2.834136 | -0.589798 |
| C | -2.138725 | -1.882063 | -0.748090 |
| H | -1.252394 | -2.074215 | -1.359064 |
| H | -2.657515 | -2.834369 | -0.590053 |
| H | -2.802915 | -1.225620 | -1.318173 |

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$^{2}S_{1}^{\bullet}$

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Number of imaginary frequencies : 0 Electronic energy : HF=-305.8357518

Zero-point correction= 0.084418 (Hartree/Particle)

Thermal correction to Energy= 0.089824

Thermal correction to Enthalpy= 0.090768

Thermal correction to Gibbs Free Energy= 0.054212

Sum of electronic and zero-point Energies= -305.751334

Sum of electronic and thermal Energies= -305.745928

Sum of electronic and thermal Enthalpies= -305.744983

Sum of electronic and thermal Free Energies= -305.781540

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 0.007129 | 1.182919 | -0.030016 |
| C | 1.418152 | 0.734432 | 0.036131 |
| C | -0.890566 | 0.040980 | -0.001908 |
| C | 1.273238 | -0.809822 | -0.040169 |
| O | -0.130662 | -1.109368 | 0.034033 |
| O | -2.103057 | 0.015152 | 0.001053 |
| H | 1.903270 | 1.055383 | 0.970439 |
| H | 2.034231 | 1.137211 | -0.778801 |
| H | 1.773269 | -1.323632 | 0.785082 |
| H | 1.658933 | -1.210176 | -0.983376 |

H -0.347673 2.203897 -0.058258

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$^{2}S_{2}^{\bullet}$

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Number of imaginary frequencies : 0 Electronic energy : HF=-444.2040657

Zero-point correction= 0.216988 (Hartree/Particle)

Thermal correction to Energy= 0.228244

Thermal correction to Enthalpy= 0.229189

Thermal correction to Gibbs Free Energy= 0.179233

Sum of electronic and zero-point Energies= -443.987078

Sum of electronic and thermal Energies= -443.975821

Sum of electronic and thermal Enthalpies= -443.974877

Sum of electronic and thermal Free Energies= -444.024833

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Cartesian Coordinates

.....

C 0.412206 -0.099359 -0.127856

C 1.084690 -1.233623 0.379307

C 2.473508 -1.259056 0.466752

C 3.240335 -0.162085 0.068999

| | | | |
|---|---|---|---|
| C | 2.583425 | 0.972071 | -0.412347 |
| C | 1.194879 | 1.012100 | -0.510808 |
| H | 0.507696 | -2.077420 | 0.737901 |
| H | 2.958881 | -2.145820 | 0.866020 |
| H | 4.323076 | -0.186036 | 0.141908 |
| H | 3.156339 | 1.842375 | -0.721349 |
| H | 0.728250 | 1.909490 | -0.898819 |
| N | -0.987873 | -0.098104 | -0.252142 |
| C | -1.701001 | 1.179418 | -0.359604 |
| H | -1.266981 | 1.769714 | -1.175248 |
| H | -2.723789 | 0.961133 | -0.666302 |
| C | -1.708316 | 1.991889 | 0.939552 |
| H | -0.691764 | 2.220016 | 1.270804 |
| H | -2.240204 | 2.937815 | 0.791133 |
| H | -2.208173 | 1.438090 | 1.740100 |
| C | -1.690758 | -1.301479 | -0.232455 |
| H | -1.149390 | -2.158143 | -0.616937 |
| C | -3.175737 | -1.367696 | -0.120208 |
| H | -3.564916 | -0.778537 | 0.720986 |
| H | -3.720476 | -1.031552 | -1.021380 |
| H | -3.472831 | -2.407474 | 0.048186 |

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**$N_2$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-109.5207179

Zero-point correction= 0.005599 (Hartree/Particle)

Thermal correction to Energy= 0.007960

Thermal correction to Enthalpy= 0.008904

Thermal correction to Gibbs Free Energy= -0.012850

Sum of electronic and zero-point Energies= -109.515119

Sum of electronic and thermal Energies= -109.512758

Sum of electronic and thermal Enthalpies= -109.511814

Sum of electronic and thermal Free Energies= -109.533568

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 0.000000 | 0.000000 | 0.552651 |
| N | 0.000000 | 0.000000 | -0.552651 |

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**$^{CSS}A$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.0320481

Zero-point correction= 0.634675 (Hartree/Particle)

Thermal correction to Energy= 0.679255

Thermal correction to Enthalpy= 0.680199

Thermal correction to Gibbs Free Energy= 0.552721

Sum of electronic and zero-point Energies= -2073.397373

Sum of electronic and thermal Energies= -2073.352793

Sum of electronic and thermal Enthalpies= -2073.351849

Sum of electronic and thermal Free Energies= -2073.479327

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | 1.073257 | -0.100949 | 0.071497 |
| N | 2.423527 | -1.562295 | -0.280672 |
| C | 2.168415 | -2.902210 | -0.454770 |
| C | 3.395669 | -3.648075 | -0.618770 |
| C | 4.422139 | -2.730495 | -0.572298 |
| C | 3.788882 | -1.432680 | -0.331240 |
| C | 0.901004 | -3.476493 | -0.481935 |
| C | -0.302139 | -2.794118 | -0.375365 |
| N | -0.423064 | -1.434326 | -0.211079 |
| C | -1.771247 | -1.187023 | -0.180851 |

| | | | |
|---|---|---|---|
| C | -2.529305 | -2.423989 | -0.310404 |
| C | -1.608036 | -3.428827 | -0.434506 |
| C | -2.344527 | 0.076309 | -0.075021 |
| C | -1.650951 | 1.278074 | 0.011558 |
| N | -0.286100 | 1.391812 | 0.051989 |
| C | -0.031846 | 2.735725 | 0.172827 |
| C | -1.270753 | 3.499513 | 0.194743 |
| C | -2.285551 | 2.588428 | 0.091378 |
| C | 1.229042 | 3.306230 | 0.264149 |
| C | 2.440864 | 2.624173 | 0.201197 |
| C | 3.753155 | 3.256588 | 0.308741 |
| C | 4.674136 | 2.232883 | 0.215193 |
| C | 3.908933 | 1.014223 | 0.052640 |
| N | 2.560588 | 1.272709 | 0.047629 |
| C | 4.476335 | -0.245970 | -0.116197 |
| H | 0.849541 | -4.552895 | -0.612252 |
| H | 5.555931 | -0.311356 | -0.075036 |
| H | 1.269247 | 4.382160 | 0.396338 |
| H | -3.428903 | 0.129333 | -0.076274 |
| C | 0.626577 | -1.197830 | 2.657907 |
| H | 0.992696 | -2.200710 | 2.352694 |
| H | -0.482234 | -1.238006 | 2.590191 |
| C | -1.358315 | 4.992314 | 0.306530 |

| | | | |
|---|---|---|---|
| H | -0.833146 | 5.361456 | 1.196213 |
| H | -0.907299 | 5.495307 | -0.559022 |
| H | -2.397070 | 5.329335 | 0.376204 |
| C | -1.841885 | -4.900733 | -0.601489 |
| H | -1.346010 | -5.290795 | -1.499385 |
| H | -1.453034 | -5.475078 | 0.249469 |
| H | -2.908117 | -5.130169 | -0.690697 |
| C | 3.478496 | -5.126278 | -0.855555 |
| H | 2.911046 | -5.686578 | -0.102585 |
| H | 3.069935 | -5.406585 | -1.835773 |
| H | 4.512044 | -5.482596 | -0.824157 |
| C | 6.168957 | 2.331054 | 0.216978 |
| H | 6.588018 | 2.281039 | 1.231788 |
| H | 6.627774 | 1.520927 | -0.358356 |
| H | 6.496735 | 3.281253 | -0.218448 |
| C | 5.836300 | -3.034518 | -0.754299 |
| C | 6.797308 | -2.262032 | -1.289193 |
| H | 6.131024 | -4.037100 | -0.438847 |
| H | 7.819861 | -2.620978 | -1.365108 |
| H | 6.595571 | -1.272300 | -1.684289 |
| C | 3.966739 | 4.689412 | 0.438089 |
| C | 5.038447 | 5.328237 | 0.941727 |
| H | 3.149360 | 5.314133 | 0.076638 |

| | | | |
|---|---|---|---|
| H | 5.078705 | 6.413702 | 0.959571 |
| H | 5.885222 | 4.803847 | 1.370682 |
| C | -4.026898 | -2.533199 | -0.266202 |
| C | -4.579071 | -2.464756 | 1.168341 |
| H | -4.356637 | -3.471707 | -0.723743 |
| H | -4.492972 | -1.737728 | -0.859332 |
| H | -4.147643 | -3.260128 | 1.788637 |
| H | -4.282923 | -1.530183 | 1.658705 |
| C | -3.764270 | 2.843233 | 0.019057 |
| C | -4.303081 | 2.780284 | -1.420741 |
| H | -4.004455 | 3.824851 | 0.440046 |
| H | -4.313787 | 2.118725 | 0.631349 |
| H | -3.785207 | 3.506079 | -2.060330 |
| H | -4.098778 | 1.803120 | -1.873552 |
| C | -6.082407 | -2.582716 | 1.240287 |
| O | -6.841186 | -2.749162 | 0.308098 |
| O | -6.535258 | -2.484811 | 2.519377 |
| H | -7.501737 | -2.564894 | 2.458705 |
| C | -5.785290 | 3.048770 | -1.523936 |
| O | -6.533938 | 3.340880 | -0.615321 |
| O | -6.230082 | 2.932698 | -2.805112 |
| H | -7.183374 | 3.116756 | -2.765207 |
| O | 1.200680 | -0.150012 | 1.963416 |

H 0.864562 -1.100633 3.736084

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**$^{OSS}$A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.0364094

Zero-point correction= 0.633760 (Hartree/Particle)

Thermal correction to Energy= 0.678710

Thermal correction to Enthalpy= 0.679655

Thermal correction to Gibbs Free Energy= 0.551417

Sum of electronic and zero-point Energies= -2073.402649

Sum of electronic and thermal Energies= -2073.357699

Sum of electronic and thermal Enthalpies= -2073.356755

Sum of electronic and thermal Free Energies= -2073.484992

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Cartesian Coordinates

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Fe 1.068471 -0.095403 0.092103

N 2.437479 -1.557406 -0.299988

C 2.185960 -2.894138 -0.476272

C 3.417395 -3.632772 -0.642157

| | | | |
|---|---|---|---|
| C | 4.438931 | -2.707350 | -0.593641 |
| C | 3.798394 | -1.414905 | -0.349948 |
| C | 0.916247 | -3.470895 | -0.499093 |
| C | -0.289481 | -2.794289 | -0.382155 |
| N | -0.419045 | -1.437413 | -0.210196 |
| C | -1.766125 | -1.192473 | -0.180957 |
| C | -2.519438 | -2.434243 | -0.314304 |
| C | -1.595007 | -3.434906 | -0.441603 |
| C | -2.346403 | 0.069093 | -0.078885 |
| C | -1.665788 | 1.281528 | 0.000888 |
| N | -0.305057 | 1.409757 | 0.033835 |
| C | -0.056087 | 2.751179 | 0.154160 |
| C | -1.300041 | 3.506991 | 0.181947 |
| C | -2.309363 | 2.587227 | 0.083866 |
| C | 1.206558 | 3.322993 | 0.250006 |
| C | 2.420321 | 2.641608 | 0.201954 |
| C | 3.732255 | 3.279767 | 0.309235 |
| C | 4.656917 | 2.260654 | 0.217323 |
| C | 3.897292 | 1.035800 | 0.056023 |
| N | 2.548057 | 1.290625 | 0.058176 |
| C | 4.473369 | -0.218759 | -0.126607 |
| H | 0.867340 | -4.547051 | -0.632785 |
| H | 5.553833 | -0.273888 | -0.088978 |

| | | | |
|---|---|---|---|
| H | 1.245659 | 4.399329 | 0.379281 |
| H | -3.431357 | 0.112748 | -0.078675 |
| C | 0.851515 | -1.333670 | 2.709516 |
| H | 1.484451 | -2.198234 | 2.411774 |
| H | -0.202223 | -1.676510 | 2.605918 |
| C | -1.398201 | 4.998959 | 0.296219 |
| H | -0.872388 | 5.370714 | 1.184412 |
| H | -0.954525 | 5.506646 | -0.570430 |
| H | -2.439109 | 5.328337 | 0.370444 |
| C | -1.822705 | -4.907101 | -0.613284 |
| H | -1.327089 | -5.291695 | -1.513680 |
| H | -1.429131 | -5.482280 | 0.234902 |
| H | -2.888050 | -5.141136 | -0.700814 |
| C | 3.511043 | -5.109972 | -0.881312 |
| H | 2.946417 | -5.675642 | -0.130304 |
| H | 3.106584 | -5.391700 | -1.862846 |
| H | 4.547150 | -5.458872 | -0.848659 |
| C | 6.151132 | 2.366367 | 0.218239 |
| H | 6.571006 | 2.302788 | 1.231795 |
| H | 6.612914 | 1.566990 | -0.369658 |
| H | 6.473017 | 3.324787 | -0.202967 |
| C | 5.856229 | -3.001197 | -0.771671 |
| C | 6.807590 | -2.221756 | -1.312849 |

| | | | |
|---|---|---|---|
| H | 6.161190 | -3.998001 | -0.447827 |
| H | 7.834740 | -2.567954 | -1.385777 |
| H | 6.592784 | -1.237598 | -1.715205 |
| C | 3.941133 | 4.714142 | 0.432708 |
| C | 5.003785 | 5.356351 | 0.950420 |
| H | 3.128746 | 5.335277 | 0.054248 |
| H | 5.043650 | 6.441889 | 0.962741 |
| H | 5.842863 | 4.834369 | 1.397235 |
| C | -4.016440 | -2.550564 | -0.267986 |
| C | -4.565941 | -2.485618 | 1.167689 |
| H | -4.342455 | -3.490255 | -0.725671 |
| H | -4.486964 | -1.756794 | -0.859753 |
| H | -4.129608 | -3.279168 | 1.786820 |
| H | -4.273342 | -1.549939 | 1.658110 |
| C | -3.790299 | 2.832382 | 0.022475 |
| C | -4.337490 | 2.770717 | -1.414175 |
| H | -4.034808 | 3.810691 | 0.448601 |
| H | -4.330219 | 2.101544 | 0.635608 |
| H | -3.827296 | 3.501086 | -2.054776 |
| H | -4.131064 | 1.796001 | -1.871230 |
| C | -6.068621 | -2.610439 | 1.241691 |
| O | -6.828060 | -2.776582 | 0.309950 |
| O | -6.519649 | -2.519535 | 2.521769 |

| | | | |
|---|---|---|---|
| H | -7.485897 | -2.603344 | 2.462581 |
| C | -5.821645 | 3.032365 | -1.507414 |
| O | -6.564994 | 3.323241 | -0.594116 |
| O | -6.274776 | 2.911813 | -2.785195 |
| H | -7.228504 | 3.092147 | -2.739177 |
| O | 1.136395 | -0.166417 | 2.031049 |
| H | 1.018109 | -1.202361 | 3.799338 |

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**$^{3}$A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.0446298

Zero-point correction= 0.632856 (Hartree/Particle)

Thermal correction to Energy= 0.678121

Thermal correction to Enthalpy= 0.679066

Thermal correction to Gibbs Free Energy= 0.548513

Sum of electronic and zero-point Energies= -2073.411774

Sum of electronic and thermal Energies= -2073.366508

Sum of electronic and thermal Enthalpies= -2073.365564

Sum of electronic and thermal Free Energies= -2073.496117

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | 1.067163 | -0.101508 | 0.190799 |
| N | 2.454674 | -1.539805 | -0.349185 |
| C | 2.219046 | -2.884868 | -0.505450 |
| C | 3.438668 | -3.595721 | -0.719665 |
| C | 4.457102 | -2.643667 | -0.715522 |
| C | 3.815012 | -1.378654 | -0.445545 |
| C | 0.946149 | -3.477013 | -0.469681 |
| C | -0.242167 | -2.799079 | -0.325463 |
| N | -0.384798 | -1.431789 | -0.157308 |
| C | -1.751465 | -1.200293 | -0.150063 |
| C | -2.479712 | -2.455989 | -0.268896 |
| C | -1.546277 | -3.445685 | -0.375023 |
| C | -2.356032 | 0.035964 | -0.090094 |
| C | -1.690071 | 1.265998 | -0.018744 |
| N | -0.323404 | 1.403263 | 0.043005 |
| C | -0.088926 | 2.748844 | 0.178317 |
| C | -1.322270 | 3.485039 | 0.175682 |
| C | -2.332863 | 2.548459 | 0.048999 |
| C | 1.178218 | 3.327322 | 0.317941 |
| C | 2.373614 | 2.641728 | 0.270427 |
| C | 3.686913 | 3.279545 | 0.375449 |

| | | | |
|---|---|---|---|
| C | 4.616735 | 2.276200 | 0.241905 |
| C | 3.876040 | 1.043432 | 0.057522 |
| N | 2.510753 | 1.282286 | 0.100576 |
| C | 4.476829 | -0.171818 | -0.194053 |
| H | 0.897094 | -4.553050 | -0.594742 |
| H | 5.558152 | -0.204912 | -0.182036 |
| H | 1.215533 | 4.399826 | 0.468697 |
| H | -3.440629 | 0.062176 | -0.110803 |
| C | 0.745978 | -1.362233 | 2.833573 |
| H | 1.310997 | -2.288571 | 2.612397 |
| H | -0.323480 | -1.597536 | 2.672386 |
| C | -1.439013 | 4.976127 | 0.291948 |
| H | -0.932526 | 5.355822 | 1.188561 |
| H | -0.992365 | 5.495617 | -0.566877 |
| H | -2.485447 | 5.291391 | 0.353089 |
| C | -1.754243 | -4.921209 | -0.535675 |
| H | -1.278368 | -5.298088 | -1.450001 |
| H | -1.321712 | -5.485238 | 0.300826 |
| H | -2.817192 | -5.174400 | -0.588971 |
| C | 3.548856 | -5.071057 | -0.966121 |
| H | 2.993243 | -5.649656 | -0.217880 |
| H | 3.151279 | -5.358482 | -1.949750 |
| H | 4.589430 | -5.407613 | -0.932583 |

| | | | |
|---|---|---|---|
| C | 6.109200 | 2.398854 | 0.209357 |
| H | 6.559191 | 2.233224 | 1.197785 |
| H | 6.557366 | 1.669046 | -0.472220 |
| H | 6.407752 | 3.399323 | -0.119160 |
| C | 5.869111 | -2.916349 | -0.940616 |
| C | 6.806143 | -2.115120 | -1.478797 |
| H | 6.189016 | -3.921198 | -0.657216 |
| H | 7.833601 | -2.452826 | -1.581442 |
| H | 6.578567 | -1.121349 | -1.849546 |
| C | 3.888916 | 4.713948 | 0.519828 |
| C | 4.928007 | 5.344531 | 1.094849 |
| H | 3.095835 | 5.338952 | 0.108355 |
| H | 4.975983 | 6.429577 | 1.118117 |
| H | 5.739486 | 4.810993 | 1.578324 |
| C | -3.975782 | -2.588733 | -0.236064 |
| C | -4.542598 | -2.483857 | 1.190237 |
| H | -4.284284 | -3.546418 | -0.667036 |
| H | -4.446838 | -1.819753 | -0.859032 |
| H | -4.102987 | -3.250601 | 1.840180 |
| H | -4.268783 | -1.527943 | 1.651343 |
| C | -3.812862 | 2.790246 | -0.046304 |
| C | -4.322163 | 2.764975 | -1.498053 |
| H | -4.072458 | 3.756761 | 0.398039 |

| | | | |
|---|---|---|---|
| H | -4.368991 | 2.043785 | 0.532768 |
| H | -3.791352 | 3.507358 | -2.107381 |
| H | -4.106616 | 1.800015 | -1.971595 |
| C | -6.044034 | -2.628188 | 1.251226 |
| O | -6.789588 | -2.837725 | 0.317188 |
| O | -6.511050 | -2.499996 | 2.522350 |
| H | -7.475278 | -2.599793 | 2.455525 |
| C | -5.801958 | 3.035135 | -1.627504 |
| O | -6.569991 | 3.312684 | -0.730433 |
| O | -6.221027 | 2.940215 | -2.919546 |
| H | -7.174549 | 3.125896 | -2.895354 |
| O | 1.185131 | -0.274089 | 2.093037 |
| H | 0.868103 | -1.170375 | 3.916511 |

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**$^{5}$A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.0685069

Zero-point correction= 0.631456 (Hartree/Particle)

Thermal correction to Energy= 0.677509

Thermal correction to Enthalpy= 0.678453

Thermal correction to Gibbs Free Energy= 0.544393

Sum of electronic and zero-point Energies= -2073.437051

Sum of electronic and thermal Energies= -2073.390998

Sum of electronic and thermal Enthalpies= -2073.390054

Sum of electronic and thermal Free Energies= -2073.524114

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 1.075982 | -0.155762 | 0.590321 |
| N | 2.452228 | -1.594957 | -0.298950 |
| C | 2.168143 | -2.913957 | -0.504950 |
| C | 3.392188 | -3.659649 | -0.738300 |
| C | 4.423640 | -2.741061 | -0.710761 |
| C | 3.801398 | -1.444476 | -0.411262 |
| C | 0.877860 | -3.468359 | -0.528144 |
| C | -0.342061 | -2.795966 | -0.407946 |
| N | -0.476554 | -1.452842 | -0.204366 |
| C | -1.809893 | -1.179989 | -0.193773 |
| C | -2.577001 | -2.412554 | -0.381797 |
| C | -1.658066 | -3.422302 | -0.515128 |
| C | -2.361990 | 0.102354 | -0.061853 |
| C | -1.673700 | 1.317637 | 0.062621 |
| N | -0.319890 | 1.443534 | 0.128819 |

| | | | |
|---|---|---|---|
| C | -0.044079 | 2.776371 | 0.223749 |
| C | -1.285638 | 3.548016 | 0.229348 |
| C | -2.305387 | 2.637082 | 0.126403 |
| C | 1.238326 | 3.331007 | 0.280487 |
| C | 2.465796 | 2.655443 | 0.193323 |
| C | 3.786391 | 3.293503 | 0.210335 |
| C | 4.705759 | 2.268522 | 0.077328 |
| C | 3.934440 | 1.038591 | -0.016734 |
| N | 2.597461 | 1.309496 | 0.070568 |
| C | 4.483696 | -0.235377 | -0.222572 |
| H | 0.821333 | -4.541128 | -0.690964 |
| H | 5.565155 | -0.294642 | -0.245520 |
| H | 1.285135 | 4.410422 | 0.387136 |
| H | -3.446765 | 0.164087 | -0.082711 |
| C | 1.101765 | -1.558835 | 3.200872 |
| H | 1.968280 | -2.216651 | 2.979240 |
| H | 0.194795 | -2.176634 | 3.029672 |
| C | -1.373907 | 5.042721 | 0.316512 |
| H | -0.836352 | 5.427068 | 1.192018 |
| H | -0.934884 | 5.530087 | -0.564022 |
| H | -2.411583 | 5.381601 | 0.394369 |
| C | -1.903712 | -4.885687 | -0.733843 |
| H | -1.377960 | -5.255089 | -1.623174 |

| | | | |
|---|---|---|---|
| H | -1.553126 | -5.488333 | 0.114160 |
| H | -2.968175 | -5.100640 | -0.869515 |
| C | 3.470772 | -5.129679 | -1.023943 |
| H | 2.895050 | -5.711542 | -0.294464 |
| H | 3.068576 | -5.374609 | -2.016243 |
| H | 4.502429 | -5.492766 | -0.997497 |
| C | 6.196940 | 2.376593 | -0.017879 |
| H | 6.676926 | 2.373120 | 0.970709 |
| H | 6.625481 | 1.544199 | -0.584413 |
| H | 6.490568 | 3.309090 | -0.512542 |
| C | 5.829648 | -3.042585 | -0.956709 |
| C | 6.757744 | -2.260606 | -1.532830 |
| H | 6.144663 | -4.044003 | -0.657110 |
| H | 7.779542 | -2.608332 | -1.656197 |
| H | 6.526960 | -1.271952 | -1.914946 |
| C | 4.006022 | 4.729158 | 0.297655 |
| C | 5.107575 | 5.378572 | 0.715143 |
| H | 3.162743 | 5.344937 | -0.016226 |
| H | 5.144322 | 6.464286 | 0.714170 |
| H | 5.984499 | 4.863735 | 1.091755 |
| C | -4.075946 | -2.515048 | -0.381227 |
| C | -4.665160 | -2.492264 | 1.039866 |
| H | -4.400181 | -3.434171 | -0.880379 |

| | | | |
|---|---|---|---|
| H | -4.520048 | -1.694926 | -0.957313 |
| H | -4.256113 | -3.311820 | 1.643626 |
| H | -4.376138 | -1.577117 | 1.569708 |
| C | -3.781367 | 2.903101 | 0.033149 |
| C | -4.296425 | 2.854952 | -1.415837 |
| H | -4.023501 | 3.882415 | 0.458709 |
| H | -4.343821 | 2.175786 | 0.629841 |
| H | -3.764704 | 3.583009 | -2.041272 |
| H | -4.089672 | 1.880313 | -1.873009 |
| C | -6.170821 | -2.600752 | 1.067744 |
| O | -6.905340 | -2.727496 | 0.110292 |
| O | -6.656566 | -2.545448 | 2.337094 |
| H | -7.621670 | -2.615589 | 2.248613 |
| C | -5.775582 | 3.131740 | -1.540265 |
| O | -6.537085 | 3.418781 | -0.640795 |
| O | -6.199953 | 3.029780 | -2.829303 |
| H | -7.152994 | 3.217588 | -2.803411 |
| O | 1.107949 | -0.377730 | 2.481543 |
| H | 1.136772 | -1.369002 | 4.293016 |

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$^{CSS}$**B'**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.7729276

Zero-point correction= 0.720260 (Hartree/Particle)

Thermal correction to Energy= 0.774189

Thermal correction to Enthalpy= 0.775133

Thermal correction to Gibbs Free Energy= 0.619990

Sum of electronic and zero-point Energies= -2488.052667

Sum of electronic and thermal Energies= -2487.998738

Sum of electronic and thermal Enthalpies= -2487.997794

Sum of electronic and thermal Free Energies= -2488.152938

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.700435 | 0.023708 | -0.741337 |
| N | -2.126640 | -1.394422 | -0.988117 |
| C | -1.928441 | -2.754458 | -1.045227 |
| C | -3.167693 | -3.448798 | -1.311521 |
| C | -4.152003 | -2.486152 | -1.374794 |
| C | -3.471919 | -1.204110 | -1.198512 |
| C | -0.710921 | -3.394953 | -0.826912 |
| C | 0.481130 | -2.778405 | -0.473107 |

| | | | |
|---|---|---|---|
| N | 0.650216 | -1.424234 | -0.321159 |
| C | 1.960829 | -1.255985 | 0.041298 |
| C | 2.644680 | -2.540346 | 0.129256 |
| C | 1.717991 | -3.492641 | -0.196381 |
| C | 2.562593 | -0.027441 | 0.294236 |
| C | 1.945654 | 1.215743 | 0.205881 |
| N | 0.634841 | 1.413382 | -0.140182 |
| C | 0.449533 | 2.771430 | -0.125661 |
| C | 1.675264 | 3.460295 | 0.249851 |
| C | 2.612463 | 2.486515 | 0.461604 |
| C | -0.742639 | 3.417986 | -0.423514 |
| C | -1.949498 | 2.802464 | -0.739457 |
| C | -3.197801 | 3.516211 | -0.996487 |
| C | -4.145839 | 2.546073 | -1.246431 |
| C | -3.461748 | 1.274265 | -1.144880 |
| N | -2.129023 | 1.449653 | -0.843736 |
| C | -4.081497 | 0.039758 | -1.310091 |
| H | -0.701576 | -4.476773 | -0.913679 |
| H | -5.131909 | 0.044669 | -1.570940 |
| H | -0.730382 | 4.502109 | -0.394337 |
| H | 3.605798 | -0.041146 | 0.594614 |
| C | -0.954506 | -0.119606 | -3.567873 |
| H | -0.472052 | 0.130600 | -4.533185 |

| | | | |
|---|---|---|---|
| H | -1.915875 | 0.433607 | -3.553180 |
| C | 1.826487 | 4.947771 | 0.363169 |
| H | 1.700412 | 5.445097 | -0.607354 |
| H | 1.080302 | 5.381027 | 1.040752 |
| H | 2.814241 | 5.222144 | 0.745625 |
| C | 1.887115 | -4.980765 | -0.269946 |
| H | 1.155824 | -5.503971 | 0.358781 |
| H | 1.752341 | -5.356382 | -1.292673 |
| H | 2.883180 | -5.287886 | 0.062648 |
| C | -3.313999 | -4.937193 | -1.417535 |
| H | -2.601943 | -5.360594 | -2.136043 |
| H | -3.131529 | -5.434952 | -0.455907 |
| H | -4.319489 | -5.220847 | -1.740314 |
| C | -5.608571 | 2.728100 | -1.514082 |
| H | -5.825863 | 2.826571 | -2.586691 |
| H | -6.194639 | 1.880329 | -1.145587 |
| H | -5.981972 | 3.634334 | -1.026002 |
| C | -5.575674 | -2.740965 | -1.567579 |
| C | -6.619026 | -2.048303 | -1.081680 |
| H | -5.805100 | -3.630080 | -2.157167 |
| H | -7.638373 | -2.352360 | -1.301217 |
| H | -6.495202 | -1.183744 | -0.438298 |
| C | -3.347541 | 4.962453 | -0.927563 |

| | | | |
|---|---|---|---|
| C | -4.262383 | 5.727568 | -1.548744 |
| H | -2.625155 | 5.475558 | -0.292374 |
| H | -4.281875 | 6.802861 | -1.396520 |
| H | -4.994129 | 5.320968 | -2.238375 |
| C | 4.098356 | -2.735183 | 0.455002 |
| C | 5.007191 | -2.514951 | -0.766829 |
| H | 4.271908 | -3.744897 | 0.840897 |
| H | 4.412941 | -2.056836 | 1.256214 |
| H | 4.717025 | -3.180661 | -1.589318 |
| H | 4.891216 | -1.501742 | -1.168316 |
| C | 4.061260 | 2.656211 | 0.821258 |
| C | 4.980262 | 2.615558 | -0.412108 |
| H | 4.381724 | 1.880842 | 1.526373 |
| H | 4.217327 | 3.607191 | 1.340826 |
| H | 4.878897 | 1.665546 | -0.949279 |
| H | 4.687029 | 3.384049 | -1.138195 |
| C | 6.470337 | -2.750619 | -0.477034 |
| O | 6.946431 | -3.143384 | 0.567239 |
| O | 7.248600 | -2.475671 | -1.558265 |
| H | 8.159812 | -2.659755 | -1.275315 |
| C | 6.438777 | 2.825068 | -0.081919 |
| O | 6.904685 | 3.073055 | 1.010280 |
| O | 7.226412 | 2.712839 | -1.185459 |

| | | | |
|---|---|---|---|
| H | 8.133576 | 2.866296 | -0.872795 |
| O | -0.099308 | 0.204981 | -2.529144 |
| H | -1.214529 | -1.198000 | -3.622685 |
| C | -2.268556 | -1.746014 | 2.460719 |
| O | -2.590580 | -2.191793 | 3.804053 |
| C | -2.532061 | -1.165198 | 4.700716 |
| C | -1.981651 | -0.008020 | 3.984486 |
| C | -1.569860 | -0.370196 | 2.582835 |
| H | -1.633171 | -2.501658 | 1.999294 |
| H | -3.201814 | -1.671909 | 1.896211 |
| H | -1.924523 | 0.329328 | 1.820145 |
| H | -0.482724 | -0.459424 | 2.479083 |
| O | -2.874768 | -1.270282 | 5.857215 |
| N | -1.799634 | 1.129498 | 4.577856 |
| N | -1.655011 | 2.131425 | 5.108915 |

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.7775281

Zero-point correction= 0.719369 (Hartree/Particle)

Thermal correction to Energy= 0.773682

Thermal correction to Enthalpy= 0.774626

Thermal correction to Gibbs Free Energy= 0.618225

Sum of electronic and zero-point Energies= -2488.058160

Sum of electronic and thermal Energies= -2488.003846

Sum of electronic and thermal Enthalpies= -2488.002902

Sum of electronic and thermal Free Energies= -2488.159303

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.656618 | -0.033488 | -0.780854 |
| N | -2.081876 | -1.481984 | -0.981310 |
| C | -1.857682 | -2.835436 | -1.007274 |
| C | -3.083501 | -3.555090 | -1.270882 |
| C | -4.081877 | -2.608635 | -1.373086 |
| C | -3.421964 | -1.312660 | -1.218382 |
| C | -0.626135 | -3.447536 | -0.772949 |
| C | 0.558043 | -2.808234 | -0.430552 |
| N | 0.710698 | -1.451447 | -0.295813 |
| C | 2.012572 | -1.256848 | 0.076180 |
| C | 2.716784 | -2.531080 | 0.179884 |
| C | 1.806096 | -3.500298 | -0.139524 |
| C | 2.590682 | -0.015653 | 0.329033 |

| | | | |
|---|---|---|---|
| C | 1.954632 | 1.219113 | 0.226992 |
| N | 0.648049 | 1.394253 | -0.138415 |
| C | 0.433862 | 2.747280 | -0.132848 |
| C | 1.641500 | 3.459511 | 0.257619 |
| C | 2.594608 | 2.503502 | 0.485409 |
| C | -0.767345 | 3.367078 | -0.457862 |
| C | -1.956556 | 2.729034 | -0.802823 |
| C | -3.209874 | 3.419360 | -1.097901 |
| C | -4.136695 | 2.432484 | -1.361811 |
| C | -3.436175 | 1.170954 | -1.228432 |
| N | -2.113825 | 1.373734 | -0.904115 |
| C | -4.039760 | -0.075480 | -1.374243 |
| H | -0.598430 | -4.530677 | -0.838145 |
| H | -5.085045 | -0.086996 | -1.654903 |
| H | -0.777294 | 4.451447 | -0.432702 |
| H | 3.630419 | -0.010579 | 0.641357 |
| C | -0.914194 | 0.255588 | -3.654081 |
| H | -0.400242 | 0.152769 | -4.632052 |
| H | -1.340984 | 1.281929 | -3.643101 |
| C | 1.765823 | 4.949982 | 0.366020 |
| H | 1.652521 | 5.439911 | -0.609733 |
| H | 0.997962 | 5.373824 | 1.024912 |
| H | 2.740362 | 5.242827 | 0.768052 |

| | | | |
|---|---|---|---|
| C | 1.999449 | -4.986067 | -0.197436 |
| H | 1.277012 | -5.514002 | 0.437419 |
| H | 1.869648 | -5.373297 | -1.216280 |
| H | 3.000552 | -5.273593 | 0.137332 |
| C | -3.207310 | -5.047418 | -1.346437 |
| H | -2.475687 | -5.475859 | -2.041719 |
| H | -3.036468 | -5.520694 | -0.370519 |
| H | -4.202269 | -5.352749 | -1.681913 |
| C | -5.595376 | 2.589701 | -1.664908 |
| H | -5.789810 | 2.661563 | -2.743929 |
| H | -6.178438 | 1.742169 | -1.291074 |
| H | -5.991277 | 3.501036 | -1.205029 |
| C | -5.498206 | -2.887905 | -1.583087 |
| C | -6.558125 | -2.193453 | -1.137138 |
| H | -5.706408 | -3.797096 | -2.149475 |
| H | -7.569815 | -2.515622 | -1.365969 |
| H | -6.455561 | -1.308486 | -0.518172 |
| C | -3.384575 | 4.864239 | -1.048588 |
| C | -4.288895 | 5.606799 | -1.710365 |
| H | -2.693480 | 5.395301 | -0.393693 |
| H | -4.331792 | 6.683211 | -1.571485 |
| H | -4.988240 | 5.179923 | -2.421070 |
| C | 4.171662 | -2.699081 | 0.514399 |

| | | | |
|---|---|---|---|
| C | 5.082459 | -2.468219 | -0.704027 |
| H | 4.360741 | -3.703690 | 0.906264 |
| H | 4.470056 | -2.011564 | 1.313988 |
| H | 4.811687 | -3.145436 | -1.523603 |
| H | 4.946446 | -1.460554 | -1.113357 |
| C | 4.034222 | 2.701814 | 0.866634 |
| C | 4.973855 | 2.670829 | -0.351373 |
| H | 4.356787 | 1.935985 | 1.581186 |
| H | 4.165128 | 3.658185 | 1.383200 |
| H | 4.901000 | 1.715327 | -0.883214 |
| H | 4.677224 | 3.428340 | -1.087651 |
| C | 6.548720 | -2.668486 | -0.403820 |
| O | 7.028098 | -3.029689 | 0.650339 |
| O | 7.325941 | -2.399644 | -1.487242 |
| H | 8.239542 | -2.558380 | -1.196770 |
| C | 6.421880 | 2.913792 | 0.001717 |
| O | 6.861824 | 3.192210 | 1.097340 |
| O | 7.232124 | 2.794975 | -1.084378 |
| H | 8.130202 | 2.972446 | -0.758445 |
| O | -0.037732 | -0.001482 | -2.616716 |
| H | -1.781329 | -0.438330 | -3.695354 |
| C | -2.048623 | -1.639009 | 2.509520 |
| O | -2.266516 | -2.120610 | 3.861888 |

| | | | |
|---|---|---|---|
| C | -2.538234 | -1.096967 | 4.720857 |
| C | -2.325577 | 0.149901 | 3.974513 |
| C | -1.780053 | -0.116961 | 2.597111 |
| H | -1.210812 | -2.192310 | 2.086107 |
| H | -2.948280 | -1.852808 | 1.926462 |
| H | -2.289111 | 0.427167 | 1.797556 |
| H | -0.709871 | 0.108572 | 2.524484 |
| O | -2.872817 | -1.263084 | 5.872584 |
| N | -2.501030 | 1.307281 | 4.529410 |
| N | -2.670964 | 2.323505 | 5.025439 |

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**$^3$B'**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.7858777

Zero-point correction= 0.718752 (Hartree/Particle)

Thermal correction to Energy= 0.773340

Thermal correction to Enthalpy= 0.774285

Thermal correction to Gibbs Free Energy= 0.615580

Sum of electronic and zero-point Energies= -2488.067126

Sum of electronic and thermal Energies= -2488.012537

Sum of electronic and thermal Enthalpies= -2488.011593

Sum of electronic and thermal Free Energies= -2488.170298

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.625312 | 0.028553 | -0.868920 |
| N | -2.025613 | -1.402094 | -1.043626 |
| C | -1.806029 | -2.773107 | -1.069415 |
| C | -3.031454 | -3.481137 | -1.362098 |
| C | -4.027153 | -2.539785 | -1.463151 |
| C | -3.381606 | -1.236469 | -1.284512 |
| C | -0.611727 | -3.405996 | -0.794704 |
| C | 0.571822 | -2.773611 | -0.405732 |
| N | 0.721146 | -1.410275 | -0.273889 |
| C | 2.026414 | -1.215787 | 0.101414 |
| C | 2.713100 | -2.472765 | 0.232204 |
| C | 1.794064 | -3.454257 | -0.090715 |
| C | 2.610574 | 0.040265 | 0.316632 |
| C | 1.964522 | 1.249682 | 0.179074 |
| N | 0.645842 | 1.420935 | -0.191047 |
| C | 0.422040 | 2.786553 | -0.147821 |
| C | 1.638011 | 3.490820 | 0.236276 |
| C | 2.593665 | 2.540678 | 0.441345 |

| | | | |
|---|---|---|---|
| C | -0.770204 | 3.422355 | -0.398404 |
| C | -1.983621 | 2.792325 | -0.711457 |
| C | -3.225043 | 3.473527 | -0.977737 |
| C | -4.154856 | 2.473984 | -1.276661 |
| C | -3.454144 | 1.234512 | -1.183043 |
| N | -2.134667 | 1.434817 | -0.829851 |
| C | -4.030354 | -0.028370 | -1.394363 |
| H | -0.594711 | -4.488268 | -0.863039 |
| H | -5.070902 | -0.055049 | -1.686087 |
| H | -0.769730 | 4.504520 | -0.345375 |
| H | 3.647409 | 0.057868 | 0.633914 |
| C | -0.849730 | -0.202376 | -3.792019 |
| H | -0.292098 | -0.020853 | -4.729478 |
| H | -1.809802 | 0.339677 | -3.885014 |
| C | 1.751342 | 4.979368 | 0.370599 |
| H | 1.577059 | 5.485643 | -0.587281 |
| H | 1.014371 | 5.377443 | 1.078911 |
| H | 2.742727 | 5.275938 | 0.724790 |
| C | 1.992932 | -4.941199 | -0.125342 |
| H | 1.232364 | -5.468595 | 0.463676 |
| H | 1.937794 | -5.341621 | -1.146530 |
| H | 2.969649 | -5.221945 | 0.280626 |
| C | -3.150394 | -4.973050 | -1.447896 |

| | | | |
|---|---|---|---|
| H | -2.416877 | -5.392771 | -2.146448 |
| H | -2.974483 | -5.449528 | -0.474784 |
| H | -4.144539 | -5.279852 | -1.783011 |
| C | -5.612500 | 2.638072 | -1.583584 |
| H | -5.791969 | 2.918012 | -2.631427 |
| H | -6.172890 | 1.717143 | -1.397667 |
| H | -6.055347 | 3.426331 | -0.964220 |
| C | -5.440726 | -2.830407 | -1.679385 |
| C | -6.513566 | -2.154538 | -1.235589 |
| H | -5.633767 | -3.740271 | -2.249574 |
| H | -7.517968 | -2.496735 | -1.467315 |
| H | -6.430221 | -1.270465 | -0.613239 |
| C | -3.402241 | 4.912530 | -0.897055 |
| C | -4.391988 | 5.667805 | -1.410717 |
| H | -2.627860 | 5.442054 | -0.342043 |
| H | -4.403085 | 6.742450 | -1.253618 |
| H | -5.196581 | 5.257973 | -2.010312 |
| C | 4.161769 | -2.647892 | 0.590025 |
| C | 5.090998 | -2.500170 | -0.627641 |
| H | 4.328855 | -3.633487 | 1.037315 |
| H | 4.466091 | -1.924990 | 1.355441 |
| H | 4.811923 | -3.210708 | -1.415793 |
| H | 4.983326 | -1.510649 | -1.087002 |

| | | | |
|---|---|---|---|
| C | 4.034976 | 2.737440 | 0.815218 |
| C | 4.971539 | 2.657377 | -0.402746 |
| H | 4.349648 | 1.991154 | 1.553571 |
| H | 4.174561 | 3.708416 | 1.300466 |
| H | 4.885294 | 1.686652 | -0.903880 |
| H | 4.682996 | 3.395774 | -1.161346 |
| C | 6.549668 | -2.720064 | -0.304881 |
| O | 7.012246 | -3.047677 | 0.767540 |
| O | 7.343213 | -2.514035 | -1.391105 |
| H | 8.249891 | -2.681939 | -1.084429 |
| C | 6.422788 | 2.893042 | -0.058890 |
| O | 6.868067 | 3.195339 | 1.028154 |
| O | 7.228848 | 2.736237 | -1.143193 |
| H | 8.129851 | 2.911219 | -0.824088 |
| O | -0.103713 | 0.212100 | -2.694789 |
| H | -1.092843 | -1.280989 | -3.769454 |
| C | -2.379796 | -1.681802 | 2.407602 |
| O | -2.714494 | -2.207423 | 3.718845 |
| C | -2.745142 | -1.222628 | 4.661855 |
| C | -2.247104 | -0.001834 | 4.015792 |
| C | -1.775359 | -0.271059 | 2.612113 |
| H | -1.683922 | -2.375321 | 1.935971 |
| H | -3.298541 | -1.640765 | 1.816402 |

| | | | |
|---|---|---|---|
| H | -2.150328 | 0.437223 | 1.868824 |
| H | -0.682013 | -0.287817 | 2.537796 |
| O | -3.113746 | -1.401659 | 5.801224 |
| N | -2.153480 | 1.115306 | 4.665361 |
| N | -2.086301 | 2.098386 | 5.245295 |

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**$^{5}$B'**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.8118892

Zero-point correction= 0.717255 (Hartree/Particle)

Thermal correction to Energy= 0.772605

Thermal correction to Enthalpy= 0.773549

Thermal correction to Gibbs Free Energy= 0.612328

Sum of electronic and zero-point Energies= -2488.094635

Sum of electronic and thermal Energies= -2488.039284

Sum of electronic and thermal Enthalpies= -2488.038340

Sum of electronic and thermal Free Energies= -2488.199561

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.625312 | 0.028553 | -0.868920 |
| N | -2.025613 | -1.402094 | -1.043626 |
| C | -1.806029 | -2.773107 | -1.069415 |
| C | -3.031454 | -3.481137 | -1.362098 |
| C | -4.027153 | -2.539785 | -1.463151 |
| C | -3.381606 | -1.236469 | -1.284512 |
| C | -0.611727 | -3.405996 | -0.794704 |
| C | 0.571822 | -2.773611 | -0.405732 |
| N | 0.721146 | -1.410275 | -0.273889 |
| C | 2.026414 | -1.215787 | 0.101414 |
| C | 2.713100 | -2.472765 | 0.232204 |
| C | 1.794064 | -3.454257 | -0.090715 |
| C | 2.610574 | 0.040265 | 0.316632 |
| C | 1.964522 | 1.249682 | 0.179074 |
| N | 0.645842 | 1.420935 | -0.191047 |
| C | 0.422040 | 2.786553 | -0.147821 |
| C | 1.638011 | 3.490820 | 0.236276 |
| C | 2.593665 | 2.540678 | 0.441345 |
| C | -0.770204 | 3.422355 | -0.398404 |
| C | -1.983621 | 2.792325 | -0.711457 |
| C | -3.225043 | 3.473527 | -0.977737 |
| C | -4.154856 | 2.473984 | -1.276661 |
| C | -3.454144 | 1.234512 | -1.183043 |

| | | | |
|---|---|---|---|
| N | -2.134667 | 1.434817 | -0.829851 |
| C | -4.030354 | -0.028370 | -1.394363 |
| H | -0.594711 | -4.488268 | -0.863039 |
| H | -5.070902 | -0.055049 | -1.686087 |
| H | -0.769730 | 4.504520 | -0.345375 |
| H | 3.647409 | 0.057868 | 0.633914 |
| C | -0.849730 | -0.202376 | -3.792019 |
| H | -0.292098 | -0.020853 | -4.729478 |
| H | -1.809802 | 0.339677 | -3.885014 |
| C | 1.751342 | 4.979368 | 0.370599 |
| H | 1.577059 | 5.485643 | -0.587281 |
| H | 1.014371 | 5.377443 | 1.078911 |
| H | 2.742727 | 5.275938 | 0.724790 |
| C | 1.992932 | -4.941199 | -0.125342 |
| H | 1.232364 | -5.468595 | 0.463676 |
| H | 1.937794 | -5.341621 | -1.146530 |
| H | 2.969649 | -5.221945 | 0.280626 |
| C | -3.150394 | -4.973050 | -1.447896 |
| H | -2.416877 | -5.392771 | -2.146448 |
| H | -2.974483 | -5.449528 | -0.474784 |
| H | -4.144539 | -5.279852 | -1.783011 |
| C | -5.612500 | 2.638072 | -1.583584 |
| H | -5.791969 | 2.918012 | -2.631427 |

| | | | |
|---|---|---|---|
| H | -6.172890 | 1.717143 | -1.397667 |
| H | -6.055347 | 3.426331 | -0.964220 |
| C | -5.440726 | -2.830407 | -1.679385 |
| C | -6.513566 | -2.154538 | -1.235589 |
| H | -5.633767 | -3.740271 | -2.249574 |
| H | -7.517968 | -2.496735 | -1.467315 |
| H | -6.430221 | -1.270465 | -0.613239 |
| C | -3.402241 | 4.912530 | -0.897055 |
| C | -4.391988 | 5.667805 | -1.410717 |
| H | -2.627860 | 5.442054 | -0.342043 |
| H | -4.403085 | 6.742450 | -1.253618 |
| H | -5.196581 | 5.257973 | -2.010312 |
| C | 4.161769 | -2.647892 | 0.590025 |
| C | 5.090998 | -2.500170 | -0.627641 |
| H | 4.328855 | -3.633487 | 1.037315 |
| H | 4.466091 | -1.924990 | 1.355441 |
| H | 4.811923 | -3.210708 | -1.415793 |
| H | 4.983326 | -1.510649 | -1.087002 |
| C | 4.034976 | 2.737440 | 0.815218 |
| C | 4.971539 | 2.657377 | -0.402746 |
| H | 4.349648 | 1.991154 | 1.553571 |
| H | 4.174561 | 3.708416 | 1.300466 |
| H | 4.885294 | 1.686652 | -0.903880 |

| | | | |
|---|---|---|---|
| H | 4.682996 | 3.395774 | -1.161346 |
| C | 6.549668 | -2.720064 | -0.304881 |
| O | 7.012246 | -3.047677 | 0.767540 |
| O | 7.343213 | -2.514035 | -1.391105 |
| H | 8.249891 | -2.681939 | -1.084429 |
| C | 6.422788 | 2.893042 | -0.058890 |
| O | 6.868067 | 3.195339 | 1.028154 |
| O | 7.228848 | 2.736237 | -1.143193 |
| H | 8.129851 | 2.911219 | -0.824088 |
| O | -0.103713 | 0.212100 | -2.694789 |
| H | -1.092843 | -1.280989 | -3.769454 |
| C | -2.379796 | -1.681802 | 2.407602 |
| O | -2.714494 | -2.207423 | 3.718845 |
| C | -2.745142 | -1.222628 | 4.661855 |
| C | -2.247104 | -0.001834 | 4.015792 |
| C | -1.775359 | -0.271059 | 2.612113 |
| H | -1.683922 | -2.375321 | 1.935971 |
| H | -3.298541 | -1.640765 | 1.816402 |
| H | -2.150328 | 0.437223 | 1.868824 |
| H | -0.682013 | -0.287817 | 2.537796 |
| O | -3.113746 | -1.401659 | 5.801224 |
| N | -2.153480 | 1.115306 | 4.665361 |
| N | -2.086301 | 2.098386 | 5.245295 |

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$^{OSS}$**B**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.7641303

Zero-point correction= 0.720852 (Hartree/Particle)

Thermal correction to Energy= 0.773342

Thermal correction to Enthalpy= 0.774286

Thermal correction to Gibbs Free Energy= 0.629372

Sum of electronic and zero-point Energies= -2488.043279

Sum of electronic and thermal Energies= -2487.990788

Sum of electronic and thermal Enthalpies= -2487.989844

Sum of electronic and thermal Free Energies= -2488.134758

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.873317 | 0.003766 | -0.135510 |
| N | -2.255308 | -1.436535 | -0.480627 |
| C | -2.053683 | -2.790885 | -0.527654 |
| C | -3.291339 | -3.482235 | -0.811908 |
| C | -4.262248 | -2.513824 | -0.917692 |

| | | | |
|---|---|---|---|
| C | -3.581328 | -1.234348 | -0.739430 |
| C | -0.827007 | -3.425268 | -0.353999 |
| C | 0.383198 | -2.789546 | -0.109234 |
| N | 0.546026 | -1.436770 | 0.046932 |
| C | 1.883473 | -1.233191 | 0.251535 |
| C | 2.596498 | -2.501831 | 0.242665 |
| C | 1.657241 | -3.473987 | 0.014924 |
| C | 2.488218 | 0.006083 | 0.449361 |
| C | 1.849569 | 1.243400 | 0.423926 |
| N | 0.514312 | 1.437279 | 0.220890 |
| C | 0.323934 | 2.790692 | 0.187499 |
| C | 1.578251 | 3.488998 | 0.419129 |
| C | 2.534411 | 2.522761 | 0.568492 |
| C | -0.879654 | 3.427650 | -0.077632 |
| C | -2.088728 | 2.795698 | -0.347144 |
| C | -3.327561 | 3.493682 | -0.682366 |
| C | -4.263653 | 2.511539 | -0.918513 |
| C | -3.580194 | 1.245769 | -0.727937 |
| N | -2.275723 | 1.449013 | -0.373902 |
| C | -4.187297 | 0.005790 | -0.892102 |
| H | -0.812693 | -4.506563 | -0.438320 |
| H | -5.229467 | 0.000232 | -1.183074 |
| H | -0.867235 | 4.511185 | -0.096772 |

| | | | |
|---|---|---|---|
| H | 3.557557 | 0.007746 | 0.632934 |
| C | -0.358434 | -0.836487 | -2.846671 |
| H | -0.150021 | -0.425753 | -3.850052 |
| H | -1.264524 | -1.461490 | -2.934365 |
| C | 1.732747 | 4.978949 | 0.475621 |
| H | 1.501090 | 5.450633 | -0.488023 |
| H | 1.060303 | 5.421550 | 1.219908 |
| H | 2.754234 | 5.265027 | 0.743414 |
| C | 1.851790 | -4.956638 | -0.101283 |
| H | 1.186995 | -5.505680 | 0.576389 |
| H | 1.640842 | -5.318240 | -1.116047 |
| H | 2.878626 | -5.245304 | 0.141941 |
| C | -3.451128 | -4.970138 | -0.893341 |
| H | -2.740358 | -5.417772 | -1.598833 |
| H | -3.282466 | -5.446913 | 0.080718 |
| H | -4.458893 | -5.244921 | -1.216942 |
| C | -5.715524 | 2.671802 | -1.248431 |
| H | -5.896890 | 2.690664 | -2.332090 |
| H | -6.312604 | 1.853306 | -0.835138 |
| H | -6.101358 | 3.611138 | -0.839816 |
| C | -5.687732 | -2.742357 | -1.143450 |
| C | -6.706649 | -2.067029 | -0.590223 |
| H | -5.931058 | -3.575495 | -1.805218 |

| | | | |
|---|---|---|---|
| H | -7.736734 | -2.323080 | -0.822467 |
| H | -6.542812 | -1.271808 | 0.129517 |
| C | -3.475419 | 4.942471 | -0.695319 |
| C | -4.352665 | 5.670318 | -1.407137 |
| H | -2.791339 | 5.486149 | -0.043788 |
| H | -4.383779 | 6.751886 | -1.311702 |
| H | -5.043938 | 5.224001 | -2.114024 |
| C | 4.081878 | -2.669784 | 0.394220 |
| C | 4.838599 | -2.428809 | -0.923410 |
| H | 4.317000 | -3.677371 | 0.751591 |
| H | 4.474319 | -1.988649 | 1.157526 |
| H | 4.462298 | -3.092592 | -1.712085 |
| H | 4.665909 | -1.413779 | -1.298763 |
| C | 4.011084 | 2.704650 | 0.776895 |
| C | 4.800324 | 2.658919 | -0.543015 |
| H | 4.406306 | 1.939207 | 1.453792 |
| H | 4.209890 | 3.661652 | 1.269801 |
| H | 4.650536 | 1.703563 | -1.059446 |
| H | 4.431187 | 3.420072 | -1.241628 |
| C | 6.328164 | -2.651008 | -0.808894 |
| O | 6.923712 | -3.067374 | 0.162112 |
| O | 6.974108 | -2.333976 | -1.962992 |
| H | 7.913767 | -2.513836 | -1.792712 |

| | | | |
|---|---|---|---|
| C | 6.284248 | 2.875988 | -0.365577 |
| O | 6.860746 | 3.119277 | 0.673280 |
| O | 6.952308 | 2.775248 | -1.546771 |
| H | 7.886439 | 2.932097 | -1.329817 |
| O | -0.503800 | 0.217810 | -1.949809 |
| H | 0.477660 | -1.513350 | -2.594811 |
| C | -0.553283 | -2.041208 | 3.165951 |
| O | -1.975415 | -2.114776 | 2.948979 |
| C | -2.449285 | -0.931472 | 2.413795 |
| C | -1.303718 | -0.018608 | 2.133394 |
| C | -0.166686 | -0.565766 | 3.003079 |
| H | -0.351223 | -2.433880 | 4.169495 |
| H | -0.055674 | -2.682081 | 2.434116 |
| H | 0.828893 | -0.444958 | 2.576933 |
| H | -0.172897 | -0.051912 | 3.975465 |
| O | -3.641751 | -0.773453 | 2.267747 |
| N | -1.693999 | 1.349132 | 2.466954 |
| N | -1.000078 | 2.163726 | 2.982115 |

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**$^{3}$B**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.7639103

Zero-point correction= 0.720859 (Hartree/Particle)

Thermal correction to Energy= 0.773348

Thermal correction to Enthalpy= 0.774292

Thermal correction to Gibbs Free Energy= 0.628357

Sum of electronic and zero-point Energies= -2488.043051

Sum of electronic and thermal Energies= -2487.990562

Sum of electronic and thermal Enthalpies= -2487.989618

Sum of electronic and thermal Free Energies= -2488.135554

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.873558 | 0.003734 | -0.134815 |
| N | -2.255323 | -1.436593 | -0.480847 |
| C | -2.053591 | -2.790920 | -0.528427 |
| C | -3.291302 | -3.482269 | -0.812334 |
| C | -4.262396 | -2.513917 | -0.917120 |
| C | -3.581515 | -1.234450 | -0.738767 |
| C | -0.826758 | -3.425235 | -0.355514 |
| C | 0.383378 | -2.789476 | -0.110509 |
| N | 0.546024 | -1.436746 | 0.046272 |
| C | 1.883357 | -1.233085 | 0.251376 |

| | | | |
|---|---|---|---|
| C | 2.596555 | -2.501646 | 0.242092 |
| C | 1.657489 | -3.473807 | 0.013580 |
| C | 2.487963 | 0.006192 | 0.449735 |
| C | 1.849267 | 1.243501 | 0.424229 |
| N | 0.514104 | 1.437391 | 0.220958 |
| C | 0.323726 | 2.790760 | 0.187280 |
| C | 1.578061 | 3.489117 | 0.418829 |
| C | 2.534168 | 2.522905 | 0.568556 |
| C | -0.879864 | 3.427679 | -0.077965 |
| C | -2.089044 | 2.795678 | -0.346961 |
| C | -3.327912 | 3.493606 | -0.682261 |
| C | -4.264180 | 2.511428 | -0.917528 |
| C | -3.580694 | 1.245683 | -0.726682 |
| N | -2.276153 | 1.449037 | -0.373008 |
| C | -4.187731 | 0.005683 | -0.890787 |
| H | -0.812338 | -4.506491 | -0.440324 |
| H | -5.230027 | 0.000051 | -1.181314 |
| H | -0.867424 | 4.511209 | -0.097386 |
| H | 3.557253 | 0.007880 | 0.633565 |
| C | -0.359483 | -0.834673 | -2.846214 |
| H | -0.150376 | -0.422951 | -3.849010 |
| H | -1.266084 | -1.458729 | -2.934793 |
| C | 1.732575 | 4.979077 | 0.474983 |

| | | | |
|---|---|---|---|
| H | 1.500759 | 5.450567 | -0.488717 |
| H | 1.060260 | 5.421829 | 1.219299 |
| H | 2.754106 | 5.265202 | 0.742552 |
| C | 1.852246 | -4.956383 | -0.103236 |
| H | 1.187504 | -5.505794 | 0.574190 |
| H | 1.641375 | -5.317597 | -1.118154 |
| H | 2.879112 | -5.245012 | 0.139902 |
| C | -3.450983 | -4.970158 | -0.894327 |
| H | -2.741245 | -5.417313 | -1.601172 |
| H | -3.280718 | -5.447425 | 0.079205 |
| H | -4.459213 | -5.244902 | -1.216496 |
| C | -5.716169 | 2.671570 | -1.246968 |
| H | -5.897989 | 2.689648 | -2.330565 |
| H | -6.313132 | 1.853414 | -0.832823 |
| H | -6.101762 | 3.611225 | -0.838869 |
| C | -5.688037 | -2.742409 | -1.141978 |
| C | -6.706471 | -2.067447 | -0.587416 |
| H | -5.931875 | -3.575081 | -1.804143 |
| H | -7.736764 | -2.323288 | -0.818972 |
| H | -6.541950 | -1.272758 | 0.132761 |
| C | -3.475619 | 4.942413 | -0.695973 |
| C | -4.352863 | 5.669969 | -1.408084 |
| H | -2.791386 | 5.486373 | -0.044838 |

| | | | |
|---|---|---|---|
| H | -4.383848 | 6.751592 | -1.313229 |
| H | -5.044249 | 5.223349 | -2.114669 |
| C | 4.081901 | -2.669521 | 0.394047 |
| C | 4.839055 | -2.427890 | -0.923216 |
| H | 4.317001 | -3.677250 | 0.751027 |
| H | 4.474016 | -1.988703 | 1.157805 |
| H | 4.462956 | -3.091267 | -1.712335 |
| H | 4.666561 | -1.412665 | -1.298117 |
| C | 4.010823 | 2.704792 | 0.777068 |
| C | 4.800201 | 2.658636 | -0.542747 |
| H | 4.405951 | 1.939557 | 1.454255 |
| H | 4.209599 | 3.661944 | 1.269694 |
| H | 4.650347 | 1.703160 | -1.058940 |
| H | 4.431231 | 3.419647 | -1.241600 |
| C | 6.328566 | -2.650302 | -0.808359 |
| O | 6.923683 | -3.067934 | 0.162366 |
| O | 6.974977 | -2.332086 | -1.961868 |
| H | 7.914542 | -2.512326 | -1.791463 |
| C | 6.284141 | 2.875535 | -0.365223 |
| O | 6.860653 | 3.118449 | 0.673713 |
| O | 6.952243 | 2.774845 | -1.546402 |
| H | 7.886398 | 2.931441 | -1.329368 |
| O | -0.504317 | 0.219006 | -1.948391 |

| | | | |
|---|---|---|---|
| H | 0.475946 | -1.512375 | -2.594666 |
| C | -0.553126 | -2.042512 | 3.164480 |
| O | -1.975230 | -2.115445 | 2.947252 |
| C | -2.448435 | -0.931579 | 2.412564 |
| C | -1.302246 | -0.019407 | 2.131078 |
| C | -0.166213 | -0.567122 | 3.002429 |
| H | -0.351338 | -2.435781 | 4.167861 |
| H | -0.055555 | -2.683172 | 2.432422 |
| H | 0.829910 | -0.446257 | 2.577540 |
| H | -0.173567 | -0.053845 | 3.975062 |
| O | -3.640905 | -0.772884 | 2.267135 |
| N | -1.692819 | 1.348500 | 2.467130 |
| N | -0.999168 | 2.163280 | 2.981948 |

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**$^{CSS}$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2488.7340614

Zero-point correction= 0.718537 (Hartree/Particle)

Thermal correction to Energy= 0.770902

Thermal correction to Enthalpy= 0.771847

Thermal correction to Gibbs Free Energy= 0.627476

Sum of electronic and zero-point Energies= -2488.015524

Sum of electronic and thermal Energies= -2487.963159

Sum of electronic and thermal Enthalpies= -2487.962215

Sum of electronic and thermal Free Energies= -2488.106586

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.895439 | -0.005865 | -0.046582 |
| N | -2.301041 | -1.451297 | -0.421081 |
| C | -2.052535 | -2.781644 | -0.620701 |
| C | -3.272776 | -3.484878 | -0.968713 |
| C | -4.277734 | -2.546066 | -0.963570 |
| C | -3.628298 | -1.266216 | -0.664717 |
| C | -0.804599 | -3.394588 | -0.517095 |
| C | 0.400816 | -2.775267 | -0.199086 |
| N | 0.557508 | -1.440459 | 0.061490 |
| C | 1.882644 | -1.255863 | 0.328257 |
| C | 2.599882 | -2.523586 | 0.266643 |
| C | 1.672033 | -3.472490 | -0.075518 |
| C | 2.473895 | -0.014609 | 0.575742 |
| C | 1.841253 | 1.221866 | 0.476989 |
| N | 0.508239 | 1.404517 | 0.205754 |

| | | | |
|---|---|---|---|
| C | 0.331424 | 2.758314 | 0.070822 |
| C | 1.587897 | 3.461992 | 0.272649 |
| C | 2.528243 | 2.505789 | 0.544499 |
| C | -0.878946 | 3.388904 | -0.192755 |
| C | -2.113490 | 2.762935 | -0.353606 |
| C | -3.361598 | 3.462744 | -0.664118 |
| C | -4.316692 | 2.480944 | -0.809225 |
| C | -3.635351 | 1.216480 | -0.598837 |
| N | -2.314826 | 1.418486 | -0.295981 |
| C | -4.247682 | -0.023344 | -0.750091 |
| H | -0.769302 | -4.462612 | -0.708860 |
| H | -5.293699 | -0.023238 | -1.028119 |
| H | -0.853196 | 4.468653 | -0.290364 |
| H | 3.535783 | -0.008994 | 0.801999 |
| C | 0.514118 | 0.083052 | -2.610611 |
| H | 0.363000 | 0.102437 | -3.708123 |
| H | 1.197037 | -0.770230 | -2.413434 |
| C | 1.761126 | 4.949700 | 0.201027 |
| H | 1.561255 | 5.336211 | -0.806650 |
| H | 1.075351 | 5.468537 | 0.882177 |
| H | 2.778891 | 5.247922 | 0.470599 |
| C | 1.877522 | -4.941138 | -0.301058 |
| H | 1.188868 | -5.545819 | 0.301971 |

| | | | |
|---|---|---|---|
| H | 1.708786 | -5.220910 | -1.349217 |
| H | 2.895381 | -5.247713 | -0.040829 |
| C | -3.377472 | -4.958317 | -1.223309 |
| H | -2.669351 | -5.286197 | -1.994327 |
| H | -3.161340 | -5.544509 | -0.320254 |
| H | -4.381667 | -5.237211 | -1.554697 |
| C | -5.780155 | 2.642764 | -1.083288 |
| H | -6.005002 | 2.646287 | -2.159034 |
| H | -6.363141 | 1.833291 | -0.633762 |
| H | -6.146951 | 3.590123 | -0.674577 |
| C | -5.694102 | -2.801785 | -1.201758 |
| C | -6.740799 | -2.172659 | -0.643060 |
| H | -5.910574 | -3.622233 | -1.888276 |
| H | -7.759410 | -2.453757 | -0.895807 |
| H | -6.614235 | -1.387832 | 0.095348 |
| C | -3.492821 | 4.909765 | -0.743220 |
| C | -4.415974 | 5.621423 | -1.413963 |
| H | -2.746904 | 5.474428 | -0.183087 |
| H | -4.418522 | 6.706895 | -1.370959 |
| H | -5.173142 | 5.157792 | -2.036839 |
| C | 4.079141 | -2.702832 | 0.459719 |
| C | 4.877996 | -2.420446 | -0.824416 |
| H | 4.300745 | -3.723192 | 0.790139 |

| | | | |
|---|---|---|---|
| H | 4.450574 | -2.049154 | 1.256961 |
| H | 4.532596 | -3.061983 | -1.644607 |
| H | 4.708298 | -1.395952 | -1.175512 |
| C | 3.998453 | 2.698205 | 0.788460 |
| C | 4.831460 | 2.568006 | -0.498417 |
| H | 4.368751 | 1.975522 | 1.524072 |
| H | 4.186066 | 3.684071 | 1.226623 |
| H | 4.692448 | 1.582879 | -0.958787 |
| H | 4.490452 | 3.285153 | -1.255341 |
| C | 6.364954 | -2.631134 | -0.667268 |
| O | 6.938373 | -3.028543 | 0.325174 |
| O | 7.040560 | -2.324978 | -1.807644 |
| H | 7.976497 | -2.492584 | -1.607258 |
| C | 6.309710 | 2.789559 | -0.284538 |
| O | 6.853603 | 3.087555 | 0.757986 |
| O | 7.016075 | 2.622250 | -1.435438 |
| H | 7.943392 | 2.786235 | -1.195812 |
| O | -0.703743 | -0.004753 | -1.968842 |
| H | 1.089898 | 1.000181 | -2.359178 |
| C | -1.162729 | -2.348588 | 2.964264 |
| O | -2.549448 | -1.965536 | 2.870330 |
| C | -2.650325 | -0.683586 | 2.384436 |
| C | -1.271147 | -0.202301 | 1.975554 |

| | | | |
|---|---|---|---|
| C | -0.373215 | -1.031315 | 2.910248 |
| H | -1.032748 | -2.894923 | 3.903855 |
| H | -0.916031 | -3.002556 | 2.125639 |
| H | 0.640476 | -1.156462 | 2.534484 |
| H | -0.326268 | -0.601851 | 3.919843 |
| O | -3.713038 | -0.112300 | 2.356869 |
| N | -1.227230 | 1.322350 | 2.666059 |
| N | -0.540574 | 2.213188 | 2.750248 |

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**$^{OSS}$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2488.7571881

Zero-point correction= 0.718756 (Hartree/Particle)

Thermal correction to Energy= 0.771273

Thermal correction to Enthalpy= 0.772218

Thermal correction to Gibbs Free Energy= 0.627656

Sum of electronic and zero-point Energies= -2488.038433

Sum of electronic and thermal Energies= -2487.985915

Sum of electronic and thermal Enthalpies= -2487.984970

Sum of electronic and thermal Free Energies= -2488.129532

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.880041 | 0.000951 | -0.130466 |
| N | -2.237568 | -1.443454 | -0.539611 |
| C | -2.027435 | -2.795648 | -0.562942 |
| C | -3.255045 | -3.499153 | -0.867407 |
| C | -4.230204 | -2.539627 | -0.998762 |
| C | -3.560441 | -1.253292 | -0.809073 |
| C | -0.805782 | -3.421722 | -0.336073 |
| C | 0.398024 | -2.778406 | -0.074605 |
| N | 0.555216 | -1.423343 | 0.048625 |
| C | 1.891210 | -1.205346 | 0.242472 |
| C | 2.611090 | -2.470553 | 0.262480 |
| C | 1.675091 | -3.453729 | 0.068498 |
| C | 2.489801 | 0.042295 | 0.411593 |
| C | 1.839527 | 1.274083 | 0.404964 |
| N | 0.496234 | 1.453867 | 0.246689 |
| C | 0.284294 | 2.801969 | 0.266098 |
| C | 1.534690 | 3.514673 | 0.486042 |
| C | 2.510547 | 2.559786 | 0.567896 |
| C | -0.934613 | 3.426445 | 0.035388 |
| C | -2.126737 | 2.785200 | -0.284908 |

| | | | |
|---|---|---|---|
| C | -3.370079 | 3.476022 | -0.618028 |
| C | -4.285876 | 2.489067 | -0.909873 |
| C | -3.587719 | 1.227383 | -0.749032 |
| N | -2.291568 | 1.437269 | -0.367560 |
| C | -4.177311 | -0.016365 | -0.950309 |
| H | -0.786462 | -4.504591 | -0.395282 |
| H | -5.214321 | -0.026676 | -1.259015 |
| H | -0.942473 | 4.510084 | 0.059677 |
| H | 3.562580 | 0.053349 | 0.574525 |
| C | -0.400956 | -0.768989 | -2.878356 |
| H | -0.059564 | -0.363915 | -3.847898 |
| H | -1.386347 | -1.237705 | -3.054667 |
| C | 1.669221 | 5.005030 | 0.578341 |
| H | 1.425133 | 5.496459 | -0.372389 |
| H | 0.995806 | 5.422980 | 1.336081 |
| H | 2.688515 | 5.298764 | 0.846493 |
| C | 1.876014 | -4.938089 | -0.006998 |
| H | 1.211974 | -5.470126 | 0.684607 |
| H | 1.668427 | -5.328083 | -1.011921 |
| H | 2.903626 | -5.215866 | 0.245617 |
| C | -3.401722 | -4.988744 | -0.937197 |
| H | -2.658073 | -5.439876 | -1.605325 |
| H | -3.272225 | -5.450846 | 0.049858 |

| | | | |
|---|---|---|---|
| H | -4.392751 | -5.275475 | -1.299956 |
| C | -5.732275 | 2.641350 | -1.266810 |
| H | -5.888626 | 2.704137 | -2.352671 |
| H | -6.326018 | 1.796826 | -0.904137 |
| H | -6.143022 | 3.556207 | -0.827886 |
| C | -5.645991 | -2.785776 | -1.260450 |
| C | -6.694476 | -2.113830 | -0.760397 |
| H | -5.857778 | -3.637075 | -1.909912 |
| H | -7.711090 | -2.392441 | -1.023666 |
| H | -6.572466 | -1.298964 | -0.054790 |
| C | -3.540897 | 4.921850 | -0.581619 |
| C | -4.417687 | 5.662375 | -1.280945 |
| H | -2.876160 | 5.452165 | 0.100314 |
| H | -4.466647 | 6.739148 | -1.146658 |
| H | -5.090320 | 5.232539 | -2.015410 |
| C | 4.098211 | -2.626922 | 0.409951 |
| C | 4.846465 | -2.413660 | -0.917281 |
| H | 4.340764 | -3.624306 | 0.790224 |
| H | 4.491320 | -1.925405 | 1.154258 |
| H | 4.471789 | -3.100322 | -1.686871 |
| H | 4.663547 | -1.410027 | -1.317698 |
| C | 3.991318 | 2.757982 | 0.725357 |
| C | 4.732356 | 2.733420 | -0.622765 |

| | | | |
|---|---|---|---|
| H | 4.420569 | 1.990661 | 1.379363 |
| H | 4.197166 | 3.712785 | 1.219749 |
| H | 4.574719 | 1.780977 | -1.142065 |
| H | 4.328848 | 3.496143 | -1.300328 |
| C | 6.338350 | -2.620282 | -0.804602 |
| O | 6.942652 | -3.003538 | 0.174636 |
| O | 6.975863 | -2.331067 | -1.970764 |
| H | 7.917754 | -2.498548 | -1.800183 |
| C | 6.218894 | 2.967094 | -0.496437 |
| O | 6.828692 | 3.210534 | 0.523372 |
| O | 6.845918 | 2.882280 | -1.700858 |
| H | 7.785304 | 3.048669 | -1.516125 |
| O | -0.440494 | 0.255321 | -1.939183 |
| H | 0.296624 | -1.583632 | -2.608566 |
| C | -0.070642 | -1.712980 | 3.349777 |
| O | -1.418954 | -2.187488 | 3.197086 |
| C | -2.154158 | -1.292858 | 2.431534 |
| C | -1.277444 | -0.168935 | 1.979465 |
| C | -0.094687 | -0.231570 | 2.942795 |
| H | 0.223964 | -1.876510 | 4.392953 |
| H | 0.588485 | -2.302120 | 2.703845 |
| H | 0.852166 | 0.085571 | 2.508858 |
| H | -0.279878 | 0.401138 | 3.822263 |

O -3.335771 -1.494221 2.254599

N -2.282444 1.226321 2.459743

N -1.849099 2.087528 3.086264

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**$^{3}$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2488.7568722

Zero-point correction= 0.718678 (Hartree/Particle)

Thermal correction to Energy= 0.771230

Thermal correction to Enthalpy= 0.772174

Thermal correction to Gibbs Free Energy= 0.626046

Sum of electronic and zero-point Energies= -2488.038194

Sum of electronic and thermal Energies= -2487.985642

Sum of electronic and thermal Enthalpies= -2487.984698

Sum of electronic and thermal Free Energies= -2488.130826

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Cartesian Coordinates

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Fe -0.874290 -0.006163 -0.130143

N -2.239929 -1.452662 -0.507114

| | | | |
|---|---|---|---|
| C | -2.034006 | -2.805866 | -0.530980 |
| C | -3.265559 | -3.504306 | -0.827143 |
| C | -4.236988 | -2.539853 | -0.960245 |
| C | -3.562137 | -1.256246 | -0.781851 |
| C | -0.809151 | -3.434915 | -0.321921 |
| C | 0.398098 | -2.793713 | -0.077231 |
| N | 0.558738 | -1.438369 | 0.048918 |
| C | 1.894817 | -1.226859 | 0.246185 |
| C | 2.612403 | -2.494108 | 0.258896 |
| C | 1.674627 | -3.473261 | 0.058687 |
| C | 2.494404 | 0.017934 | 0.430361 |
| C | 1.846870 | 1.251370 | 0.417561 |
| N | 0.508015 | 1.437751 | 0.231487 |
| C | 0.305334 | 2.789255 | 0.220892 |
| C | 1.556529 | 3.495175 | 0.451502 |
| C | 2.522889 | 2.534759 | 0.572803 |
| C | -0.904027 | 3.419507 | -0.037267 |
| C | -2.103510 | 2.781849 | -0.339454 |
| C | -3.342702 | 3.475149 | -0.686608 |
| C | -4.266886 | 2.488527 | -0.949702 |
| C | -3.576332 | 1.225564 | -0.761007 |
| N | -2.278911 | 1.435247 | -0.386802 |
| C | -4.172272 | -0.018079 | -0.939759 |

| | | | |
|---|---|---|---|
| H | -0.792850 | -4.517731 | -0.384619 |
| H | -5.210083 | -0.028746 | -1.246006 |
| H | -0.900787 | 4.503445 | -0.039172 |
| H | 3.565277 | 0.026511 | 0.605000 |
| C | -0.260341 | -0.825981 | -2.841361 |
| H | -0.113333 | -0.419069 | -3.857835 |
| H | -1.094503 | -1.548499 | -2.902290 |
| C | 1.700982 | 4.985740 | 0.522359 |
| H | 1.472107 | 5.464168 | -0.438678 |
| H | 1.021500 | 5.419350 | 1.265646 |
| H | 2.719062 | 5.276066 | 0.798577 |
| C | 1.871901 | -4.957652 | -0.026061 |
| H | 1.208325 | -5.493098 | 0.663551 |
| H | 1.661129 | -5.341249 | -1.032776 |
| H | 2.899391 | -5.239323 | 0.222693 |
| C | -3.419399 | -4.993479 | -0.896108 |
| H | -2.695585 | -5.445685 | -1.585213 |
| H | -3.265370 | -5.460094 | 0.085300 |
| H | -4.420825 | -5.275030 | -1.233298 |
| C | -5.713686 | 2.641829 | -1.304232 |
| H | -5.874496 | 2.678202 | -2.390686 |
| H | -6.311313 | 1.810943 | -0.917266 |
| H | -6.116133 | 3.570393 | -0.886898 |

| | | | |
|---|---|---|---|
| C | -5.656492 | -2.777405 | -1.212367 |
| C | -6.692428 | -2.101644 | -0.692124 |
| H | -5.880890 | -3.620503 | -1.868232 |
| H | -7.714995 | -2.367895 | -0.945141 |
| H | -6.551894 | -1.295468 | 0.020191 |
| C | -3.501285 | 4.922664 | -0.686090 |
| C | -4.376238 | 5.652856 | -1.398590 |
| H | -2.827577 | 5.464583 | -0.022254 |
| H | -4.415140 | 6.733078 | -1.291419 |
| H | -5.057267 | 5.210346 | -2.117623 |
| C | 4.099173 | -2.653807 | 0.405009 |
| C | 4.847527 | -2.427494 | -0.920001 |
| H | 4.340639 | -3.655379 | 0.774873 |
| H | 4.493041 | -1.960444 | 1.156569 |
| H | 4.471747 | -3.105339 | -1.696823 |
| H | 4.665714 | -1.419364 | -1.309512 |
| C | 4.001040 | 2.726111 | 0.761290 |
| C | 4.771779 | 2.691855 | -0.569868 |
| H | 4.411371 | 1.959947 | 1.428494 |
| H | 4.200692 | 3.682191 | 1.255703 |
| H | 4.622616 | 1.737364 | -1.087877 |
| H | 4.386238 | 3.452653 | -1.260010 |
| C | 6.339192 | -2.637001 | -0.809960 |

| | | | |
|---|---|---|---|
| O | 6.943647 | -3.028469 | 0.165939 |
| O | 6.976157 | -2.339781 | -1.974350 |
| H | 7.918038 | -2.509299 | -1.805773 |
| C | 6.255983 | 2.921599 | -0.412086 |
| O | 6.843336 | 3.173944 | 0.618595 |
| O | 6.909923 | 2.821924 | -1.601075 |
| H | 7.845340 | 2.987792 | -1.396745 |
| O | -0.502851 | 0.219086 | -1.957676 |
| H | 0.647870 | -1.407058 | -2.594536 |
| C | -0.428549 | -1.910949 | 3.301973 |
| O | -1.848887 | -2.082016 | 3.157703 |
| C | -2.379256 | -1.036761 | 2.412919 |
| C | -1.284227 | -0.119034 | 1.974158 |
| C | -0.141224 | -0.448543 | 2.930718 |
| H | -0.166048 | -2.161987 | 4.336232 |
| H | 0.082476 | -2.608767 | 2.630759 |
| H | 0.852342 | -0.322652 | 2.502938 |
| H | -0.195671 | 0.186589 | 3.825978 |
| O | -3.576992 | -0.978501 | 2.239623 |
| N | -1.973603 | 1.455964 | 2.490555 |
| N | -1.360653 | 2.190795 | 3.127534 |

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**$^{5}$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2488.745154

Zero-point correction= 0.718145 (Hartree/Particle)

Thermal correction to Energy= 0.770425

Thermal correction to Enthalpy= 0.771369

Thermal correction to Gibbs Free Energy= 0.629035

Sum of electronic and zero-point Energies= -2488.027009

Sum of electronic and thermal Energies= -2487.974729

Sum of electronic and thermal Enthalpies= -2487.973785

Sum of electronic and thermal Free Energies= -2488.116119

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.891075 | 0.007279 | -0.085674 |
| N | -2.118579 | -1.644280 | -0.519256 |
| C | -1.721088 | -2.944992 | -0.586074 |
| C | -2.861638 | -3.785059 | -0.906300 |
| C | -3.954115 | -2.946781 | -1.002176 |
| C | -3.450078 | -1.587326 | -0.775951 |
| C | -0.403475 | -3.389058 | -0.391044 |

| | | | |
|---|---|---|---|
| C | 0.734386 | -2.618744 | -0.119635 |
| N | 0.756769 | -1.259987 | 0.045752 |
| C | 2.051504 | -0.879054 | 0.240668 |
| C | 2.907845 | -2.061307 | 0.226020 |
| C | 2.088632 | -3.142327 | -0.000679 |
| C | 2.499532 | 0.441224 | 0.417103 |
| C | 1.729818 | 1.613770 | 0.416927 |
| N | 0.376449 | 1.654148 | 0.306224 |
| C | -0.003367 | 2.959876 | 0.248371 |
| C | 1.175287 | 3.816971 | 0.384494 |
| C | 2.255448 | 2.979091 | 0.486769 |
| C | -1.307279 | 3.410015 | 0.012811 |
| C | -2.451347 | 2.644131 | -0.262662 |
| C | -3.770817 | 3.188739 | -0.605844 |
| C | -4.582597 | 2.101362 | -0.859159 |
| C | -3.755705 | 0.915980 | -0.674936 |
| N | -2.498458 | 1.290462 | -0.302188 |
| C | -4.189936 | -0.401428 | -0.876495 |
| H | -0.242088 | -4.458713 | -0.486136 |
| H | -5.222875 | -0.519161 | -1.180793 |
| H | -1.435710 | 4.487200 | -0.017041 |
| H | 3.569392 | 0.571694 | 0.534730 |
| C | -0.016985 | -0.584175 | -2.789503 |

| | | | |
|---|---|---|---|
| H | -0.485867 | -1.584042 | -2.785374 |
| H | 1.057854 | -0.726724 | -2.576301 |
| C | 1.153646 | 5.315978 | 0.381916 |
| H | 0.799060 | 5.715019 | -0.577025 |
| H | 0.486282 | 5.710102 | 1.158078 |
| H | 2.149863 | 5.731883 | 0.560879 |
| C | 2.465225 | -4.589410 | -0.120755 |
| H | 1.877329 | -5.216908 | 0.559900 |
| H | 2.292032 | -4.972051 | -1.134912 |
| H | 3.522031 | -4.752609 | 0.111850 |
| C | -2.827376 | -5.278037 | -1.033279 |
| H | -2.015185 | -5.609173 | -1.691666 |
| H | -2.670580 | -5.761475 | -0.060132 |
| H | -3.764689 | -5.669192 | -1.439354 |
| C | -6.038550 | 2.095900 | -1.209902 |
| H | -6.205681 | 2.133746 | -2.295387 |
| H | -6.535640 | 1.194494 | -0.838560 |
| H | -6.544460 | 2.964338 | -0.775456 |
| C | -5.327863 | -3.362828 | -1.268035 |
| C | -6.450941 | -2.820051 | -0.772242 |
| H | -5.434896 | -4.232078 | -1.919527 |
| H | -7.426467 | -3.215802 | -1.040752 |
| H | -6.429259 | -1.996854 | -0.066085 |

| | | | |
|---|---|---|---|
| C | -4.093723 | 4.608487 | -0.612515 |
| C | -5.057151 | 5.232229 | -1.312358 |
| H | -3.471862 | 5.227690 | 0.034333 |
| H | -5.212072 | 6.302579 | -1.210907 |
| H | -5.698626 | 4.712668 | -2.015892 |
| C | 4.399475 | -2.059288 | 0.404986 |
| C | 5.165428 | -1.738784 | -0.914969 |
| H | 4.736040 | -3.034887 | 0.772882 |
| H | 4.691836 | -1.318846 | 1.157839 |
| H | 4.898268 | -2.477307 | -1.675013 |
| H | 4.883533 | -0.744740 | -1.263928 |
| C | 3.717258 | 3.318524 | 0.576256 |
| C | 4.453478 | 3.221129 | -0.794785 |
| H | 4.202017 | 2.643699 | 1.287664 |
| H | 3.847133 | 4.329598 | 0.976679 |
| H | 3.836405 | 2.625223 | -1.479001 |
| H | 4.583503 | 4.201951 | -1.257052 |
| C | 6.655255 | -1.764402 | -0.698801 |
| O | 7.369800 | -0.815613 | -0.410169 |
| O | 7.176161 | -3.006689 | -0.806316 |
| H | 8.123546 | -2.919192 | -0.605274 |
| C | 5.806959 | 2.537033 | -0.781559 |
| O | 6.783236 | 2.901262 | -1.404452 |

| | | | |
|---|---|---|---|
| O | 5.784610 | 1.407680 | -0.040437 |
| H | 6.592020 | 0.869047 | -0.196830 |
| O | -0.638265 | 0.316230 | -1.928616 |
| H | -0.091968 | -0.199558 | -3.822311 |
| C | 0.019681 | -1.774056 | 3.295231 |
| O | -1.328541 | -2.258105 | 3.163040 |
| C | -2.094796 | -1.352503 | 2.447015 |
| C | -1.240523 | -0.200242 | 2.010583 |
| C | -0.030103 | -0.281789 | 2.935261 |
| H | 0.340998 | -1.965599 | 4.325451 |
| H | 0.665903 | -2.335934 | 2.614006 |
| H | 0.899082 | 0.064225 | 2.486113 |
| H | -0.203169 | 0.321379 | 3.837014 |
| O | -3.278512 | -1.554038 | 2.298509 |
| N | -2.245043 | 1.172959 | 2.542395 |
| N | -1.791050 | 2.037622 | 3.149903 |

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$^{CSS}C$

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.2626784

Zero-point correction= 0.712602 (Hartree/Particle)

Thermal correction to Energy= 0.762137

Thermal correction to Enthalpy= 0.763081

Thermal correction to Gibbs Free Energy= 0.629105

Sum of electronic and zero-point Energies= -2378.550077

Sum of electronic and thermal Energies= -2378.500542

Sum of electronic and thermal Enthalpies= -2378.499597

Sum of electronic and thermal Free Energies= -2378.633574

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.879745 | -0.079776 | 0.006386 |
| N | -2.045750 | -1.719056 | -0.295340 |
| C | -1.616476 | -3.014835 | -0.274443 |
| C | -2.713779 | -3.921398 | -0.557851 |
| C | -3.826308 | -3.136511 | -0.748365 |
| C | -3.368866 | -1.750682 | -0.610583 |
| C | -0.302999 | -3.430466 | -0.064092 |
| C | 0.806099 | -2.611951 | 0.117619 |
| N | 0.783463 | -1.245536 | 0.178389 |
| C | 2.076549 | -0.843172 | 0.352735 |
| C | 2.964365 | -1.998716 | 0.390247 |
| C | 2.168372 | -3.104427 | 0.247226 |

| | | | |
|---|---|---|---|
| C | 2.491737 | 0.480840 | 0.494657 |
| C | 1.666248 | 1.599558 | 0.417387 |
| N | 0.318339 | 1.557635 | 0.193605 |
| C | -0.112470 | 2.854669 | 0.176207 |
| C | 1.001974 | 3.763048 | 0.399765 |
| C | 2.116383 | 2.980559 | 0.554925 |
| C | -1.420868 | 3.271950 | -0.044104 |
| C | -2.518287 | 2.455274 | -0.310472 |
| C | -3.844430 | 2.954884 | -0.682119 |
| C | -4.606804 | 1.838161 | -0.944278 |
| C | -3.742675 | 0.693296 | -0.718740 |
| N | -2.496190 | 1.097031 | -0.333243 |
| C | -4.150172 | -0.628556 | -0.856871 |
| H | -0.121135 | -4.500218 | -0.088335 |
| H | -5.163109 | -0.804091 | -1.194674 |
| H | -1.588616 | 4.343164 | -0.065035 |
| H | 3.544464 | 0.653117 | 0.685347 |
| C | 0.488857 | 0.211381 | -2.596799 |
| H | 1.323863 | -0.478745 | -2.356622 |
| H | 0.873060 | 1.233913 | -2.405010 |
| C | 0.889539 | 5.258228 | 0.434833 |
| H | 0.598460 | 5.665782 | -0.541898 |
| H | 0.132611 | 5.591014 | 1.155634 |

| | | | |
|---|---|---|---|
| H | 1.837185 | 5.729187 | 0.713200 |
| C | 2.571718 | -4.548055 | 0.198924 |
| H | 2.015831 | -5.148612 | 0.929449 |
| H | 2.381514 | -4.991524 | -0.786941 |
| H | 3.637372 | -4.675509 | 0.412931 |
| C | -2.613621 | -5.416686 | -0.584591 |
| H | -1.833448 | -5.757693 | -1.276457 |
| H | -2.365405 | -5.825984 | 0.403570 |
| H | -3.556587 | -5.875304 | -0.895131 |
| C | -6.052717 | 1.772462 | -1.328456 |
| H | -6.194815 | 1.798225 | -2.417887 |
| H | -6.523457 | 0.854841 | -0.963347 |
| H | -6.602583 | 2.622755 | -0.911572 |
| C | -5.177882 | -3.615678 | -1.019499 |
| C | -6.335960 | -3.072719 | -0.610581 |
| H | -5.235370 | -4.541391 | -1.594962 |
| H | -7.287237 | -3.525761 | -0.875859 |
| H | -6.368724 | -2.188034 | 0.016436 |
| C | -4.213718 | 4.362035 | -0.708610 |
| C | -5.193045 | 4.947632 | -1.420343 |
| H | -3.618942 | 5.010196 | -0.064183 |
| H | -5.384270 | 6.013069 | -1.328808 |
| H | -5.811882 | 4.401309 | -2.123718 |

| | | | |
|---|---|---|---|
| C | 4.462579 | -1.946388 | 0.464873 |
| C | 5.107609 | -1.769838 | -0.941227 |
| H | 4.847113 | -2.870817 | 0.912310 |
| H | 4.793014 | -1.128255 | 1.113471 |
| H | 4.784719 | -2.573695 | -1.604934 |
| H | 4.787521 | -0.815605 | -1.374617 |
| C | 3.519493 | 3.448586 | 0.827633 |
| C | 4.459465 | 3.522540 | -0.411368 |
| H | 3.999523 | 2.823440 | 1.587889 |
| H | 3.468396 | 4.455067 | 1.256258 |
| H | 3.911803 | 3.836448 | -1.301576 |
| H | 5.242070 | 4.266732 | -0.210885 |
| C | 6.610767 | -1.796720 | -0.905368 |
| O | 7.349224 | -2.616219 | -1.401181 |
| O | 7.133689 | -0.743289 | -0.186122 |
| H | 8.098937 | -0.845570 | -0.227973 |
| C | 5.185596 | 2.237197 | -0.745049 |
| O | 5.212613 | 1.698406 | -1.833127 |
| O | 5.861708 | 1.753750 | 0.324538 |
| H | 6.304516 | 0.923393 | 0.051063 |
| O | -0.679544 | -0.074790 | -1.918241 |
| H | 0.331259 | 0.138717 | -3.690593 |
| C | -0.721891 | -0.422167 | 4.165734 |

| | | | |
|---|---|---|---|
| O | -2.133681 | -0.477338 | 3.941606 |
| C | -2.409497 | -0.353373 | 2.578595 |
| C | -1.153570 | -0.102560 | 1.812335 |
| C | -0.117056 | 0.152490 | 2.875684 |
| H | -0.540217 | 0.187288 | 5.058068 |
| H | 0.858617 | -0.275964 | 2.634486 |
| H | 0.034878 | 1.239845 | 2.965746 |
| O | -3.562527 | -0.440736 | 2.212195 |
| H | -0.353983 | -1.438701 | 4.364477 |

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.2780775

Zero-point correction= 0.712154 (Hartree/Particle)

Thermal correction to Energy= 0.761919

Thermal correction to Enthalpy= 0.762863

Thermal correction to Gibbs Free Energy= 0.628043

Sum of electronic and zero-point Energies= -2378.565924

Sum of electronic and thermal Energies= -2378.516159

Sum of electronic and thermal Enthalpies= -2378.515215

Sum of electronic and thermal Free Energies= -2378.650034

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.826473 | -0.069627 | -0.051958 |
| N | -1.993303 | -1.703742 | -0.328321 |
| C | -1.570891 | -3.003334 | -0.280339 |
| C | -2.678834 | -3.907245 | -0.516258 |
| C | -3.794261 | -3.121397 | -0.691210 |
| C | -3.330535 | -1.737368 | -0.595623 |
| C | -0.259938 | -3.423800 | -0.064375 |
| C | 0.848645 | -2.607077 | 0.126592 |
| N | 0.824305 | -1.243641 | 0.200324 |
| C | 2.116623 | -0.839432 | 0.358756 |
| C | 3.007717 | -1.993794 | 0.383890 |
| C | 2.212854 | -3.099877 | 0.244068 |
| C | 2.533480 | 0.483241 | 0.496241 |
| C | 1.710828 | 1.603487 | 0.415262 |
| N | 0.364259 | 1.566872 | 0.199588 |
| C | -0.058867 | 2.863246 | 0.159337 |
| C | 1.059860 | 3.770427 | 0.372416 |
| C | 2.169559 | 2.984276 | 0.536784 |
| C | -1.363890 | 3.282800 | -0.074669 |

| | | | |
|---|---|---|---|
| C | -2.462203 | 2.466359 | -0.337730 |
| C | -3.796866 | 2.965027 | -0.667895 |
| C | -4.571441 | 1.849809 | -0.905493 |
| C | -3.704924 | 0.704450 | -0.709591 |
| N | -2.440512 | 1.106028 | -0.372074 |
| C | -4.119720 | -0.617546 | -0.825127 |
| H | -0.082748 | -4.494326 | -0.081311 |
| H | -5.145710 | -0.794601 | -1.119301 |
| H | -1.530934 | 4.353904 | -0.098740 |
| H | 3.587937 | 0.654948 | 0.677721 |
| C | -1.209900 | -0.169439 | -2.954736 |
| H | -1.998572 | 0.607095 | -2.999376 |
| H | -1.732356 | -1.146150 | -2.951467 |
| C | 0.954755 | 5.266269 | 0.387341 |
| H | 0.673756 | 5.662645 | -0.596922 |
| H | 0.194070 | 5.612017 | 1.098005 |
| H | 1.902697 | 5.735703 | 0.667226 |
| C | 2.616796 | -4.542731 | 0.184637 |
| H | 2.063716 | -5.148305 | 0.913185 |
| H | 2.423805 | -4.979632 | -0.803593 |
| H | 3.683206 | -4.670774 | 0.394366 |
| C | -2.589856 | -5.403539 | -0.507660 |
| H | -1.818052 | -5.767281 | -1.197087 |

| | | | |
|---|---|---|---|
| H | -2.336863 | -5.789494 | 0.488448 |
| H | -3.539022 | -5.861831 | -0.799111 |
| C | -6.030936 | 1.787460 | -1.235433 |
| H | -6.214308 | 1.808009 | -2.318815 |
| H | -6.490376 | 0.873630 | -0.847326 |
| H | -6.561537 | 2.641775 | -0.802510 |
| C | -5.156785 | -3.598838 | -0.909210 |
| C | -6.294253 | -3.051162 | -0.452555 |
| H | -5.239718 | -4.524434 | -1.481781 |
| H | -7.257749 | -3.500005 | -0.677866 |
| H | -6.295579 | -2.167957 | 0.177501 |
| C | -4.167138 | 4.372802 | -0.681072 |
| C | -5.162474 | 4.957338 | -1.370387 |
| H | -3.558585 | 5.019637 | -0.048737 |
| H | -5.353234 | 6.022389 | -1.274135 |
| H | -5.796169 | 4.410244 | -2.059898 |
| C | 4.506405 | -1.940219 | 0.447688 |
| C | 5.140409 | -1.763603 | -0.963042 |
| H | 4.894429 | -2.864438 | 0.892614 |
| H | 4.840827 | -1.122130 | 1.094121 |
| H | 4.810640 | -2.565555 | -1.625631 |
| H | 4.818628 | -0.808503 | -1.393425 |
| C | 3.574521 | 3.448401 | 0.806724 |

| | | | |
|---|---|---|---|
| C | 4.513063 | 3.516991 | -0.433359 |
| H | 4.052963 | 2.823649 | 1.568091 |
| H | 3.526525 | 4.455928 | 1.233342 |
| H | 3.964959 | 3.826442 | -1.324845 |
| H | 5.295282 | 4.262884 | -0.237258 |
| C | 6.643880 | -1.792647 | -0.940985 |
| O | 7.376680 | -2.604515 | -1.457324 |
| O | 7.175014 | -0.751718 | -0.209653 |
| H | 8.139685 | -0.853441 | -0.264309 |
| C | 5.241593 | 2.231848 | -0.762966 |
| O | 5.281539 | 1.698088 | -1.853027 |
| O | 5.905279 | 1.743290 | 0.312210 |
| H | 6.351194 | 0.914401 | 0.039140 |
| O | -0.334605 | -0.006577 | -1.892369 |
| H | -0.658696 | -0.110869 | -3.912237 |
| C | -0.729206 | -0.368579 | 4.241433 |
| O | -2.138508 | -0.421691 | 4.010733 |
| C | -2.393670 | -0.347429 | 2.631650 |
| C | -1.151368 | -0.096183 | 1.887153 |
| C | -0.113702 | 0.183199 | 2.944214 |
| H | -0.547159 | 0.253865 | 5.125257 |
| H | 0.861772 | -0.255493 | 2.718141 |
| H | 0.045316 | 1.270981 | 3.020925 |

O -3.545543 -0.474733 2.256547

H -0.363779 -1.383522 4.458130

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**$^3$C**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.272942

Zero-point correction= 0.711998 (Hartree/Particle)

Thermal correction to Energy= 0.761898

Thermal correction to Enthalpy= 0.762842

Thermal correction to Gibbs Free Energy= 0.626490

Sum of electronic and zero-point Energies= -2378.560944

Sum of electronic and thermal Energies= -2378.511044

Sum of electronic and thermal Enthalpies= -2378.510100

Sum of electronic and thermal Free Energies= -2378.646452

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Cartesian Coordinates

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Fe -0.841966 -0.057234 -0.084642

N -1.971032 -1.713767 -0.340175

C -1.561690 -3.016088 -0.245584

| | | | |
|---|---|---|---|
| C | -2.669643 | -3.916728 | -0.484054 |
| C | -3.771741 | -3.125589 | -0.711333 |
| C | -3.300403 | -1.742823 | -0.639433 |
| C | -0.256369 | -3.432193 | 0.003232 |
| C | 0.842540 | -2.597501 | 0.166276 |
| N | 0.798220 | -1.229689 | 0.171701 |
| C | 2.084493 | -0.800466 | 0.334071 |
| C | 2.988169 | -1.940563 | 0.417336 |
| C | 2.209301 | -3.063859 | 0.320361 |
| C | 2.484842 | 0.529990 | 0.447822 |
| C | 1.654340 | 1.645188 | 0.377140 |
| N | 0.304667 | 1.606203 | 0.178413 |
| C | -0.124331 | 2.901499 | 0.167502 |
| C | 0.992331 | 3.809737 | 0.378823 |
| C | 2.108360 | 3.026360 | 0.511020 |
| C | -1.432937 | 3.315719 | -0.049451 |
| C | -2.512477 | 2.483587 | -0.333754 |
| C | -3.847306 | 2.958907 | -0.698601 |
| C | -4.586369 | 1.830267 | -0.976653 |
| C | -3.698891 | 0.700889 | -0.764973 |
| N | -2.459341 | 1.126960 | -0.378842 |
| C | -4.086537 | -0.626981 | -0.901014 |
| H | -0.075658 | -4.501692 | 0.030866 |

| | | | |
|---|---|---|---|
| H | -5.101530 | -0.816373 | -1.224519 |
| H | -1.612941 | 4.384844 | -0.057827 |
| H | 3.537524 | 0.711993 | 0.628568 |
| C | -0.142247 | -0.941178 | -2.768220 |
| H | -0.876748 | -1.769108 | -2.783300 |
| H | 0.831786 | -1.388333 | -2.491333 |
| C | 0.877946 | 5.304378 | 0.422082 |
| H | 0.572184 | 5.715309 | -0.548673 |
| H | 0.131205 | 5.632044 | 1.155610 |
| H | 1.828594 | 5.775736 | 0.688934 |
| C | 2.631703 | -4.502714 | 0.337172 |
| H | 2.075836 | -5.078105 | 1.087504 |
| H | 2.458048 | -4.990596 | -0.630625 |
| H | 3.696459 | -4.606685 | 0.567203 |
| C | -2.594816 | -5.412762 | -0.428210 |
| H | -1.813047 | -5.805135 | -1.090358 |
| H | -2.366188 | -5.769992 | 0.584309 |
| H | -3.542606 | -5.870570 | -0.724792 |
| C | -6.031439 | 1.740081 | -1.358525 |
| H | -6.175768 | 1.766004 | -2.447622 |
| H | -6.485418 | 0.813693 | -0.994480 |
| H | -6.594702 | 2.579641 | -0.938268 |
| C | -5.133123 | -3.597151 | -0.952635 |

| | | | |
|---|---|---|---|
| C | -6.273305 | -3.038532 | -0.517370 |
| H | -5.211852 | -4.525325 | -1.521623 |
| H | -7.236600 | -3.481223 | -0.755542 |
| H | -6.276579 | -2.152457 | 0.108684 |
| C | -4.246025 | 4.358713 | -0.703686 |
| C | -5.230311 | 4.933915 | -1.416350 |
| H | -3.671473 | 5.007655 | -0.042178 |
| H | -5.446166 | 5.993215 | -1.310203 |
| H | -5.829714 | 4.385041 | -2.134506 |
| C | 4.485331 | -1.866702 | 0.497979 |
| C | 5.135754 | -1.736650 | -0.910490 |
| H | 4.877125 | -2.769039 | 0.982426 |
| H | 4.802341 | -1.021133 | 1.117040 |
| H | 4.817036 | -2.562992 | -1.548121 |
| H | 4.816926 | -0.797679 | -1.377075 |
| C | 3.515947 | 3.493367 | 0.760601 |
| C | 4.440329 | 3.548259 | -0.491422 |
| H | 4.003220 | 2.877043 | 1.523335 |
| H | 3.471998 | 4.505062 | 1.177070 |
| H | 3.879049 | 3.833300 | -1.382825 |
| H | 5.215720 | 4.306841 | -0.318920 |
| C | 6.639044 | -1.760554 | -0.868044 |
| O | 7.379540 | -2.593831 | -1.337022 |

| | | | |
|---|---|---|---|
| O | 7.157785 | -0.685753 | -0.178986 |
| H | 8.123391 | -0.787656 | -0.213014 |
| C | 5.180197 | 2.264876 | -0.801834 |
| O | 5.210514 | 1.704769 | -1.879084 |
| O | 5.864443 | 1.810372 | 0.275198 |
| H | 6.317289 | 0.980568 | 0.017334 |
| O | -0.518767 | 0.108576 | -1.942012 |
| H | -0.042607 | -0.584269 | -3.809478 |
| C | -0.778868 | -0.295949 | 4.245059 |
| O | -2.182863 | -0.357275 | 4.003509 |
| C | -2.416673 | -0.348930 | 2.609051 |
| C | -1.181783 | -0.099247 | 1.886118 |
| C | -0.146855 | 0.212663 | 2.936142 |
| H | -0.601233 | 0.356258 | 5.108766 |
| H | 0.827930 | -0.243448 | 2.737149 |
| H | 0.026080 | 1.300645 | 2.982268 |
| O | -3.564733 | -0.525806 | 2.227857 |
| H | -0.411692 | -1.302785 | 4.498645 |

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**$^{5}$C**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.2576823

Zero-point correction= 0.709910 (Hartree/Particle)

Thermal correction to Energy= 0.760315

Thermal correction to Enthalpy= 0.761259

Thermal correction to Gibbs Free Energy= 0.623187

Sum of electronic and zero-point Energies= -2378.547772

Sum of electronic and thermal Energies= -2378.497367

Sum of electronic and thermal Enthalpies= -2378.496423

Sum of electronic and thermal Free Energies= -2378.634496

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.861102 | -0.053694 | -0.056481 |
| N | -2.038288 | -1.752068 | -0.337355 |
| C | -1.596519 | -3.040014 | -0.278959 |
| C | -2.705738 | -3.943319 | -0.535087 |
| C | -3.821744 | -3.154493 | -0.727410 |
| C | -3.366369 | -1.762862 | -0.619644 |
| C | -0.267576 | -3.429544 | -0.046243 |
| C | 0.853567 | -2.612057 | 0.145630 |
| N | 0.840791 | -1.247413 | 0.188489 |
| C | 2.119905 | -0.814040 | 0.358895 |

| | | | |
|---|---|---|---|
| C | 3.012761 | -1.970006 | 0.420998 |
| C | 2.224090 | -3.087470 | 0.293269 |
| C | 2.513531 | 0.529677 | 0.475967 |
| C | 1.700746 | 1.670536 | 0.396858 |
| N | 0.354048 | 1.646276 | 0.214962 |
| C | -0.093690 | 2.929831 | 0.158068 |
| C | 1.033750 | 3.842649 | 0.331084 |
| C | 2.153216 | 3.061303 | 0.484075 |
| C | -1.419855 | 3.322911 | -0.065431 |
| C | -2.537869 | 2.511418 | -0.316946 |
| C | -3.876819 | 2.995073 | -0.679512 |
| C | -4.639635 | 1.868373 | -0.918943 |
| C | -3.767429 | 0.723040 | -0.698445 |
| N | -2.529498 | 1.157337 | -0.331831 |
| C | -4.145905 | -0.619063 | -0.835826 |
| H | -0.080148 | -4.499425 | -0.048575 |
| H | -5.166937 | -0.799038 | -1.149424 |
| H | -1.590217 | 4.394152 | -0.105903 |
| H | 3.569377 | 0.704659 | 0.651654 |
| C | -0.142219 | -0.899934 | -2.750112 |
| H | -0.821409 | -1.772283 | -2.747132 |
| H | 0.865999 | -1.275964 | -2.496355 |
| C | 0.927585 | 5.338684 | 0.322677 |

| | | | |
|---|---|---|---|
| H | 0.625842 | 5.717041 | -0.662582 |
| H | 0.179583 | 5.694391 | 1.041822 |
| H | 1.879040 | 5.816151 | 0.575983 |
| C | 2.643507 | -4.527437 | 0.277707 |
| H | 2.079398 | -5.119551 | 1.008693 |
| H | 2.475624 | -4.990590 | -0.703289 |
| H | 3.706135 | -4.641500 | 0.513264 |
| C | -2.620800 | -5.439974 | -0.527156 |
| H | -1.814735 | -5.802306 | -1.176951 |
| H | -2.419746 | -5.829495 | 0.479545 |
| H | -3.553783 | -5.897534 | -0.868352 |
| C | -6.090660 | 1.795973 | -1.281975 |
| H | -6.250116 | 1.834561 | -2.368668 |
| H | -6.546611 | 0.869173 | -0.921204 |
| H | -6.642127 | 2.635727 | -0.845925 |
| C | -5.177339 | -3.638240 | -0.971786 |
| C | -6.324735 | -3.089540 | -0.541991 |
| H | -5.246822 | -4.566251 | -1.542326 |
| H | -7.283000 | -3.539883 | -0.785787 |
| H | -6.339711 | -2.203999 | 0.084523 |
| C | -4.256458 | 4.399224 | -0.718326 |
| C | -5.256849 | 4.969889 | -1.412652 |
| H | -3.646057 | 5.059624 | -0.101576 |

| | | | |
|---|---|---|---|
| H | -5.448071 | 6.036328 | -1.334194 |
| H | -5.894057 | 4.410517 | -2.088731 |
| C | 4.510211 | -1.912225 | 0.511370 |
| C | 5.171087 | -1.770693 | -0.891262 |
| H | 4.893493 | -2.822294 | 0.988354 |
| H | 4.828726 | -1.074991 | 1.141196 |
| H | 4.864126 | -2.596811 | -1.534962 |
| H | 4.849340 | -0.831786 | -1.355811 |
| C | 3.561794 | 3.538938 | 0.707426 |
| C | 4.478180 | 3.547554 | -0.551345 |
| H | 4.054075 | 2.948966 | 1.487861 |
| H | 3.522259 | 4.565137 | 1.087590 |
| H | 3.914217 | 3.814928 | -1.446550 |
| H | 5.264059 | 4.300849 | -0.404774 |
| C | 6.673899 | -1.783356 | -0.834017 |
| O | 7.425417 | -2.616401 | -1.285672 |
| O | 7.177149 | -0.697215 | -0.151200 |
| H | 8.143743 | -0.793019 | -0.172173 |
| C | 5.199792 | 2.246828 | -0.831199 |
| O | 5.214764 | 1.656943 | -1.892853 |
| O | 5.887352 | 1.814045 | 0.252478 |
| H | 6.330136 | 0.973271 | 0.013481 |
| O | -0.569688 | 0.127835 | -1.917264 |

| | | | |
|---|---|---|---|
| H | -0.094310 | -0.534321 | -3.791515 |
| C | -0.738929 | -0.290208 | 4.242021 |
| O | -2.145981 | -0.377432 | 4.019249 |
| C | -2.400481 | -0.374177 | 2.630684 |
| C | -1.174442 | -0.103531 | 1.900720 |
| C | -0.135287 | 0.247488 | 2.931942 |
| H | -0.563435 | 0.355558 | 5.110446 |
| H | 0.851557 | -0.174231 | 2.720714 |
| H | -0.003197 | 1.340403 | 2.981232 |
| O | -3.547297 | -0.571512 | 2.261235 |
| H | -0.348327 | -1.292389 | 4.476542 |

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**$^{CSS}$TS(C-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.087931

Zero-point correction= 0.941312 (Hartree/Particle)

Thermal correction to Energy= 1.002355

Thermal correction to Enthalpy= 1.003299

Thermal correction to Gibbs Free Energy= 0.845340

Sum of electronic and zero-point Energies= -2823.146619

Sum of electronic and thermal Energies= -2823.085576

Sum of electronic and thermal Enthalpies= -2823.084632

Sum of electronic and thermal Free Energies= -2823.242591

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.049261 | 0.237958 | -0.757969 |
| N | -1.334894 | -1.180497 | -1.473060 |
| C | -1.112495 | -2.533243 | -1.555239 |
| C | -2.255653 | -3.213117 | -2.128657 |
| C | -3.190359 | -2.235040 | -2.403166 |
| C | -2.572790 | -0.967550 | -2.005738 |
| C | 0.061173 | -3.172327 | -1.155955 |
| C | 1.190578 | -2.560580 | -0.618861 |
| N | 1.314346 | -1.223535 | -0.358865 |
| C | 2.568165 | -1.044539 | 0.148455 |
| C | 3.273057 | -2.320761 | 0.223015 |
| C | 2.408842 | -3.269229 | -0.256604 |
| C | 3.104413 | 0.179140 | 0.549479 |
| C | 2.509444 | 1.427401 | 0.393787 |
| N | 1.273221 | 1.640135 | -0.140999 |
| C | 1.115768 | 2.989374 | -0.211901 |
| C | 2.280922 | 3.676003 | 0.335005 |

| | | | |
|---|---|---|---|
| C | 3.153141 | 2.700065 | 0.725750 |
| C | 0.014198 | 3.642524 | -0.752437 |
| C | -1.112569 | 3.035343 | -1.299391 |
| C | -2.239881 | 3.760392 | -1.886774 |
| C | -3.149714 | 2.798828 | -2.275708 |
| C | -2.559878 | 1.519109 | -1.924342 |
| N | -1.340049 | 1.691855 | -1.323639 |
| C | -3.154878 | 0.285941 | -2.190297 |
| H | 0.104559 | -4.248792 | -1.283520 |
| H | -4.147893 | 0.309622 | -2.624583 |
| H | 0.040617 | 4.726858 | -0.750360 |
| H | 4.092627 | 0.159527 | 0.994884 |
| C | 0.803285 | -0.445343 | -3.492268 |
| H | 1.225452 | -1.437290 | -3.224107 |
| H | 1.401230 | -0.085943 | -4.353585 |
| C | 2.427853 | 5.164694 | 0.428590 |
| H | 2.447752 | 5.634111 | -0.563621 |
| H | 1.594525 | 5.617337 | 0.979989 |
| H | 3.352810 | 5.448107 | 0.939935 |
| C | 2.635787 | -4.741680 | -0.428301 |
| H | 1.845276 | -5.333368 | 0.050094 |
| H | 2.651867 | -5.031049 | -1.487116 |
| H | 3.588812 | -5.055212 | 0.008877 |

| | | | |
|---|---|---|---|
| C | -2.344779 | -4.682151 | -2.409407 |
| H | -1.355928 | -5.119302 | -2.577816 |
| H | -2.808745 | -5.239535 | -1.583266 |
| H | -2.949989 | -4.870280 | -3.302470 |
| C | -4.450916 | 2.990603 | -2.993883 |
| H | -4.425164 | 3.900030 | -3.602964 |
| H | -4.669568 | 2.147977 | -3.657412 |
| H | -5.302165 | 3.089034 | -2.305251 |
| C | -4.508035 | -2.355999 | -3.006636 |
| C | -5.307925 | -3.438550 | -3.049609 |
| H | -4.886593 | -1.449945 | -3.479615 |
| H | -6.268445 | -3.396648 | -3.554849 |
| H | -5.046740 | -4.381386 | -2.581546 |
| C | -2.294617 | 5.206852 | -2.043471 |
| C | -3.387058 | 5.986236 | -2.129307 |
| H | -1.326062 | 5.703924 | -2.098008 |
| H | -3.294007 | 7.059310 | -2.270042 |
| H | -4.394419 | 5.593259 | -2.041539 |
| C | 4.699143 | -2.515788 | 0.649720 |
| C | 5.689462 | -2.352532 | -0.539829 |
| H | 4.826327 | -3.518692 | 1.075435 |
| H | 4.969818 | -1.808802 | 1.440366 |
| H | 5.423280 | -3.036181 | -1.347750 |

| | | | |
|---|---|---|---|
| H | 5.635855 | -1.327650 | -0.924593 |
| C | 4.489746 | 2.894016 | 1.386158 |
| C | 5.723032 | 2.883682 | 0.435590 |
| H | 4.648301 | 2.147898 | 2.171378 |
| H | 4.481508 | 3.864202 | 1.894197 |
| H | 5.484675 | 3.351225 | -0.521263 |
| H | 6.530848 | 3.459492 | 0.907247 |
| C | 7.116536 | -2.641792 | -0.163873 |
| O | 7.832487 | -3.517653 | -0.592305 |
| O | 7.586819 | -1.777640 | 0.801156 |
| H | 8.508714 | -2.036994 | 0.964520 |
| C | 6.302056 | 1.515791 | 0.149247 |
| O | 6.520505 | 1.052219 | -0.952331 |
| O | 6.601460 | 0.851255 | 1.290848 |
| H | 6.970161 | -0.021856 | 1.042547 |
| O | 0.842844 | 0.477392 | -2.467352 |
| H | -0.217077 | -0.643350 | -3.885608 |
| C | -0.806650 | 0.016105 | 1.151230 |
| C | -1.025706 | -1.381503 | 1.732735 |
| C | -0.159859 | 0.725085 | 2.302964 |
| C | 0.154295 | -1.528593 | 2.703585 |
| H | -1.046354 | -2.172694 | 0.985610 |
| H | -1.963938 | -1.435459 | 2.302638 |

| | | | |
|---|---|---|---|
| H | -3.983955 | -1.168218 | 0.376301 |
| O | -0.118273 | 1.906718 | 2.592867 |
| O | 0.439462 | -0.188492 | 3.153574 |
| H | 1.041972 | -1.932710 | 2.210871 |
| H | -0.070785 | -2.132763 | 3.589369 |
| C | -4.662034 | -1.428387 | 1.179079 |
| C | -4.627773 | -0.735438 | 2.408078 |
| C | -5.550581 | -2.481948 | 0.981060 |
| C | -5.496242 | -1.168435 | 3.431840 |
| N | -3.773433 | 0.375613 | 2.600948 |
| C | -6.416776 | -2.895074 | 1.995693 |
| H | -5.553890 | -2.979472 | 0.015381 |
| C | -6.373461 | -2.231456 | 3.221522 |
| H | -5.505463 | -0.672192 | 4.394111 |
| C | -3.233770 | 1.064857 | 1.510829 |
| C | -3.531841 | 0.867540 | 3.966785 |
| H | -7.103855 | -3.720932 | 1.836278 |
| H | -7.033577 | -2.533978 | 4.030850 |
| H | -3.712669 | 0.781882 | 0.577552 |
| C | -2.999305 | 2.553969 | 1.636804 |
| H | -2.975310 | 1.798117 | 3.881207 |
| H | -4.494867 | 1.120891 | 4.429864 |
| C | -2.742075 | -0.089998 | 4.867939 |

| | | | |
|---|---|---|---|
| H | -2.098896 | 2.789698 | 2.209774 |
| H | -2.861218 | 2.968854 | 0.639168 |
| H | -3.870568 | 3.042510 | 2.095906 |
| H | -3.198027 | -1.082518 | 4.912480 |
| H | -1.711972 | -0.189107 | 4.519496 |
| H | -2.714401 | 0.316474 | 5.885455 |
| H | -1.930062 | 0.574696 | 1.064241 |

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**$^{OSS}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.1063441

Zero-point correction= 0.940754 (Hartree/Particle)

Thermal correction to Energy= 1.002072

Thermal correction to Enthalpy= 1.003016

Thermal correction to Gibbs Free Energy= 0.843839

Sum of electronic and zero-point Energies= -2823.165590

Sum of electronic and thermal Energies= -2823.104272

Sum of electronic and thermal Enthalpies= -2823.103328

Sum of electronic and thermal Free Energies= -2823.262505

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.015076 | 0.235517 | -0.808139 |
| N | -1.295212 | -1.187153 | -1.514546 |
| C | -1.073002 | -2.538278 | -1.603028 |
| C | -2.216250 | -3.212233 | -2.181499 |
| C | -3.147973 | -2.230879 | -2.450565 |
| C | -2.531476 | -0.967104 | -2.045501 |
| C | 0.098842 | -3.178271 | -1.206089 |
| C | 1.217235 | -2.561151 | -0.655212 |
| N | 1.333996 | -1.222540 | -0.393061 |
| C | 2.577548 | -1.038873 | 0.141055 |
| C | 3.280918 | -2.312061 | 0.227946 |
| C | 2.429108 | -3.262782 | -0.270876 |
| C | 3.108205 | 0.184075 | 0.548417 |
| C | 2.517539 | 1.431831 | 0.378403 |
| N | 1.293197 | 1.647374 | -0.179998 |
| C | 1.127441 | 2.996722 | -0.233460 |
| C | 2.282305 | 3.679547 | 0.334460 |
| C | 3.151400 | 2.702491 | 0.729525 |
| C | 0.025460 | 3.653236 | -0.764731 |
| C | -1.100126 | 3.043040 | -1.307496 |
| C | -2.229595 | 3.761770 | -1.894944 |

| | | | |
|---|---|---|---|
| C | -3.129689 | 2.795818 | -2.292742 |
| C | -2.532544 | 1.518397 | -1.945250 |
| N | -1.318859 | 1.700583 | -1.340811 |
| C | -3.116426 | 0.284652 | -2.224675 |
| H | 0.145889 | -4.253864 | -1.334886 |
| H | -4.109293 | 0.305442 | -2.658115 |
| H | 0.045797 | 4.737002 | -0.749421 |
| H | 4.086007 | 0.163680 | 1.014954 |
| C | 0.979541 | -0.501528 | -3.459944 |
| H | 1.629349 | -1.322984 | -3.101637 |
| H | 1.476188 | -0.074236 | -4.350440 |
| C | 2.417950 | 5.167377 | 0.452699 |
| H | 2.425042 | 5.653993 | -0.531092 |
| H | 1.585741 | 5.600784 | 1.020382 |
| H | 3.344945 | 5.448881 | 0.960742 |
| C | 2.661175 | -4.735602 | -0.431879 |
| H | 1.866376 | -5.324849 | 0.041621 |
| H | 2.690165 | -5.030658 | -1.488648 |
| H | 3.609551 | -5.043935 | 0.018181 |
| C | -2.308141 | -4.680308 | -2.464815 |
| H | -1.321219 | -5.117804 | -2.643614 |
| H | -2.764275 | -5.236991 | -1.634462 |
| H | -2.922400 | -4.865810 | -3.352032 |

| | | | |
|---|---|---|---|
| C | -4.433185 | 2.981419 | -3.007394 |
| H | -4.416859 | 3.896455 | -3.608079 |
| H | -4.646233 | 2.142893 | -3.677615 |
| H | -5.281237 | 3.065340 | -2.313690 |
| C | -4.465289 | -2.347039 | -3.058863 |
| C | -5.269357 | -3.425272 | -3.087690 |
| H | -4.834988 | -1.445164 | -3.545971 |
| H | -6.229309 | -3.386053 | -3.593970 |
| H | -5.015724 | -4.359892 | -2.599671 |
| C | -2.294471 | 5.209489 | -2.041862 |
| C | -3.394199 | 5.978297 | -2.118233 |
| H | -1.330289 | 5.714671 | -2.096433 |
| H | -3.311955 | 7.053230 | -2.250488 |
| H | -4.397013 | 5.574923 | -2.027299 |
| C | 4.697082 | -2.506718 | 0.687316 |
| C | 5.712425 | -2.361967 | -0.483003 |
| H | 4.809764 | -3.504737 | 1.127735 |
| H | 4.952902 | -1.791920 | 1.475489 |
| H | 5.459459 | -3.053136 | -1.288819 |
| H | 5.674134 | -1.340612 | -0.878987 |
| C | 4.475918 | 2.893325 | 1.414336 |
| C | 5.725077 | 2.884619 | 0.484548 |
| H | 4.619180 | 2.145016 | 2.200264 |

| | | | |
|---|---|---|---|
| H | 4.458626 | 3.861602 | 1.925034 |
| H | 5.504707 | 3.360141 | -0.472707 |
| H | 6.526937 | 3.452604 | 0.974709 |
| C | 7.129588 | -2.656380 | -0.073363 |
| O | 7.845656 | -3.545183 | -0.473156 |
| O | 7.586528 | -1.778694 | 0.884989 |
| H | 8.501963 | -2.042426 | 1.075682 |
| C | 6.298128 | 1.513950 | 0.199749 |
| O | 6.505792 | 1.043716 | -0.901249 |
| O | 6.599472 | 0.854026 | 1.342894 |
| H | 6.967084 | -0.021065 | 1.100063 |
| O | 0.777120 | 0.494880 | -2.516370 |
| H | 0.042259 | -0.971695 | -3.815351 |
| C | -0.804444 | 0.034368 | 1.126619 |
| C | -0.965741 | -1.371216 | 1.716677 |
| C | -0.185888 | 0.792280 | 2.239430 |
| C | 0.143619 | -1.435495 | 2.776027 |
| H | -0.876511 | -2.176460 | 0.989536 |
| H | -1.943881 | -1.483534 | 2.204500 |
| H | -4.121633 | -1.155306 | 0.380655 |
| O | -0.123873 | 1.990267 | 2.459615 |
| O | 0.351439 | -0.075342 | 3.194369 |
| H | 1.080285 | -1.826457 | 2.363266 |

| | | | |
|---|---|---|---|
| H | -0.120857 | -2.020545 | 3.664448 |
| C | -4.754695 | -1.457245 | 1.204384 |
| C | -4.701983 | -0.767190 | 2.440380 |
| C | -5.594353 | -2.553318 | 1.028485 |
| C | -5.507812 | -1.269953 | 3.490865 |
| N | -3.904691 | 0.368897 | 2.610659 |
| C | -6.400317 | -3.025122 | 2.067154 |
| H | -5.606572 | -3.042403 | 0.057834 |
| C | -6.337682 | -2.372394 | 3.298838 |
| H | -5.500936 | -0.794459 | 4.463504 |
| C | -3.330906 | 1.045345 | 1.481664 |
| C | -3.684538 | 0.890912 | 3.962612 |
| H | -7.049580 | -3.884063 | 1.923749 |
| H | -6.946258 | -2.718835 | 4.131428 |
| H | -3.875447 | 0.779190 | 0.577898 |
| C | -3.172972 | 2.551533 | 1.604539 |
| H | -3.218853 | 1.869434 | 3.864778 |
| H | -4.656257 | 1.063175 | 4.446760 |
| C | -2.796868 | 0.016018 | 4.859215 |
| H | -2.324326 | 2.834972 | 2.231351 |
| H | -2.977649 | 2.960438 | 0.612788 |
| H | -4.089553 | 3.023978 | 1.988678 |
| H | -3.173387 | -1.008560 | 4.927263 |

H -1.771575 -0.011053 4.483410

H -2.774062 0.436162 5.872090

H -2.057810 0.569763 1.148428

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**$^{3}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.1023275

Zero-point correction= 0.940511 (Hartree/Particle)

Thermal correction to Energy= 1.001983

Thermal correction to Enthalpy= 1.002927

Thermal correction to Gibbs Free Energy= 0.841992

Sum of electronic and zero-point Energies= -2823.161816

Sum of electronic and thermal Energies= -2823.100345

Sum of electronic and thermal Enthalpies= -2823.099401

Sum of electronic and thermal Free Energies= -2823.260336

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Cartesian Coordinates

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Fe 0.002046 0.193886 -0.855136

N -1.257668 -1.270602 -1.506352

| | | | |
|---|---|---|---|
| C | -1.006486 | -2.616534 | -1.574607 |
| C | -2.139846 | -3.324491 | -2.130181 |
| C | -3.096375 | -2.367923 | -2.402632 |
| C | -2.504838 | -1.085246 | -2.025244 |
| C | 0.179611 | -3.224734 | -1.165743 |
| C | 1.280014 | -2.573858 | -0.622190 |
| N | 1.372059 | -1.225004 | -0.395042 |
| C | 2.604287 | -1.009208 | 0.152319 |
| C | 3.326800 | -2.267816 | 0.281752 |
| C | 2.498375 | -3.244653 | -0.205163 |
| C | 3.110420 | 0.233017 | 0.531197 |
| C | 2.497550 | 1.463486 | 0.321286 |
| N | 1.274311 | 1.640821 | -0.254196 |
| C | 1.079685 | 2.987127 | -0.337289 |
| C | 2.217105 | 3.704189 | 0.220273 |
| C | 3.101748 | 2.753825 | 0.645798 |
| C | -0.033950 | 3.611553 | -0.880123 |
| C | -1.154374 | 2.967502 | -1.396237 |
| C | -2.309305 | 3.650741 | -1.979131 |
| C | -3.196707 | 2.657850 | -2.334620 |
| C | -2.564511 | 1.401285 | -1.969758 |
| N | -1.344816 | 1.622879 | -1.393098 |
| C | -3.122662 | 0.149116 | -2.214805 |

| | | | |
|---|---|---|---|
| H | 0.247821 | -4.301697 | -1.271310 |
| H | -4.122730 | 0.137270 | -2.631766 |
| H | -0.033130 | 4.695528 | -0.889022 |
| H | 4.081938 | 0.243216 | 1.010580 |
| C | 1.163922 | -0.593314 | -3.411086 |
| H | 2.032444 | -1.123760 | -2.977949 |
| H | 1.496897 | -0.173194 | -4.377180 |
| C | 2.323025 | 5.196731 | 0.305817 |
| H | 2.320015 | 5.661795 | -0.688289 |
| H | 1.482756 | 5.625694 | 0.864873 |
| H | 3.244399 | 5.507415 | 0.806848 |
| C | 2.755252 | -4.717604 | -0.321145 |
| H | 1.965050 | -5.305154 | 0.161931 |
| H | 2.799440 | -5.042867 | -1.368453 |
| H | 3.703754 | -4.997404 | 0.146825 |
| C | -2.200914 | -4.798541 | -2.389921 |
| H | -1.207645 | -5.212736 | -2.588683 |
| H | -2.620180 | -5.354277 | -1.539816 |
| H | -2.833335 | -5.012824 | -3.257562 |
| C | -4.518787 | 2.799516 | -3.024408 |
| H | -4.534546 | 3.699739 | -3.647115 |
| H | -4.729549 | 1.940753 | -3.669216 |
| H | -5.352462 | 2.883257 | -2.313607 |

| | | | |
|---|---|---|---|
| C | -4.417969 | -2.523906 | -2.993551 |
| C | -5.202975 | -3.616045 | -2.976740 |
| H | -4.807031 | -1.644949 | -3.506750 |
| H | -6.168280 | -3.611732 | -3.474289 |
| H | -4.927573 | -4.527620 | -2.457860 |
| C | -2.405511 | 5.093009 | -2.158235 |
| C | -3.521460 | 5.838430 | -2.230937 |
| H | -1.452613 | 5.615205 | -2.243546 |
| H | -3.463034 | 6.911260 | -2.390108 |
| H | -4.514069 | 5.417994 | -2.110478 |
| C | 4.738292 | -2.427370 | 0.768152 |
| C | 5.769368 | -2.302401 | -0.390784 |
| H | 4.858615 | -3.409996 | 1.239908 |
| H | 4.970953 | -1.685637 | 1.538323 |
| H | 5.539481 | -3.022251 | -1.178214 |
| H | 5.721990 | -1.294264 | -0.818318 |
| C | 4.415936 | 2.986972 | 1.337254 |
| C | 5.673873 | 2.975583 | 0.419227 |
| H | 4.564192 | 2.262643 | 2.144358 |
| H | 4.376374 | 3.967973 | 1.821509 |
| H | 5.454457 | 3.422100 | -0.552130 |
| H | 6.461226 | 3.569537 | 0.901796 |
| C | 7.183786 | -2.562727 | 0.050351 |

| | | | |
|---|---|---|---|
| O | 7.915412 | -3.458834 | -0.302074 |
| O | 7.616200 | -1.640782 | 0.977764 |
| H | 8.530899 | -1.886167 | 1.194669 |
| C | 6.270751 | 1.607015 | 0.176409 |
| O | 6.484702 | 1.105729 | -0.909690 |
| O | 6.583478 | 0.989049 | 1.339432 |
| H | 6.965500 | 0.112591 | 1.125590 |
| O | 0.681323 | 0.427200 | -2.602483 |
| H | 0.403617 | -1.362842 | -3.643199 |
| C | -0.818397 | 0.015728 | 1.130642 |
| C | -1.022675 | -1.389387 | 1.707120 |
| C | -0.139462 | 0.733455 | 2.229796 |
| C | 0.084488 | -1.506796 | 2.765369 |
| H | -0.961606 | -2.190247 | 0.971622 |
| H | -2.004917 | -1.475598 | 2.192854 |
| H | -4.184707 | -1.000346 | 0.398732 |
| O | -0.002657 | 1.927123 | 2.446126 |
| O | 0.352554 | -0.160798 | 3.189607 |
| H | 1.002653 | -1.937331 | 2.348413 |
| H | -0.203430 | -2.085614 | 3.650788 |
| C | -4.825584 | -1.290460 | 1.220652 |
| C | -4.744833 | -0.615237 | 2.464338 |
| C | -5.699840 | -2.357792 | 1.036506 |

| | | | |
|---|---|---|---|
| C | -5.562313 | -1.105862 | 3.512831 |
| N | -3.912052 | 0.490486 | 2.642782 |
| C | -6.517232 | -2.814996 | 2.072910 |
| H | -5.727856 | -2.839052 | 0.062031 |
| C | -6.428368 | -2.178114 | 3.311526 |
| H | -5.534748 | -0.643812 | 4.491636 |
| C | -3.297267 | 1.145568 | 1.514798 |
| C | -3.663937 | 0.986288 | 3.998569 |
| H | -7.193530 | -3.651749 | 1.923117 |
| H | -7.043973 | -2.514647 | 4.143160 |
| H | -3.871415 | 0.927420 | 0.615438 |
| C | -3.064051 | 2.641342 | 1.655778 |
| H | -3.175589 | 1.954817 | 3.910589 |
| H | -4.625266 | 1.176057 | 4.496726 |
| C | -2.789736 | 0.074944 | 4.872213 |
| H | -2.207570 | 2.874182 | 2.293107 |
| H | -2.835181 | 3.047675 | 0.669790 |
| H | -3.957341 | 3.160730 | 2.034236 |
| H | -3.198362 | -0.937748 | 4.934940 |
| H | -1.771951 | 0.018071 | 4.479214 |
| H | -2.737134 | 0.482301 | 5.889329 |
| H | -2.071382 | 0.614147 | 1.187249 |

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**$^{5}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.0891609

Zero-point correction= 0.937784 (Hartree/Particle)

Thermal correction to Energy= 1.000024

Thermal correction to Enthalpy= 1.000968

Thermal correction to Gibbs Free Energy= 0.837437

Sum of electronic and zero-point Energies= -2823.151377

Sum of electronic and thermal Energies= -2823.089137

Sum of electronic and thermal Enthalpies= -2823.088193

Sum of electronic and thermal Free Energies= -2823.251724

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.040866 | 0.196662 | -0.803019 |
| N | -1.416074 | -1.302914 | -1.452366 |
| C | -1.136205 | -2.630132 | -1.573773 |
| C | -2.246873 | -3.312456 | -2.220094 |
| C | -3.190684 | -2.340530 | -2.500344 |

| | | | |
|---|---|---|---|
| C | -2.617740 | -1.070040 | -2.034537 |
| C | 0.065984 | -3.227977 | -1.159320 |
| C | 1.194794 | -2.610086 | -0.602679 |
| N | 1.334072 | -1.274069 | -0.346818 |
| C | 2.578934 | -1.069451 | 0.175240 |
| C | 3.273513 | -2.350924 | 0.272583 |
| C | 2.412983 | -3.306708 | -0.210882 |
| C | 3.123248 | 0.174417 | 0.536713 |
| C | 2.565241 | 1.446096 | 0.336778 |
| N | 1.352978 | 1.658805 | -0.233503 |
| C | 1.144602 | 2.997330 | -0.308053 |
| C | 2.297762 | 3.699204 | 0.251322 |
| C | 3.183224 | 2.734657 | 0.662498 |
| C | -0.000087 | 3.606676 | -0.835671 |
| C | -1.156780 | 2.995258 | -1.345824 |
| C | -2.290643 | 3.706652 | -1.951526 |
| C | -3.200286 | 2.735975 | -2.325769 |
| C | -2.614591 | 1.455360 | -1.948757 |
| N | -1.410242 | 1.662490 | -1.344593 |
| C | -3.185948 | 0.200666 | -2.217440 |
| H | 0.138960 | -4.302469 | -1.296297 |
| H | -4.166457 | 0.221902 | -2.681303 |
| H | 0.006623 | 4.692030 | -0.844614 |

| | | | |
|---|---|---|---|
| H | 4.102290 | 0.147714 | 1.002701 |
| C | 1.837094 | 0.055366 | -3.029550 |
| H | 2.623729 | 0.608767 | -2.485954 |
| H | 1.934206 | 0.329201 | -4.095573 |
| C | 2.421353 | 5.189719 | 0.351748 |
| H | 2.416658 | 5.664259 | -0.638002 |
| H | 1.587211 | 5.620890 | 0.918328 |
| H | 3.347864 | 5.488587 | 0.850848 |
| C | 2.644431 | -4.782393 | -0.347687 |
| H | 1.856568 | -5.362307 | 0.148426 |
| H | 2.655931 | -5.096468 | -1.399310 |
| H | 3.599750 | -5.083712 | 0.092399 |
| C | -2.296543 | -4.772017 | -2.553465 |
| H | -1.292713 | -5.182353 | -2.701188 |
| H | -2.775022 | -5.364076 | -1.760741 |
| H | -2.868576 | -4.943602 | -3.471464 |
| C | -4.503324 | 2.920379 | -3.041446 |
| H | -4.474977 | 3.813800 | -3.673772 |
| H | -4.733791 | 2.062327 | -3.680578 |
| H | -5.346768 | 3.042677 | -2.347783 |
| C | -4.480984 | -2.468136 | -3.161120 |
| C | -5.263960 | -3.559206 | -3.243645 |
| H | -4.849343 | -1.560042 | -3.638300 |

| | | | |
|---|---|---|---|
| H | -6.206429 | -3.525028 | -3.782245 |
| H | -5.009932 | -4.500426 | -2.768546 |
| C | -2.347544 | 5.149480 | -2.141208 |
| C | -3.440887 | 5.925369 | -2.239775 |
| H | -1.379494 | 5.646080 | -2.207958 |
| H | -3.349084 | 6.995693 | -2.400362 |
| H | -4.447314 | 5.533496 | -2.139531 |
| C | 4.692348 | -2.546882 | 0.723578 |
| C | 5.702315 | -2.400872 | -0.451651 |
| H | 4.809579 | -3.544221 | 1.164218 |
| H | 4.951513 | -1.830408 | 1.509578 |
| H | 5.454693 | -3.103092 | -1.249564 |
| H | 5.650661 | -1.383735 | -0.856500 |
| C | 4.507437 | 2.955674 | 1.338989 |
| C | 5.754308 | 2.912909 | 0.407414 |
| H | 4.653320 | 2.234130 | 2.149454 |
| H | 4.492223 | 3.941419 | 1.815307 |
| H | 5.539582 | 3.380520 | -0.555101 |
| H | 6.567421 | 3.471370 | 0.889537 |
| C | 7.122860 | -2.675563 | -0.040519 |
| O | 7.840817 | -3.574555 | -0.413210 |
| O | 7.579601 | -1.764532 | 0.886374 |
| H | 8.495968 | -2.019384 | 1.084525 |

| | | | |
|---|---|---|---|
| C | 6.295806 | 1.526093 | 0.139197 |
| O | 6.460661 | 1.025054 | -0.955522 |
| O | 6.617999 | 0.889161 | 1.289205 |
| H | 6.962946 | 0.001428 | 1.059290 |
| O | 0.551429 | 0.362596 | -2.593904 |
| H | 2.083277 | -1.019667 | -2.952750 |
| C | -0.834435 | 0.058381 | 1.180609 |
| C | -0.993696 | -1.345217 | 1.768854 |
| C | -0.133591 | 0.801402 | 2.261033 |
| C | 0.127757 | -1.432315 | 2.814373 |
| H | -0.933302 | -2.148976 | 1.036780 |
| H | -1.969244 | -1.438614 | 2.265940 |
| H | -4.138177 | -0.998786 | 0.398776 |
| O | -0.018784 | 1.997807 | 2.456881 |
| O | 0.383529 | -0.075052 | 3.215032 |
| H | 1.046379 | -1.856175 | 2.394428 |
| H | -0.144565 | -1.998189 | 3.712398 |
| C | -4.773116 | -1.327645 | 1.210484 |
| C | -4.733598 | -0.670410 | 2.465191 |
| C | -5.600764 | -2.426796 | 0.999928 |
| C | -5.539679 | -1.210754 | 3.497261 |
| N | -3.948235 | 0.467300 | 2.669745 |
| C | -6.408623 | -2.933945 | 2.020345 |

| | | | |
|---|---|---|---|
| H | -5.600090 | -2.891882 | 0.017334 |
| C | -6.358532 | -2.314677 | 3.269751 |
| H | -5.540189 | -0.765502 | 4.484229 |
| C | -3.326234 | 1.145156 | 1.560820 |
| C | -3.740010 | 0.956076 | 4.034204 |
| H | -7.048324 | -3.795114 | 1.850036 |
| H | -6.967219 | -2.690385 | 4.089524 |
| H | -3.879937 | 0.928895 | 0.648078 |
| C | -3.114310 | 2.642293 | 1.717173 |
| H | -3.310439 | 1.953777 | 3.965552 |
| H | -4.714592 | 1.081326 | 4.525643 |
| C | -2.822387 | 0.082836 | 4.902403 |
| H | -2.285280 | 2.884118 | 2.386595 |
| H | -2.852943 | 3.054217 | 0.741451 |
| H | -4.026751 | 3.149287 | 2.064766 |
| H | -3.178410 | -0.950299 | 4.951459 |
| H | -1.801159 | 0.081548 | 4.513807 |
| H | -2.794207 | 0.480338 | 5.924258 |
| H | -2.103236 | 0.637063 | 1.241612 |

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$^{OSS}\mathbf{D}$

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Number of imaginary frequencies : 0 Electronic energy : HF=-2824.1440158

Zero-point correction= 0.943504 (Hartree/Particle)

Thermal correction to Energy= 1.006503

Thermal correction to Enthalpy= 1.007447

Thermal correction to Gibbs Free Energy= 0.839510

Sum of electronic and zero-point Energies= -2823.200512

Sum of electronic and thermal Energies= -2823.137513

Sum of electronic and thermal Enthalpies= -2823.136569

Sum of electronic and thermal Free Energies= -2823.304506

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -2.014723 | -0.098485 | 0.216511 |
| N | -2.613443 | 1.485524 | 1.343576 |
| C | -1.898068 | 2.129940 | 2.319774 |
| C | -2.689339 | 3.176260 | 2.932713 |
| C | -3.920253 | 3.143059 | 2.309636 |
| C | -3.848386 | 2.066761 | 1.325171 |
| C | -0.597990 | 1.799612 | 2.697791 |
| C | 0.145105 | 0.736415 | 2.200907 |

| | | | |
|---|---|---|---|
| N | -0.258286 | -0.117170 | 1.209788 |
| C | 0.733421 | -1.044848 | 1.072585 |
| C | 1.809436 | -0.777506 | 2.018273 |
| C | 1.446074 | 0.343515 | 2.716136 |
| C | 0.742571 | -2.088542 | 0.151836 |
| C | -0.260975 | -2.382011 | -0.763454 |
| N | -1.429558 | -1.691700 | -0.890147 |
| C | -2.131776 | -2.298399 | -1.889087 |
| C | -1.379122 | -3.419776 | -2.434305 |
| C | -0.207520 | -3.476205 | -1.730078 |
| C | -3.398427 | -1.927845 | -2.325903 |
| C | -4.185051 | -0.916394 | -1.779711 |
| C | -5.553916 | -0.613660 | -2.195743 |
| C | -5.979639 | 0.412046 | -1.379347 |
| C | -4.864097 | 0.724599 | -0.504771 |
| N | -3.795343 | -0.085254 | -0.776604 |
| C | -4.890218 | 1.719855 | 0.468219 |
| H | -0.139728 | 2.397535 | 3.477628 |
| H | -5.802877 | 2.298658 | 0.547761 |
| H | -3.820848 | -2.500724 | -3.143594 |
| H | 1.629545 | -2.709378 | 0.124302 |
| C | -2.659663 | -1.267946 | 2.797817 |
| H | -1.610983 | -1.368105 | 3.134325 |

| | | | |
|---|---|---|---|
| H | -3.222222 | -2.099113 | 3.259184 |
| C | -1.855839 | -4.303300 | -3.547878 |
| H | -2.753489 | -4.866547 | -3.262158 |
| H | -2.113846 | -3.723104 | -4.442315 |
| H | -1.094094 | -5.032235 | -3.839035 |
| C | 2.183183 | 1.044911 | 3.817853 |
| H | 2.331203 | 2.107438 | 3.590588 |
| H | 1.639636 | 0.992377 | 4.769824 |
| H | 3.171251 | 0.605421 | 3.982287 |
| C | -2.243997 | 4.055457 | 4.061219 |
| H | -1.517122 | 3.547991 | 4.702899 |
| H | -1.771007 | 4.981913 | 3.707141 |
| H | -3.096220 | 4.346990 | 4.683429 |
| C | -7.328892 | 1.060870 | -1.331784 |
| H | -8.104599 | 0.363469 | -1.663835 |
| H | -7.581149 | 1.387285 | -0.317993 |
| H | -7.390354 | 1.945304 | -1.981144 |
| C | -5.108861 | 3.945653 | 2.564092 |
| C | -5.165704 | 5.192199 | 3.063267 |
| H | -6.056281 | 3.466284 | 2.318014 |
| H | -6.121454 | 5.680683 | 3.229281 |
| H | -4.277683 | 5.769443 | 3.297287 |
| C | -6.276337 | -1.334934 | -3.234178 |

| | | | |
|---|---|---|---|
| C | -7.295324 | -0.886758 | -3.987456 |
| H | -5.941637 | -2.357090 | -3.410734 |
| H | -7.769975 | -1.532537 | -4.720499 |
| H | -7.669982 | 0.128931 | -3.919313 |
| C | 3.025043 | -1.633294 | 2.227778 |
| C | 2.751646 | -2.791591 | 3.230843 |
| H | 3.847283 | -1.020352 | 2.614786 |
| H | 3.373406 | -2.053140 | 1.279033 |
| H | 2.384300 | -2.390268 | 4.176966 |
| H | 1.988325 | -3.462511 | 2.820381 |
| C | 0.922188 | -4.448090 | -1.929499 |
| C | 0.970217 | -5.639810 | -0.928093 |
| H | 1.887107 | -3.931827 | -1.904492 |
| H | 0.835743 | -4.870807 | -2.935581 |
| H | -0.034799 | -5.963911 | -0.652514 |
| H | 1.480426 | -6.481673 | -1.414642 |
| C | 3.980135 | -3.603389 | 3.539608 |
| O | 4.545633 | -3.712604 | 4.602827 |
| O | 4.467354 | -4.252078 | 2.426575 |
| H | 5.250959 | -4.743908 | 2.723353 |
| C | 1.736991 | -5.370730 | 0.348871 |
| O | 1.320989 | -5.541928 | 1.477417 |
| O | 2.992603 | -4.936956 | 0.091155 |

| | | | |
|---|---|---|---|
| H | 3.441534 | -4.773345 | 0.946670 |
| O | -2.800678 | -1.321890 | 1.416237 |
| H | -3.049444 | -0.332862 | 3.241993 |
| C | -1.279168 | 1.145589 | -1.414453 |
| C | -1.794802 | 2.587639 | -1.495977 |
| C | 0.182086 | 1.307971 | -1.445924 |
| C | -0.656796 | 3.374300 | -0.831280 |
| H | -2.749935 | 2.764060 | -0.998988 |
| H | -1.904688 | 2.911935 | -2.543263 |
| H | 6.517092 | 4.180696 | -3.420823 |
| O | 1.075805 | 0.532794 | -1.751688 |
| O | 0.534979 | 2.602263 | -1.071663 |
| H | -0.803030 | 3.465546 | 0.249727 |
| H | -0.499661 | 4.373568 | -1.252518 |
| C | 7.046157 | 3.578539 | -2.692353 |
| C | 6.332281 | 2.603936 | -1.950736 |
| C | 8.398199 | 3.809222 | -2.459410 |
| C | 7.045723 | 1.905394 | -0.946143 |
| N | 4.987096 | 2.343470 | -2.219529 |
| C | 9.096682 | 3.096838 | -1.481622 |
| H | 8.908564 | 4.570556 | -3.045349 |
| C | 8.397509 | 2.150401 | -0.726742 |
| H | 6.546056 | 1.161005 | -0.339169 |

| | | | |
|---|---|---|---|
| C | 4.413998 | 2.793065 | -3.406396 |
| C | 4.172805 | 1.608559 | -1.232478 |
| H | 10.151972 | 3.281606 | -1.303764 |
| H | 8.911235 | 1.587868 | 0.049460 |
| H | 5.099951 | 2.875226 | -4.243339 |
| C | 2.947082 | 2.733182 | -3.668755 |
| H | 3.229906 | 1.316287 | -1.694227 |
| H | 4.687703 | 0.672453 | -0.983535 |
| C | 3.870431 | 2.410828 | 0.035309 |
| H | 2.349089 | 3.154437 | -2.853061 |
| H | 2.729119 | 3.302624 | -4.579322 |
| H | 2.556258 | 1.714004 | -3.821086 |
| H | 4.782673 | 2.739151 | 0.543933 |
| H | 3.265843 | 3.288697 | -0.206651 |
| H | 3.285782 | 1.789847 | 0.720974 |
| H | -1.601595 | 0.514343 | -2.240871 |

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**$^3$D**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2824.138187

Zero-point correction= 0.942964 (Hartree/Particle)

Thermal correction to Energy= 1.006053

Thermal correction to Enthalpy= 1.006997

Thermal correction to Gibbs Free Energy= 0.838185

Sum of electronic and zero-point Energies= -2823.195223

Sum of electronic and thermal Energies= -2823.132134

Sum of electronic and thermal Enthalpies= -2823.131190

Sum of electronic and thermal Free Energies= -2823.300002

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.198085 | -0.082721 | -0.883297 |
| N | -0.902290 | -1.723868 | -1.372461 |
| C | -0.557259 | -3.039903 | -1.208288 |
| C | -1.624540 | -3.910835 | -1.654875 |
| C | -2.637906 | -3.084358 | -2.093845 |
| C | -2.146923 | -1.717717 | -1.928312 |
| C | 0.655861 | -3.482473 | -0.684393 |
| C | 1.680413 | -2.669320 | -0.213298 |
| N | 1.647043 | -1.300025 | -0.165642 |
| C | 2.833153 | -0.903388 | 0.383548 |
| C | 3.657226 | -2.063531 | 0.695142 |
| C | 2.935613 | -3.166625 | 0.320277 |

| | | | |
|---|---|---|---|
| C | 3.206615 | 0.417504 | 0.628088 |
| C | 2.495451 | 1.552696 | 0.251730 |
| N | 1.291391 | 1.544638 | -0.389252 |
| C | 0.991864 | 2.846544 | -0.663583 |
| C | 2.031747 | 3.728358 | -0.154652 |
| C | 2.969300 | 2.923434 | 0.430775 |
| C | -0.137559 | 3.292046 | -1.335582 |
| C | -1.169323 | 2.488948 | -1.809710 |
| C | -2.356545 | 2.985255 | -2.505460 |
| C | -3.134233 | 1.877528 | -2.765240 |
| C | -2.407640 | 0.738855 | -2.230559 |
| N | -1.232139 | 1.140850 | -1.659878 |
| C | -2.851416 | -0.579004 | -2.313171 |
| H | 0.811131 | -4.554121 | -0.626201 |
| H | -3.833763 | -0.733769 | -2.743757 |
| H | -0.231920 | 4.362301 | -1.478377 |
| H | 4.152295 | 0.575589 | 1.132923 |
| C | 1.513701 | -1.102041 | -3.275912 |
| H | 2.351413 | -1.598660 | -2.750102 |
| H | 1.903823 | -0.780902 | -4.258865 |
| C | 2.007209 | 5.223199 | -0.261558 |
| H | 2.032829 | 5.555747 | -1.307150 |
| H | 1.097911 | 5.640567 | 0.187207 |

| | | | |
|---|---|---|---|
| H | 2.863590 | 5.678044 | 0.244816 |
| C | 3.324204 | -4.612581 | 0.404910 |
| H | 2.568523 | -5.204179 | 0.936024 |
| H | 3.440189 | -5.062674 | -0.589356 |
| H | 4.273001 | -4.743041 | 0.933913 |
| C | -1.577276 | -5.408166 | -1.662444 |
| H | -0.557252 | -5.776468 | -1.811700 |
| H | -1.943253 | -5.841916 | -0.721506 |
| H | -2.201087 | -5.811058 | -2.466712 |
| C | -4.434111 | 1.809728 | -3.506614 |
| H | -4.494402 | 2.607260 | -4.254376 |
| H | -4.551271 | 0.853452 | -4.025532 |
| H | -5.300813 | 1.925835 | -2.841061 |
| C | -3.935938 | -3.430037 | -2.656435 |
| C | -4.657750 | -4.541830 | -2.429387 |
| H | -4.363161 | -2.693078 | -3.336263 |
| H | -5.611224 | -4.695570 | -2.926120 |
| H | -4.339812 | -5.313358 | -1.736465 |
| C | -2.575749 | 4.380587 | -2.859238 |
| C | -3.747488 | 4.999079 | -3.087306 |
| H | -1.672416 | 4.983780 | -2.947961 |
| H | -3.775037 | 6.048434 | -3.366162 |
| H | -4.704444 | 4.499883 | -2.981080 |

| | | | |
|---|---|---|---|
| C | 5.058090 | -2.028892 | 1.234229 |
| C | 6.116056 | -1.938017 | 0.096752 |
| H | 5.251734 | -2.934480 | 1.821642 |
| H | 5.192200 | -1.184395 | 1.917325 |
| H | 5.984000 | -2.761585 | -0.607041 |
| H | 5.990829 | -0.994868 | -0.447509 |
| C | 4.221634 | 3.361287 | 1.138241 |
| C | 5.518361 | 3.363383 | 0.276127 |
| H | 4.396861 | 2.754053 | 2.031935 |
| H | 4.069990 | 4.384174 | 1.498023 |
| H | 5.306801 | 3.671455 | -0.749212 |
| H | 6.224752 | 4.081813 | 0.712786 |
| C | 7.531441 | -2.006931 | 0.601570 |
| O | 8.360087 | -2.855776 | 0.366527 |
| O | 7.836957 | -0.955048 | 1.437005 |
| H | 8.763468 | -1.082066 | 1.700458 |
| C | 6.248822 | 2.039834 | 0.220783 |
| O | 6.570063 | 1.445634 | -0.789149 |
| O | 6.549785 | 1.586102 | 1.460520 |
| H | 7.022266 | 0.733116 | 1.364714 |
| O | 1.008611 | -0.004542 | -2.592275 |
| H | 0.755171 | -1.882829 | -3.474106 |
| C | -0.913830 | -0.067928 | 0.969279 |

| | | | |
|---|---|---|---|
| C | -0.757805 | -1.271034 | 1.906786 |
| C | -0.656743 | 1.081711 | 1.855199 |
| C | 0.255441 | -0.746108 | 2.932625 |
| H | -0.407440 | -2.185313 | 1.426609 |
| H | -1.708018 | -1.507032 | 2.410070 |
| H | -4.823721 | -0.584865 | 0.373003 |
| O | -0.980784 | 2.257476 | 1.773721 |
| O | 0.056559 | 0.678197 | 2.976282 |
| H | 1.287190 | -0.948420 | 2.625264 |
| H | 0.107103 | -1.136258 | 3.946208 |
| C | -5.297410 | -0.984969 | 1.261487 |
| C | -5.440952 | -0.160067 | 2.403210 |
| C | -5.697978 | -2.316860 | 1.286436 |
| C | -5.974078 | -0.749995 | 3.573377 |
| N | -5.079563 | 1.191071 | 2.351126 |
| C | -6.247306 | -2.883012 | 2.440707 |
| H | -5.556900 | -2.920497 | 0.393175 |
| C | -6.369338 | -2.085248 | 3.580903 |
| H | -6.087390 | -0.167763 | 4.480225 |
| C | -4.953948 | 1.840499 | 1.124583 |
| C | -4.825796 | 1.925956 | 3.596842 |
| H | -6.555476 | -3.924383 | 2.456481 |
| H | -6.779410 | -2.504849 | 4.496936 |

| | | | |
|---|---|---|---|
| H | -5.558960 | 1.435712 | 0.322709 |
| C | -4.184402 | 3.103260 | 0.941393 |
| H | -4.787398 | 2.985461 | 3.343135 |
| H | -5.688812 | 1.808057 | 4.265584 |
| C | -3.530970 | 1.519344 | 4.307012 |
| H | -3.155679 | 3.017424 | 1.315411 |
| H | -4.115749 | 3.323061 | -0.127459 |
| H | -4.645758 | 3.989911 | 1.414931 |
| H | -3.520419 | 0.448019 | 4.527868 |
| H | -2.659355 | 1.755201 | 3.691574 |
| H | -3.441012 | 2.062068 | 5.255610 |
| H | -1.907184 | 0.024711 | 0.532067 |

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**$^5$D**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2824.125271

Zero-point correction= 0.939983 (Hartree/Particle)

Thermal correction to Energy= 1.004054

Thermal correction to Enthalpy= 1.004999

Thermal correction to Gibbs Free Energy= 0.832490

Sum of electronic and zero-point Energies= -2823.185288

Sum of electronic and thermal Energies= -2823.121217

Sum of electronic and thermal Enthalpies= -2823.120272

Sum of electronic and thermal Free Energies= -2823.292781

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.171968 | -0.084981 | -0.853965 |
| N | -0.977981 | -1.736600 | -1.332045 |
| C | -0.583519 | -3.041297 | -1.221955 |
| C | -1.623251 | -3.911690 | -1.747426 |
| C | -2.643421 | -3.086897 | -2.183298 |
| C | -2.195851 | -1.711518 | -1.938520 |
| C | 0.644660 | -3.489035 | -0.701715 |
| C | 1.701961 | -2.722355 | -0.191524 |
| N | 1.681047 | -1.368104 | -0.073950 |
| C | 2.869600 | -0.966040 | 0.440144 |
| C | 3.711972 | -2.137740 | 0.686745 |
| C | 2.981648 | -3.234099 | 0.291689 |
| C | 3.211984 | 0.377337 | 0.674118 |
| C | 2.487457 | 1.525486 | 0.313677 |
| N | 1.274518 | 1.537153 | -0.314101 |
| C | 0.943341 | 2.836680 | -0.575885 |

| | | | |
|---|---|---|---|
| C | 1.992548 | 3.711109 | -0.066318 |
| C | 2.948400 | 2.901629 | 0.495494 |
| C | -0.207497 | 3.290555 | -1.234378 |
| C | -1.276571 | 2.532892 | -1.737240 |
| C | -2.456725 | 3.044917 | -2.451191 |
| C | -3.231741 | 1.937152 | -2.747587 |
| C | -2.514895 | 0.783544 | -2.213525 |
| N | -1.367945 | 1.193063 | -1.615250 |
| C | -2.909561 | -0.560609 | -2.316834 |
| H | 0.794775 | -4.564502 | -0.703575 |
| H | -3.872447 | -0.737326 | -2.784971 |
| H | -0.280008 | 4.366901 | -1.353735 |
| H | 4.166607 | 0.553171 | 1.158648 |
| C | 2.255772 | 0.026511 | -2.896132 |
| H | 2.666074 | 1.005330 | -2.591100 |
| H | 2.373794 | -0.045678 | -3.991738 |
| C | 1.969005 | 5.208087 | -0.150388 |
| H | 1.983460 | 5.556300 | -1.191118 |
| H | 1.064232 | 5.618793 | 0.313340 |
| H | 2.830396 | 5.656215 | 0.353488 |
| C | 3.387219 | -4.677931 | 0.308987 |
| H | 2.638162 | -5.300770 | 0.813210 |
| H | 3.503058 | -5.080475 | -0.705698 |

| | | | |
|---|---|---|---|
| H | 4.339376 | -4.825260 | 0.828206 |
| C | -1.545634 | -5.405638 | -1.833391 |
| H | -0.515182 | -5.744623 | -1.980995 |
| H | -1.919479 | -5.896106 | -0.923740 |
| H | -2.145705 | -5.778370 | -2.669617 |
| C | -4.517709 | 1.887170 | -3.514142 |
| H | -4.535796 | 2.653131 | -4.297330 |
| H | -4.659986 | 0.913448 | -3.992792 |
| H | -5.392885 | 2.064060 | -2.873253 |
| C | -3.910999 | -3.441439 | -2.806957 |
| C | -4.618680 | -4.573553 | -2.644140 |
| H | -4.327756 | -2.690000 | -3.477653 |
| H | -5.549916 | -4.728442 | -3.181242 |
| H | -4.311390 | -5.361847 | -1.965296 |
| C | -2.669218 | 4.445050 | -2.784481 |
| C | -3.826740 | 5.065146 | -3.076622 |
| H | -1.767278 | 5.057302 | -2.790807 |
| H | -3.840787 | 6.122819 | -3.323313 |
| H | -4.785685 | 4.559358 | -3.056644 |
| C | 5.129868 | -2.111441 | 1.179428 |
| C | 6.148198 | -1.960506 | 0.011875 |
| H | 5.356500 | -3.035994 | 1.724381 |
| H | 5.276574 | -1.290125 | 1.888601 |

| | | | |
|---|---|---|---|
| H | 6.016441 | -2.769434 | -0.708777 |
| H | 5.978499 | -1.007438 | -0.501970 |
| C | 4.209174 | 3.345972 | 1.184823 |
| C | 5.487948 | 3.375090 | 0.296648 |
| H | 4.409789 | 2.726520 | 2.064774 |
| H | 4.055104 | 4.361590 | 1.563825 |
| H | 5.253736 | 3.712092 | -0.714628 |
| H | 6.202509 | 4.081363 | 0.739418 |
| C | 7.579117 | -2.001712 | 0.473310 |
| O | 8.417931 | -2.832988 | 0.212653 |
| O | 7.886729 | -0.945608 | 1.303003 |
| H | 8.822213 | -1.055205 | 1.541273 |
| C | 6.214718 | 2.052593 | 0.188281 |
| O | 6.487950 | 1.472504 | -0.843756 |
| O | 6.570717 | 1.581537 | 1.406471 |
| H | 7.037358 | 0.729546 | 1.278376 |
| O | 0.913823 | -0.127827 | -2.565831 |
| H | 2.904151 | -0.749679 | -2.451412 |
| C | -0.945947 | -0.078800 | 1.024513 |
| C | -0.780628 | -1.307684 | 1.918301 |
| C | -0.660161 | 1.051446 | 1.935754 |
| C | 0.239559 | -0.817778 | 2.954486 |
| H | -0.438921 | -2.206208 | 1.405110 |

| | | | |
|---|---|---|---|
| H | -1.732619 | -1.550778 | 2.414083 |
| H | -4.775124 | -0.609895 | 0.319345 |
| O | -0.985287 | 2.225913 | 1.884774 |
| O | 0.054976 | 0.608587 | 3.034032 |
| H | 1.267683 | -1.021396 | 2.640060 |
| H | 0.085646 | -1.229614 | 3.958041 |
| C | -5.256147 | -1.043404 | 1.187993 |
| C | -5.437898 | -0.255698 | 2.350426 |
| C | -5.632147 | -2.382691 | 1.165892 |
| C | -5.983755 | -0.889601 | 3.491321 |
| N | -5.099707 | 1.102958 | 2.346864 |
| C | -6.193128 | -2.992880 | 2.291670 |
| H | -5.463709 | -2.956391 | 0.257857 |
| C | -6.353545 | -2.231644 | 3.451792 |
| H | -6.127113 | -0.336954 | 4.412292 |
| C | -4.947969 | 1.789691 | 1.143536 |
| C | -4.896007 | 1.805738 | 3.619496 |
| H | -6.481715 | -4.039717 | 2.270474 |
| H | -6.774144 | -2.685456 | 4.346474 |
| H | -5.516042 | 1.395726 | 0.310274 |
| C | -4.209463 | 3.078236 | 1.023183 |
| H | -4.872880 | 2.872881 | 3.398266 |
| H | -5.773739 | 1.650677 | 4.260704 |

| | | | |
|---|---|---|---|
| C | -3.612798 | 1.404453 | 4.353767 |
| H | -3.192085 | 3.011309 | 1.430003 |
| H | -4.110837 | 3.329545 | -0.036217 |
| H | -4.711986 | 3.937590 | 1.505082 |
| H | -3.587465 | 0.327997 | 4.546674 |
| H | -2.730174 | 1.672555 | 3.767829 |
| H | -3.557395 | 1.923318 | 5.318153 |
| H | -1.926546 | 0.034586 | 0.568888 |

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**$^{OSS}$TS(D-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.1071026

Zero-point correction= 0.941337 (Hartree/Particle)

Thermal correction to Energy= 1.004130

Thermal correction to Enthalpy= 1.005074

Thermal correction to Gibbs Free Energy= 0.837205

Sum of electronic and zero-point Energies= -2823.165766

Sum of electronic and thermal Energies= -2823.102972

Sum of electronic and thermal Enthalpies= -2823.102028

Sum of electronic and thermal Free Energies= -2823.269898

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.084298 | 1.610866 | 0.123944 |
| N | -1.150649 | 2.261184 | -1.466946 |
| C | -0.859631 | 2.054078 | -2.801854 |
| C | -1.821464 | 2.705994 | -3.645189 |
| C | -2.714137 | 3.345267 | -2.796802 |
| C | -2.269083 | 3.048227 | -1.444332 |
| C | 0.262628 | 1.367661 | -3.261924 |
| C | 1.246724 | 0.807017 | -2.471375 |
| N | 1.244340 | 0.785139 | -1.094830 |
| C | 2.397674 | 0.139850 | -0.730574 |
| C | 3.178052 | -0.214933 | -1.909819 |
| C | 2.449453 | 0.183820 | -2.993277 |
| C | 2.756454 | -0.200301 | 0.564495 |
| C | 2.001858 | 0.051039 | 1.708637 |
| N | 0.804836 | 0.715347 | 1.715707 |
| C | 0.393115 | 0.737997 | 3.023156 |
| C | 1.343358 | 0.054186 | 3.870557 |
| C | 2.359909 | -0.376664 | 3.049148 |
| C | -0.767992 | 1.354278 | 3.485838 |
| C | -1.661756 | 2.075937 | 2.713396 |

| | | | |
|---|---|---|---|
| C | -2.819264 | 2.787562 | 3.244253 |
| C | -3.406519 | 3.418853 | 2.170153 |
| C | -2.622149 | 3.059568 | 1.004362 |
| N | -1.576010 | 2.240522 | 1.352913 |
| C | -2.934439 | 3.459078 | -0.287656 |
| H | 0.385020 | 1.279065 | -4.335313 |
| H | -3.819563 | 4.070125 | -0.413666 |
| H | -0.969839 | 1.282286 | 4.548604 |
| H | 3.676545 | -0.756985 | 0.691903 |
| C | 1.460470 | 3.849544 | -0.621495 |
| H | 2.265177 | 3.282674 | -1.119207 |
| H | 1.910921 | 4.768842 | -0.211524 |
| C | 1.200733 | -0.109001 | 5.355086 |
| H | 1.247914 | 0.855969 | 5.876365 |
| H | 0.241789 | -0.569014 | 5.623778 |
| H | 1.992727 | -0.739502 | 5.769985 |
| C | 2.766688 | 0.028661 | -4.449576 |
| H | 1.988929 | -0.549003 | -4.963558 |
| H | 2.838799 | 0.998232 | -4.958316 |
| H | 3.717049 | -0.491240 | -4.601068 |
| C | -1.802482 | 2.723196 | -5.143307 |
| H | -0.795020 | 2.561372 | -5.537893 |
| H | -2.447124 | 1.945884 | -5.576357 |

| | | | |
|---|---|---|---|
| H | -2.160240 | 3.685807 | -5.524210 |
| C | -4.586951 | 4.340646 | 2.162145 |
| H | -4.703087 | 4.828867 | 3.134724 |
| H | -4.475898 | 5.121987 | 1.403198 |
| H | -5.528244 | 3.815051 | 1.948281 |
| C | -3.857120 | 4.184898 | -3.114886 |
| C | -4.579812 | 4.214342 | -4.250061 |
| H | -4.153417 | 4.878935 | -2.328152 |
| H | -5.400884 | 4.916127 | -4.364535 |
| H | -4.399403 | 3.539601 | -5.079437 |
| C | -3.186463 | 2.821226 | 4.653780 |
| C | -4.409941 | 3.008444 | 5.177266 |
| H | -2.363997 | 2.676713 | 5.354349 |
| H | -4.556065 | 3.035273 | 6.253309 |
| H | -5.297644 | 3.115898 | 4.562994 |
| C | 4.537344 | -0.848792 | -1.894581 |
| C | 5.666001 | 0.204859 | -1.686753 |
| H | 4.714220 | -1.369659 | -2.842345 |
| H | 4.605306 | -1.607536 | -1.107895 |
| H | 5.599592 | 0.977565 | -2.454669 |
| H | 5.550813 | 0.680307 | -0.706223 |
| C | 3.579753 | -1.157795 | 3.452105 |
| C | 4.895679 | -0.335206 | 3.591280 |

| | | | |
|---|---|---|---|
| H | 3.762589 | -1.984226 | 2.757205 |
| H | 3.383346 | -1.623003 | 4.423697 |
| H | 4.694584 | 0.668778 | 3.968848 |
| H | 5.551295 | -0.846051 | 4.309265 |
| C | 7.044394 | -0.390115 | -1.772154 |
| O | 7.885719 | -0.190586 | -2.617997 |
| O | 7.294524 | -1.274392 | -0.745407 |
| H | 8.197436 | -1.602852 | -0.889358 |
| C | 5.702234 | -0.198933 | 2.317715 |
| O | 6.111823 | 0.841280 | 1.842433 |
| O | 5.959676 | -1.406384 | 1.761953 |
| H | 6.468098 | -1.260858 | 0.937032 |
| O | 0.869363 | 3.145629 | 0.430826 |
| H | 0.739289 | 4.154839 | -1.397661 |
| C | -1.449568 | -1.021455 | -0.061317 |
| C | -2.871347 | -0.579115 | -0.248647 |
| C | -0.962126 | -1.636638 | -1.242624 |
| C | -3.195085 | -1.132976 | -1.660568 |
| H | -2.987322 | 0.510222 | -0.217086 |
| H | -3.566433 | -0.975839 | 0.507136 |
| H | -3.861003 | -3.100995 | 0.887805 |
| O | 0.121884 | -2.151363 | -1.536902 |
| O | -1.979778 | -1.660920 | -2.207687 |

| | | | |
|---|---|---|---|
| H | -3.568607 | -0.356702 | -2.337170 |
| H | -3.935404 | -1.943283 | -1.620484 |
| C | -4.155527 | -4.088000 | 0.556884 |
| C | -3.172503 | -5.005805 | 0.120299 |
| C | -5.507088 | -4.418847 | 0.518478 |
| C | -3.617031 | -6.250463 | -0.380694 |
| N | -1.803050 | -4.699288 | 0.207425 |
| C | -5.935082 | -5.659010 | 0.040077 |
| H | -6.234464 | -3.684322 | 0.854956 |
| C | -4.972421 | -6.564452 | -0.414015 |
| H | -2.904574 | -6.984486 | -0.735977 |
| C | -1.353530 | -3.684358 | 1.029352 |
| C | -0.857114 | -5.444788 | -0.644187 |
| H | -6.991389 | -5.908767 | 0.008937 |
| H | -5.276244 | -7.534753 | -0.799423 |
| H | -2.071422 | -3.358857 | 1.769254 |
| C | 0.096767 | -3.468162 | 1.300386 |
| H | 0.146436 | -5.149209 | -0.347808 |
| H | -0.947007 | -6.514188 | -0.412443 |
| C | -1.026134 | -5.187585 | -2.144511 |
| H | 0.623415 | -3.119745 | 0.401000 |
| H | 0.203826 | -2.693577 | 2.063051 |
| H | 0.599884 | -4.374918 | 1.678400 |

H -2.039312 -5.416173 -2.486137

H -0.795745 -4.143033 -2.367622

H -0.328737 -5.829034 -2.696877

H -0.870286 -0.908585 0.838149

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**$^{3}$TS(D-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.1134626

Zero-point correction= 0.941578 (Hartree/Particle)

Thermal correction to Energy= 1.004510

Thermal correction to Enthalpy= 1.005454

Thermal correction to Gibbs Free Energy= 0.836183

Sum of electronic and zero-point Energies= -2823.171884

Sum of electronic and thermal Energies= -2823.108953

Sum of electronic and thermal Enthalpies= -2823.108008

Sum of electronic and thermal Free Energies= -2823.277279

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Cartesian Coordinates

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Fe -0.009000 -1.560057 0.095495

| | | | |
|---|---|---|---|
| N | 1.054525 | -2.210242 | -1.507336 |
| C | 0.744694 | -2.037488 | -2.832496 |
| C | 1.701641 | -2.717140 | -3.679722 |
| C | 2.603280 | -3.327038 | -2.830372 |
| C | 2.167505 | -3.002389 | -1.475302 |
| C | -0.365707 | -1.337330 | -3.299967 |
| C | -1.335148 | -0.732058 | -2.513494 |
| N | -1.331945 | -0.691314 | -1.144528 |
| C | -2.447165 | 0.007425 | -0.783161 |
| C | -3.209781 | 0.395023 | -1.963822 |
| C | -2.509295 | -0.059195 | -3.046013 |
| C | -2.794335 | 0.355339 | 0.518722 |
| C | -2.079243 | 0.039554 | 1.669377 |
| N | -0.922139 | -0.686749 | 1.691163 |
| C | -0.551441 | -0.778656 | 3.004003 |
| C | -1.500234 | -0.076563 | 3.854470 |
| C | -2.457988 | 0.438724 | 3.020692 |
| C | 0.567560 | -1.453606 | 3.478561 |
| C | 1.476179 | -2.171424 | 2.704640 |
| C | 2.605741 | -2.927018 | 3.243895 |
| C | 3.228372 | -3.503904 | 2.157442 |
| C | 2.484952 | -3.076298 | 0.988382 |
| N | 1.435353 | -2.268507 | 1.346012 |

| | | | |
|---|---|---|---|
| C | 2.822525 | -3.417291 | -0.318423 |
| H | -0.492764 | -1.269552 | -4.374659 |
| H | 3.706336 | -4.031119 | -0.448340 |
| H | 0.733626 | -1.432476 | 4.549819 |
| H | -3.684148 | 0.960488 | 0.643806 |
| C | -1.666039 | -3.842906 | -0.700155 |
| H | -2.479170 | -3.237577 | -1.150126 |
| H | -2.139144 | -4.781277 | -0.348639 |
| C | -1.397740 | 0.019558 | 5.347652 |
| H | -1.499943 | -0.963919 | 5.824178 |
| H | -0.429221 | 0.426690 | 5.663426 |
| H | -2.175951 | 0.664856 | 5.765755 |
| C | -2.833537 | 0.078671 | -4.502900 |
| H | -2.020706 | 0.573135 | -5.048734 |
| H | -2.994581 | -0.896527 | -4.980070 |
| H | -3.740092 | 0.671020 | -4.658310 |
| C | 1.651851 | -2.774138 | -5.176037 |
| H | 0.623303 | -2.716254 | -5.545498 |
| H | 2.209450 | -1.950918 | -5.643741 |
| H | 2.088642 | -3.708792 | -5.542317 |
| C | 4.402003 | -4.434768 | 2.147479 |
| H | 4.448258 | -5.007687 | 3.079171 |
| H | 4.341635 | -5.145793 | 1.317594 |

| | | | |
|---|---|---|---|
| H | 5.358193 | -3.901912 | 2.048605 |
| C | 3.745419 | -4.174246 | -3.145104 |
| C | 4.491053 | -4.166755 | -4.263478 |
| H | 4.015556 | -4.896453 | -2.374617 |
| H | 5.309671 | -4.869424 | -4.389654 |
| H | 4.330639 | -3.457582 | -5.068404 |
| C | 2.915206 | -3.044048 | 4.661589 |
| C | 4.108289 | -3.301593 | 5.225363 |
| H | 2.069295 | -2.906528 | 5.335283 |
| H | 4.205681 | -3.388883 | 6.303663 |
| H | 5.018204 | -3.410274 | 4.644893 |
| C | -4.537055 | 1.095061 | -1.956992 |
| C | -5.718298 | 0.094721 | -1.788320 |
| H | -4.672470 | 1.642780 | -2.896723 |
| H | -4.579819 | 1.840522 | -1.156519 |
| H | -5.679456 | -0.665423 | -2.570467 |
| H | -5.641693 | -0.405992 | -0.816532 |
| C | -3.649226 | 1.267211 | 3.416467 |
| C | -5.003683 | 0.503544 | 3.499175 |
| H | -3.772572 | 2.119184 | 2.740083 |
| H | -3.454953 | 1.695547 | 4.405190 |
| H | -4.858983 | -0.520371 | 3.847903 |
| H | -5.651360 | 1.020988 | 4.219667 |

| | | | |
|---|---|---|---|
| C | -7.065055 | 0.758057 | -1.878128 |
| O | -7.912557 | 0.601441 | -2.726632 |
| O | -7.275434 | 1.651302 | -0.849941 |
| H | -8.162080 | 2.021116 | -0.994682 |
| C | -5.788646 | 0.444883 | 2.205931 |
| O | -6.251141 | -0.558349 | 1.701318 |
| O | -5.962185 | 1.676991 | 1.672508 |
| H | -6.465252 | 1.578695 | 0.837197 |
| O | -1.014399 | -3.206629 | 0.343330 |
| H | -0.992656 | -4.131145 | -1.533550 |
| C | 1.560687 | 0.868516 | 0.125630 |
| C | 2.938091 | 0.410266 | -0.249183 |
| C | 0.979314 | 1.622792 | -0.941289 |
| C | 3.059574 | 0.912110 | -1.711357 |
| H | 3.060185 | -0.673900 | -0.192733 |
| H | 3.723555 | 0.838564 | 0.391317 |
| H | 4.398516 | 2.780979 | 0.694493 |
| O | -0.083077 | 2.234396 | -1.040536 |
| O | 1.868582 | 1.654914 | -2.015470 |
| H | 3.135769 | 0.080363 | -2.419821 |
| H | 3.919322 | 1.576665 | -1.857596 |
| C | 4.667439 | 3.776775 | 0.368837 |
| C | 3.658285 | 4.738545 | 0.133803 |

| | | | |
|---|---|---|---|
| C | 6.008355 | 4.076333 | 0.145117 |
| C | 4.065881 | 5.999367 | -0.359257 |
| N | 2.307502 | 4.464783 | 0.405938 |
| C | 6.400704 | 5.330154 | -0.327309 |
| H | 6.753488 | 3.306886 | 0.331376 |
| C | 5.410692 | 6.282479 | -0.580341 |
| H | 3.333522 | 6.771161 | -0.559829 |
| C | 1.939288 | 3.413843 | 1.237847 |
| C | 1.276029 | 5.301825 | -0.234531 |
| H | 7.447963 | 5.555342 | -0.505298 |
| H | 5.684111 | 7.266669 | -0.953176 |
| H | 2.756883 | 3.017730 | 1.826086 |
| C | 0.565835 | 3.341219 | 1.825569 |
| H | 0.314971 | 4.996642 | 0.171458 |
| H | 1.428154 | 6.345863 | 0.071695 |
| C | 1.220727 | 5.178474 | -1.760461 |
| H | -0.187022 | 3.107610 | 1.062455 |
| H | 0.538823 | 2.537822 | 2.565441 |
| H | 0.273396 | 4.273542 | 2.338164 |
| H | 2.178980 | 5.420051 | -2.227981 |
| H | 0.929666 | 4.163327 | -2.037102 |
| H | 0.468817 | 5.876991 | -2.147016 |
| H | 1.096704 | 0.744036 | 1.087019 |

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**$^{5}$TS(D-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.1252505

Zero-point correction= 0.938092 (Hartree/Particle)

Thermal correction to Energy= 1.002268

Thermal correction to Enthalpy= 1.003212

Thermal correction to Gibbs Free Energy= 0.828382

Sum of electronic and zero-point Energies= -2823.187158

Sum of electronic and thermal Energies= -2823.122983

Sum of electronic and thermal Enthalpies= -2823.122038

Sum of electronic and thermal Free Energies= -2823.296868

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 2.157213 | 0.263589 | 0.434967 |
| N | 2.696503 | -1.618450 | 1.269810 |
| C | 1.978961 | -2.295866 | 2.212536 |
| C | 2.776442 | -3.386056 | 2.752752 |
| C | 4.000968 | -3.330744 | 2.107817 |

| | | | |
|---|---|---|---|
| C | 3.926192 | -2.191599 | 1.186667 |
| C | 0.670580 | -1.960357 | 2.605114 |
| C | -0.117505 | -0.887199 | 2.165045 |
| N | 0.243457 | 0.026201 | 1.216607 |
| C | -0.769398 | 0.929250 | 1.093691 |
| C | -1.845714 | 0.576538 | 2.018402 |
| C | -1.441595 | -0.556819 | 2.682019 |
| C | -0.785278 | 2.025740 | 0.216064 |
| C | 0.225764 | 2.445359 | -0.659997 |
| N | 1.428060 | 1.829015 | -0.787784 |
| C | 2.153024 | 2.503928 | -1.716775 |
| C | 1.370557 | 3.631581 | -2.224240 |
| C | 0.165313 | 3.596769 | -1.567342 |
| C | 3.450067 | 2.161829 | -2.128636 |
| C | 4.258512 | 1.103407 | -1.675696 |
| C | 5.626860 | 0.826998 | -2.128066 |
| C | 6.050537 | -0.283248 | -1.419708 |
| C | 4.940142 | -0.674650 | -0.563979 |
| N | 3.887906 | 0.174642 | -0.756573 |
| C | 4.951241 | -1.760564 | 0.327954 |
| H | 0.220332 | -2.595341 | 3.362229 |
| H | 5.865553 | -2.344738 | 0.346614 |
| H | 3.885203 | 2.800530 | -2.891125 |

| | | | |
|---|---|---|---|
| H | -1.700787 | 2.606921 | 0.202005 |
| C | 2.728930 | 1.214217 | 3.136935 |
| H | 1.670815 | 1.288700 | 3.452994 |
| H | 3.275672 | 2.005346 | 3.682871 |
| C | 1.847287 | 4.603896 | -3.261523 |
| H | 2.697847 | 5.195857 | -2.899434 |
| H | 2.181390 | 4.090968 | -4.171872 |
| H | 1.061757 | 5.307933 | -3.551699 |
| C | -2.166800 | -1.320169 | 3.750488 |
| H | -2.259574 | -2.382386 | 3.493987 |
| H | -1.642648 | -1.268150 | 4.713400 |
| H | -3.177626 | -0.932706 | 3.908499 |
| C | 2.345986 | -4.329002 | 3.834754 |
| H | 1.600389 | -3.870300 | 4.491528 |
| H | 1.900052 | -5.250134 | 3.433911 |
| H | 3.199442 | -4.629280 | 4.451903 |
| C | 7.394870 | -0.943621 | -1.458511 |
| H | 8.177976 | -0.216696 | -1.697974 |
| H | 7.643128 | -1.401170 | -0.495730 |
| H | 7.449864 | -1.737124 | -2.217064 |
| C | 5.181615 | -4.162493 | 2.290542 |
| C | 5.242223 | -5.425900 | 2.746877 |
| H | 6.125465 | -3.690287 | 2.017281 |

| | | | |
|---|---|---|---|
| H | 6.197424 | -5.932015 | 2.852618 |
| H | 4.358277 | -5.998885 | 3.005014 |
| C | 6.351688 | 1.637014 | -3.096884 |
| C | 7.370367 | 1.261743 | -3.890030 |
| H | 6.015443 | 2.670650 | -3.179907 |
| H | 7.841260 | 1.973060 | -4.562409 |
| H | 7.749109 | 0.245681 | -3.915225 |
| C | -3.099505 | 1.370850 | 2.246501 |
| C | -2.886021 | 2.506333 | 3.289298 |
| H | -3.899808 | 0.712277 | 2.604010 |
| H | -3.455407 | 1.808401 | 1.308223 |
| H | -2.521486 | 2.089655 | 4.229857 |
| H | -2.140016 | 3.216027 | 2.913762 |
| C | -0.994956 | 4.533326 | -1.762520 |
| C | -1.136667 | 5.658408 | -0.695618 |
| H | -1.936923 | 3.977162 | -1.808286 |
| H | -0.886863 | 5.020751 | -2.737059 |
| H | -0.158886 | 6.020983 | -0.373738 |
| H | -1.682444 | 6.497778 | -1.146761 |
| C | -4.148311 | 3.264533 | 3.597312 |
| O | -4.737736 | 3.322326 | 4.651612 |
| O | -4.637777 | 3.927884 | 2.493662 |
| H | -5.443193 | 4.383580 | 2.789712 |

| | | | |
|---|---|---|---|
| C | -1.917253 | 5.271208 | 0.542085 |
| O | -1.537693 | 5.395433 | 1.689412 |
| O | -3.141540 | 4.788571 | 0.226313 |
| H | -3.600524 | 4.553362 | 1.059531 |
| O | 2.902005 | 1.368527 | 1.768096 |
| H | 3.110175 | 0.247227 | 3.517744 |
| C | 1.273834 | -1.122455 | -1.734458 |
| C | 1.853842 | -2.505714 | -1.750978 |
| C | -0.172511 | -1.263031 | -1.700190 |
| C | 0.711671 | -3.326069 | -1.126476 |
| H | 2.790437 | -2.610224 | -1.201829 |
| H | 2.041473 | -2.831924 | -2.788551 |
| H | -6.670021 | -3.935579 | -3.573008 |
| O | -1.062630 | -0.467155 | -1.954215 |
| O | -0.493971 | -2.572855 | -1.372194 |
| H | 0.842085 | -3.429836 | -0.045414 |
| H | 0.582619 | -4.317077 | -1.572214 |
| C | -7.151886 | -3.379247 | -2.778360 |
| C | -6.384142 | -2.476659 | -2.001160 |
| C | -8.497211 | -3.600090 | -2.500687 |
| C | -7.034871 | -1.840860 | -0.916125 |
| N | -5.045767 | -2.223671 | -2.312229 |
| C | -9.134199 | -2.948974 | -1.441745 |

| | | | |
|---|---|---|---|
| H | -9.050761 | -4.305357 | -3.116673 |
| C | -8.380732 | -2.075266 | -0.652538 |
| H | -6.491861 | -1.153594 | -0.279713 |
| C | -4.535982 | -2.597808 | -3.552799 |
| C | -4.171296 | -1.581923 | -1.312394 |
| H | -10.184321 | -3.125916 | -1.229029 |
| H | -8.846024 | -1.562405 | 0.185973 |
| H | -5.257628 | -2.601399 | -4.363159 |
| C | -3.080105 | -2.554068 | -3.873745 |
| H | -3.250234 | -1.265436 | -1.800328 |
| H | -4.655078 | -0.661412 | -0.964174 |
| C | -3.822211 | -2.486881 | -0.128422 |
| H | -2.462094 | -3.054757 | -3.119811 |
| H | -2.915980 | -3.056943 | -4.833354 |
| H | -2.666598 | -1.536441 | -3.965403 |
| H | -4.715735 | -2.836061 | 0.398912 |
| H | -3.254574 | -3.357139 | -0.468611 |
| H | -3.190499 | -1.934117 | 0.573672 |
| H | 1.710512 | -0.290916 | -2.265635 |

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**$^{4}$TS(D-E)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2379.9085134

Zero-point correction= 0.720209 (Hartree/Particle)

Thermal correction to Energy= 0.770847

Thermal correction to Enthalpy= 0.771791

Thermal correction to Gibbs Free Energy= 0.631852

Sum of electronic and zero-point Energies= -2379.188305

Sum of electronic and thermal Energies= -2379.137666

Sum of electronic and thermal Enthalpies= -2379.136722

Sum of electronic and thermal Free Energies= -2379.276661

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.880163 | 0.080468 | -0.326205 |
| N | -2.187856 | -1.589813 | -0.282749 |
| C | -1.795830 | -2.896872 | -0.270722 |
| C | -2.942107 | -3.758080 | -0.515755 |
| C | -4.031981 | -2.919650 | -0.685467 |
| C | -3.520254 | -1.551675 | -0.548116 |
| C | -0.471726 | -3.328078 | -0.066798 |
| C | 0.677552 | -2.545372 | 0.113089 |

| | | | |
|---|---|---|---|
| N | 0.707479 | -1.182031 | 0.153551 |
| C | 2.002035 | -0.792608 | 0.309482 |
| C | 2.858598 | -1.976779 | 0.371413 |
| C | 2.033627 | -3.067501 | 0.253911 |
| C | 2.447880 | 0.535816 | 0.405762 |
| C | 1.687430 | 1.711513 | 0.323917 |
| N | 0.345926 | 1.742482 | 0.121020 |
| C | -0.050560 | 3.041589 | 0.097732 |
| C | 1.110450 | 3.910070 | 0.295685 |
| C | 2.196892 | 3.082619 | 0.439828 |
| C | -1.372488 | 3.478913 | -0.078085 |
| C | -2.529418 | 2.703387 | -0.280016 |
| C | -3.880848 | 3.231516 | -0.502882 |
| C | -4.701356 | 2.130364 | -0.674488 |
| C | -3.849929 | 0.957347 | -0.540282 |
| N | -2.564786 | 1.347005 | -0.294231 |
| C | -4.282856 | -0.375462 | -0.651361 |
| H | -0.313708 | -4.402510 | -0.069015 |
| H | -5.344548 | -0.511485 | -0.830565 |
| H | -1.517187 | 4.554881 | -0.061691 |
| H | 3.508486 | 0.666267 | 0.591049 |
| C | -0.303405 | -0.908235 | -3.019320 |
| H | 0.676277 | -1.356482 | -2.763466 |

| | | | |
|---|---|---|---|
| H | -0.230517 | -0.578517 | -4.072957 |
| C | 1.060657 | 5.408565 | 0.326848 |
| H | 0.755227 | 5.822761 | -0.642804 |
| H | 0.339765 | 5.773110 | 1.069194 |
| H | 2.033663 | 5.843830 | 0.573798 |
| C | 2.403516 | -4.520730 | 0.252530 |
| H | 1.844817 | -5.077947 | 1.014515 |
| H | 2.186598 | -4.995394 | -0.713211 |
| H | 3.468814 | -4.667022 | 0.455062 |
| C | -2.904843 | -5.252720 | -0.615897 |
| H | -1.921193 | -5.607030 | -0.939310 |
| H | -3.124982 | -5.742145 | 0.343396 |
| H | -3.646682 | -5.613622 | -1.336380 |
| C | -6.165380 | 2.112808 | -0.992616 |
| H | -6.446605 | 2.993881 | -1.579135 |
| H | -6.438083 | 1.223446 | -1.569347 |
| H | -6.790741 | 2.115915 | -0.088576 |
| C | -5.415730 | -3.251749 | -0.990610 |
| C | -6.070478 | -4.397878 | -0.732695 |
| H | -5.980053 | -2.462787 | -1.488288 |
| H | -7.107156 | -4.523525 | -1.031703 |
| H | -5.613815 | -5.227713 | -0.204386 |
| C | -4.208755 | 4.648051 | -0.570495 |

| | | | |
|---|---|---|---|
| C | -5.396227 | 5.235570 | -0.339708 |
| H | -3.379191 | 5.301757 | -0.840646 |
| H | -5.512540 | 6.310647 | -0.442858 |
| H | -6.272582 | 4.680716 | -0.022616 |
| C | 4.356572 | -1.969457 | 0.467300 |
| C | 5.028128 | -1.848901 | -0.932304 |
| H | 4.705664 | -2.892502 | 0.945102 |
| H | 4.698049 | -1.145111 | 1.101560 |
| H | 4.690549 | -2.659002 | -1.581132 |
| H | 4.747675 | -0.895630 | -1.394409 |
| C | 3.618570 | 3.499214 | 0.698024 |
| C | 4.556448 | 3.497477 | -0.545069 |
| H | 4.069538 | 2.872219 | 1.474084 |
| H | 3.613718 | 4.517659 | 1.100393 |
| H | 4.020353 | 3.809438 | -1.443063 |
| H | 5.371262 | 4.211975 | -0.366712 |
| C | 6.528714 | -1.924431 | -0.867964 |
| O | 7.246831 | -2.789295 | -1.314708 |
| O | 7.073873 | -0.859603 | -0.184570 |
| H | 8.035410 | -0.997772 | -0.196845 |
| C | 5.224030 | 2.171737 | -0.841630 |
| O | 5.212707 | 1.593425 | -1.909920 |
| O | 5.891731 | 1.699404 | 0.236799 |

| | | | |
|---|---|---|---|
| H | 6.295895 | 0.840988 | -0.007656 |
| O | -0.647037 | 0.158509 | -2.201752 |
| H | -1.045214 | -1.730497 | -2.998646 |
| C | -1.299289 | 0.309046 | 2.299098 |
| C | -2.571999 | -0.368804 | 2.714533 |
| C | -0.216252 | -0.315710 | 3.058024 |
| C | -2.048300 | -1.724130 | 3.222394 |
| H | -3.310991 | -0.476953 | 1.919627 |
| H | -3.052291 | 0.190720 | 3.535970 |
| O | 0.915377 | 0.062294 | 3.289518 |
| O | -0.680936 | -1.501067 | 3.611467 |
| H | -2.069965 | -2.478930 | 2.430630 |
| H | -2.588086 | -2.105061 | 4.095796 |
| H | -1.243619 | 1.367729 | 2.095028 |

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**$^{6}$TS(D-E)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2379.9106291

Zero-point correction= 0.719896 (Hartree/Particle)

Thermal correction to Energy= 0.770641

Thermal correction to Enthalpy= 0.771585

Thermal correction to Gibbs Free Energy= 0.630781

Sum of electronic and zero-point Energies= -2379.190733

Sum of electronic and thermal Energies= -2379.139988

Sum of electronic and thermal Enthalpies= -2379.139044

Sum of electronic and thermal Free Energies= -2379.279848

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.881268 | 0.163637 | -0.490889 |
| N | -2.184338 | -1.498039 | -0.439146 |
| C | -1.792034 | -2.809254 | -0.431918 |
| C | -2.949899 | -3.670393 | -0.592981 |
| C | -4.048903 | -2.833617 | -0.693453 |
| C | -3.532895 | -1.467642 | -0.604719 |
| C | -0.466751 | -3.248615 | -0.281637 |
| C | 0.683975 | -2.477695 | -0.101197 |
| N | 0.721959 | -1.111512 | -0.062734 |
| C | 2.005562 | -0.739116 | 0.171679 |
| C | 2.850812 | -1.926922 | 0.261379 |
| C | 2.028530 | -3.010302 | 0.091317 |
| C | 2.437912 | 0.586932 | 0.328025 |
| C | 1.667958 | 1.749569 | 0.275682 |

| | | | |
|---|---|---|---|
| N | 0.318290 | 1.791469 | 0.038520 |
| C | -0.075773 | 3.094896 | 0.100999 |
| C | 1.078637 | 3.941550 | 0.371335 |
| C | 2.163715 | 3.106443 | 0.485634 |
| C | -1.391798 | 3.552452 | -0.041142 |
| C | -2.541346 | 2.777308 | -0.252490 |
| C | -3.904004 | 3.295941 | -0.378468 |
| C | -4.723629 | 2.195938 | -0.560056 |
| C | -3.863626 | 1.028498 | -0.531103 |
| N | -2.558360 | 1.420023 | -0.346120 |
| C | -4.302253 | -0.293216 | -0.651999 |
| H | -0.318929 | -4.323969 | -0.280073 |
| H | -5.372896 | -0.427692 | -0.762640 |
| H | -1.536707 | 4.623822 | 0.045088 |
| H | 3.486938 | 0.720389 | 0.565690 |
| C | -0.364080 | -0.938435 | -3.241828 |
| H | 0.598599 | -1.431230 | -3.010585 |
| H | -0.296182 | -0.577337 | -4.284044 |
| C | 1.021968 | 5.434013 | 0.504907 |
| H | 0.692090 | 5.909906 | -0.427517 |
| H | 0.316344 | 5.742274 | 1.286400 |
| H | 1.998029 | 5.857545 | 0.758561 |
| C | 2.381057 | -4.466921 | 0.114457 |

| | | | |
|---|---|---|---|
| H | 1.820834 | -5.001275 | 0.891638 |
| H | 2.153900 | -4.957772 | -0.840754 |
| H | 3.445562 | -4.620557 | 0.314450 |
| C | -2.916717 | -5.166060 | -0.676063 |
| H | -1.963791 | -5.523610 | -1.078463 |
| H | -3.051970 | -5.642450 | 0.304933 |
| H | -3.716158 | -5.536722 | -1.326220 |
| C | -6.203871 | 2.179087 | -0.790682 |
| H | -6.524081 | 3.083169 | -1.318996 |
| H | -6.505973 | 1.314528 | -1.389659 |
| H | -6.771993 | 2.137081 | 0.149045 |
| C | -5.451960 | -3.167227 | -0.893454 |
| C | -6.084884 | -4.308276 | -0.569867 |
| H | -6.050657 | -2.386306 | -1.362748 |
| H | -7.140115 | -4.438959 | -0.791599 |
| H | -5.590648 | -5.127885 | -0.059885 |
| C | -4.245154 | 4.710989 | -0.353387 |
| C | -5.422962 | 5.272620 | -0.029463 |
| H | -3.436408 | 5.385798 | -0.634277 |
| H | -5.553536 | 6.350100 | -0.071587 |
| H | -6.275735 | 4.693107 | 0.306942 |
| C | 4.339895 | -1.925254 | 0.445577 |
| C | 5.090964 | -1.779169 | -0.910865 |

| | | | |
|---|---|---|---|
| H | 4.658075 | -2.858194 | 0.924678 |
| H | 4.642747 | -1.114891 | 1.116156 |
| H | 4.791364 | -2.578063 | -1.591531 |
| H | 4.837879 | -0.817734 | -1.371718 |
| C | 3.578553 | 3.508187 | 0.800393 |
| C | 4.550607 | 3.554589 | -0.415372 |
| H | 4.006156 | 2.849365 | 1.562958 |
| H | 3.561869 | 4.508554 | 1.244466 |
| H | 4.036602 | 3.885036 | -1.319654 |
| H | 5.349707 | 4.274552 | -0.193930 |
| C | 6.585182 | -1.859152 | -0.759537 |
| O | 7.324076 | -2.730515 | -1.156690 |
| O | 7.093431 | -0.790560 | -0.054452 |
| H | 8.052852 | -0.934309 | -0.003064 |
| C | 5.245335 | 2.246285 | -0.728640 |
| O | 5.275749 | 1.700043 | -1.813347 |
| O | 5.881685 | 1.751136 | 0.357578 |
| H | 6.302938 | 0.902614 | 0.107080 |
| O | -0.650243 | 0.107319 | -2.375869 |
| H | -1.139336 | -1.727599 | -3.226476 |
| C | -1.189836 | -0.056503 | 2.450027 |
| C | -2.508442 | -0.647973 | 2.846413 |
| C | -0.140364 | -0.827902 | 3.038913 |

| | | | |
|---|---|---|---|
| C | -2.081773 | -2.078590 | 3.241086 |
| H | -3.264850 | -0.659370 | 2.054275 |
| H | -2.959955 | -0.122266 | 3.708371 |
| O | 1.061196 | -0.625868 | 3.166995 |
| O | -0.686932 | -2.020406 | 3.557976 |
| H | -2.230159 | -2.772254 | 2.403712 |
| H | -2.618450 | -2.469311 | 4.114177 |
| H | -1.041783 | 0.992190 | 2.233739 |

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**$^{3}$E**

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Number of imaginary frequencies : 0 Electronic energy : HF=-750.0454499

Zero-point correction= 0.302947 (Hartree/Particle)

Thermal correction to Energy= 0.321650

Thermal correction to Enthalpy= 0.322595

Thermal correction to Gibbs Free Energy= 0.249656

Sum of electronic and zero-point Energies= -749.742503

Sum of electronic and thermal Energies= -749.723800

Sum of electronic and thermal Enthalpies= -749.722855

Sum of electronic and thermal Free Energies= -749.795794

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 2.580026 | 0.412984 | 0.584974 |
| C | 3.683391 | 0.456975 | 1.574200 |
| C | 2.956491 | -0.411450 | -0.547166 |
| C | 4.813085 | -0.317539 | 0.843590 |
| O | 4.244992 | -0.856581 | -0.363741 |
| O | 2.306301 | -0.717878 | -1.530011 |
| H | 3.398471 | -0.027724 | 2.520141 |
| H | 3.981315 | 1.480882 | 1.836479 |
| H | 5.207046 | -1.150395 | 1.431855 |
| H | 5.645731 | 0.336480 | 0.565516 |
| C | -1.324111 | -2.660380 | -0.251996 |
| C | -2.575089 | -3.069200 | 0.212673 |
| C | -3.532929 | -2.091093 | 0.480070 |
| C | -3.255856 | -0.740292 | 0.282974 |
| C | -1.997445 | -0.316950 | -0.201887 |
| C | -1.026697 | -1.314915 | -0.452656 |
| H | -0.553828 | -3.397736 | -0.462174 |
| H | -2.795483 | -4.120741 | 0.367782 |
| H | -4.514770 | -2.374478 | 0.850154 |
| H | -4.034265 | -0.023849 | 0.511753 |

| | | | |
|---|---|---|---|
| H | -0.034453 | -1.059661 | -0.800438 |
| N | -1.722134 | 1.046550 | -0.432415 |
| C | -2.682918 | 2.055097 | 0.025030 |
| C | -0.487151 | 1.465004 | -0.928846 |
| H | -2.494205 | 2.973285 | -0.531055 |
| C | -0.211398 | 2.896300 | -1.264994 |
| H | 0.826402 | 2.979216 | -1.600586 |
| H | -0.838609 | 3.293292 | -2.083539 |
| H | -0.332192 | 3.581882 | -0.415534 |
| H | 0.081069 | 0.715448 | -1.461371 |
| H | 1.605283 | 0.882883 | 0.653932 |
| H | -3.690479 | 1.740343 | -0.260431 |
| C | -2.611692 | 2.336607 | 1.530959 |
| H | -3.354207 | 3.090822 | 1.813333 |
| H | -2.803498 | 1.431482 | 2.113434 |
| H | -1.620982 | 2.711510 | 1.806117 |

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**$^{3}$TS(E-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-749.9870295

Zero-point correction= 0.302153 (Hartree/Particle)

Thermal correction to Energy= 0.319253

Thermal correction to Enthalpy= 0.320198

Thermal correction to Gibbs Free Energy= 0.255726

Sum of electronic and zero-point Energies= -749.684876

Sum of electronic and thermal Energies= -749.667776

Sum of electronic and thermal Enthalpies= -749.666832

Sum of electronic and thermal Free Energies= -749.731304

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 1.746210 | -0.082772 | -0.761666 |
| C | 2.889423 | 0.831271 | -1.135586 |
| C | 2.350473 | -1.263509 | -0.155176 |
| C | 3.997010 | 0.356885 | -0.171430 |
| H | 2.679075 | 1.902571 | -1.019838 |
| H | 3.188384 | 0.677306 | -2.181808 |
| H | -0.292790 | -1.695272 | 0.129940 |
| O | 1.849654 | -2.348292 | 0.115938 |
| O | 3.673986 | -0.995229 | 0.174857 |
| H | 4.016601 | 0.962043 | 0.744982 |
| H | 4.997092 | 0.371902 | -0.613459 |
| C | -1.324843 | -1.370000 | 0.054948 |

| | | | |
|---|---|---|---|
| C | -1.645540 | 0.038942 | -0.104279 |
| C | -2.314130 | -2.312550 | -0.000253 |
| C | -3.046233 | 0.393227 | -0.335129 |
| N | -0.700363 | 1.025929 | 0.037091 |
| C | -3.684552 | -1.949003 | -0.190206 |
| H | -2.044062 | -3.361379 | 0.076725 |
| C | -4.012188 | -0.577566 | -0.360397 |
| H | -3.338238 | 1.431989 | -0.428855 |
| C | 0.566304 | 0.860053 | 0.621078 |
| C | -0.940759 | 2.356004 | -0.572340 |
| H | -4.458670 | -2.707567 | -0.217799 |
| H | -5.049504 | -0.288929 | -0.506597 |
| H | 1.085310 | 1.814542 | 0.618825 |
| C | 0.661407 | 0.136971 | 1.948693 |
| H | 0.005586 | 2.663361 | -1.027551 |
| H | -1.660099 | 2.245228 | -1.383847 |
| C | -1.399243 | 3.402115 | 0.445991 |
| H | 0.593329 | -0.948812 | 1.866678 |
| H | 1.631771 | 0.361766 | 2.400989 |
| H | -0.122510 | 0.477366 | 2.637929 |
| H | -2.359253 | 3.128705 | 0.892834 |
| H | -0.668720 | 3.509883 | 1.252882 |
| H | -1.511399 | 4.373940 | -0.044810 |

H 0.961484 -0.272388 -1.488704

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**P**

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Number of imaginary frequencies : 0 Electronic energy : HF=-750.1423461

Zero-point correction= 0.310663 (Hartree/Particle)

Thermal correction to Energy= 0.326837

Thermal correction to Enthalpy= 0.327782

Thermal correction to Gibbs Free Energy= 0.266200

Sum of electronic and zero-point Energies= -749.831683

Sum of electronic and thermal Energies= -749.815509

Sum of electronic and thermal Enthalpies= -749.814565

Sum of electronic and thermal Free Energies= -749.876146

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Cartesian Coordinates

.....

C -1.500889 -0.620034 -0.416578

C -2.315819 -1.921487 -0.281352

C -2.577123 0.440166 -0.658522

C -3.744729 -1.439574 0.032700

| | | | |
|---|---|---|---|
| H | -1.932680 | -2.588993 | 0.496436 |
| H | -2.303563 | -2.475994 | -1.223914 |
| H | 1.020859 | -1.985113 | -0.350864 |
| O | -2.431029 | 1.589289 | -0.996938 |
| O | -3.814153 | -0.074070 | -0.415945 |
| H | -3.969987 | -1.458449 | 1.104567 |
| H | -4.519724 | -2.001988 | -0.493342 |
| C | 1.905604 | -1.373547 | -0.217695 |
| C | 1.793500 | -0.022726 | 0.186977 |
| C | 3.147533 | -1.947811 | -0.484536 |
| C | 2.994601 | 0.719208 | 0.277602 |
| N | 0.559210 | 0.562238 | 0.494151 |
| C | 4.323034 | -1.206150 | -0.378266 |
| H | 3.186656 | -2.989406 | -0.792965 |
| C | 4.226938 | 0.133628 | 0.001353 |
| H | 2.970444 | 1.757939 | 0.582244 |
| C | -0.579689 | -0.292931 | 0.817455 |
| C | 0.432900 | 2.024603 | 0.515079 |
| H | 5.286931 | -1.656304 | -0.593229 |
| H | 5.125251 | 0.738768 | 0.092299 |
| H | -0.147482 | -1.254695 | 1.106830 |
| C | -1.373725 | 0.188883 | 2.043680 |
| H | -0.573796 | 2.264650 | 0.853038 |

| | | | |
|---|---|---|---|
| H | 1.117499 | 2.448768 | 1.263786 |
| C | 0.648206 | 2.696517 | -0.846472 |
| H | -1.958179 | 1.092337 | 1.851715 |
| H | -2.071386 | -0.591552 | 2.364828 |
| H | -0.693483 | 0.389196 | 2.875767 |
| H | 1.628211 | 2.461469 | -1.269407 |
| H | -0.128854 | 2.378160 | -1.543734 |
| H | 0.579891 | 3.784245 | -0.733892 |
| H | -0.851672 | -0.642923 | -1.294708 |

**(U)B3LYP-D3(BJ) optimizations**

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**$S_1$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-414.7439657

Zero-point correction= 0.085025 (Hartree/Particle)

Thermal correction to Energy= 0.091823

Thermal correction to Enthalpy= 0.092767

Thermal correction to Gibbs Free Energy= 0.053445

Sum of electronic and zero-point Energies= -414.658940

Sum of electronic and thermal Energies= -414.652143

Sum of electronic and thermal Enthalpies= -414.651198

Sum of electronic and thermal Free Energies= -414.690521

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| N | 1.715329 | -0.329699 | 0.022765 |
| N | 2.855703 | -0.325286 | 0.052307 |
| C | 0.418158 | -0.319249 | 0.007918 |
| C | -0.483341 | -1.511050 | -0.141369 |
| C | -1.843432 | -0.827313 | 0.146357 |
| H | -0.279776 | -2.317027 | 0.569396 |
| H | -0.449309 | -1.931498 | -1.153942 |
| H | -2.156650 | -0.994477 | 1.182134 |
| H | -2.635837 | -1.161258 | -0.525380 |
| C | -0.340888 | 0.935778 | -0.015780 |
| O | 0.046239 | 2.077195 | -0.023718 |
| O | -1.668568 | 0.587823 | -0.048841 |

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**$S_2$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-444.9044636

Zero-point correction= 0.231528 (Hartree/Particle)

Thermal correction to Energy= 0.242535

Thermal correction to Enthalpy= 0.243480

Thermal correction to Gibbs Free Energy= 0.194552

Sum of electronic and zero-point Energies= -444.672936

Sum of electronic and thermal Energies= -444.661928

Sum of electronic and thermal Enthalpies= -444.660984

Sum of electronic and thermal Free Energies= -444.709912

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 2.439048 | 1.196631 | 0.107484 |
| C | 1.069455 | 1.206058 | -0.140435 |
| C | 0.344852 | -0.000010 | -0.283595 |
| C | 1.069415 | -1.206094 | -0.140343 |
| C | 2.439008 | -1.196694 | 0.107575 |
| C | 3.143868 | -0.000037 | 0.234053 |
| H | 2.957604 | 2.146382 | 0.206789 |
| H | 0.566975 | 2.160871 | -0.223699 |
| H | 0.566902 | -2.160896 | -0.223522 |
| H | 2.957534 | -2.146453 | 0.206956 |

| | | | |
|---|---|---|---|
| H | 4.210371 | -0.000049 | 0.433101 |
| N | -1.015053 | 0.000011 | -0.577760 |
| C | -1.767095 | 1.247162 | -0.598822 |
| H | -2.697218 | 1.056341 | -1.143273 |
| H | -1.217323 | 1.984621 | -1.194730 |
| C | -1.767138 | -1.247113 | -0.598879 |
| H | -2.697213 | -1.056261 | -1.143402 |
| H | -1.217346 | -1.984588 | -1.194746 |
| C | -2.091908 | -1.830225 | 0.783343 |
| H | -1.180836 | -1.980220 | 1.368480 |
| H | -2.746806 | -1.160743 | 1.347814 |
| H | -2.598424 | -2.796291 | 0.682574 |
| C | -2.091737 | 1.830284 | 0.783426 |
| H | -1.180614 | 1.980253 | 1.368490 |
| H | -2.598232 | 2.796365 | 0.682695 |
| H | -2.746608 | 1.160821 | 1.347950 |

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**$N_2$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-109.5214704

Zero-point correction= 0.005599 (Hartree/Particle)

Thermal correction to Energy= 0.007960

Thermal correction to Enthalpy= 0.008904

Thermal correction to Gibbs Free Energy= -0.012850

Sum of electronic and zero-point Energies= -109.515871

Sum of electronic and thermal Energies= -109.513511

Sum of electronic and thermal Enthalpies= -109.512566

Sum of electronic and thermal Free Energies= -109.534321

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 0.000000 | 0.000000 | 0.552651 |
| N | 0.000000 | 0.000000 | -0.552651 |

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**$^{CSS}$A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.2370986

Zero-point correction= 0.636271 (Hartree/Particle)

Thermal correction to Energy= 0.680590

Thermal correction to Enthalpy= 0.681534

Thermal correction to Gibbs Free Energy= 0.554824

Sum of electronic and zero-point Energies= -2073.600828

Sum of electronic and thermal Energies= -2073.556509

Sum of electronic and thermal Enthalpies= -2073.555565

Sum of electronic and thermal Free Energies= -2073.682275

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 1.064512 | -0.088832 | 0.017983 |
| N | 2.417997 | -1.544747 | -0.301440 |
| C | 2.169012 | -2.886678 | -0.485170 |
| C | 3.401711 | -3.627915 | -0.618202 |
| C | 4.425413 | -2.709405 | -0.536660 |
| C | 3.785676 | -1.413392 | -0.308357 |
| C | 0.907694 | -3.466339 | -0.529435 |
| C | -0.293235 | -2.786582 | -0.425478 |
| N | -0.418396 | -1.424080 | -0.271740 |
| C | -1.767518 | -1.182287 | -0.213490 |
| C | -2.520172 | -2.423230 | -0.318473 |
| C | -1.598197 | -3.425413 | -0.452738 |
| C | -2.347450 | 0.073028 | -0.095999 |
| C | -1.657510 | 1.273898 | -0.022561 |
| N | -0.292064 | 1.396795 | -0.000947 |

| | | | |
|---|---|---|---|
| C | -0.044038 | 2.744598 | 0.113986 |
| C | -1.288809 | 3.499033 | 0.141341 |
| C | -2.297652 | 2.579930 | 0.060235 |
| C | 1.209883 | 3.321384 | 0.211722 |
| C | 2.419423 | 2.638614 | 0.177863 |
| C | 3.728341 | 3.269140 | 0.319003 |
| C | 4.651435 | 2.244014 | 0.262723 |
| C | 3.892957 | 1.024466 | 0.084750 |
| N | 2.543889 | 1.284356 | 0.035688 |
| C | 4.466220 | -0.232193 | -0.063527 |
| H | 0.860515 | -4.543141 | -0.654350 |
| H | 5.542738 | -0.298498 | 0.017207 |
| H | 1.245841 | 4.397689 | 0.338626 |
| H | -3.431275 | 0.119969 | -0.076157 |
| C | 0.615387 | -1.281972 | 2.526068 |
| H | 1.051365 | -2.238739 | 2.172899 |
| H | -0.486065 | -1.385830 | 2.422941 |
| C | -1.385692 | 4.989557 | 0.238928 |
| H | -0.874114 | 5.368132 | 1.132335 |
| H | -0.923816 | 5.484280 | -0.625099 |
| H | -2.427466 | 5.319528 | 0.290150 |
| C | -1.829117 | -4.898042 | -0.590307 |
| H | -1.364378 | -5.297172 | -1.500551 |

| | | | |
|---|---|---|---|
| H | -1.403235 | -5.454999 | 0.253896 |
| H | -2.896807 | -5.132329 | -0.634627 |
| C | 3.492115 | -5.102651 | -0.858133 |
| H | 2.914613 | -5.664884 | -0.114585 |
| H | 3.096418 | -5.378597 | -1.844371 |
| H | 4.526223 | -5.454892 | -0.813423 |
| C | 6.143070 | 2.342445 | 0.308511 |
| H | 6.527417 | 2.332529 | 1.337713 |
| H | 6.617689 | 1.510312 | -0.219952 |
| H | 6.483892 | 3.275899 | -0.152133 |
| C | 5.842389 | -3.004489 | -0.682898 |
| C | 6.809064 | -2.211847 | -1.175518 |
| H | 6.133966 | -4.011110 | -0.378979 |
| H | 7.837121 | -2.557502 | -1.230998 |
| H | 6.603856 | -1.217442 | -1.555902 |
| C | 3.941403 | 4.699185 | 0.445471 |
| C | 5.011675 | 5.332160 | 0.958265 |
| H | 3.129064 | 5.324178 | 0.074321 |
| H | 5.058873 | 6.417008 | 0.975809 |
| H | 5.849630 | 4.800847 | 1.394815 |
| C | -4.011153 | -2.527381 | -0.219796 |
| C | -4.495041 | -2.374962 | 1.229883 |
| H | -4.359631 | -3.488183 | -0.611183 |

| | | | |
|---|---|---|---|
| H | -4.498090 | -1.761475 | -0.834211 |
| H | -4.059443 | -3.153292 | 1.867548 |
| H | -4.146041 | -1.428451 | 1.657979 |
| C | -3.776281 | 2.811756 | -0.004274 |
| C | -4.317195 | 2.653848 | -1.432857 |
| H | -4.027315 | 3.812053 | 0.361400 |
| H | -4.308577 | 2.113219 | 0.651472 |
| H | -3.832040 | 3.366326 | -2.110990 |
| H | -4.072055 | 1.663753 | -1.833366 |
| C | -5.994591 | -2.434250 | 1.366623 |
| O | -6.795755 | -2.589034 | 0.468515 |
| O | -6.390524 | -2.291642 | 2.659614 |
| H | -7.361084 | -2.330124 | 2.638431 |
| C | -5.808143 | 2.850175 | -1.533657 |
| O | -6.561928 | 3.137337 | -0.627784 |
| O | -6.256456 | 2.668700 | -2.805321 |
| H | -7.217440 | 2.805050 | -2.761763 |
| O | 1.137600 | -0.164179 | 1.903308 |
| H | 0.822403 | -1.229441 | 3.612917 |

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$^{OSS}$**A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.2407234

Zero-point correction= 0.635449 (Hartree/Particle)

Thermal correction to Energy= 0.680093

Thermal correction to Enthalpy= 0.681037

Thermal correction to Gibbs Free Energy= 0.553570

Sum of electronic and zero-point Energies= -2073.605274

Sum of electronic and thermal Energies= -2073.560630

Sum of electronic and thermal Enthalpies= -2073.559686

Sum of electronic and thermal Free Energies= -2073.687154

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 1.062077 | -0.083207 | 0.032842 |
| N | 2.434181 | -1.540082 | -0.322533 |
| C | 2.189305 | -2.880165 | -0.496173 |
| C | 3.426059 | -3.615240 | -0.627063 |
| C | 4.444518 | -2.687876 | -0.554222 |
| C | 3.797366 | -1.395842 | -0.332448 |
| C | 0.925901 | -3.463084 | -0.530927 |
| C | -0.277169 | -2.788163 | -0.422127 |

| | | | |
|---|---|---|---|
| N | -0.411122 | -1.427446 | -0.267718 |
| C | -1.759814 | -1.188740 | -0.215782 |
| C | -2.507152 | -2.434937 | -0.322414 |
| C | -1.581513 | -3.433316 | -0.451193 |
| C | -2.347858 | 0.064260 | -0.105030 |
| C | -1.670967 | 1.275101 | -0.032647 |
| N | -0.309403 | 1.411643 | -0.013650 |
| C | -0.067152 | 2.756623 | 0.106643 |
| C | -1.316684 | 3.503014 | 0.140749 |
| C | -2.319875 | 2.575924 | 0.057305 |
| C | 1.188188 | 3.334834 | 0.209835 |
| C | 2.399323 | 2.653557 | 0.182722 |
| C | 3.707933 | 3.290475 | 0.320361 |
| C | 4.635150 | 2.271120 | 0.256658 |
| C | 3.882484 | 1.045592 | 0.078839 |
| N | 2.531640 | 1.300507 | 0.043165 |
| C | 4.465459 | -0.204429 | -0.085959 |
| H | 0.881427 | -4.540499 | -0.651655 |
| H | 5.543261 | -0.259667 | -0.012065 |
| H | 1.222874 | 4.410915 | 0.338909 |
| H | -3.432243 | 0.101686 | -0.087644 |
| C | 0.761174 | -1.381945 | 2.565768 |
| H | 1.355768 | -2.251434 | 2.213121 |

| | | | |
|---|---|---|---|
| H | -0.305735 | -1.668376 | 2.435698 |
| C | -1.424012 | 4.992186 | 0.247924 |
| H | -0.914804 | 5.368655 | 1.143564 |
| H | -0.966261 | 5.495826 | -0.613173 |
| H | -2.468040 | 5.314611 | 0.301682 |
| C | -1.805415 | -4.906982 | -0.587554 |
| H | -1.337688 | -5.304805 | -1.496842 |
| H | -1.377701 | -5.460654 | 0.257855 |
| H | -2.871901 | -5.146420 | -0.632780 |
| C | 3.527068 | -5.091047 | -0.855881 |
| H | 2.951909 | -5.651697 | -0.109420 |
| H | 3.136063 | -5.377414 | -1.841068 |
| H | 4.563606 | -5.435648 | -0.806066 |
| C | 6.126291 | 2.378179 | 0.295125 |
| H | 6.515943 | 2.352500 | 1.321905 |
| H | 6.602739 | 1.558152 | -0.250345 |
| H | 6.457906 | 3.321849 | -0.150873 |
| C | 5.864272 | -2.973196 | -0.697141 |
| C | 6.819619 | -2.176676 | -1.204448 |
| H | 6.167146 | -3.971557 | -0.377530 |
| H | 7.852213 | -2.509087 | -1.256427 |
| H | 6.599870 | -1.190934 | -1.599329 |
| C | 3.915707 | 4.721601 | 0.446282 |

| | | | |
|---|---|---|---|
| C | 4.979341 | 5.356880 | 0.969459 |
| H | 3.105581 | 5.343926 | 0.065974 |
| H | 5.025017 | 6.441790 | 0.986028 |
| H | 5.812816 | 4.827041 | 1.416401 |
| C | -3.997851 | -2.546071 | -0.227265 |
| C | -4.485314 | -2.394300 | 1.221228 |
| H | -4.340782 | -3.508918 | -0.618434 |
| H | -4.486678 | -1.783093 | -0.843668 |
| H | -4.048192 | -3.170257 | 1.860678 |
| H | -4.140953 | -1.446080 | 1.649333 |
| C | -3.800320 | 2.798611 | 0.000655 |
| C | -4.345632 | 2.645422 | -1.426708 |
| H | -4.056757 | 3.794928 | 0.373294 |
| H | -4.324660 | 2.092337 | 0.654379 |
| H | -3.865873 | 3.363390 | -2.102946 |
| H | -4.098018 | 1.658462 | -1.833309 |
| C | -5.985006 | -2.458953 | 1.353968 |
| O | -6.783186 | -2.614090 | 0.453234 |
| O | -6.384667 | -2.320717 | 2.646121 |
| H | -7.355049 | -2.362027 | 2.622504 |
| C | -5.837730 | 2.836745 | -1.521062 |
| O | -6.588294 | 3.122430 | -0.612100 |
| O | -6.290909 | 2.652654 | -2.790553 |

H -7.252084 2.786362 -2.743176

O 1.101412 -0.189623 1.959677

H 0.929203 -1.323025 3.660781

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**$^{3}$A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.248732

Zero-point correction= 0.634369 (Hartree/Particle)

Thermal correction to Energy= 0.679312

Thermal correction to Enthalpy= 0.680256

Thermal correction to Gibbs Free Energy= 0.550819

Sum of electronic and zero-point Energies= -2073.614363

Sum of electronic and thermal Energies= -2073.569420

Sum of electronic and thermal Enthalpies= -2073.568476

Sum of electronic and thermal Free Energies= -2073.697913

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Cartesian Coordinates

.....

Fe 1.056059 -0.087048 0.141287

N 2.444037 -1.524343 -0.362494

| | | | |
|---|---|---|---|
| C | 2.210801 | -2.870942 | -0.520054 |
| C | 3.435921 | -3.581046 | -0.703525 |
| C | 4.454256 | -2.629513 | -0.674955 |
| C | 3.809064 | -1.363548 | -0.423933 |
| C | 0.942518 | -3.467247 | -0.501747 |
| C | -0.243392 | -2.787795 | -0.367942 |
| N | -0.386873 | -1.418263 | -0.215716 |
| C | -1.754533 | -1.188552 | -0.182075 |
| C | -2.480027 | -2.444652 | -0.280528 |
| C | -1.547772 | -3.434931 | -0.391277 |
| C | -2.361169 | 0.042646 | -0.106535 |
| C | -1.695591 | 1.268449 | -0.039188 |
| N | -0.326418 | 1.411709 | 0.009333 |
| C | -0.095309 | 2.759905 | 0.141093 |
| C | -1.333479 | 3.489609 | 0.146058 |
| C | -2.340196 | 2.547754 | 0.035433 |
| C | 1.165510 | 3.344443 | 0.279961 |
| C | 2.358278 | 2.656560 | 0.248947 |
| C | 3.670430 | 3.290159 | 0.377945 |
| C | 4.600900 | 2.282494 | 0.273726 |
| C | 3.864004 | 1.051733 | 0.078736 |
| N | 2.496478 | 1.295861 | 0.085557 |
| C | 4.467160 | -0.163168 | -0.153441 |

| | | | |
|---|---|---|---|
| H | 0.896974 | -4.544160 | -0.615564 |
| H | 5.546854 | -0.200710 | -0.109537 |
| H | 1.199823 | 4.416811 | 0.428626 |
| H | -3.445502 | 0.067338 | -0.108551 |
| C | 0.788839 | -1.500788 | 2.654948 |
| H | 1.409112 | -2.352943 | 2.318646 |
| H | -0.264811 | -1.787986 | 2.477071 |
| C | -1.454894 | 4.978110 | 0.254501 |
| H | -0.974290 | 5.360255 | 1.164161 |
| H | -0.981976 | 5.491967 | -0.592937 |
| H | -2.503240 | 5.290569 | 0.282664 |
| C | -1.755926 | -4.910419 | -0.523101 |
| H | -1.300532 | -5.300189 | -1.442208 |
| H | -1.300371 | -5.457196 | 0.312197 |
| H | -2.819565 | -5.164311 | -0.545468 |
| C | 3.548674 | -5.054986 | -0.941262 |
| H | 3.020919 | -5.630075 | -0.170291 |
| H | 3.118349 | -5.350201 | -1.908069 |
| H | 4.592322 | -5.382187 | -0.940408 |
| C | 6.091456 | 2.403510 | 0.275852 |
| H | 6.511669 | 2.294583 | 1.284607 |
| H | 6.556707 | 1.637333 | -0.351323 |
| H | 6.397817 | 3.385436 | -0.098267 |

| | | | |
|---|---|---|---|
| C | 5.869897 | -2.896274 | -0.865259 |
| C | 6.808261 | -2.082254 | -1.379859 |
| H | 6.189756 | -3.898888 | -0.575724 |
| H | 7.842135 | -2.404912 | -1.460475 |
| H | 6.572333 | -1.091336 | -1.752237 |
| C | 3.875285 | 4.720906 | 0.517893 |
| C | 4.922660 | 5.345832 | 1.083652 |
| H | 3.080656 | 5.346708 | 0.111686 |
| H | 4.977455 | 6.430201 | 1.106398 |
| H | 5.733646 | 4.805882 | 1.559712 |
| C | -3.970777 | -2.569321 | -0.201056 |
| C | -4.477010 | -2.394694 | 1.238095 |
| H | -4.297997 | -3.542924 | -0.577953 |
| H | -4.458045 | -1.823067 | -0.838405 |
| H | -4.037062 | -3.151546 | 1.898297 |
| H | -4.151071 | -1.432636 | 1.649113 |
| C | -3.819410 | 2.771121 | -0.054646 |
| C | -4.329856 | 2.641992 | -1.497183 |
| H | -4.084905 | 3.761694 | 0.327215 |
| H | -4.362425 | 2.056318 | 0.574371 |
| H | -3.823430 | 3.362090 | -2.151450 |
| H | -4.082573 | 1.657088 | -1.909225 |
| C | -5.976982 | -2.478805 | 1.354788 |

| | | | |
|---|---|---|---|
| O | -6.761754 | -2.666522 | 0.448672 |
| O | -6.393469 | -2.317263 | 2.638918 |
| H | -7.362801 | -2.373684 | 2.605568 |
| C | -5.816295 | 2.852666 | -1.630344 |
| O | -6.587859 | 3.144539 | -0.740951 |
| O | -6.238825 | 2.679484 | -2.912395 |
| H | -7.198743 | 2.827870 | -2.889085 |
| O | 1.137763 | -0.308593 | 2.035051 |
| H | 0.920086 | -1.421558 | 3.749955 |

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**$^{5}$A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2074.2683019

Zero-point correction= 0.633103 (Hartree/Particle)

Thermal correction to Energy= 0.678776

Thermal correction to Enthalpy= 0.679720

Thermal correction to Gibbs Free Energy= 0.547361

Sum of electronic and zero-point Energies= -2073.635199

Sum of electronic and thermal Energies= -2073.589526

Sum of electronic and thermal Enthalpies= -2073.588582

Sum of electronic and thermal Free Energies= -2073.720941

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 1.065249 | -0.137333 | 0.500677 |
| N | 2.462634 | -1.557344 | -0.338436 |
| C | 2.189554 | -2.882263 | -0.523186 |
| C | 3.424879 | -3.624198 | -0.702081 |
| C | 4.450719 | -2.699951 | -0.658195 |
| C | 3.814922 | -1.401467 | -0.401232 |
| C | 0.906453 | -3.447008 | -0.558741 |
| C | -0.315720 | -2.781751 | -0.461015 |
| N | -0.462878 | -1.433613 | -0.295059 |
| C | -1.798367 | -1.173788 | -0.257763 |
| C | -2.553974 | -2.417507 | -0.405003 |
| C | -1.628450 | -3.421764 | -0.527353 |
| C | -2.362001 | 0.098704 | -0.113014 |
| C | -1.682215 | 1.314256 | 0.022963 |
| N | -0.328570 | 1.455230 | 0.083309 |
| C | -0.065240 | 2.790324 | 0.202089 |
| C | -1.316396 | 3.546436 | 0.221493 |
| C | -2.325495 | 2.625159 | 0.113041 |
| C | 1.208338 | 3.354711 | 0.278888 |

| | | | |
|---|---|---|---|
| C | 2.437554 | 2.685371 | 0.203225 |
| C | 3.754351 | 3.326283 | 0.255325 |
| C | 4.681498 | 2.305983 | 0.134397 |
| C | 3.920690 | 1.073731 | 0.010801 |
| N | 2.579323 | 1.340199 | 0.067982 |
| C | 4.483746 | -0.192628 | -0.188184 |
| H | 0.860016 | -4.523934 | -0.691966 |
| H | 5.564943 | -0.245715 | -0.172269 |
| H | 1.246854 | 4.432272 | 0.402267 |
| H | -3.446957 | 0.150354 | -0.117603 |
| C | 0.891941 | -1.815160 | 2.848955 |
| H | 1.696235 | -2.503400 | 2.515662 |
| H | -0.063533 | -2.291156 | 2.544093 |
| C | -1.421229 | 5.036300 | 0.324892 |
| H | -0.907548 | 5.413814 | 1.217331 |
| H | -0.964470 | 5.535235 | -0.539416 |
| H | -2.464018 | 5.362571 | 0.380792 |
| C | -1.863668 | -4.891557 | -0.687400 |
| H | -1.360886 | -5.285532 | -1.579214 |
| H | -1.478024 | -5.456902 | 0.170433 |
| H | -2.929589 | -5.120113 | -0.780465 |
| C | 3.517720 | -5.097118 | -0.952677 |
| H | 2.940652 | -5.664289 | -0.212995 |

| | | | |
|---|---|---|---|
| H | 3.122142 | -5.365888 | -1.940971 |
| H | 4.552154 | -5.449667 | -0.911293 |
| C | 6.171351 | 2.422273 | 0.072775 |
| H | 6.625628 | 2.442597 | 1.072790 |
| H | 6.616955 | 1.581261 | -0.466474 |
| H | 6.468977 | 3.347450 | -0.432858 |
| C | 5.863175 | -2.991107 | -0.855792 |
| C | 6.796670 | -2.194191 | -1.400904 |
| H | 6.177948 | -3.989290 | -0.546999 |
| H | 7.827084 | -2.524501 | -1.493412 |
| H | 6.558988 | -1.209080 | -1.787133 |
| C | 3.968280 | 4.758360 | 0.362377 |
| C | 5.069663 | 5.399391 | 0.791628 |
| H | 3.124332 | 5.376066 | 0.055382 |
| H | 5.108796 | 6.484556 | 0.807975 |
| H | 5.943471 | 4.875034 | 1.160951 |
| C | -4.047144 | -2.524501 | -0.348536 |
| C | -4.568991 | -2.406404 | 1.091026 |
| H | -4.386736 | -3.474632 | -0.772741 |
| H | -4.515881 | -1.742051 | -0.956132 |
| H | -4.150495 | -3.199490 | 1.721919 |
| H | -4.232118 | -1.469925 | 1.550000 |
| C | -3.801783 | 2.864282 | 0.020309 |

| | | | |
|---|---|---|---|
| C | -4.307304 | 2.745541 | -1.424879 |
| H | -4.060674 | 3.854917 | 0.406503 |
| H | -4.349903 | 2.148781 | 0.643619 |
| H | -3.803238 | 3.473375 | -2.072228 |
| H | -4.055610 | 1.765154 | -1.844711 |
| C | -6.071825 | -2.468361 | 1.185937 |
| O | -6.848311 | -2.600113 | 0.262860 |
| O | -6.502044 | -2.357723 | 2.470851 |
| H | -7.471696 | -2.395381 | 2.423226 |
| C | -5.794750 | 2.951032 | -1.556476 |
| O | -6.568093 | 3.222469 | -0.662343 |
| O | -6.213395 | 2.798771 | -2.841718 |
| H | -7.174516 | 2.939076 | -2.818492 |
| O | 1.039595 | -0.525892 | 2.365242 |
| H | 0.906938 | -1.836801 | 3.956983 |

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**$^{CSS}$B'**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2489.0255258

Zero-point correction= 0.724322 (Hartree/Particle)

Thermal correction to Energy= 0.776597

Thermal correction to Enthalpy= 0.777541

Thermal correction to Gibbs Free Energy= 0.633788

Sum of electronic and zero-point Energies= -2488.301204

Sum of electronic and thermal Energies= -2488.248929

Sum of electronic and thermal Enthalpies= -2488.247984

Sum of electronic and thermal Free Energies= -2488.391738

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.708202 | -0.020052 | -0.623757 |
| N | -2.238981 | -1.305311 | -0.873917 |
| C | -2.145231 | -2.671690 | -1.004947 |
| C | -3.447160 | -3.256975 | -1.230676 |
| C | -4.357674 | -2.223155 | -1.186108 |
| C | -3.574933 | -1.003424 | -0.999100 |
| C | -0.979312 | -3.412443 | -0.853257 |
| C | 0.251986 | -2.905188 | -0.469718 |
| N | 0.526800 | -1.576282 | -0.260964 |
| C | 1.832472 | -1.526105 | 0.158177 |
| C | 2.399988 | -2.865804 | 0.237733 |
| C | 1.415563 | -3.725036 | -0.172708 |
| C | 2.532059 | -0.358385 | 0.430103 |

| | | | |
|---|---|---|---|
| C | 2.035147 | 0.929032 | 0.280899 |
| N | 0.750593 | 1.246590 | -0.075300 |
| C | 0.701908 | 2.616874 | -0.118595 |
| C | 2.000772 | 3.190151 | 0.205015 |
| C | 2.831559 | 2.135036 | 0.462827 |
| C | -0.427686 | 3.366539 | -0.405432 |
| C | -1.696320 | 2.855807 | -0.647153 |
| C | -2.890611 | 3.670202 | -0.852585 |
| C | -3.934962 | 2.782693 | -1.015007 |
| C | -3.362135 | 1.457753 | -0.923651 |
| N | -2.003036 | 1.522514 | -0.704095 |
| C | -4.090790 | 0.282720 | -1.048526 |
| H | -1.055209 | -4.486391 | -0.986136 |
| H | -5.149833 | 0.375546 | -1.247825 |
| H | -0.312578 | 4.444524 | -0.413280 |
| H | 3.558182 | -0.459923 | 0.759543 |
| C | -1.151734 | -0.006443 | -3.398574 |
| H | -0.702679 | 0.172627 | -4.394360 |
| H | -1.970582 | 0.732090 | -3.289245 |
| C | 2.314940 | 4.653392 | 0.220580 |
| H | 2.194823 | 5.103803 | -0.772875 |
| H | 1.651997 | 5.202137 | 0.900822 |
| H | 3.343787 | 4.835581 | 0.544646 |

| | | | |
|---|---|---|---|
| C | 1.463653 | -5.215796 | -0.300259 |
| H | 0.668010 | -5.697851 | 0.281037 |
| H | 1.334982 | -5.535955 | -1.342057 |
| H | 2.418660 | -5.618172 | 0.049874 |
| C | -3.711404 | -4.721637 | -1.388593 |
| H | -3.070399 | -5.162108 | -2.161218 |
| H | -3.516039 | -5.271233 | -0.458577 |
| H | -4.751022 | -4.914391 | -1.666454 |
| C | -5.387686 | 3.087944 | -1.196827 |
| H | -5.655094 | 3.215091 | -2.254626 |
| H | -6.018492 | 2.287339 | -0.798986 |
| H | -5.653546 | 4.017799 | -0.683620 |
| C | -5.803669 | -2.357189 | -1.287341 |
| C | -6.741904 | -1.593875 | -0.704019 |
| H | -6.147641 | -3.202628 | -1.884686 |
| H | -7.797955 | -1.797115 | -0.853782 |
| H | -6.488978 | -0.769208 | -0.046674 |
| C | -2.910741 | 5.121993 | -0.820859 |
| C | -3.811743 | 5.940977 | -1.390646 |
| H | -2.095656 | 5.587752 | -0.267377 |
| H | -3.732543 | 7.018078 | -1.278170 |
| H | -4.629883 | 5.572944 | -1.999430 |
| C | 3.798454 | -3.220881 | 0.653034 |

| | | | |
|---|---|---|---|
| C | 4.840970 | -3.115263 | -0.484620 |
| H | 3.802483 | -4.249914 | 1.025843 |
| H | 4.136603 | -2.590153 | 1.481285 |
| H | 5.638306 | -3.855675 | -0.330237 |
| H | 4.392383 | -3.328236 | -1.457341 |
| C | 4.307251 | 2.142147 | 0.719573 |
| C | 5.077754 | 1.874715 | -0.585414 |
| H | 4.584618 | 1.373239 | 1.447414 |
| H | 4.632783 | 3.098472 | 1.139172 |
| H | 4.701718 | 0.974109 | -1.074430 |
| H | 4.908526 | 2.694831 | -1.295688 |
| C | 5.548153 | -1.778803 | -0.540192 |
| O | 5.801847 | -1.086338 | 0.430718 |
| O | 5.922699 | -1.445544 | -1.786866 |
| H | 6.394054 | -0.585777 | -1.729523 |
| C | 6.561140 | 1.755329 | -0.378749 |
| O | 7.216386 | 2.209862 | 0.527501 |
| O | 7.175010 | 1.072119 | -1.410360 |
| H | 8.117737 | 1.046764 | -1.174627 |
| O | -0.171062 | 0.097694 | -2.427132 |
| H | -1.633749 | -1.004671 | -3.446613 |
| C | -1.991415 | -1.673280 | 2.284630 |
| O | -2.284570 | -1.961637 | 3.678402 |

| | | | |
|---|---|---|---|
| C | -2.138490 | -0.851027 | 4.457150 |
| C | -1.545949 | 0.186362 | 3.607524 |
| C | -1.197215 | -0.351150 | 2.248921 |
| H | -1.429092 | -2.511014 | 1.875211 |
| H | -2.939276 | -1.581569 | 1.749641 |
| H | -1.540619 | 0.304701 | 1.439570 |
| H | -0.123728 | -0.520535 | 2.130855 |
| O | -2.448216 | -0.811925 | 5.627472 |
| N | -1.276276 | 1.369510 | 4.058452 |
| N | -1.050327 | 2.416678 | 4.456831 |

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**$^{OSS}$B'**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2489.0310956

Zero-point correction= 0.723324 (Hartree/Particle)

Thermal correction to Energy= 0.775705

Thermal correction to Enthalpy= 0.776649

Thermal correction to Gibbs Free Energy= 0.632440

Sum of electronic and zero-point Energies= -2488.307771

Sum of electronic and thermal Energies= -2488.255391

Sum of electronic and thermal Enthalpies= -2488.254447

Sum of electronic and thermal Free Energies= -2488.398656

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.737898 | 0.070938 | -0.754021 |
| N | -1.940155 | -1.509776 | -0.894884 |
| C | -1.547878 | -2.809613 | -1.145312 |
| C | -2.702189 | -3.672767 | -1.261927 |
| C | -3.813215 | -2.890817 | -1.031734 |
| C | -3.330457 | -1.527928 | -0.861276 |
| C | -0.240861 | -3.264731 | -1.176842 |
| C | 0.862264 | -2.505404 | -0.782413 |
| N | 0.803011 | -1.182333 | -0.413574 |
| C | 2.068512 | -0.860128 | 0.034973 |
| C | 2.939862 | -1.996987 | -0.058630 |
| C | 2.191053 | -3.028491 | -0.591759 |
| C | 2.458757 | 0.406432 | 0.466484 |
| C | 1.690180 | 1.544048 | 0.371096 |
| N | 0.386403 | 1.586171 | -0.108750 |
| C | 0.056412 | 2.917943 | -0.176934 |
| C | 1.166109 | 3.741486 | 0.276600 |
| C | 2.168208 | 2.884567 | 0.648205 |

| | | | |
|---|---|---|---|
| C | -1.174302 | 3.425719 | -0.554239 |
| C | -2.319818 | 2.650128 | -0.742633 |
| C | -3.661022 | 3.173883 | -0.919894 |
| C | -4.505687 | 2.064254 | -0.950580 |
| C | -3.674015 | 0.913308 | -0.825766 |
| N | -2.337867 | 1.279282 | -0.702183 |
| C | -4.126754 | -0.405205 | -0.852276 |
| H | -0.075662 | -4.310321 | -1.409262 |
| H | -5.192792 | -0.562017 | -0.947768 |
| H | -1.275254 | 4.502535 | -0.603547 |
| H | 3.463935 | 0.514174 | 0.851645 |
| C | -1.414652 | 0.360115 | -3.420900 |
| H | -1.002034 | 0.316171 | -4.441835 |
| H | -1.967607 | 1.307825 | -3.321810 |
| C | 1.140027 | 5.236386 | 0.329179 |
| H | 1.026086 | 5.672918 | -0.671480 |
| H | 0.300381 | 5.604147 | 0.932276 |
| H | 2.061302 | 5.639219 | 0.759735 |
| C | 2.619500 | -4.427905 | -0.905800 |
| H | 2.010333 | -5.169808 | -0.372903 |
| H | 2.528182 | -4.655041 | -1.976231 |
| H | 3.662776 | -4.597523 | -0.621757 |
| C | -2.632099 | -5.149717 | -1.487838 |

| | | | |
|---|---|---|---|
| H | -2.055272 | -5.388647 | -2.389641 |
| H | -2.139707 | -5.661407 | -0.650696 |
| H | -3.627154 | -5.588184 | -1.599644 |
| C | -5.998387 | 2.056135 | -1.049495 |
| H | -6.347402 | 2.192134 | -2.082306 |
| H | -6.423072 | 1.116454 | -0.685009 |
| H | -6.428745 | 2.872150 | -0.458575 |
| C | -5.189940 | -3.360912 | -0.965164 |
| C | -6.189046 | -2.848871 | -0.229261 |
| H | -5.406630 | -4.248171 | -1.560900 |
| H | -7.182265 | -3.286833 | -0.254548 |
| H | -6.041130 | -2.001770 | 0.431683 |
| C | -3.986905 | 4.582470 | -0.975691 |
| C | -5.118750 | 5.163565 | -1.420371 |
| H | -3.208037 | 5.250226 | -0.608071 |
| H | -5.234953 | 6.242563 | -1.386166 |
| H | -5.941191 | 4.599786 | -1.844644 |
| C | 4.413183 | -1.969757 | 0.211836 |
| C | 5.175342 | -1.482140 | -1.045172 |
| H | 4.779470 | -2.963167 | 0.487677 |
| H | 4.650196 | -1.297617 | 1.041475 |
| H | 4.999385 | -2.195293 | -1.860125 |
| H | 4.790356 | -0.515579 | -1.370567 |

| | | | |
|---|---|---|---|
| C | 3.521838 | 3.247583 | 1.189636 |
| C | 4.632637 | 3.330956 | 0.118087 |
| H | 3.841961 | 2.531025 | 1.952490 |
| H | 3.448042 | 4.219569 | 1.687223 |
| H | 4.227795 | 3.615747 | -0.855914 |
| H | 5.362712 | 4.105080 | 0.392658 |
| C | 6.661310 | -1.361758 | -0.868694 |
| O | 7.358027 | -0.408246 | -1.191764 |
| O | 7.223115 | -2.457776 | -0.322302 |
| H | 8.171831 | -2.261047 | -0.244798 |
| C | 5.442392 | 2.058007 | -0.034489 |
| O | 5.616719 | 1.238082 | 0.852627 |
| O | 5.993037 | 1.949681 | -1.249901 |
| H | 6.534876 | 1.119276 | -1.267710 |
| O | -0.350945 | 0.259158 | -2.517416 |
| H | -2.139820 | -0.462622 | -3.318852 |
| C | -1.448985 | -2.058071 | 2.172699 |
| O | -1.438893 | -2.618200 | 3.514012 |
| C | -1.548133 | -1.648209 | 4.464138 |
| C | -1.463353 | -0.360282 | 3.767512 |
| C | -1.177341 | -0.541855 | 2.303511 |
| H | -0.687048 | -2.569512 | 1.587454 |
| H | -2.430420 | -2.252048 | 1.734361 |

| | | | |
|---|---|---|---|
| H | -1.836163 | 0.043548 | 1.655817 |
| H | -0.140925 | -0.295324 | 2.052155 |
| O | -1.675857 | -1.881420 | 5.645989 |
| N | -1.520601 | 0.762703 | 4.408317 |
| N | -1.584418 | 1.751118 | 4.979576 |

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**$^3$B'**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2489.0397931

Zero-point correction= 0.723052 (Hartree/Particle)

Thermal correction to Energy= 0.776013

Thermal correction to Enthalpy= 0.776957

Thermal correction to Gibbs Free Energy= 0.628887

Sum of electronic and zero-point Energies= -2488.316741

Sum of electronic and thermal Energies= -2488.263780

Sum of electronic and thermal Enthalpies= -2488.262836

Sum of electronic and thermal Free Energies= -2488.410906

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.716059 | 0.010119 | -0.805669 |
| N | -1.908447 | -1.597027 | -0.851791 |
| C | -1.494960 | -2.920404 | -0.941849 |
| C | -2.634388 | -3.798287 | -1.077805 |
| C | -3.760301 | -3.013071 | -1.013278 |
| C | -3.294091 | -1.628333 | -0.915736 |
| C | -0.199495 | -3.371314 | -0.829862 |
| C | 0.896286 | -2.574361 | -0.495746 |
| N | 0.832426 | -1.212068 | -0.279582 |
| C | 2.097815 | -0.832922 | 0.095660 |
| C | 2.977210 | -1.965956 | 0.125142 |
| C | 2.222670 | -3.061278 | -0.260736 |
| C | 2.491901 | 0.479604 | 0.377446 |
| C | 1.697077 | 1.586103 | 0.202882 |
| N | 0.382176 | 1.576509 | -0.224700 |
| C | -0.004878 | 2.904778 | -0.275084 |
| C | 1.105851 | 3.769477 | 0.101241 |
| C | 2.152371 | 2.954985 | 0.420733 |
| C | -1.262111 | 3.372556 | -0.562575 |
| C | -2.396242 | 2.572959 | -0.751952 |
| C | -3.732564 | 3.065814 | -0.962085 |
| C | -4.550324 | 1.934824 | -1.062103 |
| C | -3.692619 | 0.805290 | -0.926626 |

| | | | |
|---|---|---|---|
| N | -2.382466 | 1.200392 | -0.729530 |
| C | -4.114316 | -0.529963 | -0.981340 |
| H | -0.026001 | -4.435346 | -0.943387 |
| H | -5.166921 | -0.711333 | -1.143761 |
| H | -1.394509 | 4.446898 | -0.593335 |
| H | 3.501324 | 0.633701 | 0.730757 |
| C | -1.312731 | -0.260060 | -3.612388 |
| H | -0.953947 | -0.042285 | -4.634242 |
| H | -2.295524 | 0.234596 | -3.503679 |
| C | 1.034795 | 5.263783 | 0.132465 |
| H | 0.814076 | 5.673456 | -0.860892 |
| H | 0.242946 | 5.614939 | 0.805263 |
| H | 1.977651 | 5.703355 | 0.468950 |
| C | 2.665384 | -4.483713 | -0.417262 |
| H | 2.046498 | -5.170336 | 0.173674 |
| H | 2.605519 | -4.819665 | -1.460637 |
| H | 3.701363 | -4.614327 | -0.089939 |
| C | -2.545420 | -5.289218 | -1.169562 |
| H | -1.853775 | -5.597426 | -1.962118 |
| H | -2.176934 | -5.727536 | -0.233503 |
| H | -3.519164 | -5.738630 | -1.379649 |
| C | -6.036237 | 1.889980 | -1.229866 |
| H | -6.344691 | 2.060448 | -2.270774 |

| | | | |
|---|---|---|---|
| H | -6.447996 | 0.923576 | -0.925569 |
| H | -6.519583 | 2.664519 | -0.623894 |
| C | -5.132073 | -3.499366 | -1.013230 |
| C | -6.203448 | -2.948142 | -0.419979 |
| H | -5.281811 | -4.446279 | -1.532983 |
| H | -7.179058 | -3.419977 | -0.486344 |
| H | -6.136093 | -2.038689 | 0.166257 |
| C | -4.088166 | 4.469377 | -1.010634 |
| C | -5.223565 | 5.028377 | -1.470581 |
| H | -3.332603 | 5.151181 | -0.621434 |
| H | -5.363191 | 6.104466 | -1.431733 |
| H | -6.026585 | 4.450120 | -1.911629 |
| C | 4.452884 | -1.898346 | 0.370864 |
| C | 5.201196 | -1.543692 | -0.939216 |
| H | 4.830718 | -2.853645 | 0.747588 |
| H | 4.693897 | -1.139384 | 1.120988 |
| H | 5.016832 | -2.337593 | -1.673362 |
| H | 4.813711 | -0.614699 | -1.357895 |
| C | 3.526970 | 3.357910 | 0.870850 |
| C | 4.593208 | 3.325716 | -0.249023 |
| H | 3.874666 | 2.713829 | 1.685158 |
| H | 3.477318 | 4.372527 | 1.276878 |
| H | 4.141346 | 3.453456 | -1.235676 |

| | | | |
|---|---|---|---|
| H | 5.300035 | 4.157030 | -0.121498 |
| C | 6.688730 | -1.409498 | -0.786511 |
| O | 7.382191 | -0.480448 | -1.179869 |
| O | 7.255726 | -2.463960 | -0.167841 |
| H | 8.204742 | -2.261733 | -0.110996 |
| C | 5.447903 | 2.073017 | -0.258666 |
| O | 5.657360 | 1.367470 | 0.714823 |
| O | 5.991810 | 1.843641 | -1.460267 |
| H | 6.552522 | 1.028493 | -1.392390 |
| O | -0.389670 | 0.180675 | -2.669306 |
| H | -1.495215 | -1.348691 | -3.556659 |
| C | -1.526153 | -1.736540 | 2.322979 |
| O | -1.575873 | -2.240363 | 3.685532 |
| C | -1.628230 | -1.227548 | 4.594622 |
| C | -1.445174 | 0.021859 | 3.848297 |
| C | -1.156788 | -0.236257 | 2.396527 |
| H | -0.790161 | -2.321485 | 1.774709 |
| H | -2.510227 | -1.885003 | 1.872789 |
| H | -1.764626 | 0.362554 | 1.713684 |
| H | -0.104577 | -0.069041 | 2.145601 |
| O | -1.785923 | -1.403100 | 5.782837 |
| N | -1.436943 | 1.171074 | 4.443157 |
| N | -1.442069 | 2.184076 | 4.973836 |

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**$^{5}$B’**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2489.0632093

Zero-point correction= 0.721652 (Hartree/Particle)

Thermal correction to Energy= 0.775303

Thermal correction to Enthalpy= 0.776247

Thermal correction to Gibbs Free Energy= 0.626176

Sum of electronic and zero-point Energies= -2488.341557

Sum of electronic and thermal Energies= -2488.287906

Sum of electronic and thermal Enthalpies= -2488.286962

Sum of electronic and thermal Free Energies= -2488.437033

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.701968 | -0.279061 | -1.097191 |
| N | -2.024265 | -1.878286 | -0.427769 |
| C | -1.630959 | -3.172367 | -0.224891 |
| C | -2.788913 | -4.046202 | -0.188837 |
| C | -3.898383 | -3.237991 | -0.343804 |

| | | | |
|---|---|---|---|
| C | -3.385462 | -1.875023 | -0.522724 |
| C | -0.307179 | -3.597691 | -0.050528 |
| C | 0.829898 | -2.793663 | 0.022958 |
| N | 0.824506 | -1.429618 | -0.073382 |
| C | 2.098841 | -1.006639 | 0.154954 |
| C | 2.977378 | -2.153283 | 0.366508 |
| C | 2.186843 | -3.271218 | 0.279574 |
| C | 2.505189 | 0.328060 | 0.227048 |
| C | 1.715712 | 1.459303 | 0.012031 |
| N | 0.398282 | 1.438391 | -0.345917 |
| C | -0.012249 | 2.738988 | -0.437336 |
| C | 1.099789 | 3.636634 | -0.136269 |
| C | 2.178768 | 2.838608 | 0.152243 |
| C | -1.311045 | 3.160026 | -0.728445 |
| C | -2.443163 | 2.354138 | -0.894921 |
| C | -3.802938 | 2.836853 | -1.144158 |
| C | -4.609762 | 1.712679 | -1.173655 |
| C | -3.735474 | 0.574830 | -0.945500 |
| N | -2.440379 | 0.996195 | -0.803616 |
| C | -4.163453 | -0.750668 | -0.817165 |
| H | -0.155692 | -4.666121 | 0.070826 |
| H | -5.219481 | -0.933516 | -0.969215 |
| H | -1.459002 | 4.232111 | -0.803699 |

| | | | |
|---|---|---|---|
| H | 3.534626 | 0.504199 | 0.509090 |
| C | -1.639213 | -0.771757 | -3.769895 |
| H | -1.350126 | -0.878844 | -4.833302 |
| H | -2.406037 | 0.028398 | -3.734961 |
| C | 1.006629 | 5.129856 | -0.109418 |
| H | 0.654398 | 5.528706 | -1.068349 |
| H | 0.303672 | 5.468308 | 0.661360 |
| H | 1.975479 | 5.589971 | 0.102876 |
| C | 2.586361 | -4.708175 | 0.408174 |
| H | 2.009026 | -5.218198 | 1.189036 |
| H | 2.415442 | -5.259471 | -0.524943 |
| H | 3.645692 | -4.808618 | 0.662554 |
| C | -2.747991 | -5.524300 | 0.044931 |
| H | -2.037898 | -6.015425 | -0.630469 |
| H | -2.433529 | -5.763674 | 1.069029 |
| H | -3.728098 | -5.984103 | -0.108532 |
| C | -6.094769 | 1.651344 | -1.338808 |
| H | -6.390642 | 1.625663 | -2.396249 |
| H | -6.514007 | 0.758604 | -0.865554 |
| H | -6.572289 | 2.530203 | -0.892695 |
| C | -5.285115 | -3.680462 | -0.304188 |
| C | -6.347867 | -2.996132 | 0.148566 |
| H | -5.458255 | -4.698065 | -0.657365 |

| | | | |
|---|---|---|---|
| H | -7.342233 | -3.431862 | 0.128042 |
| H | -6.255416 | -2.001429 | 0.570793 |
| C | -4.167838 | 4.236889 | -1.274150 |
| C | -5.251743 | 4.749965 | -1.880976 |
| H | -3.469584 | 4.942249 | -0.824125 |
| H | -5.423154 | 5.822052 | -1.897234 |
| H | -5.978242 | 4.132460 | -2.396652 |
| C | 4.465229 | -2.059653 | 0.516821 |
| C | 5.127214 | -1.792821 | -0.856134 |
| H | 4.876027 | -2.980228 | 0.940906 |
| H | 4.737115 | -1.243269 | 1.193652 |
| H | 4.922042 | -2.642728 | -1.519460 |
| H | 4.694901 | -0.908445 | -1.324469 |
| C | 3.560463 | 3.275252 | 0.546225 |
| C | 4.606885 | 3.176960 | -0.588428 |
| H | 3.924723 | 2.685142 | 1.393435 |
| H | 3.514794 | 4.312421 | 0.890180 |
| H | 4.145221 | 3.293257 | -1.571784 |
| H | 5.342408 | 3.987245 | -0.489496 |
| C | 6.618299 | -1.615456 | -0.809629 |
| O | 7.264590 | -0.753331 | -1.389220 |
| O | 7.243734 | -2.552290 | -0.070540 |
| H | 8.189917 | -2.332512 | -0.106401 |

| | | | |
|---|---|---|---|
| C | 5.421594 | 1.897890 | -0.571752 |
| O | 5.670917 | 1.249489 | 0.432147 |
| O | 5.880500 | 1.570884 | -1.786001 |
| H | 6.423956 | 0.747430 | -1.695871 |
| O | -0.535492 | -0.502638 | -2.971743 |
| H | -2.158257 | -1.711250 | -3.491505 |
| C | -2.272342 | -0.770976 | 2.938406 |
| O | -2.163989 | -0.424025 | 4.343850 |
| C | -1.411264 | 0.705538 | 4.523658 |
| C | -0.866772 | 1.067125 | 3.215932 |
| C | -1.229230 | 0.060416 | 2.165277 |
| H | -2.105743 | -1.844939 | 2.842895 |
| H | -3.290885 | -0.540396 | 2.611638 |
| H | -1.662332 | 0.507420 | 1.271109 |
| H | -0.374625 | -0.541935 | 1.846595 |
| O | -1.269027 | 1.234368 | 5.605285 |
| N | -0.103891 | 2.103287 | 3.059458 |
| N | 0.560832 | 3.024863 | 2.933354 |

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**$^{OSS}$B**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2489.0285515

Zero-point correction= 0.724971 (Hartree/Particle)

Thermal correction to Energy= 0.775886

Thermal correction to Enthalpy= 0.776830

Thermal correction to Gibbs Free Energy= 0.640832

Sum of electronic and zero-point Energies= -2488.303580

Sum of electronic and thermal Energies= -2488.252665

Sum of electronic and thermal Enthalpies= -2488.251721

Sum of electronic and thermal Free Energies= -2488.387720

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.808475 | 0.013827 | -0.130975 |
| N | -2.321479 | -1.258743 | -0.537467 |
| C | -2.266151 | -2.626890 | -0.609486 |
| C | -3.574186 | -3.174421 | -0.888480 |
| C | -4.436852 | -2.105826 | -0.959792 |
| C | -3.621995 | -0.909940 | -0.771928 |
| C | -1.119519 | -3.392382 | -0.449046 |
| C | 0.141810 | -2.892512 | -0.171796 |
| N | 0.445516 | -1.569074 | 0.026198 |
| C | 1.789980 | -1.515450 | 0.283358 |

| | | | |
|---|---|---|---|
| C | 2.360055 | -2.853846 | 0.269739 |
| C | 1.330251 | -3.711217 | -0.024530 |
| C | 2.517371 | -0.356928 | 0.523798 |
| C | 2.007921 | 0.935344 | 0.506197 |
| N | 0.703118 | 1.279587 | 0.296692 |
| C | 0.659588 | 2.648154 | 0.298432 |
| C | 1.983032 | 3.198029 | 0.546490 |
| C | 2.825796 | 2.129082 | 0.674452 |
| C | -0.460996 | 3.418607 | 0.040320 |
| C | -1.721135 | 2.923424 | -0.261847 |
| C | -2.884283 | 3.754008 | -0.560741 |
| C | -3.916909 | 2.881144 | -0.825647 |
| C | -3.366102 | 1.546464 | -0.689952 |
| N | -2.044524 | 1.603549 | -0.341406 |
| C | -4.098935 | 0.385244 | -0.885371 |
| H | -1.219602 | -4.466584 | -0.555246 |
| H | -5.137908 | 0.494666 | -1.164443 |
| H | -0.334959 | 4.494310 | 0.061312 |
| H | 3.571798 | -0.470489 | 0.737366 |
| C | -0.271101 | -0.843494 | -2.803361 |
| H | -0.085749 | -0.461860 | -3.822239 |
| H | -1.178430 | -1.470227 | -2.848938 |
| C | 2.305777 | 4.657592 | 0.614680 |

| | | | |
|---|---|---|---|
| H | 2.113093 | 5.161356 | -0.340873 |
| H | 1.698144 | 5.164366 | 1.373456 |
| H | 3.357294 | 4.820030 | 0.868685 |
| C | 1.361168 | -5.200360 | -0.175899 |
| H | 0.636031 | -5.687070 | 0.487173 |
| H | 1.113758 | -5.507239 | -1.199841 |
| H | 2.349046 | -5.607155 | 0.058199 |
| C | -3.894225 | -4.632692 | -0.983315 |
| H | -3.240399 | -5.145191 | -1.699233 |
| H | -3.768565 | -5.132519 | -0.014696 |
| H | -4.928480 | -4.791921 | -1.300108 |
| C | -5.344798 | 3.200215 | -1.132476 |
| H | -5.521810 | 3.315944 | -2.210482 |
| H | -6.014785 | 2.412461 | -0.776049 |
| H | -5.638655 | 4.139592 | -0.653636 |
| C | -5.881899 | -2.168641 | -1.143251 |
| C | -6.788984 | -1.387247 | -0.538496 |
| H | -6.242556 | -2.954787 | -1.808319 |
| H | -7.850860 | -1.509642 | -0.731812 |
| H | -6.496261 | -0.636528 | 0.187745 |
| C | -2.887575 | 5.206283 | -0.518156 |
| C | -3.713288 | 6.038245 | -1.174905 |
| H | -2.133059 | 5.655529 | 0.126870 |

| | | | |
|---|---|---|---|
| H | -3.638312 | 7.113694 | -1.044653 |
| H | -4.465274 | 5.681749 | -1.870050 |
| C | 3.800051 | -3.210787 | 0.498442 |
| C | 4.698443 | -3.034312 | -0.748379 |
| H | 3.854510 | -4.256082 | 0.817168 |
| H | 4.229081 | -2.616353 | 1.311269 |
| H | 5.495151 | -3.791113 | -0.746183 |
| H | 4.132073 | -3.173107 | -1.671908 |
| C | 4.318491 | 2.120729 | 0.797726 |
| C | 4.966704 | 1.936370 | -0.585757 |
| H | 4.655799 | 1.308956 | 1.449433 |
| H | 4.683516 | 3.049711 | 1.244896 |
| H | 4.543165 | 1.067927 | -1.093930 |
| H | 4.737963 | 2.799516 | -1.224849 |
| C | 5.417295 | -1.703667 | -0.796373 |
| O | 5.787283 | -1.078501 | 0.182470 |
| O | 5.657122 | -1.293026 | -2.053449 |
| H | 6.147887 | -0.444142 | -1.993386 |
| C | 6.462191 | 1.804637 | -0.524453 |
| O | 7.201029 | 2.203360 | 0.342571 |
| O | 6.973628 | 1.184937 | -1.648444 |
| H | 7.933838 | 1.143589 | -1.502733 |
| O | -0.395196 | 0.232439 | -1.930854 |

| | | | |
|---|---|---|---|
| H | 0.569837 | -1.512969 | -2.548411 |
| C | -0.539186 | -2.095048 | 3.028038 |
| O | -1.955987 | -2.158780 | 2.768204 |
| C | -2.420252 | -0.947361 | 2.294533 |
| C | -1.265720 | -0.037924 | 2.056021 |
| C | -0.144627 | -0.617947 | 2.920275 |
| H | -0.369282 | -2.514751 | 4.026153 |
| H | -0.022851 | -2.715751 | 2.294642 |
| H | 0.854206 | -0.484730 | 2.510259 |
| H | -0.162804 | -0.136015 | 3.907997 |
| O | -3.610368 | -0.769889 | 2.154542 |
| N | -1.637338 | 1.328031 | 2.412773 |
| N | -0.920803 | 2.123925 | 2.924642 |

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**$^{3}$B**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2489.0283601

Zero-point correction= 0.724980 (Hartree/Particle)

Thermal correction to Energy= 0.775893

Thermal correction to Enthalpy= 0.776837

Thermal correction to Gibbs Free Energy= 0.639814

Sum of electronic and zero-point Energies= -2488.303380

Sum of electronic and thermal Energies= -2488.252468

Sum of electronic and thermal Enthalpies= -2488.251523

Sum of electronic and thermal Free Energies= -2488.388546

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.808796 | 0.013701 | -0.130679 |
| N | -2.321419 | -1.258936 | -0.537830 |
| C | -2.265779 | -2.627055 | -0.610605 |
| C | -3.573775 | -3.174741 | -0.889366 |
| C | -4.436776 | -2.106336 | -0.959513 |
| C | -3.622149 | -0.910352 | -0.771360 |
| C | -1.119009 | -3.392391 | -0.450432 |
| C | 0.142132 | -2.892435 | -0.172541 |
| N | 0.445556 | -1.568983 | 0.025815 |
| C | 1.789869 | -1.515152 | 0.283435 |
| C | 2.360182 | -2.853461 | 0.269892 |
| C | 1.330630 | -3.710968 | -0.024909 |
| C | 2.517113 | -0.356507 | 0.523939 |
| C | 2.007529 | 0.935692 | 0.506072 |
| N | 0.702766 | 1.279804 | 0.296372 |

| | | | |
|---|---|---|---|
| C | 0.659078 | 2.648322 | 0.297925 |
| C | 1.982515 | 3.198391 | 0.545896 |
| C | 2.825348 | 2.129569 | 0.674093 |
| C | -0.461539 | 3.418635 | 0.039597 |
| C | -1.721751 | 2.923287 | -0.262085 |
| C | -2.885102 | 3.753707 | -0.560691 |
| C | -3.917917 | 2.880713 | -0.824373 |
| C | -3.366930 | 1.546098 | -0.688536 |
| N | -2.045147 | 1.603410 | -0.340849 |
| C | -4.099581 | 0.384768 | -0.883802 |
| H | -1.218904 | -4.466572 | -0.557025 |
| H | -5.138782 | 0.493987 | -1.162112 |
| H | -0.335583 | 4.494352 | 0.060336 |
| H | 3.571507 | -0.469951 | 0.737734 |
| C | -0.270585 | -0.842439 | -2.802805 |
| H | -0.085259 | -0.460112 | -3.821397 |
| H | -1.177628 | -1.469504 | -2.848714 |
| C | 2.305074 | 4.658007 | 0.613839 |
| H | 2.112283 | 5.161596 | -0.341782 |
| H | 1.697398 | 5.164791 | 1.372571 |
| H | 3.356579 | 4.820626 | 0.867778 |
| C | 1.361776 | -5.200118 | -0.176195 |
| H | 0.636970 | -5.686884 | 0.487198 |

| | | | |
|---|---|---|---|
| H | 1.114041 | -5.507127 | -1.200016 |
| H | 2.349813 | -5.606716 | 0.057570 |
| C | -3.893582 | -4.633026 | -0.984816 |
| H | -3.239397 | -5.145207 | -1.700623 |
| H | -3.768292 | -5.133150 | -0.016301 |
| H | -4.927686 | -4.792264 | -1.302109 |
| C | -5.346057 | 3.199520 | -1.130298 |
| H | -5.523956 | 3.314471 | -2.208241 |
| H | -6.015700 | 2.411972 | -0.772761 |
| H | -5.639572 | 4.139217 | -0.651880 |
| C | -5.881941 | -2.169357 | -1.142047 |
| C | -6.788691 | -1.388758 | -0.535766 |
| H | -6.242915 | -2.954896 | -1.807660 |
| H | -7.850700 | -1.511130 | -0.728367 |
| H | -6.495476 | -0.638757 | 0.191020 |
| C | -2.888385 | 5.206019 | -0.518983 |
| C | -3.714510 | 6.037514 | -1.175792 |
| H | -2.133504 | 5.655700 | 0.125307 |
| H | -3.639507 | 7.113051 | -1.046291 |
| H | -4.466881 | 5.680523 | -1.870268 |
| C | 3.800106 | -3.210238 | 0.499241 |
| C | 4.698950 | -3.034178 | -0.747302 |
| H | 3.854474 | -4.255429 | 0.818349 |

| | | | |
|---|---|---|---|
| H | 4.228820 | -2.615557 | 1.312053 |
| H | 5.495919 | -3.790712 | -0.744370 |
| H | 4.133012 | -3.173647 | -1.670987 |
| C | 4.318036 | 2.121330 | 0.797399 |
| C | 4.966307 | 1.936690 | -0.585992 |
| H | 4.655360 | 1.309757 | 1.449355 |
| H | 4.682998 | 3.050451 | 1.244342 |
| H | 4.542932 | 1.068069 | -1.093994 |
| H | 4.737445 | 2.799642 | -1.225307 |
| C | 5.417466 | -1.703354 | -0.795673 |
| O | 5.787373 | -1.077879 | 0.182980 |
| O | 5.657124 | -1.292956 | -2.052891 |
| H | 6.147747 | -0.443972 | -1.993046 |
| C | 6.461809 | 1.805153 | -0.524606 |
| O | 7.200586 | 2.204010 | 0.342396 |
| O | 6.973326 | 1.185270 | -1.648491 |
| H | 7.933523 | 1.143915 | -1.502703 |
| O | -0.395356 | 0.233156 | -1.929850 |
| H | 0.570641 | -1.511505 | -2.547933 |
| C | -0.536573 | -2.094675 | 3.027269 |
| O | -1.953146 | -2.159760 | 2.766660 |
| C | -2.418414 | -0.948316 | 2.293815 |
| C | -1.264495 | -0.038092 | 2.054198 |

| | | | |
|---|---|---|---|
| C | -0.143525 | -0.617160 | 2.919896 |
| H | -0.366809 | -2.514263 | 4.025479 |
| H | -0.019153 | -2.714867 | 2.294196 |
| H | 0.855511 | -0.482814 | 2.510741 |
| H | -0.163129 | -0.135496 | 3.907666 |
| O | -3.608773 | -0.771718 | 2.154600 |
| N | -1.637912 | 1.327601 | 2.412907 |
| N | -0.922365 | 2.125014 | 2.923376 |

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**$^{CSS}$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2489.0027866

Zero-point correction= 0.723009 (Hartree/Particle)

Thermal correction to Energy= 0.773705

Thermal correction to Enthalpy= 0.774649

Thermal correction to Gibbs Free Energy= 0.638979

Sum of electronic and zero-point Energies= -2488.279778

Sum of electronic and thermal Energies= -2488.229082

Sum of electronic and thermal Enthalpies= -2488.228138

Sum of electronic and thermal Free Energies= -2488.363807

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.824416 | -0.010552 | -0.058190 |
| N | -2.026638 | -1.623238 | -0.391837 |
| C | -1.614132 | -2.921360 | -0.538075 |
| C | -2.745978 | -3.788867 | -0.802021 |
| C | -3.861870 | -2.985212 | -0.798431 |
| C | -3.373838 | -1.619711 | -0.594936 |
| C | -0.299214 | -3.363565 | -0.452229 |
| C | 0.810044 | -2.583412 | -0.153297 |
| N | 0.782419 | -1.241586 | 0.126385 |
| C | 2.066236 | -0.878977 | 0.414059 |
| C | 2.948955 | -2.031613 | 0.324857 |
| C | 2.165250 | -3.095166 | -0.041892 |
| C | 2.482320 | 0.419475 | 0.705802 |
| C | 1.700503 | 1.556922 | 0.566384 |
| N | 0.377524 | 1.561432 | 0.189915 |
| C | 0.043991 | 2.876179 | -0.016700 |
| C | 1.184656 | 3.737217 | 0.247170 |
| C | 2.208895 | 2.920289 | 0.643720 |
| C | -1.216498 | 3.342810 | -0.358185 |
| C | -2.358851 | 2.563777 | -0.499809 |

| | | | |
|---|---|---|---|
| C | -3.684470 | 3.088945 | -0.829580 |
| C | -4.516487 | 1.993332 | -0.908508 |
| C | -3.688099 | 0.831741 | -0.647342 |
| N | -2.396908 | 1.208017 | -0.375170 |
| C | -4.147315 | -0.474527 | -0.726036 |
| H | -0.125059 | -4.420936 | -0.623541 |
| H | -5.190267 | -0.618769 | -0.973873 |
| H | -1.318324 | 4.411480 | -0.507538 |
| H | 3.519105 | 0.561160 | 0.985042 |
| C | 0.682791 | 0.182226 | -2.517867 |
| H | 1.443994 | -0.585187 | -2.266545 |
| H | 1.125524 | 1.157102 | -2.226978 |
| C | 1.171949 | 5.228846 | 0.125837 |
| H | 0.989655 | 5.547907 | -0.907885 |
| H | 0.381880 | 5.675158 | 0.742084 |
| H | 2.124709 | 5.665005 | 0.439923 |
| C | 2.582830 | -4.506122 | -0.318005 |
| H | 1.997907 | -5.224678 | 0.269131 |
| H | 2.443458 | -4.770878 | -1.373801 |
| H | 3.638235 | -4.664411 | -0.075549 |
| C | -2.671614 | -5.274014 | -0.967995 |
| H | -3.642870 | -5.693381 | -1.244411 |
| H | -1.951015 | -5.556358 | -1.745184 |

| | | | |
|---|---|---|---|
| H | -2.354700 | -5.769470 | -0.041128 |
| C | -5.989324 | 1.964531 | -1.163796 |
| H | -6.223939 | 1.915615 | -2.235955 |
| H | -6.458705 | 1.098618 | -0.688108 |
| H | -6.465283 | 2.868681 | -0.770374 |
| C | -5.245121 | -3.417880 | -0.934403 |
| C | -6.311687 | -2.871451 | -0.329356 |
| H | -5.408230 | -4.293727 | -1.564286 |
| H | -7.310301 | -3.267520 | -0.489808 |
| H | -6.209845 | -2.041048 | 0.361361 |
| C | -3.992649 | 4.499536 | -0.981724 |
| C | -5.017315 | 5.047816 | -1.657658 |
| H | -3.305432 | 5.182032 | -0.481734 |
| H | -5.156179 | 6.124690 | -1.678363 |
| H | -5.725849 | 4.453547 | -2.223455 |
| C | 4.440907 | -1.982228 | 0.424487 |
| C | 5.067376 | -1.682782 | -0.961038 |
| H | 4.834238 | -2.935889 | 0.796464 |
| H | 4.764817 | -1.213448 | 1.131862 |
| H | 4.814737 | -2.469357 | -1.673917 |
| H | 4.666402 | -0.736233 | -1.340591 |
| C | 3.589855 | 3.336994 | 1.055348 |
| C | 4.629662 | 3.368116 | -0.095614 |

| | | | |
|---|---|---|---|
| H | 3.971092 | 2.692753 | 1.853489 |
| H | 3.536155 | 4.345914 | 1.477948 |
| H | 4.178751 | 3.749745 | -1.012915 |
| H | 5.452600 | 4.035822 | 0.191207 |
| C | 6.554081 | -1.515013 | -0.885298 |
| O | 7.149228 | -0.768386 | -0.117226 |
| O | 7.239314 | -2.289254 | -1.747660 |
| H | 8.177721 | -2.068030 | -1.618383 |
| C | 5.264458 | 2.031899 | -0.411191 |
| O | 5.302742 | 1.521103 | -1.515298 |
| O | 5.831306 | 1.478206 | 0.677774 |
| H | 6.287966 | 0.642292 | 0.406802 |
| O | -0.557891 | -0.050693 | -1.958742 |
| H | 0.605025 | 0.185340 | -3.622062 |
| C | -0.737729 | -2.234763 | 2.931474 |
| O | -2.171187 | -2.114096 | 2.808744 |
| C | -2.490318 | -0.872034 | 2.313858 |
| C | -1.213593 | -0.167431 | 1.924705 |
| C | -0.205961 | -0.795876 | 2.894927 |
| H | -0.530180 | -2.752792 | 3.872529 |
| H | -0.358765 | -2.823827 | 2.095848 |
| H | 0.823505 | -0.728219 | 2.551275 |
| H | -0.277973 | -0.358155 | 3.899503 |

| | | | |
|---|---|---|---|
| O | -3.636480 | -0.496106 | 2.265109 |
| N | -1.441499 | 1.363932 | 2.520048 |
| N | -0.846640 | 2.322262 | 2.592573 |

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**$^{OSS}$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2489.0232234

Zero-point correction= 0.722845 (Hartree/Particle)

Thermal correction to Energy= 0.773932

Thermal correction to Enthalpy= 0.774876

Thermal correction to Gibbs Free Energy= 0.637349

Sum of electronic and zero-point Energies= -2488.300378

Sum of electronic and thermal Energies= -2488.249291

Sum of electronic and thermal Enthalpies= -2488.248347

Sum of electronic and thermal Free Energies= -2488.385874

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.810952 | -0.007437 | -0.144574 |
| N | -1.944997 | -1.643422 | -0.480475 |

| | | | |
|---|---|---|---|
| C | -1.547156 | -2.954582 | -0.432696 |
| C | -2.672485 | -3.835795 | -0.655944 |
| C | -3.774411 | -3.029007 | -0.809479 |
| C | -3.287595 | -1.653904 | -0.721185 |
| C | -0.249603 | -3.391335 | -0.209518 |
| C | 0.845747 | -2.569089 | 0.005927 |
| N | 0.801133 | -1.201774 | 0.101938 |
| C | 2.088365 | -0.782546 | 0.299330 |
| C | 2.986290 | -1.924185 | 0.324771 |
| C | 2.210403 | -3.040686 | 0.144951 |
| C | 2.498889 | 0.532965 | 0.482639 |
| C | 1.680385 | 1.652427 | 0.430271 |
| N | 0.334328 | 1.634188 | 0.194119 |
| C | -0.067779 | 2.938370 | 0.154414 |
| C | 1.056229 | 3.826035 | 0.413776 |
| C | 2.150263 | 3.023920 | 0.593184 |
| C | -1.349320 | 3.377520 | -0.137224 |
| C | -2.430999 | 2.560366 | -0.431021 |
| C | -3.762528 | 3.049211 | -0.778635 |
| C | -4.533061 | 1.929022 | -1.002520 |
| C | -3.663026 | 0.787817 | -0.792533 |
| N | -2.404773 | 1.198850 | -0.444885 |
| C | -4.075417 | -0.530754 | -0.916558 |

| | | | |
|---|---|---|---|
| H | -0.074770 | -4.461248 | -0.225225 |
| H | -5.104404 | -0.704448 | -1.199866 |
| H | -1.509112 | 4.448734 | -0.160961 |
| H | 3.546805 | 0.696445 | 0.696189 |
| C | -0.154173 | -0.862830 | -2.798765 |
| H | -1.015566 | -1.549452 | -2.883758 |
| H | 0.710395 | -1.474398 | -2.480947 |
| C | 0.964753 | 5.319127 | 0.457633 |
| H | 0.679885 | 5.733557 | -0.517537 |
| H | 0.211308 | 5.652555 | 1.180911 |
| H | 1.919513 | 5.772226 | 0.739286 |
| C | 2.637668 | -4.472968 | 0.062809 |
| H | 2.084357 | -5.099004 | 0.772831 |
| H | 2.462658 | -4.891410 | -0.936266 |
| H | 3.703258 | -4.584494 | 0.284256 |
| C | -2.613390 | -5.330134 | -0.625493 |
| H | -1.833051 | -5.718132 | -1.291125 |
| H | -2.391694 | -5.699204 | 0.383695 |
| H | -3.565603 | -5.771772 | -0.931543 |
| C | -5.988833 | 1.857416 | -1.334990 |
| H | -6.167721 | 1.872247 | -2.418716 |
| H | -6.443093 | 0.942436 | -0.943883 |
| H | -6.522228 | 2.712251 | -0.907325 |

| | | | |
|---|---|---|---|
| C | -5.151592 | -3.472620 | -0.985595 |
| C | -6.246899 | -2.898988 | -0.465258 |
| H | -5.281863 | -4.384053 | -1.571079 |
| H | -7.234903 | -3.310356 | -0.650860 |
| H | -6.181838 | -2.033004 | 0.184454 |
| C | -4.138231 | 4.452314 | -0.813363 |
| C | -5.138079 | 5.010814 | -1.515945 |
| H | -3.534655 | 5.112543 | -0.191242 |
| H | -5.342244 | 6.074844 | -1.443010 |
| H | -5.761730 | 4.439317 | -2.194279 |
| C | 4.478832 | -1.836187 | 0.383846 |
| C | 5.068116 | -1.591041 | -1.028884 |
| H | 4.900077 | -2.761587 | 0.792974 |
| H | 4.800851 | -1.026565 | 1.045273 |
| H | 4.810527 | -2.413243 | -1.698565 |
| H | 4.647289 | -0.667074 | -1.440991 |
| C | 3.556083 | 3.455044 | 0.889255 |
| C | 4.504823 | 3.473447 | -0.339721 |
| H | 4.003718 | 2.825581 | 1.664794 |
| H | 3.526025 | 4.468681 | 1.300899 |
| H | 3.971255 | 3.786453 | -1.238434 |
| H | 5.311241 | 4.193848 | -0.149576 |
| C | 6.554609 | -1.403124 | -0.993364 |

| | | | |
|---|---|---|---|
| O | 7.154553 | -0.596531 | -0.293298 |
| O | 7.231814 | -2.232858 | -1.808862 |
| H | 8.170690 | -1.997466 | -1.711741 |
| C | 5.189210 | 2.157487 | -0.640220 |
| O | 5.213538 | 1.616065 | -1.730048 |
| O | 5.817455 | 1.661038 | 0.442658 |
| H | 6.291738 | 0.831599 | 0.182763 |
| O | -0.396879 | 0.214388 | -1.955730 |
| H | 0.070023 | -0.492446 | -3.814289 |
| C | 0.145323 | -1.569972 | 3.271111 |
| O | -1.159460 | -2.161283 | 3.132799 |
| C | -1.978710 | -1.324529 | 2.385884 |
| C | -1.194863 | -0.147526 | 1.917923 |
| C | -0.019758 | -0.094276 | 2.883799 |
| H | 0.468619 | -1.718265 | 4.307480 |
| H | 0.841888 | -2.087043 | 2.605432 |
| H | 0.890483 | 0.321384 | 2.458429 |
| H | -0.273996 | 0.504887 | 3.769162 |
| O | -3.144989 | -1.613860 | 2.231854 |
| N | -2.305399 | 1.211782 | 2.353924 |
| N | -1.894024 | 2.147435 | 2.875475 |

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**$^3$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2489.0232546

Zero-point correction= 0.722896 (Hartree/Particle)

Thermal correction to Energy= 0.773908

Thermal correction to Enthalpy= 0.774853

Thermal correction to Gibbs Free Energy= 0.636691

Sum of electronic and zero-point Energies= -2488.300358

Sum of electronic and thermal Energies= -2488.249346

Sum of electronic and thermal Enthalpies= -2488.248402

Sum of electronic and thermal Free Energies= -2488.386564

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.798499 | -0.014944 | -0.142690 |
| N | -1.948321 | -1.646751 | -0.449398 |
| C | -1.562496 | -2.962025 | -0.407869 |
| C | -2.698862 | -3.830451 | -0.620474 |
| C | -3.792983 | -3.010752 | -0.770578 |
| C | -3.291479 | -1.641976 | -0.695883 |
| C | -0.262081 | -3.410202 | -0.214982 |

| | | | |
|---|---|---|---|
| C | 0.841111 | -2.596613 | -0.011895 |
| N | 0.804621 | -1.229941 | 0.106997 |
| C | 2.094083 | -0.825103 | 0.317548 |
| C | 2.985826 | -1.972781 | 0.319663 |
| C | 2.203881 | -3.079484 | 0.114197 |
| C | 2.509335 | 0.483247 | 0.536104 |
| C | 1.700490 | 1.609746 | 0.473501 |
| N | 0.364623 | 1.607480 | 0.186656 |
| C | -0.016922 | 2.918206 | 0.109379 |
| C | 1.109847 | 3.791597 | 0.396217 |
| C | 2.182591 | 2.976347 | 0.635666 |
| C | -1.283731 | 3.371526 | -0.218240 |
| C | -2.379790 | 2.565214 | -0.492446 |
| C | -3.702727 | 3.065502 | -0.860287 |
| C | -4.489250 | 1.951454 | -1.055544 |
| C | -3.636130 | 0.803225 | -0.812149 |
| N | -2.375035 | 1.205262 | -0.468038 |
| C | -4.063971 | -0.512114 | -0.912654 |
| H | -0.095137 | -4.481176 | -0.245833 |
| H | -5.095065 | -0.679302 | -1.192652 |
| H | -1.423664 | 4.444460 | -0.272331 |
| H | 3.554249 | 0.637269 | 0.770974 |
| C | -0.003032 | -0.891332 | -2.757985 |

| | | | |
|---|---|---|---|
| H | -0.677329 | -1.765713 | -2.722540 |
| H | 1.003742 | -1.253169 | -2.478569 |
| C | 1.040847 | 5.286296 | 0.417385 |
| H | 0.792387 | 5.692198 | -0.571171 |
| H | 0.271417 | 5.640111 | 1.113568 |
| H | 1.993889 | 5.727764 | 0.722310 |
| C | 2.622082 | -4.512314 | 0.000899 |
| H | 2.069375 | -5.150080 | 0.701174 |
| H | 2.438649 | -4.909603 | -1.005249 |
| H | 3.688182 | -4.634622 | 0.214011 |
| C | -2.657074 | -5.325657 | -0.591424 |
| H | -1.905346 | -5.723148 | -1.284157 |
| H | -2.404807 | -5.699716 | 0.408723 |
| H | -3.624947 | -5.754398 | -0.864804 |
| C | -5.944949 | 1.891576 | -1.390212 |
| H | -6.121047 | 1.879926 | -2.474478 |
| H | -6.412732 | 0.994039 | -0.975411 |
| H | -6.467130 | 2.765035 | -0.987009 |
| C | -5.180700 | -3.431409 | -0.923850 |
| C | -6.246480 | -2.839773 | -0.364136 |
| H | -5.343742 | -4.331172 | -1.519002 |
| H | -7.249652 | -3.223558 | -0.526471 |
| H | -6.137518 | -1.985730 | 0.295929 |

| | | | |
|---|---|---|---|
| C | -4.055669 | 4.472683 | -0.936087 |
| C | -5.046549 | 5.027110 | -1.654594 |
| H | -3.440747 | 5.140977 | -0.333917 |
| H | -5.232781 | 6.096099 | -1.612738 |
| H | -5.680247 | 4.446559 | -2.315691 |
| C | 4.478757 | -1.893669 | 0.378800 |
| C | 5.066222 | -1.618360 | -1.028666 |
| H | 4.896320 | -2.830317 | 0.765560 |
| H | 4.805717 | -1.101276 | 1.058401 |
| H | 4.803180 | -2.422713 | -1.717685 |
| H | 4.648614 | -0.682987 | -1.417997 |
| C | 3.580442 | 3.393112 | 0.984893 |
| C | 4.565427 | 3.437619 | -0.214415 |
| H | 4.001220 | 2.742948 | 1.758164 |
| H | 3.542484 | 4.396865 | 1.419739 |
| H | 4.063591 | 3.794200 | -1.115190 |
| H | 5.380041 | 4.133038 | 0.026325 |
| C | 6.553500 | -1.436917 | -0.993786 |
| O | 7.160122 | -0.662526 | -0.263795 |
| O | 7.222877 | -2.232293 | -1.848946 |
| H | 8.162802 | -2.002055 | -1.749671 |
| C | 5.228417 | 2.117676 | -0.542571 |
| O | 5.247622 | 1.599752 | -1.643928 |

| | | | |
|---|---|---|---|
| O | 5.842142 | 1.586312 | 0.532065 |
| H | 6.306395 | 0.756887 | 0.255051 |
| O | -0.440189 | 0.165660 | -1.970009 |
| H | 0.052683 | -0.566397 | -3.811641 |
| C | -0.283315 | -1.837236 | 3.203985 |
| O | -1.695096 | -2.084313 | 3.063499 |
| C | -2.279145 | -1.053735 | 2.338780 |
| C | -1.227351 | -0.092259 | 1.906883 |
| C | -0.088474 | -0.350282 | 2.882785 |
| H | 0.000814 | -2.109066 | 4.226491 |
| H | 0.258518 | -2.475368 | 2.500786 |
| H | 0.901330 | -0.139193 | 2.483995 |
| H | -0.216564 | 0.252880 | 3.792330 |
| O | -3.479272 | -1.044936 | 2.172967 |
| N | -1.991941 | 1.485902 | 2.379151 |
| N | -1.372519 | 2.280997 | 2.927494 |

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**$^{5}$TS(B-C)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2489.0046063

Zero-point correction= 0.720726 (Hartree/Particle)

Thermal correction to Energy= 0.772285

Thermal correction to Enthalpy= 0.773229

Thermal correction to Gibbs Free Energy= 0.633337

Sum of electronic and zero-point Energies= -2488.283880

Sum of electronic and thermal Energies= -2488.232321

Sum of electronic and thermal Enthalpies= -2488.231377

Sum of electronic and thermal Free Energies= -2488.371270

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.822962 | -0.002496 | -0.106874 |
| N | -2.001113 | -1.692559 | -0.484370 |
| C | -1.580124 | -2.988374 | -0.451011 |
| C | -2.706772 | -3.869246 | -0.698368 |
| C | -3.814510 | -3.060372 | -0.848840 |
| C | -3.336020 | -1.679566 | -0.733996 |
| C | -0.259364 | -3.394043 | -0.225191 |
| C | 0.852242 | -2.583506 | 0.013643 |
| N | 0.836073 | -1.219922 | 0.142199 |
| C | 2.116909 | -0.797920 | 0.348163 |
| C | 3.005068 | -1.953347 | 0.352557 |
| C | 2.220807 | -3.062288 | 0.146533 |

| | | | |
|---|---|---|---|
| C | 2.527027 | 0.528666 | 0.537252 |
| C | 1.731943 | 1.677612 | 0.481531 |
| N | 0.389139 | 1.675858 | 0.267435 |
| C | -0.027811 | 2.968315 | 0.170472 |
| C | 1.110270 | 3.859170 | 0.382184 |
| C | 2.206313 | 3.058028 | 0.583687 |
| C | -1.325865 | 3.382120 | -0.134125 |
| C | -2.439041 | 2.581798 | -0.415616 |
| C | -3.770426 | 3.079118 | -0.779025 |
| C | -4.554441 | 1.962856 | -0.994143 |
| C | -3.699422 | 0.806333 | -0.769328 |
| N | -2.450865 | 1.226190 | -0.414762 |
| C | -4.103300 | -0.524874 | -0.906513 |
| H | -0.073353 | -4.462856 | -0.260144 |
| H | -5.133274 | -0.684583 | -1.199012 |
| H | -1.478998 | 4.454392 | -0.190234 |
| H | 3.579961 | 0.680162 | 0.740128 |
| C | 0.124485 | -0.763998 | -2.706143 |
| H | -0.376720 | -1.745525 | -2.642851 |
| H | 1.182709 | -0.919428 | -2.431511 |
| C | 1.033117 | 5.353718 | 0.362506 |
| H | 0.751589 | 5.728248 | -0.629679 |
| H | 0.281367 | 5.723599 | 1.069763 |

| | | | |
|---|---|---|---|
| H | 1.990957 | 5.811745 | 0.625614 |
| C | 2.646931 | -4.493063 | 0.033433 |
| H | 2.085713 | -5.135334 | 0.722600 |
| H | 2.479482 | -4.886826 | -0.976989 |
| H | 3.710326 | -4.613398 | 0.261254 |
| C | -2.647125 | -5.364119 | -0.700381 |
| H | -1.838318 | -5.733860 | -1.341899 |
| H | -2.465532 | -5.757966 | 0.307726 |
| H | -3.583866 | -5.802135 | -1.056135 |
| C | -6.008042 | 1.908580 | -1.339167 |
| H | -6.178270 | 1.939579 | -2.424034 |
| H | -6.471877 | 0.991585 | -0.964129 |
| H | -6.539256 | 2.761664 | -0.904656 |
| C | -5.185679 | -3.509931 | -1.049465 |
| C | -6.292830 | -2.934474 | -0.556221 |
| H | -5.302848 | -4.424359 | -1.633213 |
| H | -7.276344 | -3.347073 | -0.761700 |
| H | -6.242961 | -2.064892 | 0.090019 |
| C | -4.131756 | 4.484901 | -0.834801 |
| C | -5.130974 | 5.046947 | -1.536090 |
| H | -3.512061 | 5.147347 | -0.230810 |
| H | -5.317609 | 6.115170 | -1.478666 |
| H | -5.771009 | 4.474723 | -2.198172 |

| | | | |
|---|---|---|---|
| C | 4.498397 | -1.881132 | 0.412897 |
| C | 5.090041 | -1.636945 | -0.999813 |
| H | 4.912976 | -2.810644 | 0.819893 |
| H | 4.826591 | -1.074752 | 1.075507 |
| H | 4.832974 | -2.460258 | -1.668248 |
| H | 4.671024 | -0.712336 | -1.411850 |
| C | 3.616535 | 3.498638 | 0.842430 |
| C | 4.545873 | 3.467633 | -0.400594 |
| H | 4.074640 | 2.895676 | 1.632971 |
| H | 3.596673 | 4.527136 | 1.216570 |
| H | 4.003289 | 3.765342 | -1.299147 |
| H | 5.367306 | 4.178784 | -0.242379 |
| C | 6.576349 | -1.451138 | -0.958539 |
| O | 7.171467 | -0.621983 | -0.281069 |
| O | 7.259713 | -2.311853 | -1.736260 |
| H | 8.198524 | -2.078080 | -1.634678 |
| C | 5.202436 | 2.131964 | -0.675064 |
| O | 5.196331 | 1.558945 | -1.749022 |
| O | 5.844192 | 1.657246 | 0.409229 |
| H | 6.305619 | 0.816277 | 0.163856 |
| O | -0.503369 | 0.215264 | -1.941728 |
| H | 0.106049 | -0.457995 | -3.766572 |
| C | -0.008282 | -1.694865 | 3.248010 |

| | | | |
|---|---|---|---|
| O | -1.358329 | -2.173024 | 3.094023 |
| C | -2.106886 | -1.258209 | 2.371504 |
| C | -1.228808 | -0.130429 | 1.936340 |
| C | -0.049575 | -0.202526 | 2.894827 |
| H | 0.295536 | -1.892195 | 4.281763 |
| H | 0.643418 | -2.252979 | 2.571431 |
| H | 0.889642 | 0.150008 | 2.475682 |
| H | -0.256355 | 0.395226 | 3.792707 |
| O | -3.292814 | -1.439392 | 2.214736 |
| N | -2.224528 | 1.295867 | 2.398182 |
| N | -1.733616 | 2.196264 | 2.914952 |

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$^{CSS}C$

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.5069114

Zero-point correction= 0.714580 (Hartree/Particle)

Thermal correction to Energy= 0.763764

Thermal correction to Enthalpy= 0.764708

Thermal correction to Gibbs Free Energy= 0.631477

Sum of electronic and zero-point Energies= -2378.792332

Sum of electronic and thermal Energies= -2378.743147

Sum of electronic and thermal Enthalpies= -2378.742203

Sum of electronic and thermal Free Energies= -2378.875434

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.859685 | -0.081594 | -0.017018 |
| N | -2.021944 | -1.715424 | -0.308115 |
| C | -1.601657 | -3.014364 | -0.243222 |
| C | -2.706445 | -3.919894 | -0.497356 |
| C | -3.812516 | -3.132847 | -0.714028 |
| C | -3.346134 | -1.747243 | -0.623713 |
| C | -0.295122 | -3.433465 | -0.019226 |
| C | 0.809885 | -2.613640 | 0.153559 |
| N | 0.788160 | -1.245251 | 0.201680 |
| C | 2.080330 | -0.841346 | 0.388143 |
| C | 2.965722 | -1.996073 | 0.436085 |
| C | 2.172514 | -3.102909 | 0.291818 |
| C | 2.497954 | 0.476841 | 0.535447 |
| C | 1.673300 | 1.590179 | 0.447495 |
| N | 0.329283 | 1.549680 | 0.194362 |
| C | -0.104282 | 2.847278 | 0.181553 |
| C | 1.006100 | 3.753162 | 0.432251 |

| | | | |
|---|---|---|---|
| C | 2.116828 | 2.969464 | 0.603493 |
| C | -1.405124 | 3.266803 | -0.055254 |
| C | -2.491867 | 2.449280 | -0.344135 |
| C | -3.816081 | 2.946337 | -0.723067 |
| C | -4.573370 | 1.829406 | -1.000485 |
| C | -3.709970 | 0.684993 | -0.776116 |
| N | -2.465541 | 1.090160 | -0.380466 |
| C | -4.120396 | -0.632970 | -0.904849 |
| H | -0.116842 | -4.503666 | -0.020764 |
| H | -5.130507 | -0.811624 | -1.246936 |
| H | -1.574662 | 4.337390 | -0.067403 |
| H | 3.545210 | 0.645922 | 0.749978 |
| C | 0.606620 | 0.182322 | -2.526863 |
| H | 1.403775 | -0.537890 | -2.250715 |
| H | 1.006184 | 1.186723 | -2.282404 |
| C | 0.894093 | 5.245592 | 0.469434 |
| H | 0.604677 | 5.651683 | -0.507949 |
| H | 0.134638 | 5.575737 | 1.188445 |
| H | 1.841709 | 5.714228 | 0.750541 |
| C | 2.579760 | -4.542332 | 0.236681 |
| H | 2.035258 | -5.145256 | 0.973538 |
| H | 2.376170 | -4.982326 | -0.747590 |
| H | 3.648767 | -4.663394 | 0.435688 |

| | | | |
|---|---|---|---|
| C | -2.618510 | -5.413373 | -0.469746 |
| H | -1.843625 | -5.783680 | -1.152100 |
| H | -2.367627 | -5.785807 | 0.531787 |
| H | -3.567037 | -5.873804 | -0.759041 |
| C | -6.014753 | 1.763423 | -1.391570 |
| H | -6.151589 | 1.826625 | -2.479745 |
| H | -6.476152 | 0.828894 | -1.060085 |
| H | -6.572436 | 2.594353 | -0.947266 |
| C | -5.170660 | -3.600535 | -0.954163 |
| C | -6.308452 | -3.013817 | -0.550219 |
| H | -5.252046 | -4.546498 | -1.491790 |
| H | -7.275067 | -3.451082 | -0.783195 |
| H | -6.304469 | -2.106329 | 0.043773 |
| C | -4.191309 | 4.348705 | -0.743572 |
| C | -5.182716 | 4.923397 | -1.446591 |
| H | -3.593599 | 4.999845 | -0.105562 |
| H | -5.383367 | 5.986877 | -1.356602 |
| H | -5.801726 | 4.367089 | -2.141277 |
| C | 4.460618 | -1.930699 | 0.469594 |
| C | 5.028756 | -1.723928 | -0.959475 |
| H | 4.872212 | -2.856568 | 0.887557 |
| H | 4.804078 | -1.116840 | 1.115748 |
| H | 4.681989 | -2.519061 | -1.621055 |

| | | | |
|---|---|---|---|
| H | 4.669616 | -0.768098 | -1.357842 |
| C | 3.517163 | 3.430091 | 0.877352 |
| C | 4.445600 | 3.451644 | -0.367592 |
| H | 3.988816 | 2.817083 | 1.652035 |
| H | 3.476931 | 4.448242 | 1.277113 |
| H | 3.893333 | 3.753001 | -1.258795 |
| H | 5.249797 | 4.179224 | -0.196107 |
| C | 6.527913 | -1.712016 | -1.017000 |
| O | 7.252185 | -2.418533 | -1.678351 |
| O | 7.073162 | -0.761704 | -0.177850 |
| H | 8.034065 | -0.811243 | -0.310712 |
| C | 5.130078 | 2.138333 | -0.667843 |
| O | 5.133790 | 1.568722 | -1.740707 |
| O | 5.797930 | 1.666821 | 0.410416 |
| H | 6.232743 | 0.826784 | 0.150629 |
| O | -0.607768 | -0.084674 | -1.926286 |
| H | 0.514799 | 0.139792 | -3.628982 |
| C | -0.768291 | -0.376201 | 4.123611 |
| O | -2.177785 | -0.424001 | 3.878014 |
| C | -2.428922 | -0.321477 | 2.508344 |
| C | -1.161585 | -0.087397 | 1.768236 |
| C | -0.135450 | 0.168849 | 2.835338 |
| H | -0.596532 | 0.246467 | 5.008102 |

H 0.832313 -0.284162 2.609039

H 0.037742 1.254051 2.903983

O -3.573966 -0.412907 2.118358

H -0.413537 -1.392622 4.343380

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$^{oss}C$

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.5206301

Zero-point correction= 0.714135 (Hartree/Particle)

Thermal correction to Energy= 0.763526

Thermal correction to Enthalpy= 0.764470

Thermal correction to Gibbs Free Energy= 0.630660

Sum of electronic and zero-point Energies= -2378.806495

Sum of electronic and thermal Energies= -2378.757104

Sum of electronic and thermal Enthalpies= -2378.756160

Sum of electronic and thermal Free Energies= -2378.889970

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Cartesian Coordinates

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Fe -0.810645 -0.071420 -0.077876

| | | | |
|---|---|---|---|
| N | -1.978739 | -1.700952 | -0.324123 |
| C | -1.561492 | -3.002514 | -0.251859 |
| C | -2.677511 | -3.904056 | -0.455107 |
| C | -3.790161 | -3.115637 | -0.635079 |
| C | -3.319543 | -1.732921 | -0.578228 |
| C | -0.254380 | -3.426454 | -0.040421 |
| C | 0.851847 | -2.608736 | 0.133722 |
| N | 0.829686 | -1.242860 | 0.190093 |
| C | 2.121771 | -0.838402 | 0.360013 |
| C | 3.009341 | -1.993047 | 0.401771 |
| C | 2.216048 | -3.099546 | 0.261970 |
| C | 2.541930 | 0.478573 | 0.503078 |
| C | 1.719876 | 1.594001 | 0.415218 |
| N | 0.376253 | 1.559118 | 0.173421 |
| C | -0.050065 | 2.856431 | 0.148414 |
| C | 1.065119 | 3.760376 | 0.390825 |
| C | 2.171961 | 2.972570 | 0.564015 |
| C | -1.349577 | 3.278894 | -0.090205 |
| C | -2.441737 | 2.462062 | -0.360197 |
| C | -3.776066 | 2.958518 | -0.692466 |
| C | -4.550419 | 1.842497 | -0.929290 |
| C | -3.686041 | 0.697362 | -0.730272 |
| N | -2.420268 | 1.100631 | -0.394405 |

| | | | |
|---|---|---|---|
| C | -4.105326 | -0.620355 | -0.830469 |
| H | -0.080520 | -4.497252 | -0.040223 |
| H | -5.131145 | -0.799733 | -1.120938 |
| H | -1.517376 | 4.349575 | -0.106232 |
| H | 3.591031 | 0.646473 | 0.709541 |
| C | -1.258868 | -0.202716 | -2.936608 |
| H | -2.039858 | 0.581898 | -2.959789 |
| H | -1.791822 | -1.171697 | -2.884547 |
| C | 0.959126 | 5.253280 | 0.419421 |
| H | 0.672114 | 5.654745 | -0.560593 |
| H | 0.200772 | 5.590587 | 1.136259 |
| H | 1.908561 | 5.719570 | 0.698202 |
| C | 2.621797 | -4.539085 | 0.202947 |
| H | 2.079086 | -5.142689 | 0.940579 |
| H | 2.414919 | -4.977001 | -0.781557 |
| H | 3.691333 | -4.661324 | 0.398275 |
| C | -2.597134 | -5.397575 | -0.408868 |
| H | -1.838504 | -5.781754 | -1.101455 |
| H | -2.328201 | -5.756597 | 0.592718 |
| H | -3.554207 | -5.855870 | -0.672131 |
| C | -6.007802 | 1.779869 | -1.256735 |
| H | -6.192050 | 1.829006 | -2.338636 |
| H | -6.458760 | 0.852701 | -0.892034 |

| | | | |
|---|---|---|---|
| H | -6.540978 | 2.619848 | -0.799880 |
| C | -5.160293 | -3.579241 | -0.809751 |
| C | -6.271132 | -2.990206 | -0.340405 |
| H | -5.273080 | -4.520229 | -1.350411 |
| H | -7.251533 | -3.420006 | -0.524552 |
| H | -6.228111 | -2.089200 | 0.262029 |
| C | -4.148652 | 4.362239 | -0.710818 |
| C | -5.160288 | 4.931645 | -1.388156 |
| H | -3.530178 | 5.016984 | -0.097178 |
| H | -5.356760 | 5.996200 | -1.302372 |
| H | -5.801273 | 4.369482 | -2.057835 |
| C | 4.504295 | -1.928287 | 0.440504 |
| C | 5.081176 | -1.717272 | -0.983931 |
| H | 4.912883 | -2.855756 | 0.857920 |
| H | 4.844617 | -1.117160 | 1.091669 |
| H | 4.737596 | -2.508951 | -1.651311 |
| H | 4.726373 | -0.759642 | -1.381775 |
| C | 3.573061 | 3.428018 | 0.844064 |
| C | 4.511370 | 3.444333 | -0.393178 |
| H | 4.036386 | 2.815053 | 1.623656 |
| H | 3.533387 | 4.446928 | 1.241949 |
| H | 3.966889 | 3.738482 | -1.291553 |
| H | 5.311251 | 4.176404 | -0.219716 |

| | | | |
|---|---|---|---|
| C | 6.580806 | -1.706330 | -1.033637 |
| O | 7.306897 | -2.401879 | -1.704535 |
| O | 7.124020 | -0.771959 | -0.175464 |
| H | 8.085216 | -0.820037 | -0.306872 |
| C | 5.206514 | 2.133706 | -0.681321 |
| O | 5.241799 | 1.571419 | -1.757434 |
| O | 5.846744 | 1.656589 | 0.411258 |
| H | 6.288917 | 0.818748 | 0.156607 |
| O | -0.337686 | -0.027797 | -1.916739 |
| H | -0.750964 | -0.171714 | -3.918502 |
| C | -0.706720 | -0.321436 | 4.181895 |
| O | -2.117155 | -0.377248 | 3.952236 |
| C | -2.370625 | -0.321358 | 2.572460 |
| C | -1.128588 | -0.078019 | 1.832924 |
| C | -0.089481 | 0.212115 | 2.879305 |
| H | -0.525321 | 0.311135 | 5.057893 |
| H | 0.881171 | -0.235630 | 2.652920 |
| H | 0.075080 | 1.299815 | 2.935485 |
| O | -3.519721 | -0.455572 | 2.192253 |
| H | -0.342696 | -1.334211 | 4.408374 |

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**$^{3}$C**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.5157445

Zero-point correction= 0.714026 (Hartree/Particle)

Thermal correction to Energy= 0.763521

Thermal correction to Enthalpy= 0.764465

Thermal correction to Gibbs Free Energy= 0.629249

Sum of electronic and zero-point Energies= -2378.801718

Sum of electronic and thermal Energies= -2378.752224

Sum of electronic and thermal Enthalpies= -2378.751279

Sum of electronic and thermal Free Energies= -2378.886495

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.821843 | -0.060406 | -0.107464 |
| N | -1.950945 | -1.712365 | -0.332009 |
| C | -1.551898 | -3.014901 | -0.187412 |
| C | -2.667078 | -3.912813 | -0.398867 |
| C | -3.760513 | -3.120828 | -0.661711 |
| C | -3.278826 | -1.741038 | -0.641123 |
| C | -0.253843 | -3.433669 | 0.076332 |
| C | 0.843068 | -2.598685 | 0.218753 |

| | | | |
|---|---|---|---|
| N | 0.801988 | -1.229480 | 0.198641 |
| C | 2.089202 | -0.798948 | 0.358287 |
| C | 2.989398 | -1.938481 | 0.457952 |
| C | 2.210597 | -3.062306 | 0.376382 |
| C | 2.494097 | 0.526308 | 0.465708 |
| C | 1.663950 | 1.636240 | 0.384712 |
| N | 0.317494 | 1.598165 | 0.157487 |
| C | -0.116626 | 2.893611 | 0.164491 |
| C | 0.995169 | 3.798967 | 0.409519 |
| C | 2.109735 | 3.015033 | 0.548399 |
| C | -1.419446 | 3.309352 | -0.062571 |
| C | -2.487277 | 2.476081 | -0.371393 |
| C | -3.820595 | 2.947261 | -0.744200 |
| C | -4.552390 | 1.817745 | -1.039630 |
| C | -3.664494 | 0.689893 | -0.827991 |
| N | -2.427820 | 1.118880 | -0.431487 |
| C | -4.054863 | -0.634759 | -0.949473 |
| H | -0.078285 | -4.502453 | 0.132372 |
| H | -5.065738 | -0.828431 | -1.280653 |
| H | -1.603279 | 4.377369 | -0.055874 |
| H | 3.542024 | 0.705369 | 0.667737 |
| C | -0.064470 | -1.048921 | -2.702380 |
| H | -0.775905 | -1.894404 | -2.648399 |

| | | | |
|---|---|---|---|
| H | 0.920047 | -1.445781 | -2.389191 |
| C | 0.877951 | 5.290088 | 0.470566 |
| H | 0.569985 | 5.708922 | -0.495671 |
| H | 0.130122 | 5.605775 | 1.207877 |
| H | 1.828302 | 5.758609 | 0.742103 |
| C | 2.633690 | -4.497998 | 0.398426 |
| H | 2.095010 | -5.065561 | 1.166793 |
| H | 2.436111 | -4.992605 | -0.560833 |
| H | 3.703660 | -4.596497 | 0.603985 |
| C | -2.606378 | -5.403395 | -0.282390 |
| H | -1.827821 | -5.827398 | -0.928267 |
| H | -2.379358 | -5.718965 | 0.743822 |
| H | -3.558961 | -5.862407 | -0.560222 |
| C | -5.992513 | 1.725751 | -1.429646 |
| H | -6.131617 | 1.792381 | -2.517292 |
| H | -6.435336 | 0.780809 | -1.102572 |
| H | -6.565110 | 2.543224 | -0.979794 |
| C | -5.128431 | -3.577424 | -0.874245 |
| C | -6.246300 | -2.968659 | -0.449761 |
| H | -5.232630 | -4.527335 | -1.400822 |
| H | -7.225390 | -3.391691 | -0.655542 |
| H | -6.210192 | -2.058040 | 0.138582 |
| C | -4.227449 | 4.341326 | -0.742235 |

| | | | |
|---|---|---|---|
| C | -5.225093 | 4.904323 | -1.445252 |
| H | -3.650606 | 4.993855 | -0.086914 |
| H | -5.451905 | 5.961018 | -1.339556 |
| H | -5.824178 | 4.345109 | -2.154998 |
| C | 4.483413 | -1.854122 | 0.495402 |
| C | 5.058182 | -1.688157 | -0.936104 |
| H | 4.902002 | -2.761205 | 0.945947 |
| H | 4.813966 | -1.016119 | 1.116759 |
| H | 4.715995 | -2.502569 | -1.576334 |
| H | 4.701392 | -0.744276 | -1.363974 |
| C | 3.513332 | 3.474188 | 0.808249 |
| C | 4.435499 | 3.482187 | -0.441838 |
| H | 3.987507 | 2.867534 | 1.586327 |
| H | 3.476989 | 4.495636 | 1.199316 |
| H | 3.876447 | 3.758096 | -1.337018 |
| H | 5.230176 | 4.224289 | -0.289098 |
| C | 6.557912 | -1.676613 | -0.986506 |
| O | 7.284746 | -2.398679 | -1.627891 |
| O | 7.098572 | -0.706172 | -0.168549 |
| H | 8.060228 | -0.758176 | -0.294998 |
| C | 5.139429 | 2.173946 | -0.719115 |
| O | 5.160033 | 1.590585 | -1.784457 |
| O | 5.804058 | 1.724677 | 0.370583 |

| | | | |
|---|---|---|---|
| H | 6.251133 | 0.886728 | 0.125561 |
| O | -0.469575 | 0.049230 | -1.957464 |
| H | 0.026867 | -0.771650 | -3.767819 |
| C | -0.808777 | -0.222715 | 4.181363 |
| O | -2.211422 | -0.279847 | 3.925420 |
| C | -2.426613 | -0.297770 | 2.527769 |
| C | -1.183192 | -0.063667 | 1.825102 |
| C | -0.157880 | 0.262032 | 2.873961 |
| H | -0.637750 | 0.439930 | 5.037674 |
| H | 0.813652 | -0.205153 | 2.687849 |
| H | 0.021428 | 1.349234 | 2.898533 |
| O | -3.568078 | -0.479958 | 2.129237 |
| H | -0.450832 | -1.228483 | 4.450037 |

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**$^{5}$C**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.4989973

Zero-point correction= 0.712021 (Hartree/Particle)

Thermal correction to Energy= 0.762009

Thermal correction to Enthalpy= 0.762954

Thermal correction to Gibbs Free Energy= 0.626103

Sum of electronic and zero-point Energies= -2378.786976

Sum of electronic and thermal Energies= -2378.736988

Sum of electronic and thermal Enthalpies= -2378.736044

Sum of electronic and thermal Free Energies= -2378.872895

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.839629 | -0.056879 | -0.097591 |
| N | -2.016754 | -1.752891 | -0.333724 |
| C | -1.583116 | -3.041573 | -0.226851 |
| C | -2.698803 | -3.944983 | -0.449050 |
| C | -3.809172 | -3.156043 | -0.668234 |
| C | -3.345509 | -1.765361 | -0.615088 |
| C | -0.261032 | -3.432807 | 0.019554 |
| C | 0.855951 | -2.612736 | 0.194541 |
| N | 0.843656 | -1.246680 | 0.211568 |
| C | 2.122215 | -0.810153 | 0.383031 |
| C | 3.013054 | -1.963893 | 0.467008 |
| C | 2.226939 | -3.083469 | 0.351551 |
| C | 2.519062 | 0.528866 | 0.489869 |
| C | 1.707509 | 1.663783 | 0.389885 |
| N | 0.365770 | 1.639142 | 0.169333 |

| | | | |
|---|---|---|---|
| C | -0.086465 | 2.922824 | 0.128280 |
| C | 1.034762 | 3.834349 | 0.340053 |
| C | 2.151491 | 3.052921 | 0.507822 |
| C | -1.407091 | 3.316478 | -0.104055 |
| C | -2.515188 | 2.501743 | -0.368604 |
| C | -3.858735 | 2.979157 | -0.717879 |
| C | -4.617351 | 1.849902 | -0.959998 |
| C | -3.739574 | 0.707940 | -0.753117 |
| N | -2.498647 | 1.146917 | -0.399570 |
| C | -4.120532 | -0.631351 | -0.869168 |
| H | -0.077307 | -4.502542 | 0.045692 |
| H | -5.141500 | -0.816965 | -1.176880 |
| H | -1.581987 | 4.386988 | -0.129185 |
| H | 3.569031 | 0.702200 | 0.692064 |
| C | -0.068866 | -1.025607 | -2.698236 |
| H | -0.737029 | -1.902939 | -2.628234 |
| H | 0.940079 | -1.366605 | -2.402333 |
| C | 0.925698 | 5.327457 | 0.347329 |
| H | 0.625185 | 5.712611 | -0.635232 |
| H | 0.174075 | 5.672335 | 1.067627 |
| H | 1.875966 | 5.802530 | 0.608088 |
| C | 2.649425 | -4.519673 | 0.343998 |
| H | 2.099990 | -5.105009 | 1.091171 |

| | | | |
|---|---|---|---|
| H | 2.462793 | -4.990541 | -0.629420 |
| H | 3.716703 | -4.625750 | 0.560135 |
| C | -2.624441 | -5.438048 | -0.380932 |
| H | -1.825974 | -5.830250 | -1.022364 |
| H | -2.416043 | -5.785459 | 0.639169 |
| H | -3.564132 | -5.900501 | -0.695242 |
| C | -6.069495 | 1.772801 | -1.306455 |
| H | -6.241649 | 1.847926 | -2.388895 |
| H | -6.508193 | 0.828435 | -0.971999 |
| H | -6.623110 | 2.591312 | -0.834534 |
| C | -5.171753 | -3.628680 | -0.874948 |
| C | -6.296139 | -3.036503 | -0.443556 |
| H | -5.267306 | -4.576387 | -1.407260 |
| H | -7.270422 | -3.470409 | -0.649238 |
| H | -6.270899 | -2.128734 | 0.149594 |
| C | -4.248503 | 4.377441 | -0.744857 |
| C | -5.273121 | 4.934267 | -1.413799 |
| H | -3.627482 | 5.042730 | -0.144875 |
| H | -5.475372 | 5.998201 | -1.333763 |
| H | -5.919448 | 4.363126 | -2.070406 |
| C | 4.507367 | -1.892893 | 0.520968 |
| C | 5.099676 | -1.723042 | -0.903083 |
| H | 4.916420 | -2.804345 | 0.971801 |

| | | | |
|---|---|---|---|
| H | 4.835571 | -1.059112 | 1.149450 |
| H | 4.771650 | -2.540033 | -1.547428 |
| H | 4.742733 | -0.781078 | -1.334965 |
| C | 3.554690 | 3.523205 | 0.749816 |
| C | 4.475575 | 3.484251 | -0.500305 |
| H | 4.029521 | 2.943820 | 1.548261 |
| H | 3.520688 | 4.558427 | 1.103465 |
| H | 3.919149 | 3.742910 | -1.402280 |
| H | 5.280442 | 4.219404 | -0.368448 |
| C | 6.599785 | -1.701743 | -0.931001 |
| O | 7.342043 | -2.429528 | -1.547888 |
| O | 7.119848 | -0.713417 | -0.121207 |
| H | 8.083938 | -0.761319 | -0.229294 |
| C | 5.160976 | 2.159153 | -0.741932 |
| O | 5.170400 | 1.545768 | -1.790497 |
| O | 5.823443 | 1.732405 | 0.357915 |
| H | 6.261596 | 0.883798 | 0.134739 |
| O | -0.516605 | 0.057305 | -1.950871 |
| H | -0.014459 | -0.743712 | -3.764471 |
| C | -0.758485 | -0.199052 | 4.165856 |
| O | -2.165043 | -0.281170 | 3.933333 |
| C | -2.404689 | -0.309136 | 2.542038 |
| C | -1.172001 | -0.056476 | 1.826834 |

| | | | |
|---|---|---|---|
| C | -0.139342 | 0.310571 | 2.853301 |
| H | -0.586361 | 0.459530 | 5.024565 |
| H | 0.844076 | -0.123510 | 2.654752 |
| H | -0.000438 | 1.403039 | 2.877245 |
| O | -3.546582 | -0.513090 | 2.160737 |
| H | -0.376976 | -1.200185 | 4.417375 |

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**$^{CSS}$TS(C-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.415886

Zero-point correction= 0.944282 (Hartree/Particle)

Thermal correction to Energy= 1.004583

Thermal correction to Enthalpy= 1.005528

Thermal correction to Gibbs Free Energy= 0.850399

Sum of electronic and zero-point Energies= -2823.471604

Sum of electronic and thermal Energies= -2823.411303

Sum of electronic and thermal Enthalpies= -2823.410358

Sum of electronic and thermal Free Energies= -2823.565487

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.090560 | 0.316219 | -0.731988 |
| N | -1.437938 | -1.048666 | -1.411346 |
| C | -1.283184 | -2.414381 | -1.463294 |
| C | -2.459660 | -3.044318 | -2.025589 |
| C | -3.335867 | -2.024154 | -2.339058 |
| C | -2.660571 | -0.782217 | -1.960825 |
| C | -0.136602 | -3.100754 | -1.077519 |
| C | 1.032967 | -2.525128 | -0.599308 |
| N | 1.224083 | -1.187450 | -0.378779 |
| C | 2.499797 | -1.051622 | 0.090627 |
| C | 3.152210 | -2.353620 | 0.164981 |
| C | 2.234063 | -3.274627 | -0.263438 |
| C | 3.087341 | 0.141827 | 0.494104 |
| C | 2.520587 | 1.404077 | 0.388213 |
| N | 1.281602 | 1.666299 | -0.122110 |
| C | 1.142072 | 3.021582 | -0.112001 |
| C | 2.327341 | 3.656345 | 0.451658 |
| C | 3.188671 | 2.646274 | 0.774084 |
| C | 0.038986 | 3.718783 | -0.577646 |
| C | -1.103087 | 3.154566 | -1.129085 |
| C | -2.229535 | 3.922461 | -1.657996 |
| C | -3.149917 | 2.994674 | -2.100484 |

| | | | |
|---|---|---|---|
| C | -2.573358 | 1.690741 | -1.829538 |
| N | -1.346813 | 1.816343 | -1.228778 |
| C | -3.197407 | 0.487030 | -2.138426 |
| H | -0.147455 | -4.180492 | -1.174827 |
| H | -4.189162 | 0.548064 | -2.570188 |
| H | 0.076764 | 4.799884 | -0.507811 |
| H | 4.077566 | 0.080189 | 0.927677 |
| C | 0.754961 | -0.480247 | -3.400766 |
| H | 1.289905 | -1.388613 | -3.052440 |
| H | 1.282192 | -0.149144 | -4.317094 |
| C | 2.497941 | 5.132389 | 0.625242 |
| H | 2.473931 | 5.657067 | -0.338226 |
| H | 1.696551 | 5.556164 | 1.242398 |
| H | 3.450347 | 5.374289 | 1.105795 |
| C | 2.396995 | -4.754151 | -0.420694 |
| H | 1.613025 | -5.306589 | 0.111775 |
| H | 2.340695 | -5.056924 | -1.473898 |
| H | 3.361898 | -5.093872 | -0.032761 |
| C | -2.630308 | -4.511302 | -2.261625 |
| H | -1.666395 | -5.007920 | -2.405268 |
| H | -3.130667 | -5.012342 | -1.420922 |
| H | -3.239561 | -4.691247 | -3.153078 |
| C | -4.458879 | 3.240005 | -2.781188 |

| | | | |
|---|---|---|---|
| H | -4.433220 | 4.182602 | -3.336879 |
| H | -4.698135 | 2.437501 | -3.485602 |
| H | -5.293506 | 3.307159 | -2.069454 |
| C | -4.652668 | -2.090524 | -2.946355 |
| C | -5.503093 | -3.132173 | -2.958470 |
| H | -4.979787 | -1.179473 | -3.446203 |
| H | -6.461126 | -3.060041 | -3.464056 |
| H | -5.289479 | -4.068630 | -2.455874 |
| C | -2.285217 | 5.373314 | -1.706953 |
| C | -3.384344 | 6.146503 | -1.726634 |
| H | -1.318996 | 5.876517 | -1.727919 |
| H | -3.303382 | 7.227781 | -1.785262 |
| H | -4.385516 | 5.734805 | -1.661713 |
| C | 4.590509 | -2.582279 | 0.510359 |
| C | 5.492124 | -2.386732 | -0.736414 |
| H | 4.729401 | -3.598802 | 0.896277 |
| H | 4.915975 | -1.901417 | 1.302661 |
| H | 5.163350 | -3.039077 | -1.546756 |
| H | 5.414937 | -1.349177 | -1.081335 |
| C | 4.544934 | 2.776739 | 1.398776 |
| C | 5.732194 | 2.709157 | 0.399342 |
| H | 4.694213 | 2.016997 | 2.172301 |
| H | 4.598744 | 3.743416 | 1.909170 |

| | | | |
|---|---|---|---|
| H | 5.475045 | 3.194722 | -0.543109 |
| H | 6.591431 | 3.234740 | 0.836573 |
| C | 6.942833 | -2.676729 | -0.485977 |
| O | 7.660933 | -3.443513 | -1.084247 |
| O | 7.443179 | -1.950972 | 0.575016 |
| H | 8.385437 | -2.179753 | 0.631606 |
| C | 6.216545 | 1.313415 | 0.084837 |
| O | 6.369962 | 0.847950 | -1.027030 |
| O | 6.513370 | 0.622845 | 1.210137 |
| H | 6.840590 | -0.261481 | 0.940932 |
| O | 0.724324 | 0.538419 | -2.471799 |
| H | -0.250064 | -0.823485 | -3.726377 |
| C | -0.773139 | 0.124182 | 1.139693 |
| C | -0.877171 | -1.243926 | 1.801915 |
| C | -0.181626 | 0.952958 | 2.232910 |
| C | 0.339827 | -1.240883 | 2.734153 |
| H | -0.869120 | -2.076203 | 1.102845 |
| H | -1.785585 | -1.325999 | 2.408560 |
| H | -3.513361 | -1.334006 | 0.292184 |
| O | -0.253097 | 2.145126 | 2.462786 |
| O | 0.525850 | 0.142889 | 3.103661 |
| H | 1.241271 | -1.596421 | 2.231852 |
| H | 0.190198 | -1.808453 | 3.658382 |

| | | | |
|---|---|---|---|
| C | -4.146663 | -1.742888 | 1.065266 |
| C | -4.316237 | -1.066230 | 2.290035 |
| C | -4.756414 | -2.972962 | 0.846011 |
| C | -5.088295 | -1.688491 | 3.290805 |
| N | -3.736078 | 0.200848 | 2.500232 |
| C | -5.534057 | -3.577992 | 1.834990 |
| H | -4.606352 | -3.453096 | -0.114245 |
| C | -5.686044 | -2.925663 | 3.058403 |
| H | -5.234697 | -1.210441 | 4.251009 |
| C | -3.264078 | 0.952356 | 1.419110 |
| C | -3.603646 | 0.710847 | 3.868812 |
| H | -6.003249 | -4.541235 | 1.659224 |
| H | -6.280610 | -3.377436 | 3.848310 |
| H | -3.708489 | 0.629470 | 0.480799 |
| C | -3.191120 | 2.453380 | 1.561520 |
| H | -3.276104 | 1.745388 | 3.800808 |
| H | -4.596145 | 0.729475 | 4.336398 |
| C | -2.616068 | -0.065828 | 4.745673 |
| H | -2.339258 | 2.771411 | 2.166406 |
| H | -3.062845 | 2.890812 | 0.573581 |
| H | -4.123351 | 2.845402 | 1.991578 |
| H | -2.840158 | -1.135741 | 4.751730 |
| H | -1.591117 | 0.077129 | 4.399355 |

H -2.679323 0.301337 5.776124

H -1.950735 0.587207 1.020522

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**$^{CSS}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.4317063

Zero-point correction= 0.943681 (Hartree/Particle)

Thermal correction to Energy= 1.004259

Thermal correction to Enthalpy= 1.005204

Thermal correction to Gibbs Free Energy= 0.849096

Sum of electronic and zero-point Energies= -2823.488025

Sum of electronic and thermal Energies= -2823.427447

Sum of electronic and thermal Enthalpies= -2823.426503

Sum of electronic and thermal Free Energies= -2823.582610

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Cartesian Coordinates

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Fe -0.071448 0.318727 -0.778594

N -1.417546 -1.051825 -1.440676

C -1.258743 -2.414829 -1.505817

| | | | |
|---|---|---|---|
| C | -2.438983 | -3.041735 | -2.061835 |
| C | -3.320248 | -2.020597 | -2.354434 |
| C | -2.645851 | -0.781025 | -1.972269 |
| C | -0.106816 | -3.099514 | -1.138184 |
| C | 1.055099 | -2.518085 | -0.651900 |
| N | 1.235700 | -1.180291 | -0.415648 |
| C | 2.502570 | -1.039842 | 0.077418 |
| C | 3.159167 | -2.337318 | 0.149807 |
| C | 2.255038 | -3.259781 | -0.306036 |
| C | 3.082996 | 0.153348 | 0.490032 |
| C | 2.517882 | 1.414463 | 0.370631 |
| N | 1.289178 | 1.678387 | -0.161868 |
| C | 1.142965 | 3.033362 | -0.142211 |
| C | 2.319150 | 3.665752 | 0.438521 |
| C | 3.176889 | 2.655648 | 0.770205 |
| C | 0.038944 | 3.732200 | -0.599182 |
| C | -1.107768 | 3.163778 | -1.133507 |
| C | -2.244379 | 3.924428 | -1.647154 |
| C | -3.162381 | 2.991945 | -2.082768 |
| C | -2.574271 | 1.690951 | -1.823190 |
| N | -1.344256 | 1.826366 | -1.236650 |
| C | -3.190635 | 0.485878 | -2.136343 |
| H | -0.111243 | -4.177965 | -1.244709 |

| | | | |
|---|---|---|---|
| H | -4.188192 | 0.542406 | -2.554067 |
| H | 0.072670 | 4.812323 | -0.521040 |
| H | 4.064598 | 0.092310 | 0.941810 |
| C | 0.834056 | -0.493573 | -3.402919 |
| H | 1.512812 | -1.282298 | -3.025791 |
| H | 1.279193 | -0.115696 | -4.341204 |
| C | 2.479652 | 5.140446 | 0.630836 |
| H | 2.444897 | 5.678004 | -0.324904 |
| H | 1.678987 | 5.546787 | 1.260061 |
| H | 3.433295 | 5.382564 | 1.108259 |
| C | 2.428703 | -4.737508 | -0.468500 |
| H | 1.644090 | -5.295944 | 0.056103 |
| H | 2.382902 | -5.035988 | -1.523246 |
| H | 3.392496 | -5.072112 | -0.074083 |
| C | -2.608488 | -4.507204 | -2.306118 |
| H | -1.646746 | -4.997185 | -2.483962 |
| H | -3.079463 | -5.015993 | -1.453867 |
| H | -3.244437 | -4.681980 | -3.179558 |
| C | -4.484907 | 3.229871 | -2.738377 |
| H | -4.477776 | 4.176431 | -3.287602 |
| H | -4.731142 | 2.430134 | -3.443298 |
| H | -5.304035 | 3.284174 | -2.008379 |
| C | -4.643062 | -2.084658 | -2.951745 |

| | | | |
|---|---|---|---|
| C | -5.496736 | -3.122179 | -2.938931 |
| H | -4.968005 | -1.179477 | -3.463199 |
| H | -6.459397 | -3.054645 | -3.436185 |
| H | -5.283640 | -4.048122 | -2.417278 |
| C | -2.311044 | 5.375654 | -1.687065 |
| C | -3.417216 | 6.137893 | -1.682866 |
| H | -1.349585 | 5.886905 | -1.721840 |
| H | -3.347459 | 7.220195 | -1.735173 |
| H | -4.412757 | 5.716049 | -1.600835 |
| C | 4.590851 | -2.564301 | 0.523179 |
| C | 5.515258 | -2.380245 | -0.708454 |
| H | 4.720200 | -3.577825 | 0.919648 |
| H | 4.901827 | -1.878219 | 1.316412 |
| H | 5.198839 | -3.036926 | -1.520227 |
| H | 5.449826 | -1.344168 | -1.060320 |
| C | 4.520967 | 2.784864 | 1.420610 |
| C | 5.725865 | 2.724869 | 0.441964 |
| H | 4.656453 | 2.021317 | 2.192749 |
| H | 4.563028 | 3.748510 | 1.937229 |
| H | 5.487008 | 3.221992 | -0.499290 |
| H | 6.578441 | 3.241767 | 0.901289 |
| C | 6.959708 | -2.676136 | -0.428537 |
| O | 7.681932 | -3.456930 | -1.002825 |

| | | | |
|---|---|---|---|
| O | 7.445304 | -1.936448 | 0.628905 |
| H | 8.384304 | -2.171243 | 0.710094 |
| C | 6.206737 | 1.329253 | 0.121947 |
| O | 6.352529 | 0.864847 | -0.991514 |
| O | 6.504402 | 0.636826 | 1.245291 |
| H | 6.833039 | -0.247183 | 0.976903 |
| O | 0.660397 | 0.553229 | -2.510944 |
| H | -0.111914 | -0.997747 | -3.678898 |
| C | -0.779337 | 0.135539 | 1.132490 |
| C | -0.817677 | -1.236809 | 1.802212 |
| C | -0.206927 | 1.003630 | 2.181083 |
| C | 0.348484 | -1.156921 | 2.794321 |
| H | -0.719029 | -2.075264 | 1.116979 |
| H | -1.752766 | -1.379393 | 2.354659 |
| H | -3.591523 | -1.318190 | 0.287895 |
| O | -0.260982 | 2.210360 | 2.346312 |
| O | 0.459571 | 0.237339 | 3.138577 |
| H | 1.290068 | -1.486162 | 2.344535 |
| H | 0.180867 | -1.713976 | 3.722530 |
| C | -4.159979 | -1.784037 | 1.077960 |
| C | -4.337816 | -1.123326 | 2.315134 |
| C | -4.671342 | -3.059432 | 0.869672 |
| C | -5.017976 | -1.826352 | 3.335549 |

| | | | |
|---|---|---|---|
| N | -3.860046 | 0.172913 | 2.512757 |
| C | -5.360770 | -3.737708 | 1.876767 |
| H | -4.512866 | -3.520710 | -0.099116 |
| C | -5.519182 | -3.106120 | 3.110850 |
| H | -5.164189 | -1.375591 | 4.308853 |
| C | -3.362851 | 0.931781 | 1.407584 |
| C | -3.752385 | 0.692096 | 3.874733 |
| H | -5.752890 | -4.736289 | 1.708567 |
| H | -6.042388 | -3.611880 | 3.919010 |
| H | -3.871391 | 0.634756 | 0.492111 |
| C | -3.328400 | 2.435652 | 1.571149 |
| H | -3.549186 | 1.758610 | 3.806899 |
| H | -4.727950 | 0.600029 | 4.369933 |
| C | -2.663258 | 0.028315 | 4.725477 |
| H | -2.523852 | 2.762576 | 2.233027 |
| H | -3.132530 | 2.884473 | 0.598404 |
| H | -4.290633 | 2.826625 | 1.934253 |
| H | -2.785421 | -1.058187 | 4.748386 |
| H | -1.668795 | 0.257103 | 4.338080 |
| H | -2.721113 | 0.399154 | 5.755608 |
| H | -2.065654 | 0.567339 | 1.094646 |

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**$^3$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.4263262

Zero-point correction= 0.943241 (Hartree/Particle)

Thermal correction to Energy= 1.004044

Thermal correction to Enthalpy= 1.004988

Thermal correction to Gibbs Free Energy= 0.846785

Sum of electronic and zero-point Energies= -2823.483085

Sum of electronic and thermal Energies= -2823.422282

Sum of electronic and thermal Enthalpies= -2823.421338

Sum of electronic and thermal Free Energies= -2823.579541

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.054012 | 0.297172 | -0.827036 |
| N | -1.395722 | -1.098297 | -1.446859 |
| C | -1.221150 | -2.458416 | -1.502534 |
| C | -2.400172 | -3.103858 | -2.037657 |
| C | -3.296844 | -2.095059 | -2.329018 |
| C | -2.633983 | -0.845357 | -1.963590 |
| C | -0.056964 | -3.125427 | -1.135563 |

| | | | |
|---|---|---|---|
| C | 1.094916 | -2.525180 | -0.653421 |
| N | 1.261016 | -1.181093 | -0.431678 |
| C | 2.519793 | -1.025402 | 0.076677 |
| C | 3.187597 | -2.315482 | 0.170275 |
| C | 2.298424 | -3.251005 | -0.287741 |
| C | 3.084659 | 0.177867 | 0.480816 |
| C | 2.506725 | 1.430241 | 0.337719 |
| N | 1.281452 | 1.673708 | -0.213601 |
| C | 1.116871 | 3.028841 | -0.205379 |
| C | 2.279437 | 3.679289 | 0.379561 |
| C | 3.144913 | 2.682408 | 0.731385 |
| C | 0.008149 | 3.712792 | -0.670337 |
| C | -1.136479 | 3.126286 | -1.191250 |
| C | -2.290567 | 3.868628 | -1.695393 |
| C | -3.205117 | 2.920156 | -2.100718 |
| C | -2.594943 | 1.629299 | -1.836576 |
| N | -1.356994 | 1.787276 | -1.274537 |
| C | -3.198578 | 0.413185 | -2.127635 |
| H | -0.048160 | -4.204801 | -1.230564 |
| H | -4.203528 | 0.452158 | -2.529167 |
| H | 0.031277 | 4.793779 | -0.602111 |
| H | 4.060161 | 0.132821 | 0.947002 |
| C | 0.973514 | -0.545675 | -3.381898 |

| | | | |
|---|---|---|---|
| H | 1.828668 | -1.107910 | -2.963360 |
| H | 1.287685 | -0.172559 | -4.372632 |
| C | 2.419672 | 5.157179 | 0.562978 |
| H | 2.377247 | 5.688668 | -0.395742 |
| H | 1.613708 | 5.555462 | 1.190493 |
| H | 3.369954 | 5.414939 | 1.038702 |
| C | 2.486453 | -4.729251 | -0.427839 |
| H | 1.706282 | -5.286770 | 0.104265 |
| H | 2.445116 | -5.044117 | -1.477924 |
| H | 3.452654 | -5.048587 | -0.026895 |
| C | -2.561017 | -4.573708 | -2.258420 |
| H | -1.595326 | -5.067182 | -2.400047 |
| H | -3.056352 | -5.064024 | -1.409242 |
| H | -3.172797 | -4.766964 | -3.145450 |
| C | -4.543811 | 3.133619 | -2.731025 |
| H | -4.560270 | 4.073468 | -3.291448 |
| H | -4.795359 | 2.322401 | -3.420755 |
| H | -5.347092 | 3.186576 | -1.983678 |
| C | -4.624136 | -2.178871 | -2.913722 |
| C | -5.456441 | -3.233838 | -2.910890 |
| H | -4.973590 | -1.272906 | -3.406823 |
| H | -6.425717 | -3.175625 | -3.396197 |
| H | -5.219989 | -4.165289 | -2.409833 |

| | | | |
|---|---|---|---|
| C | -2.374086 | 5.318456 | -1.750412 |
| C | -3.488483 | 6.068362 | -1.733869 |
| H | -1.419095 | 5.839662 | -1.809153 |
| H | -3.431977 | 7.150667 | -1.799961 |
| H | -4.477349 | 5.636418 | -1.627627 |
| C | 4.616088 | -2.524877 | 0.565413 |
| C | 5.554723 | -2.349499 | -0.656857 |
| H | 4.748833 | -3.531732 | 0.977267 |
| H | 4.910455 | -1.825387 | 1.353177 |
| H | 5.254274 | -3.020150 | -1.463263 |
| H | 5.485588 | -1.318690 | -1.023210 |
| C | 4.479011 | 2.833884 | 1.397180 |
| C | 5.696307 | 2.778772 | 0.433582 |
| H | 4.613219 | 2.079324 | 2.178227 |
| H | 4.503161 | 3.802691 | 1.904984 |
| H | 5.464070 | 3.267270 | -0.513840 |
| H | 6.538296 | 3.306283 | 0.899983 |
| C | 6.997426 | -2.630418 | -0.353206 |
| O | 7.730733 | -3.420020 | -0.900718 |
| O | 7.465346 | -1.863758 | 0.692623 |
| H | 8.404139 | -2.091904 | 0.792902 |
| C | 6.191322 | 1.384488 | 0.129811 |
| O | 6.339689 | 0.907388 | -0.978021 |

| | | | |
|---|---|---|---|
| O | 6.495702 | 0.709510 | 1.261591 |
| H | 6.832820 | -0.175006 | 1.005857 |
| O | 0.577104 | 0.519679 | -2.584965 |
| H | 0.165105 | -1.279957 | -3.556083 |
| C | -0.796762 | 0.122165 | 1.140258 |
| C | -0.848295 | -1.259398 | 1.789988 |
| C | -0.171369 | 0.960798 | 2.174827 |
| C | 0.322122 | -1.217259 | 2.781218 |
| H | -0.764751 | -2.089493 | 1.091938 |
| H | -1.785331 | -1.399305 | 2.340935 |
| H | -3.671034 | -1.218634 | 0.297119 |
| O | -0.170900 | 2.170302 | 2.341590 |
| O | 0.473084 | 0.169448 | 3.133495 |
| H | 1.253666 | -1.571320 | 2.327252 |
| H | 0.141554 | -1.776840 | 3.705781 |
| C | -4.225263 | -1.688950 | 1.094602 |
| C | -4.377016 | -1.034416 | 2.339696 |
| C | -4.741592 | -2.962673 | 0.888052 |
| C | -5.041554 | -1.744095 | 3.367210 |
| N | -3.891551 | 0.256218 | 2.536982 |
| C | -5.414353 | -3.646259 | 1.903029 |
| H | -4.601418 | -3.418952 | -0.086145 |
| C | -5.549649 | -3.021026 | 3.143274 |

| | | | |
|---|---|---|---|
| H | -5.168120 | -1.300460 | 4.346548 |
| C | -3.368437 | 1.004533 | 1.428485 |
| C | -3.755668 | 0.763892 | 3.899879 |
| H | -5.810823 | -4.643393 | 1.736098 |
| H | -6.059153 | -3.530681 | 3.957888 |
| H | -3.909245 | 0.741258 | 0.520187 |
| C | -3.275635 | 2.504887 | 1.605996 |
| H | -3.553657 | 1.831179 | 3.837238 |
| H | -4.721089 | 0.668857 | 4.414093 |
| C | -2.650747 | 0.091474 | 4.723415 |
| H | -2.455531 | 2.792817 | 2.267592 |
| H | -3.062598 | 2.952417 | 0.635795 |
| H | -4.218618 | 2.936446 | 1.974210 |
| H | -2.780272 | -0.994237 | 4.746330 |
| H | -1.663786 | 0.312258 | 4.312950 |
| H | -2.680875 | 0.459772 | 5.755796 |
| H | -2.098246 | 0.597107 | 1.124326 |

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**$^{5}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.4115821

Zero-point correction= 0.940544 (Hartree/Particle)

Thermal correction to Energy= 1.002127

Thermal correction to Enthalpy= 1.003071

Thermal correction to Gibbs Free Energy= 0.842195

Sum of electronic and zero-point Energies= -2823.471038

Sum of electronic and thermal Energies= -2823.409455

Sum of electronic and thermal Enthalpies= -2823.408511

Sum of electronic and thermal Free Energies= -2823.569387

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.074938 | 0.279065 | -0.815887 |
| N | -1.522501 | -1.152143 | -1.426292 |
| C | -1.315459 | -2.495432 | -1.522626 |
| C | -2.486145 | -3.131838 | -2.105657 |
| C | -3.385922 | -2.117504 | -2.382706 |
| C | -2.734345 | -0.869331 | -1.967537 |
| C | -0.129523 | -3.144991 | -1.152396 |
| C | 1.042151 | -2.570983 | -0.649580 |
| N | 1.241222 | -1.241882 | -0.396519 |
| C | 2.501189 | -1.087550 | 0.106110 |
| C | 3.149652 | -2.392923 | 0.174977 |

| | | | |
|---|---|---|---|
| C | 2.244665 | -3.313108 | -0.293998 |
| C | 3.087559 | 0.121520 | 0.500090 |
| C | 2.561362 | 1.409127 | 0.351446 |
| N | 1.359130 | 1.678655 | -0.219760 |
| C | 1.174482 | 3.024087 | -0.215146 |
| C | 2.337250 | 3.668209 | 0.389586 |
| C | 3.199754 | 2.664139 | 0.750820 |
| C | 0.038083 | 3.683806 | -0.685315 |
| C | -1.138120 | 3.120599 | -1.195215 |
| C | -2.283643 | 3.882432 | -1.706424 |
| C | -3.223443 | 2.949833 | -2.103540 |
| C | -2.646410 | 1.640897 | -1.831585 |
| N | -1.412003 | 1.793183 | -1.271596 |
| C | -3.263331 | 0.417210 | -2.120459 |
| H | -0.112263 | -4.223060 | -1.274173 |
| H | -4.260818 | 0.478308 | -2.541190 |
| H | 0.060618 | 4.766613 | -0.622925 |
| H | 4.061586 | 0.048485 | 0.968640 |
| C | 1.816476 | 0.144676 | -2.978026 |
| H | 2.572561 | 0.705585 | -2.401239 |
| H | 1.954226 | 0.416027 | -4.039324 |
| C | 2.485106 | 5.144487 | 0.581430 |
| H | 2.452140 | 5.680045 | -0.375504 |

| | | | |
|---|---|---|---|
| H | 1.674586 | 5.543487 | 1.202736 |
| H | 3.431988 | 5.397880 | 1.066577 |
| C | 2.422271 | -4.790748 | -0.455384 |
| H | 1.640870 | -5.349693 | 0.073512 |
| H | 2.370596 | -5.090092 | -1.509582 |
| H | 3.388549 | -5.124199 | -0.066049 |
| C | -2.636373 | -4.594399 | -2.376589 |
| H | -1.664443 | -5.076351 | -2.517652 |
| H | -3.140597 | -5.115050 | -1.550628 |
| H | -3.234314 | -4.764656 | -3.277890 |
| C | -4.557660 | 3.195712 | -2.731870 |
| H | -4.545317 | 4.121069 | -3.316518 |
| H | -4.841616 | 2.375873 | -3.398518 |
| H | -5.354563 | 3.296462 | -1.982506 |
| C | -4.706051 | -2.193829 | -2.982724 |
| C | -5.536049 | -3.250756 | -3.008261 |
| H | -5.054290 | -1.276184 | -3.455671 |
| H | -6.502547 | -3.185431 | -3.498352 |
| H | -5.298728 | -4.191950 | -2.525732 |
| C | -2.336727 | 5.332566 | -1.782772 |
| C | -3.432680 | 6.109894 | -1.781462 |
| H | -1.369487 | 5.830762 | -1.842784 |
| H | -3.348680 | 7.189652 | -1.859602 |

| | | | |
|---|---|---|---|
| H | -4.432729 | 5.704476 | -1.676002 |
| C | 4.580915 | -2.624948 | 0.546957 |
| C | 5.505928 | -2.414978 | -0.680657 |
| H | 4.714376 | -3.644578 | 0.925902 |
| H | 4.888865 | -1.950712 | 1.351880 |
| H | 5.199052 | -3.066533 | -1.500159 |
| H | 5.428152 | -1.375557 | -1.019893 |
| C | 4.530102 | 2.814234 | 1.424300 |
| C | 5.749797 | 2.739227 | 0.465374 |
| H | 4.655410 | 2.062933 | 2.210355 |
| H | 4.562838 | 3.786843 | 1.924747 |
| H | 5.535721 | 3.252618 | -0.473200 |
| H | 6.606223 | 3.229566 | 0.945481 |
| C | 6.952219 | -2.697536 | -0.397517 |
| O | 7.680593 | -3.480320 | -0.961199 |
| O | 7.430467 | -1.941711 | 0.651838 |
| H | 8.370415 | -2.170130 | 0.739884 |
| C | 6.194146 | 1.333396 | 0.137571 |
| O | 6.294613 | 0.859562 | -0.977006 |
| O | 6.507818 | 0.641519 | 1.256326 |
| H | 6.812575 | -0.250573 | 0.986569 |
| O | 0.511671 | 0.440491 | -2.593115 |
| H | 2.066650 | -0.927540 | -2.883049 |

| | | | |
|---|---|---|---|
| C | -0.816533 | 0.143031 | 1.141762 |
| C | -0.859963 | -1.236093 | 1.793596 |
| C | -0.157625 | 0.984344 | 2.166156 |
| C | 0.315947 | -1.198885 | 2.777957 |
| H | -0.793062 | -2.068272 | 1.096490 |
| H | -1.796263 | -1.360455 | 2.349261 |
| H | -3.692661 | -1.183926 | 0.298158 |
| O | -0.157463 | 2.191687 | 2.326734 |
| O | 0.488415 | 0.190989 | 3.113137 |
| H | 1.240538 | -1.570489 | 2.326683 |
| H | 0.128290 | -1.741915 | 3.710454 |
| C | -4.245226 | -1.659511 | 1.093520 |
| C | -4.393828 | -1.015618 | 2.344129 |
| C | -4.763336 | -2.931097 | 0.876735 |
| C | -5.054002 | -1.733611 | 3.368134 |
| N | -3.908981 | 0.275718 | 2.550460 |
| C | -5.432797 | -3.622639 | 1.888487 |
| H | -4.626085 | -3.378190 | -0.102447 |
| C | -5.563069 | -3.008708 | 3.134726 |
| H | -5.176982 | -1.299004 | 4.351995 |
| C | -3.380368 | 1.029075 | 1.448953 |
| C | -3.773431 | 0.774821 | 3.916116 |
| H | -5.830670 | -4.617955 | 1.714382 |

| | | | |
|---|---|---|---|
| H | -6.069315 | -3.525589 | 3.946762 |
| H | -3.915618 | 0.771485 | 0.535823 |
| C | -3.283467 | 2.528744 | 1.631026 |
| H | -3.585113 | 1.845185 | 3.861063 |
| H | -4.735013 | 0.664197 | 4.433572 |
| C | -2.657275 | 0.108378 | 4.729526 |
| H | -2.473857 | 2.814053 | 2.306555 |
| H | -3.052774 | 2.976333 | 0.664604 |
| H | -4.230240 | 2.962737 | 1.985749 |
| H | -2.777086 | -0.978597 | 4.746565 |
| H | -1.674776 | 0.340475 | 4.314313 |
| H | -2.683221 | 0.470220 | 5.764178 |
| H | -2.119811 | 0.622596 | 1.140774 |

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**$^{OSS}$D**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2824.4564687

Zero-point correction= 0.946947 (Hartree/Particle)

Thermal correction to Energy= 1.008916

Thermal correction to Enthalpy= 1.009861

Thermal correction to Gibbs Free Energy= 0.848394

Sum of electronic and zero-point Energies= -2823.509521

Sum of electronic and thermal Energies= -2823.447552

Sum of electronic and thermal Enthalpies= -2823.446608

Sum of electronic and thermal Free Energies= -2823.608075

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.029685 | -0.102297 | -0.848847 |
| N | 1.230311 | 1.448938 | -1.370769 |
| C | 0.938697 | 2.788433 | -1.309160 |
| C | 2.056810 | 3.576927 | -1.780422 |
| C | 3.041125 | 2.678114 | -2.138266 |
| C | 2.490001 | 1.349658 | -1.883814 |
| C | -0.270606 | 3.318673 | -0.875427 |
| C | -1.354157 | 2.581175 | -0.424224 |
| N | -1.393461 | 1.215036 | -0.303705 |
| C | -2.627118 | 0.905413 | 0.196801 |
| C | -3.407086 | 2.117698 | 0.395047 |
| C | -2.612679 | 3.163366 | 0.005068 |
| C | -3.075999 | -0.372388 | 0.509888 |
| C | -2.394815 | -1.553720 | 0.257269 |
| N | -1.162036 | -1.641595 | -0.323214 |

| | | | |
|---|---|---|---|
| C | -0.895033 | -2.973023 | -0.464116 |
| C | -1.992707 | -3.770446 | 0.061717 |
| C | -2.925426 | -2.886616 | 0.527212 |
| C | 0.257615 | -3.514963 | -1.004951 |
| C | 1.349426 | -2.789231 | -1.458303 |
| C | 2.571773 | -3.381867 | -1.997495 |
| C | 3.405992 | -2.327563 | -2.298669 |
| C | 2.679824 | -1.121389 | -1.943569 |
| N | 1.449852 | -1.433497 | -1.430304 |
| C | 3.172135 | 0.163887 | -2.129570 |
| H | -0.375863 | 4.397232 | -0.884129 |
| H | 4.180003 | 0.248707 | -2.517161 |
| H | 0.323484 | -4.595641 | -1.041735 |
| H | -4.046662 | -0.451971 | 0.981931 |
| C | -1.086095 | 0.858711 | -3.328370 |
| H | -1.926962 | 1.401255 | -2.856625 |
| H | -1.434354 | 0.535250 | -4.325543 |
| C | -2.016834 | -5.265993 | 0.087855 |
| H | -1.965394 | -5.687942 | -0.923471 |
| H | -1.164147 | -5.665760 | 0.649215 |
| H | -2.930088 | -5.645221 | 0.554886 |
| C | -2.938348 | 4.624053 | -0.022493 |
| H | -2.199022 | 5.212626 | 0.533895 |

| | | | |
|---|---|---|---|
| H | -2.953464 | 5.015621 | -1.047247 |
| H | -3.919053 | 4.822719 | 0.419266 |
| C | 2.088645 | 5.068626 | -1.872795 |
| H | 1.088103 | 5.482522 | -2.029367 |
| H | 2.491519 | 5.527953 | -0.959573 |
| H | 2.723398 | 5.391091 | -2.704078 |
| C | 4.776019 | -2.370187 | -2.895062 |
| H | 4.892268 | -3.251275 | -3.533650 |
| H | 4.977825 | -1.482186 | -3.501520 |
| H | 5.557027 | -2.422244 | -2.123830 |
| C | 4.364907 | 2.927769 | -2.683578 |
| C | 5.114570 | 4.031426 | -2.524960 |
| H | 4.786622 | 2.118795 | -3.278805 |
| H | 6.091480 | 4.111387 | -2.991596 |
| H | 4.798658 | 4.867132 | -1.910801 |
| C | 2.790208 | -4.809394 | -2.156645 |
| C | 3.969134 | -5.453633 | -2.166381 |
| H | 1.889123 | -5.410559 | -2.273704 |
| H | 4.014082 | -6.529147 | -2.308442 |
| H | 4.912115 | -4.942860 | -2.006866 |
| C | -4.843617 | 2.166134 | 0.813074 |
| C | -5.777786 | 2.008960 | -0.414893 |
| H | -5.059638 | 3.120066 | 1.307549 |

| | | | |
|---|---|---|---|
| H | -5.065862 | 1.381080 | 1.541607 |
| H | -5.547575 | 2.767320 | -1.164701 |
| H | -5.622053 | 1.022032 | -0.865774 |
| C | -4.230995 | -3.212321 | 1.187511 |
| C | -5.463133 | -3.180071 | 0.242213 |
| H | -4.418382 | -2.543905 | 2.033339 |
| H | -4.163471 | -4.220567 | 1.607276 |
| H | -5.204633 | -3.563924 | -0.745698 |
| H | -6.250053 | -3.816099 | 0.667772 |
| C | -7.236155 | 2.133523 | -0.083181 |
| O | -8.044715 | 2.891538 | -0.565472 |
| O | -7.620423 | 1.250769 | 0.903777 |
| H | -8.575099 | 1.383239 | 1.024148 |
| C | -6.079925 | -1.812973 | 0.063765 |
| O | -6.290419 | -1.260447 | -0.997912 |
| O | -6.418866 | -1.262948 | 1.252139 |
| H | -6.836211 | -0.393459 | 1.075120 |
| O | -0.669192 | -0.243433 | -2.595757 |
| H | -0.283009 | 1.601088 | -3.493785 |
| C | 0.975221 | -0.042020 | 1.052370 |
| C | 0.791164 | 1.223804 | 1.890448 |
| C | 0.528441 | -1.116667 | 1.947128 |
| C | -0.365779 | 0.827046 | 2.815380 |

| | | | |
|---|---|---|---|
| H | 0.560175 | 2.119913 | 1.316176 |
| H | 1.688517 | 1.439690 | 2.483654 |
| H | 4.103582 | 0.997867 | 0.270468 |
| O | 0.771654 | -2.315980 | 1.955967 |
| O | -0.288878 | -0.607133 | 2.941465 |
| H | -1.339753 | 1.087168 | 2.391886 |
| H | -0.292320 | 1.252044 | 3.822504 |
| C | 4.233149 | 1.524559 | 1.204449 |
| C | 4.369688 | 0.812696 | 2.419771 |
| C | 4.189740 | 2.912869 | 1.189500 |
| C | 4.448094 | 1.574670 | 3.610225 |
| N | 4.414412 | -0.582949 | 2.443519 |
| C | 4.276294 | 3.655094 | 2.369740 |
| H | 4.066551 | 3.410183 | 0.233977 |
| C | 4.400425 | 2.965345 | 3.576095 |
| H | 4.527253 | 1.087556 | 4.572829 |
| C | 4.536869 | -1.352724 | 1.288184 |
| C | 4.368716 | -1.272174 | 3.736367 |
| H | 4.232922 | 4.739845 | 2.349873 |
| H | 4.455750 | 3.512153 | 4.514454 |
| H | 4.737768 | -0.804991 | 0.380861 |
| C | 3.979113 | -2.735139 | 1.191393 |
| H | 4.733893 | -2.286188 | 3.575679 |

| | | | |
|---|---|---|---|
| H | 5.088769 | -0.798528 | 4.413937 |
| C | 2.971889 | -1.314474 | 4.358859 |
| H | 2.888456 | -2.752143 | 1.341784 |
| H | 4.177411 | -3.128595 | 0.192982 |
| H | 4.420507 | -3.442799 | 1.908699 |
| H | 2.552901 | -0.309843 | 4.459146 |
| H | 2.288439 | -1.899120 | 3.740514 |
| H | 3.020010 | -1.766000 | 5.356978 |
| H | 1.997463 | -0.221224 | 0.727466 |

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**$^3$D**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2824.4564585

Zero-point correction= 0.946959 (Hartree/Particle)

Thermal correction to Energy= 1.008921

Thermal correction to Enthalpy= 1.009865

Thermal correction to Gibbs Free Energy= 0.847413

Sum of electronic and zero-point Energies= -2823.509499

Sum of electronic and thermal Energies= -2823.447538

Sum of electronic and thermal Enthalpies= -2823.446594

Sum of electronic and thermal Free Energies= -2823.609045

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.029445 | -0.099318 | -0.849522 |
| N | 1.228790 | 1.453903 | -1.368619 |
| C | 0.935832 | 2.793040 | -1.305123 |
| C | 2.053004 | 3.583305 | -1.775595 |
| C | 3.038123 | 2.685960 | -2.134939 |
| C | 2.488474 | 1.356619 | -1.882032 |
| C | -0.273888 | 3.321425 | -0.870276 |
| C | -1.356651 | 2.582174 | -0.420065 |
| N | -1.394811 | 1.215763 | -0.302159 |
| C | -2.628086 | 0.904178 | 0.198071 |
| C | -3.408949 | 2.115452 | 0.398939 |
| C | -2.615520 | 3.162509 | 0.010678 |
| C | -3.075891 | -0.374609 | 0.508706 |
| C | -2.393790 | -1.554870 | 0.253647 |
| N | -1.160934 | -1.640578 | -0.327037 |
| C | -0.892708 | -2.971516 | -0.470283 |
| C | -1.989756 | -3.770870 | 0.053926 |
| C | -2.923233 | -2.888735 | 0.521083 |
| C | 0.260750 | -3.511515 | -1.011298 |

| | | | |
|---|---|---|---|
| C | 1.352296 | -2.784026 | -1.462520 |
| C | 2.575797 | -3.374654 | -2.001319 |
| C | 3.409243 | -2.319086 | -2.300148 |
| C | 2.681382 | -1.114134 | -1.944287 |
| N | 1.451287 | -1.428262 | -1.432482 |
| C | 3.172099 | 0.171933 | -2.128915 |
| H | -0.380141 | 4.399901 | -0.877135 |
| H | 4.179984 | 0.258434 | -2.516086 |
| H | 0.327614 | -4.592068 | -1.049849 |
| H | -4.046374 | -0.455900 | 0.980824 |
| C | -1.087333 | 0.864886 | -3.327256 |
| H | -1.929671 | 1.404289 | -2.854555 |
| H | -1.434400 | 0.542929 | -4.325325 |
| C | -2.012558 | -5.266484 | 0.077269 |
| H | -1.959749 | -5.686480 | -0.934794 |
| H | -1.160052 | -5.666538 | 0.638709 |
| H | -2.925917 | -5.647409 | 0.542704 |
| C | -2.942355 | 4.622989 | -0.013994 |
| H | -2.203554 | 5.211032 | 0.543653 |
| H | -2.957667 | 5.016588 | -1.037965 |
| H | -3.923261 | 4.819999 | 0.428056 |
| C | 2.083275 | 5.075149 | -1.866146 |
| H | 1.082225 | 5.488228 | -2.021623 |

| | | | |
|---|---|---|---|
| H | 2.486267 | 5.533791 | -0.952639 |
| H | 2.717200 | 5.399254 | -2.697432 |
| C | 4.780110 | -2.359538 | -2.894730 |
| H | 4.898094 | -3.239561 | -3.534471 |
| H | 4.981994 | -1.470449 | -3.499562 |
| H | 5.560045 | -2.412049 | -2.122439 |
| C | 4.361335 | 2.937709 | -2.680674 |
| C | 5.109962 | 4.041916 | -2.520947 |
| H | 4.783502 | 2.129991 | -3.277285 |
| H | 6.086490 | 4.123569 | -2.988087 |
| H | 4.793514 | 4.876422 | -1.905427 |
| C | 2.795933 | -4.801753 | -2.161973 |
| C | 3.975562 | -5.444722 | -2.171218 |
| H | 1.895618 | -5.403747 | -2.280673 |
| H | 4.021806 | -6.520023 | -2.314469 |
| H | 4.917830 | -4.933123 | -2.010159 |
| C | -4.845385 | 2.161962 | 0.817505 |
| C | -5.779818 | 2.006466 | -0.410498 |
| H | -5.061992 | 3.114784 | 1.313855 |
| H | -5.066815 | 1.375340 | 1.544595 |
| H | -5.550415 | 2.766504 | -1.158852 |
| H | -5.623478 | 1.020558 | -0.863382 |
| C | -4.228513 | -3.216851 | 1.180787 |

| | | | |
|---|---|---|---|
| C | -5.460691 | -3.183588 | 0.235614 |
| H | -4.416357 | -2.550346 | 2.028019 |
| H | -4.160140 | -4.225906 | 1.598456 |
| H | -5.201889 | -3.564920 | -0.753195 |
| H | -6.247025 | -3.821338 | 0.659691 |
| C | -7.238149 | 2.129311 | -0.077996 |
| O | -8.047344 | 2.888033 | -0.558103 |
| O | -7.621469 | 1.244030 | 0.907070 |
| H | -8.576165 | 1.375658 | 1.028190 |
| C | -6.078847 | -1.816695 | 0.060303 |
| O | -6.290180 | -1.262134 | -1.000159 |
| O | -6.417779 | -1.269434 | 1.249923 |
| H | -6.835994 | -0.399958 | 1.074883 |
| O | -0.668123 | -0.238027 | -2.597064 |
| H | -0.285927 | 1.609513 | -3.490588 |
| C | 0.974490 | -0.041706 | 1.052283 |
| C | 0.791386 | 1.223432 | 1.891602 |
| C | 0.526448 | -1.116850 | 1.945770 |
| C | -0.366007 | 0.826748 | 2.816034 |
| H | 0.561192 | 2.120306 | 1.318209 |
| H | 1.688900 | 1.437917 | 2.485097 |
| H | 4.104632 | 0.989385 | 0.271557 |
| O | 0.768568 | -2.316382 | 1.953246 |

| | | | |
|---|---|---|---|
| O | -0.290557 | -0.607624 | 2.940541 |
| H | -1.339685 | 1.088352 | 2.392754 |
| H | -0.292231 | 1.250567 | 3.823634 |
| C | 4.235244 | 1.515793 | 1.205582 |
| C | 4.370989 | 0.803470 | 2.420696 |
| C | 4.193714 | 2.904160 | 1.190938 |
| C | 4.450632 | 1.564983 | 3.611335 |
| N | 4.413865 | -0.592263 | 2.444058 |
| C | 4.281429 | 3.645931 | 2.371403 |
| H | 4.071022 | 3.401993 | 0.235625 |
| C | 4.404796 | 2.955746 | 3.577563 |
| H | 4.529467 | 1.077478 | 4.573769 |
| C | 4.537282 | -1.361959 | 1.288726 |
| C | 4.366188 | -1.281817 | 3.736686 |
| H | 4.239469 | 4.730743 | 2.351803 |
| H | 4.461026 | 3.502256 | 4.516042 |
| H | 4.740069 | -0.813991 | 0.381905 |
| C | 3.975815 | -2.742812 | 1.190310 |
| H | 4.729581 | -2.296440 | 3.575813 |
| H | 5.086765 | -0.809788 | 4.414865 |
| C | 2.968942 | -1.321715 | 4.358350 |
| H | 2.884816 | -2.756598 | 1.338696 |
| H | 4.175070 | -3.136681 | 0.192269 |

| | | | |
|---|---|---|---|
| H | 4.413602 | -3.451826 | 1.908467 |
| H | 2.551900 | -0.316309 | 4.459014 |
| H | 2.284677 | -1.904566 | 3.739203 |
| H | 3.015573 | -1.773940 | 5.356219 |
| H | 1.996618 | -0.221616 | 0.727618 |

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**$^5$D**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2824.4422398

Zero-point correction= 0.944068 (Hartree/Particle)

Thermal correction to Energy= 1.006990

Thermal correction to Enthalpy= 1.007934

Thermal correction to Gibbs Free Energy= 0.841582

Sum of electronic and zero-point Energies= -2823.498172

Sum of electronic and thermal Energies= -2823.435250

Sum of electronic and thermal Enthalpies= -2823.434306

Sum of electronic and thermal Free Energies= -2823.600658

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | 0.034995 | -0.069327 | -0.828660 |
| N | 1.273893 | 1.515902 | -1.334620 |
| C | 0.927242 | 2.837957 | -1.300136 |
| C | 2.015107 | 3.640404 | -1.834448 |
| C | 3.012544 | 2.755904 | -2.203351 |
| C | 2.507210 | 1.413871 | -1.897459 |
| C | -0.299296 | 3.350381 | -0.850903 |
| C | -1.399424 | 2.640531 | -0.359350 |
| N | -1.436176 | 1.291547 | -0.178618 |
| C | -2.662697 | 0.956875 | 0.298406 |
| C | -3.468157 | 2.167297 | 0.445716 |
| C | -2.681073 | 3.216733 | 0.035087 |
| C | -3.072892 | -0.350430 | 0.593845 |
| C | -2.381871 | -1.539455 | 0.331471 |
| N | -1.151935 | -1.628323 | -0.252618 |
| C | -0.848882 | -2.949788 | -0.411274 |
| C | -1.942707 | -3.758376 | 0.113932 |
| C | -2.891222 | -2.886092 | 0.584786 |
| C | 0.320333 | -3.473626 | -0.968258 |
| C | 1.433469 | -2.773864 | -1.448997 |
| C | 2.652353 | -3.364674 | -2.018005 |
| C | 3.477152 | -2.302943 | -2.343567 |
| C | 2.753241 | -1.093218 | -1.971833 |

| | | | |
|---|---|---|---|
| N | 1.550758 | -1.428019 | -1.433259 |
| C | 3.197962 | 0.221733 | -2.159896 |
| H | -0.412920 | 4.428517 | -0.902423 |
| H | 4.189456 | 0.332616 | -2.585550 |
| H | 0.378045 | -4.556378 | -1.002864 |
| H | -4.048204 | -0.456082 | 1.054224 |
| C | -2.013634 | -0.142963 | -2.856119 |
| H | -2.522729 | -1.018798 | -2.418939 |
| H | -2.141620 | -0.203560 | -3.950538 |
| C | -1.961386 | -5.254698 | 0.128896 |
| H | -1.919619 | -5.668459 | -0.886305 |
| H | -1.099722 | -5.654938 | 0.675995 |
| H | -2.866783 | -5.643173 | 0.603722 |
| C | -3.039918 | 4.667625 | -0.049461 |
| H | -2.308106 | 5.293808 | 0.475020 |
| H | -3.069778 | 5.016115 | -1.089528 |
| H | -4.021483 | 4.865981 | 0.391382 |
| C | 2.009416 | 5.128884 | -1.976384 |
| H | 0.995285 | 5.512518 | -2.123490 |
| H | 2.419643 | 5.628731 | -1.087908 |
| H | 2.618149 | 5.439559 | -2.831353 |
| C | 4.834269 | -2.345418 | -2.968775 |
| H | 4.922783 | -3.195704 | -3.652993 |

| | | | |
|---|---|---|---|
| H | 5.042600 | -1.431425 | -3.533030 |
| H | 5.628713 | -2.451463 | -2.216855 |
| C | 4.309727 | 3.030335 | -2.798273 |
| C | 5.040056 | 4.151984 | -2.678595 |
| H | 4.729480 | 2.222376 | -3.396721 |
| H | 5.998708 | 4.247548 | -3.179161 |
| H | 4.725919 | 4.988341 | -2.064194 |
| C | 2.874184 | -4.790334 | -2.179056 |
| C | 4.052285 | -5.432493 | -2.261222 |
| H | 1.970340 | -5.397393 | -2.226170 |
| H | 4.089585 | -6.509945 | -2.390495 |
| H | 5.003146 | -4.919001 | -2.175854 |
| C | -4.917251 | 2.201984 | 0.818704 |
| C | -5.807825 | 1.996421 | -0.435161 |
| H | -5.169849 | 3.162095 | 1.283615 |
| H | -5.147458 | 1.427159 | 1.556377 |
| H | -5.578718 | 2.751576 | -1.188470 |
| H | -5.605201 | 1.008486 | -0.864724 |
| C | -4.198372 | -3.239805 | 1.227681 |
| C | -5.414018 | -3.229963 | 0.260650 |
| H | -4.413156 | -2.573600 | 2.068870 |
| H | -4.120645 | -4.246618 | 1.649479 |
| H | -5.134861 | -3.632603 | -0.714128 |

| | | | |
|---|---|---|---|
| H | -6.207728 | -3.857801 | 0.685092 |
| C | -7.277910 | 2.078929 | -0.146341 |
| O | -8.092704 | 2.821718 | -0.641852 |
| O | -7.665729 | 1.174135 | 0.819245 |
| H | -8.626228 | 1.280761 | 0.916323 |
| C | -6.021866 | -1.864204 | 0.045081 |
| O | -6.168056 | -1.310641 | -1.026763 |
| O | -6.428697 | -1.315959 | 1.212482 |
| H | -6.838757 | -0.447582 | 1.014396 |
| O | -0.656975 | -0.097314 | -2.551634 |
| H | -2.561392 | 0.753103 | -2.514075 |
| C | 1.022217 | -0.023750 | 1.069303 |
| C | 0.834002 | 1.244393 | 1.896024 |
| C | 0.589067 | -1.104307 | 1.976126 |
| C | -0.297187 | 0.842341 | 2.849169 |
| H | 0.584186 | 2.131585 | 1.317297 |
| H | 1.745388 | 1.468261 | 2.463699 |
| H | 4.140920 | 1.006760 | 0.214579 |
| O | 0.852797 | -2.296171 | 1.984349 |
| O | -0.204391 | -0.592045 | 2.980553 |
| H | -1.281940 | 1.089526 | 2.446330 |
| H | -0.200794 | 1.270978 | 3.852206 |
| C | 4.258575 | 1.538303 | 1.147289 |

| | | | |
|---|---|---|---|
| C | 4.413252 | 0.834716 | 2.365136 |
| C | 4.183105 | 2.925229 | 1.125895 |
| C | 4.480253 | 1.603483 | 3.551880 |
| N | 4.482868 | -0.560332 | 2.395181 |
| C | 4.255947 | 3.674114 | 2.302890 |
| H | 4.044642 | 3.415007 | 0.168305 |
| C | 4.401115 | 2.992814 | 3.511599 |
| H | 4.573894 | 1.123098 | 4.516546 |
| C | 4.595339 | -1.335530 | 1.241857 |
| C | 4.481372 | -1.242160 | 3.692576 |
| H | 4.186826 | 4.757372 | 2.278633 |
| H | 4.447719 | 3.544840 | 4.447347 |
| H | 4.755586 | -0.790552 | 0.325023 |
| C | 4.062039 | -2.729040 | 1.166999 |
| H | 4.871569 | -2.246739 | 3.531169 |
| H | 5.200504 | -0.743948 | 4.353063 |
| C | 3.098788 | -1.319155 | 4.343214 |
| H | 2.974626 | -2.763805 | 1.334492 |
| H | 4.250467 | -3.127745 | 0.168780 |
| H | 4.527115 | -3.421609 | 1.883784 |
| H | 2.655482 | -0.325581 | 4.449246 |
| H | 2.418188 | -1.922976 | 3.740393 |
| H | 3.178184 | -1.765920 | 5.341400 |

H 2.030649 -0.197755 0.706555

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**$^{3}$TS(D-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2824.4331811

Zero-point correction= 0.945655 (Hartree/Particle)

Thermal correction to Energy= 1.007304

Thermal correction to Enthalpy= 1.008248

Thermal correction to Gibbs Free Energy= 0.844861

Sum of electronic and zero-point Energies= -2823.487526

Sum of electronic and thermal Energies= -2823.425877

Sum of electronic and thermal Enthalpies= -2823.424933

Sum of electronic and thermal Free Energies= -2823.588320

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Cartesian Coordinates

.....

Fe 0.150420 -1.446944 0.188525

N 1.269769 -2.134866 -1.347830

C 0.996439 -2.029961 -2.689381

C 2.016296 -2.692225 -3.473057

| | | | |
|---|---|---|---|
| C | 2.910258 | -3.231550 | -2.568205 |
| C | 2.413012 | -2.877833 | -1.243390 |
| C | -0.139387 | -1.428350 | -3.219678 |
| C | -1.177393 | -0.885768 | -2.483579 |
| N | -1.212845 | -0.783168 | -1.117378 |
| C | -2.397478 | -0.178415 | -0.810269 |
| C | -3.167609 | 0.070463 | -2.021555 |
| C | -2.401663 | -0.359250 | -3.068118 |
| C | -2.791023 | 0.240149 | 0.452311 |
| C | -2.052500 | 0.099929 | 1.617619 |
| N | -0.851484 | -0.545604 | 1.707363 |
| C | -0.456650 | -0.450400 | 3.013872 |
| C | -1.438663 | 0.292830 | 3.788586 |
| C | -2.438167 | 0.636883 | 2.916850 |
| C | 0.707153 | -0.989722 | 3.543592 |
| C | 1.638583 | -1.747042 | 2.841618 |
| C | 2.805953 | -2.388853 | 3.443564 |
| C | 3.444997 | -3.053884 | 2.418337 |
| C | 2.680517 | -2.783498 | 1.216837 |
| N | 1.593321 | -1.995123 | 1.501951 |
| C | 3.052336 | -3.205096 | -0.053077 |
| H | -0.237318 | -1.410300 | -4.298849 |
| H | 3.964611 | -3.784589 | -0.127757 |

| | | | |
|---|---|---|---|
| H | 0.886517 | -0.829359 | 4.600360 |
| H | -3.719739 | 0.791024 | 0.518155 |
| C | -1.344793 | -3.801294 | -0.568483 |
| H | -2.211838 | -3.258878 | -0.995632 |
| H | -1.725025 | -4.786788 | -0.236907 |
| C | -1.318888 | 0.588211 | 5.251196 |
| H | -1.309591 | -0.332240 | 5.848222 |
| H | -0.390807 | 1.126379 | 5.479948 |
| H | -2.151517 | 1.201088 | 5.607702 |
| C | -2.709129 | -0.335018 | -4.532077 |
| H | -1.947311 | 0.221846 | -5.090952 |
| H | -2.744485 | -1.346452 | -4.955760 |
| H | -3.675241 | 0.138101 | -4.729726 |
| C | 2.029574 | -2.803872 | -4.964455 |
| H | 1.016271 | -2.779603 | -5.376005 |
| H | 2.590978 | -1.986372 | -5.436743 |
| H | 2.499921 | -3.741652 | -5.276725 |
| C | 4.658010 | -3.925069 | 2.494336 |
| H | 4.719290 | -4.414353 | 3.471592 |
| H | 4.637932 | -4.703284 | 1.725547 |
| H | 5.588328 | -3.356497 | 2.358769 |
| C | 4.098858 | -4.031307 | -2.812127 |
| C | 4.870193 | -4.030382 | -3.912333 |

| | | | |
|---|---|---|---|
| H | 4.383383 | -4.703181 | -2.002774 |
| H | 5.727629 | -4.691925 | -3.990951 |
| H | 4.690029 | -3.363522 | -4.748102 |
| C | 3.134809 | -2.335827 | 4.857457 |
| C | 4.343279 | -2.501678 | 5.421767 |
| H | 2.295467 | -2.140039 | 5.524315 |
| H | 4.463455 | -2.463055 | 6.500245 |
| H | 5.242552 | -2.656070 | 4.835943 |
| C | -4.566846 | 0.599060 | -2.053423 |
| C | -5.585689 | -0.524764 | -1.726576 |
| H | -4.791502 | 1.009983 | -3.043699 |
| H | -4.690114 | 1.419828 | -1.340037 |
| H | -5.453660 | -1.363557 | -2.411648 |
| H | -5.414917 | -0.887761 | -0.706642 |
| C | -3.680382 | 1.417865 | 3.225559 |
| C | -4.969845 | 0.561898 | 3.358694 |
| H | -3.851467 | 2.191148 | 2.470196 |
| H | -3.532020 | 1.945106 | 4.172875 |
| H | -4.750737 | -0.407780 | 3.807946 |
| H | -5.678138 | 1.091340 | 4.009313 |
| C | -7.017032 | -0.085245 | -1.824671 |
| O | -7.893797 | -0.557670 | -2.509714 |
| O | -7.284631 | 1.000427 | -1.016677 |

| | | | |
|---|---|---|---|
| H | -8.231018 | 1.187889 | -1.128963 |
| C | -5.703145 | 0.316942 | 2.059653 |
| O | -6.065494 | -0.764792 | 1.642262 |
| O | -5.956596 | 1.473598 | 1.406387 |
| H | -6.437322 | 1.254739 | 0.579718 |
| O | -0.743697 | -3.131816 | 0.485064 |
| H | -0.654497 | -4.000400 | -1.412729 |
| C | 1.473176 | 0.818024 | 0.191940 |
| C | 2.844598 | 0.470493 | -0.304445 |
| C | 0.733774 | 1.501951 | -0.826758 |
| C | 2.780018 | 0.927730 | -1.782280 |
| H | 3.071921 | -0.592281 | -0.232575 |
| H | 3.639867 | 0.987820 | 0.250476 |
| H | 4.143546 | 2.815851 | 0.160428 |
| O | -0.370553 | 2.037489 | -0.829628 |
| O | 1.505177 | 1.561577 | -1.983599 |
| H | 2.850231 | 0.078633 | -2.468429 |
| H | 3.558288 | 1.657199 | -2.032012 |
| C | 4.254481 | 3.832434 | -0.187198 |
| C | 3.127236 | 4.679643 | -0.245874 |
| C | 5.503966 | 4.274558 | -0.610218 |
| C | 3.317514 | 5.983199 | -0.755762 |
| N | 1.872854 | 4.261336 | 0.213280 |

| | | | |
|---|---|---|---|
| C | 5.682427 | 5.565222 | -1.110515 |
| H | 6.345590 | 3.588750 | -0.558832 |
| C | 4.572080 | 6.410130 | -1.178016 |
| H | 2.485061 | 6.673143 | -0.806743 |
| C | 1.749684 | 3.206545 | 1.112135 |
| C | 0.675577 | 4.959110 | -0.285008 |
| H | 6.658214 | 5.901662 | -1.446827 |
| H | 4.680585 | 7.422321 | -1.559358 |
| H | 2.688601 | 2.931707 | 1.576681 |
| C | 0.512440 | 3.072705 | 1.945491 |
| H | -0.185484 | 4.476253 | 0.167268 |
| H | 0.693086 | 5.999598 | 0.070921 |
| C | 0.506495 | 4.900238 | -1.804321 |
| H | -0.342231 | 2.746524 | 1.342438 |
| H | 0.677593 | 2.311692 | 2.711339 |
| H | 0.245559 | 4.012518 | 2.455494 |
| H | 1.360411 | 5.327084 | -2.335369 |
| H | 0.370097 | 3.863271 | -2.110961 |
| H | -0.387772 | 5.469823 | -2.082746 |
| H | 1.138505 | 0.710171 | 1.203054 |

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**$^{4}$TS(D-E)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2380.1582292

Zero-point correction= 0.722123 (Hartree/Particle)

Thermal correction to Energy= 0.772399

Thermal correction to Enthalpy= 0.773344

Thermal correction to Gibbs Free Energy= 0.634666

Sum of electronic and zero-point Energies= -2379.436106

Sum of electronic and thermal Energies= -2379.385830

Sum of electronic and thermal Enthalpies= -2379.384886

Sum of electronic and thermal Free Energies= -2379.523564

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.866526 | 0.059296 | -0.469379 |
| N | -2.185567 | -1.597386 | -0.252301 |
| C | -1.797254 | -2.905878 | -0.190124 |
| C | -2.947044 | -3.772703 | -0.384513 |
| C | -4.038657 | -2.940470 | -0.569217 |
| C | -3.524483 | -1.570035 | -0.496178 |
| C | -0.480711 | -3.335687 | 0.036347 |
| C | 0.659557 | -2.545764 | 0.204299 |

| | | | |
|---|---|---|---|
| N | 0.685631 | -1.180464 | 0.202677 |
| C | 1.981519 | -0.787292 | 0.348031 |
| C | 2.837928 | -1.966353 | 0.453832 |
| C | 2.016252 | -3.060845 | 0.365319 |
| C | 2.430925 | 0.536789 | 0.396984 |
| C | 1.669492 | 1.701405 | 0.264186 |
| N | 0.334119 | 1.725779 | 0.014272 |
| C | -0.067153 | 3.025907 | -0.006893 |
| C | 1.085448 | 3.896707 | 0.222311 |
| C | 2.168789 | 3.072385 | 0.394337 |
| C | -1.384759 | 3.461992 | -0.182541 |
| C | -2.536733 | 2.680181 | -0.361580 |
| C | -3.898086 | 3.199365 | -0.525741 |
| C | -4.719225 | 2.092887 | -0.657552 |
| C | -3.857638 | 0.925777 | -0.557113 |
| N | -2.561850 | 1.322095 | -0.379916 |
| C | -4.292936 | -0.405377 | -0.619221 |
| H | -0.324096 | -4.409152 | 0.071538 |
| H | -5.359207 | -0.548864 | -0.757087 |
| H | -1.533503 | 4.536757 | -0.158224 |
| H | 3.484231 | 0.672849 | 0.609197 |
| C | -0.231456 | -1.210083 | -2.979683 |
| H | 0.729321 | -1.621596 | -2.611877 |

| | | | |
|---|---|---|---|
| H | -0.105837 | -1.045936 | -4.066743 |
| C | 1.029149 | 5.392133 | 0.257024 |
| H | 0.713469 | 5.804012 | -0.709821 |
| H | 0.311695 | 5.750238 | 1.005533 |
| H | 2.002598 | 5.829324 | 0.497116 |
| C | 2.389821 | -4.509918 | 0.394013 |
| H | 1.842608 | -5.049803 | 1.176316 |
| H | 2.158968 | -5.004761 | -0.557749 |
| H | 3.458494 | -4.646077 | 0.584130 |
| C | -2.913283 | -5.267559 | -0.422230 |
| H | -1.929736 | -5.635467 | -0.729090 |
| H | -3.136895 | -5.714343 | 0.556479 |
| H | -3.655951 | -5.654259 | -1.127991 |
| C | -6.194452 | 2.067147 | -0.902696 |
| H | -6.501545 | 2.928159 | -1.505632 |
| H | -6.494238 | 1.158072 | -1.432527 |
| H | -6.773234 | 2.105487 | 0.030572 |
| C | -5.424827 | -3.284224 | -0.832982 |
| C | -6.062427 | -4.426909 | -0.524507 |
| H | -6.003911 | -2.512597 | -1.339975 |
| H | -7.104666 | -4.571197 | -0.792979 |
| H | -5.582541 | -5.234496 | 0.016708 |
| C | -4.238478 | 4.610469 | -0.575382 |

| | | | |
|---|---|---|---|
| C | -5.428024 | 5.179921 | -0.314558 |
| H | -3.421168 | 5.273847 | -0.857659 |
| H | -5.561266 | 6.253809 | -0.405166 |
| H | -6.288252 | 4.608524 | 0.015376 |
| C | 4.333289 | -1.943043 | 0.512502 |
| C | 4.937198 | -1.813834 | -0.910996 |
| H | 4.709366 | -2.860742 | 0.978784 |
| H | 4.683540 | -1.112103 | 1.132354 |
| H | 4.577535 | -2.623054 | -1.548313 |
| H | 4.622635 | -0.862581 | -1.355347 |
| C | 3.581215 | 3.484865 | 0.681464 |
| C | 4.536314 | 3.419837 | -0.541916 |
| H | 4.004002 | 2.878727 | 1.488717 |
| H | 3.578478 | 4.517303 | 1.044615 |
| H | 4.018747 | 3.711708 | -1.456905 |
| H | 5.367616 | 4.117621 | -0.376662 |
| C | 6.436861 | -1.856996 | -0.931740 |
| O | 7.150216 | -2.622911 | -1.536900 |
| O | 6.995108 | -0.883465 | -0.130186 |
| H | 7.956757 | -0.974791 | -0.231137 |
| C | 5.168363 | 2.067258 | -0.776717 |
| O | 5.157618 | 1.450107 | -1.823317 |
| O | 5.802777 | 1.617332 | 0.329291 |

| | | | |
|---|---|---|---|
| H | 6.203231 | 0.748014 | 0.115571 |
| O | -0.599629 | -0.035018 | -2.341929 |
| H | -0.981809 | -2.017901 | -2.867971 |
| C | -1.289626 | 0.516058 | 2.286426 |
| C | -2.451949 | -0.336315 | 2.666386 |
| C | -0.109840 | 0.005925 | 2.967464 |
| C | -1.743894 | -1.626716 | 3.119076 |
| H | -3.162285 | -0.508285 | 1.857517 |
| H | -3.006316 | 0.121650 | 3.503860 |
| O | 0.974001 | 0.520491 | 3.164910 |
| O | -0.405553 | -1.242066 | 3.490173 |
| H | -1.683761 | -2.346901 | 2.300976 |
| H | -2.208293 | -2.099946 | 3.989493 |
| H | -1.352861 | 1.545090 | 1.972859 |

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**$^{6}$TS(D-E)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2380.1579337

Zero-point correction= 0.721885 (Hartree/Particle)

Thermal correction to Energy= 0.772208

Thermal correction to Enthalpy= 0.773152

Thermal correction to Gibbs Free Energy= 0.634141

Sum of electronic and zero-point Energies= -2379.436048

Sum of electronic and thermal Energies= -2379.385726

Sum of electronic and thermal Enthalpies= -2379.384782

Sum of electronic and thermal Free Energies= -2379.523792

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.824935 | 0.208740 | -0.564953 |
| N | -2.142235 | -1.428341 | -0.461877 |
| C | -1.757472 | -2.740875 | -0.406651 |
| C | -2.918799 | -3.597383 | -0.554980 |
| C | -4.010603 | -2.756420 | -0.707511 |
| C | -3.487024 | -1.393126 | -0.656601 |
| C | -0.438679 | -3.185829 | -0.239594 |
| C | 0.714216 | -2.421259 | -0.083566 |
| N | 0.765195 | -1.055192 | -0.066236 |
| C | 2.048064 | -0.694492 | 0.194545 |
| C | 2.882438 | -1.889402 | 0.299917 |
| C | 2.053967 | -2.963833 | 0.127491 |
| C | 2.478954 | 0.620369 | 0.386802 |
| C | 1.701973 | 1.779960 | 0.356715 |

| | | | |
|---|---|---|---|
| N | 0.351279 | 1.824054 | 0.120636 |
| C | -0.040894 | 3.128990 | 0.216337 |
| C | 1.111218 | 3.967260 | 0.513276 |
| C | 2.196082 | 3.128637 | 0.606527 |
| C | -1.349848 | 3.596037 | 0.070050 |
| C | -2.488636 | 2.831914 | -0.199209 |
| C | -3.847316 | 3.356143 | -0.344655 |
| C | -4.657758 | 2.266149 | -0.604761 |
| C | -3.798610 | 1.097176 | -0.595366 |
| N | -2.498055 | 1.478691 | -0.354480 |
| C | -4.245117 | -0.217440 | -0.737313 |
| H | -0.300816 | -4.260907 | -0.198320 |
| H | -5.313468 | -0.343699 | -0.873463 |
| H | -1.493311 | 4.664496 | 0.187180 |
| H | 3.523483 | 0.749736 | 0.641375 |
| C | -0.201095 | -0.996598 | -3.172614 |
| H | 0.779788 | -1.403973 | -2.863653 |
| H | -0.123866 | -0.755592 | -4.248355 |
| C | 1.055682 | 5.453661 | 0.683673 |
| H | 0.708820 | 5.948783 | -0.231884 |
| H | 0.362398 | 5.741618 | 1.483553 |
| H | 2.035987 | 5.870970 | 0.930314 |
| C | 2.385455 | -4.420253 | 0.190188 |

| | | | |
|---|---|---|---|
| H | 1.871877 | -4.898790 | 1.033007 |
| H | 2.078607 | -4.947560 | -0.721316 |
| H | 3.459221 | -4.583238 | 0.319825 |
| C | -2.898155 | -5.092480 | -0.574263 |
| H | -1.936642 | -5.473094 | -0.931124 |
| H | -3.065629 | -5.519825 | 0.423551 |
| H | -3.682480 | -5.483262 | -1.230615 |
| C | -6.127216 | 2.258818 | -0.883380 |
| H | -6.426860 | 3.177606 | -1.397841 |
| H | -6.408558 | 1.409983 | -1.513475 |
| H | -6.724631 | 2.194876 | 0.036405 |
| C | -5.410380 | -3.088752 | -0.910287 |
| C | -6.044772 | -4.218656 | -0.554321 |
| H | -6.001853 | -2.320067 | -1.407560 |
| H | -7.098284 | -4.358079 | -0.777396 |
| H | -5.550041 | -5.018906 | -0.015740 |
| C | -4.194687 | 4.763991 | -0.257963 |
| C | -5.392482 | 5.298314 | 0.035867 |
| H | -3.376639 | 5.455784 | -0.457772 |
| H | -5.532078 | 6.375102 | 0.048472 |
| H | -6.253940 | 4.692419 | 0.292954 |
| C | 4.368009 | -1.888058 | 0.475406 |
| C | 5.082034 | -1.702753 | -0.890891 |

| | | | |
|---|---|---|---|
| H | 4.697396 | -2.829883 | 0.927329 |
| H | 4.676378 | -1.090008 | 1.157817 |
| H | 4.771891 | -2.485632 | -1.584547 |
| H | 4.805142 | -0.732882 | -1.319497 |
| C | 3.612264 | 3.517715 | 0.912078 |
| C | 4.566922 | 3.509485 | -0.313388 |
| H | 4.035779 | 2.870528 | 1.686625 |
| H | 3.613281 | 4.529602 | 1.328298 |
| H | 4.043406 | 3.815438 | -1.220288 |
| H | 5.381489 | 4.222441 | -0.129970 |
| C | 6.578090 | -1.756112 | -0.791126 |
| O | 7.332957 | -2.531899 | -1.329483 |
| O | 7.075936 | -0.780071 | 0.046707 |
| H | 8.041503 | -0.883740 | 0.034045 |
| C | 5.234997 | 2.181232 | -0.588445 |
| O | 5.273951 | 1.617035 | -1.663701 |
| O | 5.839668 | 1.691148 | 0.516666 |
| H | 6.263149 | 0.838178 | 0.281201 |
| O | -0.571234 | 0.122585 | -2.440134 |
| H | -0.930702 | -1.823988 | -3.081885 |
| C | -0.994718 | -0.288596 | 2.413755 |
| C | -2.468006 | -0.346480 | 2.629458 |
| C | -0.392533 | -1.515491 | 2.834264 |

| | | | |
|---|---|---|---|
| C | -2.688648 | -1.861418 | 2.842085 |
| H | -3.053227 | 0.035594 | 1.788974 |
| H | -2.777546 | 0.229721 | 3.519429 |
| O | 0.777249 | -1.842473 | 2.978720 |
| O | -1.405906 | -2.436544 | 3.130810 |
| H | -3.089620 | -2.333357 | 1.940541 |
| H | -3.357871 | -2.084690 | 3.680573 |
| H | -0.418957 | 0.607444 | 2.239746 |

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Number of imaginary frequencies : 0 Electronic energy : HF=-444.2486452

Zero-point correction= 0.217080 (Hartree/Particle)

Thermal correction to Energy= 0.228361

Thermal correction to Enthalpy= 0.229306

Thermal correction to Gibbs Free Energy= 0.179419

Sum of electronic and zero-point Energies= -444.031565

Sum of electronic and thermal Energies= -444.020284

Sum of electronic and thermal Enthalpies= -444.019340

Sum of electronic and thermal Free Energies= -444.069226

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -2.267136 | -1.344292 | 0.430618 |
| C | -0.889021 | -1.236830 | 0.261025 |
| C | -0.318468 | -0.035339 | -0.201508 |
| C | -1.174839 | 1.046285 | -0.488582 |
| C | -2.547900 | 0.929583 | -0.300825 |
| C | -3.108668 | -0.263905 | 0.160685 |
| H | -2.683362 | -2.280875 | 0.790730 |
| H | -0.254859 | -2.080789 | 0.507381 |
| H | -0.748821 | 1.956319 | -0.895369 |
| H | -3.187934 | 1.775156 | -0.536747 |
| H | -4.180915 | -0.351149 | 0.302929 |
| N | 1.064527 | 0.089990 | -0.392011 |
| C | 1.862886 | -1.082754 | -0.750710 |
| H | 2.562784 | -0.778689 | -1.539546 |
| H | 1.199095 | -1.832016 | -1.189599 |
| C | 1.721695 | 1.313513 | -0.298682 |
| H | 2.706574 | 1.311281 | -0.755927 |
| C | 1.471185 | 2.260718 | 0.833608 |
| H | 0.407110 | 2.395264 | 1.045945 |
| H | 1.938378 | 1.911541 | 1.770938 |

| | | | |
|---|---|---|---|
| H | 1.895743 | 3.243563 | 0.606429 |
| C | 2.643781 | -1.665527 | 0.429627 |
| H | 1.970518 | -2.008769 | 1.220446 |
| H | 3.257797 | -2.512779 | 0.106426 |
| H | 3.305109 | -0.906698 | 0.858501 |

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**$^3$E**

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Number of imaginary frequencies : 0 Electronic energy : HF=-750.1197216

Zero-point correction= 0.303439 (Hartree/Particle)

Thermal correction to Energy= 0.321723

Thermal correction to Enthalpy= 0.322668

Thermal correction to Gibbs Free Energy= 0.254843

Sum of electronic and zero-point Energies= -749.816283

Sum of electronic and thermal Energies= -749.797998

Sum of electronic and thermal Enthalpies= -749.797054

Sum of electronic and thermal Free Energies= -749.864879

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 1.046897 | 1.123573 | 1.204520 |
| C | 1.951927 | 0.078286 | 1.730799 |
| C | 1.660879 | 1.801406 | 0.080576 |
| C | 3.235223 | 0.301639 | 0.892069 |
| O | 2.930974 | 1.307022 | -0.092395 |
| O | 1.200154 | 2.657279 | -0.652189 |
| H | 1.531706 | -0.923042 | 1.562044 |
| H | 2.135094 | 0.169929 | 2.809515 |
| H | 3.540553 | -0.602845 | 0.361985 |
| H | 4.071552 | 0.664077 | 1.497603 |
| C | 1.346651 | -1.244111 | -1.642428 |
| C | 1.550974 | -2.432081 | -0.934540 |
| C | 0.563738 | -2.852793 | -0.039691 |
| C | -0.591626 | -2.101739 | 0.163606 |
| C | -0.802354 | -0.896704 | -0.544125 |
| C | 0.191942 | -0.491467 | -1.464310 |
| H | 2.092477 | -0.894962 | -2.349914 |
| H | 2.450316 | -3.020320 | -1.084557 |
| H | 0.694174 | -3.774970 | 0.519856 |
| H | -1.316147 | -2.450159 | 0.888523 |
| H | 0.050309 | 0.412420 | -2.041644 |
| N | -1.945140 | -0.117082 | -0.350732 |
| C | -3.084453 | -0.672301 | 0.382268 |

| | | | |
|---|---|---|---|
| C | -1.959380 | 1.239637 | -0.663858 |
| H | -3.997056 | -0.239927 | -0.034242 |
| C | -3.232021 | 1.994490 | -0.837417 |
| H | -2.997291 | 3.013861 | -1.153224 |
| H | -3.888286 | 1.556217 | -1.606031 |
| H | -3.838274 | 2.076339 | 0.079236 |
| H | -1.005874 | 1.724929 | -0.812146 |
| H | 0.030491 | 1.319704 | 1.514705 |
| H | -3.135105 | -1.744939 | 0.183502 |
| C | -3.019006 | -0.388579 | 1.886000 |
| H | -3.894979 | -0.800547 | 2.397372 |
| H | -2.121737 | -0.826335 | 2.332889 |
| H | -2.991325 | 0.690189 | 2.065507 |

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**$^{3}$TS(E-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-750.0607554

Zero-point correction= 0.302647 (Hartree/Particle)

Thermal correction to Energy= 0.319678

Thermal correction to Enthalpy= 0.320622

Thermal correction to Gibbs Free Energy= 0.256402

Sum of electronic and zero-point Energies= -749.758109

Sum of electronic and thermal Energies= -749.741077

Sum of electronic and thermal Enthalpies= -749.740133

Sum of electronic and thermal Free Energies= -749.804354

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 1.720770 | -0.102855 | -0.795315 |
| C | 2.864011 | 0.812212 | -1.157898 |
| C | 2.319180 | -1.270884 | -0.162410 |
| C | 3.932765 | 0.379286 | -0.134644 |
| H | 2.635270 | 1.882575 | -1.083257 |
| H | 3.207274 | 0.626725 | -2.184727 |
| H | -0.266994 | -1.690943 | 0.084065 |
| O | 1.823898 | -2.357822 | 0.105586 |
| O | 3.625458 | -0.977412 | 0.210891 |
| H | 3.884564 | 0.994694 | 0.773560 |
| H | 4.953482 | 0.414904 | -0.523284 |
| C | -1.298900 | -1.363479 | 0.030714 |
| C | -1.620991 | 0.044444 | -0.125852 |
| C | -2.290159 | -2.301948 | 0.002174 |
| C | -3.023728 | 0.404590 | -0.337027 |

| | | | |
|---|---|---|---|
| N | -0.679678 | 1.029773 | 0.026438 |
| C | -3.664994 | -1.933568 | -0.159759 |
| H | -2.021966 | -3.351095 | 0.075348 |
| C | -3.991852 | -0.562184 | -0.335511 |
| H | -3.310332 | 1.443677 | -0.437621 |
| C | 0.583649 | 0.854383 | 0.605608 |
| C | -0.919110 | 2.361988 | -0.568517 |
| H | -4.441748 | -2.689285 | -0.166300 |
| H | -5.030535 | -0.272537 | -0.466613 |
| H | 1.114904 | 1.801832 | 0.605812 |
| C | 0.680586 | 0.118040 | 1.921543 |
| H | 0.028092 | 2.677359 | -1.015687 |
| H | -1.636170 | 2.259301 | -1.382577 |
| C | -1.383299 | 3.381641 | 0.470231 |
| H | 0.529545 | -0.957938 | 1.834198 |
| H | 1.682434 | 0.267410 | 2.333216 |
| H | -0.050473 | 0.509605 | 2.640400 |
| H | -2.339402 | 3.085743 | 0.910440 |
| H | -0.651988 | 3.470747 | 1.278476 |
| H | -1.503562 | 4.364653 | 0.005255 |
| H | 0.932935 | -0.293959 | -1.517618 |

**(U)ωB97XD optimizations**

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**$S_1$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-414.5892421

Zero-point correction= 0.086251 (Hartree/Particle)

Thermal correction to Energy= 0.092981

Thermal correction to Enthalpy= 0.093926

Thermal correction to Gibbs Free Energy= 0.054724

Sum of electronic and zero-point Energies= -414.502991

Sum of electronic and thermal Energies= -414.496261

Sum of electronic and thermal Enthalpies= -414.495317

Sum of electronic and thermal Free Energies= -414.534518

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| N | 1.709485 | -0.333369 | 0.022278 |
| N | 2.843219 | -0.327316 | 0.048898 |
| C | 0.413989 | -0.325154 | 0.010820 |
| C | -0.490767 | -1.509700 | -0.136319 |

| | | | |
|---|---|---|---|
| C | -1.842223 | -0.811434 | 0.140995 |
| H | -0.299381 | -2.309884 | 0.583151 |
| H | -0.455856 | -1.935806 | -1.145305 |
| H | -2.165277 | -0.977077 | 1.173400 |
| H | -2.632385 | -1.136752 | -0.536577 |
| C | -0.337437 | 0.931111 | -0.014471 |
| O | 0.058411 | 2.065577 | -0.023106 |
| O | -1.655586 | 0.593846 | -0.049276 |

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**$S_2$**

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---

Number of imaginary frequencies : 0 Electronic energy : HF=-444.718553

Zero-point correction= 0.233390 (Hartree/Particle)

Thermal correction to Energy= 0.244369

Thermal correction to Enthalpy= 0.245313

Thermal correction to Gibbs Free Energy= 0.195573

Sum of electronic and zero-point Energies= -444.485163

Sum of electronic and thermal Energies= -444.474184

Sum of electronic and thermal Enthalpies= -444.473240

Sum of electronic and thermal Free Energies= -444.522980

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 2.434207 | 1.193022 | 0.107708 |
| C | 1.067850 | 1.202229 | -0.142145 |
| C | 0.344210 | -0.000006 | -0.285667 |
| C | 1.067773 | -1.202270 | -0.141998 |
| C | 2.434130 | -1.193120 | 0.107850 |
| C | 3.137381 | -0.000064 | 0.235110 |
| H | 2.952077 | 2.142650 | 0.207579 |
| H | 0.568718 | 2.159675 | -0.224962 |
| H | 0.568572 | -2.159692 | -0.224684 |
| H | 2.951940 | -2.142769 | 0.207840 |
| H | 4.203332 | -0.000087 | 0.435026 |
| N | -1.013646 | 0.000018 | -0.580109 |
| C | -1.764301 | 1.243142 | -0.596899 |
| H | -2.696617 | 1.053834 | -1.137933 |
| H | -1.220907 | 1.982602 | -1.196032 |
| C | -1.764321 | -1.243092 | -0.596983 |
| H | -2.696538 | -1.053792 | -1.138192 |
| H | -1.220824 | -1.982573 | -1.195994 |
| C | -2.086572 | -1.823364 | 0.783718 |
| H | -1.175840 | -1.968304 | 1.370866 |

| | | | |
|---|---|---|---|
| H | -2.744994 | -1.155406 | 1.345429 |
| H | -2.588968 | -2.790755 | 0.683963 |
| C | -2.086298 | 1.823468 | 0.783839 |
| H | -1.175457 | 1.968450 | 1.370806 |
| H | -2.588728 | 2.790846 | 0.684136 |
| H | -2.744599 | 1.155522 | 1.345706 |

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**$N_2$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-109.4823772

Zero-point correction= 0.005703 (Hartree/Particle)

Thermal correction to Energy= 0.008064

Thermal correction to Enthalpy= 0.009008

Thermal correction to Gibbs Free Energy= -0.012740

Sum of electronic and zero-point Energies= -109.476674

Sum of electronic and thermal Energies= -109.474314

Sum of electronic and thermal Enthalpies= -109.473369

Sum of electronic and thermal Free Energies= -109.495117

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 0.000000 | 0.000000 | 0.550767 |
| N | 0.000000 | 0.000000 | -0.550767 |

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**$^5$A**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2073.4427797

Zero-point correction= 0.639976 (Hartree/Particle)

Thermal correction to Energy= 0.684973

Thermal correction to Enthalpy= 0.685917

Thermal correction to Gibbs Free Energy= 0.556183

Sum of electronic and zero-point Energies= -2072.802803

Sum of electronic and thermal Energies= -2072.757807

Sum of electronic and thermal Enthalpies= -2072.756863

Sum of electronic and thermal Free Energies= -2072.886597

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | 1.062520 | -0.143839 | 0.554944 |
| N | 2.447525 | -1.557199 | -0.320128 |

| | | | |
|---|---|---|---|
| C | 2.175324 | -2.869830 | -0.522601 |
| C | 3.403193 | -3.612819 | -0.718181 |
| C | 4.423207 | -2.697223 | -0.661351 |
| C | 3.793847 | -1.407078 | -0.388279 |
| C | 0.890904 | -3.430885 | -0.564266 |
| C | -0.322714 | -2.762528 | -0.460838 |
| N | -0.463062 | -1.421425 | -0.279896 |
| C | -1.789119 | -1.161143 | -0.246621 |
| C | -2.550086 | -2.397220 | -0.410037 |
| C | -1.633939 | -3.397429 | -0.538847 |
| C | -2.351160 | 0.109461 | -0.096839 |
| C | -1.666745 | 1.318186 | 0.044937 |
| N | -0.321321 | 1.450377 | 0.116530 |
| C | -0.055455 | 2.779490 | 0.226965 |
| C | -1.300350 | 3.541569 | 0.232419 |
| C | -2.306085 | 2.629871 | 0.122379 |
| C | 1.214012 | 3.340468 | 0.298484 |
| C | 2.440512 | 2.665995 | 0.219557 |
| C | 3.752164 | 3.304188 | 0.243436 |
| C | 4.672547 | 2.291832 | 0.115823 |
| C | 3.909015 | 1.062002 | 0.019127 |
| N | 2.575379 | 1.327215 | 0.099019 |
| C | 4.466644 | -0.201620 | -0.181860 |

| | | | |
|---|---|---|---|
| H | 0.840796 | -4.506921 | -0.711999 |
| H | 5.549827 | -0.256442 | -0.186650 |
| H | 1.257098 | 4.420244 | 0.410905 |
| H | -3.437116 | 0.165005 | -0.108757 |
| C | 0.824990 | -1.854764 | 2.847268 |
| H | 1.589784 | -2.568706 | 2.476299 |
| H | -0.156333 | -2.273026 | 2.538202 |
| C | -1.392449 | 5.032247 | 0.324032 |
| H | -0.905089 | 5.404679 | 1.232089 |
| H | -0.899497 | 5.514782 | -0.528008 |
| H | -2.432302 | 5.370815 | 0.341603 |
| C | -1.866680 | -4.864977 | -0.714993 |
| H | -1.384575 | -5.238591 | -1.625640 |
| H | -1.454302 | -5.434768 | 0.125649 |
| H | -2.933054 | -5.098297 | -0.783305 |
| C | 3.488912 | -5.082561 | -0.987493 |
| H | 2.980926 | -5.659114 | -0.206180 |
| H | 3.014541 | -5.341565 | -1.941458 |
| H | 4.526885 | -5.422763 | -1.035501 |
| C | 6.160993 | 2.403493 | 0.021697 |
| H | 6.638796 | 2.316652 | 1.005411 |
| H | 6.580291 | 1.617610 | -0.613821 |
| H | 6.450145 | 3.372361 | -0.398101 |

| | | | |
|---|---|---|---|
| C | 5.844505 | -2.979139 | -0.859097 |
| C | 6.731125 | -2.206274 | -1.495214 |
| H | 6.196196 | -3.932560 | -0.462320 |
| H | 7.770923 | -2.505767 | -1.585846 |
| H | 6.442993 | -1.266425 | -1.955985 |
| C | 3.976627 | 4.742535 | 0.330330 |
| C | 5.038753 | 5.358061 | 0.863421 |
| H | 3.187444 | 5.368861 | -0.086064 |
| H | 5.116149 | 6.441118 | 0.859606 |
| H | 5.843955 | 4.808516 | 1.340399 |
| C | -4.043840 | -2.496491 | -0.359812 |
| C | -4.560857 | -2.406647 | 1.078803 |
| H | -4.387091 | -3.435170 | -0.805676 |
| H | -4.503848 | -1.698914 | -0.953800 |
| H | -4.138089 | -3.211045 | 1.691678 |
| H | -4.227261 | -1.477800 | 1.555098 |
| C | -3.780619 | 2.872680 | 0.015050 |
| C | -4.263198 | 2.764593 | -1.434121 |
| H | -4.040524 | 3.861138 | 0.405944 |
| H | -4.334605 | 2.154609 | 0.629626 |
| H | -3.743738 | 3.492352 | -2.068509 |
| H | -4.014054 | 1.783904 | -1.854704 |
| C | -6.060461 | -2.479152 | 1.177279 |

| | | | |
|---|---|---|---|
| O | -6.834459 | -2.620973 | 0.258301 |
| O | -6.488494 | -2.369134 | 2.453175 |
| H | -7.452860 | -2.416515 | 2.410467 |
| C | -5.743843 | 2.984453 | -1.588477 |
| O | -6.523417 | 3.269891 | -0.709101 |
| O | -6.145396 | 2.830760 | -2.869193 |
| H | -7.100078 | 2.981441 | -2.863135 |
| O | 1.028237 | -0.563404 | 2.410565 |
| H | 0.852696 | -1.919835 | 3.952794 |

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**$^{3}$B**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.0389651

Zero-point correction= 0.732969 (Hartree/Particle)

Thermal correction to Energy= 0.783147

Thermal correction to Enthalpy= 0.784091

Thermal correction to Gibbs Free Energy= 0.648816

Sum of electronic and zero-point Energies= -2487.305996

Sum of electronic and thermal Energies= -2487.255818

Sum of electronic and thermal Enthalpies= -2487.254874

Sum of electronic and thermal Free Energies= -2487.390149

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.809515 | 0.017311 | -0.122285 |
| N | -2.318666 | -1.242171 | -0.546465 |
| C | -2.273747 | -2.600698 | -0.623796 |
| C | -3.578860 | -3.139999 | -0.914094 |
| C | -4.425202 | -2.071379 | -0.991527 |
| C | -3.607668 | -0.887969 | -0.789638 |
| C | -1.133372 | -3.373349 | -0.460511 |
| C | 0.126347 | -2.881462 | -0.176753 |
| N | 0.431810 | -1.568397 | 0.030558 |
| C | 1.767078 | -1.523824 | 0.284925 |
| C | 2.333725 | -2.859916 | 0.261144 |
| C | 1.307079 | -3.706082 | -0.037211 |
| C | 2.500555 | -0.371797 | 0.530031 |
| C | 1.998450 | 0.921056 | 0.518873 |
| N | 0.703418 | 1.270065 | 0.313424 |
| C | 0.671595 | 2.630924 | 0.307759 |
| C | 1.995177 | 3.173277 | 0.551823 |
| C | 2.825072 | 2.105260 | 0.683723 |
| C | -0.439629 | 3.407902 | 0.045095 |

| | | | |
|---|---|---|---|
| C | -1.701410 | 2.919444 | -0.259372 |
| C | -2.853735 | 3.755068 | -0.557893 |
| C | -3.887066 | 2.898118 | -0.817429 |
| C | -3.342764 | 1.562526 | -0.683364 |
| N | -2.028991 | 1.610041 | -0.338410 |
| C | -4.079823 | 0.409344 | -0.887418 |
| H | -1.239162 | -4.447443 | -0.573530 |
| H | -5.121682 | 0.524858 | -1.160272 |
| H | -0.307076 | 4.484118 | 0.062099 |
| H | 3.557165 | -0.492087 | 0.738193 |
| C | -0.215651 | -0.820578 | -2.776841 |
| H | -0.065325 | -0.431959 | -3.797781 |
| H | -1.084513 | -1.501378 | -2.812265 |
| C | 2.323667 | 4.631178 | 0.608622 |
| H | 2.109951 | 5.126490 | -0.345509 |
| H | 1.733012 | 5.138253 | 1.379272 |
| H | 3.380647 | 4.792165 | 0.838504 |
| C | 1.326227 | -5.193067 | -0.203534 |
| H | 0.627635 | -5.679856 | 0.486175 |
| H | 1.033860 | -5.482595 | -1.219258 |
| H | 2.321060 | -5.606380 | -0.016506 |
| C | -3.905809 | -4.595365 | -1.020001 |
| H | -3.293995 | -5.091298 | -1.782404 |

| | | | |
|---|---|---|---|
| H | -3.726106 | -5.109021 | -0.068862 |
| H | -4.956750 | -4.744924 | -1.280876 |
| C | -5.314645 | 3.220675 | -1.120550 |
| H | -5.515137 | 3.212432 | -2.199004 |
| H | -5.990467 | 2.496751 | -0.655516 |
| H | -5.569675 | 4.215707 | -0.744332 |
| C | -5.876140 | -2.110450 | -1.185714 |
| C | -6.758807 | -1.393851 | -0.484465 |
| H | -6.246770 | -2.805567 | -1.939973 |
| H | -7.825115 | -1.474706 | -0.674582 |
| H | -6.435790 | -0.733763 | 0.315163 |
| C | -2.853166 | 5.213896 | -0.516910 |
| C | -3.585591 | 6.026201 | -1.286391 |
| H | -2.191774 | 5.667685 | 0.220812 |
| H | -3.539181 | 7.104176 | -1.165149 |
| H | -4.233459 | 5.644646 | -2.069510 |
| C | 3.774857 | -3.217303 | 0.480601 |
| C | 4.657799 | -3.035105 | -0.770445 |
| H | 3.831186 | -4.262703 | 0.798039 |
| H | 4.205637 | -2.626099 | 1.294902 |
| H | 5.437866 | -3.807135 | -0.798465 |
| H | 4.075160 | -3.140490 | -1.688284 |
| C | 4.316878 | 2.087012 | 0.813974 |

| | | | |
|---|---|---|---|
| C | 4.966121 | 1.905207 | -0.563515 |
| H | 4.644431 | 1.271747 | 1.466533 |
| H | 4.683241 | 3.012275 | 1.267756 |
| H | 4.550862 | 1.030141 | -1.069104 |
| H | 4.731103 | 2.763999 | -1.205325 |
| C | 5.404496 | -1.721977 | -0.803631 |
| O | 5.782541 | -1.114243 | 0.178119 |
| O | 5.660451 | -1.309075 | -2.048440 |
| H | 6.157264 | -0.470246 | -1.980023 |
| C | 6.460974 | 1.788795 | -0.499730 |
| O | 7.189036 | 2.199827 | 0.366537 |
| O | 6.980225 | 1.176590 | -1.609979 |
| H | 7.936151 | 1.148904 | -1.465763 |
| O | -0.392907 | 0.241437 | -1.907468 |
| H | 0.667214 | -1.439109 | -2.531565 |
| C | -0.572696 | -2.092579 | 3.029348 |
| O | -1.978362 | -2.154364 | 2.770822 |
| C | -2.439378 | -0.956755 | 2.293515 |
| C | -1.286476 | -0.043741 | 2.042592 |
| C | -0.178976 | -0.618564 | 2.926571 |
| H | -0.402025 | -2.513211 | 4.026190 |
| H | -0.052488 | -2.711567 | 2.295551 |
| H | 0.827357 | -0.485038 | 2.532452 |

H -0.213202 -0.139022 3.914629

O -3.626377 -0.779556 2.158642

N -1.676520 1.313527 2.421127

N -0.974407 2.100620 2.953190

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**$^{3}$TS(B-C)**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2488.0389651

Zero-point correction= 0.732975 (Hartree/Particle)

Thermal correction to Energy= 0.783149

Thermal correction to Enthalpy= 0.784093

Thermal correction to Gibbs Free Energy= 0.648863

Sum of electronic and zero-point Energies= -2487.305990

Sum of electronic and thermal Energies= -2487.255816

Sum of electronic and thermal Enthalpies= -2487.254872

Sum of electronic and thermal Free Energies= -2487.390102

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Cartesian Coordinates

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Fe -0.809376 0.017259 -0.122042

| | | | |
|---|---|---|---|
| N | -2.318449 | -1.242365 | -0.546151 |
| C | -2.273352 | -2.600864 | -0.623710 |
| C | -3.578333 | -3.140269 | -0.914463 |
| C | -4.424754 | -2.071728 | -0.992039 |
| C | -3.607403 | -0.888251 | -0.789774 |
| C | -1.132924 | -3.373425 | -0.460365 |
| C | 0.126730 | -2.881442 | -0.176456 |
| N | 0.432063 | -1.568368 | 0.030949 |
| C | 1.767294 | -1.523698 | 0.285536 |
| C | 2.334008 | -2.859769 | 0.261923 |
| C | 1.307498 | -3.705990 | -0.036709 |
| C | 2.500683 | -0.371617 | 0.530582 |
| C | 1.998544 | 0.921238 | 0.519079 |
| N | 0.703521 | 1.270139 | 0.313486 |
| C | 0.671621 | 2.630999 | 0.307601 |
| C | 1.995168 | 3.173467 | 0.551543 |
| C | 2.825118 | 2.105511 | 0.683663 |
| C | -0.439683 | 3.407867 | 0.044944 |
| C | -1.701464 | 2.919317 | -0.259351 |
| C | -2.853860 | 3.754833 | -0.557872 |
| C | -3.887114 | 2.897789 | -0.817405 |
| C | -3.342702 | 1.562252 | -0.683331 |
| N | -2.028954 | 1.609875 | -0.338337 |

| | | | |
|---|---|---|---|
| C | -4.079642 | 0.409012 | -0.887563 |
| H | -1.238597 | -4.447515 | -0.573539 |
| H | -5.121462 | 0.524474 | -1.160590 |
| H | -0.307199 | 4.484095 | 0.061856 |
| H | 3.557286 | -0.491824 | 0.738847 |
| C | -0.216351 | -0.820971 | -2.776730 |
| H | -0.065307 | -0.432371 | -3.797569 |
| H | -1.085990 | -1.500770 | -2.812469 |
| C | 2.323582 | 4.631393 | 0.608135 |
| H | 2.109110 | 5.126723 | -0.345814 |
| H | 1.733459 | 5.138389 | 1.379248 |
| H | 3.380717 | 4.792462 | 0.837233 |
| C | 1.326791 | -5.192964 | -0.203108 |
| H | 0.627755 | -5.679808 | 0.486109 |
| H | 1.035103 | -5.482446 | -1.219042 |
| H | 2.321509 | -5.606267 | -0.015445 |
| C | -3.905118 | -4.595648 | -1.020721 |
| H | -3.293396 | -5.091284 | -1.783392 |
| H | -3.725167 | -5.109574 | -0.069775 |
| H | -4.956095 | -4.745249 | -1.281430 |
| C | -5.314729 | 3.220201 | -1.120513 |
| H | -5.515288 | 3.211713 | -2.198952 |
| H | -5.990471 | 2.496330 | -0.655277 |

| | | | |
|---|---|---|---|
| H | -5.569805 | 4.215290 | -0.744484 |
| C | -5.875636 | -2.110899 | -1.186686 |
| C | -6.758559 | -1.394541 | -0.485517 |
| H | -6.245975 | -2.805850 | -1.941239 |
| H | -7.824807 | -1.475423 | -0.675959 |
| H | -6.435814 | -0.734598 | 0.314344 |
| C | -2.853400 | 5.213661 | -0.516917 |
| C | -3.585875 | 6.025905 | -1.286413 |
| H | -2.192045 | 5.667512 | 0.220802 |
| H | -3.539536 | 7.103884 | -1.165182 |
| H | -4.233724 | 5.644296 | -2.069524 |
| C | 3.775096 | -3.217123 | 0.481726 |
| C | 4.658193 | -3.035465 | -0.769259 |
| H | 3.831336 | -4.262413 | 0.799547 |
| H | 4.205793 | -2.625634 | 1.295861 |
| H | 5.438602 | -3.807200 | -0.796426 |
| H | 4.075808 | -3.141855 | -1.687139 |
| C | 4.316956 | 2.087369 | 0.813610 |
| C | 4.965836 | 1.905194 | -0.564014 |
| H | 4.644729 | 1.272323 | 1.466332 |
| H | 4.683393 | 3.012797 | 1.266989 |
| H | 4.550427 | 1.029995 | -1.069246 |
| H | 4.730615 | 2.763809 | -1.205986 |

| | | | |
|---|---|---|---|
| C | 5.404450 | -1.722133 | -0.803252 |
| O | 5.782721 | -1.114000 | 0.178161 |
| O | 5.659755 | -1.309541 | -2.048297 |
| H | 6.156444 | -0.470607 | -1.980325 |
| C | 6.460708 | 1.788818 | -0.500649 |
| O | 7.189015 | 2.200049 | 0.365323 |
| O | 6.979653 | 1.176433 | -1.610936 |
| H | 7.935619 | 1.148790 | -1.466982 |
| O | -0.392588 | 0.241094 | -1.907226 |
| H | 0.665720 | -1.440580 | -2.531319 |
| C | -0.574687 | -2.092909 | 3.029336 |
| O | -1.980461 | -2.153322 | 2.770974 |
| C | -2.440290 | -0.955316 | 2.293546 |
| C | -1.286492 | -0.043375 | 2.042729 |
| C | -0.179646 | -0.619245 | 2.926854 |
| H | -0.404290 | -2.513982 | 4.026031 |
| H | -0.055161 | -2.712151 | 2.295282 |
| H | 0.826884 | -0.486567 | 2.532942 |
| H | -0.213671 | -0.139811 | 3.914970 |
| O | -3.627102 | -0.776984 | 2.158535 |
| N | -1.675346 | 1.314245 | 2.421316 |
| N | -0.972586 | 2.100649 | 2.953536 |

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$^{oss}C$

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Number of imaginary frequencies : 0 Electronic energy : HF=-2378.5176066

Zero-point correction= 0.717672 (Hartree/Particle)

Thermal correction to Energy= 0.767175

Thermal correction to Enthalpy= 0.768119

Thermal correction to Gibbs Free Energy= 0.633893

Sum of electronic and zero-point Energies= -2377.799934

Sum of electronic and thermal Energies= -2377.750432

Sum of electronic and thermal Enthalpies= -2377.749488

Sum of electronic and thermal Free Energies= -2377.883714

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.822861 | -0.053778 | -0.137715 |
| N | -1.944189 | -1.694646 | -0.339230 |
| C | -1.554700 | -3.001414 | -0.190787 |
| C | -2.677320 | -3.896404 | -0.405882 |
| C | -3.747711 | -3.110901 | -0.692399 |

| | | | |
|---|---|---|---|
| C | -3.266550 | -1.730410 | -0.673999 |
| C | -0.275403 | -3.423970 | 0.073167 |
| C | 0.862530 | -2.594819 | 0.221741 |
| N | 0.809099 | -1.235008 | 0.203476 |
| C | 2.097609 | -0.818254 | 0.353839 |
| C | 2.984760 | -1.923644 | 0.445577 |
| C | 2.193744 | -3.060758 | 0.362660 |
| C | 2.479883 | 0.538134 | 0.471629 |
| C | 1.651847 | 1.632482 | 0.405929 |
| N | 0.303701 | 1.585192 | 0.172522 |
| C | -0.124671 | 2.881690 | 0.187458 |
| C | 0.983846 | 3.784927 | 0.456252 |
| C | 2.089934 | 3.010368 | 0.591715 |
| C | -1.412343 | 3.301145 | -0.057262 |
| C | -2.511179 | 2.485464 | -0.386595 |
| C | -3.812806 | 2.955179 | -0.748037 |
| C | -4.550155 | 1.815046 | -1.059953 |
| C | -3.669068 | 0.720070 | -0.868093 |
| N | -2.437250 | 1.131693 | -0.465790 |
| C | -4.033560 | -0.639297 | -0.997454 |
| H | -0.110861 | -4.495925 | 0.135282 |
| H | -5.040460 | -0.846052 | -1.340327 |
| H | -1.585326 | 4.372570 | -0.032819 |

| | | | |
|---|---|---|---|
| H | 3.527685 | 0.726462 | 0.679487 |
| C | 0.218741 | -0.938659 | -2.651291 |
| H | -0.157263 | -1.964785 | -2.475100 |
| H | 1.292560 | -0.944643 | -2.384187 |
| C | 0.853049 | 5.272900 | 0.533235 |
| H | 0.510324 | 5.688082 | -0.421337 |
| H | 0.124501 | 5.569647 | 1.296108 |
| H | 1.805537 | 5.750428 | 0.777687 |
| C | 2.620887 | -4.496618 | 0.377283 |
| H | 2.102263 | -5.069581 | 1.155530 |
| H | 2.417611 | -4.993555 | -0.579432 |
| H | 3.694490 | -4.589920 | 0.567801 |
| C | -2.617134 | -5.384132 | -0.274760 |
| H | -1.885491 | -5.816613 | -0.967254 |
| H | -2.321792 | -5.680082 | 0.738312 |
| H | -3.589241 | -5.838689 | -0.481295 |
| C | -5.995347 | 1.731425 | -1.438496 |
| H | -6.153534 | 1.869887 | -2.516197 |
| H | -6.429265 | 0.764411 | -1.166395 |
| H | -6.571364 | 2.507742 | -0.923854 |
| C | -5.125686 | -3.552915 | -0.919270 |
| C | -6.214440 | -2.970298 | -0.409711 |
| H | -5.249749 | -4.448527 | -1.528546 |

| | | | |
|---|---|---|---|
| H | -7.206483 | -3.361636 | -0.614499 |
| H | -6.139154 | -2.107481 | 0.245630 |
| C | -4.226285 | 4.348719 | -0.739762 |
| C | -5.234944 | 4.908770 | -1.422432 |
| H | -3.645663 | 5.007616 | -0.092550 |
| H | -5.461384 | 5.964898 | -1.311403 |
| H | -5.847388 | 4.345810 | -2.118688 |
| C | 4.478912 | -1.843137 | 0.483853 |
| C | 5.055709 | -1.682305 | -0.942143 |
| H | 4.895164 | -2.749697 | 0.938651 |
| H | 4.814065 | -1.006554 | 1.107165 |
| H | 4.709179 | -2.496063 | -1.580755 |
| H | 4.701630 | -0.737790 | -1.372662 |
| C | 3.493917 | 3.461141 | 0.864175 |
| C | 4.410421 | 3.492889 | -0.381734 |
| H | 3.960584 | 2.836051 | 1.632299 |
| H | 3.457466 | 4.472713 | 1.279338 |
| H | 3.850914 | 3.786508 | -1.271053 |
| H | 5.204785 | 4.231944 | -0.218425 |
| C | 6.553802 | -1.674666 | -0.991044 |
| O | 7.278529 | -2.412956 | -1.609788 |
| O | 7.091919 | -0.689616 | -0.206329 |
| H | 8.049423 | -0.743345 | -0.325323 |

| | | | |
|---|---|---|---|
| C | 5.119325 | 2.195423 | -0.691117 |
| O | 5.168636 | 1.663436 | -1.777316 |
| O | 5.752482 | 1.701557 | 0.386994 |
| H | 6.206570 | 0.878434 | 0.120350 |
| O | -0.508292 | 0.030184 | -1.985039 |
| H | 0.158681 | -0.761148 | -3.738962 |
| C | -0.829578 | -0.249231 | 4.167271 |
| O | -2.216207 | -0.397865 | 3.903570 |
| C | -2.433145 | -0.398183 | 2.525587 |
| C | -1.207469 | -0.073076 | 1.821266 |
| C | -0.208155 | 0.297619 | 2.875189 |
| H | -0.710498 | 0.412237 | 5.031763 |
| H | 0.788797 | -0.109973 | 2.681110 |
| H | -0.097217 | 1.393045 | 2.916355 |
| O | -3.556633 | -0.634717 | 2.121021 |
| H | -0.406312 | -1.230808 | 4.423443 |

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**$^{3}$C**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2378.5661948

Zero-point correction= 0.721613 (Hartree/Particle)

Thermal correction to Energy= 0.770552

Thermal correction to Enthalpy= 0.771496

Thermal correction to Gibbs Free Energy= 0.637639

Sum of electronic and zero-point Energies= -2377.844581

Sum of electronic and thermal Energies= -2377.795643

Sum of electronic and thermal Enthalpies= -2377.794699

Sum of electronic and thermal Free Energies= -2377.928555

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.822569 | -0.057297 | -0.105332 |
| N | -1.953422 | -1.699175 | -0.339428 |
| C | -1.567355 | -2.995393 | -0.198870 |
| C | -2.680892 | -3.886482 | -0.424995 |
| C | -3.757353 | -3.091121 | -0.696949 |
| C | -3.270316 | -1.720589 | -0.660926 |
| C | -0.274274 | -3.421879 | 0.073641 |
| C | 0.823000 | -2.594365 | 0.227396 |
| N | 0.787037 | -1.233133 | 0.214845 |
| C | 2.068005 | -0.814020 | 0.371994 |
| C | 2.963757 | -1.953416 | 0.464455 |
| C | 2.184527 | -3.066691 | 0.380356 |

| | | | |
|---|---|---|---|
| C | 2.479932 | 0.507718 | 0.479116 |
| C | 1.656432 | 1.620146 | 0.397539 |
| N | 0.319176 | 1.589723 | 0.169762 |
| C | -0.101910 | 2.881290 | 0.169601 |
| C | 1.011870 | 3.779159 | 0.415084 |
| C | 2.113287 | 2.992061 | 0.559739 |
| C | -1.397553 | 3.305551 | -0.064783 |
| C | -2.468652 | 2.477929 | -0.375882 |
| C | -3.792893 | 2.955932 | -0.749695 |
| C | -4.529836 | 1.840716 | -1.038837 |
| C | -3.647347 | 0.710562 | -0.826756 |
| N | -2.416005 | 1.129443 | -0.432729 |
| C | -4.042683 | -0.608852 | -0.955357 |
| H | -0.104762 | -4.493046 | 0.125365 |
| H | -5.057514 | -0.797188 | -1.283508 |
| H | -1.575831 | 4.375844 | -0.061727 |
| H | 3.530771 | 0.682216 | 0.678833 |
| C | -0.006579 | -1.022217 | -2.675166 |
| H | -0.661456 | -1.911918 | -2.603110 |
| H | 1.006518 | -1.352752 | -2.373375 |
| C | 0.899985 | 5.270282 | 0.468953 |
| H | 0.563913 | 5.676094 | -0.492009 |
| H | 0.175510 | 5.589302 | 1.226639 |

| | | | |
|---|---|---|---|
| H | 1.858670 | 5.739320 | 0.707045 |
| C | 2.595078 | -4.505337 | 0.390981 |
| H | 2.076057 | -5.062868 | 1.178773 |
| H | 2.358454 | -4.993354 | -0.561312 |
| H | 3.670113 | -4.614416 | 0.559909 |
| C | -2.627881 | -5.377561 | -0.318188 |
| H | -1.889889 | -5.803204 | -1.008063 |
| H | -2.349462 | -5.694149 | 0.693469 |
| H | -3.599242 | -5.824257 | -0.545944 |
| C | -5.971169 | 1.750518 | -1.423883 |
| H | -6.099121 | 1.683395 | -2.511277 |
| H | -6.443824 | 0.868139 | -0.982556 |
| H | -6.515427 | 2.635449 | -1.080922 |
| C | -5.134906 | -3.529194 | -0.929216 |
| C | -6.224591 | -2.958171 | -0.407616 |
| H | -5.260420 | -4.412806 | -1.556189 |
| H | -7.216824 | -3.343928 | -0.622816 |
| H | -6.148570 | -2.110327 | 0.266828 |
| C | -4.197372 | 4.357550 | -0.753256 |
| C | -5.093981 | 4.923976 | -1.568451 |
| H | -3.715335 | 4.992098 | -0.009295 |
| H | -5.348889 | 5.975298 | -1.475305 |
| H | -5.580798 | 4.366375 | -2.362365 |

| | | | |
|---|---|---|---|
| C | 4.458378 | -1.871321 | 0.494005 |
| C | 5.013021 | -1.686852 | -0.935550 |
| H | 4.877471 | -2.784655 | 0.930957 |
| H | 4.791331 | -1.042839 | 1.127493 |
| H | 4.657413 | -2.487861 | -1.585388 |
| H | 4.654699 | -0.735185 | -1.346955 |
| C | 3.520731 | 3.435892 | 0.827600 |
| C | 4.441972 | 3.440846 | -0.415129 |
| H | 3.980461 | 2.820014 | 1.606966 |
| H | 3.491654 | 4.454451 | 1.226431 |
| H | 3.885364 | 3.708152 | -1.314477 |
| H | 5.232793 | 4.187767 | -0.269444 |
| C | 6.510374 | -1.677411 | -1.014096 |
| O | 7.214725 | -2.363577 | -1.710841 |
| O | 7.070941 | -0.760868 | -0.166012 |
| H | 8.024313 | -0.802964 | -0.319476 |
| C | 5.160260 | 2.141309 | -0.688563 |
| O | 5.239574 | 1.594558 | -1.766150 |
| O | 5.770271 | 1.662338 | 0.409823 |
| H | 6.224464 | 0.834229 | 0.161772 |
| O | -0.468418 | 0.052317 | -1.941567 |
| H | 0.052361 | -0.754247 | -3.744500 |
| C | -0.828504 | -0.183743 | 4.197196 |

| | | | |
|---|---|---|---|
| O | -2.218322 | -0.297256 | 3.938693 |
| C | -2.434860 | -0.328246 | 2.558040 |
| C | -1.202866 | -0.059678 | 1.843128 |
| C | -0.192686 | 0.308398 | 2.890108 |
| H | -0.687117 | 0.496587 | 5.044029 |
| H | 0.792931 | -0.131059 | 2.707679 |
| H | -0.049585 | 1.400652 | 2.900073 |
| O | -3.566600 | -0.545502 | 2.163318 |
| H | -0.434168 | -1.170505 | 4.480499 |

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**$^{OSS}$TS(C-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2823.2739218

Zero-point correction= 0.954652 (Hartree/Particle)

Thermal correction to Energy= 1.014074

Thermal correction to Enthalpy= 1.015018

Thermal correction to Gibbs Free Energy= 0.862404

Sum of electronic and zero-point Energies= -2822.319270

Sum of electronic and thermal Energies= -2822.259848

Sum of electronic and thermal Enthalpies= -2822.258904

Sum of electronic and thermal Free Energies= -2822.411518

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.076686 | 0.310909 | -0.715713 |
| N | -1.447703 | -1.041116 | -1.386140 |
| C | -1.304299 | -2.397361 | -1.440136 |
| C | -2.477488 | -3.018691 | -2.016518 |
| C | -3.332824 | -1.995587 | -2.335438 |
| C | -2.651176 | -0.765986 | -1.952224 |
| C | -0.164394 | -3.092709 | -1.051724 |
| C | 1.011608 | -2.529386 | -0.577331 |
| N | 1.212487 | -1.202796 | -0.353781 |
| C | 2.483405 | -1.081840 | 0.103292 |
| C | 3.128380 | -2.384878 | 0.167378 |
| C | 2.205863 | -3.291537 | -0.256053 |
| C | 3.080811 | 0.104889 | 0.510918 |
| C | 2.525265 | 1.371151 | 0.412371 |
| N | 1.297380 | 1.641425 | -0.095221 |
| C | 1.173008 | 2.989373 | -0.089011 |
| C | 2.359771 | 3.615444 | 0.476222 |
| C | 3.205126 | 2.603345 | 0.800642 |
| C | 0.082811 | 3.695054 | -0.569730 |

| | | | |
|---|---|---|---|
| C | -1.055422 | 3.142361 | -1.140259 |
| C | -2.151061 | 3.921684 | -1.704043 |
| C | -3.069619 | 3.014071 | -2.158809 |
| C | -2.521807 | 1.705351 | -1.854313 |
| N | -1.317459 | 1.816216 | -1.228879 |
| C | -3.163135 | 0.510419 | -2.154676 |
| H | -0.183080 | -4.173265 | -1.154626 |
| H | -4.144902 | 0.583788 | -2.610715 |
| H | 0.132771 | 4.777756 | -0.509029 |
| H | 4.074895 | 0.034004 | 0.939083 |
| C | 0.660886 | -0.447406 | -3.424586 |
| H | 1.064551 | -1.436516 | -3.107681 |
| H | 1.238249 | -0.168018 | -4.329790 |
| C | 2.541083 | 5.090513 | 0.642217 |
| H | 2.509113 | 5.605410 | -0.325057 |
| H | 1.748187 | 5.518219 | 1.266086 |
| H | 3.500265 | 5.329708 | 1.110186 |
| C | 2.353327 | -4.769930 | -0.431799 |
| H | 1.585788 | -5.319676 | 0.125342 |
| H | 2.254936 | -5.055538 | -1.485399 |
| H | 3.329756 | -5.119953 | -0.084513 |
| C | -2.650865 | -4.483249 | -2.265735 |
| H | -1.695289 | -4.961109 | -2.500599 |

| | | | |
|---|---|---|---|
| H | -3.070193 | -5.004438 | -1.394786 |
| H | -3.329096 | -4.652610 | -3.107485 |
| C | -4.351929 | 3.267333 | -2.885448 |
| H | -4.336697 | 4.253233 | -3.359234 |
| H | -4.517474 | 2.517888 | -3.665606 |
| H | -5.219331 | 3.237931 | -2.213589 |
| C | -4.642562 | -2.053967 | -2.972843 |
| C | -5.533611 | -3.049596 | -2.893070 |
| H | -4.911460 | -1.187561 | -3.576477 |
| H | -6.477130 | -2.997349 | -3.427371 |
| H | -5.365178 | -3.932560 | -2.284480 |
| C | -2.183686 | 5.378456 | -1.778874 |
| C | -3.272994 | 6.151136 | -1.701119 |
| H | -1.219066 | 5.868287 | -1.909922 |
| H | -3.201524 | 7.230886 | -1.790252 |
| H | -4.260381 | 5.734813 | -1.525872 |
| C | 4.570313 | -2.618720 | 0.495178 |
| C | 5.450142 | -2.382316 | -0.751223 |
| H | 4.714590 | -3.644976 | 0.852074 |
| H | 4.896929 | -1.959607 | 1.306074 |
| H | 5.112490 | -3.008529 | -1.578377 |
| H | 5.363104 | -1.335403 | -1.066900 |
| C | 4.559986 | 2.715414 | 1.433158 |

| | | | |
|---|---|---|---|
| C | 5.745027 | 2.647190 | 0.441587 |
| H | 4.692918 | 1.946939 | 2.200973 |
| H | 4.617882 | 3.675430 | 1.955478 |
| H | 5.490940 | 3.126860 | -0.504768 |
| H | 6.602733 | 3.178344 | 0.874250 |
| C | 6.906550 | -2.667018 | -0.538076 |
| O | 7.623522 | -3.372014 | -1.202839 |
| O | 7.410686 | -2.019187 | 0.557492 |
| H | 8.354103 | -2.228134 | 0.578709 |
| C | 6.246635 | 1.257946 | 0.131510 |
| O | 6.480591 | 0.824485 | -0.975005 |
| O | 6.470550 | 0.541185 | 1.247298 |
| H | 6.806748 | -0.333799 | 0.974167 |
| O | 0.750228 | 0.527382 | -2.468492 |
| H | -0.376053 | -0.649507 | -3.780790 |
| C | -0.793767 | 0.131103 | 1.204316 |
| C | -0.912684 | -1.229923 | 1.855367 |
| C | -0.214731 | 0.950117 | 2.313609 |
| C | 0.315287 | -1.231572 | 2.768064 |
| H | -0.916524 | -2.058212 | 1.149494 |
| H | -1.812598 | -1.306885 | 2.478788 |
| H | -3.348981 | -1.455134 | 0.365017 |
| O | -0.298278 | 2.134694 | 2.557638 |

| | | | |
|---|---|---|---|
| O | 0.493292 | 0.138037 | 3.155101 |
| H | 1.210347 | -1.573572 | 2.244510 |
| H | 0.180019 | -1.816267 | 3.682898 |
| C | -4.088037 | -1.775860 | 1.089120 |
| C | -4.322209 | -1.031729 | 2.254729 |
| C | -4.771747 | -2.962092 | 0.863823 |
| C | -5.233747 | -1.529790 | 3.195887 |
| N | -3.659176 | 0.198529 | 2.468199 |
| C | -5.685312 | -3.449563 | 1.794240 |
| H | -4.566102 | -3.503039 | -0.053843 |
| C | -5.903107 | -2.726864 | 2.962249 |
| H | -5.434259 | -0.986169 | 4.111784 |
| C | -3.186364 | 0.926398 | 1.387995 |
| C | -3.522313 | 0.727831 | 3.825144 |
| H | -6.212536 | -4.381187 | 1.615319 |
| H | -6.607725 | -3.089428 | 3.705371 |
| H | -3.600260 | 0.571064 | 0.444378 |
| C | -3.143506 | 2.432425 | 1.490096 |
| H | -3.038008 | 1.699380 | 3.745295 |
| H | -4.520330 | 0.907483 | 4.245912 |
| C | -2.695051 | -0.146663 | 4.767385 |
| H | -2.260216 | 2.782709 | 2.029731 |
| H | -3.101479 | 2.850821 | 0.485908 |

| | | | |
|---|---|---|---|
| H | -4.055110 | 2.793785 | 1.979987 |
| H | -3.040961 | -1.183864 | 4.768211 |
| H | -1.639933 | -0.124760 | 4.486870 |
| H | -2.779316 | 0.242384 | 5.786920 |
| H | -1.924728 | 0.605210 | 0.987352 |

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**$^{3}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2823.2920704

Zero-point correction= 0.953825 (Hartree/Particle)

Thermal correction to Energy= 1.013468

Thermal correction to Enthalpy= 1.014413

Thermal correction to Gibbs Free Energy= 0.859826

Sum of electronic and zero-point Energies= -2822.338246

Sum of electronic and thermal Energies= -2822.278602

Sum of electronic and thermal Enthalpies= -2822.277658

Sum of electronic and thermal Free Energies= -2822.432245

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.070067 | 0.304898 | -0.804050 |
| N | -1.450654 | -1.023855 | -1.472959 |
| C | -1.279677 | -2.368555 | -1.586955 |
| C | -2.454621 | -2.989927 | -2.160023 |
| C | -3.337549 | -1.973780 | -2.410416 |
| C | -2.671862 | -0.749300 | -1.994040 |
| C | -0.124039 | -3.060399 | -1.246857 |
| C | 1.032315 | -2.507023 | -0.723659 |
| N | 1.218804 | -1.192259 | -0.420590 |
| C | 2.467844 | -1.092518 | 0.100170 |
| C | 3.113028 | -2.391197 | 0.122086 |
| C | 2.216141 | -3.275578 | -0.395184 |
| C | 3.050626 | 0.079909 | 0.559839 |
| C | 2.500113 | 1.343428 | 0.428045 |
| N | 1.304013 | 1.612181 | -0.157666 |
| C | 1.172186 | 2.963318 | -0.155112 |
| C | 2.327920 | 3.585327 | 0.462944 |
| C | 3.152286 | 2.573720 | 0.843287 |
| C | 0.090823 | 3.675085 | -0.638791 |
| C | -1.068987 | 3.129489 | -1.168636 |
| C | -2.185432 | 3.917827 | -1.671895 |
| C | -3.128409 | 3.019344 | -2.089061 |
| C | -2.570573 | 1.706822 | -1.830328 |

| | | | |
|---|---|---|---|
| N | -1.339511 | 1.808218 | -1.262875 |
| C | -3.212717 | 0.519415 | -2.139490 |
| H | -0.126981 | -4.134595 | -1.399809 |
| H | -4.212738 | 0.590014 | -2.552746 |
| H | 0.143800 | 4.756076 | -0.567821 |
| H | 4.020091 | 0.003300 | 1.038138 |
| C | 1.875991 | 0.327531 | -2.900498 |
| H | 2.527961 | 1.019212 | -2.336039 |
| H | 2.014302 | 0.556518 | -3.970901 |
| C | 2.496975 | 5.059114 | 0.649168 |
| H | 2.460782 | 5.588314 | -0.309705 |
| H | 1.699806 | 5.466107 | 1.280624 |
| H | 3.454071 | 5.297865 | 1.120728 |
| C | 2.379117 | -4.743519 | -0.632554 |
| H | 1.607076 | -5.320362 | -0.111064 |
| H | 2.300792 | -4.984640 | -1.698559 |
| H | 3.352389 | -5.099333 | -0.283334 |
| C | -2.607915 | -4.447407 | -2.455484 |
| H | -1.662293 | -4.888432 | -2.785032 |
| H | -2.941667 | -5.008931 | -1.573655 |
| H | -3.348333 | -4.602431 | -3.245531 |
| C | -4.455198 | 3.283805 | -2.724256 |
| H | -4.473458 | 4.280107 | -3.175153 |

| | | | |
|---|---|---|---|
| H | -4.673645 | 2.551613 | -3.507564 |
| H | -5.270675 | 3.235658 | -1.992143 |
| C | -4.664622 | -2.031763 | -3.015312 |
| C | -5.550455 | -3.025710 | -2.893249 |
| H | -4.946437 | -1.172709 | -3.623402 |
| H | -6.510050 | -2.982731 | -3.398847 |
| H | -5.364691 | -3.892211 | -2.266720 |
| C | -2.217954 | 5.376463 | -1.720838 |
| C | -3.299639 | 6.144276 | -1.553871 |
| H | -1.264312 | 5.868677 | -1.910122 |
| H | -3.235617 | 7.225583 | -1.626932 |
| H | -4.270425 | 5.721664 | -1.313960 |
| C | 4.540612 | -2.638724 | 0.497776 |
| C | 5.463748 | -2.380423 | -0.713106 |
| H | 4.666772 | -3.672885 | 0.837370 |
| H | 4.840198 | -1.999167 | 1.333958 |
| H | 5.153359 | -2.990690 | -1.562620 |
| H | 5.392237 | -1.326339 | -1.008630 |
| C | 4.464530 | 2.688549 | 1.558778 |
| C | 5.704947 | 2.662305 | 0.635463 |
| H | 4.562373 | 1.903259 | 2.314440 |
| H | 4.476647 | 3.635446 | 2.106751 |
| H | 5.512049 | 3.207013 | -0.289997 |

| | | | |
|---|---|---|---|
| H | 6.543187 | 3.144481 | 1.153403 |
| C | 6.909745 | -2.678386 | -0.450851 |
| O | 7.637559 | -3.403932 | -1.080239 |
| O | 7.383981 | -2.014805 | 0.647407 |
| H | 8.322177 | -2.237593 | 0.713282 |
| C | 6.183854 | 1.279496 | 0.267572 |
| O | 6.373077 | 0.872652 | -0.857571 |
| O | 6.427076 | 0.531554 | 1.357501 |
| H | 6.754247 | -0.338775 | 1.059846 |
| O | 0.539158 | 0.443186 | -2.565942 |
| H | 2.279564 | -0.690284 | -2.736693 |
| C | -0.846614 | 0.135098 | 1.128928 |
| C | -0.865646 | -1.239820 | 1.791690 |
| C | -0.263925 | 0.993478 | 2.175923 |
| C | 0.285116 | -1.148958 | 2.795002 |
| H | -0.748040 | -2.077582 | 1.105111 |
| H | -1.805291 | -1.399437 | 2.334087 |
| H | -3.533982 | -1.347293 | 0.292219 |
| O | -0.304083 | 2.198852 | 2.334140 |
| O | 0.382721 | 0.234171 | 3.136414 |
| H | 1.234998 | -1.476042 | 2.357975 |
| H | 0.107441 | -1.708200 | 3.719894 |
| C | -4.138159 | -1.817046 | 1.056001 |

| | | | |
|---|---|---|---|
| C | -4.389997 | -1.148426 | 2.272014 |
| C | -4.603862 | -3.105131 | 0.839243 |
| C | -5.099894 | -1.858537 | 3.262667 |
| N | -3.950434 | 0.153647 | 2.478567 |
| C | -5.324660 | -3.788933 | 1.814917 |
| H | -4.374827 | -3.575506 | -0.112375 |
| C | -5.557961 | -3.149505 | 3.028677 |
| H | -5.301616 | -1.404007 | 4.225382 |
| C | -3.425561 | 0.912141 | 1.376712 |
| C | -3.849791 | 0.660461 | 3.838582 |
| H | -5.681878 | -4.799027 | 1.640028 |
| H | -6.106759 | -3.659928 | 3.816315 |
| H | -3.946942 | 0.630024 | 0.460611 |
| C | -3.398857 | 2.414646 | 1.548701 |
| H | -3.650368 | 1.729234 | 3.782659 |
| H | -4.824338 | 0.565137 | 4.335910 |
| C | -2.760211 | -0.003709 | 4.683444 |
| H | -2.602991 | 2.739412 | 2.223344 |
| H | -3.182336 | 2.866669 | 0.580031 |
| H | -4.366303 | 2.806090 | 1.894929 |
| H | -2.881981 | -1.091024 | 4.701673 |
| H | -1.767216 | 0.226311 | 4.290536 |
| H | -2.811733 | 0.363076 | 5.714584 |

H -2.146874 0.556345 1.102835

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**$^3$D**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2823.3218885

Zero-point correction= 0.957254 (Hartree/Particle)

Thermal correction to Energy= 1.018102

Thermal correction to Enthalpy= 1.019046

Thermal correction to Gibbs Free Energy= 0.860275

Sum of electronic and zero-point Energies= -2822.364635

Sum of electronic and thermal Energies= -2822.303786

Sum of electronic and thermal Enthalpies= -2822.302842

Sum of electronic and thermal Free Energies= -2822.461614

.....

Cartesian Coordinates

.....

Fe 0.030238 -0.137496 -0.821415

N 1.241126 1.382843 -1.380330

C 0.973921 2.717787 -1.344127

C 2.090794 3.478737 -1.853001

| | | | |
|---|---|---|---|
| C | 3.046757 | 2.561325 | -2.203304 |
| C | 2.481679 | 1.254803 | -1.911424 |
| C | -0.221093 | 3.275443 | -0.908234 |
| C | -1.310494 | 2.564236 | -0.438225 |
| N | -1.366904 | 1.209315 | -0.292677 |
| C | -2.599092 | 0.929582 | 0.201210 |
| C | -3.364828 | 2.150483 | 0.371957 |
| C | -2.558904 | 3.172189 | -0.029340 |
| C | -3.067102 | -0.334810 | 0.536185 |
| C | -2.402246 | -1.527822 | 0.310192 |
| N | -1.178717 | -1.644938 | -0.264251 |
| C | -0.940426 | -2.975162 | -0.388069 |
| C | -2.047984 | -3.744668 | 0.149912 |
| C | -2.956721 | -2.842368 | 0.603085 |
| C | 0.194850 | -3.544799 | -0.930215 |
| C | 1.290901 | -2.841996 | -1.406434 |
| C | 2.487438 | -3.461177 | -1.958897 |
| C | 3.327881 | -2.436068 | -2.290731 |
| C | 2.629485 | -1.215670 | -1.934480 |
| N | 1.412890 | -1.497032 | -1.396195 |
| C | 3.140080 | 0.054098 | -2.147520 |
| H | -0.310752 | 4.356166 | -0.939964 |
| H | 4.142995 | 0.116501 | -2.555976 |

| | | | |
|---|---|---|---|
| H | 0.242653 | -4.627890 | -0.955738 |
| H | -4.043228 | -0.392578 | 1.003797 |
| C | -1.145584 | 0.782134 | -3.277374 |
| H | -2.029690 | 1.263330 | -2.816033 |
| H | -1.453804 | 0.451667 | -4.284459 |
| C | -2.096602 | -5.238449 | 0.192958 |
| H | -2.027744 | -5.667163 | -0.813231 |
| H | -1.263329 | -5.640377 | 0.779550 |
| H | -3.026934 | -5.598293 | 0.640790 |
| C | -2.860486 | 4.636116 | -0.093017 |
| H | -2.136973 | 5.218726 | 0.488264 |
| H | -2.821980 | 5.005276 | -1.124093 |
| H | -3.856854 | 4.856912 | 0.299839 |
| C | 2.140989 | 4.967250 | -1.979159 |
| H | 1.158459 | 5.380636 | -2.225704 |
| H | 2.472213 | 5.441808 | -1.046495 |
| H | 2.841356 | 5.262951 | -2.765788 |
| C | 4.685115 | -2.503941 | -2.912483 |
| H | 4.819434 | -3.451615 | -3.441652 |
| H | 4.837693 | -1.690078 | -3.627872 |
| H | 5.478050 | -2.430722 | -2.156944 |
| C | 4.369572 | 2.784746 | -2.778539 |
| C | 5.170402 | 3.828145 | -2.536858 |

| | | | |
|---|---|---|---|
| H | 4.726863 | 2.017582 | -3.464782 |
| H | 6.136633 | 3.915325 | -3.023688 |
| H | 4.904448 | 4.608076 | -1.830111 |
| C | 2.686540 | -4.899709 | -2.103936 |
| C | 3.848140 | -5.548450 | -1.971116 |
| H | 1.796703 | -5.484362 | -2.336107 |
| H | 3.908684 | -6.623198 | -2.112236 |
| H | 4.762952 | -5.035199 | -1.691101 |
| C | -4.805431 | 2.220272 | 0.773185 |
| C | -5.715831 | 2.023532 | -0.458301 |
| H | -5.020199 | 3.191707 | 1.232484 |
| H | -5.036719 | 1.463080 | 1.528720 |
| H | -5.465778 | 2.748681 | -1.234268 |
| H | -5.560845 | 1.019006 | -0.871019 |
| C | -4.263685 | -3.129537 | 1.279284 |
| C | -5.494015 | -3.108836 | 0.342268 |
| H | -4.431221 | -2.433989 | 2.107151 |
| H | -4.204897 | -4.124442 | 1.730718 |
| H | -5.243774 | -3.514172 | -0.639230 |
| H | -6.284433 | -3.731143 | 0.780346 |
| C | -7.179349 | 2.168133 | -0.165109 |
| O | -7.973228 | 2.884630 | -0.720757 |
| O | -7.584265 | 1.364175 | 0.865019 |

| | | | |
|---|---|---|---|
| H | -8.537860 | 1.496305 | 0.950980 |
| C | -6.111836 | -1.747624 | 0.135891 |
| O | -6.376940 | -1.247725 | -0.935148 |
| O | -6.392414 | -1.143889 | 1.303691 |
| H | -6.809255 | -0.283760 | 1.104791 |
| O | -0.672675 | -0.294293 | -2.553789 |
| H | -0.390798 | 1.579178 | -3.419461 |
| C | 0.995732 | -0.061966 | 1.057190 |
| C | 0.816423 | 1.200239 | 1.899510 |
| C | 0.566240 | -1.131280 | 1.971364 |
| C | -0.330821 | 0.796478 | 2.826338 |
| H | 0.579810 | 2.098414 | 1.328558 |
| H | 1.714929 | 1.417424 | 2.491422 |
| H | 4.053659 | 1.107709 | 0.225485 |
| O | 0.820765 | -2.323738 | 1.985091 |
| O | -0.233412 | -0.624704 | 2.963541 |
| H | -1.308820 | 1.041482 | 2.400593 |
| H | -0.261811 | 1.231901 | 3.828634 |
| C | 4.184916 | 1.639285 | 1.158275 |
| C | 4.384270 | 0.937137 | 2.364781 |
| C | 4.073842 | 3.021065 | 1.146459 |
| C | 4.455521 | 1.700581 | 3.549533 |
| N | 4.487310 | -0.452995 | 2.388061 |

| | | | |
|---|---|---|---|
| C | 4.153031 | 3.765565 | 2.320684 |
| H | 3.896022 | 3.509417 | 0.193904 |
| C | 4.340029 | 3.084868 | 3.518742 |
| H | 4.577552 | 1.219921 | 4.511770 |
| C | 4.610550 | -1.218972 | 1.229997 |
| C | 4.478511 | -1.143945 | 3.673738 |
| H | 4.054017 | 4.846319 | 2.302945 |
| H | 4.391014 | 3.633289 | 4.455887 |
| H | 4.807941 | -0.669094 | 0.320971 |
| C | 4.031274 | -2.591849 | 1.130792 |
| H | 4.885982 | -2.141927 | 3.509853 |
| H | 5.182710 | -0.647408 | 4.351494 |
| C | 3.089595 | -1.246451 | 4.299539 |
| H | 2.937731 | -2.592613 | 1.266474 |
| H | 4.237648 | -2.994904 | 0.137267 |
| H | 4.449680 | -3.301305 | 1.858478 |
| H | 2.623912 | -0.260882 | 4.391444 |
| H | 2.433114 | -1.866451 | 3.684884 |
| H | 3.157209 | -1.688465 | 5.299764 |
| H | 2.025200 | -0.239956 | 0.743001 |

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**$^{6}$TS(D-E)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2379.2247583

Zero-point correction= 0.729080 (Hartree/Particle)

Thermal correction to Energy= 0.779145

Thermal correction to Enthalpy= 0.780089

Thermal correction to Gibbs Free Energy= 0.641361

Sum of electronic and zero-point Energies= -2378.495678

Sum of electronic and thermal Energies= -2378.445614

Sum of electronic and thermal Enthalpies= -2378.444670

Sum of electronic and thermal Free Energies= -2378.583397

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.765133 | 0.532438 | -0.881581 |
| N | -2.134401 | -1.143421 | -0.666918 |
| C | -1.805309 | -2.456221 | -0.787727 |
| C | -2.997488 | -3.277912 | -0.883018 |
| C | -4.058723 | -2.411974 | -0.816860 |
| C | -3.488757 | -1.073406 | -0.688539 |
| C | -0.504286 | -2.960069 | -0.742551 |
| C | 0.663144 | -2.245573 | -0.483321 |

| | | | |
|---|---|---|---|
| N | 0.733659 | -0.903208 | -0.280876 |
| C | 2.013966 | -0.626041 | 0.074010 |
| C | 2.811296 | -1.846184 | 0.065483 |
| C | 1.966717 | -2.860311 | -0.280304 |
| C | 2.491054 | 0.629556 | 0.452289 |
| C | 1.758312 | 1.812970 | 0.541478 |
| N | 0.434937 | 1.921809 | 0.270130 |
| C | 0.087706 | 3.214022 | 0.500543 |
| C | 1.253759 | 3.981740 | 0.918887 |
| C | 2.297199 | 3.104312 | 0.959852 |
| C | -1.202362 | 3.731121 | 0.411617 |
| C | -2.376482 | 3.025066 | 0.133038 |
| C | -3.719151 | 3.597244 | 0.145881 |
| C | -4.578310 | 2.561712 | -0.123591 |
| C | -3.747991 | 1.381976 | -0.288711 |
| N | -2.435030 | 1.699795 | -0.131040 |
| C | -4.232891 | 0.098032 | -0.540525 |
| H | -0.399102 | -4.037112 | -0.829710 |
| H | -5.312796 | -0.009239 | -0.585941 |
| H | -1.312013 | 4.788741 | 0.634358 |
| H | 3.533313 | 0.680099 | 0.748911 |
| C | -1.524353 | 1.894547 | -3.300441 |
| H | -2.591258 | 1.614266 | -3.184675 |

| | | | |
|---|---|---|---|
| H | -1.344042 | 1.980452 | -4.389104 |
| C | 1.235229 | 5.442905 | 1.242402 |
| H | 0.906097 | 6.032687 | 0.379437 |
| H | 0.544791 | 5.660954 | 2.065298 |
| H | 2.224147 | 5.808467 | 1.532365 |
| C | 2.239398 | -4.327486 | -0.382716 |
| H | 1.622217 | -4.881288 | 0.335175 |
| H | 2.002816 | -4.706885 | -1.382922 |
| H | 3.289588 | -4.557492 | -0.181179 |
| C | -2.999012 | -4.767122 | -1.004827 |
| H | -2.228809 | -5.105483 | -1.705302 |
| H | -2.789689 | -5.233758 | -0.035267 |
| H | -3.967258 | -5.129310 | -1.360832 |
| C | -6.065340 | 2.606105 | -0.276285 |
| H | -6.390310 | 3.603813 | -0.587010 |
| H | -6.407672 | 1.888113 | -1.027449 |
| H | -6.581675 | 2.370093 | 0.662759 |
| C | -5.489450 | -2.709005 | -0.844978 |
| C | -6.080390 | -3.767350 | -0.281241 |
| H | -6.117520 | -1.989303 | -1.370901 |
| H | -7.151718 | -3.923047 | -0.366187 |
| H | -5.516854 | -4.494296 | 0.295764 |
| C | -4.020433 | 5.007288 | 0.369965 |

| | | | |
|---|---|---|---|
| C | -5.125094 | 5.507427 | 0.935247 |
| H | -3.258473 | 5.711455 | 0.035686 |
| H | -5.265142 | 6.579404 | 1.035922 |
| H | -5.908218 | 4.869017 | 1.332029 |
| C | 4.290612 | -1.914198 | 0.290421 |
| C | 5.047872 | -1.577558 | -1.013026 |
| H | 4.575984 | -2.917203 | 0.626580 |
| H | 4.596081 | -1.221136 | 1.081250 |
| H | 4.735819 | -2.248384 | -1.814747 |
| H | 4.812045 | -0.550968 | -1.319197 |
| C | 3.714214 | 3.393362 | 1.360301 |
| C | 4.715974 | 3.472517 | 0.184215 |
| H | 4.071420 | 2.647532 | 2.077607 |
| H | 3.737499 | 4.352459 | 1.886518 |
| H | 4.240217 | 3.871494 | -0.712829 |
| H | 5.536282 | 4.147993 | 0.459265 |
| C | 6.539069 | -1.682040 | -0.895115 |
| O | 7.287962 | -2.334647 | -1.577228 |
| O | 7.034766 | -0.922353 | 0.130662 |
| H | 7.995043 | -1.028259 | 0.101151 |
| C | 5.381133 | 2.169757 | -0.192285 |
| O | 5.543681 | 1.767774 | -1.322931 |
| O | 5.839993 | 1.505579 | 0.882469 |

| | | | |
|---|---|---|---|
| H | 6.264375 | 0.683803 | 0.568328 |
| O | -0.656948 | 0.994382 | -2.715579 |
| H | -1.429861 | 2.920748 | -2.889437 |
| C | -0.127819 | -2.816978 | 2.422017 |
| C | -1.101332 | -1.712142 | 2.530778 |
| C | -0.819547 | -4.067732 | 2.196376 |
| C | -2.448133 | -2.464319 | 2.536985 |
| H | -1.019172 | -1.040343 | 1.663630 |
| H | -0.956356 | -1.094786 | 3.425241 |
| O | -0.371732 | -5.174685 | 1.965648 |
| O | -2.162062 | -3.845900 | 2.269347 |
| H | -3.128668 | -2.106741 | 1.762405 |
| H | -2.948921 | -2.412232 | 3.509024 |
| H | 0.947820 | -2.721963 | 2.372582 |

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**$^2S_2^\bullet$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-444.0603958

Zero-point correction= 0.219132 (Hartree/Particle)

Thermal correction to Energy= 0.230300

Thermal correction to Enthalpy= 0.231244

Thermal correction to Gibbs Free Energy= 0.181537

Sum of electronic and zero-point Energies= -443.841264

Sum of electronic and thermal Energies= -443.830096

Sum of electronic and thermal Enthalpies= -443.829152

Sum of electronic and thermal Free Energies= -443.878859

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -2.263394 | -1.336016 | 0.448199 |
| C | -0.887856 | -1.227709 | 0.279835 |
| C | -0.321599 | -0.037030 | -0.201702 |
| C | -1.176935 | 1.034493 | -0.506548 |
| C | -2.547370 | 0.919353 | -0.317474 |
| C | -3.104246 | -0.264973 | 0.160100 |
| H | -2.678009 | -2.267085 | 0.823000 |
| H | -0.252457 | -2.067067 | 0.541736 |
| H | -0.751892 | 1.941877 | -0.922529 |
| H | -3.188342 | 1.760305 | -0.565071 |
| H | -4.176261 | -0.352595 | 0.301510 |
| N | 1.059922 | 0.088311 | -0.393554 |
| C | 1.858527 | -1.075814 | -0.756287 |
| H | 2.544918 | -0.774617 | -1.557914 |

| | | | |
|---|---|---|---|
| H | 1.195988 | -1.834365 | -1.181722 |
| C | 1.709678 | 1.314230 | -0.296768 |
| H | 2.693073 | 1.321077 | -0.758435 |
| C | 1.467600 | 2.241706 | 0.852882 |
| H | 0.404517 | 2.371663 | 1.074514 |
| H | 1.942313 | 1.872946 | 1.776672 |
| H | 1.889599 | 3.227576 | 0.638383 |
| C | 2.659344 | -1.645238 | 0.413524 |
| H | 1.999570 | -1.984077 | 1.217371 |
| H | 3.271191 | -2.491875 | 0.087371 |
| H | 3.323831 | -0.879952 | 0.825429 |

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**$^3$E**

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Number of imaginary frequencies : 0 Electronic energy : HF=-749.8200722

Zero-point correction= 0.306795 (Hartree/Particle)

Thermal correction to Energy= 0.324726

Thermal correction to Enthalpy= 0.325670

Thermal correction to Gibbs Free Energy= 0.258921

Sum of electronic and zero-point Energies= -749.513278

Sum of electronic and thermal Energies= -749.495347

Sum of electronic and thermal Enthalpies= -749.494402

Sum of electronic and thermal Free Energies= -749.561151

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 1.046184 | 1.152805 | 1.197288 |
| C | 1.938122 | 0.096329 | 1.718465 |
| C | 1.670793 | 1.816968 | 0.069055 |
| C | 3.215016 | 0.303029 | 0.872942 |
| O | 2.921150 | 1.306195 | -0.102959 |
| O | 1.221527 | 2.674790 | -0.660227 |
| H | 1.501385 | -0.897640 | 1.550197 |
| H | 2.128349 | 0.188387 | 2.794552 |
| H | 3.504160 | -0.606034 | 0.341454 |
| H | 4.059517 | 0.652862 | 1.473283 |
| C | 1.330949 | -1.289052 | -1.631409 |
| C | 1.529886 | -2.464944 | -0.909680 |
| C | 0.545415 | -2.866844 | -0.010544 |
| C | -0.602723 | -2.106927 | 0.185171 |
| C | -0.809450 | -0.915246 | -0.537723 |
| C | 0.181116 | -0.530775 | -1.463757 |
| H | 2.077167 | -0.953295 | -2.344710 |

| | | | |
|---|---|---|---|
| H | 2.425618 | -3.059815 | -1.053783 |
| H | 0.671443 | -3.781798 | 0.561058 |
| H | -1.325883 | -2.444397 | 0.917718 |
| H | 0.043616 | 0.364095 | -2.057823 |
| N | -1.946902 | -0.128525 | -0.355696 |
| C | -3.072708 | -0.647512 | 0.412172 |
| C | -1.949050 | 1.220921 | -0.699311 |
| H | -3.989847 | -0.215702 | 0.004206 |
| C | -3.216816 | 1.982336 | -0.870018 |
| H | -2.980086 | 2.985318 | -1.231350 |
| H | -3.891689 | 1.518314 | -1.604165 |
| H | -3.796344 | 2.105808 | 0.058915 |
| H | -0.991404 | 1.711001 | -0.814740 |
| H | 0.029902 | 1.358056 | 1.504289 |
| H | -3.146299 | -1.724456 | 0.244197 |
| C | -2.972298 | -0.324094 | 1.903151 |
| H | -3.836256 | -0.718692 | 2.446003 |
| H | -2.064991 | -0.751654 | 2.340157 |
| H | -2.938070 | 0.759462 | 2.051083 |

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**$^{3}$TS(E-P)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-749.8129555

Zero-point correction= 0.306101 (Hartree/Particle)

Thermal correction to Energy= 0.323505

Thermal correction to Enthalpy= 0.324449

Thermal correction to Gibbs Free Energy= 0.258397

Sum of electronic and zero-point Energies= -749.506855

Sum of electronic and thermal Energies= -749.489451

Sum of electronic and thermal Enthalpies= -749.488507

Sum of electronic and thermal Free Energies= -749.554558

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 1.629365 | -1.044537 | -1.178616 |
| C | 2.389942 | 0.005507 | -1.890452 |
| C | 2.252623 | -1.323258 | 0.102410 |
| C | 3.382288 | 0.468083 | -0.800149 |
| H | 1.753571 | 0.821043 | -2.252128 |
| H | 2.910133 | -0.401161 | -2.769290 |
| H | -0.396073 | -1.612264 | 0.785289 |
| O | 1.959240 | -2.151473 | 0.935347 |

| | | | |
|---|---|---|---|
| O | 3.326637 | -0.491604 | 0.253262 |
| H | 3.097872 | 1.443916 | -0.391400 |
| H | 4.413710 | 0.524394 | -1.153153 |
| C | -1.324811 | -1.253952 | 0.354599 |
| C | -1.464562 | 0.104269 | 0.018245 |
| C | -2.350909 | -2.151173 | 0.089021 |
| C | -2.654549 | 0.519762 | -0.600376 |
| N | -0.422544 | 1.010336 | 0.268420 |
| C | -3.529531 | -1.733858 | -0.525444 |
| H | -2.214727 | -3.195468 | 0.353576 |
| C | -3.666869 | -0.393811 | -0.872373 |
| H | -2.804269 | 1.562556 | -0.857554 |
| C | 0.455204 | 0.878007 | 1.340266 |
| C | -0.281088 | 2.205002 | -0.552869 |
| H | -4.324838 | -2.441841 | -0.733240 |
| H | -4.577615 | -0.045230 | -1.350213 |
| H | 1.315162 | 1.536923 | 1.273620 |
| C | 0.030658 | 0.403306 | 2.690784 |
| H | 0.792379 | 2.363495 | -0.724309 |
| H | -0.729686 | 2.012324 | -1.531717 |
| C | -0.872708 | 3.461407 | 0.084893 |
| H | -0.366570 | -0.615520 | 2.695371 |
| H | 0.891888 | 0.418502 | 3.362134 |

| | | | |
|---|---|---|---|
| H | -0.749587 | 1.051437 | 3.120279 |
| H | -1.948414 | 3.355822 | 0.249343 |
| H | -0.402508 | 3.646627 | 1.054889 |
| H | -0.703596 | 4.334445 | -0.552727 |
| H | 0.743635 | -1.556259 | -1.526216 |

**(U)M06 optimizations**

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$^{oss}$**C**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2377.77077

Zero-point correction= 0.711032 (Hartree/Particle)

Thermal correction to Energy= 0.760323

Thermal correction to Enthalpy= 0.761267

Thermal correction to Gibbs Free Energy= 0.627897

Sum of electronic and zero-point Energies= -2377.059738

Sum of electronic and thermal Energies= -2377.010447

Sum of electronic and thermal Enthalpies= -2377.009503

Sum of electronic and thermal Free Energies= -2377.142873

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.825030 | -0.091655 | -0.031013 |
| N | -1.987727 | -1.712376 | -0.272197 |
| C | -1.594335 | -3.011132 | -0.172075 |
| C | -2.698088 | -3.905011 | -0.423153 |
| C | -3.783612 | -3.111362 | -0.680262 |
| C | -3.299179 | -1.740807 | -0.618444 |
| C | -0.298725 | -3.442225 | 0.072472 |
| C | 0.802039 | -2.622493 | 0.252897 |
| N | 0.771639 | -1.261103 | 0.318219 |
| C | 2.062081 | -0.864615 | 0.493351 |
| C | 2.947524 | -2.007904 | 0.511347 |
| C | 2.157533 | -3.110772 | 0.364152 |
| C | 2.487715 | 0.447861 | 0.638926 |
| C | 1.672807 | 1.562226 | 0.512677 |
| N | 0.344892 | 1.525887 | 0.210102 |
| C | -0.065860 | 2.823783 | 0.162258 |
| C | 1.034276 | 3.718544 | 0.441562 |
| C | 2.124959 | 2.928558 | 0.667827 |
| C | -1.348331 | 3.255533 | -0.132166 |
| C | -2.424275 | 2.437158 | -0.443768 |
| C | -3.722750 | 2.929136 | -0.874695 |

| | | | |
|---|---|---|---|
| C | -4.477044 | 1.815131 | -1.143673 |
| C | -3.629607 | 0.681363 | -0.862086 |
| N | -2.398266 | 1.082933 | -0.443238 |
| C | -4.052132 | -0.632335 | -0.960336 |
| H | -0.124899 | -4.517712 | 0.075872 |
| H | -5.057626 | -0.813933 | -1.328225 |
| H | -1.508421 | 4.331588 | -0.170695 |
| H | 3.539318 | 0.613274 | 0.863820 |
| C | 0.759672 | -0.033755 | -2.445800 |
| H | 1.442680 | -0.876456 | -2.184592 |
| H | 1.295393 | 0.893589 | -2.143237 |
| C | 0.941540 | 5.204724 | 0.444823 |
| H | 0.648518 | 5.592080 | -0.540354 |
| H | 0.193357 | 5.566580 | 1.162884 |
| H | 1.899962 | 5.669166 | 0.704611 |
| C | 2.566629 | -4.539036 | 0.264885 |
| H | 2.074938 | -5.159837 | 1.026117 |
| H | 2.304670 | -4.967735 | -0.711876 |
| H | 3.649067 | -4.656662 | 0.394309 |
| C | -2.629867 | -5.390344 | -0.358708 |
| H | -1.874402 | -5.792296 | -1.047577 |
| H | -2.362970 | -5.741928 | 0.647324 |
| H | -3.591952 | -5.846372 | -0.616476 |

| | | | |
|---|---|---|---|
| C | -5.902555 | 1.741831 | -1.561820 |
| H | -6.016098 | 1.706242 | -2.655038 |
| H | -6.394984 | 0.849962 | -1.156285 |
| H | -6.453822 | 2.622175 | -1.208563 |
| C | -5.142588 | -3.559569 | -0.932553 |
| C | -6.268579 | -2.948417 | -0.544361 |
| H | -5.235168 | -4.511660 | -1.463619 |
| H | -7.244245 | -3.368431 | -0.777490 |
| H | -6.247397 | -2.033250 | 0.044132 |
| C | -4.090501 | 4.329002 | -0.944348 |
| C | -5.025642 | 4.879449 | -1.730537 |
| H | -3.541769 | 4.995600 | -0.273656 |
| H | -5.241812 | 5.944044 | -1.683783 |
| H | -5.583575 | 4.297592 | -2.460509 |
| C | 4.435682 | -1.932165 | 0.464103 |
| C | 4.896043 | -1.745173 | -0.993020 |
| H | 4.882656 | -2.849222 | 0.874363 |
| H | 4.813720 | -1.104839 | 1.080478 |
| H | 4.493822 | -2.544426 | -1.624464 |
| H | 4.500911 | -0.790804 | -1.376677 |
| C | 3.514334 | 3.377350 | 0.981343 |
| C | 4.452370 | 3.424514 | -0.240397 |
| H | 3.971674 | 2.747884 | 1.756116 |

| | | | |
|---|---|---|---|
| H | 3.467603 | 4.388209 | 1.407210 |
| H | 3.919121 | 3.790843 | -1.123509 |
| H | 5.284907 | 4.110214 | -0.027448 |
| C | 6.376530 | -1.725880 | -1.178150 |
| O | 7.035159 | -2.384420 | -1.942294 |
| O | 6.987475 | -0.830168 | -0.341429 |
| H | 7.929971 | -0.868052 | -0.563966 |
| C | 5.078596 | 2.103682 | -0.590175 |
| O | 5.019518 | 1.548831 | -1.663746 |
| O | 5.772276 | 1.603243 | 0.449434 |
| H | 6.174958 | 0.761016 | 0.153926 |
| O | -0.496021 | -0.154168 | -1.910056 |
| H | 0.712314 | -0.014718 | -3.552430 |
| C | -0.946409 | -0.102578 | 4.232148 |
| O | -2.329863 | -0.167240 | 3.927801 |
| C | -2.514421 | -0.209072 | 2.549662 |
| C | -1.230805 | -0.024840 | 1.863129 |
| C | -0.244319 | 0.301715 | 2.936894 |
| H | -0.804819 | 0.605959 | 5.058415 |
| H | 0.720220 | -0.202860 | 2.797109 |
| H | -0.028004 | 1.385524 | 2.915861 |
| O | -3.636635 | -0.365324 | 2.120693 |
| H | -0.610278 | -1.093168 | 4.577253 |

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$^{3}$C

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Number of imaginary frequencies : 0 Electronic energy : HF=-2377.7664397

Zero-point correction= 0.711080 (Hartree/Particle)

Thermal correction to Energy= 0.760455

Thermal correction to Enthalpy= 0.761399

Thermal correction to Gibbs Free Energy= 0.626822

Sum of electronic and zero-point Energies= -2377.055360

Sum of electronic and thermal Energies= -2377.005984

Sum of electronic and thermal Enthalpies= -2377.005040

Sum of electronic and thermal Free Energies= -2377.139618

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.808506 | -0.060723 | -0.079304 |
| N | -1.920079 | -1.698830 | -0.321094 |
| C | -1.535128 | -2.991718 | -0.120923 |
| C | -2.633782 | -3.893451 | -0.348497 |
| C | -3.707257 | -3.112546 | -0.686728 |

| | | | |
|---|---|---|---|
| C | -3.225978 | -1.743101 | -0.688251 |
| C | -0.247467 | -3.406731 | 0.185643 |
| C | 0.846384 | -2.568102 | 0.304796 |
| N | 0.801698 | -1.205756 | 0.249127 |
| C | 2.087583 | -0.781520 | 0.378282 |
| C | 2.985509 | -1.910071 | 0.488740 |
| C | 2.207844 | -3.030691 | 0.448992 |
| C | 2.496553 | 0.541358 | 0.455697 |
| C | 1.657148 | 1.641349 | 0.389624 |
| N | 0.313596 | 1.585673 | 0.187214 |
| C | -0.127531 | 2.872171 | 0.220460 |
| C | 0.970105 | 3.783383 | 0.461541 |
| C | 2.092363 | 3.012281 | 0.562192 |
| C | -1.430803 | 3.281877 | -0.000931 |
| C | -2.477895 | 2.444029 | -0.354601 |
| C | -3.791202 | 2.912999 | -0.765370 |
| C | -4.497146 | 1.791466 | -1.120358 |
| C | -3.611099 | 0.673758 | -0.899225 |
| N | -2.399641 | 1.095174 | -0.442481 |
| C | -3.990297 | -0.647587 | -1.050418 |
| H | -0.074110 | -4.478178 | 0.275629 |
| H | -4.987218 | -0.849000 | -1.431015 |
| H | -1.626541 | 4.352082 | 0.024695 |

| | | | |
|---|---|---|---|
| H | 3.551645 | 0.724586 | 0.643861 |
| C | 0.003637 | -1.045869 | -2.655734 |
| H | -0.699212 | -1.907406 | -2.620627 |
| H | 0.990083 | -1.437908 | -2.320614 |
| C | 0.834358 | 5.263726 | 0.547681 |
| H | 0.473424 | 5.692347 | -0.397162 |
| H | 0.118608 | 5.561967 | 1.325440 |
| H | 1.790865 | 5.745996 | 0.779273 |
| C | 2.628059 | -4.458542 | 0.489846 |
| H | 2.154688 | -5.001414 | 1.319233 |
| H | 2.354726 | -4.987841 | -0.433013 |
| H | 3.713548 | -4.553955 | 0.611316 |
| C | -2.579548 | -5.371655 | -0.183141 |
| H | -1.814921 | -5.826600 | -0.827651 |
| H | -2.336990 | -5.655781 | 0.849841 |
| H | -3.541394 | -5.834642 | -0.428984 |
| C | -5.913711 | 1.692745 | -1.562100 |
| H | -6.013130 | 1.728998 | -2.656569 |
| H | -6.375508 | 0.756836 | -1.225545 |
| H | -6.502256 | 2.524986 | -1.156546 |
| C | -5.065921 | -3.565787 | -0.940918 |
| C | -6.184943 | -2.947811 | -0.545396 |
| H | -5.161918 | -4.517845 | -1.471213 |

| | | | |
|---|---|---|---|
| H | -7.165596 | -3.360601 | -0.770633 |
| H | -6.149046 | -2.034659 | 0.046244 |
| C | -4.213246 | 4.298951 | -0.741614 |
| C | -5.159707 | 4.867416 | -1.501000 |
| H | -3.700322 | 4.936097 | -0.016238 |
| H | -5.419428 | 5.916412 | -1.381304 |
| H | -5.684785 | 4.318184 | -2.279096 |
| C | 4.473915 | -1.818787 | 0.489280 |
| C | 5.002663 | -1.703096 | -0.950651 |
| H | 4.910966 | -2.706864 | 0.967981 |
| H | 4.815345 | -0.956029 | 1.077715 |
| H | 4.644153 | -2.541236 | -1.557493 |
| H | 4.619058 | -0.776542 | -1.405761 |
| C | 3.494604 | 3.474970 | 0.790425 |
| C | 4.394586 | 3.439792 | -0.460860 |
| H | 3.977263 | 2.896334 | 1.589289 |
| H | 3.461394 | 4.510678 | 1.152074 |
| H | 3.823066 | 3.676586 | -1.363618 |
| H | 5.184778 | 4.197294 | -0.353224 |
| C | 6.490923 | -1.671368 | -1.063494 |
| O | 7.191027 | -2.349901 | -1.771212 |
| O | 7.052833 | -0.738676 | -0.233258 |
| H | 8.005102 | -0.776574 | -0.409775 |

| | | | |
|---|---|---|---|
| C | 5.114859 | 2.142548 | -0.704593 |
| O | 5.166792 | 1.549739 | -1.758536 |
| O | 5.764927 | 1.718544 | 0.395071 |
| H | 6.219778 | 0.884706 | 0.157036 |
| O | -0.430505 | 0.038213 | -1.935528 |
| H | 0.121972 | -0.781293 | -3.723924 |
| C | -0.907995 | -0.168468 | 4.171955 |
| O | -2.290275 | -0.244611 | 3.880046 |
| C | -2.469086 | -0.301477 | 2.490178 |
| C | -1.209232 | -0.057087 | 1.824347 |
| C | -0.224809 | 0.306594 | 2.889840 |
| H | -0.765886 | 0.502800 | 5.029358 |
| H | 0.762981 | -0.152186 | 2.744633 |
| H | -0.056721 | 1.400210 | 2.904451 |
| O | -3.590575 | -0.517408 | 2.067601 |
| H | -0.543961 | -1.168477 | 4.462698 |

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**$^{OSS}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2822.267995

Zero-point correction= 0.938227 (Hartree/Particle)

Thermal correction to Energy= 0.998705

Thermal correction to Enthalpy= 0.999649

Thermal correction to Gibbs Free Energy= 0.844216

Sum of electronic and zero-point Energies= -2821.329768

Sum of electronic and thermal Energies= -2821.269290

Sum of electronic and thermal Enthalpies= -2821.268346

Sum of electronic and thermal Free Energies= -2821.423779

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.053019 | 0.255029 | -0.737548 |
| N | -1.370221 | -1.134624 | -1.361536 |
| C | -1.203549 | -2.492072 | -1.377151 |
| C | -2.366505 | -3.153610 | -1.913422 |
| C | -3.246442 | -2.157168 | -2.256025 |
| C | -2.592780 | -0.906986 | -1.910117 |
| C | -0.052677 | -3.157504 | -0.982091 |
| C | 1.099123 | -2.548605 | -0.508286 |
| N | 1.254892 | -1.209105 | -0.300397 |
| C | 2.518789 | -1.047463 | 0.174468 |
| C | 3.195287 | -2.321652 | 0.265598 |
| C | 2.305671 | -3.263992 | -0.165598 |

| | | | |
|---|---|---|---|
| C | 3.087264 | 0.161216 | 0.551892 |
| C | 2.505869 | 1.405966 | 0.386138 |
| N | 1.282543 | 1.629327 | -0.163070 |
| C | 1.140210 | 2.976782 | -0.216289 |
| C | 2.302374 | 3.643696 | 0.336293 |
| C | 3.154461 | 2.659045 | 0.730522 |
| C | 0.046796 | 3.651541 | -0.726526 |
| C | -1.087195 | 3.052887 | -1.249989 |
| C | -2.199811 | 3.784636 | -1.828347 |
| C | -3.106460 | 2.836800 | -2.236557 |
| C | -2.530372 | 1.559410 | -1.893080 |
| N | -1.322411 | 1.716888 | -1.280086 |
| C | -3.138707 | 0.342465 | -2.162915 |
| H | -0.038673 | -4.241503 | -1.081855 |
| H | -4.113926 | 0.370383 | -2.644704 |
| H | 0.082853 | 4.738901 | -0.713141 |
| H | 4.075782 | 0.125245 | 1.004901 |
| C | 0.796133 | -0.604099 | -3.355635 |
| H | 1.374843 | -1.480701 | -2.988004 |
| H | 1.295981 | -0.275253 | -4.287391 |
| C | 2.463436 | 5.119393 | 0.437133 |
| H | 2.408631 | 5.600867 | -0.548632 |
| H | 1.677463 | 5.568375 | 1.058813 |

| | | | |
|---|---|---|---|
| H | 3.429899 | 5.390480 | 0.877449 |
| C | 2.506526 | -4.731747 | -0.316353 |
| H | 1.758250 | -5.307686 | 0.244670 |
| H | 2.428313 | -5.045920 | -1.366089 |
| H | 3.495229 | -5.039936 | 0.043493 |
| C | -2.550773 | -4.627327 | -2.001586 |
| H | -2.063723 | -5.142675 | -1.165203 |
| H | -3.616376 | -4.887691 | -1.983210 |
| H | -2.133921 | -5.045660 | -2.929167 |
| C | -4.396465 | 3.038464 | -2.949511 |
| H | -4.378116 | 3.974141 | -3.521475 |
| H | -4.603049 | 2.219819 | -3.648700 |
| H | -5.250196 | 3.098989 | -2.258846 |
| C | -4.598476 | -2.262305 | -2.772459 |
| C | -5.086166 | -3.238282 | -3.549418 |
| H | -5.281647 | -1.464730 | -2.466426 |
| H | -6.129756 | -3.245452 | -3.853730 |
| H | -4.458136 | -4.041310 | -3.929114 |
| C | -2.259295 | 5.227895 | -1.955806 |
| C | -3.364531 | 5.983464 | -1.999049 |
| H | -1.294947 | 5.737284 | -2.023761 |
| H | -3.302240 | 7.062239 | -2.118682 |
| H | -4.359976 | 5.559461 | -1.887620 |

| | | | |
|---|---|---|---|
| C | 4.633752 | -2.510027 | 0.611911 |
| C | 5.510001 | -2.356748 | -0.643055 |
| H | 4.793114 | -3.506407 | 1.048813 |
| H | 4.952947 | -1.787985 | 1.375764 |
| H | 5.177462 | -3.042993 | -1.428841 |
| H | 5.410040 | -1.331466 | -1.032080 |
| C | 4.485961 | 2.824103 | 1.386196 |
| C | 5.689897 | 2.744346 | 0.427270 |
| H | 4.620720 | 2.091762 | 2.192635 |
| H | 4.509608 | 3.807462 | 1.872862 |
| H | 5.456150 | 3.213779 | -0.533651 |
| H | 6.538058 | 3.282503 | 0.874656 |
| C | 6.964328 | -2.606245 | -0.416948 |
| O | 7.691930 | -3.338698 | -1.037886 |
| O | 7.453092 | -1.882478 | 0.636703 |
| H | 8.399816 | -2.086253 | 0.675879 |
| C | 6.187837 | 1.353084 | 0.153583 |
| O | 6.365195 | 0.862970 | -0.939088 |
| O | 6.469770 | 0.698375 | 1.294891 |
| H | 6.811291 | -0.185224 | 1.047754 |
| O | 0.741779 | 0.430401 | -2.456989 |
| H | -0.200513 | -0.995082 | -3.658697 |
| C | -0.803096 | 0.132864 | 1.163621 |

| | | | |
|---|---|---|---|
| C | -0.930486 | -1.212541 | 1.857971 |
| C | -0.198659 | 0.986037 | 2.202924 |
| C | 0.216718 | -1.173675 | 2.859570 |
| H | -0.875910 | -2.080176 | 1.195431 |
| H | -1.886433 | -1.285154 | 2.401978 |
| H | -3.781908 | -1.126902 | 0.261305 |
| O | -0.189719 | 2.192484 | 2.341586 |
| O | 0.394176 | 0.205777 | 3.180718 |
| H | 1.149559 | -1.564963 | 2.427120 |
| H | 0.010264 | -1.710956 | 3.795062 |
| C | -4.359333 | -1.561931 | 1.071600 |
| C | -4.468222 | -0.894700 | 2.309326 |
| C | -4.950280 | -2.800988 | 0.872582 |
| C | -5.162319 | -1.561316 | 3.339406 |
| N | -3.913022 | 0.368753 | 2.500497 |
| C | -5.658843 | -3.436626 | 1.888530 |
| H | -4.838462 | -3.272174 | -0.103982 |
| C | -5.747384 | -2.802127 | 3.122823 |
| H | -5.253823 | -1.112787 | 4.324139 |
| C | -3.342842 | 1.085783 | 1.405357 |
| C | -3.813745 | 0.898363 | 3.853889 |
| H | -6.115912 | -4.410095 | 1.726781 |
| H | -6.281176 | -3.278067 | 3.944553 |

| | | | |
|---|---|---|---|
| H | -3.852325 | 0.826019 | 0.471971 |
| C | -3.199049 | 2.573531 | 1.569785 |
| H | -3.620949 | 1.970816 | 3.781982 |
| H | -4.794588 | 0.810285 | 4.343789 |
| C | -2.730873 | 0.250484 | 4.704864 |
| H | -2.414533 | 2.844318 | 2.284839 |
| H | -2.895875 | 3.003386 | 0.610755 |
| H | -4.148800 | 3.047084 | 1.866649 |
| H | -2.855746 | -0.838376 | 4.751235 |
| H | -1.732359 | 0.462805 | 4.304344 |
| H | -2.770933 | 0.640055 | 5.729540 |
| H | -2.055641 | 0.631938 | 1.100530 |

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**$^{3}$TS(C-D)**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2822.2636835

Zero-point correction= 0.937997 (Hartree/Particle)

Thermal correction to Energy= 0.998596

Thermal correction to Enthalpy= 0.999540

Thermal correction to Gibbs Free Energy= 0.842229

Sum of electronic and zero-point Energies= -2821.325687

Sum of electronic and thermal Energies= -2821.265088

Sum of electronic and thermal Enthalpies= -2821.264144

Sum of electronic and thermal Free Energies= -2821.421454

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.036881 | 0.221116 | -0.767001 |
| N | -1.379389 | -1.156494 | -1.403207 |
| C | -1.199667 | -2.507940 | -1.451247 |
| C | -2.345703 | -3.162994 | -2.027958 |
| C | -3.232508 | -2.164291 | -2.354319 |
| C | -2.588171 | -0.919831 | -1.972682 |
| C | -0.050514 | -3.170457 | -1.041022 |
| C | 1.077605 | -2.572728 | -0.506711 |
| N | 1.230905 | -1.239519 | -0.257852 |
| C | 2.476439 | -1.100079 | 0.272625 |
| C | 3.147595 | -2.379022 | 0.345928 |
| C | 2.270174 | -3.303017 | -0.140871 |
| C | 3.042634 | 0.097233 | 0.681836 |
| C | 2.488239 | 1.347472 | 0.461299 |
| N | 1.301970 | 1.572717 | -0.169052 |
| C | 1.184214 | 2.923167 | -0.273626 |

| | | | |
|---|---|---|---|
| C | 2.326142 | 3.583234 | 0.314485 |
| C | 3.135216 | 2.597171 | 0.796033 |
| C | 0.116836 | 3.603051 | -0.831285 |
| C | -1.030145 | 3.015408 | -1.337457 |
| C | -2.152883 | 3.761622 | -1.881764 |
| C | -3.088085 | 2.827142 | -2.244843 |
| C | -2.512304 | 1.541571 | -1.920550 |
| N | -1.283096 | 1.684055 | -1.351675 |
| C | -3.139219 | 0.335092 | -2.184455 |
| H | -0.030918 | -4.253520 | -1.147122 |
| H | -4.135809 | 0.379279 | -2.618131 |
| H | 0.171954 | 4.689692 | -0.839432 |
| H | 4.011224 | 0.053655 | 1.175456 |
| C | 1.978205 | 0.075725 | -2.810152 |
| H | 2.658798 | 0.781627 | -2.286382 |
| H | 2.163471 | 0.209259 | -3.892622 |
| C | 2.518212 | 5.057666 | 0.375829 |
| H | 2.499306 | 5.510358 | -0.624444 |
| H | 1.727102 | 5.541409 | 0.963859 |
| H | 3.479279 | 5.319889 | 0.833083 |
| C | 2.475276 | -4.764847 | -0.335142 |
| H | 1.715824 | -5.357622 | 0.192168 |
| H | 2.417660 | -5.044375 | -1.395829 |

| | | | |
|---|---|---|---|
| H | 3.456324 | -5.084524 | 0.035115 |
| C | -2.482634 | -4.625702 | -2.259812 |
| H | -1.507873 | -5.110451 | -2.384745 |
| H | -2.992805 | -5.131501 | -1.426617 |
| H | -3.072838 | -4.820614 | -3.164018 |
| C | -4.414534 | 3.039439 | -2.882819 |
| H | -4.441124 | 3.999899 | -3.411142 |
| H | -4.646337 | 2.248753 | -3.606287 |
| H | -5.229719 | 3.051184 | -2.144189 |
| C | -4.530347 | -2.255562 | -2.992684 |
| C | -5.352884 | -3.313762 | -3.016641 |
| H | -4.863589 | -1.353942 | -3.511640 |
| H | -6.302286 | -3.269704 | -3.544023 |
| H | -5.128946 | -4.241651 | -2.495378 |
| C | -2.201117 | 5.206421 | -2.004995 |
| C | -3.298070 | 5.972303 | -1.950117 |
| H | -1.239750 | 5.704017 | -2.155328 |
| H | -3.238039 | 7.050794 | -2.073515 |
| H | -4.282367 | 5.554822 | -1.749138 |
| C | 4.590908 | -2.568538 | 0.667350 |
| C | 5.428254 | -2.372178 | -0.609043 |
| H | 4.767992 | -3.575349 | 1.071938 |
| H | 4.923760 | -1.864279 | 1.441946 |

| | | | |
|---|---|---|---|
| H | 5.076825 | -3.039934 | -1.402706 |
| H | 5.301519 | -1.337824 | -0.967504 |
| C | 4.431219 | 2.767371 | 1.517311 |
| C | 5.673369 | 2.726816 | 0.606293 |
| H | 4.542291 | 2.017670 | 2.311140 |
| H | 4.420388 | 3.739050 | 2.027442 |
| H | 5.485044 | 3.265233 | -0.328297 |
| H | 6.514497 | 3.207704 | 1.124924 |
| C | 6.891560 | -2.610840 | -0.437219 |
| O | 7.608067 | -3.312155 | -1.104953 |
| O | 7.403480 | -1.917373 | 0.625927 |
| H | 8.353500 | -2.109309 | 0.630269 |
| C | 6.124821 | 1.336017 | 0.261849 |
| O | 6.220525 | 0.870133 | -0.851341 |
| O | 6.449678 | 0.645049 | 1.369495 |
| H | 6.759258 | -0.238898 | 1.084928 |
| O | 0.648778 | 0.286806 | -2.530077 |
| H | 2.338528 | -0.946228 | -2.556897 |
| C | -0.883359 | 0.159781 | 1.136764 |
| C | -0.990897 | -1.180662 | 1.846520 |
| C | -0.276798 | 1.028021 | 2.159043 |
| C | 0.128523 | -1.114104 | 2.878265 |
| H | -0.907269 | -2.056658 | 1.196541 |

| | | | |
|---|---|---|---|
| H | -1.960166 | -1.264561 | 2.364955 |
| H | -3.848100 | -1.079971 | 0.189533 |
| O | -0.255360 | 2.238656 | 2.265226 |
| O | 0.293594 | 0.271296 | 3.171431 |
| H | 1.074411 | -1.512934 | 2.481087 |
| H | -0.101786 | -1.631698 | 3.819308 |
| C | -4.382174 | -1.550285 | 1.009087 |
| C | -4.523985 | -0.883993 | 2.245280 |
| C | -4.884306 | -2.829259 | 0.822958 |
| C | -5.162506 | -1.594024 | 3.284192 |
| N | -4.052263 | 0.411192 | 2.424223 |
| C | -5.536480 | -3.509375 | 1.848016 |
| H | -4.751021 | -3.292517 | -0.154441 |
| C | -5.659828 | -2.874150 | 3.079143 |
| H | -5.273384 | -1.151116 | 4.269490 |
| C | -3.443585 | 1.119842 | 1.333615 |
| C | -4.004003 | 0.964379 | 3.769060 |
| H | -5.925070 | -4.513728 | 1.695565 |
| H | -6.150521 | -3.381997 | 3.908841 |
| H | -3.953989 | 0.874510 | 0.395371 |
| C | -3.293027 | 2.607042 | 1.502049 |
| H | -3.917792 | 2.050289 | 3.685439 |
| H | -4.971373 | 0.787832 | 4.260585 |

| | | | |
|---|---|---|---|
| C | -2.863419 | 0.430400 | 4.623640 |
| H | -2.545754 | 2.870345 | 2.259232 |
| H | -2.928712 | 3.028347 | 0.559337 |
| H | -4.248844 | 3.101136 | 1.742670 |
| H | -2.899383 | -0.663817 | 4.695384 |
| H | -1.889503 | 0.709690 | 4.203997 |
| H | -2.921596 | 0.839317 | 5.640041 |
| H | -2.164097 | 0.656516 | 1.073134 |

**Interconversion Scan**

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**Scanpoint_1**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2379.9241959

Zero-point correction= 0.725386 (Hartree/Particle)

Thermal correction to Energy= 0.774045

Thermal correction to Enthalpy= 0.774989

Thermal correction to Gibbs Free Energy= 0.643181

Sum of electronic and zero-point Energies= -2379.198810

Sum of electronic and thermal Energies= -2379.150151

Sum of electronic and thermal Enthalpies= -2379.149207

Sum of electronic and thermal Free Energies= -2379.281015

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| Fe | -0.852328 | 0.089443 | -0.063422 |
| N | -2.050935 | -1.518149 | -0.345036 |
| C | -1.686257 | -2.838204 | -0.316098 |
| C | -2.823541 | -3.692084 | -0.584193 |
| C | -3.895779 | -2.849909 | -0.798790 |
| C | -3.379616 | -1.491194 | -0.654520 |
| C | -0.385927 | -3.295540 | -0.112374 |
| C | 0.735441 | -2.497658 | 0.059346 |
| N | 0.735540 | -1.131336 | 0.105150 |
| C | 2.029724 | -0.753917 | 0.301910 |
| C | 2.897146 | -1.926014 | 0.351277 |
| C | 2.085542 | -3.015691 | 0.207289 |
| C | 2.476289 | 0.554668 | 0.466570 |
| C | 1.691511 | 1.702707 | 0.416302 |
| N | 0.343987 | 1.717685 | 0.206338 |
| C | -0.034587 | 3.028304 | 0.211103 |

| | | | |
|---|---|---|---|
| C | 1.115197 | 3.890817 | 0.441251 |
| C | 2.198200 | 3.063739 | 0.574080 |
| C | -1.328663 | 3.494511 | 0.016037 |
| C | -2.444275 | 2.706422 | -0.256557 |
| C | -3.776759 | 3.232853 | -0.549830 |
| C | -4.571021 | 2.134093 | -0.799966 |
| C | -3.717960 | 0.971889 | -0.637477 |
| N | -2.445662 | 1.347439 | -0.297752 |
| C | -4.153472 | -0.341543 | -0.788118 |
| H | -0.232392 | -4.368601 | -0.102001 |
| H | -5.203577 | -0.482515 | -1.015933 |
| H | -1.473744 | 4.568250 | 0.054674 |
| H | 3.532140 | 0.690614 | 0.667675 |
| C | -0.232061 | -0.719803 | -2.783537 |
| H | 0.767208 | -1.141311 | -2.565628 |
| H | -0.198448 | -0.342122 | -3.821629 |
| C | 1.057748 | 5.387907 | 0.505120 |
| H | 0.756965 | 5.822965 | -0.456646 |
| H | 0.332715 | 5.734207 | 1.251961 |
| H | 2.028685 | 5.818923 | 0.766576 |
| C | 2.452826 | -4.468627 | 0.203347 |
| H | 1.919558 | -5.015270 | 0.990515 |
| H | 2.204011 | -4.951461 | -0.750275 |

| | | | |
|---|---|---|---|
| H | 3.524129 | -4.612572 | 0.371925 |
| C | -2.787765 | -5.187344 | -0.664111 |
| H | -1.812343 | -5.548166 | -1.004750 |
| H | -2.984566 | -5.658607 | 0.308562 |
| H | -3.546117 | -5.556483 | -1.362136 |
| C | -6.009189 | 2.104986 | -1.218059 |
| H | -6.268679 | 3.012575 | -1.772645 |
| H | -6.222060 | 1.245210 | -1.860991 |
| H | -6.693262 | 2.044693 | -0.359955 |
| C | -5.271558 | -3.173311 | -1.150854 |
| C | -5.949691 | -4.298005 | -0.864784 |
| H | -5.801441 | -2.404931 | -1.713912 |
| H | -6.972781 | -4.430980 | -1.204563 |
| H | -5.525963 | -5.100760 | -0.271075 |
| C | -4.107682 | 4.649359 | -0.605860 |
| C | -5.310020 | 5.221677 | -0.420310 |
| H | -3.272461 | 5.314013 | -0.826773 |
| H | -5.433078 | 6.297021 | -0.511683 |
| H | -6.193599 | 4.652471 | -0.152124 |
| C | 4.393260 | -1.906762 | 0.466133 |
| C | 5.079555 | -1.773246 | -0.925140 |
| H | 4.739818 | -2.831764 | 0.941284 |
| H | 4.724355 | -1.086743 | 1.111056 |

| | | | |
|---|---|---|---|
| H | 4.745704 | -2.575367 | -1.585644 |
| H | 4.806320 | -0.814390 | -1.380166 |
| C | 3.619307 | 3.472195 | 0.847641 |
| C | 4.557330 | 3.523167 | -0.394302 |
| H | 4.074586 | 2.819518 | 1.599535 |
| H | 3.608189 | 4.474213 | 1.288925 |
| H | 4.016284 | 3.851336 | -1.283426 |
| H | 5.359205 | 4.246737 | -0.195247 |
| C | 6.579384 | -1.853909 | -0.850024 |
| O | 7.299305 | -2.709474 | -1.311008 |
| O | 7.121963 | -0.805598 | -0.138770 |
| H | 8.083299 | -0.945556 | -0.147287 |
| C | 5.249295 | 2.218955 | -0.728100 |
| O | 5.257704 | 1.677523 | -1.815491 |
| O | 5.913883 | 1.721693 | 0.340879 |
| H | 6.335534 | 0.878382 | 0.073404 |
| O | -0.593339 | 0.310142 | -1.923871 |
| H | -0.943624 | -1.567100 | -2.776149 |
| C | -1.135474 | 0.066554 | 2.103823 |
| C | -2.558133 | 0.266523 | 2.645859 |
| C | -0.695154 | -1.169362 | 2.790604 |
| C | -3.002015 | -1.175963 | 2.930524 |
| H | -3.244897 | 0.773146 | 1.966296 |

| | | | |
|---|---|---|---|
| H | -2.548527 | 0.839568 | 3.587344 |
| O | 0.417023 | -1.600268 | 3.032417 |
| O | -1.798602 | -1.899469 | 3.227166 |
| H | -3.486817 | -1.629873 | 2.059500 |
| H | -3.674618 | -1.270078 | 3.791806 |
| H | -0.456122 | 0.879978 | 2.355798 |

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**Scanpoint_2**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.925539

Zero-point correction= 0.725466 (Hartree/Particle)

Thermal correction to Energy= 0.775045

Thermal correction to Enthalpy= 0.775989

Thermal correction to Gibbs Free Energy= 0.640630

Sum of electronic and zero-point Energies= -2379.200073

Sum of electronic and thermal Energies= -2379.150494

Sum of electronic and thermal Enthalpies= -2379.149550

Sum of electronic and thermal Free Energies= -2379.284909

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.893598 | 0.082428 | -0.051539 |
| N | -2.088295 | -1.537649 | -0.316426 |
| C | -1.718934 | -2.857172 | -0.275741 |
| C | -2.849309 | -3.716752 | -0.556207 |
| C | -3.922421 | -2.879169 | -0.786329 |
| C | -3.413637 | -1.518130 | -0.640318 |
| C | -0.422997 | -3.309883 | -0.035209 |
| C | 0.697178 | -2.507693 | 0.133418 |
| N | 0.695339 | -1.139551 | 0.148755 |
| C | 1.994688 | -0.754879 | 0.297313 |
| C | 2.863707 | -1.923348 | 0.363403 |
| C | 2.050635 | -3.019312 | 0.272530 |
| C | 2.442598 | 0.558219 | 0.407406 |
| C | 1.652032 | 1.700575 | 0.361056 |
| N | 0.300035 | 1.708252 | 0.187453 |
| C | -0.085104 | 3.016400 | 0.196430 |
| C | 1.066535 | 3.886173 | 0.391430 |
| C | 2.156627 | 3.065215 | 0.494596 |
| C | -1.385995 | 3.476080 | 0.029001 |
| C | -2.501929 | 2.683831 | -0.231750 |
| C | -3.840117 | 3.203564 | -0.512579 |
| C | -4.627622 | 2.101748 | -0.769437 |

| | | | |
|---|---|---|---|
| C | -3.766307 | 0.943426 | -0.619503 |
| N | -2.495447 | 1.325572 | -0.283925 |
| C | -4.192380 | -0.371645 | -0.783259 |
| H | -0.267404 | -4.382689 | -0.012168 |
| H | -5.240649 | -0.517828 | -1.015987 |
| H | -1.535475 | 4.548962 | 0.073381 |
| H | 3.502319 | 0.701267 | 0.579543 |
| C | -0.284997 | -0.787494 | -2.761921 |
| H | 0.694349 | -1.242606 | -2.521117 |
| H | -0.216780 | -0.421091 | -3.802465 |
| C | 1.001905 | 5.382916 | 0.453388 |
| H | 0.664974 | 5.813671 | -0.498297 |
| H | 0.301416 | 5.726347 | 1.224619 |
| H | 1.978629 | 5.820401 | 0.679935 |
| C | 2.423047 | -4.471245 | 0.293635 |
| H | 1.885286 | -5.011472 | 1.082232 |
| H | 2.185804 | -4.968539 | -0.655700 |
| H | 3.493303 | -4.608177 | 0.474270 |
| C | -2.806297 | -5.212327 | -0.635204 |
| H | -1.822047 | -5.569290 | -0.953697 |
| H | -3.025075 | -5.687574 | 0.331094 |
| H | -3.546710 | -5.583361 | -1.351316 |
| C | -6.067694 | 2.066246 | -1.180161 |

| | | | |
|---|---|---|---|
| H | -6.337072 | 2.977698 | -1.723553 |
| H | -6.277681 | 1.211780 | -1.831138 |
| H | -6.746476 | 1.991451 | -0.318995 |
| C | -5.292002 | -3.209364 | -1.154949 |
| C | -5.967241 | -4.339203 | -0.881966 |
| H | -5.819949 | -2.441530 | -1.720423 |
| H | -6.985677 | -4.475960 | -1.233923 |
| H | -5.546048 | -5.143215 | -0.288110 |
| C | -4.181175 | 4.618229 | -0.553548 |
| C | -5.386479 | 5.180106 | -0.356080 |
| H | -3.351761 | 5.290859 | -0.772041 |
| H | -5.517566 | 6.255401 | -0.436087 |
| H | -6.264471 | 4.602049 | -0.088482 |
| C | 4.362032 | -1.897937 | 0.442781 |
| C | 5.015407 | -1.793925 | -0.966801 |
| H | 4.722458 | -2.811332 | 0.930016 |
| H | 4.704333 | -1.062796 | 1.061758 |
| H | 4.666808 | -2.610082 | -1.602055 |
| H | 4.731420 | -0.844934 | -1.435590 |
| C | 3.582798 | 3.480221 | 0.728017 |
| C | 4.491086 | 3.513709 | -0.536727 |
| H | 4.055376 | 2.839425 | 1.479289 |
| H | 3.580092 | 4.488676 | 1.154240 |

| | | | |
|---|---|---|---|
| H | 3.927797 | 3.823629 | -1.418589 |
| H | 5.293663 | 4.244400 | -0.369149 |
| C | 6.516598 | -1.874081 | -0.923154 |
| O | 7.224904 | -2.745033 | -1.373444 |
| O | 7.075485 | -0.805596 | -0.256877 |
| H | 8.036250 | -0.947585 | -0.280833 |
| C | 5.181697 | 2.207070 | -0.863735 |
| O | 5.164100 | 1.643750 | -1.939949 |
| O | 5.877251 | 1.734452 | 0.196596 |
| H | 6.293830 | 0.886864 | -0.064482 |
| O | -0.626123 | 0.260966 | -1.917469 |
| H | -1.025524 | -1.610015 | -2.762812 |
| C | -1.268840 | 0.184696 | 2.079374 |
| C | -2.640916 | -0.285229 | 2.579305 |
| C | -0.322700 | -0.592173 | 2.909927 |
| C | -2.342340 | -1.710563 | 3.068955 |
| H | -3.433906 | -0.275842 | 1.829846 |
| H | -2.985919 | 0.330790 | 3.425393 |
| O | 0.845191 | -0.397457 | 3.189307 |
| O | -0.955680 | -1.714817 | 3.439938 |
| H | -2.501734 | -2.452322 | 2.278975 |
| H | -2.928706 | -2.006903 | 3.947359 |
| H | -1.097174 | 1.250465 | 2.224948 |

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**Scanpoint_3**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2379.9198205

Zero-point correction= 0.724868 (Hartree/Particle)

Thermal correction to Energy= 0.773737

Thermal correction to Enthalpy= 0.774681

Thermal correction to Gibbs Free Energy= 0.641866

Sum of electronic and zero-point Energies= -2379.194952

Sum of electronic and thermal Energies= -2379.146084

Sum of electronic and thermal Enthalpies= -2379.145139

Sum of electronic and thermal Free Energies= -2379.277954

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.936512 | 0.087845 | -0.086087 |
| N | 2.091721 | 1.762537 | -0.227647 |
| C | 1.676410 | 3.063353 | -0.126656 |
| C | 2.796200 | 3.972555 | -0.249209 |
| C | 3.915131 | 3.183919 | -0.424938 |

| | | | |
|---|---|---|---|
| C | 3.441588 | 1.801581 | -0.417374 |
| C | 0.352453 | 3.458192 | 0.055252 |
| C | -0.740832 | 2.609523 | 0.155278 |
| N | -0.691672 | 1.244080 | 0.124258 |
| C | -1.973884 | 0.810445 | 0.278850 |
| C | -2.884807 | 1.945274 | 0.376433 |
| C | -2.112118 | 3.069757 | 0.305301 |
| C | -2.372638 | -0.519738 | 0.373572 |
| C | -1.544776 | -1.632197 | 0.262235 |
| N | -0.196573 | -1.582964 | 0.061311 |
| C | 0.218874 | -2.874444 | -0.097064 |
| C | -0.902335 | -3.790845 | 0.046581 |
| C | -2.006994 | -3.017182 | 0.281241 |
| C | 1.518887 | -3.278522 | -0.378693 |
| C | 2.618025 | -2.436783 | -0.533489 |
| C | 3.975216 | -2.891878 | -0.829794 |
| C | 4.755360 | -1.755722 | -0.868915 |
| C | 3.864143 | -0.642849 | -0.596570 |
| N | 2.586898 | -1.085626 | -0.385789 |
| C | 4.265389 | 0.690243 | -0.576291 |
| H | 0.156217 | 4.522578 | 0.121919 |
| H | 5.324324 | 0.880927 | -0.706305 |
| H | 1.688707 | -4.344486 | -0.480420 |

| | | | |
|---|---|---|---|
| H | -3.424748 | -0.706381 | 0.551864 |
| C | 0.365571 | 1.063844 | -2.766676 |
| H | -0.632209 | 1.479082 | -2.529433 |
| H | 0.333132 | 0.746590 | -3.825121 |
| C | -0.802201 | -5.283618 | -0.054331 |
| H | -0.507993 | -5.603072 | -1.062422 |
| H | -0.054208 | -5.687367 | 0.639030 |
| H | -1.756195 | -5.768079 | 0.173867 |
| C | -2.535849 | 4.506403 | 0.363679 |
| H | -2.021339 | 5.043422 | 1.169922 |
| H | -2.311985 | 5.038059 | -0.570124 |
| H | -3.611072 | 4.600442 | 0.542394 |
| C | 2.706501 | 5.467963 | -0.238425 |
| H | 1.743196 | 5.814819 | -0.625214 |
| H | 2.818097 | 5.885664 | 0.771883 |
| H | 3.495678 | 5.907684 | -0.857045 |
| C | 6.213918 | -1.644191 | -1.191826 |
| H | 6.525371 | -2.455417 | -1.857924 |
| H | 6.443820 | -0.695592 | -1.686851 |
| H | 6.846529 | -1.702805 | -0.294935 |
| C | 5.301097 | 3.577229 | -0.635795 |
| C | 5.906136 | 4.707578 | -0.231463 |
| H | 5.909183 | 2.862025 | -1.189718 |

| | | | |
|---|---|---|---|
| H | 6.948519 | 4.895754 | -0.472010 |
| H | 5.401121 | 5.460471 | 0.363991 |
| C | 4.340764 | -4.279794 | -1.072634 |
| C | 5.544357 | -4.856036 | -0.908033 |
| H | 3.532540 | -4.916355 | -1.433114 |
| H | 5.695577 | -5.904407 | -1.148736 |
| H | 6.400386 | -4.319830 | -0.512661 |
| C | -4.380370 | 1.865813 | 0.468033 |
| C | -5.044641 | 1.787836 | -0.937986 |
| H | -4.766500 | 2.749078 | 0.989992 |
| H | -4.688271 | 0.999140 | 1.061148 |
| H | -4.731338 | 2.636871 | -1.548022 |
| H | -4.733115 | 0.865959 | -1.442168 |
| C | -3.410453 | -3.497420 | 0.527880 |
| C | -4.348739 | -3.507668 | -0.714823 |
| H | -3.887695 | -2.912260 | 1.320255 |
| H | -3.358710 | -4.524431 | 0.904396 |
| H | -3.799199 | -3.769627 | -1.620577 |
| H | -5.128506 | -4.264393 | -0.555531 |
| C | -6.547092 | 1.812900 | -0.878749 |
| O | -7.291119 | 2.667554 | -1.301876 |
| O | -7.060621 | 0.709249 | -0.233142 |
| H | -8.026120 | 0.816098 | -0.246479 |

| | | | |
|---|---|---|---|
| C | -5.077716 | -2.207105 | -0.974959 |
| O | -5.089756 | -1.597184 | -2.025608 |
| O | -5.769974 | -1.800234 | 0.114206 |
| H | -6.215559 | -0.955345 | -0.104830 |
| O | 0.718661 | -0.013882 | -1.965528 |
| H | 1.081676 | 1.905688 | -2.709159 |
| C | 1.301120 | 0.097908 | 2.042775 |
| C | 2.093758 | -1.107530 | 2.578097 |
| C | 0.134152 | 0.200567 | 2.965821 |
| C | 1.497887 | -1.359541 | 3.969933 |
| H | 3.174071 | -0.933891 | 2.618317 |
| H | 1.932854 | -1.992401 | 1.959283 |
| O | -0.773221 | 1.005463 | 3.026838 |
| O | 0.175218 | -0.812483 | 3.927023 |
| H | 2.063627 | -0.847071 | 4.765150 |
| H | 1.420705 | -2.419565 | 4.236326 |
| H | 1.859044 | 1.035482 | 2.109467 |

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**Scanpoint_4**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.919546

Zero-point correction= 0.724782 (Hartree/Particle)

Thermal correction to Energy= 0.774648

Thermal correction to Enthalpy= 0.775592

Thermal correction to Gibbs Free Energy= 0.638212

Sum of electronic and zero-point Energies= -2379.194764

Sum of electronic and thermal Energies= -2379.144898

Sum of electronic and thermal Enthalpies= -2379.143954

Sum of electronic and thermal Free Energies= -2379.281334

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.889296 | -0.096673 | -0.076163 |
| N | -2.034768 | -1.776478 | -0.226860 |
| C | -1.631933 | -3.071723 | -0.033803 |
| C | -2.739701 | -3.986323 | -0.212283 |
| C | -3.834942 | -3.207757 | -0.528966 |
| C | -3.361257 | -1.825787 | -0.535696 |
| C | -0.324050 | -3.458580 | 0.256212 |
| C | 0.772724 | -2.610151 | 0.344565 |
| N | 0.730183 | -1.247124 | 0.236533 |
| C | 2.016385 | -0.810195 | 0.341561 |
| C | 2.922118 | -1.940408 | 0.502140 |

| | | | |
|---|---|---|---|
| C | 2.142692 | -3.065135 | 0.519336 |
| C | 2.419178 | 0.521733 | 0.345335 |
| C | 1.586948 | 1.628677 | 0.233728 |
| N | 0.233173 | 1.578517 | 0.072951 |
| C | -0.191006 | 2.870196 | -0.034624 |
| C | 0.930550 | 3.789547 | 0.097067 |
| C | 2.046145 | 3.014968 | 0.261783 |
| C | -1.496300 | 3.272477 | -0.290693 |
| C | -2.573924 | 2.424008 | -0.530847 |
| C | -3.919768 | 2.871928 | -0.887190 |
| C | -4.668904 | 1.725983 | -1.048571 |
| C | -3.777055 | 0.615039 | -0.771316 |
| N | -2.523897 | 1.067243 | -0.457824 |
| C | -4.168595 | -0.720472 | -0.794163 |
| H | -0.136870 | -4.518815 | 0.386552 |
| H | -5.212325 | -0.916589 | -1.010514 |
| H | -1.679314 | 4.339814 | -0.342626 |
| H | 3.474498 | 0.714110 | 0.494351 |
| C | -0.216536 | -1.147007 | -2.698599 |
| H | 0.761537 | -1.571208 | -2.401689 |
| H | -0.127305 | -0.860511 | -3.762401 |
| C | 0.816466 | 5.283653 | 0.046334 |
| H | 0.472982 | 5.631393 | -0.936522 |

| | | | |
|---|---|---|---|
| H | 0.099650 | 5.659226 | 0.786829 |
| H | 1.776769 | 5.768602 | 0.244649 |
| C | 2.562636 | -4.497606 | 0.659953 |
| H | 2.031249 | -4.994848 | 1.480718 |
| H | 2.357187 | -5.075740 | -0.250272 |
| H | 3.633946 | -4.583285 | 0.864846 |
| C | -2.657938 | -5.479767 | -0.124969 |
| H | -1.662142 | -5.844048 | -0.395997 |
| H | -2.873816 | -5.851872 | 0.886377 |
| H | -3.382161 | -5.947343 | -0.800126 |
| C | -6.098568 | 1.605706 | -1.479450 |
| H | -6.382770 | 2.450299 | -2.115500 |
| H | -6.269849 | 0.684998 | -2.045904 |
| H | -6.792890 | 1.595676 | -0.627495 |
| C | -5.196277 | -3.611142 | -0.850973 |
| C | -5.839237 | -4.725973 | -0.461956 |
| H | -5.748692 | -2.918349 | -1.485791 |
| H | -6.855314 | -4.923878 | -0.790954 |
| H | -5.393813 | -5.455789 | 0.205432 |
| C | -4.300113 | 4.264907 | -1.071518 |
| C | -5.525362 | 4.806118 | -0.955428 |
| H | -3.484708 | 4.938323 | -1.335694 |
| H | -5.684748 | 5.864324 | -1.141544 |

| | | | |
|---|---|---|---|
| H | -6.393042 | 4.229795 | -0.652744 |
| C | 4.419524 | -1.860365 | 0.561682 |
| C | 5.055892 | -1.837374 | -0.859322 |
| H | 4.815856 | -2.723560 | 1.109115 |
| H | 4.739351 | -0.971047 | 1.113820 |
| H | 4.727716 | -2.707549 | -1.430524 |
| H | 4.737003 | -0.933856 | -1.391201 |
| C | 3.457423 | 3.492627 | 0.463237 |
| C | 4.364484 | 3.471955 | -0.802867 |
| H | 3.950505 | 2.920663 | 1.255634 |
| H | 3.420187 | 4.526927 | 0.820194 |
| H | 3.791378 | 3.704453 | -1.702050 |
| H | 5.142754 | 4.237850 | -0.685276 |
| C | 6.559246 | -1.866976 | -0.826901 |
| O | 7.290836 | -2.746187 | -1.220607 |
| O | 7.089457 | -0.736096 | -0.246213 |
| H | 8.054057 | -0.848873 | -0.271513 |
| C | 5.097337 | 2.169929 | -1.044652 |
| O | 5.094607 | 1.533486 | -2.079484 |
| O | 5.812826 | 1.793843 | 0.041095 |
| H | 6.255346 | 0.944479 | -0.165112 |
| O | -0.589300 | -0.041530 | -1.945203 |
| H | -0.948918 | -1.975500 | -2.652388 |

| | | | |
|---|---|---|---|
| C | -1.310174 | -0.153255 | 2.036256 |
| C | -2.637966 | 0.451917 | 2.522557 |
| C | -0.293848 | 0.402724 | 2.977521 |
| C | -2.315417 | 0.959921 | 3.934339 |
| H | -3.466543 | -0.263819 | 2.519993 |
| H | -2.939817 | 1.297032 | 1.899404 |
| O | 0.906588 | 0.242042 | 3.050999 |
| O | -0.905636 | 1.213532 | 3.938115 |
| H | -2.539116 | 0.207608 | 4.708201 |
| H | -2.829846 | 1.889226 | 4.203359 |
| H | -1.289413 | -1.240771 | 2.158462 |

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**Scanpoint_5**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.9255672

Zero-point correction= 0.725508 (Hartree/Particle)

Thermal correction to Energy= 0.775070

Thermal correction to Enthalpy= 0.776014

Thermal correction to Gibbs Free Energy= 0.641050

Sum of electronic and zero-point Energies= -2379.200059

Sum of electronic and thermal Energies= -2379.150498

Sum of electronic and thermal Enthalpies= -2379.149553

Sum of electronic and thermal Free Energies= -2379.284517

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.865931 | 0.131594 | -0.045635 |
| N | 1.991802 | 1.821504 | -0.157769 |
| C | 1.574590 | 3.111423 | 0.038929 |
| C | 2.671693 | 4.039430 | -0.140435 |
| C | 3.773117 | 3.275415 | -0.469121 |
| C | 3.315461 | 1.888351 | -0.479984 |
| C | 0.261376 | 3.486667 | 0.320283 |
| C | -0.830624 | 2.630849 | 0.392461 |
| N | -0.778001 | 1.268687 | 0.269526 |
| C | -2.059509 | 0.819593 | 0.390918 |
| C | -2.972491 | 1.940980 | 0.573205 |
| C | -2.201975 | 3.072659 | 0.585373 |
| C | -2.449684 | -0.516665 | 0.382345 |
| C | -1.609802 | -1.612592 | 0.229266 |
| N | -0.259946 | -1.546962 | 0.053360 |
| C | 0.174848 | -2.833401 | -0.072684 |
| C | -0.938592 | -3.764710 | 0.045565 |

| | | | |
|---|---|---|---|
| C | -2.057974 | -3.003076 | 0.234338 |
| C | 1.485480 | -3.223098 | -0.315786 |
| C | 2.565282 | -2.366384 | -0.513816 |
| C | 3.913513 | -2.800176 | -0.877178 |
| C | 4.656530 | -1.647167 | -1.018653 |
| C | 3.758998 | -0.546370 | -0.722310 |
| N | 2.510766 | -1.011865 | -0.405762 |
| C | 4.134398 | 0.794395 | -0.749258 |
| H | 0.066210 | 4.544547 | 0.457544 |
| H | 5.173614 | 1.003874 | -0.974149 |
| H | 1.674071 | -4.288187 | -0.387054 |
| H | -3.500586 | -0.721919 | 0.545018 |
| C | 0.200270 | 1.211759 | -2.657465 |
| H | -0.802318 | 1.586090 | -2.375881 |
| H | 0.150244 | 0.947966 | -3.729591 |
| C | -0.810527 | -5.256504 | -0.026579 |
| H | -0.445990 | -5.585832 | -1.008144 |
| H | -0.104466 | -5.635813 | 0.722149 |
| H | -1.769943 | -5.752545 | 0.146546 |
| C | -2.633375 | 4.500552 | 0.738570 |
| H | -2.094701 | 4.999880 | 1.553286 |
| H | -2.446419 | 5.084040 | -0.172153 |
| H | -3.702386 | 4.575385 | 0.959177 |

| | | | |
|---|---|---|---|
| C | 2.573990 | 5.531446 | -0.045382 |
| H | 1.575380 | 5.886961 | -0.317767 |
| H | 2.782678 | 5.899978 | 0.968714 |
| H | 3.295504 | 6.009937 | -0.715641 |
| C | 6.084581 | -1.511830 | -1.450356 |
| H | 6.372120 | -2.344668 | -2.100157 |
| H | 6.249571 | -0.581428 | -2.002621 |
| H | 6.780516 | -1.511249 | -0.599713 |
| C | 5.127416 | 3.696117 | -0.799137 |
| C | 5.762551 | 4.812155 | -0.401250 |
| H | 5.680351 | 3.017193 | -1.448351 |
| H | 6.773329 | 5.025180 | -0.737013 |
| H | 5.315922 | 5.527868 | 0.280492 |
| C | 4.302215 | -4.187422 | -1.087154 |
| C | 5.530735 | -4.722491 | -0.979315 |
| H | 3.491404 | -4.860952 | -1.364275 |
| H | 5.697091 | -5.776190 | -1.183743 |
| H | 6.394168 | -4.146277 | -0.664548 |
| C | -4.468692 | 1.848609 | 0.649038 |
| C | -5.121240 | 1.845962 | -0.764570 |
| H | -4.865044 | 2.698961 | 1.216389 |
| H | -4.775939 | 0.947151 | 1.188487 |
| H | -4.806466 | 2.728512 | -1.324191 |

| | | | |
|---|---|---|---|
| H | -4.801881 | 0.954202 | -1.315801 |
| C | -3.462548 | -3.495642 | 0.444204 |
| C | -4.387568 | -3.454495 | -0.808394 |
| H | -3.947722 | -2.945505 | 1.256638 |
| H | -3.412303 | -4.536995 | 0.777783 |
| H | -3.826061 | -3.666654 | -1.719861 |
| H | -5.160553 | -4.226261 | -0.694747 |
| C | -6.624459 | 1.862700 | -0.715338 |
| O | -7.367275 | 2.739609 | -1.092663 |
| O | -7.138581 | 0.721521 | -0.140717 |
| H | -8.104423 | 0.825313 | -0.155724 |
| C | -5.129303 | -2.151629 | -1.014186 |
| O | -5.138270 | -1.490720 | -2.033707 |
| O | -5.838006 | -1.804371 | 0.085685 |
| H | -6.288656 | -0.954396 | -0.098794 |
| O | 0.599814 | 0.104337 | -1.920658 |
| H | 0.894770 | 2.069401 | -2.572983 |
| C | 1.197006 | 0.194967 | 2.093624 |
| C | 2.652041 | 0.144040 | 2.578216 |
| C | 0.554078 | -0.902414 | 2.849927 |
| C | 2.823700 | -1.337443 | 2.946438 |
| H | 2.792309 | 0.766150 | 3.477075 |
| H | 3.394589 | 0.464434 | 1.845741 |

| | | | |
|---|---|---|---|
| O | -0.612703 | -1.104710 | 3.129422 |
| O | 1.513068 | -1.806111 | 3.299091 |
| H | 3.484939 | -1.505312 | 3.805283 |
| H | 3.195295 | -1.925268 | 2.100524 |
| H | 0.697830 | 1.137635 | 2.315363 |

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**Scanpoint_6**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2379.9189022

Zero-point correction= 0.724825 (Hartree/Particle)

Thermal correction to Energy= 0.773723

Thermal correction to Enthalpy= 0.774668

Thermal correction to Gibbs Free Energy= 0.641668

Sum of electronic and zero-point Energies= -2379.194077

Sum of electronic and thermal Energies= -2379.145179

Sum of electronic and thermal Enthalpies= -2379.144235

Sum of electronic and thermal Free Energies= -2379.277235

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.827140 | 0.094992 | -0.089434 |
| N | 1.957877 | 1.788470 | -0.233388 |
| C | 1.543807 | 3.084855 | -0.070671 |
| C | 2.639463 | 4.006646 | -0.287281 |
| C | 3.738537 | 3.232330 | -0.598598 |
| C | 3.279867 | 1.846164 | -0.563458 |
| C | 0.237901 | 3.470705 | 0.225327 |
| C | -0.853537 | 2.618907 | 0.345609 |
| N | -0.807057 | 1.254304 | 0.246314 |
| C | -2.085992 | 0.810029 | 0.415391 |
| C | -2.989356 | 1.935937 | 0.611583 |
| C | -2.216330 | 3.066631 | 0.574366 |
| C | -2.478992 | -0.527186 | 0.425690 |
| C | -1.652894 | -1.625954 | 0.217635 |
| N | -0.311907 | -1.566515 | -0.009431 |
| C | 0.109850 | -2.851801 | -0.162085 |
| C | -1.007198 | -3.777954 | -0.033469 |
| C | -2.112847 | -3.014351 | 0.209950 |
| C | 1.417941 | -3.251480 | -0.396255 |
| C | 2.513174 | -2.405547 | -0.544325 |
| C | 3.866341 | -2.849647 | -0.874588 |
| C | 4.621331 | -1.703478 | -0.999050 |
| C | 3.724487 | -0.594767 | -0.728649 |

| | | | |
|---|---|---|---|
| N | 2.467180 | -1.051076 | -0.435271 |
| C | 4.101625 | 0.744133 | -0.787375 |
| H | 0.047531 | 4.532233 | 0.339769 |
| H | 5.143399 | 0.946467 | -1.006595 |
| H | 1.596858 | -4.317342 | -0.477452 |
| H | -3.525055 | -0.729384 | 0.622599 |
| C | 0.219011 | 1.203633 | -2.713124 |
| H | -0.702391 | 1.717090 | -2.378527 |
| H | 0.053818 | 0.912959 | -3.766774 |
| C | -0.889506 | -5.268795 | -0.129954 |
| H | -0.519975 | -5.584379 | -1.113953 |
| H | -0.191021 | -5.662547 | 0.618433 |
| H | -1.853246 | -5.761516 | 0.028449 |
| C | -2.642485 | 4.498046 | 0.710417 |
| H | -2.071364 | 5.017953 | 1.489390 |
| H | -2.493741 | 5.059059 | -0.221257 |
| H | -3.701744 | 4.578489 | 0.972670 |
| C | 2.542272 | 5.501026 | -0.239287 |
| H | 1.541321 | 5.847640 | -0.514641 |
| H | 2.759973 | 5.902807 | 0.760286 |
| H | 3.257828 | 5.957409 | -0.931040 |
| C | 6.061028 | -1.580417 | -1.393521 |
| H | 6.359983 | -2.419178 | -2.030403 |

| | | | |
|---|---|---|---|
| H | 6.248168 | -0.654544 | -1.946491 |
| H | 6.733160 | -1.579611 | -0.524034 |
| C | 5.090882 | 3.641246 | -0.950415 |
| C | 5.728692 | 4.770142 | -0.595102 |
| H | 5.639752 | 2.940048 | -1.579043 |
| H | 6.737575 | 4.970844 | -0.943930 |
| H | 5.286285 | 5.509580 | 0.063725 |
| C | 4.249599 | -4.239899 | -1.074181 |
| C | 5.470437 | -4.784168 | -0.932431 |
| H | 3.441669 | -4.907375 | -1.373312 |
| H | 5.634103 | -5.839360 | -1.131369 |
| H | 6.328555 | -4.214992 | -0.591596 |
| C | -4.483089 | 1.851761 | 0.735332 |
| C | -5.181415 | 1.861471 | -0.655964 |
| H | -4.856184 | 2.700958 | 1.320333 |
| H | -4.779289 | 0.948766 | 1.278472 |
| H | -4.880771 | 2.745826 | -1.220411 |
| H | -4.884341 | 0.971532 | -1.222483 |
| C | -3.512806 | -3.502486 | 0.457711 |
| C | -4.479354 | -3.433688 | -0.761848 |
| H | -3.969640 | -2.965677 | 1.295428 |
| H | -3.457829 | -4.550035 | 0.770385 |
| H | -3.950322 | -3.636137 | -1.694661 |

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|---|---|---|---|
| H | -5.254884 | -4.200850 | -0.634395 |
| C | -6.682254 | 1.883957 | -0.559311 |
| O | -7.433873 | 2.760464 | -0.919587 |
| O | -7.181859 | 0.748446 | 0.039371 |
| H | -8.147547 | 0.854270 | 0.050768 |
| C | -5.216643 | -2.122426 | -0.923029 |
| O | -5.258543 | -1.448393 | -1.933080 |
| O | -5.881890 | -1.782957 | 0.206695 |
| H | -6.335456 | -0.929683 | 0.046090 |
| O | 0.526484 | 0.078507 | -1.960146 |
| H | 1.022670 | 1.964696 | -2.715636 |
| C | 1.148145 | 0.034449 | 2.045096 |
| C | 2.439873 | 0.719148 | 2.527683 |
| C | 1.154124 | -1.280033 | 2.752196 |
| C | 2.858138 | -0.100280 | 3.755799 |
| H | 2.308999 | 1.779672 | 2.765205 |
| H | 3.228738 | 0.652357 | 1.775234 |
| O | 0.354162 | -2.193304 | 2.755892 |
| O | 2.284408 | -1.398121 | 3.565406 |
| H | 2.463387 | 0.324341 | 4.693464 |
| H | 3.942009 | -0.218190 | 3.864835 |
| H | 0.248635 | 0.571454 | 2.358919 |

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**Scanpoint_7**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.9195193

Zero-point correction= 0.724769 (Hartree/Particle)

Thermal correction to Energy= 0.774545

Thermal correction to Enthalpy= 0.775489

Thermal correction to Gibbs Free Energy= 0.639402

Sum of electronic and zero-point Energies= -2379.194750

Sum of electronic and thermal Energies= -2379.144975

Sum of electronic and thermal Enthalpies= -2379.144030

Sum of electronic and thermal Free Energies= -2379.280117

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.824288 | 0.063376 | -0.123598 |
| N | 1.962901 | 1.737119 | -0.320603 |
| C | 1.545379 | 3.041954 | -0.273268 |
| C | 2.660579 | 3.945773 | -0.461444 |
| C | 3.779278 | 3.152423 | -0.614446 |

| | | | |
|---|---|---|---|
| C | 3.309644 | 1.771295 | -0.532971 |
| C | 0.230866 | 3.449899 | -0.056491 |
| C | -0.858775 | 2.608870 | 0.136918 |
| N | -0.806730 | 1.241506 | 0.156932 |
| C | -2.079488 | 0.807268 | 0.392624 |
| C | -2.983471 | 1.943515 | 0.514817 |
| C | -2.218918 | 3.069295 | 0.353531 |
| C | -2.468232 | -0.527391 | 0.507231 |
| C | -1.654733 | -1.640665 | 0.311189 |
| N | -0.321436 | -1.597682 | 0.030171 |
| C | 0.075416 | -2.885721 | -0.164126 |
| C | -1.044672 | -3.798191 | 0.011579 |
| C | -2.127599 | -3.024305 | 0.326360 |
| C | 1.366882 | -3.294466 | -0.462970 |
| C | 2.473946 | -2.461474 | -0.575269 |
| C | 3.832112 | -2.925463 | -0.855181 |
| C | 4.620979 | -1.796950 | -0.880500 |
| C | 3.732482 | -0.676733 | -0.624353 |
| N | 2.451281 | -1.110796 | -0.423330 |
| C | 4.135019 | 0.655499 | -0.643770 |
| H | 0.039415 | 4.517133 | -0.032737 |
| H | 5.193985 | 0.841611 | -0.778654 |
| H | 1.530337 | -4.359643 | -0.578306 |

| | | | |
|---|---|---|---|
| H | -3.508754 | -0.716743 | 0.744054 |
| C | 0.225036 | 1.047550 | -2.802828 |
| H | -0.696853 | 1.577526 | -2.495957 |
| H | 0.061685 | 0.706519 | -3.841835 |
| C | -0.955195 | -5.289356 | -0.112953 |
| H | -0.674906 | -5.595158 | -1.129032 |
| H | -0.200396 | -5.702770 | 0.566707 |
| H | -1.908816 | -5.772496 | 0.119853 |
| C | -2.651736 | 4.505120 | 0.370721 |
| H | -2.062576 | 5.096918 | 1.082012 |
| H | -2.533549 | 4.979414 | -0.612123 |
| H | -3.703757 | 4.604178 | 0.655067 |
| C | 2.566462 | 5.439694 | -0.526350 |
| H | 1.596529 | 5.763721 | -0.916615 |
| H | 2.692659 | 5.910644 | 0.458672 |
| H | 3.344877 | 5.848051 | -1.179086 |
| C | 6.085693 | -1.696130 | -1.175962 |
| H | 6.404965 | -2.513575 | -1.830574 |
| H | 6.332498 | -0.752086 | -1.671836 |
| H | 6.697798 | -1.753293 | -0.265175 |
| C | 5.160716 | 3.537689 | -0.866058 |
| C | 5.768110 | 4.688882 | -0.529791 |
| H | 5.762626 | 2.795890 | -1.390744 |

| | | | |
|---|---|---|---|
| H | 6.806426 | 4.866387 | -0.794680 |
| H | 5.269811 | 5.470728 | 0.033194 |
| C | 4.191622 | -4.315333 | -1.097239 |
| C | 5.387313 | -4.899916 | -0.909797 |
| H | 3.386789 | -4.944546 | -1.477214 |
| H | 5.536092 | -5.948684 | -1.150339 |
| H | 6.236471 | -4.372391 | -0.489076 |
| C | -4.473213 | 1.869740 | 0.686317 |
| C | -5.212302 | 1.806497 | -0.681907 |
| H | -4.828169 | 2.750310 | 1.235481 |
| H | -4.754419 | 0.998569 | 1.286176 |
| H | -4.929352 | 2.658969 | -1.301781 |
| H | -4.931372 | 0.887386 | -1.208831 |
| C | -3.517602 | -3.502169 | 0.643259 |
| C | -4.527119 | -3.479751 | -0.542298 |
| H | -3.946041 | -2.934178 | 1.475370 |
| H | -3.450647 | -4.537776 | 0.992423 |
| H | -4.032888 | -3.727259 | -1.483240 |
| H | -5.302776 | -4.234018 | -0.353376 |
| C | -6.709851 | 1.833868 | -0.544835 |
| O | -7.474501 | 2.681258 | -0.944867 |
| O | -7.189069 | 0.741735 | 0.145177 |
| H | -8.154656 | 0.845492 | 0.173167 |

| | | | |
|---|---|---|---|
| C | -5.259788 | -2.170267 | -0.734732 |
| O | -5.332213 | -1.541264 | -1.771698 |
| O | -5.882901 | -1.776349 | 0.401250 |
| H | -6.339741 | -0.929253 | 0.217746 |
| O | 0.532191 | -0.038091 | -1.995238 |
| H | 1.028914 | 1.807770 | -2.841215 |
| C | 1.058537 | 0.057838 | 2.001117 |
| C | 1.724438 | 1.269908 | 2.672569 |
| C | 1.687778 | -1.117624 | 2.676053 |
| C | 2.312508 | 0.690000 | 3.964780 |
| H | 1.032673 | 2.096116 | 2.865069 |
| H | 2.537452 | 1.664935 | 2.057412 |
| O | 1.545032 | -2.310557 | 2.512402 |
| O | 2.557756 | -0.693675 | 3.685482 |
| H | 1.607008 | 0.759456 | 4.808871 |
| H | 3.259146 | 1.148415 | 4.272312 |
| H | -0.011043 | 0.010428 | 2.232974 |

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**Scanpoint_8**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.925088

Zero-point correction= 0.725450 (Hartree/Particle)

Thermal correction to Energy= 0.774960

Thermal correction to Enthalpy= 0.775905

Thermal correction to Gibbs Free Energy= 0.641084

Sum of electronic and zero-point Energies= -2379.199638

Sum of electronic and thermal Energies= -2379.150128

Sum of electronic and thermal Enthalpies= -2379.149183

Sum of electronic and thermal Free Energies= -2379.284004

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.797905 | 0.019138 | -0.083141 |
| N | 1.953403 | 1.676161 | -0.285210 |
| C | 1.545521 | 2.985701 | -0.273937 |
| C | 2.666750 | 3.874524 | -0.491485 |
| C | 3.777246 | 3.067412 | -0.637367 |
| C | 3.296641 | 1.693053 | -0.522141 |
| C | 0.230732 | 3.407793 | -0.082264 |
| C | -0.864927 | 2.579328 | 0.129120 |
| N | -0.822363 | 1.211709 | 0.191417 |
| C | -2.100990 | 0.795218 | 0.426175 |
| C | -2.996269 | 1.941982 | 0.513622 |

| | | | |
|---|---|---|---|
| C | -2.222189 | 3.056502 | 0.325273 |
| C | -2.508531 | -0.532464 | 0.557440 |
| C | -1.709025 | -1.658056 | 0.378502 |
| N | -0.375248 | -1.632174 | 0.094286 |
| C | 0.015743 | -2.928931 | -0.054409 |
| C | -1.110259 | -3.828366 | 0.150226 |
| C | -2.190146 | -3.037207 | 0.434751 |
| C | 1.305415 | -3.352770 | -0.344974 |
| C | 2.413968 | -2.529692 | -0.505710 |
| C | 3.764753 | -3.013112 | -0.791058 |
| C | 4.562434 | -1.893906 | -0.853709 |
| C | 3.686820 | -0.759539 | -0.611791 |
| N | 2.403342 | -1.176097 | -0.393600 |
| C | 4.105859 | 0.566175 | -0.642876 |
| H | 0.045600 | 4.476271 | -0.091779 |
| H | 5.165100 | 0.737771 | -0.792898 |
| H | 1.464229 | -4.422066 | -0.423424 |
| H | -3.551957 | -0.704579 | 0.794497 |
| C | 0.144028 | 0.976077 | -2.762314 |
| H | -0.829490 | 1.425600 | -2.487507 |
| H | 0.050433 | 0.637252 | -3.810512 |
| C | -1.031537 | -5.323296 | 0.068417 |
| H | -0.773300 | -5.660261 | -0.943684 |

| | | | |
|---|---|---|---|
| H | -0.265539 | -5.722568 | 0.743933 |
| H | -1.982958 | -5.793597 | 0.334188 |
| C | -2.643071 | 4.495736 | 0.301398 |
| H | -2.057146 | 5.100343 | 1.004554 |
| H | -2.509693 | 4.944020 | -0.691610 |
| H | -3.697348 | 4.610383 | 0.570960 |
| C | 2.585435 | 5.367256 | -0.591442 |
| H | 1.615406 | 5.690912 | -0.981710 |
| H | 2.723853 | 5.860292 | 0.380991 |
| H | 3.362138 | 5.752587 | -1.259925 |
| C | 6.024853 | -1.811985 | -1.164072 |
| H | 6.334553 | -2.653672 | -1.791930 |
| H | 6.273066 | -0.887029 | -1.694314 |
| H | 6.641611 | -1.840412 | -0.255366 |
| C | 5.159383 | 3.435365 | -0.911434 |
| C | 5.778911 | 4.588455 | -0.605899 |
| H | 5.750019 | 2.677400 | -1.425385 |
| H | 6.816182 | 4.751373 | -0.883748 |
| H | 5.292572 | 5.386080 | -0.054737 |
| C | 4.108551 | -4.411781 | -1.004632 |
| C | 5.298452 | -5.003747 | -0.805720 |
| H | 3.296801 | -5.040160 | -1.371415 |
| H | 5.437317 | -6.058635 | -1.024653 |

| | | | |
|---|---|---|---|
| H | 6.151927 | -4.475417 | -0.394927 |
| C | -4.487543 | 1.885442 | 0.678606 |
| C | -5.219815 | 1.795704 | -0.691856 |
| H | -4.837257 | 2.782303 | 1.204196 |
| H | -4.779955 | 1.031872 | 1.298055 |
| H | -4.925553 | 2.630313 | -1.330475 |
| H | -4.944647 | 0.861684 | -1.194992 |
| C | -3.585040 | -3.495957 | 0.758603 |
| C | -4.589842 | -3.493401 | -0.430922 |
| H | -4.011750 | -2.903966 | 1.574772 |
| H | -3.528218 | -4.523355 | 1.133011 |
| H | -4.094653 | -3.768563 | -1.363642 |
| H | -5.373260 | -4.235427 | -0.226438 |
| C | -6.717720 | 1.840705 | -0.563389 |
| O | -7.471740 | 2.687169 | -0.984789 |
| O | -7.211357 | 0.768045 | 0.146862 |
| H | -8.175952 | 0.882188 | 0.168142 |
| C | -5.308936 | -2.181758 | -0.657781 |
| O | -5.371079 | -1.577458 | -1.709886 |
| O | -5.931998 | -1.754708 | 0.466085 |
| H | -6.379869 | -0.907661 | 0.261074 |
| O | 0.505246 | -0.092633 | -1.954522 |
| H | 0.884649 | 1.798727 | -2.760291 |

| | | | |
|---|---|---|---|
| C | 1.004789 | -0.026563 | 2.062853 |
| C | 1.159328 | 1.308681 | 2.800469 |
| C | 2.148416 | -0.822781 | 2.562077 |
| C | 2.676399 | 1.380519 | 3.030892 |
| H | 0.639884 | 1.289457 | 3.772423 |
| H | 0.793172 | 2.179885 | 2.255486 |
| O | 2.335598 | -2.023828 | 2.592768 |
| O | 3.127050 | 0.018601 | 3.086025 |
| H | 2.958406 | 1.867897 | 3.972198 |
| H | 3.188212 | 1.892012 | 2.208299 |
| H | 0.072653 | -0.543446 | 2.288201 |

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**Scanpoint_9**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.9242935

Zero-point correction= 0.725508 (Hartree/Particle)

Thermal correction to Energy= 0.775052

Thermal correction to Enthalpy= 0.775996

Thermal correction to Gibbs Free Energy= 0.640810

Sum of electronic and zero-point Energies= -2379.198786

Sum of electronic and thermal Energies= -2379.149242

Sum of electronic and thermal Enthalpies= -2379.148297

Sum of electronic and thermal Free Energies= -2379.283483

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | 0.808667 | 0.091316 | -0.050093 |
| N | 1.919971 | 1.765824 | -0.241775 |
| C | 1.508453 | 3.060943 | -0.078377 |
| C | 2.604719 | 3.981986 | -0.304060 |
| C | 3.699316 | 3.206042 | -0.616702 |
| C | 3.240207 | 1.819859 | -0.568983 |
| C | 0.204061 | 3.448897 | 0.219692 |
| C | -0.887282 | 2.598878 | 0.353572 |
| N | -0.838683 | 1.233156 | 0.273200 |
| C | -2.117288 | 0.789505 | 0.447429 |
| C | -3.022014 | 1.917583 | 0.626285 |
| C | -2.249924 | 3.048504 | 0.576097 |
| C | -2.512037 | -0.547517 | 0.476036 |
| C | -1.683071 | -1.650757 | 0.296663 |
| N | -0.332216 | -1.593436 | 0.102864 |
| C | 0.090294 | -2.881850 | -0.051174 |
| C | -1.027695 | -3.805031 | 0.068852 |

| | | | |
|---|---|---|---|
| C | -2.140252 | -3.037668 | 0.290968 |
| C | 1.400229 | -3.277980 | -0.297952 |
| C | 2.487046 | -2.427300 | -0.481657 |
| C | 3.837534 | -2.872947 | -0.824264 |
| C | 4.586320 | -1.727234 | -0.975987 |
| C | 3.688900 | -0.617320 | -0.710830 |
| N | 2.437728 | -1.071471 | -0.393678 |
| C | 4.059977 | 0.719537 | -0.793411 |
| H | 0.015187 | 4.511285 | 0.327631 |
| H | 5.100394 | 0.922130 | -1.016869 |
| H | 1.582828 | -4.343596 | -0.378437 |
| H | -3.561462 | -0.746064 | 0.658616 |
| C | 0.088441 | 1.084072 | -2.680494 |
| H | -0.904142 | 1.478431 | -2.390464 |
| H | 0.012239 | 0.783738 | -3.741369 |
| C | -0.917610 | -5.296239 | -0.045910 |
| H | -0.605636 | -5.602709 | -1.052543 |
| H | -0.177593 | -5.702992 | 0.654219 |
| H | -1.871555 | -5.789724 | 0.162433 |
| C | -2.677239 | 4.481103 | 0.694646 |
| H | -2.103567 | 5.011115 | 1.464709 |
| H | -2.532185 | 5.030049 | -0.244700 |
| H | -3.735669 | 4.564067 | 0.959630 |

| | | | |
|---|---|---|---|
| C | 2.509288 | 5.475860 | -0.254144 |
| H | 1.508048 | 5.825502 | -0.525328 |
| H | 2.731579 | 5.872481 | 0.746137 |
| H | 3.223682 | 5.932221 | -0.947133 |
| C | 6.021934 | -1.603896 | -1.382989 |
| H | 6.326831 | -2.460839 | -1.992119 |
| H | 6.196713 | -0.694993 | -1.967215 |
| H | 6.694112 | -1.564657 | -0.515063 |
| C | 5.049656 | 3.612265 | -0.979390 |
| C | 5.688945 | 4.741770 | -0.630888 |
| H | 5.594118 | 2.909310 | -1.609650 |
| H | 6.696411 | 4.940664 | -0.984860 |
| H | 5.252743 | 5.479137 | 0.034053 |
| C | 4.222466 | -4.265169 | -1.007851 |
| C | 5.442965 | -4.806191 | -0.852363 |
| H | 3.417410 | -4.936303 | -1.308020 |
| H | 5.610789 | -5.862417 | -1.042716 |
| H | 6.296672 | -4.231418 | -0.509858 |
| C | -4.516144 | 1.834972 | 0.746833 |
| C | -5.210395 | 1.837322 | -0.646721 |
| H | -4.890697 | 2.687799 | 1.325559 |
| H | -4.815070 | 0.935340 | 1.294171 |
| H | -4.911696 | 2.721541 | -1.212349 |

| | | | |
|---|---|---|---|
| H | -4.907228 | 0.947424 | -1.209921 |
| C | -3.547198 | -3.525886 | 0.500347 |
| C | -4.479421 | -3.451930 | -0.744783 |
| H | -4.028442 | -2.989977 | 1.325043 |
| H | -3.502066 | -4.574596 | 0.811765 |
| H | -3.923518 | -3.639414 | -1.664945 |
| H | -5.251431 | -4.227278 | -0.648531 |
| C | -6.711509 | 1.853824 | -0.554362 |
| O | -7.465663 | 2.729201 | -0.911488 |
| O | -7.208999 | 0.712850 | 0.037051 |
| H | -8.175028 | 0.815885 | 0.046540 |
| C | -5.225488 | -2.145862 | -0.913097 |
| O | -5.268597 | -1.478091 | -1.926803 |
| O | -5.898996 | -1.807587 | 0.211979 |
| H | -6.358318 | -0.957936 | 0.046672 |
| O | 0.492218 | -0.002013 | -1.914379 |
| H | 0.793097 | 1.936129 | -2.640031 |
| C | 1.150452 | 0.214573 | 2.088511 |
| C | 0.496624 | -0.833805 | 2.996342 |
| C | 2.576919 | 0.145522 | 2.480236 |
| C | 1.635939 | -1.846544 | 3.174625 |
| H | -0.402222 | -1.301619 | 2.591257 |
| H | 0.232480 | -0.402160 | 3.975817 |

| | | | |
|---|---|---|---|
| O | 3.478198 | 0.955386 | 2.378020 |
| O | 2.846993 | -1.080706 | 3.084466 |
| H | 1.630000 | -2.601345 | 2.380457 |
| H | 1.630070 | -2.357003 | 4.145215 |
| H | 0.781249 | 1.226397 | 2.255105 |

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**Scanpoint_10**

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Number of imaginary frequencies : 1 Electronic energy : HF=-2379.9236011

Zero-point correction= 0.725427 (Hartree/Particle)

Thermal correction to Energy= 0.774074

Thermal correction to Enthalpy= 0.775018

Thermal correction to Gibbs Free Energy= 0.643127

Sum of electronic and zero-point Energies= -2379.198174

Sum of electronic and thermal Energies= -2379.149527

Sum of electronic and thermal Enthalpies= -2379.148583

Sum of electronic and thermal Free Energies= -2379.280474

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.786784 | -0.047953 | -0.077623 |
| N | -1.919508 | -1.701711 | -0.306015 |
| C | -1.518311 | -3.005735 | -0.212312 |
| C | -2.634230 | -3.906738 | -0.425690 |
| C | -3.733819 | -3.109864 | -0.645869 |
| C | -3.255842 | -1.730409 | -0.566162 |
| C | -0.213763 | -3.421732 | 0.033500 |
| C | 0.883497 | -2.588558 | 0.213403 |
| N | 0.843964 | -1.221198 | 0.206064 |
| C | 2.121341 | -0.795077 | 0.431513 |
| C | 3.015768 | -1.937611 | 0.568594 |
| C | 2.239574 | -3.058527 | 0.434824 |
| C | 2.521938 | 0.535756 | 0.535971 |
| C | 1.711890 | 1.654428 | 0.358341 |
| N | 0.371280 | 1.619954 | 0.104661 |
| C | -0.023638 | 2.915848 | -0.062261 |
| C | 1.103027 | 3.819675 | 0.108625 |
| C | 2.190699 | 3.033707 | 0.383425 |
| C | -1.320939 | 3.334150 | -0.334328 |
| C | -2.424449 | 2.502781 | -0.502878 |
| C | -3.774981 | 2.972091 | -0.807758 |
| C | -4.557391 | 1.840795 | -0.900722 |
| C | -3.675398 | 0.716412 | -0.650544 |

| | | | |
|---|---|---|---|
| N | -2.403380 | 1.146478 | -0.390511 |
| C | -4.073206 | -0.615898 | -0.713682 |
| H | -0.034908 | -4.489797 | 0.087346 |
| H | -5.126381 | -0.801728 | -0.886794 |
| H | -1.483015 | 4.402287 | -0.425175 |
| H | 3.566717 | 0.717809 | 0.759100 |
| C | -0.118928 | -0.991645 | -2.745561 |
| H | 0.841940 | -1.459424 | -2.458524 |
| H | -0.005073 | -0.649894 | -3.790465 |
| C | 1.024379 | 5.312763 | -0.007394 |
| H | 0.764399 | 5.626270 | -1.026594 |
| H | 0.260577 | 5.731984 | 0.659057 |
| H | 1.976592 | 5.788604 | 0.245367 |
| C | 2.656233 | -4.498271 | 0.481827 |
| H | 2.064630 | -5.065443 | 1.210593 |
| H | 2.525556 | -4.993296 | -0.489081 |
| H | 3.708981 | -4.603050 | 0.761359 |
| C | -2.552153 | -5.401638 | -0.437139 |
| H | -1.577460 | -5.749796 | -0.794048 |
| H | -2.703438 | -5.828767 | 0.563557 |
| H | -3.321277 | -5.826606 | -1.090183 |
| C | -6.010234 | 1.744866 | -1.251155 |
| H | -6.313542 | 2.588520 | -1.879437 |

| | | | |
|---|---|---|---|
| H | -6.231454 | 0.821911 | -1.795960 |
| H | -6.652494 | 1.755525 | -0.359861 |
| C | -5.105920 | -3.487958 | -0.954236 |
| C | -5.743629 | -4.616001 | -0.599007 |
| H | -5.668687 | -2.763932 | -1.543591 |
| H | -6.769051 | -4.795419 | -0.909335 |
| H | -5.285896 | -5.371180 | 0.030561 |
| C | -4.133033 | 4.368840 | -1.010406 |
| C | -5.335114 | 4.943582 | -0.832251 |
| H | -3.321192 | 5.013114 | -1.348586 |
| H | -5.482409 | 5.999247 | -1.041594 |
| H | -6.193369 | 4.397997 | -0.455042 |
| C | 4.507018 | -1.873934 | 0.729785 |
| C | 5.236593 | -1.830029 | -0.644574 |
| H | 4.858747 | -2.751906 | 1.284854 |
| H | 4.799637 | -0.999152 | 1.318990 |
| H | 4.943973 | -2.688006 | -1.252219 |
| H | 4.956732 | -0.915491 | -1.179850 |
| C | 3.592234 | 3.500187 | 0.665871 |
| C | 4.572471 | 3.463660 | -0.543450 |
| H | 4.035644 | 2.930172 | 1.488757 |
| H | 3.543564 | 4.537486 | 1.013444 |
| H | 4.056476 | 3.700869 | -1.475302 |

| | | | |
|---|---|---|---|
| H | 5.352906 | 4.219493 | -0.382392 |
| C | 6.734818 | -1.865056 | -0.517347 |
| O | 7.490956 | -2.726073 | -0.903862 |
| O | 7.226547 | -0.761705 | 0.146174 |
| H | 8.191382 | -0.872892 | 0.171586 |
| C | 5.300876 | 2.151661 | -0.738856 |
| O | 5.360042 | 1.519453 | -1.774424 |
| O | 5.936921 | 1.762015 | 0.391165 |
| H | 6.389084 | 0.912195 | 0.207547 |
| O | -0.469243 | 0.083223 | -1.938717 |
| H | -0.875292 | -1.798906 | -2.754378 |
| C | -1.088568 | -0.108048 | 2.084504 |
| C | -1.039505 | 1.215215 | 2.861606 |
| C | -2.379792 | -0.690734 | 2.520120 |
| C | -2.527955 | 1.564025 | 3.002519 |
| H | -0.481879 | 2.016311 | 2.374564 |
| H | -0.600629 | 1.072193 | 3.862733 |
| O | -2.775694 | -1.841045 | 2.532615 |
| O | -3.218157 | 0.305861 | 3.012561 |
| H | -2.884910 | 2.161413 | 2.156881 |
| H | -2.773812 | 2.091929 | 3.931975 |
| H | -0.281810 | -0.794204 | 2.339759 |

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**Scanpoint_11**

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Number of imaginary frequencies : 0 Electronic energy : HF=-2379.9258798

Zero-point correction= 0.725492 (Hartree/Particle)

Thermal correction to Energy= 0.775002

Thermal correction to Enthalpy= 0.775946

Thermal correction to Gibbs Free Energy= 0.641151

Sum of electronic and zero-point Energies= -2379.200388

Sum of electronic and thermal Energies= -2379.150878

Sum of electronic and thermal Enthalpies= -2379.149934

Sum of electronic and thermal Free Energies= -2379.284729

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| Fe | -0.796926 | 0.003778 | -0.084920 |
| N | -1.959812 | -1.632911 | -0.327156 |
| C | -1.563919 | -2.942898 | -0.312717 |
| C | -2.693269 | -3.825780 | -0.523029 |
| C | -3.796544 | -3.013668 | -0.662716 |

| | | | |
|---|---|---|---|
| C | -3.304755 | -1.641452 | -0.548996 |
| C | -0.255886 | -3.377423 | -0.127934 |
| C | 0.846153 | -2.561113 | 0.085348 |
| N | 0.815868 | -1.195735 | 0.147047 |
| C | 2.095043 | -0.789000 | 0.394104 |
| C | 2.982076 | -1.943599 | 0.477110 |
| C | 2.199603 | -3.050287 | 0.282659 |
| C | 2.505975 | 0.533660 | 0.556017 |
| C | 1.709331 | 1.667205 | 0.410508 |
| N | 0.372101 | 1.655260 | 0.140066 |
| C | -0.006692 | 2.958441 | -0.002168 |
| C | 1.128348 | 3.844935 | 0.203303 |
| C | 2.202747 | 3.040667 | 0.475978 |
| C | -1.295484 | 3.396667 | -0.283574 |
| C | -2.410646 | 2.580881 | -0.460006 |
| C | -3.755751 | 3.071164 | -0.753685 |
| C | -4.555525 | 1.951664 | -0.849901 |
| C | -3.688339 | 0.813023 | -0.612887 |
| N | -2.407128 | 1.223351 | -0.360735 |
| C | -4.109488 | -0.513027 | -0.664402 |
| H | -0.083246 | -4.447636 | -0.129774 |
| H | -5.168217 | -0.681572 | -0.821695 |
| H | -1.443957 | 4.467914 | -0.359524 |

| | | | |
|---|---|---|---|
| H | 3.550858 | 0.697016 | 0.792898 |
| C | -0.186474 | -0.880314 | -2.794309 |
| H | 0.757492 | -1.389916 | -2.522838 |
| H | -0.059133 | -0.507124 | -3.827069 |
| C | 1.067825 | 5.341163 | 0.122816 |
| H | 0.822476 | 5.682456 | -0.891090 |
| H | 0.301561 | 5.752679 | 0.791292 |
| H | 2.022615 | 5.799616 | 0.397096 |
| C | 2.605003 | -4.493664 | 0.263889 |
| H | 2.015186 | -5.084757 | 0.974631 |
| H | 2.460638 | -4.945785 | -0.725789 |
| H | 3.659507 | -4.618392 | 0.528053 |
| C | -2.622521 | -5.319170 | -0.602386 |
| H | -1.667722 | -5.655402 | -1.019196 |
| H | -2.727863 | -5.787043 | 0.385746 |
| H | -3.424080 | -5.712320 | -1.235923 |
| C | -6.011365 | 1.879595 | -1.195483 |
| H | -6.300942 | 2.725219 | -1.827680 |
| H | -6.250100 | 0.958181 | -1.735393 |
| H | -6.653363 | 1.907350 | -0.304076 |
| C | -5.183165 | -3.371617 | -0.927869 |
| C | -5.813988 | -4.509102 | -0.590499 |
| H | -5.765298 | -2.621791 | -1.463805 |

| | | | |
|---|---|---|---|
| H | -6.852653 | -4.670340 | -0.864627 |
| H | -5.335412 | -5.292189 | -0.012571 |
| C | -4.095036 | 4.473979 | -0.945148 |
| C | -5.289722 | 5.063789 | -0.765572 |
| H | -3.273773 | 5.110022 | -1.275809 |
| H | -5.421735 | 6.123094 | -0.966393 |
| H | -6.157108 | 4.527237 | -0.396320 |
| C | 4.472722 | -1.899038 | 0.649731 |
| C | 5.211799 | -1.803716 | -0.716851 |
| H | 4.813259 | -2.802488 | 1.169696 |
| H | 4.768453 | -1.052570 | 1.277386 |
| H | 4.916743 | -2.633164 | -1.361789 |
| H | 4.942713 | -0.865507 | -1.215480 |
| C | 3.604586 | 3.484886 | 0.791095 |
| C | 4.598066 | 3.485938 | -0.407703 |
| H | 4.033919 | 2.880857 | 1.596900 |
| H | 3.559902 | 4.508900 | 1.176714 |
| H | 4.095306 | 3.766288 | -1.334812 |
| H | 5.384780 | 4.225756 | -0.207591 |
| C | 6.708861 | -1.855434 | -0.582423 |
| O | 7.461773 | -2.702439 | -1.004516 |
| O | 7.204036 | -0.787640 | 0.134862 |
| H | 8.167903 | -0.906794 | 0.160602 |

| | | | |
|---|---|---|---|
| C | 5.313936 | 2.174482 | -0.647835 |
| O | 5.376085 | 1.583183 | -1.707175 |
| O | 5.934489 | 1.733787 | 0.471707 |
| H | 6.379861 | 0.886983 | 0.259307 |
| O | -0.505074 | 0.175027 | -1.950396 |
| H | -0.969064 | -1.661892 | -2.832753 |
| C | -0.996372 | -0.000656 | 2.062952 |
| C | -1.573759 | 1.254212 | 2.728369 |
| C | -1.831949 | -1.090666 | 2.614903 |
| C | -3.036872 | 0.852140 | 2.964464 |
| H | -1.498137 | 2.165505 | 2.133473 |
| H | -1.085580 | 1.453494 | 3.696332 |
| O | -1.627717 | -2.286033 | 2.712733 |
| O | -3.030501 | -0.577265 | 3.102259 |
| H | -3.672771 | 1.124866 | 2.115122 |
| H | -3.472178 | 1.277274 | 3.876904 |
| H | 0.049967 | -0.182172 | 2.306502 |

**QM cluster 1**

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**Conf1$^{L9}$**

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Number of imaginary frequencies : 3 Electronic energy : HF=-188.1141314

Zero-point correction= 0.981196 (Hartree/Particle)

Thermal correction to Energy= 1.049728

Thermal correction to Enthalpy= 1.050672

Thermal correction to Gibbs Free Energy= 0.869325

Sum of electronic and zero-point Energies= -187.132936

Sum of electronic and thermal Energies= -187.064403

Sum of electronic and thermal Enthalpies= -187.063459

Sum of electronic and thermal Free Energies= -187.244806

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -2.820202 | -4.278550 | 2.178932 |
| H | -2.313067 | -3.320705 | 2.300144 |
| C | -2.825201 | -4.637578 | 0.675894 |
| H | -2.676665 | -5.714220 | 0.545245 |
| H | -3.804274 | -4.376202 | 0.245555 |
| O | -1.805766 | -4.007810 | -0.045703 |
| H | -1.962127 | -3.042320 | 0.027228 |
| C | -4.236863 | -4.145426 | 2.686188 |

| | | | |
|---|---|---|---|
| O | -4.796560 | -4.978705 | 3.380284 |
| N | -4.833850 | -3.021478 | 2.249658 |
| H | -4.285976 | -2.359142 | 1.708774 |
| C | -6.206321 | -2.722847 | 2.558295 |
| H | -6.595518 | -3.553896 | 3.146174 |
| H | -6.285430 | -1.799973 | 3.138500 |
| C | 4.488569 | -0.525174 | 5.107601 |
| H | 5.426045 | -1.036997 | 4.906117 |
| C | 3.295127 | -1.348224 | 4.632253 |
| H | 3.331314 | -2.338404 | 5.094235 |
| H | 2.378080 | -0.860437 | 4.971952 |
| C | 3.220055 | -1.507456 | 3.108828 |
| H | 3.210556 | -0.508531 | 2.657988 |
| C | 4.421964 | -2.279404 | 2.568443 |
| H | 4.329402 | -2.424854 | 1.495578 |
| H | 5.351237 | -1.746849 | 2.756403 |
| H | 4.484422 | -3.259113 | 3.039636 |
| C | 1.925788 | -2.220322 | 2.720499 |
| H | 1.808240 | -2.246531 | 1.640336 |
| H | 1.925174 | -3.242247 | 3.095841 |
| C | 1.080079 | 2.041394 | -3.048257 |
| H | 1.468043 | 1.022212 | -3.226005 |
| H | 1.873415 | 2.602509 | -2.521796 |

| | | | |
|---|---|---|---|
| O | -0.084123 | 2.039888 | -2.336738 |
| C | 2.379471 | -0.485745 | -0.423993 |
| C | 0.785390 | 3.888287 | 0.797243 |
| C | -3.615085 | 2.686934 | -0.724989 |
| C | -1.867235 | -1.445437 | -2.466321 |
| C | 2.340572 | 0.827107 | 0.018955 |
| C | 3.487560 | 1.559595 | 0.505871 |
| C | 3.035831 | 2.802646 | 0.839331 |
| C | 1.618476 | 2.808448 | 0.562478 |
| C | 3.803848 | 3.964461 | 1.371489 |
| C | 4.898958 | 1.070032 | 0.464407 |
| C | 5.458727 | 1.319815 | -0.951353 |
| C | 6.898922 | 0.890233 | -1.105246 |
| O | 7.124315 | -0.431506 | -1.071113 |
| O | 7.810608 | 1.653545 | -1.280947 |
| C | -0.577156 | 3.921865 | 0.539917 |
| C | -1.432513 | 5.028525 | 0.882856 |
| C | -2.704363 | 4.663087 | 0.525386 |
| C | -2.584307 | 3.350358 | -0.083668 |
| C | -0.983112 | 6.280558 | 1.556395 |
| C | -3.914264 | 5.431474 | 0.725308 |
| C | -5.099112 | 4.938610 | 1.070975 |
| C | -3.505133 | 1.470048 | -1.376529 |

| | | | |
|---|---|---|---|
| C | -4.597462 | 0.842130 | -2.079629 |
| C | -4.101393 | -0.324183 | -2.598918 |
| C | -2.712137 | -0.388461 | -2.181236 |
| C | -4.779291 | -1.344529 | -3.365798 |
| C | -5.748923 | -1.132717 | -4.250994 |
| C | -0.566797 | -1.565777 | -2.011671 |
| C | 0.245410 | -2.747849 | -2.190953 |
| C | 1.425706 | -2.501891 | -1.557856 |
| C | 1.336714 | -1.154148 | -1.038600 |
| C | -0.206889 | -3.988548 | -2.876159 |
| C | 2.573180 | -3.448833 | -1.396933 |
| C | 3.630261 | -3.312283 | -2.508674 |
| C | 4.805695 | -2.472224 | -2.109982 |
| O | 5.091904 | -2.164260 | -0.972245 |
| O | 5.554899 | -2.097269 | -3.143922 |
| N | 1.235063 | 1.607804 | 0.055625 |
| N | -1.300415 | 2.929885 | -0.038939 |
| N | -2.384065 | 0.709348 | -1.464679 |
| N | 0.115773 | -0.625753 | -1.314689 |
| H | 4.855466 | 3.713195 | 1.488998 |
| H | 3.411108 | 4.273045 | 2.340999 |
| H | 3.728503 | 4.814057 | 0.692311 |
| H | -0.605998 | 6.065043 | 2.557227 |

| | | | |
|---|---|---|---|
| H | -1.807071 | 6.984418 | 1.648112 |
| H | -0.180937 | 6.753272 | 0.989030 |
| H | 0.622961 | -4.673045 | -3.036845 |
| H | -0.658525 | -3.758270 | -3.840097 |
| H | -0.951878 | -4.477377 | -2.248938 |
| H | -5.958079 | 5.575811 | 1.207944 |
| H | -5.247370 | 3.888022 | 1.252207 |
| H | -6.220848 | -1.947014 | -4.777044 |
| H | -6.087724 | -0.143019 | -4.504389 |
| H | 5.398399 | 2.385411 | -1.176797 |
| H | 4.837356 | 0.778732 | -1.670815 |
| H | 4.941111 | 0.006288 | 0.703871 |
| H | 5.510766 | 1.606947 | 1.192743 |
| H | 3.196825 | -2.888099 | -3.416187 |
| H | 4.037304 | -4.292833 | -2.772762 |
| H | 2.177425 | -4.464841 | -1.404002 |
| H | 3.057302 | -3.293015 | -0.431804 |
| H | 3.308001 | -1.018650 | -0.305649 |
| H | 1.230784 | 4.773871 | 1.227333 |
| H | -4.572950 | 3.183849 | -0.758085 |
| H | -2.266771 | -2.268410 | -3.038754 |
| H | -3.806821 | 6.505717 | 0.609944 |
| H | -4.445161 | -2.359262 | -3.185818 |

| | | | |
|---|---|---|---|
| Fe | -0.590137 | 1.151465 | -0.714478 |
| H | -6.795303 | -2.614411 | 1.643754 |
| H | 4.505989 | 0.438934 | 4.603230 |
| H | 6.329409 | -1.579165 | -2.853106 |
| H | 6.325956 | -0.965413 | -0.824103 |
| H | 0.924652 | 2.524411 | -4.028457 |
| H | -2.290856 | -5.036267 | 2.756171 |
| H | 4.423498 | -0.350451 | 6.180062 |
| C | -1.119481 | 0.386222 | 0.979879 |
| C | -0.625643 | 0.899916 | 2.306045 |
| C | -1.447125 | 0.126377 | 3.349940 |
| H | -2.167425 | 0.777497 | 3.864003 |
| O | -2.159557 | -0.863610 | 2.651363 |
| C | -1.991771 | -0.672825 | 1.267000 |
| O | -2.628177 | -1.448531 | 0.537948 |
| H | -0.827191 | -0.365511 | 4.109139 |
| H | -0.762946 | 1.978195 | 2.401476 |
| H | 0.444728 | 0.698688 | 2.410688 |
| C | -5.993342 | 1.360592 | -2.135018 |
| H | -6.091667 | 2.132354 | -2.900710 |
| H | -6.682690 | 0.551681 | -2.369361 |
| H | -6.279142 | 1.796862 | -1.179153 |
| H | 1.061542 | -1.705915 | 3.132140 |

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**Conf2$^{L9}$**

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Number of imaginary frequencies : 3 Electronic energy : HF=-188.1113916

Zero-point correction= 0.981264 (Hartree/Particle)

Thermal correction to Energy= 1.049648

Thermal correction to Enthalpy= 1.050592

Thermal correction to Gibbs Free Energy= 0.870183

Sum of electronic and zero-point Energies= -187.130127

Sum of electronic and thermal Energies= -187.061744

Sum of electronic and thermal Enthalpies= -187.060800

Sum of electronic and thermal Free Energies= -187.241208

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.883436 | -1.899844 | 2.788086 |
| H | -4.280158 | -1.051980 | 2.458561 |
| C | -4.404079 | -3.137330 | 2.006332 |
| H | -4.856216 | -4.044990 | 2.421578 |
| H | -4.728019 | -3.039870 | 0.957122 |

| | | | |
|---|---|---|---|
| O | -3.019934 | -3.309186 | 2.069944 |
| H | -2.627256 | -2.457955 | 1.776705 |
| C | -6.344828 | -1.663441 | 2.527956 |
| O | -7.241345 | -1.975236 | 3.291506 |
| N | -6.580604 | -1.095608 | 1.324227 |
| H | -5.801398 | -0.855907 | 0.730461 |
| C | -7.912681 | -0.880918 | 0.834819 |
| H | -8.598935 | -1.253312 | 1.594601 |
| H | -8.103867 | 0.182386 | 0.666088 |
| C | 1.583788 | 3.615563 | 4.747204 |
| H | 2.056638 | 4.554447 | 5.026858 |
| C | 2.617442 | 2.508440 | 4.576206 |
| H | 3.207088 | 2.416366 | 5.492759 |
| H | 2.093556 | 1.562038 | 4.426219 |
| C | 3.564181 | 2.723103 | 3.390495 |
| H | 2.962438 | 2.882598 | 2.488969 |
| C | 4.464102 | 3.939556 | 3.596715 |
| H | 5.159894 | 4.037336 | 2.765967 |
| H | 3.879842 | 4.854029 | 3.657694 |
| H | 5.040941 | 3.834574 | 4.514362 |
| C | 4.416984 | 1.474004 | 3.180692 |
| H | 5.100958 | 1.616956 | 2.348951 |
| H | 4.998433 | 1.254747 | 4.075004 |

| | | | |
|---|---|---|---|
| C | 1.451593 | -0.274431 | -3.367917 |
| H | 1.630183 | -1.274485 | -2.934832 |
| H | 2.369040 | 0.319520 | -3.205309 |
| O | 0.358467 | 0.340899 | -2.830891 |
| C | 2.386117 | -1.401060 | 0.164211 |
| C | 1.879212 | 3.230965 | -1.028884 |
| C | -2.822672 | 2.491449 | -1.730398 |
| C | -2.122576 | -2.247031 | -1.277942 |
| C | 2.677105 | -0.084168 | -0.159521 |
| C | 4.003339 | 0.489590 | -0.142996 |
| C | 3.858352 | 1.802454 | -0.483178 |
| C | 2.446251 | 2.012377 | -0.700411 |
| C | 4.905710 | 2.852693 | -0.633296 |
| C | 5.264607 | -0.295376 | 0.017510 |
| C | 5.589909 | -0.964281 | -1.334353 |
| C | 6.872722 | -1.761551 | -1.306916 |
| O | 6.845054 | -2.891973 | -0.585852 |
| O | 7.868089 | -1.451028 | -1.904920 |
| C | 0.529458 | 3.447392 | -1.265247 |
| C | -0.047323 | 4.745433 | -1.500254 |
| C | -1.399035 | 4.554633 | -1.625619 |
| C | -1.610076 | 3.122103 | -1.518074 |
| C | 0.712755 | 6.028028 | -1.524153 |

| | | | |
|---|---|---|---|
| C | -2.402360 | 5.579809 | -1.819165 |
| C | -3.607961 | 5.603527 | -1.260492 |
| C | -3.032524 | 1.122077 | -1.708803 |
| C | -4.310773 | 0.507139 | -1.965968 |
| C | -4.109579 | -0.847977 | -1.889352 |
| C | -2.707309 | -1.023324 | -1.551996 |
| C | -5.065313 | -1.921407 | -2.028686 |
| C | -6.158093 | -1.906384 | -2.788463 |
| C | -0.848465 | -2.415258 | -0.767305 |
| C | -0.348657 | -3.668830 | -0.249017 |
| C | 0.901425 | -3.415128 | 0.229468 |
| C | 1.167293 | -2.019872 | -0.044180 |
| C | -1.135575 | -4.930385 | -0.183870 |
| C | 1.808475 | -4.374768 | 0.933000 |
| C | 2.716372 | -5.160134 | -0.031933 |
| C | 4.059051 | -4.523831 | -0.228358 |
| O | 4.581846 | -3.743970 | 0.540445 |
| O | 4.669396 | -4.924315 | -1.341261 |
| N | 1.766734 | 0.849532 | -0.521874 |
| N | -0.435390 | 2.492789 | -1.286598 |
| N | -2.090304 | 0.175511 | -1.464569 |
| N | 0.082028 | -1.441641 | -0.623124 |
| H | 5.893885 | 2.448844 | -0.424093 |

| | | | |
|---|---|---|---|
| H | 4.717422 | 3.681385 | 0.050304 |
| H | 4.906337 | 3.248621 | -1.649146 |
| H | 1.153119 | 6.232752 | -0.547176 |
| H | 0.058435 | 6.857458 | -1.782409 |
| H | 1.521196 | 5.979849 | -2.254167 |
| H | -0.510563 | -5.766916 | 0.120629 |
| H | -1.579704 | -5.163621 | -1.150885 |
| H | -1.936823 | -4.806048 | 0.545798 |
| H | -4.302265 | 6.406774 | -1.448467 |
| H | -3.934595 | 4.837345 | -0.578646 |
| H | -6.829458 | -2.749483 | -2.822601 |
| H | -6.406291 | -1.075853 | -3.425751 |
| H | 5.688238 | -0.192111 | -2.098608 |
| H | 4.756793 | -1.617804 | -1.608003 |
| H | 5.148248 | -1.052963 | 0.795436 |
| H | 6.092705 | 0.357982 | 0.300320 |
| H | 2.244554 | -5.285201 | -1.007701 |
| H | 2.915064 | -6.159473 | 0.367546 |
| H | 1.192054 | -5.080934 | 1.490970 |
| H | 2.436204 | -3.843505 | 1.649742 |
| H | 3.182448 | -1.996994 | 0.580172 |
| H | 2.538495 | 4.084558 | -1.094914 |
| H | -3.665462 | 3.119875 | -1.975854 |

| | | | |
|---|---|---|---|
| H | -2.732406 | -3.132259 | -1.375246 |
| H | -2.103074 | 6.408021 | -2.454336 |
| H | -4.848813 | -2.814414 | -1.454048 |
| Fe | -0.172389 | 0.506888 | -1.003421 |
| H | -8.075661 | -1.420993 | -0.101790 |
| H | 1.034394 | 3.764840 | 3.821161 |
| H | 5.556670 | -4.525800 | -1.425043 |
| H | 6.015105 | -3.003438 | -0.052622 |
| H | 1.321759 | -0.392211 | -4.457924 |
| H | -4.721467 | -2.062836 | 3.854121 |
| H | 0.873170 | 3.351115 | 5.527258 |
| C | -0.672804 | 0.784626 | 0.831507 |
| C | -0.041351 | 1.765440 | 1.777954 |
| C | -0.891440 | 1.662405 | 3.056751 |
| H | -1.458002 | 2.583837 | 3.247253 |
| O | -1.805739 | 0.611709 | 2.858495 |
| C | -1.673171 | 0.120015 | 1.557306 |
| O | -2.438512 | -0.791518 | 1.222445 |
| H | -0.296832 | 1.432218 | 3.947496 |
| H | -0.040245 | 2.778225 | 1.368867 |
| H | 1.000228 | 1.489100 | 1.964839 |
| C | -5.589885 | 1.243982 | -2.173570 |
| H | -5.702691 | 1.543112 | -3.217344 |

H -6.435547 0.613691 -1.903635

H -5.617194 2.144002 -1.561412

H 3.788022 0.616116 2.956014

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**Conf3$^{L9}$**

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Number of imaginary frequencies : 4 Electronic energy : HF=-188.1139571

Zero-point correction= 0.981145 (Hartree/Particle)

Thermal correction to Energy= 1.048808

Thermal correction to Enthalpy= 1.049753

Thermal correction to Gibbs Free Energy= 0.872311

Sum of electronic and zero-point Energies= -187.132812

Sum of electronic and thermal Energies= -187.065149

Sum of electronic and thermal Enthalpies= -187.064204

Sum of electronic and thermal Free Energies= -187.241646

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Cartesian Coordinates

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C -4.077618 -3.687650 1.834667

H -3.478731 -2.813582 2.099260

| | | | |
|---|---|---|---|
| C | -3.790140 | -4.007514 | 0.354950 |
| H | -4.124036 | -5.022661 | 0.115915 |
| H | -4.348162 | -3.300034 | -0.277100 |
| O | -2.426351 | -3.948434 | 0.053323 |
| H | -2.149367 | -3.027704 | 0.234929 |
| C | -5.540418 | -3.389856 | 2.029730 |
| O | -6.349396 | -4.171210 | 2.498269 |
| N | -5.878769 | -2.156978 | 1.595928 |
| H | -5.156163 | -1.557359 | 1.226029 |
| C | -7.234667 | -1.684275 | 1.612784 |
| H | -7.847443 | -2.479005 | 2.037244 |
| H | -7.329828 | -0.785882 | 2.227966 |
| C | 3.223603 | -0.657499 | 5.521660 |
| H | 4.230816 | -1.064374 | 5.477366 |
| C | 2.225555 | -1.574166 | 4.821754 |
| H | 2.274123 | -2.570951 | 5.268372 |
| H | 1.217888 | -1.188585 | 4.993395 |
| C | 2.444614 | -1.692718 | 3.308708 |
| H | 2.465723 | -0.685091 | 2.877729 |
| C | 3.769610 | -2.382254 | 2.990112 |
| H | 3.887824 | -2.495916 | 1.915981 |
| H | 4.613645 | -1.805941 | 3.361897 |
| H | 3.800205 | -3.372260 | 3.442825 |

| | | | |
|---|---|---|---|
| C | 1.286128 | -2.460023 | 2.674690 |
| H | 1.385430 | -2.482033 | 1.593133 |
| H | 1.259153 | -3.484158 | 3.043569 |
| C | 1.327056 | 1.597882 | -3.198389 |
| H | 1.602346 | 0.531240 | -3.283171 |
| H | 2.184833 | 2.116463 | -2.733228 |
| O | 0.181953 | 1.783939 | -2.481175 |
| C | 2.540798 | -0.655867 | -0.310705 |
| C | 1.252109 | 3.929965 | 0.378857 |
| C | -3.271378 | 2.801045 | -0.807704 |
| C | -1.790209 | -1.561113 | -2.199359 |
| C | 2.584647 | 0.692012 | 0.007612 |
| C | 3.771361 | 1.388849 | 0.448765 |
| C | 3.411545 | 2.694128 | 0.613469 |
| C | 2.005098 | 2.771914 | 0.295135 |
| C | 4.255470 | 3.850580 | 1.029921 |
| C | 5.136588 | 0.789008 | 0.546176 |
| C | 5.797302 | 0.834223 | -0.847175 |
| C | 7.209997 | 0.298673 | -0.848797 |
| O | 7.338628 | -1.021665 | -0.649408 |
| O | 8.183110 | 0.977059 | -1.042400 |
| C | -0.109985 | 4.019905 | 0.133273 |
| C | -0.886744 | 5.213491 | 0.345916 |

| | | | |
|---|---|---|---|
| C | -2.192211 | 4.878488 | 0.095594 |
| C | -2.172120 | 3.489347 | -0.326564 |
| C | -0.340140 | 6.518125 | 0.817410 |
| C | -3.346696 | 5.740603 | 0.232856 |
| C | -4.535119 | 5.380313 | 0.706133 |
| C | -3.254946 | 1.508773 | -1.306119 |
| C | -4.417754 | 0.849510 | -1.848037 |
| C | -3.995476 | -0.378540 | -2.286718 |
| C | -2.579751 | -0.449049 | -1.970585 |
| C | -4.758771 | -1.446459 | -2.890198 |
| C | -5.818449 | -1.295468 | -3.680153 |
| C | -0.481554 | -1.701304 | -1.775169 |
| C | 0.261680 | -2.938398 | -1.860378 |
| C | 1.468598 | -2.701440 | -1.274978 |
| C | 1.460132 | -1.310645 | -0.872899 |
| C | -0.281156 | -4.204789 | -2.421838 |
| C | 2.582309 | -3.679155 | -1.064900 |
| C | 3.667694 | -3.596633 | -2.154568 |
| C | 4.920488 | -2.911348 | -1.698213 |
| O | 5.160909 | -2.568189 | -0.559421 |
| O | 5.790720 | -2.709288 | -2.686300 |
| N | 1.540586 | 1.550440 | -0.075268 |
| N | -0.910792 | 3.004551 | -0.278950 |

| | | | |
|---|---|---|---|
| N | -2.167146 | 0.701081 | -1.393170 |
| N | 0.265797 | -0.741177 | -1.179610 |
| H | 5.281822 | 3.537695 | 1.207217 |
| H | 3.867310 | 4.300027 | 1.944623 |
| H | 4.260061 | 4.617072 | 0.254491 |
| H | 0.047222 | 6.428672 | 1.833541 |
| H | -1.114327 | 7.282002 | 0.815623 |
| H | 0.476243 | 6.845680 | 0.173406 |
| H | 0.483061 | -4.977752 | -2.460353 |
| H | -0.664887 | -4.047574 | -3.429409 |
| H | -1.099619 | -4.546686 | -1.788158 |
| H | -5.349113 | 6.083067 | 0.784395 |
| H | -4.730279 | 4.380355 | 1.053459 |
| H | -6.346251 | -2.145256 | -4.082108 |
| H | -6.179994 | -0.326697 | -3.978526 |
| H | 5.828204 | 1.867976 | -1.194047 |
| H | 5.184316 | 0.254443 | -1.543065 |
| H | 5.073183 | -0.241092 | 0.901966 |
| H | 5.749606 | 1.354404 | 1.251623 |
| H | 3.297750 | -3.063756 | -3.033549 |
| H | 3.964601 | -4.593586 | -2.490659 |
| H | 2.159719 | -4.684200 | -1.054078 |
| H | 3.049276 | -3.511717 | -0.092857 |

| | | | |
|---|---|---|---|
| H | 3.430356 | -1.235240 | -0.130096 |
| H | 1.761478 | 4.831696 | 0.686997 |
| H | -4.208423 | 3.335839 | -0.844382 |
| H | -2.246026 | -2.415412 | -2.675455 |
| H | -3.188316 | 6.776787 | -0.050320 |
| H | -4.412640 | -2.448845 | -2.668266 |
| Fe | -0.320304 | 1.125355 | -0.758164 |
| H | -7.582948 | -1.457705 | 0.601419 |
| H | 3.228061 | 0.324268 | 5.052037 |
| H | 6.601299 | -2.272627 | -2.361936 |
| H | 6.488535 | -1.472457 | -0.409906 |
| H | 1.206003 | 2.001999 | -4.218526 |
| H | -3.783108 | -4.530840 | 2.459809 |
| H | 2.954779 | -0.535332 | 6.569524 |
| C | -0.823267 | 0.590397 | 1.020766 |
| C | -0.336861 | 1.243638 | 2.284727 |
| C | -1.191820 | 0.608622 | 3.392852 |
| H | -1.930675 | 1.319219 | 3.789158 |
| O | -1.878617 | -0.471206 | 2.808346 |
| C | -1.693843 | -0.437723 | 1.414948 |
| O | -2.311782 | -1.280050 | 0.755328 |
| H | -0.596855 | 0.228082 | 4.230959 |
| H | -0.448513 | 2.328591 | 2.256025 |

| | | | |
|---|---|---|---|
| H | 0.726231 | 1.029475 | 2.432190 |
| C | -5.801666 | 1.402782 | -1.832569 |
| H | -5.961963 | 2.076836 | -2.676092 |
| H | -6.528072 | 0.594446 | -1.895420 |
| H | -5.980919 | 1.962907 | -0.916062 |
| H | 0.334595 | -1.989565 | 2.905239 |

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**Conf4$^{L9}$**

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Number of imaginary frequencies : 2 Electronic energy : HF=-188.1138867

Zero-point correction= 0.981363 (Hartree/Particle)

Thermal correction to Energy= 1.050969

Thermal correction to Enthalpy= 1.051913

Thermal correction to Gibbs Free Energy= 0.865166

Sum of electronic and zero-point Energies= -187.132524

Sum of electronic and thermal Energies= -187.062917

Sum of electronic and thermal Enthalpies= -187.061973

Sum of electronic and thermal Free Energies= -187.248721

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -2.190572 | -4.791781 | 1.855163 |
| H | -1.659433 | -3.850496 | 1.998749 |
| C | -2.498960 | -4.938460 | 0.349174 |
| H | -2.622920 | -5.995257 | 0.093524 |
| H | -3.439627 | -4.415193 | 0.126478 |
| O | -1.473592 | -4.440673 | -0.462712 |
| H | -1.471857 | -3.471785 | -0.328179 |
| C | -3.487189 | -4.766490 | 2.628396 |
| O | -3.996559 | -5.747201 | 3.145586 |
| N | -4.054134 | -3.546310 | 2.634758 |
| H | -3.537593 | -2.765354 | 2.249872 |
| C | -5.330528 | -3.291929 | 3.240942 |
| H | -5.708846 | -4.241130 | 3.620540 |
| H | -5.238214 | -2.583268 | 4.068453 |
| C | 5.758777 | -1.696099 | 3.673486 |
| H | 5.945832 | -2.504582 | 2.972033 |
| C | 4.326856 | -1.744142 | 4.196809 |
| H | 4.151573 | -2.709589 | 4.679032 |
| H | 4.207273 | -0.969689 | 4.959432 |
| C | 3.264111 | -1.528492 | 3.112666 |
| H | 3.471890 | -0.581848 | 2.602628 |
| C | 3.267429 | -2.651683 | 2.079412 |

| | | | |
|---|---|---|---|
| H | 2.427853 | -2.524409 | 1.400180 |
| H | 4.185345 | -2.650337 | 1.496457 |
| H | 3.167670 | -3.619003 | 2.569125 |
| C | 1.878427 | -1.426875 | 3.746089 |
| H | 1.130005 | -1.262127 | 2.975426 |
| H | 1.631564 | -2.346712 | 4.273716 |
| C | 0.787016 | 2.313169 | -2.954362 |
| H | 1.185390 | 1.324855 | -3.247930 |
| H | 1.586129 | 2.825254 | -2.387799 |
| O | -0.360206 | 2.209640 | -2.227067 |
| C | 2.306768 | -0.285760 | -0.496567 |
| C | 0.506801 | 3.901966 | 1.050740 |
| C | -3.847165 | 2.583086 | -0.517219 |
| C | -1.896359 | -1.285214 | -2.611575 |
| C | 2.199487 | 0.976553 | 0.063862 |
| C | 3.306254 | 1.711847 | 0.633360 |
| C | 2.798721 | 2.905234 | 1.054943 |
| C | 1.386791 | 2.877262 | 0.750676 |
| C | 3.509160 | 4.049514 | 1.694247 |
| C | 4.737538 | 1.282935 | 0.588367 |
| C | 5.332040 | 1.702507 | -0.771862 |
| C | 6.796332 | 1.356518 | -0.910202 |
| O | 7.086561 | 0.049602 | -0.992023 |

| | | | |
|---|---|---|---|
| O | 7.674049 | 2.174877 | -0.976813 |
| C | -0.854931 | 3.892787 | 0.787588 |
| C | -1.758734 | 4.935220 | 1.197626 |
| C | -3.015480 | 4.528991 | 0.829120 |
| C | -2.839086 | 3.260788 | 0.145271 |
| C | -1.364516 | 6.167559 | 1.938611 |
| C | -4.258091 | 5.226304 | 1.082421 |
| C | -5.413666 | 4.660424 | 1.415197 |
| C | -3.687444 | 1.416832 | -1.246922 |
| C | -4.754731 | 0.783741 | -1.983614 |
| C | -4.201543 | -0.306298 | -2.601861 |
| C | -2.802796 | -0.321398 | -2.209514 |
| C | -4.831363 | -1.298741 | -3.442792 |
| C | -5.830218 | -1.074371 | -4.291673 |
| C | -0.581348 | -1.363026 | -2.190765 |
| C | 0.300475 | -2.465768 | -2.501072 |
| C | 1.470865 | -2.215714 | -1.850226 |
| C | 1.303199 | -0.941667 | -1.186187 |
| C | -0.074803 | -3.654518 | -3.314128 |
| C | 2.684332 | -3.090619 | -1.811733 |
| C | 3.731142 | -2.715093 | -2.877269 |
| C | 4.881157 | -1.923882 | -2.330924 |
| O | 5.131598 | -1.765292 | -1.154896 |

| | | | |
|---|---|---|---|
| O | 5.650964 | -1.402581 | -3.284319 |
| N | 1.061464 | 1.707726 | 0.140928 |
| N | -1.534635 | 2.902661 | 0.154391 |
| N | -2.529194 | 0.727309 | -1.403203 |
| N | 0.052078 | -0.460450 | -1.403347 |
| H | 4.566772 | 3.828684 | 1.818549 |
| H | 3.083179 | 4.266914 | 2.674299 |
| H | 3.416201 | 4.946186 | 1.080856 |
| H | -0.976348 | 5.914729 | 2.926418 |
| H | -2.218892 | 6.827903 | 2.068197 |
| H | -0.585316 | 6.705637 | 1.398277 |
| H | 0.807120 | -4.215935 | -3.614768 |
| H | -0.618471 | -3.358380 | -4.209635 |
| H | -0.714695 | -4.302155 | -2.714427 |
| H | -6.299717 | 5.248040 | 1.594563 |
| H | -5.510732 | 3.595950 | 1.542354 |
| H | -6.261418 | -1.869577 | -4.878308 |
| H | -6.234605 | -0.090258 | -4.454206 |
| H | 5.227780 | 2.781826 | -0.890327 |
| H | 4.763082 | 1.210814 | -1.566183 |
| H | 4.816367 | 0.201085 | 0.713290 |
| H | 5.303994 | 1.761654 | 1.390657 |
| H | 3.279762 | -2.139587 | -3.688071 |

| | | | |
|---|---|---|---|
| H | 4.166422 | -3.612255 | -3.326419 |
| H | 2.365010 | -4.121038 | -1.968704 |
| H | 3.153427 | -3.038048 | -0.829022 |
| H | 3.257515 | -0.785230 | -0.415510 |
| H | 0.910605 | 4.774080 | 1.544470 |
| H | -4.828732 | 3.032478 | -0.507507 |
| H | -2.254842 | -2.072886 | -3.256542 |
| H | -4.203420 | 6.309001 | 1.022604 |
| H | -4.431607 | -2.301962 | -3.355784 |
| Fe | -0.740657 | 1.216888 | -0.645102 |
| H | -6.033273 | -2.886833 | 2.508275 |
| H | 5.945929 | -0.751434 | 3.167055 |
| H | 6.406007 | -0.913544 | -2.905208 |
| H | 6.308028 | -0.543722 | -0.831379 |
| H | 0.603689 | 2.893981 | -3.875179 |
| H | -1.564114 | -5.616907 | 2.193808 |
| H | 6.465756 | -1.789461 | 4.495888 |
| C | -1.199638 | 0.303851 | 0.988130 |
| C | -1.047447 | 0.862214 | 2.377094 |
| C | -1.729154 | -0.174404 | 3.287385 |
| H | -2.661845 | 0.216712 | 3.716540 |
| O | -2.040986 | -1.283504 | 2.479917 |
| C | -1.752642 | -0.974131 | 1.127160 |

| | | | |
|---|---|---|---|
| O | -2.026054 | -1.849170 | 0.301204 |
| H | -1.086560 | -0.514954 | 4.107204 |
| H | -1.513008 | 1.844444 | 2.473137 |
| H | 0.011868 | 0.982065 | 2.624388 |
| C | -6.178082 | 1.225041 | -1.981415 |
| H | -6.333894 | 2.039491 | -2.691279 |
| H | -6.826179 | 0.396079 | -2.259717 |
| H | -6.469157 | 1.579852 | -0.993858 |
| H | 1.834955 | -0.600704 | 4.454112 |

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**Conf5$^{L9}$**

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Number of imaginary frequencies : 4 Electronic energy : HF=-188.1136897

Zero-point correction= 0.981128 (Hartree/Particle)

Thermal correction to Energy= 1.048787

Thermal correction to Enthalpy= 1.049731

Thermal correction to Gibbs Free Energy= 0.872247

Sum of electronic and zero-point Energies= -187.132561

Sum of electronic and thermal Energies= -187.064903

Sum of electronic and thermal Enthalpies= -187.063958

Sum of electronic and thermal Free Energies= -187.241442

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.302175 | -3.467632 | 1.724536 |
| H | -3.685377 | -2.604667 | 1.985046 |
| C | -3.966061 | -3.844902 | 0.270310 |
| H | -4.392434 | -4.823491 | 0.025064 |
| H | -4.407080 | -3.093613 | -0.402132 |
| O | -2.588070 | -3.939049 | 0.053317 |
| H | -2.217798 | -3.061201 | 0.273000 |
| C | -5.762364 | -3.134261 | 1.860569 |
| O | -6.602263 | -3.884008 | 2.325655 |
| N | -6.064108 | -1.907501 | 1.382406 |
| H | -5.323716 | -1.332238 | 1.010963 |
| C | -7.410356 | -1.410626 | 1.353168 |
| H | -8.045825 | -2.178063 | 1.794033 |
| H | -7.501444 | -0.488168 | 1.932302 |
| C | 2.908662 | -0.516412 | 5.645854 |
| H | 3.962165 | -0.781813 | 5.602117 |
| C | 2.046013 | -1.561167 | 4.945618 |
| H | 2.216661 | -2.539177 | 5.403825 |
| H | 0.994915 | -1.307771 | 5.101617 |

| | | | |
|---|---|---|---|
| C | 2.300338 | -1.663319 | 3.436777 |
| H | 2.246021 | -0.658719 | 3.002564 |
| C | 3.683640 | -2.240907 | 3.144986 |
| H | 3.833253 | -2.338036 | 2.073270 |
| H | 4.469415 | -1.599475 | 3.537363 |
| H | 3.785444 | -3.227651 | 3.594658 |
| C | 1.220337 | -2.522315 | 2.782680 |
| H | 1.346145 | -2.540602 | 1.703746 |
| H | 1.264576 | -3.543775 | 3.157722 |
| C | 1.388763 | 1.642902 | -3.171719 |
| H | 1.891702 | 0.658667 | -3.136166 |
| H | 2.102848 | 2.380592 | -2.761521 |
| O | 0.204922 | 1.674636 | -2.499026 |
| C | 2.587793 | -0.675648 | -0.239829 |
| C | 1.294034 | 3.933067 | 0.261945 |
| C | -3.239428 | 2.728307 | -0.802852 |
| C | -1.724619 | -1.637717 | -2.140850 |
| C | 2.634925 | 0.687390 | 0.007026 |
| C | 3.826942 | 1.407927 | 0.391906 |
| C | 3.465643 | 2.718702 | 0.500304 |
| C | 2.053111 | 2.777058 | 0.206306 |
| C | 4.312917 | 3.896291 | 0.844633 |
| C | 5.196758 | 0.818188 | 0.484522 |

| | | | |
|---|---|---|---|
| C | 5.820653 | 0.799263 | -0.926391 |
| C | 7.233448 | 0.264437 | -0.940690 |
| O | 7.367831 | -1.046736 | -0.691262 |
| O | 8.200944 | 0.934412 | -1.185244 |
| C | -0.074148 | 4.003640 | 0.045130 |
| C | -0.859856 | 5.193108 | 0.245291 |
| C | -2.167325 | 4.836453 | 0.036553 |
| C | -2.140526 | 3.437948 | -0.352675 |
| C | -0.317758 | 6.515497 | 0.670182 |
| C | -3.328479 | 5.687742 | 0.181802 |
| C | -4.502956 | 5.322579 | 0.685515 |
| C | -3.212842 | 1.431654 | -1.290535 |
| C | -4.367353 | 0.763481 | -1.838119 |
| C | -3.931373 | -0.458198 | -2.283886 |
| C | -2.519054 | -0.522080 | -1.948868 |
| C | -4.675270 | -1.518406 | -2.922692 |
| C | -5.743367 | -1.362780 | -3.701106 |
| C | -0.426654 | -1.769762 | -1.682322 |
| C | 0.310685 | -3.012728 | -1.708721 |
| C | 1.510735 | -2.759873 | -1.115119 |
| C | 1.505025 | -1.353975 | -0.769039 |
| C | -0.231177 | -4.296180 | -2.231464 |
| C | 2.613272 | -3.737284 | -0.850858 |

| | | | |
|---|---|---|---|
| C | 3.687742 | -3.744590 | -1.954138 |
| C | 4.932955 | -2.999895 | -1.577124 |
| O | 5.198536 | -2.589891 | -0.466231 |
| O | 5.767650 | -2.831669 | -2.601470 |
| N | 1.587316 | 1.538212 | -0.100245 |
| N | -0.872569 | 2.969106 | -0.322255 |
| N | -2.118818 | 0.631781 | -1.370391 |
| N | 0.315809 | -0.792813 | -1.108775 |
| H | 5.345027 | 3.596190 | 1.010021 |
| H | 3.944953 | 4.383717 | 1.748217 |
| H | 4.294108 | 4.628106 | 0.036590 |
| H | 0.091217 | 6.457332 | 1.680108 |
| H | -1.099793 | 7.271319 | 0.663980 |
| H | 0.481824 | 6.833812 | 0.000963 |
| H | 0.516833 | -5.084701 | -2.190571 |
| H | -0.558235 | -4.183942 | -3.264984 |
| H | -1.089715 | -4.589577 | -1.627202 |
| H | -5.323320 | 6.017397 | 0.767796 |
| H | -4.679357 | 4.326918 | 1.054520 |
| H | -6.249846 | -2.209899 | -4.134750 |
| H | -6.132900 | -0.393538 | -3.959202 |
| H | 5.840396 | 1.815954 | -1.321098 |
| H | 5.190024 | 0.187874 | -1.577982 |

| | | | |
|---|---|---|---|
| H | 5.147551 | -0.194165 | 0.890246 |
| H | 5.824999 | 1.418645 | 1.146150 |
| H | 3.302277 | -3.311365 | -2.879549 |
| H | 4.000467 | -4.766268 | -2.186807 |
| H | 2.176438 | -4.733321 | -0.770785 |
| H | 3.094165 | -3.514009 | 0.102855 |
| H | 3.478703 | -1.245941 | -0.037354 |
| H | 1.802923 | 4.848774 | 0.526654 |
| H | -4.182932 | 3.251987 | -0.834107 |
| H | -2.169150 | -2.502771 | -2.607968 |
| H | -3.188064 | 6.720418 | -0.122793 |
| H | -4.303602 | -2.520828 | -2.748495 |
| Fe | -0.273663 | 1.079630 | -0.751295 |
| H | -7.735310 | -1.216593 | 0.327264 |
| H | 2.779993 | 0.456412 | 5.175193 |
| H | 6.578593 | -2.363223 | -2.326034 |
| H | 6.524304 | -1.486627 | -0.410351 |
| H | 1.226046 | 1.898155 | -4.234135 |
| H | -4.052844 | -4.300459 | 2.383117 |
| H | 2.625055 | -0.430780 | 6.693505 |
| C | -0.758836 | 0.611217 | 1.045720 |
| C | -0.307638 | 1.328241 | 2.286829 |
| C | -1.119457 | 0.676934 | 3.418153 |

| | | | |
|---|---|---|---|
| H | -1.877356 | 1.363894 | 3.819576 |
| O | -1.776924 | -0.436142 | 2.861658 |
| C | -1.591367 | -0.436470 | 1.469644 |
| O | -2.178226 | -1.313150 | 0.828239 |
| H | -0.493930 | 0.330903 | 4.248625 |
| H | -0.485593 | 2.403275 | 2.226384 |
| H | 0.767430 | 1.186061 | 2.434017 |
| C | -5.756418 | 1.304397 | -1.824051 |
| H | -5.926053 | 1.969215 | -2.673055 |
| H | -6.475934 | 0.489107 | -1.876923 |
| H | -5.938063 | 1.871478 | -0.912205 |
| H | 0.230631 | -2.124596 | 2.989035 |

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**Conf6$^{L9}$**

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Number of imaginary frequencies : 3 Electronic energy : HF=-188.0990368

Zero-point correction= 0.979666 (Hartree/Particle)

Thermal correction to Energy= 1.049002

Thermal correction to Enthalpy= 1.049947

Thermal correction to Gibbs Free Energy= 0.865277

Sum of electronic and zero-point Energies= -187.119371

Sum of electronic and thermal Energies= -187.050034

Sum of electronic and thermal Enthalpies= -187.049090

Sum of electronic and thermal Free Energies= -187.233760

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.906850 | -2.294552 | 2.394159 |
| H | -4.351213 | -1.403187 | 2.093648 |
| C | -4.367566 | -3.511349 | 1.623568 |
| H | -4.849952 | -4.419839 | 1.993359 |
| H | -4.609705 | -3.399180 | 0.557393 |
| O | -2.990162 | -3.713119 | 1.796827 |
| H | -2.507899 | -2.956581 | 1.436568 |
| C | -6.377796 | -2.120128 | 2.106327 |
| O | -7.262884 | -2.548372 | 2.819780 |
| N | -6.612567 | -1.459690 | 0.954883 |
| H | -5.847074 | -1.152909 | 0.373811 |
| C | -7.945252 | -1.253526 | 0.466933 |
| H | -8.628303 | -1.725916 | 1.171492 |
| H | -8.176548 | -0.187340 | 0.401228 |
| C | 1.244872 | 3.328241 | 4.967673 |
| H | 2.082285 | 4.022064 | 5.008733 |

| | | | |
|---|---|---|---|
| C | 1.722096 | 1.881693 | 4.932222 |
| H | 2.328554 | 1.661161 | 5.817713 |
| H | 0.840045 | 1.239427 | 4.962721 |
| C | 2.519262 | 1.542272 | 3.667568 |
| H | 1.980012 | 1.943216 | 2.805368 |
| C | 3.914832 | 2.160498 | 3.693203 |
| H | 4.445554 | 1.918121 | 2.775262 |
| H | 3.857439 | 3.242681 | 3.775069 |
| H | 4.489096 | 1.778300 | 4.537537 |
| C | 2.625823 | 0.027452 | 3.506126 |
| H | 3.202896 | -0.219394 | 2.619239 |
| H | 3.110082 | -0.419414 | 4.374947 |
| C | 1.455094 | 0.157118 | -3.452871 |
| H | 1.894499 | -0.794476 | -3.103190 |
| H | 2.212631 | 0.942513 | -3.284519 |
| O | 0.279210 | 0.442332 | -2.817613 |
| C | 2.534393 | -1.247588 | 0.035390 |
| C | 1.730284 | 3.407673 | -0.875124 |
| C | -2.926080 | 2.433891 | -1.588485 |
| C | -1.987574 | -2.274907 | -1.266664 |
| C | 2.722533 | 0.111006 | -0.157882 |
| C | 3.999272 | 0.778831 | -0.019901 |
| C | 3.772182 | 2.096372 | -0.281576 |

| | | | |
|---|---|---|---|
| C | 2.361035 | 2.216192 | -0.569691 |
| C | 4.736460 | 3.232165 | -0.280754 |
| C | 5.310343 | 0.092930 | 0.194437 |
| C | 5.830047 | -0.399000 | -1.172877 |
| C | 7.179260 | -1.074058 | -1.094553 |
| O | 7.207792 | -2.261052 | -0.469171 |
| O | 8.182681 | -0.624915 | -1.580150 |
| C | 0.375453 | 3.547054 | -1.121035 |
| C | -0.275315 | 4.817783 | -1.315666 |
| C | -1.612848 | 4.555214 | -1.434827 |
| C | -1.741959 | 3.108745 | -1.367217 |
| C | 0.409976 | 6.139973 | -1.289554 |
| C | -2.674774 | 5.526981 | -1.587609 |
| C | -3.869803 | 5.472098 | -1.008971 |
| C | -3.082594 | 1.054241 | -1.604420 |
| C | -4.327070 | 0.386669 | -1.872630 |
| C | -4.060987 | -0.964932 | -1.829340 |
| C | -2.650941 | -1.078164 | -1.495029 |
| C | -4.941791 | -2.084342 | -2.049602 |
| C | -6.092769 | -2.082111 | -2.722526 |
| C | -0.673072 | -2.399473 | -0.847358 |
| C | -0.061454 | -3.658417 | -0.490156 |
| C | 1.203498 | -3.366327 | -0.070432 |

| | | | |
|---|---|---|---|
| C | 1.359570 | -1.936784 | -0.210682 |
| C | -0.744003 | -4.982538 | -0.549982 |
| C | 2.232216 | -4.320376 | 0.449157 |
| C | 3.212284 | -4.792861 | -0.640911 |
| C | 4.545050 | -4.107525 | -0.578614 |
| O | 4.939003 | -3.418554 | 0.339442 |
| O | 5.299522 | -4.342487 | -1.651422 |
| N | 1.761775 | 1.001881 | -0.503185 |
| N | -0.528906 | 2.539526 | -1.170788 |
| N | -2.095847 | 0.151070 | -1.379585 |
| N | 0.208412 | -1.382097 | -0.665384 |
| H | 5.739737 | 2.891296 | -0.034871 |
| H | 4.433851 | 3.980100 | 0.451874 |
| H | 4.767036 | 3.710181 | -1.260329 |
| H | 0.807110 | 6.331918 | -0.292808 |
| H | -0.283632 | 6.939084 | -1.541633 |
| H | 1.240126 | 6.158611 | -1.996228 |
| H | -0.041687 | -5.789662 | -0.354924 |
| H | -1.184086 | -5.142419 | -1.533933 |
| H | -1.540658 | -5.030222 | 0.193524 |
| H | -4.609367 | 6.241476 | -1.164080 |
| H | -4.138249 | 4.676864 | -0.335245 |
| H | -6.675337 | -2.983201 | -2.829031 |

| | | | |
|---|---|---|---|
| H | -6.475436 | -1.209179 | -3.219074 |
| H | 5.918868 | 0.453985 | -1.846897 |
| H | 5.098404 | -1.095566 | -1.592478 |
| H | 5.197319 | -0.749394 | 0.880554 |
| H | 6.036461 | 0.785369 | 0.625792 |
| H | 2.796763 | -4.633039 | -1.638066 |
| H | 3.413304 | -5.863583 | -0.546015 |
| H | 1.721492 | -5.186963 | 0.871340 |
| H | 2.802287 | -3.849723 | 1.252204 |
| H | 3.375036 | -1.820681 | 0.390268 |
| H | 2.332925 | 4.303623 | -0.878309 |
| H | -3.795145 | 3.034694 | -1.810088 |
| H | -2.541845 | -3.193321 | -1.394993 |
| H | -2.432200 | 6.384738 | -2.207784 |
| H | -4.604790 | -3.030033 | -1.639284 |
| Fe | -0.148446 | 0.592058 | -0.952511 |
| H | -8.068487 | -1.704445 | -0.520765 |
| H | 0.663709 | 3.533166 | 4.072075 |
| H | 6.167762 | -3.902327 | -1.577065 |
| H | 6.354950 | -2.495190 | -0.020992 |
| H | 1.287339 | 0.074334 | -4.540648 |
| H | -4.761627 | -2.457574 | 3.462538 |
| H | 0.615764 | 3.500212 | 5.839556 |

| | | | |
|---|---|---|---|
| C | -0.669914 | 0.722713 | 0.895684 |
| C | -1.382234 | -0.352013 | 1.669219 |
| C | -1.731620 | 0.305279 | 3.015468 |
| H | -1.356871 | -0.267842 | 3.872830 |
| O | -1.125194 | 1.570485 | 3.020995 |
| C | -0.514578 | 1.817621 | 1.780828 |
| O | 0.051197 | 2.893158 | 1.634451 |
| H | -2.815923 | 0.436373 | 3.140718 |
| H | -0.731489 | -1.221242 | 1.808422 |
| H | -2.275922 | -0.688686 | 1.137182 |
| C | -5.635484 | 1.071176 | -2.078555 |
| H | -5.789066 | 1.304845 | -3.133696 |
| H | -6.456731 | 0.438235 | -1.745798 |
| H | -5.670798 | 2.005047 | -1.520476 |
| H | 1.637863 | -0.412702 | 3.394034 |

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**Conf7$^{L9}$**

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Number of imaginary frequencies : 2 Electronic energy : HF=-188.1004437

Zero-point correction= 0.979945 (Hartree/Particle)

Thermal correction to Energy= 1.049882

Thermal correction to Enthalpy= 1.050826

Thermal correction to Gibbs Free Energy= 0.864428

Sum of electronic and zero-point Energies= -187.120498

Sum of electronic and thermal Energies= -187.050562

Sum of electronic and thermal Enthalpies= -187.049618

Sum of electronic and thermal Free Energies= -187.236016

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.741860 | -2.021634 | 2.207550 |
| H | -4.174063 | -1.294313 | 1.622976 |
| C | -4.309639 | -3.443924 | 1.816428 |
| H | -4.816043 | -4.167799 | 2.459811 |
| H | -4.610051 | -3.637186 | 0.776157 |
| O | -2.936765 | -3.674786 | 1.983932 |
| H | -2.439516 | -3.063017 | 1.421333 |
| C | -6.221917 | -1.867849 | 1.956052 |
| O | -7.079277 | -2.200648 | 2.750952 |
| N | -6.499342 | -1.360010 | 0.739934 |
| H | -5.753563 | -1.123163 | 0.101497 |
| C | -7.848871 | -1.211891 | 0.278646 |
| H | -8.505870 | -1.582700 | 1.064472 |

| | | | |
|---|---|---|---|
| H | -8.082004 | -0.162800 | 0.080546 |
| C | 1.220606 | 3.974448 | 4.347530 |
| H | 2.043183 | 4.678328 | 4.235522 |
| C | 1.727877 | 2.555042 | 4.570703 |
| H | 2.353108 | 2.513129 | 5.469643 |
| H | 0.859740 | 1.914944 | 4.736777 |
| C | 2.513818 | 2.001413 | 3.376937 |
| H | 1.941743 | 2.203761 | 2.466852 |
| C | 3.883950 | 2.662293 | 3.247819 |
| H | 4.418931 | 2.247827 | 2.396713 |
| H | 3.784272 | 3.733867 | 3.096972 |
| H | 4.476938 | 2.492265 | 4.146682 |
| C | 2.680645 | 0.489278 | 3.511522 |
| H | 3.229913 | 0.090913 | 2.662279 |
| H | 3.221034 | 0.241978 | 4.425611 |
| C | 1.262901 | 0.364712 | -3.485422 |
| H | 2.007643 | -0.446023 | -3.358223 |
| H | 1.787887 | 1.312024 | -3.274091 |
| O | 0.158159 | 0.200809 | -2.703328 |
| C | 2.584982 | -1.234002 | 0.154763 |
| C | 1.618901 | 3.341629 | -0.975448 |
| C | -3.008061 | 2.187627 | -1.594903 |
| C | -1.930962 | -2.462269 | -0.980419 |

| | | | |
|---|---|---|---|
| C | 2.731647 | 0.110505 | -0.145071 |
| C | 3.997881 | 0.812504 | -0.119557 |
| C | 3.725250 | 2.107091 | -0.444339 |
| C | 2.297564 | 2.180592 | -0.655021 |
| C | 4.661287 | 3.259012 | -0.575921 |
| C | 5.333818 | 0.166992 | 0.061980 |
| C | 5.781316 | -0.414226 | -1.295713 |
| C | 7.147834 | -1.056259 | -1.251106 |
| O | 7.239834 | -2.194579 | -0.545901 |
| O | 8.110948 | -0.624454 | -1.825807 |
| C | 0.253242 | 3.432612 | -1.183308 |
| C | -0.440559 | 4.671108 | -1.421491 |
| C | -1.770535 | 4.359621 | -1.515984 |
| C | -1.851124 | 2.914920 | -1.387599 |
| C | 0.200140 | 6.015181 | -1.455026 |
| C | -2.865862 | 5.287171 | -1.697180 |
| C | -4.060865 | 5.201309 | -1.121814 |
| C | -3.111918 | 0.804199 | -1.553009 |
| C | -4.313049 | 0.078496 | -1.870024 |
| C | -4.007331 | -1.257552 | -1.734912 |
| C | -2.620251 | -1.302906 | -1.301461 |
| C | -4.829217 | -2.420048 | -1.973612 |
| C | -5.869725 | -2.501774 | -2.801458 |

| | | | |
|---|---|---|---|
| C | -0.615001 | -2.521878 | -0.545939 |
| C | 0.041195 | -3.738647 | -0.131046 |
| C | 1.306534 | -3.385795 | 0.240977 |
| C | 1.417224 | -1.964367 | 0.011150 |
| C | -0.593876 | -5.087791 | -0.111205 |
| C | 2.373182 | -4.280382 | 0.789036 |
| C | 3.315181 | -4.823689 | -0.301574 |
| C | 4.626412 | -4.098637 | -0.367602 |
| O | 5.050034 | -3.335219 | 0.475145 |
| O | 5.325620 | -4.390167 | -1.463148 |
| N | 1.733296 | 0.957109 | -0.491961 |
| N | -0.619684 | 2.394551 | -1.177583 |
| N | -2.113517 | -0.050230 | -1.220113 |
| N | 0.237019 | -1.469374 | -0.437043 |
| H | 5.683728 | 2.956509 | -0.360814 |
| H | 4.381610 | 4.053857 | 0.115167 |
| H | 4.629382 | 3.663629 | -1.588060 |
| H | 0.591640 | 6.262016 | -0.468236 |
| H | -0.520461 | 6.779136 | -1.738154 |
| H | 1.027972 | 6.032456 | -2.164640 |
| H | 0.140507 | -5.857078 | 0.116000 |
| H | -1.037741 | -5.315357 | -1.080161 |
| H | -1.380578 | -5.127858 | 0.642986 |

| | | | |
|---|---|---|---|
| H | -4.827791 | 5.938767 | -1.297998 |
| H | -4.300853 | 4.413813 | -0.428792 |
| H | -6.422556 | -3.420528 | -2.913401 |
| H | -6.184369 | -1.680190 | -3.419584 |
| H | 5.809662 | 0.388560 | -2.033650 |
| H | 5.041838 | -1.153282 | -1.617354 |
| H | 5.279615 | -0.625013 | 0.812347 |
| H | 6.069462 | 0.901283 | 0.397445 |
| H | 2.847805 | -4.769408 | -1.286846 |
| H | 3.556243 | -5.874485 | -0.117694 |
| H | 1.895816 | -5.118650 | 1.298712 |
| H | 2.967991 | -3.740266 | 1.527720 |
| H | 3.455529 | -1.762440 | 0.507269 |
| H | 2.194841 | 4.252902 | -1.039160 |
| H | -3.893647 | 2.744212 | -1.862048 |
| H | -2.453154 | -3.403525 | -1.077311 |
| H | -2.652349 | 6.138008 | -2.337343 |
| H | -4.538961 | -3.317031 | -1.437788 |
| Fe | -0.184862 | 0.475147 | -0.840234 |
| H | -8.010786 | -1.790512 | -0.634345 |
| H | 0.610410 | 3.999564 | 3.447691 |
| H | 6.183252 | -3.923468 | -1.471361 |
| H | 6.419846 | -2.411382 | -0.032296 |

| | | | |
|---|---|---|---|
| H | 0.970319 | 0.372856 | -4.551117 |
| H | -4.532128 | -1.870782 | 3.267310 |
| H | 0.610400 | 4.294730 | 5.190371 |
| C | -0.654290 | 0.729287 | 1.008277 |
| C | -1.120779 | -0.374883 | 1.914097 |
| C | -1.573096 | 0.335976 | 3.199640 |
| H | -1.079953 | -0.059110 | 4.096364 |
| O | -1.227378 | 1.689369 | 3.057178 |
| C | -0.702144 | 1.921435 | 1.779426 |
| O | -0.359539 | 3.065256 | 1.511418 |
| H | -2.659325 | 0.264849 | 3.347531 |
| H | -0.312224 | -1.084076 | 2.113168 |
| H | -1.936596 | -0.935548 | 1.453818 |
| C | -5.615922 | 0.713129 | -2.221176 |
| H | -5.627083 | 1.010999 | -3.271075 |
| H | -6.441610 | 0.025296 | -2.051976 |
| H | -5.778593 | 1.606811 | -1.619805 |
| H | 1.709356 | 0.001853 | 3.540344 |

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**Conf8$^{L9}$**

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Number of imaginary frequencies : 2 Electronic energy : HF=-188.1108964

Zero-point correction= 0.980734 (Hartree/Particle)

Thermal correction to Energy= 1.050702

Thermal correction to Enthalpy= 1.051646

Thermal correction to Gibbs Free Energy= 0.863265

Sum of electronic and zero-point Energies= -187.130162

Sum of electronic and thermal Energies= -187.060195

Sum of electronic and thermal Enthalpies= -187.059250

Sum of electronic and thermal Free Energies= -187.247631

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -3.916041 | -2.853343 | 2.616984 |
| H | -3.396821 | -1.957389 | 2.958212 |
| C | -3.535950 | -3.119678 | 1.152053 |
| H | -3.956683 | -4.076888 | 0.829131 |
| H | -3.935679 | -2.321542 | 0.515180 |
| O | -2.142375 | -3.230877 | 0.981330 |
| H | -1.764161 | -2.343726 | 1.035317 |
| C | -5.403775 | -2.651418 | 2.767202 |
| O | -6.156934 | -3.499514 | 3.219841 |
| N | -5.817577 | -1.441639 | 2.353366 |

| | | | |
|---|---|---|---|
| H | -5.140692 | -0.785476 | 1.968536 |
| C | -7.207425 | -1.076232 | 2.419452 |
| H | -7.744779 | -1.918111 | 2.855102 |
| H | -7.346697 | -0.191134 | 3.045177 |
| C | 3.418627 | 1.017358 | 5.319322 |
| H | 4.430506 | 1.164644 | 5.688520 |
| C | 3.242086 | -0.375408 | 4.724653 |
| H | 3.519601 | -1.124955 | 5.470992 |
| H | 2.186839 | -0.521809 | 4.483070 |
| C | 4.060897 | -0.606029 | 3.450357 |
| H | 3.776197 | 0.158589 | 2.719865 |
| C | 5.562124 | -0.502142 | 3.714264 |
| H | 6.122621 | -0.761465 | 2.818718 |
| H | 5.842063 | 0.506809 | 4.005306 |
| H | 5.855595 | -1.187037 | 4.508304 |
| C | 3.732129 | -1.977576 | 2.864441 |
| H | 4.329176 | -2.163829 | 1.974982 |
| H | 3.946024 | -2.762023 | 3.588858 |
| C | 0.782930 | 2.101400 | -3.217755 |
| H | 1.816222 | 2.161899 | -2.830807 |
| H | 0.308413 | 3.079711 | -3.024890 |
| O | 0.097792 | 1.065776 | -2.650411 |
| C | 2.530602 | -0.704952 | -0.374470 |

| | | | |
|---|---|---|---|
| C | 0.755186 | 3.734237 | 0.179089 |
| C | -3.533868 | 2.199220 | -1.373104 |
| C | -1.774541 | -2.256277 | -1.846145 |
| C | 2.439012 | 0.661095 | -0.159384 |
| C | 3.559336 | 1.507980 | 0.181005 |
| C | 3.054474 | 2.763585 | 0.356090 |
| C | 1.635060 | 2.666330 | 0.112427 |
| C | 3.774546 | 4.022251 | 0.702755 |
| C | 4.990773 | 1.077641 | 0.180075 |
| C | 5.519763 | 1.112107 | -1.267970 |
| C | 6.973303 | 0.716993 | -1.380577 |
| O | 7.264147 | -0.555584 | -1.065065 |
| O | 7.842996 | 1.456456 | -1.755319 |
| C | -0.590541 | 3.683555 | -0.144711 |
| C | -1.474685 | 4.818502 | -0.058282 |
| C | -2.708990 | 4.381015 | -0.455833 |
| C | -2.542261 | 2.984298 | -0.815986 |
| C | -1.085793 | 6.171861 | 0.432312 |
| C | -3.938030 | 5.147097 | -0.483407 |
| C | -5.130100 | 4.694190 | -0.111566 |
| C | -3.413203 | 0.853469 | -1.674199 |
| C | -4.497000 | 0.047227 | -2.178349 |
| C | -4.006856 | -1.226285 | -2.298270 |

| | | | |
|---|---|---|---|
| C | -2.623558 | -1.164771 | -1.860556 |
| C | -4.684724 | -2.432184 | -2.717901 |
| C | -5.637431 | -2.502767 | -3.642996 |
| C | -0.449913 | -2.231927 | -1.446296 |
| C | 0.409226 | -3.394289 | -1.414116 |
| C | 1.624884 | -2.959444 | -0.980764 |
| C | 1.494236 | -1.532756 | -0.767095 |
| C | -0.038093 | -4.772128 | -1.757685 |
| C | 2.863843 | -3.769870 | -0.761395 |
| C | 3.851561 | -3.669692 | -1.939124 |
| C | 5.059430 | -2.832074 | -1.643783 |
| O | 5.333178 | -2.341004 | -0.567820 |
| O | 5.843945 | -2.665494 | -2.705679 |
| N | 1.297951 | 1.391208 | -0.204611 |
| N | -1.262712 | 2.595655 | -0.607047 |
| N | -2.298025 | 0.100145 | -1.503417 |
| N | 0.226567 | -1.135015 | -1.037419 |
| H | 4.833441 | 3.831804 | 0.862308 |
| H | 3.361686 | 4.463984 | 1.610346 |
| H | 3.675364 | 4.752221 | -0.101296 |
| H | -0.768288 | 6.125242 | 1.474702 |
| H | -1.925571 | 6.859323 | 0.362645 |
| H | -0.257588 | 6.570765 | -0.154847 |

| | | | |
|---|---|---|---|
| H | 0.775554 | -5.487033 | -1.656684 |
| H | -0.406922 | -4.811954 | -2.782601 |
| H | -0.848030 | -5.065738 | -1.090797 |
| H | -6.009199 | 5.317835 | -0.147982 |
| H | -5.260839 | 3.695347 | 0.267492 |
| H | -6.112692 | -3.437496 | -3.893250 |
| H | -5.959398 | -1.640487 | -4.200937 |
| H | 5.412677 | 2.121375 | -1.667686 |
| H | 4.913542 | 0.434418 | -1.876438 |
| H | 5.081525 | 0.069324 | 0.587673 |
| H | 5.590566 | 1.748776 | 0.798742 |
| H | 3.361734 | -3.237910 | -2.815323 |
| H | 4.217923 | -4.655483 | -2.236239 |
| H | 2.579085 | -4.813007 | -0.619752 |
| H | 3.366430 | -3.440721 | 0.149515 |
| H | 3.492174 | -1.162728 | -0.218200 |
| H | 1.155341 | 4.688806 | 0.488770 |
| H | -4.482072 | 2.673922 | -1.574710 |
| H | -2.174933 | -3.206222 | -2.165064 |
| H | -3.838773 | 6.179755 | -0.804474 |
| H | -4.367302 | -3.341568 | -2.221322 |
| Fe | -0.526709 | 0.737015 | -0.859150 |
| H | -7.604270 | -0.867706 | 1.422479 |

| | | | |
|---|---|---|---|
| H | 3.209571 | 1.775495 | 4.567493 |
| H | 6.618194 | -2.109223 | -2.493309 |
| H | 6.499050 | -1.056818 | -0.684822 |
| H | 0.844543 | 1.959600 | -4.310807 |
| H | -3.605685 | -3.704101 | 3.226794 |
| H | 2.731128 | 1.161230 | 6.150475 |
| C | -1.044017 | 0.299052 | 0.961575 |
| C | -0.019318 | 0.109006 | 2.049148 |
| C | -0.832597 | -0.244167 | 3.304144 |
| H | -0.639250 | 0.438913 | 4.140044 |
| O | -2.187957 | -0.139679 | 2.949444 |
| C | -2.306688 | 0.140778 | 1.567285 |
| O | -3.456816 | 0.158467 | 1.121421 |
| H | -0.640053 | -1.271114 | 3.645292 |
| H | 0.555086 | 1.027084 | 2.197515 |
| H | 0.692896 | -0.677963 | 1.790225 |
| C | -5.888170 | 0.527874 | -2.404854 |
| H | -5.971281 | 1.047342 | -3.361424 |
| H | -6.578040 | -0.313747 | -2.406342 |
| H | -6.181953 | 1.219209 | -1.617149 |
| H | 2.681304 | -2.036502 | 2.590866 |

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**Conf9$^{L9}$**

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Number of imaginary frequencies : 3 Electronic energy : HF=-188.1141314

Zero-point correction= 0.981196 (Hartree/Particle)

Thermal correction to Energy= 1.049728

Thermal correction to Enthalpy= 1.050672

Thermal correction to Gibbs Free Energy= 0.869325

Sum of electronic and zero-point Energies= -187.132936

Sum of electronic and thermal Energies= -187.064403

Sum of electronic and thermal Enthalpies= -187.063459

Sum of electronic and thermal Free Energies= -187.244806

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -2.820202 | -4.278550 | 2.178932 |
| H | -2.313067 | -3.320705 | 2.300144 |
| C | -2.825201 | -4.637578 | 0.675894 |
| H | -2.676665 | -5.714220 | 0.545245 |
| H | -3.804274 | -4.376202 | 0.245555 |
| O | -1.805766 | -4.007810 | -0.045703 |
| H | -1.962127 | -3.042320 | 0.027228 |

| | | | |
|---|---|---|---|
| C | -4.236863 | -4.145426 | 2.686188 |
| O | -4.796560 | -4.978705 | 3.380284 |
| N | -4.833850 | -3.021478 | 2.249658 |
| H | -4.285976 | -2.359142 | 1.708774 |
| C | -6.206321 | -2.722847 | 2.558295 |
| H | -6.595518 | -3.553896 | 3.146174 |
| H | -6.285430 | -1.799973 | 3.138500 |
| C | 4.488569 | -0.525174 | 5.107601 |
| H | 5.426045 | -1.036997 | 4.906117 |
| C | 3.295127 | -1.348224 | 4.632253 |
| H | 3.331314 | -2.338404 | 5.094235 |
| H | 2.378080 | -0.860437 | 4.971952 |
| C | 3.220055 | -1.507456 | 3.108828 |
| H | 3.210556 | -0.508531 | 2.657988 |
| C | 4.421964 | -2.279404 | 2.568443 |
| H | 4.329402 | -2.424854 | 1.495578 |
| H | 5.351237 | -1.746849 | 2.756403 |
| H | 4.484422 | -3.259113 | 3.039636 |
| C | 1.925788 | -2.220322 | 2.720499 |
| H | 1.808240 | -2.246531 | 1.640336 |
| H | 1.925174 | -3.242247 | 3.095841 |
| C | 1.080079 | 2.041394 | -3.048257 |
| H | 1.468043 | 1.022212 | -3.226005 |

| | | | |
|---|---|---|---|
| H | 1.873415 | 2.602509 | -2.521796 |
| O | -0.084123 | 2.039888 | -2.336738 |
| C | 2.379471 | -0.485745 | -0.423993 |
| C | 0.785390 | 3.888287 | 0.797243 |
| C | -3.615085 | 2.686934 | -0.724989 |
| C | -1.867235 | -1.445437 | -2.466321 |
| C | 2.340572 | 0.827107 | 0.018955 |
| C | 3.487560 | 1.559595 | 0.505871 |
| C | 3.035831 | 2.802646 | 0.839331 |
| C | 1.618476 | 2.808448 | 0.562478 |
| C | 3.803848 | 3.964461 | 1.371489 |
| C | 4.898958 | 1.070032 | 0.464407 |
| C | 5.458727 | 1.319815 | -0.951353 |
| C | 6.898922 | 0.890233 | -1.105246 |
| O | 7.124315 | -0.431506 | -1.071113 |
| O | 7.810608 | 1.653545 | -1.280947 |
| C | -0.577156 | 3.921865 | 0.539917 |
| C | -1.432513 | 5.028525 | 0.882856 |
| C | -2.704363 | 4.663087 | 0.525386 |
| C | -2.584307 | 3.350358 | -0.083668 |
| C | -0.983112 | 6.280558 | 1.556395 |
| C | -3.914264 | 5.431474 | 0.725308 |
| C | -5.099112 | 4.938610 | 1.070975 |

| | | | |
|---|---|---|---|
| C | -3.505133 | 1.470048 | -1.376529 |
| C | -4.597462 | 0.842130 | -2.079629 |
| C | -4.101393 | -0.324183 | -2.598918 |
| C | -2.712137 | -0.388461 | -2.181236 |
| C | -4.779291 | -1.344529 | -3.365798 |
| C | -5.748923 | -1.132717 | -4.250994 |
| C | -0.566797 | -1.565777 | -2.011671 |
| C | 0.245410 | -2.747849 | -2.190953 |
| C | 1.425706 | -2.501891 | -1.557856 |
| C | 1.336714 | -1.154148 | -1.038600 |
| C | -0.206889 | -3.988548 | -2.876159 |
| C | 2.573180 | -3.448833 | -1.396933 |
| C | 3.630261 | -3.312283 | -2.508674 |
| C | 4.805695 | -2.472224 | -2.109982 |
| O | 5.091904 | -2.164260 | -0.972245 |
| O | 5.554899 | -2.097269 | -3.143922 |
| N | 1.235063 | 1.607804 | 0.055625 |
| N | -1.300415 | 2.929885 | -0.038939 |
| N | -2.384065 | 0.709348 | -1.464679 |
| N | 0.115773 | -0.625753 | -1.314689 |
| H | 4.855466 | 3.713195 | 1.488998 |
| H | 3.411108 | 4.273045 | 2.340999 |
| H | 3.728503 | 4.814057 | 0.692311 |

| | | | |
|---|---|---|---|
| H | -0.605998 | 6.065043 | 2.557227 |
| H | -1.807071 | 6.984418 | 1.648112 |
| H | -0.180937 | 6.753272 | 0.989030 |
| H | 0.622961 | -4.673045 | -3.036845 |
| H | -0.658525 | -3.758270 | -3.840097 |
| H | -0.951878 | -4.477377 | -2.248938 |
| H | -5.958079 | 5.575811 | 1.207944 |
| H | -5.247370 | 3.888022 | 1.252207 |
| H | -6.220848 | -1.947014 | -4.777044 |
| H | -6.087724 | -0.143019 | -4.504389 |
| H | 5.398399 | 2.385411 | -1.176797 |
| H | 4.837356 | 0.778732 | -1.670815 |
| H | 4.941111 | 0.006288 | 0.703871 |
| H | 5.510766 | 1.606947 | 1.192743 |
| H | 3.196825 | -2.888099 | -3.416187 |
| H | 4.037304 | -4.292833 | -2.772762 |
| H | 2.177425 | -4.464841 | -1.404002 |
| H | 3.057302 | -3.293015 | -0.431804 |
| H | 3.308001 | -1.018650 | -0.305649 |
| H | 1.230784 | 4.773871 | 1.227333 |
| H | -4.572950 | 3.183849 | -0.758085 |
| H | -2.266771 | -2.268410 | -3.038754 |
| H | -3.806821 | 6.505717 | 0.609944 |

| | | | |
|---|---|---|---|
| H | -4.445161 | -2.359262 | -3.185818 |
| Fe | -0.590137 | 1.151465 | -0.714478 |
| H | -6.795303 | -2.614411 | 1.643754 |
| H | 4.505989 | 0.438934 | 4.603230 |
| H | 6.329409 | -1.579165 | -2.853106 |
| H | 6.325956 | -0.965413 | -0.824103 |
| H | 0.924652 | 2.524411 | -4.028457 |
| H | -2.290856 | -5.036267 | 2.756171 |
| H | 4.423498 | -0.350451 | 6.180062 |
| C | -1.119481 | 0.386222 | 0.979879 |
| C | -0.625643 | 0.899916 | 2.306045 |
| C | -1.447125 | 0.126377 | 3.349940 |
| H | -2.167425 | 0.777497 | 3.864003 |
| O | -2.159557 | -0.863610 | 2.651363 |
| C | -1.991771 | -0.672825 | 1.267000 |
| O | -2.628177 | -1.448531 | 0.537948 |
| H | -0.827191 | -0.365511 | 4.109139 |
| H | -0.762946 | 1.978195 | 2.401476 |
| H | 0.444728 | 0.698688 | 2.410688 |
| C | -5.993342 | 1.360592 | -2.135018 |
| H | -6.091667 | 2.132354 | -2.900710 |
| H | -6.682690 | 0.551681 | -2.369361 |
| H | -6.279142 | 1.796862 | -1.179153 |

H 1.061542 -1.705915 3.132140

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**Conf1$^{L10}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-197.617012

Zero-point correction= 1.019152 (Hartree/Particle)

Thermal correction to Energy= 1.091931

Thermal correction to Enthalpy= 1.092875

Thermal correction to Gibbs Free Energy= 0.903877

Sum of electronic and zero-point Energies= -196.597860

Sum of electronic and thermal Energies= -196.525081

Sum of electronic and thermal Enthalpies= -196.524137

Sum of electronic and thermal Free Energies= -196.713134

.....

Cartesian Coordinates

.....

C 4.785638 2.435564 3.131704

H 5.394739 3.336008 3.191223

C 3.823920 2.391893 4.324870

H 4.343632 1.953353 5.190123

| | | | |
|---|---|---|---|
| H | 3.513202 | 3.406767 | 4.592864 |
| O | 2.626416 | 1.701134 | 4.064098 |
| H | 2.831534 | 0.851396 | 3.641528 |
| C | 5.775070 | 1.234650 | 3.187668 |
| O | 6.720172 | 1.276825 | 3.961139 |
| N | 5.549275 | 0.187151 | 2.371641 |
| H | 4.711954 | 0.119279 | 1.785753 |
| C | 6.376904 | -1.023144 | 2.320057 |
| H | 5.775431 | -1.886488 | 2.601624 |
| H | 6.749372 | -1.160397 | 1.305553 |
| C | -3.580094 | -4.843183 | 3.076117 |
| H | -4.016815 | -5.460364 | 3.857686 |
| C | -3.640455 | -3.368826 | 3.456452 |
| H | -3.074404 | -3.219926 | 4.380090 |
| H | -3.168724 | -2.782659 | 2.664794 |
| C | -5.083379 | -2.909793 | 3.662143 |
| H | -5.641849 | -3.050780 | 2.735261 |
| H | -5.550613 | -3.530204 | 4.428443 |
| C | -5.205981 | -1.445822 | 4.097734 |
| H | -6.252003 | -1.224179 | 4.322160 |
| H | -4.627609 | -1.268231 | 5.007160 |
| N | -4.785335 | -0.522808 | 3.064846 |
| H | -5.438728 | -0.352691 | 2.302400 |

| | | | |
|---|---|---|---|
| C | -3.585968 | 0.028999 | 2.913155 |
| N | -3.423698 | 0.882653 | 1.909233 |
| N | -2.592132 | -0.168785 | 3.783290 |
| H | -2.655541 | -0.889112 | 4.480427 |
| C | 0.153038 | -0.840342 | -4.088620 |
| H | 1.053529 | -1.450195 | -4.271817 |
| H | -0.121197 | -0.340220 | -5.031506 |
| O | 0.364241 | 0.089077 | -3.109569 |
| C | -2.615019 | 0.281978 | -0.874031 |
| C | 0.286529 | -3.522742 | -1.344543 |
| C | 4.006263 | -0.556708 | -2.035023 |
| C | 1.245703 | 3.150308 | -0.726140 |
| C | -2.157182 | -1.027699 | -0.884142 |
| C | -2.975760 | -2.203144 | -0.674394 |
| C | -2.142450 | -3.278133 | -0.808461 |
| C | -0.830832 | -2.746460 | -1.085387 |
| C | -2.444129 | -4.734359 | -0.707284 |
| C | -4.411398 | -2.240406 | -0.246457 |
| C | -5.401139 | -1.567748 | -1.208213 |
| C | -5.832172 | -0.190399 | -0.765012 |
| O | -6.280053 | 0.527455 | -1.760147 |
| O | -5.786308 | 0.206695 | 0.391226 |
| C | 1.546921 | -3.037501 | -1.645087 |

| | | | |
|---|---|---|---|
| C | 2.659783 | -3.875870 | -2.022974 |
| C | 3.709374 | -3.032712 | -2.269012 |
| C | 3.218931 | -1.691456 | -1.999163 |
| C | 2.637149 | -5.364094 | -2.065254 |
| C | 5.061624 | -3.352736 | -2.671251 |
| C | 5.405379 | -4.340489 | -3.491103 |
| C | 3.589835 | 0.704666 | -1.646358 |
| C | 4.488463 | 1.818477 | -1.443655 |
| C | 3.716310 | 2.860650 | -1.009451 |
| C | 2.348523 | 2.366637 | -0.997350 |
| C | 5.955133 | 1.790665 | -1.685496 |
| C | 4.116016 | 4.201093 | -0.637571 |
| C | 5.253101 | 4.518810 | -0.027543 |
| C | -0.069773 | 2.712703 | -0.760799 |
| C | -1.215081 | 3.578925 | -0.640900 |
| C | -2.315657 | 2.772376 | -0.718490 |
| C | -1.820897 | 1.421419 | -0.876667 |
| C | -1.145398 | 5.058475 | -0.484460 |
| C | -3.745005 | 3.201190 | -0.667548 |
| C | -4.320889 | 3.413315 | -2.087209 |
| C | -5.743975 | 3.856116 | -1.955382 |
| O | -5.928450 | 5.131678 | -2.263586 |
| O | -6.655267 | 3.158966 | -1.551836 |

| | | | |
|---|---|---|---|
| N | -0.867199 | -1.391038 | -1.096318 |
| N | 1.912582 | -1.728238 | -1.652693 |
| N | 2.317084 | 1.058058 | -1.351098 |
| N | -0.465861 | 1.425684 | -0.901985 |
| H | -3.505821 | -4.912987 | -0.553459 |
| H | -2.146120 | -5.243655 | -1.623048 |
| H | 3.652001 | -5.752459 | -2.014695 |
| H | 2.176544 | -5.720703 | -2.988100 |
| H | 2.068560 | -5.764294 | -1.227069 |
| H | 6.334359 | 2.803042 | -1.809119 |
| H | 6.189133 | 1.216120 | -2.580280 |
| H | 6.468236 | 1.329525 | -0.840755 |
| H | -0.553064 | 5.323470 | 0.391075 |
| H | -2.137160 | 5.490951 | -0.375119 |
| H | -0.671933 | 5.506983 | -1.357336 |
| H | 6.435567 | -4.531769 | -3.741330 |
| H | 4.674659 | -4.973160 | -3.964563 |
| H | 5.493987 | 5.540371 | 0.215660 |
| H | 5.965576 | 3.773633 | 0.279099 |
| H | -6.318341 | -2.158658 | -1.282203 |
| H | -4.986700 | -1.488487 | -2.213391 |
| H | -4.508717 | -1.757627 | 0.730725 |
| H | -4.697579 | -3.285162 | -0.120127 |

| | | | |
|---|---|---|---|
| H | -4.271347 | 2.469997 | -2.632657 |
| H | -3.745409 | 4.171756 | -2.614520 |
| H | -3.822891 | 4.139517 | -0.113628 |
| H | -4.366734 | 2.465312 | -0.154848 |
| H | -3.681258 | 0.428645 | -0.859729 |
| H | 0.153544 | -4.594179 | -1.347127 |
| H | 5.044801 | -0.677746 | -2.301793 |
| H | 1.411768 | 4.195195 | -0.511282 |
| H | 5.834284 | -2.714857 | -2.260311 |
| H | 3.408494 | 4.986743 | -0.876313 |
| Fe | 0.734392 | -0.153390 | -1.282482 |
| H | -4.124492 | -5.020582 | 2.152593 |
| H | 7.206800 | -0.899211 | 3.013466 |
| H | 4.220836 | 2.435491 | 2.198091 |
| H | -6.527183 | 1.467737 | -1.528948 |
| H | -0.659114 | -1.537610 | -3.820769 |
| H | -6.853364 | 5.399580 | -2.135296 |
| H | -2.548996 | -5.152013 | 2.929491 |
| C | 1.015980 | -0.343029 | 0.614205 |
| C | 2.243849 | -0.529704 | 1.253707 |
| C | -0.028260 | -0.307054 | 1.702527 |
| H | -1.677513 | 0.201782 | 3.578518 |
| H | -2.507047 | 1.166688 | 1.591009 |

| | | | |
|---|---|---|---|
| H | -4.173529 | 0.936699 | 1.228367 |
| O | 2.096699 | -0.714727 | 2.651944 |
| O | 3.393822 | -0.533240 | 0.814885 |
| C | 0.729962 | -0.755124 | 2.967572 |
| H | 0.570049 | -0.098569 | 3.831766 |
| H | 0.463764 | -1.785473 | 3.247243 |
| H | -0.390875 | 0.725764 | 1.804254 |
| H | -0.877192 | -0.956534 | 1.478433 |
| H | -1.894913 | -5.183529 | 0.120254 |

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**Conf2$^{L10}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-197.614567

Zero-point correction= 1.019231 (Hartree/Particle)

Thermal correction to Energy= 1.092093

Thermal correction to Enthalpy= 1.093037

Thermal correction to Gibbs Free Energy= 0.903939

Sum of electronic and zero-point Energies= -196.595336

Sum of electronic and thermal Energies= -196.522474

Sum of electronic and thermal Enthalpies= -196.521530

Sum of electronic and thermal Free Energies= -196.710628

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 5.616642 | 1.631048 | 3.101372 |
| H | 6.167584 | 2.523508 | 3.386835 |
| C | 5.030655 | 0.908420 | 4.329713 |
| H | 5.205287 | -0.172383 | 4.239168 |
| H | 5.523112 | 1.255875 | 5.241445 |
| O | 3.657958 | 1.157368 | 4.515845 |
| H | 3.171082 | 0.680658 | 3.824002 |
| C | 6.592625 | 0.693929 | 2.328156 |
| O | 7.799393 | 0.865431 | 2.391173 |
| N | 6.032939 | -0.312187 | 1.619854 |
| H | 5.018090 | -0.356054 | 1.517620 |
| C | 6.767367 | -1.322981 | 0.842430 |
| H | 6.561287 | -2.314068 | 1.245914 |
| H | 6.441815 | -1.280489 | -0.195213 |
| C | -3.113233 | -5.154538 | 2.256293 |
| H | -3.396276 | -5.951661 | 2.940007 |
| C | -3.371407 | -3.789957 | 2.882840 |
| H | -2.787053 | -3.710067 | 3.803763 |
| H | -3.030805 | -3.019232 | 2.188136 |

| | | | |
|---|---|---|---|
| C | -4.854163 | -3.596449 | 3.198516 |
| H | -5.429683 | -3.668719 | 2.274290 |
| H | -5.187698 | -4.397641 | 3.859841 |
| C | -5.170897 | -2.259999 | 3.879084 |
| H | -6.231961 | -2.230270 | 4.137006 |
| H | -4.602634 | -2.159182 | 4.806538 |
| N | -4.905966 | -1.122256 | 3.023284 |
| H | -5.598339 | -0.906800 | 2.310767 |
| C | -3.779652 | -0.419175 | 2.948329 |
| N | -3.744331 | 0.602765 | 2.099561 |
| N | -2.746705 | -0.637224 | 3.768390 |
| H | -2.706780 | -1.472499 | 4.325407 |
| C | -0.535650 | 1.108220 | -3.695813 |
| H | -1.614293 | 0.893834 | -3.588434 |
| H | -0.288108 | 1.029043 | -4.767026 |
| O | 0.209916 | 0.216756 | -2.982610 |
| C | -2.722765 | 0.314580 | -0.681802 |
| C | 0.244381 | -3.347799 | -1.616249 |
| C | 3.930748 | -0.278542 | -1.915892 |
| C | 1.074283 | 3.263625 | -0.371759 |
| C | -2.241887 | -0.975781 | -0.847254 |
| C | -3.054471 | -2.175399 | -0.863794 |
| C | -2.205893 | -3.205616 | -1.153730 |

| | | | |
|---|---|---|---|
| C | -0.889388 | -2.627297 | -1.279449 |
| C | -2.498062 | -4.651922 | -1.363799 |
| C | -4.507471 | -2.289525 | -0.516562 |
| C | -5.461419 | -1.489771 | -1.415209 |
| C | -5.948780 | -0.209695 | -0.781023 |
| O | -6.374424 | 0.648608 | -1.669348 |
| O | -5.959309 | -0.000384 | 0.424324 |
| C | 1.504832 | -2.816520 | -1.816729 |
| C | 2.634535 | -3.597519 | -2.267399 |
| C | 3.676205 | -2.721820 | -2.402349 |
| C | 3.162226 | -1.423125 | -1.995505 |
| C | 2.630365 | -5.072284 | -2.472783 |
| C | 5.036074 | -2.980077 | -2.822943 |
| C | 5.401001 | -3.872190 | -3.737847 |
| C | 3.484632 | 0.939274 | -1.434437 |
| C | 4.355095 | 2.053305 | -1.138192 |
| C | 3.552323 | 3.047764 | -0.647951 |
| C | 2.196123 | 2.526948 | -0.692209 |
| C | 5.824924 | 2.077211 | -1.357157 |
| C | 3.918907 | 4.365509 | -0.175785 |
| C | 5.049137 | 4.664023 | 0.456588 |
| C | -0.232373 | 2.798054 | -0.423466 |
| C | -1.394459 | 3.619400 | -0.208862 |

| | | | |
|---|---|---|---|
| C | -2.476964 | 2.790041 | -0.317483 |
| C | -1.955114 | 1.470381 | -0.593923 |
| C | -1.361355 | 5.084107 | 0.059919 |
| C | -3.913004 | 3.181644 | -0.197116 |
| C | -4.507636 | 3.574239 | -1.570215 |
| C | -5.936082 | 3.970798 | -1.364936 |
| O | -6.139721 | 5.275864 | -1.472948 |
| O | -6.833916 | 3.206061 | -1.067562 |
| N | -0.940716 | -1.293908 | -1.061546 |
| N | 1.855445 | -1.513637 | -1.664762 |
| N | 2.196917 | 1.244082 | -1.140402 |
| N | -0.600312 | 1.514882 | -0.660492 |
| H | -3.554855 | -4.871331 | -1.229462 |
| H | -2.221513 | -4.940222 | -2.377653 |
| H | 3.648695 | -5.453946 | -2.446607 |
| H | 2.190304 | -5.329054 | -3.437617 |
| H | 2.052037 | -5.567861 | -1.694372 |
| H | 6.174231 | 3.104574 | -1.439785 |
| H | 6.090494 | 1.542245 | -2.267335 |
| H | 6.342870 | 1.605239 | -0.521456 |
| H | -0.750095 | 5.299407 | 0.936172 |
| H | -2.361309 | 5.475807 | 0.230952 |
| H | -0.927716 | 5.613997 | -0.787959 |

| | | | |
|---|---|---|---|
| H | 6.435998 | -4.021053 | -3.996694 |
| H | 4.683438 | -4.461220 | -4.281951 |
| H | 5.263406 | 5.670291 | 0.776427 |
| H | 5.781895 | 3.917178 | 0.705334 |
| H | -6.357813 | -2.076012 | -1.635163 |
| H | -4.995733 | -1.243323 | -2.369602 |
| H | -4.659676 | -1.956129 | 0.514363 |
| H | -4.782140 | -3.344003 | -0.559744 |
| H | -4.451581 | 2.714190 | -2.238814 |
| H | -3.950579 | 4.407110 | -1.995120 |
| H | -4.001495 | 4.035054 | 0.479548 |
| H | -4.516235 | 2.371464 | 0.214352 |
| H | -3.791442 | 0.438075 | -0.645777 |
| H | 0.121987 | -4.407667 | -1.782536 |
| H | 4.973441 | -0.353916 | -2.183671 |
| H | 1.215924 | 4.293858 | -0.082068 |
| H | 5.798923 | -2.378932 | -2.343641 |
| H | 3.191755 | 5.149570 | -0.354168 |
| Fe | 0.647536 | -0.007269 | -1.161781 |
| H | -3.686354 | -5.265625 | 1.340671 |
| H | 7.830646 | -1.102437 | 0.919012 |
| H | 4.799025 | 1.906648 | 2.431700 |
| H | -6.660114 | 1.533083 | -1.302707 |

| | | | |
|---|---|---|---|
| H | -0.372245 | 2.153380 | -3.382555 |
| H | -7.067031 | 5.507669 | -1.299702 |
| H | -2.059239 | -5.262598 | 2.017346 |
| C | 0.931506 | -0.306917 | 0.722014 |
| C | 2.161136 | -0.411311 | 1.378282 |
| C | -0.132094 | -0.294852 | 1.792896 |
| H | -1.879307 | -0.151710 | 3.603799 |
| H | -2.868522 | 1.015211 | 1.808668 |
| H | -4.518613 | 0.673394 | 1.445139 |
| O | 2.004898 | -0.502910 | 2.787270 |
| O | 3.313036 | -0.446307 | 0.952024 |
| C | 0.640377 | -0.550639 | 3.103675 |
| H | 0.447436 | 0.205416 | 3.876990 |
| H | 0.415306 | -1.544174 | 3.519500 |
| H | -0.625685 | 0.685344 | 1.806720 |
| H | -0.889406 | -1.060011 | 1.602819 |
| H | -1.924506 | -5.268298 | -0.672616 |

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**Conf3$^{L10}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-197.6539329

Zero-point correction= 1.020595 (Hartree/Particle)

Thermal correction to Energy= 1.092809

Thermal correction to Enthalpy= 1.093753

Thermal correction to Gibbs Free Energy= 0.907997

Sum of electronic and zero-point Energies= -196.633338

Sum of electronic and thermal Energies= -196.561124

Sum of electronic and thermal Enthalpies= -196.560180

Sum of electronic and thermal Free Energies= -196.745936

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -1.219934 | 5.137111 | 1.988540 |
| H | -1.550049 | 6.164332 | 2.129949 |
| C | -2.368397 | 4.143244 | 2.221283 |
| H | -2.210964 | 3.597827 | 3.162726 |
| H | -3.319034 | 4.678246 | 2.296810 |
| O | -2.533697 | 3.238607 | 1.156715 |
| H | -1.707528 | 2.742605 | 1.050184 |
| C | -0.019141 | 4.939780 | 2.957175 |
| O | 0.362425 | 5.869509 | 3.645636 |
| N | 0.567112 | 3.721263 | 2.998569 |
| H | 0.228034 | 2.968029 | 2.405267 |

| | | | |
|---|---|---|---|
| C | 1.712391 | 3.388537 | 3.858798 |
| H | 1.443090 | 2.565100 | 4.519748 |
| H | 2.561362 | 3.099720 | 3.238937 |
| C | -3.829562 | -5.633590 | 2.377456 |
| H | -4.514803 | -6.169371 | 3.030384 |
| C | -3.727048 | -4.169890 | 2.792203 |
| H | -3.370798 | -4.119504 | 3.824983 |
| H | -2.999101 | -3.666295 | 2.153165 |
| C | -5.083157 | -3.474194 | 2.689190 |
| H | -5.442852 | -3.528591 | 1.660333 |
| H | -5.801312 | -4.001181 | 3.320150 |
| C | -5.057682 | -2.005033 | 3.122608 |
| H | -6.088127 | -1.646104 | 3.205779 |
| H | -4.593648 | -1.906769 | 4.106635 |
| N | -4.375334 | -1.141856 | 2.183476 |
| H | -4.873084 | -0.920478 | 1.326096 |
| C | -3.167586 | -0.579439 | 2.325370 |
| N | -2.800197 | 0.373633 | 1.499640 |
| N | -2.338715 | -0.934380 | 3.311188 |
| H | -2.498484 | -1.780711 | 3.826558 |
| C | 1.640981 | -1.605362 | -3.550471 |
| H | 2.117474 | -2.572033 | -3.313848 |
| H | 1.968780 | -1.304192 | -4.558115 |

| | | | |
|---|---|---|---|
| O | 1.989815 | -0.648634 | -2.641922 |
| C | -1.688295 | -0.442244 | -1.164719 |
| C | 1.641354 | -3.845263 | -0.514673 |
| C | 5.054615 | -0.456884 | -0.349844 |
| C | 1.745653 | 2.931194 | -1.177894 |
| C | -1.097561 | -1.667884 | -0.913902 |
| C | -1.809125 | -2.920335 | -0.768206 |
| C | -0.856025 | -3.883412 | -0.613378 |
| C | 0.420623 | -3.204567 | -0.642504 |
| C | -1.013623 | -5.354433 | -0.432651 |
| C | -3.294351 | -3.091050 | -0.709948 |
| C | -4.046883 | -2.637236 | -1.968943 |
| C | -4.787695 | -1.329658 | -1.782247 |
| O | -5.073519 | -0.770945 | -2.935809 |
| O | -5.093308 | -0.855188 | -0.705740 |
| C | 2.878812 | -3.221984 | -0.459189 |
| C | 4.131779 | -3.923086 | -0.327251 |
| C | 5.106747 | -2.961262 | -0.266543 |
| C | 4.419747 | -1.686767 | -0.361190 |
| C | 4.283339 | -5.399821 | -0.215038 |
| C | 6.537401 | -3.117818 | -0.117509 |
| C | 7.261031 | -4.108361 | -0.628242 |
| C | 4.438152 | 0.771061 | -0.515732 |

| | | | |
|---|---|---|---|
| C | 5.147145 | 2.031152 | -0.503200 |
| C | 4.210740 | 3.001166 | -0.735250 |
| C | 2.945052 | 2.305221 | -0.897930 |
| C | 6.618471 | 2.185485 | -0.340113 |
| C | 4.383097 | 4.434877 | -0.835079 |
| C | 5.240604 | 5.155785 | -0.120929 |
| C | 0.524465 | 2.294231 | -1.311344 |
| C | -0.715889 | 2.975795 | -1.597204 |
| C | -1.691687 | 2.023147 | -1.567001 |
| C | -1.029790 | 0.768156 | -1.292951 |
| C | -0.870710 | 4.428482 | -1.883331 |
| C | -3.157713 | 2.242935 | -1.733280 |
| C | -3.566888 | 2.321933 | -3.221777 |
| C | -5.037366 | 2.595408 | -3.280599 |
| O | -5.321158 | 3.859846 | -3.562384 |
| O | -5.908495 | 1.782579 | -3.047833 |
| N | 0.237057 | -1.871643 | -0.811585 |
| N | 3.086849 | -1.879854 | -0.481780 |
| N | 3.113962 | 0.973671 | -0.735071 |
| N | 0.303767 | 0.966327 | -1.146250 |
| H | -2.056664 | -5.651142 | -0.506056 |
| H | -0.453017 | -5.891411 | -1.197110 |
| H | 5.232254 | -5.641738 | 0.258971 |

| | | | |
|---|---|---|---|
| H | 4.261199 | -5.868321 | -1.200141 |
| H | 3.477467 | -5.827740 | 0.379408 |
| H | 6.935179 | 3.154855 | -0.718602 |
| H | 7.149441 | 1.407522 | -0.886424 |
| H | 6.902931 | 2.115513 | 0.710886 |
| H | -1.881211 | 4.756309 | -1.649002 |
| H | -0.682005 | 4.629033 | -2.939288 |
| H | -0.167698 | 5.022957 | -1.303985 |
| H | 8.324578 | -4.168496 | -0.468154 |
| H | 6.827969 | -4.874261 | -1.247460 |
| H | 5.325237 | 6.221508 | -0.251165 |
| H | 5.863777 | 4.717047 | 0.638657 |
| H | -4.804000 | -3.374072 | -2.249426 |
| H | -3.374639 | -2.527049 | -2.820171 |
| H | -3.684604 | -2.515676 | 0.133146 |
| H | -3.511273 | -4.142666 | -0.521292 |
| H | -3.345374 | 1.369930 | -3.705583 |
| H | -3.024420 | 3.126126 | -3.714853 |
| H | -3.428343 | 3.175171 | -1.234061 |
| H | -3.725202 | 1.441099 | -1.261159 |
| H | -2.757041 | -0.431498 | -1.279665 |
| H | 1.627082 | -4.923110 | -0.450618 |
| H | 6.126602 | -0.456287 | -0.221128 |

| | | | |
|---|---|---|---|
| H | 1.763295 | 4.003602 | -1.300479 |
| H | 7.034985 | -2.344693 | 0.456161 |
| H | 3.742963 | 4.934862 | -1.551966 |
| Fe | 1.679951 | -0.427363 | -0.808409 |
| H | -4.197504 | -5.716105 | 1.357882 |
| H | 1.955453 | 4.275069 | 4.440089 |
| H | -0.858044 | 5.021013 | 0.966650 |
| H | -5.518458 | 0.117510 | -2.860829 |
| H | 0.551607 | -1.775455 | -3.576567 |
| H | -6.278711 | 4.021327 | -3.542509 |
| H | -2.856519 | -6.114444 | 2.431375 |
| C | 1.375545 | -0.306099 | 1.107369 |
| C | 0.436859 | 0.416647 | 1.806655 |
| C | 1.985988 | -1.273788 | 2.095967 |
| H | -1.401395 | -0.523492 | 3.331905 |
| H | -1.836304 | 0.791027 | 1.519217 |
| H | -3.442315 | 0.733778 | 0.815660 |
| O | 0.326936 | 0.015731 | 3.174338 |
| O | -0.359427 | 1.344900 | 1.489875 |
| C | 1.371047 | -0.891102 | 3.451818 |
| H | 0.953278 | -1.746763 | 3.992961 |
| H | 2.101368 | -0.392076 | 4.100435 |
| H | 1.731491 | -2.301692 | 1.824334 |

H 3.073119 -1.197577 2.114355

H -0.635503 -5.664744 0.541929

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**Conf4$^{L10}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-197.6539338

Zero-point correction= 1.020600 (Hartree/Particle)

Thermal correction to Energy= 1.092811

Thermal correction to Enthalpy= 1.093755

Thermal correction to Gibbs Free Energy= 0.908059

Sum of electronic and zero-point Energies= -196.633334

Sum of electronic and thermal Energies= -196.561123

Sum of electronic and thermal Enthalpies= -196.560179

Sum of electronic and thermal Free Energies= -196.745875

.....

Cartesian Coordinates

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C -1.219580 5.136574 1.988550

H -1.549514 6.163891 2.129703

C -2.368209 4.142955 2.221527

| | | | |
|---|---|---|---|
| H | -2.210674 | 3.597440 | 3.162894 |
| H | -3.318712 | 4.678155 | 2.297303 |
| O | -2.533954 | 3.238416 | 1.156939 |
| H | -1.707888 | 2.742290 | 1.050168 |
| C | -0.018836 | 4.939238 | 2.957202 |
| O | 0.362898 | 5.868996 | 3.645519 |
| N | 0.567242 | 3.720631 | 2.998760 |
| H | 0.228015 | 2.967396 | 2.405566 |
| C | 1.712463 | 3.387841 | 3.859058 |
| H | 1.442878 | 2.564831 | 4.520429 |
| H | 2.561233 | 3.098352 | 3.239237 |
| C | -3.829529 | -5.634086 | 2.376754 |
| H | -4.514784 | -6.170037 | 3.029529 |
| C | -3.727207 | -4.170432 | 2.791713 |
| H | -3.371028 | -4.120166 | 3.824525 |
| H | -2.999282 | -3.666694 | 2.152764 |
| C | -5.083378 | -3.474857 | 2.688729 |
| H | -5.443033 | -3.529178 | 1.659854 |
| H | -5.801498 | -4.001992 | 3.319604 |
| C | -5.058113 | -2.005738 | 3.122313 |
| H | -6.088616 | -1.646997 | 3.205524 |
| H | -4.594065 | -1.907496 | 4.106332 |
| N | -4.375909 | -1.142300 | 2.183304 |

| | | | |
|---|---|---|---|
| H | -4.873778 | -0.920419 | 1.326132 |
| C | -3.168144 | -0.579952 | 2.325346 |
| N | -2.800943 | 0.373826 | 1.500364 |
| N | -2.339080 | -0.935621 | 3.310742 |
| H | -2.498571 | -1.782528 | 3.825261 |
| C | 1.641851 | -1.605792 | -3.550352 |
| H | 2.115428 | -2.573179 | -3.310886 |
| H | 1.973468 | -1.306709 | -4.557360 |
| O | 1.989690 | -0.648484 | -2.642030 |
| C | -1.688313 | -0.441592 | -1.164346 |
| C | 1.641013 | -3.845138 | -0.515261 |
| C | 5.054546 | -0.457090 | -0.349395 |
| C | 1.746117 | 2.931347 | -1.177948 |
| C | -1.097658 | -1.667332 | -0.913827 |
| C | -1.809358 | -2.919732 | -0.768287 |
| C | -0.856357 | -3.882950 | -0.613773 |
| C | 0.420364 | -3.204257 | -0.642934 |
| C | -1.014017 | -5.354008 | -0.433353 |
| C | -3.294588 | -3.090385 | -0.710079 |
| C | -4.047057 | -2.636350 | -1.969017 |
| C | -4.787787 | -1.328756 | -1.782175 |
| O | -5.073484 | -0.769893 | -2.935689 |
| O | -5.093447 | -0.854430 | -0.705618 |

| | | | |
|---|---|---|---|
| C | 2.878542 | -3.221998 | -0.459688 |
| C | 4.131445 | -3.923225 | -0.327915 |
| C | 5.106471 | -2.961476 | -0.266832 |
| C | 4.419564 | -1.686922 | -0.361164 |
| C | 4.282896 | -5.400001 | -0.216181 |
| C | 6.537103 | -3.118152 | -0.117696 |
| C | 7.260792 | -4.108495 | -0.628718 |
| C | 4.438217 | 0.770912 | -0.515249 |
| C | 5.147313 | 2.030933 | -0.502339 |
| C | 4.211086 | 3.001050 | -0.734614 |
| C | 2.945372 | 2.305237 | -0.897717 |
| C | 6.618620 | 2.185062 | -0.338891 |
| C | 4.383522 | 4.434778 | -0.834029 |
| C | 5.240736 | 5.155422 | -0.119269 |
| C | 0.524867 | 2.294503 | -1.311449 |
| C | -0.715363 | 2.976244 | -1.597334 |
| C | -1.691342 | 2.023779 | -1.566857 |
| C | -1.029638 | 0.768702 | -1.292772 |
| C | -0.869805 | 4.428924 | -1.883682 |
| C | -3.157314 | 2.243769 | -1.733232 |
| C | -3.566477 | 2.322214 | -3.221768 |
| C | -5.036838 | 2.596280 | -3.280528 |
| O | -5.320131 | 3.860880 | -3.562104 |

| | | | |
|---|---|---|---|
| O | -5.908295 | 1.783789 | -3.047798 |
| N | 0.236953 | -1.871284 | -0.811808 |
| N | 3.086663 | -1.879869 | -0.481862 |
| N | 3.114095 | 0.973649 | -0.734964 |
| N | 0.303983 | 0.966647 | -1.146206 |
| H | -2.057191 | -5.650516 | -0.505613 |
| H | -0.454412 | -5.890806 | -1.198677 |
| H | 5.231839 | -5.642154 | 0.257648 |
| H | 4.260604 | -5.868190 | -1.201427 |
| H | 3.477054 | -5.828047 | 0.378216 |
| H | 6.935453 | 3.154674 | -0.716631 |
| H | 7.149611 | 1.407449 | -0.885681 |
| H | 6.902922 | 2.114291 | 0.712096 |
| H | -1.880555 | 4.756816 | -1.650653 |
| H | -0.679718 | 4.629457 | -2.939365 |
| H | -0.167529 | 5.023381 | -1.303445 |
| H | 8.324317 | -4.168697 | -0.468512 |
| H | 6.827808 | -4.874153 | -1.248292 |
| H | 5.325478 | 6.221176 | -0.249133 |
| H | 5.863543 | 4.716393 | 0.640449 |
| H | -4.804241 | -3.373085 | -2.249594 |
| H | -3.374799 | -2.526108 | -2.820225 |
| H | -3.684863 | -2.515138 | 0.133089 |

| | | | |
|---|---|---|---|
| H | -3.511553 | -4.142027 | -0.521618 |
| H | -3.345350 | 1.369921 | -3.705158 |
| H | -3.023695 | 3.125994 | -3.715179 |
| H | -3.427802 | 3.176276 | -1.234444 |
| H | -3.724952 | 1.442274 | -1.260705 |
| H | -2.757100 | -0.430646 | -1.278875 |
| H | 1.626621 | -4.922994 | -0.451407 |
| H | 6.126507 | -0.456664 | -0.220464 |
| H | 1.763860 | 4.003743 | -1.300593 |
| H | 7.034596 | -2.345228 | 0.456331 |
| H | 3.743745 | 4.934984 | -1.551071 |
| Fe | 1.679913 | -0.427202 | -0.808419 |
| H | -4.197359 | -5.716504 | 1.357130 |
| H | 1.955942 | 4.274545 | 4.439884 |
| H | -0.857733 | 5.020166 | 0.966676 |
| H | -5.518410 | 0.118577 | -2.860707 |
| H | 0.552178 | -1.773547 | -3.579659 |
| H | -6.277617 | 4.022738 | -3.542108 |
| H | -2.856440 | -6.114842 | 2.430712 |
| C | 1.375436 | -0.306483 | 1.107366 |
| C | 0.436496 | 0.416018 | 1.806574 |
| C | 1.985837 | -1.274243 | 2.095889 |
| H | -1.401743 | -0.524762 | 3.331501 |

| | | | |
|---|---|---|---|
| H | -1.836838 | 0.790740 | 1.519675 |
| H | -3.443060 | 0.734754 | 0.816786 |
| O | 0.326462 | 0.014882 | 3.174218 |
| O | -0.359775 | 1.344262 | 1.489840 |
| C | 1.370756 | -0.891705 | 3.451723 |
| H | 0.953173 | -1.747464 | 3.992855 |
| H | 2.100968 | -0.392533 | 4.100355 |
| H | 1.731434 | -2.302144 | 1.824167 |
| H | 3.072966 | -1.197968 | 2.114373 |
| H | -0.634789 | -5.664712 | 0.540663 |

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**Conf5$^{L10}$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-197.6491251

Zero-point correction= 1.019564 (Hartree/Particle)

Thermal correction to Energy= 1.093130

Thermal correction to Enthalpy= 1.094074

Thermal correction to Gibbs Free Energy= 0.901543

Sum of electronic and zero-point Energies= -196.629561

Sum of electronic and thermal Energies= -196.555995

Sum of electronic and thermal Enthalpies= -196.555051

Sum of electronic and thermal Free Energies= -196.747582

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 3.821859 | 3.607438 | 2.906725 |
| H | 3.788311 | 4.359060 | 3.692796 |
| C | 2.395570 | 3.256388 | 2.457909 |
| H | 2.410943 | 2.395906 | 1.773522 |
| H | 1.781429 | 2.998876 | 3.322751 |
| O | 1.759855 | 4.351639 | 1.845457 |
| H | 2.224771 | 4.542278 | 1.022472 |
| C | 4.529569 | 2.356054 | 3.485079 |
| O | 4.586780 | 2.160985 | 4.681854 |
| N | 5.082087 | 1.487382 | 2.592195 |
| H | 4.973764 | 1.667113 | 1.604399 |
| C | 5.800207 | 0.255257 | 2.959222 |
| H | 5.310653 | -0.609977 | 2.513933 |
| H | 6.833696 | 0.315718 | 2.617963 |
| C | -3.794683 | -4.431290 | 3.488449 |
| H | -4.129128 | -4.953087 | 4.382462 |
| C | -3.774107 | -2.925177 | 3.718792 |
| H | -3.082719 | -2.703832 | 4.535423 |

| | | | |
|---|---|---|---|
| H | -3.402518 | -2.433053 | 2.817915 |
| C | -5.163448 | -2.396548 | 4.073176 |
| H | -5.848435 | -2.594720 | 3.245880 |
| H | -5.537274 | -2.930786 | 4.948757 |
| C | -5.183162 | -0.895578 | 4.386797 |
| H | -6.169042 | -0.618629 | 4.769402 |
| H | -4.449724 | -0.662654 | 5.161733 |
| N | -4.922602 | -0.075287 | 3.225140 |
| H | -5.683223 | 0.031079 | 2.569500 |
| C | -3.718813 | 0.343070 | 2.794671 |
| N | -3.670103 | 1.017554 | 1.646503 |
| N | -2.601492 | 0.217966 | 3.478333 |
| H | -2.558628 | -0.325237 | 4.320922 |
| C | 0.377819 | -1.461675 | -3.932180 |
| H | 1.005821 | -2.368791 | -3.917146 |
| H | 0.393480 | -1.051300 | -4.954180 |
| O | 0.831544 | -0.526110 | -3.043732 |
| C | -2.347076 | 0.193375 | -1.033482 |
| C | 0.261805 | -3.836825 | -0.907814 |
| C | 4.279691 | -1.245710 | -1.428069 |
| C | 1.696377 | 2.795607 | -1.086797 |
| C | -1.985865 | -1.131474 | -0.854981 |
| C | -2.906494 | -2.213598 | -0.567167 |

| | | | |
|---|---|---|---|
| C | -2.158184 | -3.352426 | -0.534319 |
| C | -0.792986 | -2.950655 | -0.789988 |
| C | -2.579587 | -4.761277 | -0.292347 |
| C | -4.367282 | -2.083738 | -0.269637 |
| C | -5.207695 | -1.575199 | -1.452541 |
| C | -5.647222 | -0.137855 | -1.292921 |
| O | -5.902501 | 0.433730 | -2.445980 |
| O | -5.767540 | 0.425533 | -0.221079 |
| C | 1.581359 | -3.486682 | -1.146525 |
| C | 2.649535 | -4.436337 | -1.336427 |
| C | 3.793204 | -3.700993 | -1.508698 |
| C | 3.396538 | -2.308450 | -1.398262 |
| C | 2.501599 | -5.916720 | -1.283374 |
| C | 5.147501 | -4.159948 | -1.728173 |
| C | 5.490527 | -5.239107 | -2.423695 |
| C | 3.934996 | 0.090868 | -1.287706 |
| C | 4.892226 | 1.162974 | -1.170030 |
| C | 4.161619 | 2.318667 | -1.044119 |
| C | 2.767162 | 1.919166 | -1.114253 |
| C | 6.371372 | 1.004695 | -1.243944 |
| C | 4.621597 | 3.680191 | -0.883313 |
| C | 5.717961 | 4.061972 | -0.232783 |
| C | 0.363255 | 2.430839 | -1.117453 |

| | | | |
|---|---|---|---|
| C | -0.724133 | 3.383071 | -1.154692 |
| C | -1.870455 | 2.648470 | -1.173044 |
| C | -1.466794 | 1.257220 | -1.138648 |
| C | -0.555451 | 4.862295 | -1.136074 |
| C | -3.272149 | 3.159627 | -1.220522 |
| C | -3.787500 | 3.218269 | -2.679129 |
| C | -5.181789 | 3.759881 | -2.661613 |
| O | -5.229976 | 5.074172 | -2.840882 |
| O | -6.185346 | 3.109285 | -2.454142 |
| N | -0.721426 | -1.604959 | -0.949897 |
| N | 2.056958 | -2.216237 | -1.207862 |
| N | 2.668911 | 0.575133 | -1.224443 |
| N | -0.117351 | 1.164458 | -1.110056 |
| H | -3.651112 | -4.829939 | -0.122435 |
| H | -2.332571 | -5.382730 | -1.153001 |
| H | 3.462777 | -6.380501 | -1.071703 |
| H | 2.133690 | -6.304347 | -2.234560 |
| H | 1.795631 | -6.206177 | -0.506426 |
| H | 6.838076 | 1.954519 | -1.496318 |
| H | 6.637443 | 0.275228 | -2.007084 |
| H | 6.781262 | 0.658895 | -0.292973 |
| H | -0.109003 | 5.171765 | -0.190605 |
| H | -1.512051 | 5.366166 | -1.247895 |

| | | | |
|---|---|---|---|
| H | 0.097084 | 5.185067 | -1.946626 |
| H | 6.521382 | -5.529483 | -2.539675 |
| H | 4.762968 | -5.852003 | -2.926197 |
| H | 5.998829 | 5.099983 | -0.167732 |
| H | 6.369912 | 3.364844 | 0.265460 |
| H | -6.125148 | -2.161866 | -1.548387 |
| H | -4.665224 | -1.664589 | -2.393819 |
| H | -4.506812 | -1.396035 | 0.569054 |
| H | -4.741554 | -3.058656 | 0.044877 |
| H | -3.778186 | 2.214655 | -3.104331 |
| H | -3.145761 | 3.875556 | -3.263653 |
| H | -3.307805 | 4.163452 | -0.793324 |
| H | -3.938455 | 2.524569 | -0.636112 |
| H | -3.399588 | 0.419036 | -1.052798 |
| H | 0.034723 | -4.889270 | -0.827942 |
| H | 5.328606 | -1.475195 | -1.541851 |
| H | 1.911831 | 3.853881 | -1.072221 |
| H | 5.927497 | -3.550731 | -1.286698 |
| H | 3.991765 | 4.440661 | -1.330709 |
| Fe | 0.962587 | -0.515310 | -1.157926 |
| H | -4.467187 | -4.684577 | 2.672330 |
| H | 5.774598 | 0.181270 | 4.043835 |
| H | 4.388787 | 3.988726 | 2.053334 |

| | | | |
|---|---|---|---|
| H | -6.146225 | 1.397081 | -2.365629 |
| H | -0.652851 | -1.778930 | -3.700243 |
| H | -6.140382 | 5.406097 | -2.776461 |
| H | -2.799614 | -4.785678 | 3.234514 |
| C | 1.158285 | -0.472554 | 0.766681 |
| C | 0.243156 | -0.047095 | 1.721820 |
| C | 2.351314 | -0.977688 | 1.537836 |
| H | -1.723850 | 0.370706 | 2.873909 |
| H | -2.745247 | 1.153910 | 1.249514 |
| H | -4.465218 | 0.984628 | 1.019744 |
| O | 0.680042 | -0.216294 | 3.029653 |
| O | -0.903099 | 0.449995 | 1.589075 |
| C | 2.000634 | -0.717027 | 3.013629 |
| H | 2.026992 | -1.627916 | 3.621553 |
| H | 2.657211 | 0.028968 | 3.475942 |
| H | 2.512085 | -2.042058 | 1.347269 |
| H | 3.262974 | -0.456559 | 1.238908 |
| H | -2.065869 | -5.170483 | 0.577185 |

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**Conf6$^{L10}$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-197.6408189

Zero-point correction= 1.019354 (Hartree/Particle)

Thermal correction to Energy= 1.092953

Thermal correction to Enthalpy= 1.093897

Thermal correction to Gibbs Free Energy= 0.898951

Sum of electronic and zero-point Energies= -196.621465

Sum of electronic and thermal Energies= -196.547866

Sum of electronic and thermal Enthalpies= -196.546922

Sum of electronic and thermal Free Energies= -196.741868

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 5.868665 | 1.407112 | 2.935723 |
| H | 6.517358 | 2.238353 | 3.206616 |
| C | 5.214232 | 0.832308 | 4.195957 |
| H | 4.680463 | -0.095749 | 3.938278 |
| H | 5.982915 | 0.593862 | 4.933487 |
| O | 4.347359 | 1.742506 | 4.823160 |
| H | 3.653011 | 1.994122 | 4.202762 |
| C | 6.745958 | 0.305848 | 2.286314 |
| O | 7.844630 | 0.045116 | 2.730744 |
| N | 6.222573 | -0.368709 | 1.226298 |

| | | | |
|---|---|---|---|
| H | 5.309793 | -0.121288 | 0.873008 |
| C | 6.904097 | -1.461900 | 0.516959 |
| H | 6.245083 | -2.326220 | 0.460066 |
| H | 7.182851 | -1.138970 | -0.486243 |
| C | -2.989260 | -5.207311 | 2.065983 |
| H | -3.135657 | -6.059650 | 2.726465 |
| C | -3.264968 | -3.901686 | 2.799560 |
| H | -2.580791 | -3.825742 | 3.648063 |
| H | -3.059575 | -3.071089 | 2.122020 |
| C | -4.707126 | -3.832924 | 3.301584 |
| H | -5.389033 | -3.874861 | 2.449388 |
| H | -4.909308 | -4.701668 | 3.931156 |
| C | -5.010279 | -2.571940 | 4.121077 |
| H | -6.012237 | -2.648653 | 4.550203 |
| H | -4.302349 | -2.480510 | 4.947940 |
| N | -4.972351 | -1.362746 | 3.327390 |
| H | -5.775632 | -1.188571 | 2.740507 |
| C | -3.865227 | -0.662191 | 3.018247 |
| N | -3.976746 | 0.315231 | 2.117282 |
| N | -2.706082 | -0.802070 | 3.625461 |
| H | -2.553941 | -1.551322 | 4.276256 |
| C | -0.492223 | 1.271359 | -3.686020 |
| H | -1.561810 | 1.006468 | -3.609917 |

| | | | |
|---|---|---|---|
| H | -0.213544 | 1.224718 | -4.751400 |
| O | 0.274330 | 0.400239 | -2.969236 |
| C | -2.685913 | 0.382647 | -0.708653 |
| C | 0.278330 | -3.237090 | -1.778090 |
| C | 4.000029 | -0.189958 | -1.787944 |
| C | 1.095879 | 3.323036 | -0.243422 |
| C | -2.200000 | -0.897980 | -0.909091 |
| C | -3.013234 | -2.097726 | -0.964115 |
| C | -2.167867 | -3.115545 | -1.290932 |
| C | -0.849205 | -2.529884 | -1.399979 |
| C | -2.462176 | -4.553719 | -1.547232 |
| C | -4.470957 | -2.201085 | -0.641825 |
| C | -5.388150 | -1.446810 | -1.617848 |
| C | -5.952059 | -0.171409 | -1.035146 |
| O | -6.318860 | 0.678301 | -1.965463 |
| O | -6.068511 | 0.044348 | 0.156661 |
| C | 1.545008 | -2.704153 | -1.942607 |
| C | 2.679558 | -3.462620 | -2.412298 |
| C | 3.737291 | -2.593027 | -2.447851 |
| C | 3.224348 | -1.319751 | -1.971023 |
| C | 2.668333 | -4.918232 | -2.723857 |
| C | 5.105860 | -2.836593 | -2.847909 |
| C | 5.491318 | -3.679450 | -3.800495 |

| | | | |
|---|---|---|---|
| C | 3.543417 | 1.026209 | -1.303363 |
| C | 4.398420 | 2.149042 | -1.005264 |
| C | 3.579758 | 3.139957 | -0.525231 |
| C | 2.230909 | 2.606714 | -0.575093 |
| C | 5.864462 | 2.210834 | -1.260943 |
| C | 3.929766 | 4.466397 | -0.067496 |
| C | 5.065102 | 4.796980 | 0.540113 |
| C | -0.202492 | 2.844988 | -0.315759 |
| C | -1.372626 | 3.654488 | -0.066908 |
| C | -2.446166 | 2.829214 | -0.223839 |
| C | -1.915639 | 1.525678 | -0.562762 |
| C | -1.344700 | 5.102689 | 0.280347 |
| C | -3.888443 | 3.187708 | -0.082722 |
| C | -4.489336 | 3.601757 | -1.447852 |
| C | -5.921863 | 3.977894 | -1.234079 |
| O | -6.090783 | 5.277985 | -1.027138 |
| O | -6.852465 | 3.200191 | -1.192168 |
| N | -0.901973 | -1.204764 | -1.136367 |
| N | 1.901436 | -1.417743 | -1.693890 |
| N | 2.247395 | 1.325821 | -1.023126 |
| N | -0.564211 | 1.576462 | -0.622212 |
| H | -3.515069 | -4.776279 | -1.392622 |
| H | -2.211989 | -4.805994 | -2.577772 |

| | | | |
|---|---|---|---|
| H | 3.678804 | -5.318825 | -2.675676 |
| H | 2.274176 | -5.096521 | -3.725242 |
| H | 2.044113 | -5.459578 | -2.014590 |
| H | 6.173341 | 3.247060 | -1.383476 |
| H | 6.117694 | 1.664199 | -2.167637 |
| H | 6.435117 | 1.781797 | -0.435411 |
| H | -0.773645 | 5.265153 | 1.194180 |
| H | -2.350197 | 5.488308 | 0.428773 |
| H | -0.872780 | 5.675921 | -0.517688 |
| H | 6.532280 | -3.816806 | -4.041117 |
| H | 4.786908 | -4.235677 | -4.393233 |
| H | 5.262110 | 5.810256 | 0.847231 |
| H | 5.825722 | 4.073215 | 0.775339 |
| H | -6.250779 | -2.062670 | -1.885461 |
| H | -4.867045 | -1.199915 | -2.542968 |
| H | -4.648207 | -1.808967 | 0.363714 |
| H | -4.746117 | -3.256380 | -0.631787 |
| H | -4.420075 | 2.763317 | -2.140988 |
| H | -3.940727 | 4.456092 | -1.841292 |
| H | -3.990174 | 4.022890 | 0.613260 |
| H | -4.461294 | 2.349987 | 0.315811 |
| H | -3.753810 | 0.498548 | -0.636479 |
| H | 0.150440 | -4.285913 | -2.000360 |

| | | | |
|---|---|---|---|
| H | 5.050416 | -0.262772 | -2.026850 |
| H | 1.225533 | 4.346736 | 0.073911 |
| H | 5.860253 | -2.263715 | -2.322331 |
| H | 3.182617 | 5.232567 | -0.235263 |
| Fe | 0.669034 | 0.081197 | -1.147256 |
| H | -3.655785 | -5.314953 | 1.214401 |
| H | 7.800724 | -1.705624 | 1.082285 |
| H | 5.101500 | 1.753400 | 2.237569 |
| H | -6.651096 | 1.544773 | -1.602058 |
| H | -0.382603 | 2.316120 | -3.347905 |
| H | -7.021189 | 5.488476 | -0.844706 |
| H | -1.964766 | -5.221628 | 1.705337 |
| C | 0.963395 | -0.331374 | 0.716524 |
| C | 0.048680 | -0.341840 | 1.756678 |
| C | 2.290608 | -0.705610 | 1.334902 |
| H | -1.881517 | -0.428199 | 3.027565 |
| H | -3.101784 | 0.681730 | 1.757391 |
| H | -4.788704 | 0.338754 | 1.511176 |
| O | 0.572839 | -0.814951 | 2.957910 |
| O | -1.158883 | 0.009833 | 1.788042 |
| C | 1.916026 | -1.192404 | 2.745068 |
| H | 1.986643 | -2.285219 | 2.822537 |
| H | 2.522523 | -0.748651 | 3.540498 |

| | | | |
|---|---|---|---|
| H | 2.807575 | -1.477594 | 0.763621 |
| H | 2.946299 | 0.171147 | 1.380219 |
| H | -1.872693 | -5.193720 | -0.892173 |

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**Conf7$^{L10}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-197.6408409

Zero-point correction= 1.019327 (Hartree/Particle)

Thermal correction to Energy= 1.092039

Thermal correction to Enthalpy= 1.092983

Thermal correction to Gibbs Free Energy= 0.902369

Sum of electronic and zero-point Energies= -196.621514

Sum of electronic and thermal Energies= -196.548802

Sum of electronic and thermal Enthalpies= -196.547857

Sum of electronic and thermal Free Energies= -196.738472

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 5.879562 | 1.414929 | 2.938352 |
| H | 6.525651 | 2.233355 | 3.250448 |

| | | | |
|---|---|---|---|
| C | 5.188298 | 0.804011 | 4.161674 |
| H | 4.666624 | -0.118376 | 3.861738 |
| H | 5.933978 | 0.547598 | 4.916654 |
| O | 4.298544 | 1.693257 | 4.786614 |
| H | 3.619486 | 1.955993 | 4.153994 |
| C | 6.766130 | 0.328427 | 2.276104 |
| O | 7.879188 | 0.091738 | 2.697192 |
| N | 6.231721 | -0.363258 | 1.232333 |
| H | 5.308969 | -0.130964 | 0.895115 |
| C | 6.916466 | -1.448842 | 0.514002 |
| H | 6.270888 | -2.324230 | 0.475580 |
| H | 7.168249 | -1.126725 | -0.496539 |
| C | -2.971533 | -5.207990 | 2.063951 |
| H | -3.111921 | -6.059400 | 2.726907 |
| C | -3.250704 | -3.901874 | 2.795501 |
| H | -2.564395 | -3.820817 | 3.641790 |
| H | -3.051123 | -3.071654 | 2.115697 |
| C | -4.691731 | -3.838560 | 3.301381 |
| H | -5.375708 | -3.886159 | 2.451124 |
| H | -4.888084 | -4.706457 | 3.933944 |
| C | -4.998724 | -2.576713 | 4.118021 |
| H | -6.000072 | -2.656125 | 4.548178 |
| H | -4.290438 | -2.480541 | 4.943996 |

| | | | |
|---|---|---|---|
| N | -4.965729 | -1.369431 | 3.321317 |
| H | -5.768535 | -1.201627 | 2.731949 |
| C | -3.862050 | -0.662632 | 3.013423 |
| N | -3.976605 | 0.311297 | 2.109715 |
| N | -2.703908 | -0.794472 | 3.624111 |
| H | -2.546224 | -1.542759 | 4.274530 |
| C | -0.485960 | 1.283123 | -3.678961 |
| H | -1.557477 | 1.026067 | -3.602363 |
| H | -0.208047 | 1.233538 | -4.744444 |
| O | 0.274577 | 0.407131 | -2.961886 |
| C | -2.686970 | 0.383048 | -0.706376 |
| C | 0.276827 | -3.234737 | -1.781740 |
| C | 3.999353 | -0.188516 | -1.780350 |
| C | 1.095092 | 3.321070 | -0.229317 |
| C | -2.201421 | -0.897776 | -0.906831 |
| C | -3.014542 | -2.097496 | -0.964110 |
| C | -2.169007 | -3.114717 | -1.292514 |
| C | -0.850507 | -2.528794 | -1.400673 |
| C | -2.463386 | -4.552459 | -1.551169 |
| C | -4.472510 | -2.201586 | -0.643388 |
| C | -5.388488 | -1.448517 | -1.621465 |
| C | -5.953373 | -0.172930 | -1.040264 |
| O | -6.319734 | 0.675994 | -1.971499 |

| | | | |
|---|---|---|---|
| O | -6.070234 | 0.043734 | 0.151287 |
| C | 1.543291 | -2.701093 | -1.945390 |
| C | 2.677319 | -3.457701 | -2.419087 |
| C | 3.735433 | -2.588425 | -2.450756 |
| C | 3.223252 | -1.317188 | -1.968069 |
| C | 2.665583 | -4.911733 | -2.737919 |
| C | 5.103893 | -2.831307 | -2.851760 |
| C | 5.488245 | -3.668101 | -3.810069 |
| C | 3.543186 | 1.026048 | -1.291368 |
| C | 4.398220 | 2.148208 | -0.990645 |
| C | 3.579557 | 3.137922 | -0.508020 |
| C | 2.230567 | 2.604873 | -0.559621 |
| C | 5.863937 | 2.211166 | -1.247787 |
| C | 3.929283 | 4.463505 | -0.047834 |
| C | 5.066360 | 4.795058 | 0.556091 |
| C | -0.203423 | 2.844091 | -0.306625 |
| C | -1.373847 | 3.654074 | -0.060685 |
| C | -2.447359 | 2.829546 | -0.221369 |
| C | -1.916533 | 1.525925 | -0.559580 |
| C | -1.346007 | 5.101904 | 0.288036 |
| C | -3.889866 | 3.188555 | -0.083889 |
| C | -4.488027 | 3.600435 | -1.450838 |
| C | -5.921051 | 3.976735 | -1.240618 |

| | | | |
|---|---|---|---|
| O | -6.090290 | 5.277015 | -1.034903 |
| O | -6.851857 | 3.199227 | -1.200393 |
| N | -0.903268 | -1.204233 | -1.134076 |
| N | 1.900249 | -1.415848 | -1.690972 |
| N | 2.247195 | 1.324964 | -1.010480 |
| N | -0.564958 | 1.576267 | -0.615529 |
| H | -3.515363 | -4.776271 | -1.392180 |
| H | -2.217871 | -4.801864 | -2.583552 |
| H | 3.676159 | -5.312492 | -2.693511 |
| H | 2.269717 | -5.084951 | -3.739514 |
| H | 2.042582 | -5.456730 | -2.030362 |
| H | 6.171825 | 3.247663 | -1.370631 |
| H | 6.116609 | 1.664897 | -2.154848 |
| H | 6.436052 | 1.782612 | -0.423055 |
| H | -0.780223 | 5.262562 | 1.205463 |
| H | -2.351819 | 5.488807 | 0.430836 |
| H | -0.868488 | 5.675234 | -0.506578 |
| H | 6.529051 | -3.805884 | -4.051105 |
| H | 4.782962 | -4.218588 | -4.407141 |
| H | 5.262050 | 5.808066 | 0.864934 |
| H | 5.829968 | 4.072894 | 0.786455 |
| H | -6.250448 | -2.064830 | -1.890113 |
| H | -4.865939 | -1.202032 | -2.545887 |

| | | | |
|---|---|---|---|
| H | -4.651504 | -1.808631 | 0.361483 |
| H | -4.747122 | -3.257016 | -0.632892 |
| H | -4.417247 | 2.760992 | -2.142620 |
| H | -3.938771 | 4.454271 | -1.844472 |
| H | -3.992815 | 4.024844 | 0.610550 |
| H | -4.463742 | 2.351602 | 0.314839 |
| H | -3.754984 | 0.499391 | -0.636614 |
| H | 0.148765 | -4.282733 | -2.007759 |
| H | 5.049628 | -0.260841 | -2.019792 |
| H | 1.224322 | 4.344115 | 0.090283 |
| H | 5.859086 | -2.263995 | -2.321236 |
| H | 3.180078 | 5.228773 | -0.210416 |
| Fe | 0.668070 | 0.082118 | -1.140468 |
| H | -3.640451 | -5.320592 | 1.214871 |
| H | 7.828756 | -1.674447 | 1.061459 |
| H | 5.131923 | 1.785799 | 2.231689 |
| H | -6.651700 | 1.542889 | -1.609008 |
| H | -0.368548 | 2.327385 | -3.341897 |
| H | -7.021089 | 5.487725 | -0.854756 |
| H | -1.948213 | -5.218630 | 1.699848 |
| C | 0.956159 | -0.334814 | 0.723201 |
| C | 0.045810 | -0.326791 | 1.767525 |
| C | 2.276329 | -0.743965 | 1.334875 |

| | | | |
|---|---|---|---|
| H | -1.880660 | -0.401637 | 3.038224 |
| H | -3.103583 | 0.683426 | 1.750641 |
| H | -4.791542 | 0.337597 | 1.507927 |
| O | 0.561753 | -0.827759 | 2.961660 |
| O | -1.149127 | 0.063928 | 1.812449 |
| C | 1.892634 | -1.240722 | 2.739016 |
| H | 1.931781 | -2.336281 | 2.799123 |
| H | 2.514022 | -0.827350 | 3.539308 |
| H | 2.778261 | -1.518471 | 0.754039 |
| H | 2.949111 | 0.119420 | 1.390932 |
| H | -1.870306 | -5.193675 | -0.900573 |

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**Conf8$^{L10}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-197.6364458

Zero-point correction= 1.021228 (Hartree/Particle)

Thermal correction to Energy= 1.094231

Thermal correction to Enthalpy= 1.095175

Thermal correction to Gibbs Free Energy= 0.905171

Sum of electronic and zero-point Energies= -196.615218

Sum of electronic and thermal Energies= -196.542215

Sum of electronic and thermal Enthalpies= -196.541271

Sum of electronic and thermal Free Energies= -196.731275

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 6.286443 | 2.047017 | 2.138754 |
| H | 6.957862 | 2.744531 | 2.633922 |
| C | 5.284982 | 1.449976 | 3.130796 |
| H | 4.806232 | 0.565894 | 2.682506 |
| H | 5.795576 | 1.137801 | 4.043753 |
| O | 4.302359 | 2.370753 | 3.540815 |
| H | 3.891878 | 2.757603 | 2.758141 |
| C | 7.150731 | 0.919082 | 1.510519 |
| O | 8.316043 | 0.777058 | 1.810701 |
| N | 6.531711 | 0.101550 | 0.612940 |
| H | 5.558238 | 0.252598 | 0.392855 |
| C | 7.168546 | -1.039788 | -0.062958 |
| H | 6.608722 | -1.950312 | 0.145633 |
| H | 7.206645 | -0.860024 | -1.137281 |
| C | -2.214620 | -4.994496 | 3.196309 |
| H | -3.062502 | -5.612803 | 3.485376 |
| C | -2.439296 | -3.542849 | 3.604428 |

| | | | |
|---|---|---|---|
| H | -2.547603 | -3.497753 | 4.693249 |
| H | -1.572072 | -2.956592 | 3.299851 |
| C | -3.685908 | -2.965854 | 2.936084 |
| H | -3.497023 | -2.886839 | 1.865872 |
| H | -4.517371 | -3.658800 | 3.087102 |
| C | -4.122358 | -1.592186 | 3.466643 |
| H | -5.175698 | -1.440978 | 3.214219 |
| H | -4.037453 | -1.556766 | 4.555576 |
| N | -3.433481 | -0.439874 | 2.920910 |
| H | -3.627063 | -0.269792 | 1.942780 |
| C | -2.191413 | -0.032936 | 3.292016 |
| N | -1.868452 | 1.249476 | 2.922200 |
| N | -1.729847 | -0.406962 | 4.522863 |
| H | -1.871272 | -1.381596 | 4.740118 |
| C | -0.848097 | 0.863411 | -3.520184 |
| H | -1.919212 | 0.642015 | -3.371200 |
| H | -0.620443 | 0.720647 | -4.588129 |
| O | -0.072000 | 0.033550 | -2.763053 |
| C | -2.936537 | 0.212327 | -0.344088 |
| C | -0.012177 | -3.501328 | -1.208186 |
| C | 3.632264 | -0.436990 | -1.900282 |
| C | 0.840494 | 3.200087 | -0.424194 |
| C | -2.465741 | -1.067440 | -0.571863 |

| | | | |
|---|---|---|---|
| C | -3.310805 | -2.244081 | -0.620712 |
| C | -2.475902 | -3.299736 | -0.830382 |
| C | -1.137976 | -2.749882 | -0.923630 |
| C | -2.803735 | -4.744587 | -0.983323 |
| C | -4.802046 | -2.247008 | -0.499559 |
| C | -5.498363 | -1.626980 | -1.723450 |
| C | -6.088051 | -0.262018 | -1.435966 |
| O | -6.479517 | 0.352492 | -2.538204 |
| O | -6.188695 | 0.224797 | -0.333918 |
| C | 1.249556 | -2.990213 | -1.463330 |
| C | 2.377228 | -3.795894 | -1.870087 |
| C | 3.407137 | -2.925507 | -2.108811 |
| C | 2.889018 | -1.600093 | -1.809394 |
| C | 2.382424 | -5.282007 | -1.944011 |
| C | 4.757285 | -3.205715 | -2.546643 |
| C | 5.112126 | -4.189175 | -3.367039 |
| C | 3.188470 | 0.834755 | -1.568807 |
| C | 4.021715 | 2.011297 | -1.588380 |
| C | 3.247781 | 3.041241 | -1.111874 |
| C | 1.936772 | 2.473496 | -0.856477 |
| C | 5.409710 | 2.078821 | -2.124950 |
| C | 3.597100 | 4.430796 | -0.919451 |
| C | 4.809807 | 4.897081 | -0.635312 |

| | | | |
|---|---|---|---|
| C | -0.444411 | 2.702064 | -0.281818 |
| C | -1.600968 | 3.518919 | 0.008316 |
| C | -2.676041 | 2.678635 | -0.001975 |
| C | -2.157312 | 1.356587 | -0.284760 |
| C | -1.571347 | 4.989435 | 0.239346 |
| C | -4.122485 | 3.018313 | 0.143378 |
| C | -4.726621 | 3.300036 | -1.247908 |
| C | -6.205192 | 3.541218 | -1.161672 |
| O | -6.516728 | 4.565530 | -0.374221 |
| O | -7.053574 | 2.899143 | -1.738119 |
| N | -1.170122 | -1.407523 | -0.761304 |
| N | 1.591957 | -1.678627 | -1.429925 |
| N | 1.941132 | 1.144184 | -1.126357 |
| N | -0.812922 | 1.406687 | -0.450281 |
| H | -3.846819 | -4.935251 | -0.743536 |
| H | -2.624162 | -5.066463 | -2.009442 |
| H | 3.402086 | -5.656183 | -1.880525 |
| H | 1.948010 | -5.624428 | -2.884189 |
| H | 1.801653 | -5.708857 | -1.128086 |
| H | 5.609097 | 3.080947 | -2.500245 |
| H | 5.536633 | 1.372296 | -2.942889 |
| H | 6.154208 | 1.850430 | -1.360376 |
| H | -0.875247 | 5.238829 | 1.039597 |

| | | | |
|---|---|---|---|
| H | -2.557512 | 5.355196 | 0.513260 |
| H | -1.249254 | 5.511676 | -0.661863 |
| H | 6.141171 | -4.344328 | -3.644707 |
| H | 4.391916 | -4.851551 | -3.813381 |
| H | 4.988509 | 5.952131 | -0.515667 |
| H | 5.662232 | 4.255808 | -0.494255 |
| H | -6.324551 | -2.255364 | -2.062476 |
| H | -4.808977 | -1.523536 | -2.562833 |
| H | -5.114391 | -1.680507 | 0.382315 |
| H | -5.143486 | -3.274065 | -0.367684 |
| H | -4.538449 | 2.457775 | -1.914360 |
| H | -4.255637 | 4.192276 | -1.665281 |
| H | -4.246256 | 3.901350 | 0.771604 |
| H | -4.670006 | 2.194619 | 0.604206 |
| H | -3.997086 | 0.333044 | -0.199095 |
| H | -0.140124 | -4.569734 | -1.297593 |
| H | 4.651067 | -0.527407 | -2.246769 |
| H | 0.980410 | 4.253342 | -0.233234 |
| H | 5.522838 | -2.537828 | -2.170969 |
| H | 2.778657 | 5.134206 | -1.009983 |
| Fe | 0.384495 | -0.139579 | -0.953279 |
| H | -2.088573 | -5.062822 | 2.118938 |
| H | 8.179309 | -1.123990 | 0.329432 |

| | | | |
|---|---|---|---|
| H | 5.740874 | 2.565627 | 1.344933 |
| H | -6.825218 | 1.258399 | -2.332921 |
| H | -0.692846 | 1.926368 | -3.271144 |
| H | -7.479196 | 4.679212 | -0.320290 |
| H | -1.321206 | -5.391252 | 3.672687 |
| C | 0.870385 | -0.402020 | 0.900835 |
| C | 0.085747 | -0.751736 | 1.977421 |
| C | 2.267599 | -0.219866 | 1.450727 |
| H | -0.776478 | -0.123256 | 4.701773 |
| H | -0.900427 | 1.495387 | 3.071817 |
| H | -2.180414 | 1.513394 | 1.996184 |
| O | 0.772515 | -0.777608 | 3.199008 |
| O | -1.151160 | -1.030365 | 2.039972 |
| C | 2.138924 | -0.515240 | 2.955287 |
| H | 2.715218 | -1.397494 | 3.256440 |
| H | 2.441106 | 0.330018 | 3.583605 |
| H | 2.966488 | -0.902694 | 0.961574 |
| H | 2.620148 | 0.798980 | 1.276181 |
| H | -2.182456 | -5.353055 | -0.327307 |

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**Conf9$^{L10}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-197.6170155

Zero-point correction= 1.019148 (Hartree/Particle)

Thermal correction to Energy= 1.091929

Thermal correction to Enthalpy= 1.092873

Thermal correction to Gibbs Free Energy= 0.903876

Sum of electronic and zero-point Energies= -196.597867

Sum of electronic and thermal Energies= -196.525087

Sum of electronic and thermal Enthalpies= -196.524142

Sum of electronic and thermal Free Energies= -196.713140

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 4.785645 | 2.435382 | 3.132035 |
| H | 5.394770 | 3.335813 | 3.191581 |
| C | 3.823882 | 2.391758 | 4.325161 |
| H | 4.343576 | 1.953291 | 5.190459 |
| H | 3.513107 | 3.406637 | 4.593076 |
| O | 2.626421 | 1.700916 | 4.064383 |
| H | 2.831605 | 0.851243 | 3.641714 |
| C | 5.774993 | 1.234443 | 3.188048 |

| | | | |
|---|---|---|---|
| O | 6.719992 | 1.276464 | 3.961649 |
| N | 5.549180 | 0.187062 | 2.371893 |
| H | 4.711972 | 0.119348 | 1.785826 |
| C | 6.376720 | -1.023260 | 2.320316 |
| H | 5.775302 | -1.886553 | 2.602187 |
| H | 6.748931 | -1.160720 | 1.305748 |
| C | -3.580273 | -4.843218 | 3.075742 |
| H | -4.017145 | -5.460500 | 3.857146 |
| C | -3.640654 | -3.368916 | 3.456281 |
| H | -3.074659 | -3.220137 | 4.379971 |
| H | -3.168874 | -2.782635 | 2.664738 |
| C | -5.083588 | -2.909912 | 3.661950 |
| H | -5.642002 | -3.050765 | 2.735014 |
| H | -5.550870 | -3.530434 | 4.428131 |
| C | -5.206217 | -1.446008 | 4.097752 |
| H | -6.252249 | -1.224403 | 4.322169 |
| H | -4.627888 | -1.268558 | 5.007235 |
| N | -4.785544 | -0.522819 | 3.065035 |
| H | -5.438854 | -0.352735 | 2.302508 |
| C | -3.586129 | 0.028890 | 2.913362 |
| N | -3.423768 | 0.882486 | 1.909408 |
| N | -2.592291 | -0.168985 | 3.783455 |
| H | -2.655864 | -0.888974 | 4.480916 |

| | | | |
|---|---|---|---|
| C | 0.153435 | -0.840268 | -4.088720 |
| H | 1.053758 | -1.450601 | -4.271095 |
| H | -0.119801 | -0.340149 | -5.031894 |
| O | 0.364259 | 0.089212 | -3.109629 |
| C | -2.614983 | 0.281903 | -0.873990 |
| C | 0.286654 | -3.522730 | -1.344783 |
| C | 4.006323 | -0.556558 | -2.034969 |
| C | 1.245608 | 3.150420 | -0.726278 |
| C | -2.157099 | -1.027752 | -0.884225 |
| C | -2.975671 | -2.203228 | -0.674632 |
| C | -2.142365 | -3.278196 | -0.808889 |
| C | -0.830743 | -2.746479 | -1.085691 |
| C | -2.444110 | -4.734423 | -0.707897 |
| C | -4.411279 | -2.240558 | -0.246609 |
| C | -5.401130 | -1.567914 | -1.208269 |
| C | -5.832052 | -0.190517 | -0.765097 |
| O | -6.279766 | 0.527402 | -1.760247 |
| O | -5.786294 | 0.206515 | 0.391169 |
| C | 1.547069 | -3.037463 | -1.645185 |
| C | 2.659993 | -3.875780 | -2.022977 |
| C | 3.709561 | -3.032570 | -2.268981 |
| C | 3.219030 | -1.691335 | -1.999171 |
| C | 2.637456 | -5.364005 | -2.065211 |

| | | | |
|---|---|---|---|
| C | 5.061822 | -3.352538 | -2.671201 |
| C | 5.405659 | -4.340480 | -3.490797 |
| C | 3.589839 | 0.704817 | -1.646371 |
| C | 4.488417 | 1.818678 | -1.443720 |
| C | 3.716206 | 2.860853 | -1.009628 |
| C | 2.348442 | 2.366778 | -0.997511 |
| C | 5.955103 | 1.790905 | -1.685463 |
| C | 4.115856 | 4.201349 | -0.637884 |
| C | 5.252879 | 4.519157 | -0.027791 |
| C | -0.069848 | 2.712750 | -0.760807 |
| C | -1.215184 | 3.578905 | -0.640768 |
| C | -2.315730 | 2.772310 | -0.718294 |
| C | -1.820915 | 1.421382 | -0.876566 |
| C | -1.145595 | 5.058450 | -0.484240 |
| C | -3.745085 | 3.201091 | -0.667312 |
| C | -4.320794 | 3.413781 | -2.086957 |
| C | -5.743990 | 3.856258 | -1.955239 |
| O | -5.928764 | 5.131744 | -2.263569 |
| O | -6.655152 | 3.158910 | -1.551733 |
| N | -0.867107 | -1.391055 | -1.096423 |
| N | 1.912664 | -1.728177 | -1.652792 |
| N | 2.317066 | 1.058176 | -1.351164 |
| N | -0.465881 | 1.425714 | -0.902022 |

| | | | |
|---|---|---|---|
| H | -3.506007 | -4.913051 | -0.555484 |
| H | -2.144853 | -5.243849 | -1.623172 |
| H | 3.652305 | -5.752313 | -2.014078 |
| H | 2.177392 | -5.720680 | -2.988302 |
| H | 2.068426 | -5.764211 | -1.227331 |
| H | 6.334289 | 2.803286 | -1.809179 |
| H | 6.189198 | 1.216268 | -2.580163 |
| H | 6.468169 | 1.329892 | -0.840631 |
| H | -0.552936 | 5.323440 | 0.391074 |
| H | -2.137365 | 5.490799 | -0.374463 |
| H | -0.672533 | 5.507087 | -1.357271 |
| H | 6.435861 | -4.531681 | -3.741031 |
| H | 4.675009 | -4.973385 | -3.964042 |
| H | 5.493737 | 5.540752 | 0.215297 |
| H | 5.965333 | 3.774025 | 0.279011 |
| H | -6.318369 | -2.158793 | -1.282056 |
| H | -4.986840 | -1.488738 | -2.213512 |
| H | -4.508541 | -1.757820 | 0.730601 |
| H | -4.697405 | -3.285331 | -0.120286 |
| H | -4.270991 | 2.470705 | -2.632808 |
| H | -3.745366 | 4.172544 | -2.613860 |
| H | -3.823055 | 4.139187 | -0.113010 |
| H | -4.366874 | 2.464995 | -0.155010 |

| | | | |
|---|---|---|---|
| H | -3.681229 | 0.428506 | -0.859672 |
| H | 0.153686 | -4.594169 | -1.347412 |
| H | 5.044904 | -0.677584 | -2.301556 |
| H | 1.411649 | 4.195326 | -0.511495 |
| H | 5.834438 | -2.714441 | -2.260523 |
| H | 3.408349 | 4.986961 | -0.876801 |
| Fe | 0.734389 | -0.153333 | -1.282543 |
| H | -4.124516 | -5.020464 | 2.152095 |
| H | 7.206780 | -0.899246 | 3.013518 |
| H | 4.220878 | 2.435337 | 2.198398 |
| H | -6.526899 | 1.467687 | -1.529031 |
| H | -0.659294 | -1.537069 | -3.821402 |
| H | -6.853763 | 5.399416 | -2.135405 |
| H | -2.549157 | -5.152057 | 2.929252 |
| C | 1.015970 | -0.343136 | 0.614166 |
| C | 2.243902 | -0.529563 | 1.253618 |
| C | -0.028247 | -0.307458 | 1.702509 |
| H | -1.677735 | 0.201826 | 3.578893 |
| H | -2.507089 | 1.166621 | 1.591366 |
| H | -4.173514 | 0.936530 | 1.228457 |
| O | 2.096837 | -0.714666 | 2.651866 |
| O | 3.393865 | -0.532876 | 0.814777 |
| C | 0.730134 | -0.755187 | 2.967587 |

| | | | |
|---|---|---|---|
| H | 0.570164 | -0.098462 | 3.831641 |
| H | 0.464089 | -1.785503 | 3.247509 |
| H | -0.391240 | 0.725230 | 1.804168 |
| H | -0.876964 | -0.957238 | 1.478471 |
| H | -1.895993 | -5.183455 | 0.120454 |

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**$C^{L9}$**

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Number of imaginary frequencies : 3 Electronic energy : HF=-2940.1400115

Zero-point correction= 1.011919 (Hartree/Particle)

Thermal correction to Energy= 1.078595

Thermal correction to Enthalpy= 1.079539

Thermal correction to Gibbs Free Energy= 0.899622

Sum of electronic and zero-point Energies= -2939.128093

Sum of electronic and thermal Energies= -2939.061417

Sum of electronic and thermal Enthalpies= -2939.060473

Sum of electronic and thermal Free Energies= -2939.240390

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.524470 | -3.153217 | 2.052682 |
| H | -3.991199 | -2.617725 | 1.260492 |
| C | -3.560024 | -4.151964 | 2.735056 |
| H | -4.136201 | -4.753371 | 3.447739 |
| H | -3.169583 | -4.845780 | 1.966352 |
| O | -2.533969 | -3.518801 | 3.450309 |
| H | -2.062708 | -2.912824 | 2.836897 |
| C | -5.765466 | -3.831346 | 1.558894 |
| O | -6.626485 | -4.289550 | 2.309954 |
| N | -5.839893 | -3.927841 | 0.200772 |
| H | -5.067955 | -3.607485 | -0.365727 |
| C | -6.909648 | -4.649426 | -0.417557 |
| H | -7.561516 | -5.009414 | 0.379880 |
| H | -7.496789 | -4.015635 | -1.095490 |
| C | -1.971229 | 5.181597 | 1.743807 |
| H | -1.879029 | 6.255982 | 1.548170 |
| C | -3.427043 | 4.708079 | 1.669624 |
| H | -3.825759 | 4.905619 | 0.665026 |
| H | -3.445845 | 3.616785 | 1.787686 |
| C | -4.371217 | 5.327718 | 2.719008 |
| H | -3.933658 | 5.141599 | 3.712299 |
| C | -4.521168 | 6.847617 | 2.549799 |

| | | | |
|---|---|---|---|
| H | -5.198398 | 7.263670 | 3.304808 |
| H | -3.563154 | 7.368511 | 2.643205 |
| H | -4.936462 | 7.088555 | 1.562877 |
| C | -5.746334 | 4.644512 | 2.677408 |
| H | -6.419170 | 5.049702 | 3.442146 |
| H | -6.225260 | 4.792506 | 1.701405 |
| H | -5.660329 | 3.565263 | 2.842912 |
| C | 2.311146 | -0.052221 | -2.966699 |
| H | 2.711345 | -0.995118 | -2.548349 |
| H | 2.995029 | 0.754853 | -2.641574 |
| O | 0.987320 | 0.184280 | -2.622024 |
| C | 3.310926 | -0.643188 | 0.656246 |
| C | 1.320646 | 3.476579 | -0.909884 |
| C | -2.726921 | 1.096597 | -2.048678 |
| C | -0.412130 | -3.068923 | -1.242347 |
| C | 3.117658 | 0.703131 | 0.355187 |
| C | 4.105585 | 1.751017 | 0.577677 |
| C | 3.547811 | 2.912658 | 0.112331 |
| C | 2.224028 | 2.563515 | -0.379217 |
| C | 4.145872 | 4.287194 | 0.072665 |
| C | 5.509997 | 1.530191 | 1.068080 |
| C | 6.445190 | 1.131957 | -0.107684 |
| C | 7.903890 | 0.906153 | 0.257171 |

| | | | |
|---|---|---|---|
| O | 8.172696 | -0.178591 | 1.044360 |
| O | 8.815988 | 1.595941 | -0.132507 |
| C | 0.023023 | 3.196192 | -1.337857 |
| C | -0.902142 | 4.197058 | -1.831431 |
| C | -2.093977 | 3.546600 | -2.064890 |
| C | -1.843350 | 2.134067 | -1.771809 |
| C | -0.589607 | 5.654450 | -1.992716 |
| C | -3.331500 | 4.171344 | -2.520610 |
| C | -4.592990 | 3.815742 | -2.225548 |
| C | -2.450072 | -0.263907 | -1.939721 |
| C | -3.368560 | -1.310478 | -2.344164 |
| C | -2.702959 | -2.503276 | -2.146099 |
| C | -1.391492 | -2.147990 | -1.603983 |
| C | -3.160417 | -3.869205 | -2.351832 |
| C | -4.167425 | -4.300504 | -3.135612 |
| C | 0.801739 | -2.773017 | -0.637832 |
| C | 1.718232 | -3.779161 | -0.123082 |
| C | 2.748129 | -3.099555 | 0.471053 |
| C | 2.463022 | -1.681528 | 0.280168 |
| C | 1.498543 | -5.259033 | -0.218396 |
| C | 3.924066 | -3.689264 | 1.204572 |
| C | 5.233240 | -3.816257 | 0.384142 |
| C | 6.247249 | -2.728304 | 0.642767 |

| | | | |
|---|---|---|---|
| O | 6.218163 | -1.956227 | 1.595011 |
| O | 7.230773 | -2.701552 | -0.268492 |
| N | 1.998139 | 1.222224 | -0.227438 |
| N | -0.569541 | 1.965158 | -1.316339 |
| N | -1.275491 | -0.799642 | -1.488351 |
| N | 1.280829 | -1.520194 | -0.384247 |
| H | 5.124789 | 4.312924 | 0.559930 |
| H | 3.506850 | 5.020732 | 0.579273 |
| H | 4.283183 | 4.641112 | -0.956927 |
| H | -0.455440 | 6.153013 | -1.024010 |
| H | -1.392015 | 6.181270 | -2.516326 |
| H | 0.334546 | 5.804527 | -2.562856 |
| H | 2.302170 | -5.819364 | 0.268064 |
| H | 1.451781 | -5.595271 | -1.261838 |
| H | 0.556178 | -5.554085 | 0.257928 |
| H | -5.435651 | 4.368294 | -2.630666 |
| H | -4.823311 | 2.987415 | -1.563900 |
| H | -4.414386 | -5.356824 | -3.183944 |
| H | -4.745785 | -3.637524 | -3.768957 |
| H | 6.430179 | 1.919156 | -0.863464 |
| H | 6.048996 | 0.221674 | -0.573528 |
| H | 5.528102 | 0.754175 | 1.841416 |
| H | 5.898526 | 2.442732 | 1.534139 |

| | | | |
|---|---|---|---|
| H | 5.038017 | -3.852901 | -0.691969 |
| H | 5.751962 | -4.754511 | 0.625618 |
| H | 3.646598 | -4.690232 | 1.547835 |
| H | 4.141423 | -3.110131 | 2.107576 |
| H | 4.216728 | -0.910494 | 1.183747 |
| H | 1.647322 | 4.508979 | -0.977273 |
| H | -3.683670 | 1.373136 | -2.470873 |
| H | -0.633860 | -4.118593 | -1.395284 |
| H | -3.197709 | 5.052471 | -3.149942 |
| H | -2.615732 | -4.629324 | -1.792863 |
| Fe | 0.357838 | 0.207568 | -0.844898 |
| H | -6.542334 | -5.507701 | -0.995350 |
| H | -1.541197 | 4.989115 | 2.734366 |
| H | 7.858616 | -1.992829 | -0.018864 |
| H | 7.357623 | -0.610444 | 1.392797 |
| H | 2.405707 | -0.124543 | -4.065106 |
| H | -4.815277 | -2.420615 | 2.812767 |
| H | -1.357351 | 4.658799 | 1.005729 |
| C | -0.385838 | 0.311910 | 1.003821 |
| C | -0.217602 | 1.497845 | 1.917978 |
| C | -1.185268 | 1.219260 | 3.082603 |
| H | -2.132433 | 1.764091 | 2.963087 |
| O | -1.457496 | -0.185634 | 3.031949 |

| | | | |
|---|---|---|---|
| C | -1.070010 | -0.687899 | 1.792463 |
| O | -1.333884 | -1.871002 | 1.550400 |
| H | -0.778117 | 1.453179 | 4.072018 |
| H | -0.417220 | 2.453266 | 1.423945 |
| H | 0.823403 | 1.548756 | 2.274845 |
| C | -4.765168 | -1.095130 | -2.841291 |
| H | -4.819919 | -1.101233 | -3.938590 |
| H | -5.435912 | -1.884222 | -2.484032 |
| H | -5.171440 | -0.138441 | -2.501971 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(R)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 4 Electronic energy : HF=-3384.950482

Zero-point correction= 1.238635 (Hartree/Particle)

Thermal correction to Energy= 1.317707

Thermal correction to Enthalpy= 1.318651

Thermal correction to Gibbs Free Energy= 1.113553

Sum of electronic and zero-point Energies= -3383.711847

Sum of electronic and thermal Energies= -3383.632775

Sum of electronic and thermal Enthalpies= -3383.631831

Sum of electronic and thermal Free Energies= -3383.836929

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -5.601030 | -0.967829 | 2.473657 |
| H | -5.094153 | -0.788902 | 1.517983 |
| C | -4.825320 | -2.037223 | 3.268906 |
| H | -5.306023 | -2.176301 | 4.241729 |
| H | -4.880296 | -3.000563 | 2.735221 |
| O | -3.483459 | -1.668896 | 3.531253 |
| H | -3.015166 | -1.602777 | 2.687672 |
| C | -7.029935 | -1.390874 | 2.260512 |
| O | -7.898394 | -1.305005 | 3.126162 |
| N | -7.270305 | -1.936377 | 1.039354 |
| H | -6.516133 | -2.098606 | 0.386537 |
| C | -8.551241 | -2.527302 | 0.772504 |
| H | -8.797780 | -3.305023 | 1.505649 |
| H | -9.347824 | -1.776723 | 0.816799 |
| C | -0.985124 | 5.545855 | -1.040554 |
| H | -0.370340 | 6.264073 | -1.597818 |
| C | -1.242334 | 6.011484 | 0.397744 |
| H | -1.720136 | 7.004908 | 0.400084 |
| H | -1.955036 | 5.314616 | 0.853103 |

| | | | |
|---|---|---|---|
| C | 0.016932 | 6.045673 | 1.286161 |
| H | 0.474054 | 5.050471 | 1.221335 |
| C | 1.048667 | 7.080052 | 0.811786 |
| H | 1.940054 | 7.065249 | 1.449701 |
| H | 1.377505 | 6.885652 | -0.213910 |
| H | 0.632319 | 8.096964 | 0.842546 |
| C | -0.358929 | 6.300770 | 2.753041 |
| H | 0.524012 | 6.262173 | 3.401690 |
| H | -0.825118 | 7.287938 | 2.880239 |
| H | -1.071160 | 5.549087 | 3.112272 |
| C | 1.221981 | -2.054095 | -3.340332 |
| H | 1.518963 | -2.833300 | -2.612716 |
| H | 2.095489 | -1.388535 | -3.470686 |
| O | 0.064433 | -1.377243 | -2.980308 |
| C | 2.611865 | -1.874469 | 0.102595 |
| C | 1.701748 | 2.005878 | -2.627128 |
| C | -2.971221 | 0.827501 | -2.844933 |
| C | -2.013364 | -3.211517 | -0.360422 |
| C | 2.774104 | -0.698608 | -0.624620 |
| C | 4.062764 | -0.062427 | -0.881128 |
| C | 3.799348 | 1.039953 | -1.647872 |
| C | 2.358272 | 1.059072 | -1.854951 |
| C | 4.759899 | 2.046528 | -2.205753 |

| | | | |
|---|---|---|---|
| C | 5.402701 | -0.627943 | -0.496713 |
| C | 5.880841 | -1.665542 | -1.550316 |
| C | 7.238191 | -2.300456 | -1.292349 |
| O | 7.332013 | -3.111821 | -0.194724 |
| O | 8.199832 | -2.163947 | -2.010081 |
| C | 0.335625 | 2.052373 | -2.887715 |
| C | -0.291706 | 3.061528 | -3.719821 |
| C | -1.637601 | 2.783490 | -3.721801 |
| C | -1.794997 | 1.559639 | -2.932379 |
| C | 0.424061 | 4.204123 | -4.372471 |
| C | -2.674928 | 3.568518 | -4.382585 |
| C | -3.940788 | 3.760535 | -3.977793 |
| C | -3.123773 | -0.408718 | -2.217405 |
| C | -4.352506 | -1.172781 | -2.219831 |
| C | -4.083820 | -2.336620 | -1.522020 |
| C | -2.686585 | -2.239866 | -1.101592 |
| C | -4.952490 | -3.462326 | -1.219618 |
| C | -6.114102 | -3.807918 | -1.811554 |
| C | -0.674685 | -3.181695 | 0.015827 |
| C | -0.025196 | -4.237446 | 0.777859 |
| C | 1.285303 | -3.861342 | 0.924479 |
| C | 1.418924 | -2.580240 | 0.240194 |
| C | -0.710574 | -5.474170 | 1.277982 |

| | | | |
|---|---|---|---|
| C | 2.369113 | -4.602070 | 1.663527 |
| C | 3.343447 | -5.422158 | 0.779355 |
| C | 4.685818 | -4.767721 | 0.552954 |
| O | 5.104688 | -3.798402 | 1.175686 |
| O | 5.409370 | -5.374969 | -0.398010 |
| N | 1.767420 | 0.000849 | -1.223628 |
| N | -0.592750 | 1.169493 | -2.416565 |
| N | -2.141553 | -1.068850 | -1.530043 |
| N | 0.219292 | -2.191465 | -0.283973 |
| H | 5.787272 | 1.835465 | -1.895619 |
| H | 4.513453 | 3.060244 | -1.868614 |
| H | 4.744882 | 2.058356 | -3.302659 |
| H | 0.785196 | 4.923583 | -3.627550 |
| H | -0.231172 | 4.748795 | -5.057576 |
| H | 1.293918 | 3.860818 | -4.944459 |
| H | -0.037222 | -6.095964 | 1.874755 |
| H | -1.079859 | -6.094433 | 0.451529 |
| H | -1.575228 | -5.230860 | 1.907109 |
| H | -4.622226 | 4.377975 | -4.555572 |
| H | -4.323831 | 3.340745 | -3.053611 |
| H | -6.661229 | -4.684468 | -1.477751 |
| H | -6.526247 | -3.271345 | -2.658177 |
| H | 5.942503 | -1.185026 | -2.528269 |

| | | | |
|---|---|---|---|
| H | 5.128424 | -2.460357 | -1.623311 |
| H | 5.352880 | -1.091070 | 0.494999 |
| H | 6.146486 | 0.173170 | -0.426436 |
| H | 2.909936 | -5.653939 | -0.198514 |
| H | 3.567421 | -6.392630 | 1.242797 |
| H | 1.895282 | -5.290360 | 2.369564 |
| H | 2.961103 | -3.908025 | 2.268547 |
| H | 3.490264 | -2.291228 | 0.576509 |
| H | 2.310752 | 2.786776 | -3.068751 |
| H | -3.825869 | 1.222007 | -3.378110 |
| H | -2.571335 | -4.096828 | -0.077184 |
| H | -2.357420 | 4.081869 | -5.291160 |
| H | -4.609185 | -4.110426 | -0.413363 |
| Fe | -0.184989 | -0.501524 | -1.329519 |
| H | -8.537241 | -2.970086 | -0.225808 |
| H | -0.471348 | 4.582000 | -1.031248 |
| H | 6.265177 | -4.904513 | -0.476801 |
| H | 6.532309 | -3.072718 | 0.379027 |
| H | 1.065077 | -2.565429 | -4.306912 |
| H | -5.588943 | -0.034292 | 3.042991 |
| H | -1.924324 | 5.426897 | -1.591610 |
| C | -0.640392 | 0.536916 | 0.490180 |
| C | -0.490565 | 2.004377 | 0.444172 |

| | | | |
|---|---|---|---|
| C | -2.010268 | 0.347414 | 1.152767 |
| C | 1.020479 | 0.124185 | 2.645677 |
| H | 0.281789 | 0.263577 | 1.491707 |
| N | 1.148763 | 1.343996 | 3.387230 |
| C | 2.232763 | 2.213001 | 3.208222 |
| C | 3.161835 | 2.042914 | 2.157341 |
| C | 2.449824 | 3.297948 | 4.089784 |
| C | 4.257480 | 2.889850 | 2.027018 |
| H | 3.001378 | 1.286823 | 1.402443 |
| C | 3.548019 | 4.143027 | 3.939548 |
| H | 1.769689 | 3.482028 | 4.911771 |
| C | 4.473358 | 3.946032 | 2.915034 |
| H | 4.939692 | 2.728645 | 1.195931 |
| H | 3.679146 | 4.960508 | 4.644922 |
| H | 5.329560 | 4.604738 | 2.802132 |
| C | 0.010062 | 1.792665 | 4.192535 |
| H | -0.896407 | 1.354272 | 3.768621 |
| C | 0.407943 | -1.047986 | 3.398441 |
| H | -0.597035 | -0.847062 | 3.781580 |
| H | 0.332686 | -1.904731 | 2.724123 |
| H | 1.031449 | -1.346178 | 4.254405 |
| H | -0.098350 | 2.874716 | 4.067585 |
| C | 0.091517 | 1.438315 | 5.685731 |

| | | | |
|---|---|---|---|
| H | 0.996028 | 1.843304 | 6.148431 |
| H | -0.776377 | 1.848382 | 6.215813 |
| H | 0.097974 | 0.355572 | 5.835486 |
| H | 1.982148 | -0.161177 | 2.226379 |
| C | -5.644236 | -0.743823 | -2.845919 |
| H | -5.795691 | -1.201384 | -3.833060 |
| H | -6.499880 | -1.032829 | -2.225134 |
| H | -5.687589 | 0.339805 | -2.982215 |
| H | -3.402972 | 2.000029 | 1.672303 |
| H | -3.311122 | 1.622548 | -0.066745 |
| C | -2.737120 | 1.672256 | 0.866250 |
| O | 0.497885 | 2.692441 | 0.250297 |
| O | -1.698248 | 2.648414 | 0.724218 |
| H | -1.917351 | 0.220706 | 2.241124 |
| H | -2.571306 | -0.506081 | 0.767877 |

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$$\left[ {}^{3}\mathbf{D}^{\mathbf{A}}_{(R)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 2 Electronic energy : HF=-3384.9915357

Zero-point correction= 1.241936 (Hartree/Particle)

Thermal correction to Energy= 1.323360

Thermal correction to Enthalpy= 1.324304

Thermal correction to Gibbs Free Energy= 1.108466

Sum of electronic and zero-point Energies= -3383.749600

Sum of electronic and thermal Energies= -3383.668176

Sum of electronic and thermal Enthalpies= -3383.667232

Sum of electronic and thermal Free Energies= -3383.883069

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.947809 | -2.944501 | 1.448762 |
| H | -4.444443 | -2.454285 | 0.606893 |
| C | -3.996207 | -3.934351 | 2.136647 |
| H | -4.547833 | -4.462252 | 2.918219 |
| H | -3.652590 | -4.687842 | 1.409020 |
| O | -2.903750 | -3.291000 | 2.773805 |
| H | -2.395035 | -2.810560 | 2.105930 |
| C | -6.231256 | -3.602794 | 1.023635 |
| O | -6.914400 | -4.293215 | 1.778731 |
| N | -6.585280 | -3.364228 | -0.262164 |
| H | -5.972434 | -2.866764 | -0.892274 |
| C | -7.797351 | -3.935723 | -0.770793 |
| H | -7.811933 | -5.023119 | -0.634695 |

| | | | |
|---|---|---|---|
| H | -8.676573 | -3.533120 | -0.254429 |
| C | -2.003726 | 5.245842 | 2.029516 |
| H | -1.555061 | 6.242618 | 2.126763 |
| C | -2.438327 | 4.679764 | 3.386471 |
| H | -3.161149 | 5.356374 | 3.870790 |
| H | -2.960792 | 3.733913 | 3.204598 |
| C | -1.275929 | 4.396426 | 4.358101 |
| H | -0.563753 | 3.760865 | 3.816247 |
| C | -0.547916 | 5.677162 | 4.794016 |
| H | 0.279980 | 5.448292 | 5.475816 |
| H | -0.129614 | 6.219700 | 3.940374 |
| H | -1.230956 | 6.358295 | 5.320576 |
| C | -1.772580 | 3.617113 | 5.584367 |
| H | -0.949432 | 3.376832 | 6.267664 |
| H | -2.514646 | 4.197847 | 6.149738 |
| H | -2.242569 | 2.674321 | 5.284925 |
| C | 1.113667 | 0.748654 | -4.133011 |
| H | 1.599583 | -0.223582 | -3.926723 |
| H | 1.857479 | 1.533899 | -3.902798 |
| O | -0.087854 | 0.918339 | -3.455991 |
| C | 2.812141 | -0.721450 | -1.032043 |
| C | 1.103704 | 3.788282 | -1.308511 |
| C | -3.363372 | 2.091421 | -1.986833 |

| | | | |
|---|---|---|---|
| C | -1.550506 | -2.382589 | -2.300731 |
| C | 2.738883 | 0.668965 | -1.036654 |
| C | 3.883916 | 1.555929 | -0.859972 |
| C | 3.399423 | 2.831545 | -0.952320 |
| C | 1.965855 | 2.709463 | -1.176710 |
| C | 4.145231 | 4.127792 | -0.852699 |
| C | 5.317089 | 1.113213 | -0.753336 |
| C | 5.924177 | 0.881010 | -2.165052 |
| C | 7.381675 | 0.449498 | -2.200636 |
| O | 7.662789 | -0.787785 | -1.689287 |
| O | 8.273508 | 1.106456 | -2.682183 |
| C | -0.278013 | 3.720774 | -1.467567 |
| C | -1.135146 | 4.885309 | -1.578402 |
| C | -2.422143 | 4.413815 | -1.683761 |
| C | -2.314014 | 2.953468 | -1.697165 |
| C | -0.668893 | 6.307270 | -1.509379 |
| C | -3.630202 | 5.228095 | -1.762754 |
| C | -4.846731 | 4.940067 | -1.272186 |
| C | -3.267003 | 0.711260 | -2.161770 |
| C | -4.368145 | -0.131231 | -2.574909 |
| C | -3.853627 | -1.410110 | -2.687486 |
| C | -2.441664 | -1.309388 | -2.320186 |
| C | -4.512934 | -2.647837 | -3.070195 |

| | | | |
|---|---|---|---|
| C | -5.683091 | -2.808122 | -3.721703 |
| C | -0.201978 | -2.325769 | -1.966040 |
| C | 0.660345 | -3.493119 | -1.866524 |
| C | 1.889685 | -3.036107 | -1.463164 |
| C | 1.767066 | -1.587444 | -1.350553 |
| C | 0.229949 | -4.900226 | -2.159063 |
| C | 3.118584 | -3.858845 | -1.174587 |
| C | 4.178633 | -3.900562 | -2.304859 |
| C | 5.375361 | -3.007678 | -2.077304 |
| O | 5.647000 | -2.458839 | -1.015623 |
| O | 6.150919 | -2.887424 | -3.164458 |
| N | 1.600430 | 1.394502 | -1.235133 |
| N | -1.014049 | 2.572456 | -1.532257 |
| N | -2.124407 | -0.024951 | -1.998940 |
| N | 0.495022 | -1.191968 | -1.652887 |
| H | 5.205455 | 3.965095 | -0.639436 |
| H | 3.740574 | 4.759658 | -0.053225 |
| H | 4.082547 | 4.706009 | -1.783138 |
| H | -0.337211 | 6.568289 | -0.496675 |
| H | -1.467560 | 7.004343 | -1.777336 |
| H | 0.173756 | 6.489002 | -2.186304 |
| H | 1.027136 | -5.618739 | -1.948070 |
| H | -0.051341 | -5.025558 | -3.212388 |

| | | | |
|---|---|---|---|
| H | -0.640776 | -5.192148 | -1.559768 |
| H | -5.672759 | 5.635453 | -1.388707 |
| H | -5.047219 | 4.028751 | -0.718682 |
| H | -6.055704 | -3.803524 | -3.944177 |
| H | -6.271604 | -1.975796 | -4.089632 |
| H | 5.858436 | 1.804571 | -2.742870 |
| H | 5.320446 | 0.126436 | -2.684052 |
| H | 5.391269 | 0.198833 | -0.154349 |
| H | 5.910695 | 1.872926 | -0.233258 |
| H | 3.747093 | -3.646907 | -3.278234 |
| H | 4.589000 | -4.913389 | -2.417020 |
| H | 2.803778 | -4.886698 | -0.971672 |
| H | 3.605676 | -3.507220 | -0.259536 |
| H | 3.768111 | -1.167976 | -0.794075 |
| H | 1.542959 | 4.778259 | -1.253929 |
| H | -4.325152 | 2.548924 | -2.176637 |
| H | -1.939264 | -3.358432 | -2.568727 |
| H | -3.503795 | 6.196274 | -2.249278 |
| H | -3.982528 | -3.560006 | -2.797603 |
| Fe | -0.253719 | 0.691589 | -1.595527 |
| H | -7.878139 | -3.708486 | -1.836145 |
| H | -1.270750 | 4.579695 | 1.567017 |
| H | 6.908379 | -2.309864 | -2.935438 |

| | | | |
|---|---|---|---|
| H | 6.893185 | -1.194722 | -1.228139 |
| H | 0.933476 | 0.790014 | -5.222197 |
| H | -5.193217 | -2.163170 | 2.178458 |
| H | -2.857860 | 5.338277 | 1.350710 |
| C | -0.418797 | 0.371608 | 0.544514 |
| C | -0.606743 | 1.603839 | 1.328578 |
| C | -1.550438 | -0.532578 | 1.043000 |
| C | 1.458880 | -3.098248 | 2.786952 |
| H | 0.579147 | -0.028770 | 0.712397 |
| N | 1.719371 | -2.803481 | 4.122779 |
| C | 2.105317 | -1.510697 | 4.518719 |
| C | 1.733113 | -0.390459 | 3.745335 |
| C | 2.863353 | -1.284049 | 5.687837 |
| C | 2.106187 | 0.896958 | 4.118925 |
| H | 1.116130 | -0.524814 | 2.865906 |
| C | 3.223898 | 0.011208 | 6.056777 |
| H | 3.191125 | -2.115013 | 6.302607 |
| C | 2.856868 | 1.110987 | 5.279092 |
| H | 1.779232 | 1.726664 | 3.497978 |
| H | 3.809418 | 0.154991 | 6.962057 |
| H | 3.144114 | 2.116112 | 5.573402 |
| C | 1.707612 | -3.895221 | 5.096128 |
| H | 0.844275 | -4.532955 | 4.880994 |

| | | | |
|---|---|---|---|
| C | 0.586083 | -4.233876 | 2.363509 |
| H | -0.438689 | -4.169326 | 2.764262 |
| H | 0.510404 | -4.222736 | 1.272129 |
| H | 0.970592 | -5.228311 | 2.645861 |
| H | 1.534231 | -3.468007 | 6.086976 |
| C | 2.984125 | -4.747748 | 5.086233 |
| H | 3.864920 | -4.150922 | 5.340950 |
| H | 2.903554 | -5.569744 | 5.806990 |
| H | 3.148953 | -5.176177 | 4.093004 |
| H | 1.822888 | -2.384987 | 2.061286 |
| C | -5.776340 | 0.326093 | -2.803236 |
| H | -5.986982 | 0.497773 | -3.867666 |
| H | -6.496350 | -0.421967 | -2.452562 |
| H | -5.988397 | 1.260482 | -2.277074 |
| H | -3.236732 | 0.183400 | 2.291825 |
| H | -3.284778 | 0.726853 | 0.593205 |
| C | -2.626639 | 0.489631 | 1.435647 |
| O | 0.173377 | 2.501658 | 1.611258 |
| O | -1.905532 | 1.676765 | 1.807948 |
| H | -1.233929 | -1.093783 | 1.938649 |
| H | -1.917628 | -1.246072 | 0.301007 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(S)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 3 Electronic energy : HF=-3384.9667917

Zero-point correction= 1.239658 (Hartree/Particle)

Thermal correction to Energy= 1.319322

Thermal correction to Enthalpy= 1.320266

Thermal correction to Gibbs Free Energy= 1.111739

Sum of electronic and zero-point Energies= -3383.727134

Sum of electronic and thermal Energies= -3383.647469

Sum of electronic and thermal Enthalpies= -3383.646525

Sum of electronic and thermal Free Energies= -3383.855053

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -5.433775 | -0.784936 | 2.374323 |
| H | -4.787120 | -1.127936 | 1.562007 |
| C | -4.857043 | -1.268850 | 3.716969 |
| H | -5.501501 | -0.919146 | 4.530315 |
| H | -4.883859 | -2.374303 | 3.739759 |
| O | -3.555103 | -0.776809 | 3.945950 |
| H | -3.052467 | -0.913345 | 3.113807 |

| | | | |
|---|---|---|---|
| C | -6.861407 | -1.196855 | 2.177465 |
| O | -7.750646 | -0.994928 | 3.004438 |
| N | -7.085404 | -1.816640 | 0.984061 |
| H | -6.309276 | -1.991819 | 0.363558 |
| C | -8.397763 | -2.247688 | 0.612268 |
| H | -9.041577 | -2.126399 | 1.485050 |
| H | -8.814554 | -1.653028 | -0.213002 |
| C | -0.411866 | 5.427025 | -1.129444 |
| H | -0.270192 | 6.221924 | -1.870529 |
| C | -0.838036 | 5.986424 | 0.232683 |
| H | -1.792409 | 6.524498 | 0.128770 |
| H | -1.034188 | 5.145524 | 0.909761 |
| C | 0.187502 | 6.919538 | 0.907284 |
| H | 1.138986 | 6.372545 | 0.976643 |
| C | 0.432010 | 8.203733 | 0.099887 |
| H | 1.164042 | 8.848920 | 0.599399 |
| H | 0.811060 | 7.992850 | -0.904996 |
| H | -0.496702 | 8.779339 | -0.008615 |
| C | -0.255420 | 7.258347 | 2.338218 |
| H | 0.470118 | 7.912235 | 2.835939 |
| H | -1.223512 | 7.776147 | 2.338156 |
| H | -0.356633 | 6.351780 | 2.943426 |
| C | 1.512222 | -2.317616 | -3.188015 |

| | | | |
|---|---|---|---|
| H | 1.634948 | -3.149413 | -2.469276 |
| H | 2.432782 | -1.707052 | -3.130639 |
| O | 0.352423 | -1.581467 | -2.985870 |
| C | 2.763054 | -1.774342 | 0.235116 |
| C | 1.696658 | 1.929329 | -2.684465 |
| C | -2.870132 | 0.391921 | -3.040528 |
| C | -1.711173 | -3.491425 | -0.411298 |
| C | 2.866237 | -0.597043 | -0.501104 |
| C | 4.102674 | 0.153245 | -0.686410 |
| C | 3.795691 | 1.202469 | -1.512497 |
| C | 2.379806 | 1.078268 | -1.823423 |
| C | 4.704529 | 2.268018 | -2.048910 |
| C | 5.459320 | -0.267695 | -0.190944 |
| C | 6.124132 | -1.256627 | -1.188538 |
| C | 7.517751 | -1.737998 | -0.815472 |
| O | 7.609630 | -2.540947 | 0.287010 |
| O | 8.514467 | -1.486404 | -1.449818 |
| C | 0.354095 | 1.834430 | -3.045364 |
| C | -0.301853 | 2.747141 | -3.960884 |
| C | -1.624327 | 2.368647 | -4.009319 |
| C | -1.732600 | 1.182166 | -3.157425 |
| C | 0.364760 | 3.892750 | -4.660810 |
| C | -2.677306 | 3.035516 | -4.770122 |

| | | | |
|---|---|---|---|
| C | -3.972734 | 3.166715 | -4.443039 |
| C | -2.967039 | -0.802264 | -2.330761 |
| C | -4.161110 | -1.623587 | -2.292312 |
| C | -3.838400 | -2.735906 | -1.542401 |
| C | -2.443018 | -2.559967 | -1.141148 |
| C | -4.672484 | -3.858353 | -1.137007 |
| C | -5.800797 | -4.306313 | -1.719138 |
| C | -0.387565 | -3.365349 | -0.010344 |
| C | 0.315703 | -4.363020 | 0.780893 |
| C | 1.579222 | -3.874680 | 0.989144 |
| C | 1.633347 | -2.585776 | 0.307429 |
| C | -0.287675 | -5.649052 | 1.260507 |
| C | 2.686128 | -4.514973 | 1.785239 |
| C | 3.784899 | -5.226006 | 0.953819 |
| C | 5.076039 | -4.453312 | 0.827213 |
| O | 5.359551 | -3.450907 | 1.473765 |
| O | 5.920753 | -4.990299 | -0.065112 |
| N | 1.844264 | -0.010589 | -1.191541 |
| N | -0.531049 | 0.905437 | -2.573673 |
| N | -1.956725 | -1.379737 | -1.611369 |
| N | 0.432102 | -2.305259 | -0.277688 |
| H | 5.709001 | 2.189628 | -1.623260 |
| H | 4.326785 | 3.271986 | -1.821022 |

| | | | |
|---|---|---|---|
| H | 4.805879 | 2.204507 | -3.139697 |
| H | 0.680142 | 4.671065 | -3.954657 |
| H | -0.305808 | 4.365695 | -5.383255 |
| H | 1.260559 | 3.565433 | -5.201595 |
| H | 0.414675 | -6.222102 | 1.872549 |
| H | -0.590199 | -6.290860 | 0.423690 |
| H | -1.182804 | -5.469227 | 1.867539 |
| H | -4.660768 | 3.694362 | -5.096968 |
| H | -4.380338 | 2.780711 | -3.514514 |
| H | -6.343000 | -5.147087 | -1.296851 |
| H | -6.197141 | -3.883672 | -2.635536 |
| H | 6.210989 | -0.779303 | -2.166161 |
| H | 5.467655 | -2.127278 | -1.306024 |
| H | 5.379310 | -0.728019 | 0.799904 |
| H | 6.109238 | 0.606656 | -0.074559 |
| H | 3.437774 | -5.469596 | -0.055381 |
| H | 4.062697 | -6.185465 | 1.410804 |
| H | 2.242213 | -5.253978 | 2.458455 |
| H | 3.171422 | -3.773792 | 2.428323 |
| H | 3.643403 | -2.104798 | 0.769724 |
| H | 2.267000 | 2.737888 | -3.129063 |
| H | -3.736442 | 0.700232 | -3.610227 |
| H | -2.219922 | -4.403164 | -0.120696 |

| | | | |
|---|---|---|---|
| H | -2.347514 | 3.507743 | -5.696603 |
| H | -4.336453 | -4.386020 | -0.244927 |
| Fe | -0.055002 | -0.689795 | -1.380874 |
| H | -8.400001 | -3.300204 | 0.303505 |
| H | 0.528322 | 4.870708 | -1.047872 |
| H | 6.734218 | -4.445420 | -0.080771 |
| H | 6.764828 | -2.597358 | 0.791328 |
| H | 1.491082 | -2.767772 | -4.196297 |
| H | -5.382196 | 0.310255 | 2.365259 |
| H | -1.163669 | 4.740337 | -1.529071 |
| C | -0.634971 | 0.403196 | 0.373905 |
| C | -0.765115 | 1.929403 | 0.293978 |
| C | -2.285442 | 2.154121 | 0.302489 |
| H | -2.700131 | 2.183502 | -0.710785 |
| O | -2.833874 | 1.009685 | 0.986401 |
| C | -1.892443 | 0.000234 | 1.002390 |
| O | -2.186853 | -1.052903 | 1.575619 |
| H | -2.608818 | 3.048565 | 0.844686 |
| H | -0.294513 | 2.373543 | -0.581530 |
| H | -0.317765 | 2.404604 | 1.177207 |
| C | 0.900927 | 0.155440 | 2.640006 |
| H | 0.233627 | 0.171691 | 1.430715 |
| N | 0.719738 | 1.388980 | 3.352626 |

| | | | |
|---|---|---|---|
| C | 1.580186 | 2.472361 | 3.166939 |
| C | 2.565599 | 2.479909 | 2.148853 |
| C | 1.502084 | 3.621629 | 3.992020 |
| C | 3.425739 | 3.562909 | 1.991322 |
| H | 2.641707 | 1.657188 | 1.450641 |
| C | 2.368470 | 4.698070 | 3.816104 |
| H | 0.776508 | 3.669315 | 4.794160 |
| C | 3.345710 | 4.685250 | 2.818865 |
| H | 4.162454 | 3.525860 | 1.192509 |
| H | 2.278622 | 5.554518 | 4.480199 |
| H | 4.022336 | 5.524744 | 2.689615 |
| C | -0.521835 | 1.579082 | 4.116554 |
| H | -1.294857 | 0.937039 | 3.689948 |
| C | 0.466697 | -1.100562 | 3.376785 |
| H | -0.590646 | -1.101866 | 3.646177 |
| H | 0.625517 | -1.964338 | 2.729458 |
| H | 1.059302 | -1.244441 | 4.292770 |
| H | -0.867772 | 2.606573 | 3.961367 |
| C | -0.405428 | 1.287940 | 5.619085 |
| H | 0.353432 | 1.913836 | 6.098862 |
| H | -1.368981 | 1.475041 | 6.105570 |
| H | -0.139327 | 0.243082 | 5.795436 |
| H | 1.932875 | 0.063357 | 2.307190 |

| | | | |
|---|---|---|---|
| C | -5.472759 | -1.274375 | -2.926085 |
| H | -5.582439 | -1.722463 | -3.923161 |
| H | -6.311279 | -1.636113 | -2.321308 |
| H | -5.590008 | -0.193412 | -3.041892 |

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$$\left[ {}^{3}\mathbf{D}^{\mathbf{A}}_{(S)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 3 Electronic energy : HF=-3385.0064664

Zero-point correction= 1.242564 (Hartree/Particle)

Thermal correction to Energy= 1.322745

Thermal correction to Enthalpy= 1.323689

Thermal correction to Gibbs Free Energy= 1.111089

Sum of electronic and zero-point Energies= -3383.763903

Sum of electronic and thermal Energies= -3383.683722

Sum of electronic and thermal Enthalpies= -3383.682778

Sum of electronic and thermal Free Energies= -3383.895377

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.934763 | -2.503615 | 1.235991 |

| | | | |
|---|---|---|---|
| H | -4.148914 | -2.437299 | 0.476921 |
| C | -4.336799 | -3.026495 | 2.560913 |
| H | -5.152458 | -3.156635 | 3.280974 |
| H | -3.897418 | -4.025139 | 2.384969 |
| O | -3.406383 | -2.143192 | 3.134494 |
| H | -2.669697 | -1.980898 | 2.498337 |
| C | -6.094251 | -3.344360 | 0.792948 |
| O | -7.189806 | -3.326422 | 1.353312 |
| N | -5.811748 | -4.158931 | -0.263003 |
| H | -4.868406 | -4.202487 | -0.621452 |
| C | -6.773286 | -5.115625 | -0.720262 |
| H | -7.694545 | -4.942895 | -0.161924 |
| H | -6.980353 | -5.005690 | -1.792324 |
| C | -1.629005 | 4.704441 | -2.397279 |
| H | -1.528854 | 5.168244 | -3.384377 |
| C | -2.267139 | 5.655939 | -1.378694 |
| H | -3.262103 | 5.963529 | -1.734205 |
| H | -2.435940 | 5.111221 | -0.440916 |
| C | -1.442938 | 6.919891 | -1.061283 |
| H | -0.449100 | 6.588467 | -0.723636 |
| C | -1.245891 | 7.817690 | -2.292622 |
| H | -0.660687 | 8.709402 | -2.039731 |
| H | -0.723067 | 7.298696 | -3.101907 |

| | | | |
|---|---|---|---|
| H | -2.213369 | 8.157331 | -2.684952 |
| C | -2.087589 | 7.712233 | 0.085733 |
| H | -1.491173 | 8.595150 | 0.344357 |
| H | -3.088762 | 8.062189 | -0.197893 |
| H | -2.191696 | 7.099914 | 0.987540 |
| C | 3.172627 | -1.986570 | -2.705938 |
| H | 3.447923 | -2.569727 | -1.807538 |
| H | 3.814168 | -1.085828 | -2.712999 |
| O | 1.815540 | -1.692727 | -2.776606 |
| C | 3.443223 | -0.749018 | 0.872684 |
| C | 2.057402 | 2.065151 | -2.805781 |
| C | -1.774641 | -0.776147 | -3.571674 |
| C | -0.041573 | -3.884887 | -0.301707 |
| C | 3.392270 | 0.290029 | -0.052584 |
| C | 4.378017 | 1.359187 | -0.149017 |
| C | 3.989171 | 2.148361 | -1.198428 |
| C | 2.769479 | 1.555678 | -1.726393 |
| C | 4.658934 | 3.371964 | -1.748307 |
| C | 5.643833 | 1.448881 | 0.658072 |
| C | 6.763851 | 0.581326 | 0.019145 |
| C | 8.107903 | 0.607945 | 0.729972 |
| O | 8.151493 | 0.034273 | 1.970037 |
| O | 9.119605 | 1.063053 | 0.251865 |

| | | | |
|---|---|---|---|
| C | 0.873395 | 1.547241 | -3.328263 |
| C | 0.169721 | 2.124072 | -4.456193 |
| C | -0.973391 | 1.376455 | -4.627894 |
| C | -0.905619 | 0.307038 | -3.630144 |
| C | 0.622207 | 3.325592 | -5.229872 |
| C | -2.018182 | 1.624898 | -5.616743 |
| C | -3.336259 | 1.400133 | -5.494583 |
| C | -1.648366 | -1.883243 | -2.734834 |
| C | -2.522114 | -3.037713 | -2.787263 |
| C | -2.023078 | -3.939305 | -1.867967 |
| C | -0.854534 | -3.297439 | -1.267558 |
| C | -2.521423 | -5.251855 | -1.486277 |
| C | -3.346745 | -6.062458 | -2.176774 |
| C | 1.060742 | -3.301433 | 0.307811 |
| C | 1.796239 | -3.909833 | 1.405376 |
| C | 2.755746 | -3.006383 | 1.778182 |
| C | 2.611187 | -1.866528 | 0.879852 |
| C | 1.486221 | -5.251990 | 1.996922 |
| C | 3.742777 | -3.139526 | 2.908041 |
| C | 5.170406 | -3.588800 | 2.503556 |
| C | 6.184956 | -2.472944 | 2.431874 |
| O | 6.020458 | -1.346754 | 2.888068 |
| O | 7.327495 | -2.842017 | 1.834811 |

| | | | |
|---|---|---|---|
| N | 2.437960 | 0.433068 | -1.019139 |
| N | 0.201102 | 0.458456 | -2.845612 |
| N | -0.667456 | -2.058016 | -1.797240 |
| N | 1.579464 | -2.073534 | 0.010195 |
| H | 5.525503 | 3.659579 | -1.146232 |
| H | 3.975581 | 4.229412 | -1.772115 |
| H | 5.011296 | 3.215598 | -2.775706 |
| H | 0.612324 | 4.233114 | -4.613445 |
| H | -0.023976 | 3.514416 | -6.091253 |
| H | 1.645912 | 3.199796 | -5.602003 |
| H | 2.152757 | -5.490216 | 2.830751 |
| H | 1.590493 | -6.055089 | 1.256623 |
| H | 0.457947 | -5.293400 | 2.375137 |
| H | -4.018264 | 1.634657 | -6.306522 |
| H | -3.776717 | 1.003726 | -4.585638 |
| H | -3.653978 | -7.017986 | -1.762492 |
| H | -3.709009 | -5.825461 | -3.170561 |
| H | 6.944352 | 0.919998 | -1.002553 |
| H | 6.411577 | -0.455790 | -0.036131 |
| H | 5.463099 | 1.129169 | 1.690329 |
| H | 5.988440 | 2.487683 | 0.710423 |
| H | 5.175488 | -4.115689 | 1.544333 |
| H | 5.575978 | -4.300288 | 3.236084 |

| | | | |
|---|---|---|---|
| H | 3.350927 | -3.870486 | 3.621261 |
| H | 3.824489 | -2.196041 | 3.456973 |
| H | 4.215621 | -0.703981 | 1.628626 |
| H | 2.458605 | 2.951617 | -3.285465 |
| H | -2.572154 | -0.797180 | -4.302081 |
| H | -0.306821 | -4.881089 | 0.032391 |
| H | -1.674501 | 2.079539 | -6.546878 |
| H | -2.181834 | -5.612265 | -0.515787 |
| Fe | 0.888258 | -0.813602 | -1.399844 |
| H | -6.441780 | -6.148179 | -0.545871 |
| H | -0.631944 | 4.387017 | -2.073116 |
| H | 7.938904 | -2.077203 | 1.847151 |
| H | 7.259270 | -0.209673 | 2.310787 |
| H | 3.463644 | -2.592450 | -3.582255 |
| H | -5.298403 | -1.487558 | 1.417028 |
| H | -2.231375 | 3.800759 | -2.527683 |
| C | -0.149412 | 0.219720 | 0.228955 |
| C | -0.773712 | 1.582662 | -0.091983 |
| C | -2.235870 | 1.204373 | -0.363322 |
| H | -2.406916 | 0.958676 | -1.415794 |
| O | -2.474427 | 0.015669 | 0.424355 |
| C | -1.267478 | -0.531768 | 0.794047 |
| O | -1.278930 | -1.520007 | 1.532319 |

| | | | |
|---|---|---|---|
| H | -2.961908 | 1.960399 | -0.048394 |
| H | -0.328327 | 2.097379 | -0.944223 |
| H | -0.720434 | 2.260437 | 0.773413 |
| C | -1.680384 | 1.362261 | 5.032017 |
| H | 0.679268 | 0.256916 | 0.932945 |
| N | -2.632648 | 2.000140 | 4.242642 |
| C | -2.638071 | 3.389454 | 4.117088 |
| C | -1.475979 | 4.144611 | 4.412166 |
| C | -3.787175 | 4.101104 | 3.694932 |
| C | -1.477051 | 5.530889 | 4.303769 |
| H | -0.563024 | 3.626338 | 4.680037 |
| C | -3.768044 | 5.488315 | 3.586906 |
| H | -4.704143 | 3.572078 | 3.466593 |
| C | -2.620351 | 6.224711 | 3.896064 |
| H | -0.562507 | 6.075269 | 4.527283 |
| H | -4.671286 | 6.000746 | 3.264398 |
| H | -2.617247 | 7.307787 | 3.819479 |
| C | -3.706618 | 1.197763 | 3.634745 |
| H | -3.296806 | 0.237999 | 3.320659 |
| C | -1.363252 | -0.090540 | 4.908569 |
| H | -1.018027 | -0.368125 | 3.902761 |
| H | -0.561642 | -0.336890 | 5.611969 |
| H | -2.207403 | -0.763052 | 5.123256 |

| | | | |
|---|---|---|---|
| H | -4.036708 | 1.702185 | 2.723414 |
| C | -4.883232 | 0.940487 | 4.583130 |
| H | -5.370982 | 1.868591 | 4.898761 |
| H | -5.626211 | 0.305531 | 4.089889 |
| H | -4.539058 | 0.417858 | 5.480627 |
| H | -1.251253 | 1.958000 | 5.828071 |
| C | -3.730976 | -3.171778 | -3.661909 |
| H | -3.519356 | -3.745664 | -4.574399 |
| H | -4.541421 | -3.690609 | -3.138360 |
| H | -4.114076 | -2.196539 | -3.973434 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{C}_{(R)} \right]^{L9}$$

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Number of imaginary frequencies : 3 Electronic energy : HF=-3384.968801

Zero-point correction= 1.239129 (Hartree/Particle)

Thermal correction to Energy= 1.318995

Thermal correction to Enthalpy= 1.319939

Thermal correction to Gibbs Free Energy= 1.109959

Sum of electronic and zero-point Energies= -3383.729672

Sum of electronic and thermal Energies= -3383.649806

Sum of electronic and thermal Enthalpies= -3383.648862

Sum of electronic and thermal Free Energies= -3383.858842

.....

Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 0.215488 | 3.511243 | -4.124604 |
| H | -0.302269 | 2.574418 | -3.894456 |
| C | 1.263316 | 3.751435 | -3.018782 |
| H | 1.869806 | 4.629662 | -3.269176 |
| H | 0.753535 | 3.944916 | -2.066089 |
| O | 2.155206 | 2.654174 | -2.900628 |
| H | 1.611299 | 1.906010 | -2.594803 |
| C | -0.777387 | 4.634979 | -4.248300 |
| O | -0.731107 | 5.496271 | -5.127312 |
| N | -1.721294 | 4.612733 | -3.267234 |
| H | -1.694805 | 3.868295 | -2.579554 |
| C | -2.775507 | 5.585872 | -3.241923 |
| H | -2.647819 | 6.225092 | -4.116874 |
| H | -3.760502 | 5.105954 | -3.283302 |
| C | 0.441973 | -5.153348 | -3.152182 |
| H | 1.172999 | -5.961437 | -3.263924 |
| C | -0.995456 | -5.681252 | -3.083061 |
| H | -1.091759 | -6.377081 | -2.236276 |

| | | | |
|---|---|---|---|
| H | -1.667262 | -4.842549 | -2.859830 |
| C | -1.497218 | -6.383076 | -4.360720 |
| H | -1.367423 | -5.678683 | -5.196875 |
| C | -0.695775 | -7.652520 | -4.687388 |
| H | -1.072954 | -8.132951 | -5.597417 |
| H | 0.366330 | -7.439884 | -4.842858 |
| H | -0.773919 | -8.382104 | -3.871097 |
| C | -2.994629 | -6.705697 | -4.247320 |
| H | -3.375041 | -7.168816 | -5.164974 |
| H | -3.182376 | -7.403435 | -3.421525 |
| H | -3.584193 | -5.802389 | -4.056959 |
| C | 2.378822 | -0.748527 | 3.537652 |
| H | 2.815055 | 0.227269 | 3.255218 |
| H | 2.958144 | -1.526017 | 3.006423 |
| O | 1.009193 | -0.825238 | 3.300086 |
| C | 3.026944 | 0.595913 | 0.064534 |
| C | 1.017039 | -3.725323 | 0.887490 |
| C | -2.653221 | -1.617543 | 3.206492 |
| C | -0.433352 | 2.650266 | 2.737023 |
| C | 2.818736 | -0.779451 | 0.112480 |
| C | 3.758231 | -1.773677 | -0.389205 |
| C | 3.192557 | -2.997119 | -0.143813 |
| C | 1.913627 | -2.735568 | 0.499264 |

| | | | |
|---|---|---|---|
| C | 3.751931 | -4.359354 | -0.427464 |
| C | 5.136787 | -1.475673 | -0.911676 |
| C | 6.143534 | -1.316821 | 0.261442 |
| C | 7.585076 | -1.040716 | -0.138888 |
| O | 7.831500 | 0.165821 | -0.725697 |
| O | 8.501007 | -1.802601 | 0.065275 |
| C | -0.214869 | -3.522490 | 1.509578 |
| C | -1.111905 | -4.593768 | 1.891713 |
| C | -2.201069 | -3.998519 | 2.487878 |
| C | -1.913884 | -2.562810 | 2.503216 |
| C | -0.875613 | -6.050007 | 1.627064 |
| C | -3.380926 | -4.688609 | 2.998555 |
| C | -4.644203 | -4.235700 | 3.046668 |
| C | -2.340748 | -0.266682 | 3.339728 |
| C | -3.102466 | 0.667711 | 4.147807 |
| C | -2.477424 | 1.890052 | 4.014096 |
| C | -1.344571 | 1.666616 | 3.115985 |
| C | -2.830948 | 3.183372 | 4.583354 |
| C | -3.525981 | 3.424608 | 5.708134 |
| C | 0.685674 | 2.467978 | 1.935687 |
| C | 1.563763 | 3.547918 | 1.511589 |
| C | 2.526357 | 2.981360 | 0.719919 |
| C | 2.235854 | 1.552135 | 0.693924 |

| | | | |
|---|---|---|---|
| C | 1.375896 | 4.989719 | 1.876383 |
| C | 3.627377 | 3.685938 | -0.029248 |
| C | 5.010524 | 3.709131 | 0.667434 |
| C | 5.976131 | 2.643595 | 0.210240 |
| O | 5.866687 | 1.996331 | -0.824574 |
| O | 7.020460 | 2.490037 | 1.040173 |
| N | 1.718846 | -1.388274 | 0.648564 |
| N | -0.735617 | -2.308241 | 1.863418 |
| N | -1.295536 | 0.365332 | 2.724269 |
| N | 1.114935 | 1.276195 | 1.424952 |
| H | 4.709522 | -4.296694 | -0.951884 |
| H | 3.074455 | -4.955046 | -1.051288 |
| H | 3.920236 | -4.928402 | 0.495382 |
| H | -0.884464 | -6.273595 | 0.552262 |
| H | -1.644295 | -6.672836 | 2.092233 |
| H | 0.096972 | -6.377112 | 2.013779 |
| H | 2.133041 | 5.624683 | 1.408097 |
| H | 1.442754 | 5.146337 | 2.960485 |
| H | 0.393715 | 5.358301 | 1.557499 |
| H | -5.440876 | -4.853129 | 3.451189 |
| H | -4.926865 | -3.259635 | 2.666670 |
| H | -3.744432 | 4.442637 | 6.016861 |
| H | -3.873139 | 2.633086 | 6.363091 |

| | | | |
|---|---|---|---|
| H | 6.154173 | -2.232211 | 0.855811 |
| H | 5.793435 | -0.506176 | 0.911649 |
| H | 5.125601 | -0.566998 | -1.523145 |
| H | 5.479144 | -2.286417 | -1.564322 |
| H | 4.924988 | 3.650319 | 1.756927 |
| H | 5.523833 | 4.658838 | 0.459779 |
| H | 3.319913 | 4.725410 | -0.178535 |
| H | 3.723159 | 3.259141 | -1.032498 |
| H | 3.889028 | 0.952443 | -0.482156 |
| H | 1.305546 | -4.752962 | 0.693550 |
| H | -3.509082 | -1.984256 | 3.757859 |
| H | -0.606314 | 3.654784 | 3.105774 |
| H | -3.203222 | -5.705535 | 3.351136 |
| H | -2.485874 | 4.050253 | 4.020038 |
| Fe | 0.189630 | -0.499337 | 1.641387 |
| H | -2.736761 | 6.212825 | -2.340104 |
| H | 0.571412 | -4.470379 | -4.000093 |
| H | 7.615618 | 1.814497 | 0.656925 |
| H | 7.005928 | 0.667179 | -0.930823 |
| H | 2.569849 | -0.886724 | 4.616058 |
| H | 0.727794 | 3.398099 | -5.083508 |
| H | 0.695274 | -4.599746 | -2.242527 |
| C | -0.865835 | -0.194879 | -0.239886 |

| | | | |
|---|---|---|---|
| C | -0.581889 | 1.016802 | -1.010745 |
| C | -0.726559 | -1.318620 | -1.274328 |
| C | -3.574223 | 0.179489 | 0.101686 |
| H | -2.235372 | -0.010147 | -0.019710 |
| N | -4.065607 | 1.371035 | -0.523566 |
| C | -4.328899 | 1.481734 | -1.888997 |
| C | -5.235180 | 2.455185 | -2.371749 |
| C | -3.713771 | 0.640621 | -2.841894 |
| C | -5.509194 | 2.570887 | -3.732504 |
| H | -5.747909 | 3.105884 | -1.671505 |
| C | -4.005123 | 0.759955 | -4.198385 |
| H | -2.971725 | -0.075726 | -2.516251 |
| C | -4.904644 | 1.721869 | -4.662404 |
| H | -6.216507 | 3.326959 | -4.065331 |
| H | -3.500995 | 0.103134 | -4.903013 |
| H | -5.121231 | 1.814885 | -5.722251 |
| C | -4.046531 | 2.581441 | 0.306637 |
| H | -3.124209 | 2.564498 | 0.895918 |
| C | -4.296884 | -1.118615 | -0.225230 |
| H | -5.353324 | -1.065495 | 0.075978 |
| H | -4.279019 | -1.371491 | -1.287959 |
| H | -3.826606 | -1.937702 | 0.325363 |
| H | -3.574161 | 0.345177 | 1.177839 |

| | | | |
|---|---|---|---|
| C | -4.339009 | 0.337491 | 4.926543 |
| H | -4.111306 | 0.050246 | 5.962120 |
| H | -5.010587 | 1.201015 | 4.972005 |
| H | -4.889626 | -0.494447 | 4.477096 |
| H | -1.695759 | -1.559294 | -1.739597 |
| C | 0.225146 | -0.729565 | -2.329229 |
| O | 0.081938 | 0.700922 | -2.216257 |
| O | -0.853078 | 2.195603 | -0.818311 |
| H | -0.340164 | -2.251662 | -0.866453 |
| H | 1.267371 | -0.995815 | -2.129234 |
| H | -0.020200 | -1.005885 | -3.360301 |
| H | -3.970540 | 3.451123 | -0.351199 |
| C | -5.262017 | 2.716476 | 1.231062 |
| H | -5.163112 | 3.605941 | 1.863661 |
| H | -6.194921 | 2.797957 | 0.662884 |
| H | -5.345137 | 1.849172 | 1.893180 |

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$$\left[ {}^{3}\mathbf{D}^{C}_{(R)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 2 Electronic energy : HF=-3385.0061503

Zero-point correction= 1.242598 (Hartree/Particle)

Thermal correction to Energy= 1.323735

Thermal correction to Enthalpy= 1.324680

Thermal correction to Gibbs Free Energy= 1.106786

Sum of electronic and zero-point Energies= -3383.763552

Sum of electronic and thermal Energies= -3383.682415

Sum of electronic and thermal Enthalpies= -3383.681471

Sum of electronic and thermal Free Energies= -3383.899364

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -0.607648 | -3.247519 | 4.205972 |
| H | -0.821263 | -2.208048 | 3.937046 |
| C | 0.357547 | -3.813148 | 3.142789 |
| H | 0.677084 | -4.820789 | 3.432932 |
| H | -0.159208 | -3.882888 | 2.176327 |
| O | 1.528930 | -3.021809 | 3.033642 |
| H | 1.234216 | -2.170635 | 2.663127 |
| C | -1.888650 | -4.027824 | 4.316216 |
| O | -2.125845 | -4.830265 | 5.219055 |
| N | -2.754491 | -3.768128 | 3.295745 |
| H | -2.472805 | -3.120924 | 2.566339 |
| C | -4.020192 | -4.441764 | 3.227560 |

| | | | |
|---|---|---|---|
| H | -4.076887 | -5.111464 | 4.087027 |
| H | -4.861971 | -3.738081 | 3.270787 |
| C | 2.020618 | 5.002517 | 3.156733 |
| H | 2.871350 | 5.690695 | 3.207636 |
| C | 0.681888 | 5.744721 | 3.075297 |
| H | 0.675123 | 6.394804 | 2.187790 |
| H | -0.117568 | 5.010244 | 2.914433 |
| C | 0.326864 | 6.591971 | 4.313356 |
| H | 0.365547 | 5.927534 | 5.190442 |
| C | 1.323960 | 7.737190 | 4.547405 |
| H | 1.048631 | 8.324680 | 5.430755 |
| H | 2.343544 | 7.370293 | 4.700211 |
| H | 1.340351 | 8.419607 | 3.687904 |
| C | -1.104282 | 7.138323 | 4.201537 |
| H | -1.385505 | 7.709976 | 5.093411 |
| H | -1.201055 | 7.805611 | 3.335908 |
| H | -1.831743 | 6.328923 | 4.077351 |
| C | 2.907581 | 0.100587 | -3.407710 |
| H | 3.088544 | -0.945608 | -3.099434 |
| H | 3.651903 | 0.725239 | -2.880286 |
| O | 1.594998 | 0.515315 | -3.195993 |
| C | 3.180219 | -1.199551 | 0.159382 |
| C | 2.213135 | 3.418996 | -0.907042 |

| | | | |
|---|---|---|---|
| C | -1.900847 | 2.082641 | -3.054740 |
| C | -0.561177 | -2.536927 | -2.588526 |
| C | 3.292006 | 0.183870 | 0.043433 |
| C | 4.425609 | 0.963984 | 0.520329 |
| C | 4.158270 | 2.269473 | 0.200029 |
| C | 2.861012 | 2.272616 | -0.458223 |
| C | 5.012061 | 3.481148 | 0.428441 |
| C | 5.690846 | 0.390102 | 1.096321 |
| C | 6.658246 | -0.052591 | -0.036251 |
| C | 7.989479 | -0.628353 | 0.422280 |
| O | 7.939752 | -1.826267 | 1.074425 |
| O | 9.060166 | -0.108911 | 0.211607 |
| C | 0.961681 | 3.468990 | -1.520376 |
| C | 0.298998 | 4.696256 | -1.911352 |
| C | -0.918676 | 4.332249 | -2.441751 |
| C | -0.944237 | 2.868697 | -2.419249 |
| C | 0.848584 | 6.075112 | -1.703662 |
| C | -1.948041 | 5.245612 | -2.926314 |
| C | -3.279274 | 5.072634 | -2.901267 |
| C | -1.868409 | 0.695323 | -3.177977 |
| C | -2.811929 | -0.073296 | -3.969135 |
| C | -2.418806 | -1.390564 | -3.863415 |
| C | -1.250447 | -1.393588 | -2.983613 |

| | | | |
|---|---|---|---|
| C | -3.012370 | -2.587107 | -4.445873 |
| C | -3.734399 | -2.676127 | -5.575680 |
| C | 0.543385 | -2.578018 | -1.747260 |
| C | 1.153728 | -3.808602 | -1.268926 |
| C | 2.183439 | -3.440706 | -0.443915 |
| C | 2.209130 | -1.982310 | -0.458300 |
| C | 0.677587 | -5.186368 | -1.619497 |
| C | 3.073746 | -4.348888 | 0.364063 |
| C | 4.437239 | -4.705406 | -0.277423 |
| C | 5.601995 | -3.862187 | 0.179725 |
| O | 5.608697 | -3.162612 | 1.186234 |
| O | 6.678355 | -3.980715 | -0.613639 |
| N | 2.366517 | 0.998461 | -0.546780 |
| N | 0.184176 | 2.385618 | -1.823621 |
| N | -0.942202 | -0.126628 | -2.597075 |
| N | 1.196935 | -1.492272 | -1.235759 |
| H | 5.922309 | 3.230463 | 0.980346 |
| H | 4.481540 | 4.250239 | 1.002810 |
| H | 5.319381 | 3.943736 | -0.517787 |
| H | 0.904069 | 6.333776 | -0.638018 |
| H | 0.225979 | 6.832850 | -2.186883 |
| H | 1.862842 | 6.169548 | -2.109222 |
| H | 1.254471 | -5.955808 | -1.098947 |

| | | | |
|---|---|---|---|
| H | 0.764931 | -5.384257 | -2.695383 |
| H | -0.376243 | -5.326670 | -1.351391 |
| H | -3.947355 | 5.833846 | -3.293189 |
| H | -3.741507 | 4.189434 | -2.472779 |
| H | -4.144416 | -3.628579 | -5.898339 |
| H | -3.918376 | -1.823818 | -6.220667 |
| H | 6.890057 | 0.804824 | -0.670591 |
| H | 6.145979 | -0.794727 | -0.660214 |
| H | 5.462146 | -0.459822 | 1.748426 |
| H | 6.195661 | 1.135068 | 1.721389 |
| H | 4.399437 | -4.674060 | -1.370743 |
| H | 4.719946 | -5.735825 | -0.018700 |
| H | 2.535081 | -5.287369 | 0.526528 |
| H | 3.229188 | -3.925423 | 1.360413 |
| H | 3.931566 | -1.715258 | 0.741622 |
| H | 2.723391 | 4.363967 | -0.753400 |
| H | -2.691605 | 2.606312 | -3.575851 |
| H | -0.929385 | -3.489155 | -2.952626 |
| H | -1.576035 | 6.190788 | -3.324326 |
| H | -2.843253 | -3.509972 | -3.891603 |
| Fe | 0.703172 | 0.433909 | -1.546996 |
| H | -4.120050 | -5.034924 | 2.308542 |
| H | 2.062107 | 4.358755 | 4.043339 |

| | | | |
|---|---|---|---|
| H | 7.398407 | -3.438313 | -0.232545 |
| H | 7.017096 | -2.113867 | 1.276136 |
| H | 3.140483 | 0.164248 | -4.484754 |
| H | -0.112440 | -3.259333 | 5.180149 |
| H | 2.162381 | 4.363676 | 2.279268 |
| C | -0.595680 | 0.518541 | 0.255956 |
| C | -0.697334 | -0.720549 | 1.018029 |
| C | -0.173555 | 1.553206 | 1.306511 |
| C | -5.042041 | 0.538534 | -0.355115 |
| H | -1.530158 | 0.742799 | -0.253742 |
| N | -5.505899 | -0.581811 | 0.330822 |
| C | -6.594470 | -0.531423 | 1.208687 |
| C | -7.369319 | -1.678621 | 1.488866 |
| C | -6.939482 | 0.673541 | 1.860831 |
| C | -8.441075 | -1.613802 | 2.375883 |
| H | -7.143168 | -2.617478 | 0.995644 |
| C | -8.020152 | 0.725335 | 2.735551 |
| H | -6.317166 | 1.547670 | 1.704783 |
| C | -8.785452 | -0.413516 | 3.002398 |
| H | -9.019740 | -2.513662 | 2.569592 |
| H | -8.252847 | 1.664633 | 3.231501 |
| H | -9.625921 | -0.368287 | 3.688547 |
| C | -4.719175 | -1.820515 | 0.205412 |

| | | | |
|---|---|---|---|
| H | -3.655902 | -1.554910 | 0.223791 |
| C | -5.965238 | 1.466263 | -1.086335 |
| H | -6.335815 | 1.021053 | -2.027067 |
| H | -6.848165 | 1.747674 | -0.504558 |
| H | -5.433259 | 2.385478 | -1.353375 |
| H | -4.031658 | 0.429202 | -0.734814 |
| C | -3.982548 | 0.491749 | -4.713597 |
| H | -3.718897 | 0.783722 | -5.739328 |
| H | -4.788908 | -0.244991 | -4.784953 |
| H | -4.382751 | 1.382064 | -4.219020 |
| H | -1.049163 | 1.995464 | 1.807416 |
| C | 0.621930 | 0.702904 | 2.305357 |
| O | 0.087148 | -0.634961 | 2.176182 |
| O | -1.328739 | -1.758712 | 0.843857 |
| H | 0.427883 | 2.375102 | 0.916643 |
| H | 1.687018 | 0.673972 | 2.063486 |
| H | 0.499107 | 1.007124 | 3.349807 |
| H | -4.905628 | -2.430526 | 1.093288 |
| C | -5.025509 | -2.613358 | -1.068737 |
| H | -4.394195 | -3.507600 | -1.110834 |
| H | -6.073778 | -2.928325 | -1.113135 |
| H | -4.810611 | -2.013262 | -1.957328 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{C}_{(S)} \right]^{L9}$$

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Number of imaginary frequencies : 3 Electronic energy : HF=-3384.9562733

Zero-point correction= 1.238315 (Hartree/Particle)

Thermal correction to Energy= 1.318719

Thermal correction to Enthalpy= 1.319664

Thermal correction to Gibbs Free Energy= 1.109608

Sum of electronic and zero-point Energies= -3383.718351

Sum of electronic and thermal Energies= -3383.637946

Sum of electronic and thermal Enthalpies= -3383.637002

Sum of electronic and thermal Free Energies= -3383.847058

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 2.334860 | 4.670599 | 2.084692 |
| H | 2.098768 | 3.605417 | 2.182201 |
| C | 1.515765 | 5.281262 | 0.930139 |
| H | 1.708586 | 6.356805 | 0.901432 |
| H | 1.861644 | 4.860849 | -0.025136 |

| | | | |
|---|---|---|---|
| O | 0.115009 | 5.105338 | 1.088734 |
| H | -0.117935 | 4.228435 | 0.751971 |
| C | 3.797906 | 4.902970 | 1.841969 |
| O | 4.264915 | 6.026051 | 1.653666 |
| N | 4.533587 | 3.763169 | 1.790537 |
| H | 4.102805 | 2.872217 | 1.989268 |
| C | 5.924785 | 3.804804 | 1.458561 |
| H | 6.216710 | 4.853846 | 1.393865 |
| H | 6.532342 | 3.306344 | 2.222129 |
| C | -3.619438 | -1.221587 | 4.513755 |
| H | -4.078572 | -1.017660 | 5.488136 |
| C | -2.567219 | -2.334454 | 4.580117 |
| H | -3.036752 | -3.267962 | 4.928953 |
| H | -2.192175 | -2.522917 | 3.568321 |
| C | -1.351220 | -2.021436 | 5.474025 |
| H | -0.924407 | -1.076759 | 5.109959 |
| C | -1.727397 | -1.850762 | 6.953645 |
| H | -0.842955 | -1.627239 | 7.562421 |
| H | -2.445925 | -1.038717 | 7.108368 |
| H | -2.176019 | -2.771219 | 7.351432 |
| C | -0.276688 | -3.104873 | 5.300845 |
| H | 0.613472 | -2.884807 | 5.903359 |
| H | -0.653722 | -4.086948 | 5.618297 |

| | | | |
|---|---|---|---|
| H | 0.022542 | -3.172942 | 4.251018 |
| C | -2.306008 | -0.593791 | -3.597235 |
| H | -2.363329 | 0.510820 | -3.585742 |
| H | -3.148391 | -0.963341 | -2.982810 |
| O | -1.071443 | -1.083075 | -3.188371 |
| C | -2.948709 | 1.024758 | -0.250017 |
| C | -1.848841 | -3.669244 | -0.551053 |
| C | 2.285826 | -2.610482 | -2.796671 |
| C | 1.056778 | 2.065942 | -2.756488 |
| C | -3.030277 | -0.361271 | -0.169652 |
| C | -4.185012 | -1.089451 | 0.342913 |
| C | -3.870152 | -2.417947 | 0.256323 |
| C | -2.530830 | -2.485490 | -0.311056 |
| C | -4.701807 | -3.605828 | 0.636104 |
| C | -5.502124 | -0.466513 | 0.715866 |
| C | -6.365495 | -0.223464 | -0.553808 |
| C | -7.735981 | 0.393299 | -0.321975 |
| O | -7.753631 | 1.681640 | 0.134874 |
| O | -8.780755 | -0.166840 | -0.554488 |
| C | -0.579882 | -3.789501 | -1.109286 |
| C | 0.069101 | -5.061076 | -1.363597 |
| C | 1.277097 | -4.772178 | -1.954816 |
| C | 1.316469 | -3.312923 | -2.089388 |

| | | | |
|---|---|---|---|
| C | -0.488830 | -6.400658 | -0.990050 |
| C | 2.286685 | -5.745166 | -2.358633 |
| C | 3.620463 | -5.591622 | -2.381537 |
| C | 2.311152 | -1.231993 | -3.002577 |
| C | 3.312000 | -0.549872 | -3.801227 |
| C | 2.974138 | 0.787429 | -3.781793 |
| C | 1.764542 | 0.884754 | -2.965828 |
| C | 3.647264 | 1.925782 | -4.392738 |
| C | 4.436595 | 1.926804 | -5.480348 |
| C | -0.144068 | 2.198031 | -2.064724 |
| C | -0.794182 | 3.470875 | -1.793010 |
| C | -1.904800 | 3.185115 | -1.032822 |
| C | -1.932157 | 1.737724 | -0.882367 |
| C | -0.340415 | 4.813267 | -2.288901 |
| C | -2.885922 | 4.175571 | -0.459104 |
| C | -4.168455 | 4.412387 | -1.295260 |
| C | -5.369331 | 3.626941 | -0.823362 |
| O | -5.469555 | 3.109409 | 0.283608 |
| O | -6.356357 | 3.576012 | -1.728590 |
| N | -2.055336 | -1.230092 | -0.569075 |
| N | 0.204722 | -2.755133 | -1.530689 |
| N | 1.405204 | -0.341987 | -2.495215 |
| N | -0.850159 | 1.171832 | -1.497125 |

| | | | |
|---|---|---|---|
| H | -5.659108 | -3.302673 | 1.069180 |
| H | -4.188457 | -4.231004 | 1.376217 |
| H | -4.919832 | -4.243361 | -0.229743 |
| H | -0.570338 | -6.511223 | 0.098467 |
| H | 0.143871 | -7.215044 | -1.352856 |
| H | -1.493265 | -6.548657 | -1.404396 |
| H | -0.604531 | 5.605399 | -1.582443 |
| H | -0.792299 | 5.062337 | -3.258210 |
| H | 0.744461 | 4.851944 | -2.423146 |
| H | 4.268121 | -6.401964 | -2.703053 |
| H | 4.105812 | -4.676623 | -2.059045 |
| H | 4.902993 | 2.844672 | -5.825896 |
| H | 4.621859 | 1.035464 | -6.069715 |
| H | -6.533411 | -1.174071 | -1.063067 |
| H | -5.800712 | 0.420231 | -1.239195 |
| H | -5.342944 | 0.476328 | 1.250829 |
| H | -6.052843 | -1.121348 | 1.399726 |
| H | -4.013337 | 4.202588 | -2.357689 |
| H | -4.474233 | 5.466358 | -1.237187 |
| H | -2.372054 | 5.133530 | -0.338925 |
| H | -3.192277 | 3.871010 | 0.546490 |
| H | -3.755663 | 1.597158 | 0.187123 |
| H | -2.352640 | -4.589474 | -0.276511 |

| | | | |
|---|---|---|---|
| H | 3.055472 | -3.197707 | -3.280331 |
| H | 1.467635 | 2.967933 | -3.194507 |
| H | 1.894446 | -6.722136 | -2.644362 |
| H | 3.486253 | 2.883541 | -3.897694 |
| Fe | -0.313607 | -0.788997 | -1.490397 |
| H | 6.128948 | 3.323368 | 0.492917 |
| H | -3.168189 | -0.291652 | 4.150414 |
| H | -7.103579 | 3.078890 | -1.336284 |
| H | -6.860250 | 2.008638 | 0.392265 |
| H | -2.503707 | -0.914572 | -4.635237 |
| H | 2.036282 | 5.162806 | 3.017028 |
| H | -4.425391 | -1.487273 | 3.820616 |
| C | 0.653887 | -0.509682 | 0.410332 |
| C | 0.997261 | 0.903048 | 0.901477 |
| C | 0.021206 | -1.140443 | 1.584357 |
| C | 3.109297 | -1.734803 | 0.543256 |
| H | 1.859312 | -1.164715 | 0.405841 |
| N | 4.123362 | -0.801051 | 0.959520 |
| C | 4.301118 | -0.370647 | 2.271768 |
| C | 5.514068 | 0.231257 | 2.691217 |
| C | 3.272389 | -0.487103 | 3.239544 |
| C | 5.680155 | 0.685797 | 3.999493 |
| H | 6.346566 | 0.315126 | 2.002367 |

| | | | |
|---|---|---|---|
| C | 3.459405 | -0.035338 | 4.542356 |
| H | 2.312761 | -0.902261 | 2.965008 |
| C | 4.660463 | 0.556888 | 4.943227 |
| H | 6.630818 | 1.132741 | 4.281704 |
| H | 2.639129 | -0.138461 | 5.247961 |
| H | 4.795908 | 0.909288 | 5.961201 |
| C | 4.966119 | -0.258299 | -0.108003 |
| H | 4.335293 | -0.118423 | -0.992051 |
| C | 2.983251 | -3.035184 | 1.320071 |
| H | 3.930615 | -3.594274 | 1.298163 |
| H | 2.705212 | -2.898178 | 2.366037 |
| H | 2.205980 | -3.647678 | 0.858673 |
| H | 3.265484 | -1.940283 | -0.513674 |
| C | 4.484025 | -1.201812 | -4.469263 |
| H | 4.254211 | -1.511658 | -5.497782 |
| H | 5.332673 | -0.512147 | -4.523284 |
| H | 4.810035 | -2.096752 | -3.930599 |
| H | 5.313245 | 0.738267 | 0.182731 |
| C | 6.160371 | -1.149640 | -0.474979 |
| H | 6.730295 | -0.706074 | -1.299548 |
| H | 6.835514 | -1.291010 | 0.374856 |
| H | 5.816335 | -2.138117 | -0.795626 |
| C | 0.051387 | 1.116782 | 2.098760 |

| | | | |
|---|---|---|---|
| O | -0.285645 | -0.196013 | 2.568063 |
| O | -0.202606 | -2.315669 | 1.833038 |
| H | -0.870680 | 1.630409 | 1.801223 |
| H | 0.503998 | 1.663439 | 2.933649 |
| H | 0.872697 | 1.678152 | 0.145090 |
| H | 2.041920 | 0.951585 | 1.239711 |

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$$\left[ {}^{3}\mathbf{D}^{C}_{(S)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 2 Electronic energy : HF=-3384.9905086

Zero-point correction= 1.241528 (Hartree/Particle)

Thermal correction to Energy= 1.323114

Thermal correction to Enthalpy= 1.324058

Thermal correction to Gibbs Free Energy= 1.106281

Sum of electronic and zero-point Energies= -3383.748980

Sum of electronic and thermal Energies= -3383.667395

Sum of electronic and thermal Enthalpies= -3383.666450

Sum of electronic and thermal Free Energies= -3383.884228

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 2.011699 | 4.604562 | 2.318049 |
| H | 1.841005 | 3.524275 | 2.250121 |
| C | 1.087653 | 5.337101 | 1.324194 |
| H | 1.217588 | 6.413719 | 1.461809 |
| H | 1.395837 | 5.098625 | 0.295717 |
| O | -0.288296 | 5.049186 | 1.526317 |
| H | -0.489217 | 4.208899 | 1.089472 |
| C | 3.441385 | 4.968932 | 2.041270 |
| O | 3.841317 | 6.132732 | 2.059058 |
| N | 4.221799 | 3.907705 | 1.717401 |
| H | 3.835914 | 2.975884 | 1.734699 |
| C | 5.581788 | 4.090342 | 1.308473 |
| H | 5.849407 | 5.129068 | 1.506808 |
| H | 6.251873 | 3.426857 | 1.864776 |
| C | -3.273044 | -1.949865 | 4.594634 |
| H | -3.672859 | -1.923367 | 5.615015 |
| C | -2.167523 | -2.997932 | 4.423238 |
| H | -2.566671 | -3.998194 | 4.654909 |
| H | -1.857724 | -3.013888 | 3.372702 |
| C | -0.906978 | -2.753655 | 5.275806 |
| H | -0.550737 | -1.742601 | 5.033845 |
| C | -1.185922 | -2.824159 | 6.784917 |

| | | | |
|---|---|---|---|
| H | -0.271796 | -2.644474 | 7.363567 |
| H | -1.928105 | -2.085178 | 7.105544 |
| H | -1.563024 | -3.816836 | 7.066117 |
| C | 0.201275 | -3.737647 | 4.873735 |
| H | 1.118965 | -3.560989 | 5.448568 |
| H | -0.108973 | -4.775101 | 5.060527 |
| H | 0.431000 | -3.631120 | 3.809624 |
| C | -2.746181 | -0.417582 | -3.485088 |
| H | -2.919452 | 0.662518 | -3.317462 |
| H | -3.510055 | -0.958083 | -2.894523 |
| O | -1.446569 | -0.816500 | -3.197723 |
| C | -3.252068 | 0.921615 | 0.022183 |
| C | -1.926709 | -3.657814 | -0.764682 |
| C | 2.113951 | -2.158045 | -2.935467 |
| C | 0.533522 | 2.399538 | -2.605256 |
| C | -3.253652 | -0.469029 | -0.014018 |
| C | -4.340908 | -1.304244 | 0.482267 |
| C | -3.965012 | -2.600032 | 0.254064 |
| C | -2.655516 | -2.541035 | -0.379830 |
| C | -4.716455 | -3.861718 | 0.555360 |
| C | -5.666238 | -0.793177 | 0.976601 |
| C | -6.610905 | -0.489375 | -0.220083 |
| C | -7.996376 | 0.025231 | 0.137347 |

| | | | |
|---|---|---|---|
| O | -8.055452 | 1.266172 | 0.708032 |
| O | -9.021962 | -0.571774 | -0.088785 |
| C | -0.672641 | -3.652535 | -1.367748 |
| C | 0.067749 | -4.853964 | -1.700308 |
| C | 1.258435 | -4.439963 | -2.249765 |
| C | 1.191149 | -2.975875 | -2.291480 |
| C | -0.390040 | -6.251290 | -1.413635 |
| C | 2.340355 | -5.310509 | -2.695767 |
| C | 3.659921 | -5.061183 | -2.695658 |
| C | 2.019800 | -0.774384 | -3.082722 |
| C | 2.955383 | 0.028157 | -3.848112 |
| C | 2.505374 | 1.329019 | -3.764205 |
| C | 1.301346 | 1.285633 | -2.935389 |
| C | 3.077740 | 2.547529 | -4.319830 |
| C | 3.859838 | 2.667721 | -5.406173 |
| C | -0.623634 | 2.404228 | -1.830610 |
| C | -1.324878 | 3.609724 | -1.416943 |
| C | -2.371429 | 3.197650 | -0.623815 |
| C | -2.311179 | 1.744139 | -0.595326 |
| C | -0.976962 | 5.013389 | -1.821085 |
| C | -3.367726 | 4.079276 | 0.085195 |
| C | -4.707148 | 4.312377 | -0.657697 |
| C | -5.835639 | 3.421109 | -0.195371 |

| | | | |
|---|---|---|---|
| O | -5.845463 | 2.806169 | 0.865337 |
| O | -6.868200 | 3.390433 | -1.049288 |
| N | -2.256671 | -1.242201 | -0.536688 |
| N | 0.030288 | -2.539596 | -1.725953 |
| N | 1.038461 | 0.008707 | -2.542723 |
| N | -1.234578 | 1.295412 | -1.308957 |
| H | -5.662190 | -3.653248 | 1.063404 |
| H | -4.134296 | -4.527964 | 1.202999 |
| H | -4.950593 | -4.423229 | -0.357654 |
| H | -0.421019 | -6.447328 | -0.334487 |
| H | 0.277909 | -6.993354 | -1.859345 |
| H | -1.398287 | -6.433386 | -1.803974 |
| H | -1.217455 | 5.724966 | -1.025706 |
| H | -1.519272 | 5.323210 | -2.724249 |
| H | 0.089844 | 5.121764 | -2.036672 |
| H | 4.366071 | -5.803706 | -3.055499 |
| H | 4.076488 | -4.134439 | -2.315548 |
| H | 4.244480 | 3.637577 | -5.707593 |
| H | 4.118320 | 1.824756 | -6.037601 |
| H | -6.757126 | -1.399701 | -0.804111 |
| H | -6.119784 | 0.243100 | -0.872219 |
| H | -5.527446 | 0.106820 | 1.585962 |
| H | -6.142981 | -1.536112 | 1.625186 |

| | | | |
|---|---|---|---|
| H | -4.602398 | 4.204129 | -1.741273 |
| H | -5.064702 | 5.337935 | -0.489852 |
| H | -2.898567 | 5.051900 | 0.259376 |
| H | -3.598707 | 3.675225 | 1.075725 |
| H | -4.064911 | 1.407015 | 0.545369 |
| H | -2.365770 | -4.626694 | -0.553646 |
| H | 2.936028 | -2.653850 | -3.435043 |
| H | 0.866049 | 3.356779 | -2.989067 |
| H | 2.022695 | -6.295381 | -3.041086 |
| H | 2.838011 | 3.463793 | -3.780278 |
| Fe | -0.607663 | -0.624855 | -1.520332 |
| H | 5.715523 | 3.894429 | 0.236065 |
| H | -2.892655 | -0.951375 | 4.352684 |
| H | -7.564499 | 2.819132 | -0.664401 |
| H | -7.167167 | 1.620444 | 0.946182 |
| H | -2.967527 | -0.615891 | -4.548810 |
| H | 1.744223 | 4.920251 | 3.332514 |
| H | -4.110774 | -2.152357 | 3.918102 |
| C | 0.631297 | -0.531569 | 0.276939 |
| C | 0.836741 | 0.830114 | 0.951561 |
| C | 0.167960 | -1.385385 | 1.384500 |
| C | 4.136230 | -1.908640 | 0.653091 |
| H | 1.541709 | -0.945541 | -0.151005 |

| | | | |
|---|---|---|---|
| N | 5.283800 | -1.112827 | 0.654760 |
| C | 5.677738 | -0.348015 | 1.758215 |
| C | 7.021019 | 0.052368 | 1.933082 |
| C | 4.733561 | 0.060782 | 2.728847 |
| C | 7.396295 | 0.828627 | 3.027237 |
| H | 7.777116 | -0.263499 | 1.222136 |
| C | 5.126573 | 0.828637 | 3.821919 |
| H | 3.692736 | -0.212585 | 2.598335 |
| C | 6.458462 | 1.222451 | 3.985970 |
| H | 8.439107 | 1.116425 | 3.136629 |
| H | 4.377176 | 1.131873 | 4.548589 |
| H | 6.757778 | 1.820379 | 4.841239 |
| C | 5.971129 | -0.946127 | -0.631158 |
| H | 5.199343 | -0.848958 | -1.405183 |
| C | 3.778907 | -2.852614 | 1.757078 |
| H | 4.301890 | -3.819463 | 1.647808 |
| H | 4.032330 | -2.468784 | 2.749292 |
| H | 2.703507 | -3.056661 | 1.733277 |
| H | 3.728667 | -2.094639 | -0.335020 |
| C | 4.172211 | -0.488100 | -4.553584 |
| H | 3.963224 | -0.751522 | -5.599444 |
| H | 4.964326 | 0.267938 | -4.565202 |
| H | 4.569266 | -1.387409 | -4.072452 |

| | | | |
|---|---|---|---|
| H | 6.518682 | 0.000250 | -0.614691 |
| C | 6.906998 | -2.107378 | -0.982519 |
| H | 7.345151 | -1.959249 | -1.976057 |
| H | 7.722188 | -2.199841 | -0.257553 |
| H | 6.356615 | -3.053233 | -0.989836 |
| C | -0.185833 | 0.783042 | 2.097468 |
| O | -0.332582 | -0.608974 | 2.422622 |
| O | 0.180948 | -2.599741 | 1.525111 |
| H | -1.159442 | 1.176379 | 1.788316 |
| H | 0.133578 | 1.308246 | 3.004846 |
| H | 0.679452 | 1.692246 | 0.300011 |
| H | 1.855392 | 0.913907 | 1.367482 |

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**$C^{L10}$**

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Number of imaginary frequencies : 0 Electronic energy : HF=-3105.5375686

Zero-point correction= 1.056843 (Hartree/Particle)

Thermal correction to Energy= 1.127827

Thermal correction to Enthalpy= 1.128771

Thermal correction to Gibbs Free Energy= 0.944221

Sum of electronic and zero-point Energies= -3104.480726

Sum of electronic and thermal Energies= -3104.409742

Sum of electronic and thermal Enthalpies= -3104.408798

Sum of electronic and thermal Free Energies= -3104.593347

.....

Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -1.415390 | 5.369681 | 2.325663 |
| H | -1.908978 | 6.176240 | 2.876864 |
| C | -2.358147 | 4.165585 | 2.204413 |
| H | -2.246784 | 3.503131 | 3.076573 |
| H | -3.391697 | 4.527231 | 2.210726 |
| O | -2.231266 | 3.439750 | 0.986305 |
| H | -1.356145 | 3.024283 | 0.936526 |
| C | -0.051909 | 5.217979 | 3.052883 |
| O | 0.506330 | 6.227390 | 3.475485 |
| N | 0.472738 | 3.968108 | 3.226558 |
| H | 0.076916 | 3.163614 | 2.750666 |
| C | 1.767159 | 3.761268 | 3.886788 |
| H | 1.774457 | 2.767451 | 4.341114 |
| H | 2.603381 | 3.839625 | 3.181339 |
| C | -3.404267 | -5.530236 | 2.778134 |
| H | -4.051647 | -6.099500 | 3.454156 |

| | | | |
|---|---|---|---|
| C | -3.483530 | -4.027848 | 3.067765 |
| H | -3.134570 | -3.844045 | 4.095843 |
| H | -2.797745 | -3.500090 | 2.392603 |
| C | -4.901777 | -3.465288 | 2.909790 |
| H | -5.265790 | -3.663823 | 1.893816 |
| H | -5.582493 | -3.996495 | 3.588097 |
| C | -5.044149 | -1.964938 | 3.204443 |
| H | -6.104923 | -1.691994 | 3.184660 |
| H | -4.681532 | -1.729692 | 4.210079 |
| N | -4.357321 | -1.080552 | 2.258552 |
| H | -4.754461 | -0.976919 | 1.323082 |
| C | -3.226248 | -0.395251 | 2.502165 |
| N | -2.916681 | 0.661095 | 1.762727 |
| N | -2.417027 | -0.734524 | 3.530850 |
| H | -2.415688 | -1.701728 | 3.817015 |
| C | 1.110473 | -1.052303 | -3.585258 |
| H | 0.922413 | -2.139944 | -3.550560 |
| H | 1.483225 | -0.814293 | -4.593334 |
| O | 2.046155 | -0.638037 | -2.638526 |
| C | -1.716639 | -0.526688 | -1.131292 |
| C | 1.688296 | -3.912603 | -0.616482 |
| C | 5.065298 | -0.469688 | -0.273869 |
| C | 1.745674 | 2.842684 | -1.399243 |

| | | | |
|---|---|---|---|
| C | -1.109265 | -1.760097 | -0.919870 |
| C | -1.802772 | -3.040040 | -0.818924 |
| C | -0.822156 | -3.997162 | -0.732639 |
| C | 0.448885 | -3.290864 | -0.741446 |
| C | -0.955766 | -5.488421 | -0.638729 |
| C | -3.291913 | -3.270326 | -0.740870 |
| C | -4.150715 | -2.801520 | -1.936414 |
| C | -4.887429 | -1.490124 | -1.724350 |
| O | -5.288100 | -0.968010 | -2.875181 |
| O | -5.109085 | -0.964731 | -0.635362 |
| C | 2.920507 | -3.274458 | -0.502381 |
| C | 4.182534 | -3.966351 | -0.317415 |
| C | 5.143610 | -2.987860 | -0.186946 |
| C | 4.441441 | -1.712185 | -0.302417 |
| C | 4.355741 | -5.452223 | -0.243240 |
| C | 6.576841 | -3.118412 | 0.051797 |
| C | 7.372485 | -4.131506 | -0.325796 |
| C | 4.453996 | 0.755647 | -0.519739 |
| C | 5.166615 | 2.020667 | -0.607891 |
| C | 4.227139 | 2.965483 | -0.948971 |
| C | 2.955896 | 2.249206 | -1.061442 |
| C | 6.642462 | 2.199313 | -0.426953 |
| C | 4.394179 | 4.390699 | -1.211041 |

| | | | |
|---|---|---|---|
| C | 5.300150 | 5.211582 | -0.657172 |
| C | 0.514976 | 2.200621 | -1.480729 |
| C | -0.732041 | 2.880575 | -1.778626 |
| C | -1.721243 | 1.937507 | -1.669253 |
| C | -1.060598 | 0.685714 | -1.334090 |
| C | -0.866374 | 4.337687 | -2.102658 |
| C | -3.198934 | 2.155020 | -1.822031 |
| C | -3.697769 | 2.064454 | -3.294169 |
| C | -5.174304 | 2.351848 | -3.351525 |
| O | -5.460433 | 3.596084 | -3.760917 |
| O | -6.066402 | 1.581079 | -3.012565 |
| N | 0.245365 | -1.944810 | -0.853758 |
| N | 3.105609 | -1.916913 | -0.488462 |
| N | 3.123576 | 0.928814 | -0.777525 |
| N | 0.286159 | 0.876687 | -1.229527 |
| H | -1.997635 | -5.811438 | -0.710863 |
| H | -0.405897 | -5.988247 | -1.444874 |
| H | 5.226582 | -5.709031 | 0.367303 |
| H | 4.510978 | -5.899942 | -1.233750 |
| H | 3.480467 | -5.940553 | 0.196816 |
| H | 6.994691 | 3.072244 | -0.984067 |
| H | 7.200003 | 1.326896 | -0.781835 |
| H | 6.916815 | 2.353598 | 0.625264 |

| | | | |
|---|---|---|---|
| H | -1.914906 | 4.630574 | -2.198949 |
| H | -0.362747 | 4.591273 | -3.043415 |
| H | -0.424323 | 4.965884 | -1.321040 |
| H | 8.428528 | -4.132112 | -0.073953 |
| H | 7.012478 | -4.968540 | -0.914197 |
| H | 5.349022 | 6.258503 | -0.939998 |
| H | 5.996743 | 4.880737 | 0.105864 |
| H | -4.932050 | -3.541749 | -2.155119 |
| H | -3.561496 | -2.713309 | -2.852891 |
| H | -3.693874 | -2.791253 | 0.158528 |
| H | -3.456314 | -4.342685 | -0.604123 |
| H | -3.526486 | 1.055017 | -3.677436 |
| H | -3.157949 | 2.777215 | -3.920182 |
| H | -3.454236 | 3.137918 | -1.413774 |
| H | -3.764422 | 1.423074 | -1.235900 |
| H | -2.794710 | -0.503088 | -1.158074 |
| H | 1.690687 | -4.996136 | -0.583019 |
| H | 6.136410 | -0.459328 | -0.112230 |
| H | 1.753287 | 3.908599 | -1.595152 |
| H | 7.039658 | -2.296345 | 0.597455 |
| H | 3.702638 | 4.821322 | -1.934756 |
| Fe | 1.681397 | -0.497583 | -0.824275 |
| H | -3.719965 | -5.748584 | 1.752541 |

| | | | |
|---|---|---|---|
| H | 1.892275 | 4.526231 | 4.654374 |
| H | -1.219768 | 5.765116 | 1.321830 |
| H | -5.694227 | -0.066533 | -2.751556 |
| H | 0.134154 | -0.550145 | -3.475409 |
| H | -6.427718 | 3.694802 | -3.718519 |
| H | -2.383209 | -5.904249 | 2.897929 |
| C | 1.356435 | -0.338138 | 1.156616 |
| C | 0.497651 | 0.508933 | 1.922308 |
| C | 1.866754 | -1.376001 | 2.128502 |
| H | -1.517623 | -0.254629 | 3.612018 |
| H | -1.959132 | 1.039871 | 1.741761 |
| H | -3.574806 | 1.044332 | 1.102302 |
| O | 0.426709 | 0.118827 | 3.277697 |
| O | -0.237339 | 1.479939 | 1.633321 |
| C | 1.398050 | -0.919915 | 3.521841 |
| H | 0.916089 | -1.705607 | 4.112962 |
| H | 2.209616 | -0.489458 | 4.119193 |
| H | 1.460974 | -2.363141 | 1.865937 |
| H | 2.954666 | -1.479923 | 2.074982 |
| H | -0.556499 | -5.876985 | 0.306508 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{A}_{(R)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 2 Electronic energy : HF=-3550.3513294

Zero-point correction= 1.282422 (Hartree/Particle)

Thermal correction to Energy= 1.365334

Thermal correction to Enthalpy= 1.366278

Thermal correction to Gibbs Free Energy= 1.155776

Sum of electronic and zero-point Energies= -3549.068907

Sum of electronic and thermal Energies= -3548.985996

Sum of electronic and thermal Enthalpies= -3548.985052

Sum of electronic and thermal Free Energies= -3549.195554

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -5.611991 | -0.975498 | 2.776512 |
| H | -6.313307 | -1.816784 | 2.830958 |
| C | -4.935048 | -0.831618 | 4.143469 |
| H | -4.138083 | -0.072598 | 4.088952 |
| H | -5.677183 | -0.475102 | 4.859933 |
| O | -4.440309 | -2.063748 | 4.654101 |
| H | -3.831875 | -2.442378 | 4.007496 |
| C | -6.444170 | 0.289978 | 2.447119 |

| | | | |
|---|---|---|---|
| O | -7.153274 | 0.804138 | 3.307942 |
| N | -6.362488 | 0.781267 | 1.170324 |
| H | -5.725359 | 0.343245 | 0.519173 |
| C | -7.110341 | 1.960856 | 0.708421 |
| H | -6.428825 | 2.755931 | 0.395905 |
| H | -7.757322 | 1.704726 | -0.135990 |
| C | 2.355880 | 6.712105 | 2.166284 |
| H | 2.815823 | 6.976314 | 1.208094 |
| C | 3.331834 | 5.933272 | 3.055157 |
| H | 4.199221 | 6.560341 | 3.300125 |
| H | 2.843882 | 5.700287 | 4.011864 |
| C | 3.794162 | 4.632524 | 2.388821 |
| H | 2.913006 | 4.071396 | 2.055513 |
| H | 4.367793 | 4.859972 | 1.482270 |
| C | 4.640629 | 3.730463 | 3.301737 |
| H | 5.631238 | 4.160126 | 3.474265 |
| H | 4.182814 | 3.641097 | 4.294890 |
| N | 4.848620 | 2.384094 | 2.758760 |
| H | 5.657693 | 2.233031 | 2.171746 |
| C | 3.839026 | 1.494526 | 2.600836 |
| N | 4.018433 | 0.436167 | 1.800284 |
| N | 2.689981 | 1.610628 | 3.264133 |
| H | 2.520158 | 2.421117 | 3.835511 |

| | | | |
|---|---|---|---|
| C | 0.297790 | 0.548323 | -4.083943 |
| H | 0.632272 | 1.590467 | -3.938934 |
| H | 0.086962 | 0.424376 | -5.159075 |
| O | -0.849179 | 0.239140 | -3.360046 |
| C | 2.524850 | 0.192525 | -1.183332 |
| C | -0.933801 | 3.548831 | -1.529304 |
| C | -4.293635 | 0.111147 | -1.999017 |
| C | -0.815019 | -3.231714 | -1.905917 |
| C | 1.883154 | 1.427355 | -1.205880 |
| C | 2.550318 | 2.726222 | -1.184379 |
| C | 1.556674 | 3.664909 | -1.295692 |
| C | 0.303192 | 2.933712 | -1.369476 |
| C | 1.664546 | 5.158182 | -1.386189 |
| C | 4.025722 | 3.001600 | -1.040245 |
| C | 4.962247 | 2.393684 | -2.107701 |
| C | 5.763768 | 1.194769 | -1.634632 |
| O | 6.351472 | 0.565997 | -2.642778 |
| O | 5.876391 | 0.835290 | -0.464282 |
| C | -2.161586 | 2.914927 | -1.691619 |
| C | -3.395473 | 3.607533 | -2.016390 |
| C | -4.354215 | 2.629998 | -2.171631 |
| C | -3.675904 | 1.357396 | -1.925883 |
| C | -3.537269 | 5.083499 | -2.226969 |

| | | | |
|---|---|---|---|
| C | -5.737858 | 2.754400 | -2.614278 |
| C | -6.547042 | 3.819529 | -2.486258 |
| C | -3.649629 | -1.123123 | -1.942407 |
| C | -4.312401 | -2.395476 | -2.182957 |
| C | -3.319296 | -3.348220 | -2.187084 |
| C | -2.067772 | -2.628744 | -1.944770 |
| C | -5.774707 | -2.577839 | -2.451312 |
| C | -3.411547 | -4.783711 | -2.432852 |
| C | -4.442540 | -5.588386 | -2.130833 |
| C | 0.402719 | -2.590100 | -1.697381 |
| C | 1.680817 | -3.279366 | -1.640632 |
| C | 2.625633 | -2.318785 | -1.392099 |
| C | 1.914582 | -1.049865 | -1.328622 |
| C | 1.878081 | -4.754336 | -1.823782 |
| C | 4.102876 | -2.521401 | -1.210780 |
| C | 4.890035 | -2.554609 | -2.555262 |
| C | 6.355990 | -2.783785 | -2.300518 |
| O | 6.672724 | -4.083478 | -2.195629 |
| O | 7.207116 | -1.915719 | -2.142893 |
| N | 0.528141 | 1.586646 | -1.308995 |
| N | -2.361554 | 1.561705 | -1.628056 |
| N | -2.305738 | -1.299537 | -1.763455 |
| N | 0.573048 | -1.249434 | -1.490341 |

| | | | |
|---|---|---|---|
| H | 2.700274 | 5.499708 | -1.311714 |
| H | 1.098134 | 5.657965 | -0.591932 |
| H | 1.269796 | 5.527383 | -2.340436 |
| H | -4.290592 | 5.291223 | -2.993365 |
| H | -2.597148 | 5.538381 | -2.551309 |
| H | -3.854388 | 5.605425 | -1.314086 |
| H | -5.947201 | -3.482736 | -3.040826 |
| H | -6.190802 | -1.731541 | -3.006838 |
| H | -6.359555 | -2.676772 | -1.527015 |
| H | 2.909244 | -5.049793 | -1.610392 |
| H | 1.652952 | -5.068833 | -2.850534 |
| H | 1.226803 | -5.337790 | -1.162726 |
| H | -7.553874 | 3.801902 | -2.891785 |
| H | -6.250207 | 4.723453 | -1.965709 |
| H | -4.416121 | -6.644686 | -2.380071 |
| H | -5.326992 | -5.232728 | -1.612732 |
| H | 5.702028 | 3.132911 | -2.441495 |
| H | 4.417204 | 2.097644 | -3.008473 |
| H | 4.378983 | 2.659948 | -0.061736 |
| H | 4.163891 | 4.085966 | -1.040646 |
| H | 4.772518 | -1.604300 | -3.079899 |
| H | 4.502711 | -3.357639 | -3.186722 |
| H | 4.280233 | -3.461916 | -0.678234 |

| | | | |
|---|---|---|---|
| H | 4.529014 | -1.732185 | -0.583697 |
| H | 3.598531 | 0.194662 | -1.069072 |
| H | -0.933057 | 4.631729 | -1.574259 |
| H | -5.358996 | 0.098215 | -2.198732 |
| H | -0.779760 | -4.305324 | -2.051482 |
| H | -6.143895 | 1.879938 | -3.121657 |
| H | -2.544982 | -5.236457 | -2.914140 |
| Fe | -0.884479 | 0.138363 | -1.509234 |
| H | 1.460856 | 6.117974 | 1.953870 |
| H | -7.719158 | 2.301350 | 1.546453 |
| H | -4.885009 | -1.198340 | 1.987480 |
| H | 6.779482 | -0.279935 | -2.332998 |
| H | 1.154500 | -0.105832 | -3.845115 |
| H | 7.620962 | -4.129689 | -1.982467 |
| H | 2.034567 | 7.640747 | 2.648003 |
| C | -1.122753 | -0.002618 | 0.665047 |
| C | -2.415672 | 0.544741 | 1.279450 |
| C | -0.106168 | 0.571426 | 1.517008 |
| N | -0.153559 | -2.536887 | 2.827081 |
| C | -0.859307 | -2.586122 | 1.583018 |
| H | -0.994029 | -1.360572 | 1.043063 |
| C | 1.180351 | -2.955735 | 2.918417 |
| C | 2.094170 | -2.349016 | 3.807934 |

| | | | |
|---|---|---|---|
| C | 1.652641 | -4.038429 | 2.142926 |
| C | 3.412651 | -2.793187 | 3.896034 |
| H | 1.782028 | -1.513357 | 4.422076 |
| C | 2.972732 | -4.468713 | 2.235792 |
| H | 0.969416 | -4.565125 | 1.486514 |
| C | 3.870984 | -3.851509 | 3.110644 |
| H | 4.088590 | -2.297742 | 4.588341 |
| H | 3.294149 | -5.314287 | 1.632702 |
| H | 4.897300 | -4.197018 | 3.188547 |
| C | -0.741321 | -1.760146 | 3.922325 |
| H | -0.157096 | -0.849374 | 4.106814 |
| H | -0.235933 | -3.034296 | 0.815139 |
| C | -2.242499 | -3.215961 | 1.619751 |
| H | -2.928797 | -2.679106 | 2.282873 |
| H | -2.688164 | -3.201399 | 0.622993 |
| H | -2.198698 | -4.257909 | 1.964454 |
| C | -1.955984 | 1.856719 | 1.929758 |
| O | -0.569004 | 1.624287 | 2.276008 |
| H | -2.001205 | 2.694314 | 1.226168 |
| H | -2.484595 | 2.125528 | 2.848781 |
| H | -3.216359 | 0.711722 | 0.560984 |
| H | -2.804243 | -0.127652 | 2.058931 |
| O | 1.073570 | 0.222973 | 1.722714 |

| | | | |
|---|---|---|---|
| H | 1.875398 | 1.100927 | 2.826115 |
| H | -1.717227 | -1.411297 | 3.581295 |
| C | -0.924243 | -2.560186 | 5.215724 |
| H | 0.032880 | -2.908534 | 5.613098 |
| H | -1.410322 | -1.940619 | 5.975716 |
| H | -1.554032 | -3.438018 | 5.042634 |
| H | 4.722755 | 0.489425 | 1.066710 |
| H | 3.191370 | -0.123949 | 1.607780 |

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$$\left[ {}^{3}\mathbf{D}^{A}_{(R)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 1 Electronic energy : HF=-3550.3959077

Zero-point correction= 1.287004 (Hartree/Particle)

Thermal correction to Energy= 1.371029

Thermal correction to Enthalpy= 1.371973

Thermal correction to Gibbs Free Energy= 1.155084

Sum of electronic and zero-point Energies= -3549.108904

Sum of electronic and thermal Energies= -3549.024879

Sum of electronic and thermal Enthalpies= -3549.023935

Sum of electronic and thermal Free Energies= -3549.240824

.....

Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.996777 | -3.147470 | 2.149647 |
| H | -5.547756 | -4.079560 | 2.314400 |
| C | -3.824826 | -3.096254 | 3.131422 |
| H | -3.233072 | -2.182978 | 2.965832 |
| H | -4.208421 | -3.065779 | 4.153677 |
| O | -3.008049 | -4.259915 | 3.035084 |
| H | -2.772004 | -4.377501 | 2.105458 |
| C | -6.000592 | -1.989295 | 2.369316 |
| O | -6.537188 | -1.833932 | 3.461537 |
| N | -6.266223 | -1.184815 | 1.288140 |
| H | -5.702763 | -1.297808 | 0.457190 |
| C | -7.219945 | -0.063953 | 1.316746 |
| H | -6.739208 | 0.859578 | 0.982954 |
| H | -8.084213 | -0.268996 | 0.675205 |
| C | 1.262923 | 5.775060 | 4.190061 |
| H | 1.532136 | 6.414106 | 3.341913 |
| C | 2.462288 | 4.944448 | 4.658856 |
| H | 3.263995 | 5.607781 | 5.009593 |
| H | 2.168217 | 4.335955 | 5.525349 |
| C | 2.985268 | 4.030674 | 3.545565 |

| | | | |
|---|---|---|---|
| H | 2.152211 | 3.433634 | 3.154343 |
| H | 3.340891 | 4.637464 | 2.704388 |
| C | 4.116435 | 3.088346 | 3.990054 |
| H | 5.034940 | 3.644551 | 4.196470 |
| H | 3.860610 | 2.579568 | 4.927514 |
| N | 4.446963 | 2.072583 | 2.984963 |
| H | 5.112703 | 2.321755 | 2.262721 |
| C | 3.597213 | 1.075261 | 2.657800 |
| N | 3.823228 | 0.362265 | 1.542672 |
| N | 2.575618 | 0.722857 | 3.439018 |
| H | 2.293545 | 1.335685 | 4.186307 |
| C | -0.176619 | 1.895792 | -3.820700 |
| H | 0.088334 | 2.908428 | -3.471866 |
| H | -0.447843 | 1.977900 | -4.885399 |
| O | -1.256491 | 1.345988 | -3.126191 |
| C | 2.184646 | 1.239243 | -1.157152 |
| C | -1.585137 | 4.203965 | -0.573715 |
| C | -4.624742 | 0.609734 | -1.662686 |
| C | -0.870084 | -2.398176 | -2.069238 |
| C | 1.433286 | 2.372057 | -0.860053 |
| C | 1.976776 | 3.688565 | -0.537163 |
| C | 0.895611 | 4.519431 | -0.390363 |
| C | -0.287262 | 3.704705 | -0.611166 |

| | | | |
|---|---|---|---|
| C | 0.859881 | 5.985081 | -0.073105 |
| C | 3.420598 | 4.061998 | -0.312408 |
| C | 4.411395 | 3.825239 | -1.473875 |
| C | 5.274501 | 2.586987 | -1.315840 |
| O | 5.795724 | 2.194903 | -2.466777 |
| O | 5.483431 | 2.010790 | -0.247909 |
| C | -2.752955 | 3.486411 | -0.816134 |
| C | -4.080591 | 4.075128 | -0.832856 |
| C | -4.947634 | 3.053940 | -1.147612 |
| C | -4.122880 | 1.860933 | -1.324791 |
| C | -4.390471 | 5.523921 | -0.612633 |
| C | -6.395090 | 3.090428 | -1.333762 |
| C | -7.268404 | 3.880267 | -0.688804 |
| C | -3.870679 | -0.544231 | -1.864015 |
| C | -4.432462 | -1.839979 | -2.209744 |
| C | -3.364556 | -2.706314 | -2.302214 |
| C | -2.170921 | -1.904675 | -2.038162 |
| C | -5.880764 | -2.116144 | -2.485681 |
| C | -3.345919 | -4.124462 | -2.644097 |
| C | -4.310623 | -5.025746 | -2.399048 |
| C | 0.294524 | -1.662853 | -1.877828 |
| C | 1.629624 | -2.224679 | -1.992600 |
| C | 2.501755 | -1.194800 | -1.756717 |

| | | | |
|---|---|---|---|
| C | 1.684609 | -0.017739 | -1.488455 |
| C | 1.937239 | -3.655170 | -2.315834 |
| C | 4.002373 | -1.258785 | -1.772273 |
| C | 4.615191 | -0.997468 | -3.180647 |
| C | 6.115998 | -1.096019 | -3.113713 |
| O | 6.591223 | -2.278251 | -3.527336 |
| O | 6.870205 | -0.231789 | -2.678290 |
| N | 0.064278 | 2.410057 | -0.875915 |
| N | -2.808204 | 2.147104 | -1.091822 |
| N | -2.510252 | -0.614349 | -1.761169 |
| N | 0.358834 | -0.331243 | -1.570451 |
| H | 1.862589 | 6.416253 | -0.013788 |
| H | 0.360786 | 6.182522 | 0.883642 |
| H | 0.312531 | 6.545185 | -0.840131 |
| H | -5.332839 | 5.793773 | -1.097532 |
| H | -3.605434 | 6.168614 | -1.020456 |
| H | -4.491290 | 5.770439 | 0.452863 |
| H | -5.984132 | -2.964775 | -3.168067 |
| H | -6.370917 | -1.252917 | -2.946593 |
| H | -6.449012 | -2.364833 | -1.578820 |
| H | 2.999661 | -3.876921 | -2.186669 |
| H | 1.669535 | -3.902473 | -3.350934 |
| H | 1.383258 | -4.339370 | -1.663884 |

| | | | |
|---|---|---|---|
| H | -8.328348 | 3.845677 | -0.920966 |
| H | -6.963318 | 4.566087 | 0.094792 |
| H | -4.201741 | -6.057992 | -2.716856 |
| H | -5.221752 | -4.775324 | -1.865652 |
| H | 5.114022 | 4.665819 | -1.550152 |
| H | 3.906640 | 3.769399 | -2.441709 |
| H | 3.810214 | 3.527391 | 0.560935 |
| H | 3.452356 | 5.122060 | -0.047385 |
| H | 4.349116 | 0.008705 | -3.515016 |
| H | 4.228308 | -1.723350 | -3.898192 |
| H | 4.331268 | -2.242042 | -1.419963 |
| H | 4.437921 | -0.530060 | -1.082338 |
| H | 3.258338 | 1.334549 | -1.115065 |
| H | -1.695578 | 5.260132 | -0.355834 |
| H | -5.697612 | 0.526522 | -1.792266 |
| H | -0.745994 | -3.453158 | -2.283892 |
| H | -6.793705 | 2.400890 | -2.077665 |
| H | -2.447595 | -4.476328 | -3.150245 |
| Fe | -1.209284 | 0.901337 | -1.328607 |
| H | 0.438888 | 5.128277 | 3.870405 |
| H | -7.558528 | 0.047148 | 2.347546 |
| H | -4.620008 | -3.159482 | 1.117782 |
| H | 6.291187 | 1.333149 | -2.375909 |

| | | | |
|---|---|---|---|
| H | 0.736012 | 1.278133 | -3.762650 |
| H | 7.555588 | -2.260847 | -3.397440 |
| H | 0.890071 | 6.423032 | 4.989284 |
| C | -1.362809 | 0.123683 | 0.811728 |
| C | -2.447976 | 0.780714 | 1.672729 |
| C | -0.173826 | 0.284918 | 1.603326 |
| N | 1.276900 | -4.815788 | 1.503387 |
| C | 0.629892 | -5.894867 | 0.909290 |
| H | -1.527204 | -0.909671 | 0.521143 |
| C | 2.667406 | -4.679830 | 1.387848 |
| C | 3.314804 | -3.452004 | 1.656350 |
| C | 3.472282 | -5.770788 | 0.984160 |
| C | 4.692558 | -3.324289 | 1.501224 |
| H | 2.741481 | -2.591727 | 1.976939 |
| C | 4.847712 | -5.623569 | 0.826610 |
| H | 3.019298 | -6.743707 | 0.837877 |
| C | 5.475868 | -4.401456 | 1.075868 |
| H | 5.153498 | -2.363838 | 1.716798 |
| H | 5.436153 | -6.485360 | 0.521875 |
| H | 6.550246 | -4.295444 | 0.960221 |
| C | 0.523402 | -3.835477 | 2.304125 |
| H | 0.736878 | -2.825121 | 1.941079 |
| H | 1.135441 | -6.317448 | 0.048778 |

| | | | |
|---|---|---|---|
| C | -0.820566 | -6.182318 | 1.099761 |
| H | -1.491722 | -5.484932 | 0.560664 |
| H | -1.040563 | -7.177945 | 0.701582 |
| H | -1.127130 | -6.177900 | 2.152586 |
| C | -1.640245 | 1.862660 | 2.397110 |
| O | -0.299975 | 1.314511 | 2.506458 |
| H | -1.583989 | 2.786688 | 1.814477 |
| H | -1.985675 | 2.088299 | 3.409946 |
| H | -3.277914 | 1.210523 | 1.112672 |
| H | -2.870438 | 0.077291 | 2.406744 |
| O | 0.900384 | -0.355885 | 1.634640 |
| H | 1.813464 | 0.210011 | 2.935001 |
| H | -0.536928 | -3.999993 | 2.125292 |
| C | 0.787780 | -3.946258 | 3.808681 |
| H | 1.841861 | -3.779952 | 4.047915 |
| H | 0.190828 | -3.200220 | 4.342704 |
| H | 0.505104 | -4.935585 | 4.180730 |
| H | 4.447923 | 0.766759 | 0.850059 |
| H | 3.024976 | -0.162371 | 1.190836 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{A}_{(S)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 1 Electronic energy : HF=-3550.3429256

Zero-point correction= 1.284783 (Hartree/Particle)

Thermal correction to Energy= 1.367556

Thermal correction to Enthalpy= 1.368500

Thermal correction to Gibbs Free Energy= 1.160663

Sum of electronic and zero-point Energies= -3549.058143

Sum of electronic and thermal Energies= -3548.975370

Sum of electronic and thermal Enthalpies= -3548.974425

Sum of electronic and thermal Free Energies= -3549.182263

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -6.743691 | -2.494739 | 1.694163 |
| H | -7.093809 | -2.988868 | 2.604081 |
| C | -5.260959 | -2.148911 | 1.799836 |
| H | -5.108631 | -1.364013 | 2.553741 |
| H | -4.711728 | -3.042911 | 2.139511 |
| O | -4.777267 | -1.722617 | 0.532972 |
| H | -4.088269 | -1.035196 | 0.684240 |
| C | -7.707671 | -1.290697 | 1.479418 |

| | | | |
|---|---|---|---|
| O | -8.833029 | -1.302548 | 1.971934 |
| N | -7.237915 | -0.255828 | 0.712175 |
| H | -6.288836 | -0.352588 | 0.365057 |
| C | -7.997604 | 0.973095 | 0.446804 |
| H | -7.452612 | 1.852766 | 0.805555 |
| H | -8.198692 | 1.089748 | -0.624778 |
| C | 1.505370 | 4.641403 | 3.693929 |
| H | 1.328117 | 4.739377 | 2.619027 |
| C | 2.889185 | 4.042076 | 3.972967 |
| H | 3.666702 | 4.750537 | 3.656044 |
| H | 3.023868 | 3.905622 | 5.054837 |
| C | 3.106097 | 2.711251 | 3.241161 |
| H | 2.320575 | 2.002122 | 3.532926 |
| H | 2.980557 | 2.865482 | 2.164170 |
| C | 4.493139 | 2.103769 | 3.500745 |
| H | 5.262915 | 2.870485 | 3.371055 |
| H | 4.587396 | 1.742098 | 4.531548 |
| N | 4.853508 | 1.012896 | 2.588811 |
| H | 5.343600 | 1.239878 | 1.721588 |
| C | 4.471138 | -0.259233 | 2.702841 |
| N | 4.989320 | -1.172585 | 1.868053 |
| N | 3.645431 | -0.658786 | 3.687688 |
| H | 3.022531 | 0.018757 | 4.098074 |

| | | | |
|---|---|---|---|
| C | -0.335255 | 0.558536 | -4.131473 |
| H | 0.409934 | -0.256819 | -4.106992 |
| H | -0.104659 | 1.179508 | -5.013174 |
| O | -0.309435 | 1.358344 | -2.994512 |
| C | 2.826443 | 0.586942 | -0.983350 |
| C | -0.493099 | 4.070669 | -0.534538 |
| C | -3.927814 | 0.939792 | -1.811130 |
| C | -0.628992 | -2.552692 | -2.285317 |
| C | 2.244859 | 1.835432 | -0.763733 |
| C | 2.971988 | 3.087265 | -0.538352 |
| C | 2.014427 | 4.069003 | -0.447947 |
| C | 0.729492 | 3.406507 | -0.588414 |
| C | 2.181930 | 5.552751 | -0.292120 |
| C | 4.457798 | 3.312959 | -0.383748 |
| C | 5.396236 | 2.760664 | -1.474533 |
| C | 6.064914 | 1.438119 | -1.160319 |
| O | 6.612369 | 0.902140 | -2.236877 |
| O | 6.119133 | 0.910886 | -0.045795 |
| C | -1.741008 | 3.504902 | -0.763448 |
| C | -2.978926 | 4.264570 | -0.801902 |
| C | -3.958131 | 3.380016 | -1.185892 |
| C | -3.292470 | 2.087621 | -1.354219 |
| C | -3.114677 | 5.714343 | -0.452385 |

| | | | |
|---|---|---|---|
| C | -5.387287 | 3.599579 | -1.375822 |
| C | -5.986619 | 4.741575 | -1.748118 |
| C | -3.329860 | -0.292115 | -2.052155 |
| C | -4.046548 | -1.452801 | -2.555947 |
| C | -3.114487 | -2.454366 | -2.682768 |
| C | -1.840162 | -1.875857 | -2.265287 |
| C | -5.508160 | -1.493236 | -2.869137 |
| C | -3.281306 | -3.824741 | -3.158523 |
| C | -4.360131 | -4.603633 | -2.986758 |
| C | 0.610069 | -2.007650 | -1.958193 |
| C | 1.865872 | -2.719938 | -2.077773 |
| C | 2.845246 | -1.833195 | -1.703454 |
| C | 2.172317 | -0.586176 | -1.364162 |
| C | 2.016425 | -4.136732 | -2.548431 |
| C | 4.324391 | -2.090494 | -1.688278 |
| C | 5.003411 | -1.937785 | -3.080928 |
| C | 6.462704 | -2.295510 | -2.979734 |
| O | 6.773245 | -3.458187 | -3.566774 |
| O | 7.312948 | -1.647589 | -2.375751 |
| N | 0.896677 | 2.066653 | -0.774571 |
| N | -1.965138 | 2.188851 | -1.065670 |
| N | -2.004443 | -0.578590 | -1.869445 |
| N | 0.821916 | -0.729449 | -1.517049 |

| | | | |
|---|---|---|---|
| H | 3.232356 | 5.845806 | -0.216767 |
| H | 1.675959 | 5.934146 | 0.603004 |
| H | 1.755578 | 6.088113 | -1.148488 |
| H | -4.124066 | 5.928353 | -0.089018 |
| H | -2.934686 | 6.368648 | -1.315941 |
| H | -2.407024 | 6.006744 | 0.329890 |
| H | -5.732301 | -2.298437 | -3.574014 |
| H | -5.853636 | -0.552800 | -3.310685 |
| H | -6.094788 | -1.668844 | -1.959296 |
| H | 1.362695 | -4.819950 | -1.994411 |
| H | 3.042712 | -4.496785 | -2.426433 |
| H | 1.759962 | -4.241786 | -3.609979 |
| H | -7.067104 | 4.798520 | -1.837435 |
| H | -5.430005 | 5.638711 | -1.997173 |
| H | -4.395322 | -5.606987 | -3.400485 |
| H | -5.222733 | -4.278441 | -2.415001 |
| H | 6.219719 | 3.464134 | -1.657072 |
| H | 4.882903 | 2.653044 | -2.434069 |
| H | 4.807686 | 2.927859 | 0.581773 |
| H | 4.618677 | 4.392447 | -0.328317 |
| H | 4.921114 | -0.898659 | -3.411616 |
| H | 4.514152 | -2.579361 | -3.815103 |
| H | 4.518254 | -3.110168 | -1.330948 |

| | | | |
|---|---|---|---|
| H | 4.830429 | -1.416264 | -0.992417 |
| H | 3.897422 | 0.519722 | -0.872255 |
| H | -0.464684 | 5.139195 | -0.353552 |
| H | -4.987015 | 1.015456 | -2.024532 |
| H | -0.642335 | -3.586206 | -2.611582 |
| H | -6.024816 | 2.736050 | -1.191754 |
| H | -2.436209 | -4.244653 | -3.704648 |
| Fe | -0.576993 | 0.713933 | -1.269925 |
| H | 0.707887 | 4.016547 | 4.104948 |
| H | -8.946464 | 0.890380 | 0.978961 |
| H | -6.884807 | -3.197761 | 0.863390 |
| H | 6.972929 | -0.012066 | -2.069198 |
| H | -1.318915 | 0.092658 | -4.313376 |
| H | 7.723281 | -3.610885 | -3.418718 |
| H | 1.411929 | 5.634460 | 4.144664 |
| C | -0.830675 | 0.136946 | 0.817026 |
| C | -2.060575 | 0.630590 | 1.456976 |
| C | 0.252927 | 0.566255 | 1.812341 |
| N | -0.490950 | -2.515351 | 2.930378 |
| C | -1.359011 | -2.337380 | 1.788513 |
| H | -0.985977 | -1.229218 | 1.033420 |
| C | 0.783149 | -3.038291 | 2.838178 |
| C | 1.507983 | -3.468248 | 3.984598 |

| | | | |
|---|---|---|---|
| C | 1.439402 | -3.150288 | 1.585215 |
| C | 2.787973 | -4.011249 | 3.870507 |
| H | 1.051177 | -3.428264 | 4.966101 |
| C | 2.706359 | -3.716491 | 1.488377 |
| H | 0.957337 | -2.779015 | 0.691138 |
| C | 3.406545 | -4.154417 | 2.622035 |
| H | 3.292584 | -4.354646 | 4.770148 |
| H | 3.146764 | -3.815570 | 0.500298 |
| H | 4.381175 | -4.625185 | 2.535244 |
| C | -1.039551 | -2.110995 | 4.230794 |
| H | -0.219332 | -1.790177 | 4.881579 |
| H | -2.292300 | -1.918595 | 2.159653 |
| C | -1.657171 | -3.556602 | 0.930009 |
| H | -2.484685 | -3.312010 | 0.259986 |
| H | -0.817545 | -3.892181 | 0.318728 |
| H | -1.967052 | -4.401739 | 1.561146 |
| H | 3.330145 | -1.624829 | 3.714515 |
| H | 4.508545 | -2.060219 | 1.766530 |
| H | 5.584733 | -0.845883 | 1.114864 |
| H | -1.656575 | -1.222779 | 4.061302 |
| C | -1.875588 | -3.196702 | 4.917757 |
| H | -2.271390 | -2.827147 | 5.869912 |
| H | -2.723975 | -3.483854 | 4.289548 |

| | | | |
|---|---|---|---|
| H | -1.284126 | -4.095791 | 5.116227 |
| C | -0.379705 | 1.787292 | 2.497948 |
| O | -1.796966 | 1.566924 | 2.433383 |
| O | -3.235260 | 0.302368 | 1.302953 |
| H | -0.144757 | 2.715521 | 1.969710 |
| H | -0.119212 | 1.902014 | 3.555862 |
| H | 1.208501 | 0.804688 | 1.347050 |
| H | 0.431411 | -0.223304 | 2.558265 |

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$$\left[ {}^{3}\mathbf{D}^{A}_{(S)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 0 Electronic energy : HF=-3550.3800444

Zero-point correction= 1.287344 (Hartree/Particle)

Thermal correction to Energy= 1.371594

Thermal correction to Enthalpy= 1.372538

Thermal correction to Gibbs Free Energy= 1.156734

Sum of electronic and zero-point Energies= -3549.092701

Sum of electronic and thermal Energies= -3549.008451

Sum of electronic and thermal Enthalpies= -3549.007506

Sum of electronic and thermal Free Energies= -3549.223310

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | -6.708394 | -2.587154 | 1.370356 |
| H | -7.093924 | -3.185418 | 2.200238 |
| C | -5.235217 | -2.253390 | 1.577510 |
| H | -5.119599 | -1.536937 | 2.403203 |
| H | -4.704212 | -3.175525 | 1.868692 |
| O | -4.694012 | -1.727654 | 0.375858 |
| H | -4.011222 | -1.052534 | 0.610270 |
| C | -7.676848 | -1.375348 | 1.255607 |
| O | -8.829529 | -1.463758 | 1.670906 |
| N | -7.182308 | -0.239556 | 0.666359 |
| H | -6.216469 | -0.275085 | 0.357036 |
| C | -7.955653 | 1.002148 | 0.524434 |
| H | -7.451786 | 1.833369 | 1.029318 |
| H | -8.099222 | 1.259588 | -0.531430 |
| C | 1.560954 | 4.259328 | 4.148380 |
| H | 1.390962 | 4.504678 | 3.095769 |
| C | 2.938342 | 3.615555 | 4.352282 |
| H | 3.724769 | 4.351554 | 4.136371 |
| H | 3.063820 | 3.336079 | 5.407564 |
| C | 3.145631 | 2.389438 | 3.454166 |

| | | | |
|---|---|---|---|
| H | 2.340252 | 1.666651 | 3.635215 |
| H | 3.047395 | 2.685155 | 2.404052 |
| C | 4.510517 | 1.716642 | 3.658776 |
| H | 5.307361 | 2.464426 | 3.604008 |
| H | 4.585561 | 1.254664 | 4.650385 |
| N | 4.834267 | 0.703663 | 2.648011 |
| H | 5.337838 | 0.990523 | 1.806035 |
| C | 4.410599 | -0.558932 | 2.648967 |
| N | 4.903784 | -1.413624 | 1.736757 |
| N | 3.569228 | -1.020285 | 3.591785 |
| H | 2.955407 | -0.370103 | 4.056537 |
| C | -0.301015 | 1.089667 | -4.084610 |
| H | 0.394308 | 0.231951 | -4.119753 |
| H | -0.034155 | 1.755542 | -4.922434 |
| O | -0.227599 | 1.805821 | -2.893462 |
| C | 2.882627 | 0.706148 | -0.971427 |
| C | -0.281238 | 4.259772 | -0.119883 |
| C | -3.853898 | 1.429551 | -1.693211 |
| C | -0.729912 | -2.177918 | -2.424829 |
| C | 2.358031 | 1.951903 | -0.626287 |
| C | 3.139899 | 3.139679 | -0.274254 |
| C | 2.225912 | 4.144846 | -0.064371 |
| C | 0.912704 | 3.557235 | -0.263397 |

| | | | |
|---|---|---|---|
| C | 2.458807 | 5.591048 | 0.264336 |
| C | 4.634861 | 3.287373 | -0.108981 |
| C | 5.550911 | 2.767061 | -1.233604 |
| C | 6.142989 | 1.389428 | -1.019270 |
| O | 6.673879 | 0.908395 | -2.129313 |
| O | 6.154274 | 0.774577 | 0.051120 |
| C | -1.553804 | 3.773442 | -0.394667 |
| C | -2.761891 | 4.578007 | -0.323835 |
| C | -3.779561 | 3.780746 | -0.790361 |
| C | -3.166730 | 2.493460 | -1.120230 |
| C | -2.837415 | 5.980148 | 0.196498 |
| C | -5.203236 | 4.071084 | -0.919723 |
| C | -5.763823 | 5.267095 | -1.158063 |
| C | -3.313192 | 0.200357 | -2.052919 |
| C | -4.087520 | -0.893743 | -2.618370 |
| C | -3.207125 | -1.931952 | -2.799664 |
| C | -1.903843 | -1.439341 | -2.366469 |
| C | -5.549815 | -0.848064 | -2.929403 |
| C | -3.447714 | -3.271426 | -3.330147 |
| C | -4.547111 | -4.014078 | -3.130266 |
| C | 0.538908 | -1.710755 | -2.090720 |
| C | 1.754656 | -2.483588 | -2.241410 |
| C | 2.779014 | -1.667904 | -1.828549 |

| | | | |
|---|---|---|---|
| C | 2.173105 | -0.402838 | -1.435058 |
| C | 1.833101 | -3.881868 | -2.780482 |
| C | 4.241408 | -2.005470 | -1.820506 |
| C | 4.940623 | -1.805894 | -3.197111 |
| C | 6.383220 | -2.228129 | -3.106716 |
| O | 6.657569 | -3.355076 | -3.775643 |
| O | 7.249246 | -1.659930 | -2.447319 |
| N | 1.020911 | 2.240300 | -0.599045 |
| N | -1.832528 | 2.511934 | -0.845100 |
| N | -2.000182 | -0.155782 | -1.908498 |
| N | 0.818602 | -0.463915 | -1.601523 |
| H | 3.522251 | 5.842339 | 0.296658 |
| H | 2.032691 | 5.868697 | 1.236414 |
| H | 1.993453 | 6.243475 | -0.483196 |
| H | -3.836562 | 6.190304 | 0.589199 |
| H | -2.632041 | 6.724726 | -0.584313 |
| H | -2.116607 | 6.148164 | 1.003113 |
| H | -5.810179 | -1.607338 | -3.672050 |
| H | -5.848749 | 0.128416 | -3.324575 |
| H | -6.149537 | -1.043353 | -2.032217 |
| H | 1.122675 | -4.552067 | -2.283185 |
| H | 2.831911 | -4.310273 | -2.650320 |
| H | 1.603026 | -3.917288 | -3.852809 |

| | | | |
|---|---|---|---|
| H | -6.842786 | 5.374997 | -1.211894 |
| H | -5.175892 | 6.162447 | -1.330142 |
| H | -4.650950 | -4.994617 | -3.585459 |
| H | -5.358910 | -3.676707 | -2.494550 |
| H | 6.413574 | 3.435546 | -1.357324 |
| H | 5.041266 | 2.761756 | -2.201130 |
| H | 4.967681 | 2.828192 | 0.830623 |
| H | 4.843578 | 4.353042 | 0.014675 |
| H | 4.904863 | -0.746868 | -3.468331 |
| H | 4.432069 | -2.382821 | -3.970770 |
| H | 4.376376 | -3.053468 | -1.522266 |
| H | 4.776697 | -1.399607 | -1.085045 |
| H | 3.948691 | 0.578785 | -0.871536 |
| H | -0.207587 | 5.298620 | 0.181604 |
| H | -4.911188 | 1.570913 | -1.882504 |
| H | -0.800864 | -3.194410 | -2.794364 |
| H | -5.870132 | 3.217085 | -0.805977 |
| H | -2.649992 | -3.695441 | -3.941079 |
| Fe | -0.510335 | 1.023382 | -1.229809 |
| H | 0.755724 | 3.590042 | 4.463860 |
| H | -8.929627 | 0.831641 | 0.985162 |
| H | -6.807628 | -3.190513 | 0.459113 |
| H | 6.983449 | -0.033744 | -2.028471 |

| | | | |
|---|---|---|---|
| H | -1.310874 | 0.697277 | -4.293880 |
| H | 7.599601 | -3.553774 | -3.630968 |
| H | 1.471025 | 5.182084 | 4.730076 |
| C | -0.778544 | 0.057480 | 0.737424 |
| C | -1.975945 | 0.483618 | 1.451817 |
| C | 0.337064 | 0.304459 | 1.756297 |
| N | -0.869334 | -3.424186 | 2.314741 |
| C | -1.578542 | -3.670967 | 1.137763 |
| H | -0.867275 | -0.967241 | 0.384704 |
| C | 0.478610 | -3.731458 | 2.462619 |
| C | 1.067041 | -3.919923 | 3.738103 |
| C | 1.321045 | -3.848401 | 1.328805 |
| C | 2.416448 | -4.245563 | 3.863879 |
| H | 0.457100 | -3.852638 | 4.631663 |
| C | 2.662379 | -4.188736 | 1.468743 |
| H | 0.916895 | -3.626084 | 0.348835 |
| C | 3.234058 | -4.395513 | 2.733577 |
| H | 2.825934 | -4.418211 | 4.856171 |
| H | 3.267920 | -4.300239 | 0.571609 |
| H | 4.271271 | -4.700267 | 2.837019 |
| C | -1.593939 | -2.725259 | 3.390713 |
| H | -0.869343 | -2.172985 | 3.996179 |
| H | -2.442559 | -3.033537 | 0.987161 |

| | | | |
|---|---|---|---|
| C | -1.519661 | -4.975688 | 0.407546 |
| H | -2.038669 | -4.875537 | -0.549734 |
| H | -0.503606 | -5.333557 | 0.210213 |
| H | -2.025614 | -5.777252 | 0.972745 |
| H | 3.253637 | -1.985414 | 3.543303 |
| H | 4.378891 | -2.256000 | 1.537293 |
| H | 5.516771 | -1.039947 | 1.019725 |
| H | -2.236659 | -1.978353 | 2.914324 |
| C | -2.439919 | -3.655140 | 4.265438 |
| H | -2.988728 | -3.072600 | 5.012741 |
| H | -3.170460 | -4.195539 | 3.656498 |
| H | -1.826188 | -4.394686 | 4.789722 |
| C | -0.235443 | 1.490064 | 2.545337 |
| O | -1.662392 | 1.344161 | 2.477512 |
| O | -3.165810 | 0.194078 | 1.313349 |
| H | 0.041474 | 2.446397 | 2.092844 |
| H | 0.036669 | 1.504221 | 3.606564 |
| H | 1.306398 | 0.540878 | 1.315737 |
| H | 0.476089 | -0.562968 | 2.424543 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{C}_{(R)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 1 Electronic energy : HF=-3550.3240547

Zero-point correction= 1.283812 (Hartree/Particle)

Thermal correction to Energy= 1.367277

Thermal correction to Enthalpy= 1.368222

Thermal correction to Gibbs Free Energy= 1.155429

Sum of electronic and zero-point Energies= -3549.051884

Sum of electronic and thermal Energies= -3548.968419

Sum of electronic and thermal Enthalpies= -3548.967475

Sum of electronic and thermal Free Energies= -3549.180267

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Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 5.630455 | 0.133068 | -2.959325 |
| H | 6.149770 | -0.383764 | -3.768448 |
| C | 5.101229 | 1.511432 | -3.410736 |
| H | 5.023315 | 2.159140 | -2.525232 |
| H | 5.813749 | 1.985081 | -4.092993 |
| O | 3.856914 | 1.447262 | -4.095110 |
| H | 3.253025 | 0.927130 | -3.535288 |
| C | 6.637083 | 0.328299 | -1.782658 |

| | | | |
|---|---|---|---|
| O | 7.839369 | 0.478687 | -1.986497 |
| N | 6.074574 | 0.384169 | -0.529550 |
| H | 5.064693 | 0.283973 | -0.465973 |
| C | 6.809074 | 0.712357 | 0.704444 |
| H | 6.228129 | 1.417379 | 1.305365 |
| H | 7.010270 | -0.183061 | 1.305782 |
| C | -2.802702 | 5.144098 | 2.211861 |
| H | -3.037429 | 6.213833 | 2.243917 |
| C | -3.244051 | 4.515003 | 0.886180 |
| H | -2.700201 | 5.001963 | 0.067999 |
| H | -2.947774 | 3.458748 | 0.876513 |
| C | -4.748056 | 4.631101 | 0.610852 |
| H | -5.316352 | 4.097481 | 1.383671 |
| H | -5.058241 | 5.682463 | 0.673521 |
| C | -5.175900 | 4.118972 | -0.774591 |
| H | -6.244359 | 4.303351 | -0.927690 |
| H | -4.651112 | 4.659773 | -1.568100 |
| N | -4.956752 | 2.682849 | -0.976381 |
| H | -5.584817 | 2.028367 | -0.509907 |
| C | -3.987151 | 2.106588 | -1.693640 |
| N | -4.069281 | 0.783333 | -1.933907 |
| N | -2.986597 | 2.807224 | -2.244398 |
| H | -2.694194 | 3.713752 | -1.901732 |

| | | | |
|---|---|---|---|
| C | -0.806609 | -3.646719 | 2.388908 |
| H | -1.751437 | -3.093055 | 2.538066 |
| H | -0.676862 | -4.305023 | 3.263769 |
| O | 0.303565 | -2.815257 | 2.278418 |
| C | -2.928743 | -1.150276 | 0.513140 |
| C | 0.179217 | 0.582868 | 3.786658 |
| C | 3.798462 | -1.810937 | 1.690648 |
| C | 0.696872 | -3.635430 | -1.524199 |
| C | -2.401672 | -0.392637 | 1.559976 |
| C | -3.165314 | 0.467596 | 2.461774 |
| C | -2.273252 | 0.913957 | 3.406074 |
| C | -0.981754 | 0.354801 | 3.053840 |
| C | -2.509791 | 1.799120 | 4.594505 |
| C | -4.609223 | 0.892539 | 2.359610 |
| C | -5.695334 | -0.205111 | 2.378253 |
| C | -6.215042 | -0.608979 | 1.014218 |
| O | -6.740956 | -1.819089 | 1.020347 |
| O | -6.176181 | 0.104521 | 0.006393 |
| C | 1.449242 | 0.095328 | 3.499729 |
| C | 2.614004 | 0.318991 | 4.342713 |
| C | 3.649410 | -0.362036 | 3.748722 |
| C | 3.087814 | -0.975629 | 2.542715 |
| C | 2.639227 | 1.157042 | 5.583545 |

| | | | |
|---|---|---|---|
| C | 5.043847 | -0.478247 | 4.160229 |
| C | 5.523898 | -0.423762 | 5.412765 |
| C | 3.277977 | -2.488056 | 0.595476 |
| C | 4.057048 | -3.377712 | -0.249569 |
| C | 3.179848 | -3.894341 | -1.173401 |
| C | 1.873576 | -3.315739 | -0.858048 |
| C | 5.515418 | -3.667827 | -0.076738 |
| C | 3.417058 | -4.862228 | -2.240531 |
| C | 4.533083 | -4.986889 | -2.974566 |
| C | -0.575514 | -3.151870 | -1.225671 |
| C | -1.774055 | -3.533947 | -1.945867 |
| C | -2.807969 | -2.834689 | -1.372361 |
| C | -2.222918 | -2.035835 | -0.303289 |
| C | -1.825254 | -4.515878 | -3.078315 |
| C | -4.259894 | -2.906882 | -1.749682 |
| C | -5.047499 | -4.017617 | -0.993382 |
| C | -6.482160 | -4.027286 | -1.450013 |
| O | -6.781737 | -5.050217 | -2.260032 |
| O | -7.318440 | -3.169418 | -1.181995 |
| N | -1.084100 | -0.413609 | 1.929305 |
| N | 1.770389 | -0.664708 | 2.412180 |
| N | 1.972985 | -2.445631 | 0.188315 |
| N | -0.872689 | -2.247587 | -0.241547 |

| | | | |
|---|---|---|---|
| H | -3.565263 | 2.058498 | 4.713011 |
| H | -1.947310 | 2.738041 | 4.523628 |
| H | -2.193794 | 1.308449 | 5.522383 |
| H | 3.641319 | 1.561561 | 5.754223 |
| H | 2.365370 | 0.581682 | 6.477923 |
| H | 1.943360 | 1.999623 | 5.516562 |
| H | 5.787263 | -4.601275 | -0.576074 |
| H | 5.781689 | -3.761593 | 0.981263 |
| H | 6.138777 | -2.868882 | -0.498025 |
| H | -1.101554 | -4.267474 | -3.863014 |
| H | -2.814857 | -4.546267 | -3.543700 |
| H | -1.592349 | -5.533743 | -2.741918 |
| H | 6.589870 | -0.502975 | 5.602657 |
| H | 4.881032 | -0.327947 | 6.281172 |
| H | 4.617386 | -5.758163 | -3.734115 |
| H | 5.380197 | -4.318457 | -2.861688 |
| H | -6.576760 | 0.151133 | 2.929203 |
| H | -5.359185 | -1.105529 | 2.897955 |
| H | -4.757027 | 1.490558 | 1.453829 |
| H | -4.810279 | 1.573154 | 3.190786 |
| H | -5.026004 | -3.809616 | 0.079912 |
| H | -4.591808 | -4.992698 | -1.172440 |
| H | -4.351443 | -3.093912 | -2.826001 |

| | | | |
|---|---|---|---|
| H | -4.771626 | -1.957863 | -1.561123 |
| H | -3.989757 | -1.069818 | 0.331554 |
| H | 0.076770 | 1.181775 | 4.684622 |
| H | 4.845559 | -1.974165 | 1.913983 |
| H | 0.772212 | -4.335701 | -2.348119 |
| H | 5.762308 | -0.626747 | 3.355343 |
| H | 2.594685 | -5.545945 | -2.451869 |
| Fe | 0.452893 | -1.419657 | 1.061761 |
| H | -3.300954 | 4.667597 | 3.062924 |
| H | 7.764927 | 1.159724 | 0.424010 |
| H | 4.784652 | -0.476483 | -2.626156 |
| H | -7.028198 | -2.123237 | 0.113540 |
| H | -0.946540 | -4.299947 | 1.509399 |
| H | -7.712228 | -4.944417 | -2.525891 |
| H | -1.724093 | 5.032391 | 2.356178 |
| C | 0.770070 | 0.244395 | -0.350781 |
| C | -0.180405 | 0.436720 | -1.539828 |
| C | 2.084227 | 0.225998 | -0.977576 |
| N | 1.452921 | 3.500383 | -0.832730 |
| C | 0.869137 | 2.904390 | 0.331960 |
| H | 0.844166 | 1.549001 | 0.213476 |
| C | 0.671231 | 4.126435 | -1.810762 |
| C | 0.924088 | 3.949962 | -3.191606 |

| | | | |
|---|---|---|---|
| C | -0.385623 | 4.991126 | -1.444374 |
| C | 0.132792 | 4.588701 | -4.145665 |
| H | 1.732981 | 3.304964 | -3.521129 |
| C | -1.166890 | 5.628684 | -2.409803 |
| H | -0.539889 | 5.206855 | -0.392643 |
| C | -0.923833 | 5.425003 | -3.772733 |
| H | 0.348450 | 4.426544 | -5.198340 |
| H | -1.938505 | 6.328482 | -2.093796 |
| H | -1.523860 | 5.928660 | -4.524184 |
| C | 2.909090 | 3.431419 | -1.041580 |
| H | 3.123346 | 3.003543 | -2.023788 |
| H | -0.204388 | 3.104121 | 0.341736 |
| C | 1.521958 | 3.225447 | 1.665061 |
| H | 2.550646 | 2.859648 | 1.720541 |
| H | 1.536698 | 4.308539 | 1.853542 |
| H | 0.966125 | 2.736569 | 2.467490 |
| H | -2.287250 | 2.317664 | -2.783961 |
| H | -3.204114 | 0.261555 | -2.013833 |
| H | -4.821714 | 0.291068 | -1.458997 |
| H | 3.311285 | 2.718807 | -0.324157 |
| C | 3.591130 | 4.795842 | -0.903090 |
| H | 3.445710 | 5.211419 | 0.099113 |
| H | 4.667364 | 4.695515 | -1.079463 |

| | | | |
|---|---|---|---|
| H | 3.197800 | 5.514049 | -1.629637 |
| O | 1.999849 | 0.056688 | -2.368140 |
| O | 3.198004 | 0.383086 | -0.495953 |
| C | 0.619092 | -0.091351 | -2.744762 |
| H | 0.466736 | 0.471406 | -3.671958 |
| H | 0.421713 | -1.151127 | -2.930652 |
| H | -0.405159 | 1.504620 | -1.688113 |
| H | -1.123410 | -0.100964 | -1.422941 |

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$$\left[ {}^{3}\mathbf{D}^{C}_{(R)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 1 Electronic energy : HF=-3550.3845592

Zero-point correction= 1.287195 (Hartree/Particle)

Thermal correction to Energy= 1.370956

Thermal correction to Enthalpy= 1.371900

Thermal correction to Gibbs Free Energy= 1.157989

Sum of electronic and zero-point Energies= -3549.097365

Sum of electronic and thermal Energies= -3549.013604

Sum of electronic and thermal Enthalpies= -3549.012659

Sum of electronic and thermal Free Energies= -3549.226570

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | 5.711154 | 1.357193 | -2.351969 |
| H | 6.311300 | 1.181392 | -3.246127 |
| C | 4.997482 | 2.718095 | -2.414682 |
| H | 4.666578 | 2.994324 | -1.403437 |
| H | 5.689971 | 3.492847 | -2.759535 |
| O | 3.900660 | 2.713794 | -3.320947 |
| H | 3.270015 | 2.067257 | -2.958841 |
| C | 6.665903 | 1.266464 | -1.121272 |
| O | 7.887032 | 1.338372 | -1.245085 |
| N | 6.061235 | 1.131013 | 0.101983 |
| H | 5.046015 | 1.072739 | 0.139681 |
| C | 6.806694 | 1.097650 | 1.373390 |
| H | 6.085955 | 1.096673 | 2.191377 |
| H | 7.437927 | 0.204037 | 1.442221 |
| C | -3.223487 | 4.009186 | 3.656943 |
| H | -3.589952 | 4.981460 | 4.005084 |
| C | -3.615169 | 3.754030 | 2.198226 |
| H | -3.154648 | 4.521773 | 1.562222 |
| H | -3.194924 | 2.792031 | 1.880781 |
| C | -5.133893 | 3.754985 | 1.977343 |

| | | | |
|---|---|---|---|
| H | -5.599043 | 2.979934 | 2.600892 |
| H | -5.557550 | 4.710927 | 2.312601 |
| C | -5.576932 | 3.551260 | 0.519354 |
| H | -6.667322 | 3.617251 | 0.447815 |
| H | -5.179661 | 4.341654 | -0.125251 |
| N | -5.190835 | 2.253422 | -0.042623 |
| H | -5.707904 | 1.425704 | 0.250879 |
| C | -4.138198 | 2.006515 | -0.830728 |
| N | -3.994534 | 0.765298 | -1.336891 |
| N | -3.263042 | 2.954562 | -1.171383 |
| H | -3.264626 | 3.886421 | -0.779344 |
| C | -0.316040 | -4.289188 | 1.662494 |
| H | -1.038824 | -3.802659 | 2.340720 |
| H | -0.004055 | -5.231486 | 2.141726 |
| O | 0.812621 | -3.511830 | 1.416188 |
| C | -2.655838 | -1.734940 | 0.366486 |
| C | 0.486941 | -0.537592 | 3.838928 |
| C | 4.165685 | -1.980786 | 1.074032 |
| C | 1.050838 | -3.148670 | -2.416927 |
| C | -2.135860 | -1.225214 | 1.557019 |
| C | -2.910621 | -0.660257 | 2.660279 |
| C | -2.003348 | -0.358681 | 3.645884 |
| C | -0.695195 | -0.711949 | 3.127533 |

| | | | |
|---|---|---|---|
| C | -2.237534 | 0.226053 | 5.007632 |
| C | -4.383174 | -0.335757 | 2.705459 |
| C | -5.389492 | -1.488115 | 2.496111 |
| C | -5.948214 | -1.593969 | 1.092225 |
| O | -6.387927 | -2.808383 | 0.821321 |
| O | -6.008905 | -0.659888 | 0.286405 |
| C | 1.771244 | -0.841022 | 3.400302 |
| C | 2.955541 | -0.748255 | 4.237249 |
| C | 4.003114 | -1.197939 | 3.467959 |
| C | 3.431935 | -1.513566 | 2.157063 |
| C | 2.983309 | -0.241976 | 5.646264 |
| C | 5.410390 | -1.357486 | 3.813933 |
| C | 5.928426 | -1.549420 | 5.038111 |
| C | 3.646955 | -2.350344 | -0.160332 |
| C | 4.452109 | -2.864740 | -1.256770 |
| C | 3.567951 | -3.196650 | -2.256009 |
| C | 2.235157 | -2.888560 | -1.735897 |
| C | 5.939836 | -3.032096 | -1.230046 |
| C | 3.825837 | -3.788785 | -3.565083 |
| C | 4.902474 | -3.584001 | -4.339199 |
| C | -0.238556 | -2.917195 | -1.943999 |
| C | -1.441324 | -3.221264 | -2.694344 |
| C | -2.496804 | -2.821330 | -1.912242 |

| | | | |
|---|---|---|---|
| C | -1.922155 | -2.283705 | -0.686290 |
| C | -1.472315 | -3.856734 | -4.052314 |
| C | -3.957434 | -2.927693 | -2.244630 |
| C | -4.616848 | -4.250367 | -1.752042 |
| C | -6.067724 | -4.276572 | -2.152803 |
| O | -6.318404 | -5.062864 | -3.207426 |
| O | -6.961227 | -3.612590 | -1.635680 |
| N | -0.803034 | -1.225908 | 1.865362 |
| N | 2.088856 | -1.296018 | 2.151816 |
| N | 2.318854 | -2.343400 | -0.489405 |
| N | -0.555832 | -2.349032 | -0.738636 |
| H | -3.301778 | 0.339752 | 5.230618 |
| H | -1.772680 | 1.213874 | 5.113621 |
| H | -1.811839 | -0.411911 | 5.790686 |
| H | 3.957116 | 0.199892 | 5.877341 |
| H | 2.807883 | -1.041358 | 6.378627 |
| H | 2.219756 | 0.524059 | 5.814606 |
| H | 6.257763 | -3.774396 | -1.966982 |
| H | 6.287368 | -3.364092 | -0.246438 |
| H | 6.463839 | -2.094928 | -1.456806 |
| H | -0.840329 | -3.316845 | -4.766809 |
| H | -2.485115 | -3.882127 | -4.464755 |
| H | -1.106931 | -4.890541 | -4.022251 |

| | | | |
|---|---|---|---|
| H | 7.000982 | -1.645061 | 5.175687 |
| H | 5.314772 | -1.644942 | 5.927013 |
| H | 5.008711 | -4.093835 | -5.291906 |
| H | 5.693061 | -2.893641 | -4.064565 |
| H | -6.264082 | -1.343033 | 3.145224 |
| H | -4.967195 | -2.457211 | 2.772521 |
| H | -4.613836 | 0.444129 | 1.970890 |
| H | -4.589922 | 0.115060 | 3.679348 |
| H | -4.555809 | -4.303724 | -0.661809 |
| H | -4.097017 | -5.110622 | -2.176963 |
| H | -4.091299 | -2.861510 | -3.330394 |
| H | -4.526543 | -2.095302 | -1.817611 |
| H | -3.729252 | -1.726842 | 0.250238 |
| H | 0.393626 | -0.155236 | 4.848913 |
| H | 5.235656 | -2.083237 | 1.203222 |
| H | 1.136459 | -3.583407 | -3.406118 |
| H | 6.108761 | -1.327313 | 2.980056 |
| H | 3.056733 | -4.464535 | -3.939423 |
| Fe | 0.765577 | -1.800754 | 0.695851 |
| H | -3.637438 | 3.241176 | 4.319276 |
| H | 7.461347 | 1.970861 | 1.460152 |
| H | 4.948165 | 0.574194 | -2.272753 |
| H | -6.693796 | -2.906735 | -0.124398 |

| | | | |
|---|---|---|---|
| H | -0.864500 | -4.559855 | 0.742143 |
| H | -7.266883 | -4.979164 | -3.409776 |
| H | -2.136218 | 3.999005 | 3.777535 |
| C | 0.790114 | 0.317024 | -0.004700 |
| C | -0.145160 | 0.674226 | -1.163295 |
| C | 2.086292 | 0.793876 | -0.459313 |
| N | 0.531625 | 4.855730 | -0.914887 |
| C | 0.789683 | 4.788822 | 0.450982 |
| H | 0.532133 | 0.752147 | 0.957952 |
| C | -0.693570 | 5.318270 | -1.382869 |
| C | -1.105164 | 5.133512 | -2.730289 |
| C | -1.599484 | 5.990421 | -0.518068 |
| C | -2.349449 | 5.578246 | -3.168772 |
| H | -0.443631 | 4.659946 | -3.444558 |
| C | -2.839954 | 6.432171 | -0.979064 |
| H | -1.290865 | 6.229058 | 0.492114 |
| C | -3.240865 | 6.223678 | -2.303254 |
| H | -2.621734 | 5.423488 | -4.209470 |
| H | -3.486984 | 6.976458 | -0.294938 |
| H | -4.201746 | 6.581114 | -2.658771 |
| C | 1.578489 | 4.458224 | -1.877615 |
| H | 1.148090 | 3.758100 | -2.599568 |
| H | -0.080203 | 4.651842 | 1.082792 |

| | | | |
|---|---|---|---|
| C | 2.148671 | 4.531722 | 1.010292 |
| H | 2.500027 | 3.495388 | 0.881362 |
| H | 2.911345 | 5.189465 | 0.574568 |
| H | 2.127849 | 4.726311 | 2.087163 |
| H | -2.543768 | 2.767115 | -1.853134 |
| H | -3.055571 | 0.434306 | -1.524234 |
| H | -4.628620 | 0.060464 | -0.970119 |
| H | 2.323393 | 3.882294 | -1.335172 |
| C | 2.241898 | 5.630679 | -2.599788 |
| H | 2.732147 | 6.300677 | -1.886599 |
| H | 2.995668 | 5.229442 | -3.282038 |
| H | 1.519946 | 6.219577 | -3.173567 |
| O | 2.094318 | 0.920408 | -1.855951 |
| O | 3.100822 | 1.113074 | 0.147509 |
| C | 0.795556 | 0.561308 | -2.369387 |
| H | 0.562673 | 1.242938 | -3.194364 |
| H | 0.840642 | -0.462172 | -2.750903 |
| H | -0.522700 | 1.708321 | -1.076243 |
| H | -0.996113 | -0.002719 | -1.268851 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{C}_{(S)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 1 Electronic energy : HF=-3550.3487303

Zero-point correction= 1.283882 (Hartree/Particle)

Thermal correction to Energy= 1.367348

Thermal correction to Enthalpy= 1.368292

Thermal correction to Gibbs Free Energy= 1.154014

Sum of electronic and zero-point Energies= -3549.064848

Sum of electronic and thermal Energies= -3548.981382

Sum of electronic and thermal Enthalpies= -3548.980438

Sum of electronic and thermal Free Energies= -3549.194716

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 5.546935 | -0.925324 | -2.559110 |
| H | 6.272008 | -1.672275 | -2.905080 |
| C | 5.116975 | -0.075936 | -3.757931 |
| H | 4.378506 | 0.675481 | -3.445480 |
| H | 5.983662 | 0.463962 | -4.143384 |
| O | 4.628322 | -0.877762 | -4.827454 |
| H | 3.861794 | -1.368963 | -4.504887 |
| C | 6.243488 | -0.075916 | -1.468511 |

| | | | |
|---|---|---|---|
| O | 7.023857 | 0.822976 | -1.774720 |
| N | 5.966722 | -0.389966 | -0.159555 |
| H | 5.258840 | -1.085778 | 0.032971 |
| C | 6.600501 | 0.273286 | 0.991556 |
| H | 5.843413 | 0.653521 | 1.681564 |
| H | 7.258737 | -0.418507 | 1.529464 |
| C | -2.474288 | 5.924653 | 0.862474 |
| H | -2.635310 | 7.006607 | 0.795977 |
| C | -2.909635 | 5.215857 | -0.422625 |
| H | -2.288875 | 5.576720 | -1.256699 |
| H | -2.706582 | 4.144019 | -0.318662 |
| C | -4.389839 | 5.439373 | -0.764155 |
| H | -5.014230 | 5.123513 | 0.082262 |
| H | -4.577748 | 6.512775 | -0.899631 |
| C | -4.883317 | 4.720930 | -2.032119 |
| H | -5.908743 | 5.029588 | -2.257637 |
| H | -4.286426 | 5.007076 | -2.905095 |
| N | -4.893726 | 3.260933 | -1.933110 |
| H | -5.650303 | 2.827403 | -1.414065 |
| C | -3.879563 | 2.434010 | -2.248913 |
| N | -4.023691 | 1.120933 | -2.044904 |
| N | -2.745558 | 2.861737 | -2.829294 |
| H | -2.517318 | 3.841055 | -2.773666 |

| | | | |
|---|---|---|---|
| C | -1.558823 | -2.799364 | 2.947477 |
| H | -2.010560 | -1.915516 | 3.430739 |
| H | -1.494702 | -3.590705 | 3.711867 |
| O | -0.282572 | -2.554371 | 2.444593 |
| C | -3.207293 | -0.663515 | 0.500879 |
| C | 0.166137 | 1.038335 | 3.503757 |
| C | 3.353890 | -2.177045 | 1.830965 |
| C | -0.024246 | -3.911496 | -1.152275 |
| C | -2.549511 | 0.159717 | 1.410122 |
| C | -3.159367 | 1.263101 | 2.148048 |
| C | -2.205486 | 1.699998 | 3.031394 |
| C | -1.020730 | 0.891040 | 2.794179 |
| C | -2.286426 | 2.800288 | 4.047602 |
| C | -4.507774 | 1.897279 | 1.913841 |
| C | -5.763938 | 1.039148 | 2.191760 |
| C | -6.409331 | 0.448098 | 0.953510 |
| O | -7.121795 | -0.632011 | 1.228974 |
| O | -6.307433 | 0.915820 | -0.181800 |
| C | 1.345586 | 0.327166 | 3.306669 |
| C | 2.526797 | 0.469525 | 4.139372 |
| C | 3.437755 | -0.452974 | 3.673438 |
| C | 2.789370 | -1.122482 | 2.544313 |
| C | 2.684256 | 1.446149 | 5.264202 |

| | | | |
|---|---|---|---|
| C | 4.778359 | -0.763720 | 4.154626 |
| C | 5.278528 | -0.548488 | 5.382701 |
| C | 2.716973 | -2.931862 | 0.849788 |
| C | 3.327791 | -4.062184 | 0.168762 |
| C | 2.371333 | -4.553248 | -0.690690 |
| C | 1.187523 | -3.715799 | -0.497787 |
| C | 4.701696 | -4.597403 | 0.436612 |
| C | 2.433071 | -5.700555 | -1.590247 |
| C | 3.517566 | -6.163148 | -2.231690 |
| C | -1.193105 | -3.183774 | -0.953351 |
| C | -2.450954 | -3.486111 | -1.613195 |
| C | -3.363273 | -2.580946 | -1.137336 |
| C | -2.646614 | -1.730205 | -0.195635 |
| C | -2.656373 | -4.591197 | -2.605084 |
| C | -4.817217 | -2.485502 | -1.500650 |
| C | -5.748913 | -3.279961 | -0.536156 |
| C | -7.179080 | -3.158852 | -0.989770 |
| O | -7.574468 | -4.172805 | -1.772502 |
| O | -7.930688 | -2.219857 | -0.749518 |
| N | -1.247797 | -0.008602 | 1.792637 |
| N | 1.541203 | -0.619587 | 2.337630 |
| N | 1.435914 | -2.732510 | 0.412435 |
| N | -1.336974 | -2.113767 | -0.112422 |

| | | | |
|---|---|---|---|
| H | -3.289638 | 3.230781 | 4.105413 |
| H | -1.589890 | 3.616904 | 3.821077 |
| H | -2.035627 | 2.434857 | 5.050263 |
| H | 3.728686 | 1.757764 | 5.362848 |
| H | 2.382494 | 1.017638 | 6.229153 |
| H | 2.081070 | 2.345383 | 5.107204 |
| H | 4.761984 | -5.654117 | 0.161771 |
| H | 4.966114 | -4.510606 | 1.495343 |
| H | 5.477622 | -4.070660 | -0.135517 |
| H | -1.947147 | -4.521107 | -3.437846 |
| H | -3.663520 | -4.570222 | -3.030451 |
| H | -2.516420 | -5.577682 | -2.146285 |
| H | 6.304480 | -0.815700 | 5.616031 |
| H | 4.689943 | -0.133207 | 6.192752 |
| H | 3.457323 | -7.042835 | -2.864950 |
| H | 4.485031 | -5.676211 | -2.166772 |
| H | -6.543659 | 1.656995 | 2.657868 |
| H | -5.560198 | 0.229232 | 2.896265 |
| H | -4.573500 | 2.255442 | 0.879862 |
| H | -4.564814 | 2.792235 | 2.538940 |
| H | -5.667838 | -2.872542 | 0.474335 |
| H | -5.454385 | -4.331132 | -0.519480 |
| H | -4.965914 | -2.868560 | -2.515936 |

| | | | |
|---|---|---|---|
| H | -5.156667 | -1.445216 | -1.515972 |
| H | -4.252577 | -0.462640 | 0.318438 |
| H | 0.163286 | 1.767639 | 4.305803 |
| H | 4.351316 | -2.490956 | 2.116641 |
| H | -0.073541 | -4.723793 | -1.868130 |
| H | 5.441559 | -1.233368 | 3.429754 |
| H | 1.492432 | -6.227231 | -1.749110 |
| Fe | 0.095535 | -1.344018 | 1.085537 |
| H | -3.041544 | 5.556881 | 1.724692 |
| H | 7.196928 | 1.099251 | 0.602541 |
| H | 4.691068 | -1.472554 | -2.144308 |
| H | -7.484280 | -1.057513 | 0.402259 |
| H | -2.269318 | -3.148133 | 2.177157 |
| H | -8.486583 | -3.980077 | -2.051861 |
| H | -1.414507 | 5.753460 | 1.065063 |
| C | 0.730625 | 0.033685 | -0.549203 |
| C | -0.232947 | 0.289278 | -1.604958 |
| C | 2.001899 | -0.294728 | -1.342924 |
| N | 2.571380 | 2.946069 | -0.326948 |
| C | 1.173473 | 2.690314 | -0.201441 |
| H | 0.939368 | 1.344877 | -0.095632 |
| C | 3.126645 | 3.514336 | -1.482193 |
| C | 4.478787 | 3.302521 | -1.833237 |

| | | | |
|---|---|---|---|
| C | 2.355545 | 4.337556 | -2.334387 |
| C | 5.014443 | 3.863842 | -2.990859 |
| H | 5.123758 | 2.683530 | -1.222919 |
| C | 2.902874 | 4.887059 | -3.490534 |
| H | 1.329372 | 4.571728 | -2.073364 |
| C | 4.236160 | 4.656484 | -3.835592 |
| H | 6.053853 | 3.657862 | -3.229943 |
| H | 2.279462 | 5.516851 | -4.120586 |
| H | 4.658542 | 5.088294 | -4.737530 |
| C | 3.438877 | 2.481343 | 0.758820 |
| H | 4.172953 | 1.766801 | 0.368529 |
| H | 0.672559 | 2.869277 | -1.151729 |
| C | 0.467369 | 3.393660 | 0.944022 |
| H | 0.911992 | 3.152678 | 1.912702 |
| H | 0.518428 | 4.485087 | 0.815155 |
| H | -0.581784 | 3.088803 | 0.981231 |
| H | -1.961540 | 2.201773 | -2.707139 |
| H | -3.142947 | 0.604907 | -1.946601 |
| H | -4.807449 | 0.831914 | -1.468602 |
| O | 0.165087 | -0.175154 | -2.830166 |
| O | -1.306385 | 0.924877 | -1.564155 |
| C | 1.459141 | -0.801150 | -2.689639 |
| H | 2.053586 | -0.507269 | -3.561091 |

| | | | |
|---|---|---|---|
| H | 1.317363 | -1.886621 | -2.693898 |
| H | 2.603574 | 0.611003 | -1.504913 |
| H | 2.641607 | -1.033727 | -0.862581 |
| H | 2.810662 | 1.913229 | 1.446942 |
| C | 4.146695 | 3.614329 | 1.509529 |
| H | 3.418679 | 4.293633 | 1.963956 |
| H | 4.776218 | 3.203957 | 2.306555 |
| H | 4.784081 | 4.200308 | 0.841497 |

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$$\left[ {}^{3}\mathbf{D}^{C}_{(S)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 0 Electronic energy : HF=-3550.3955239

Zero-point correction= 1.286998 (Hartree/Particle)

Thermal correction to Energy= 1.371812

Thermal correction to Enthalpy= 1.372756

Thermal correction to Gibbs Free Energy= 1.151155

Sum of electronic and zero-point Energies= -3549.108526

Sum of electronic and thermal Energies= -3549.023712

Sum of electronic and thermal Enthalpies= -3549.022768

Sum of electronic and thermal Free Energies= -3549.244368

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | 5.531251 | 1.099684 | -2.478223 |
| H | 6.470490 | 0.795254 | -2.957494 |
| C | 4.735466 | 1.948971 | -3.469089 |
| H | 3.778786 | 2.253883 | -3.019051 |
| H | 5.292140 | 2.860582 | -3.692507 |
| O | 4.534098 | 1.279864 | -4.707869 |
| H | 4.100210 | 0.436297 | -4.525498 |
| C | 5.896084 | 1.890040 | -1.196432 |
| O | 6.072322 | 3.107178 | -1.237995 |
| N | 6.055083 | 1.163162 | -0.045719 |
| H | 5.790634 | 0.187977 | -0.056562 |
| C | 6.464760 | 1.741708 | 1.245798 |
| H | 5.683655 | 1.597920 | 1.997266 |
| H | 7.390048 | 1.276778 | 1.600198 |
| C | -3.779384 | 4.551703 | 2.457769 |
| H | -4.010671 | 5.608967 | 2.632512 |
| C | -3.843875 | 4.201433 | 0.969577 |
| H | -3.087663 | 4.775745 | 0.419916 |
| H | -3.570671 | 3.147404 | 0.847349 |
| C | -5.224248 | 4.463854 | 0.351628 |

| | | | |
|---|---|---|---|
| H | -5.996296 | 3.927202 | 0.921604 |
| H | -5.471376 | 5.530708 | 0.436872 |
| C | -5.345250 | 4.074119 | -1.130484 |
| H | -6.323674 | 4.369493 | -1.522272 |
| H | -4.602199 | 4.607424 | -1.729838 |
| N | -5.204673 | 2.633027 | -1.368657 |
| H | -5.946998 | 2.056715 | -0.992637 |
| C | -4.021039 | 1.985980 | -1.508837 |
| N | -3.960542 | 0.679905 | -1.216659 |
| N | -2.934192 | 2.583211 | -1.984423 |
| H | -2.918964 | 3.544916 | -2.290638 |
| C | -0.419814 | -3.815190 | 2.497057 |
| H | -0.842555 | -3.104077 | 3.227633 |
| H | -0.191175 | -4.745058 | 3.043417 |
| O | 0.745006 | -3.349161 | 1.892741 |
| C | -2.608300 | -1.580437 | 0.677912 |
| C | 0.879016 | 0.197688 | 3.507269 |
| C | 4.192045 | -2.349613 | 1.083426 |
| C | 0.751348 | -3.865724 | -1.949443 |
| C | -1.958167 | -0.851498 | 1.669240 |
| C | -2.610046 | 0.025772 | 2.638415 |
| C | -1.609611 | 0.519149 | 3.434623 |
| C | -0.365852 | -0.051464 | 2.939513 |

| | | | |
|---|---|---|---|
| C | -1.698239 | 1.464463 | 4.595446 |
| C | -4.068091 | 0.408035 | 2.692993 |
| C | -5.087536 | -0.727341 | 2.938098 |
| C | -5.832093 | -1.194213 | 1.700929 |
| O | -6.432968 | -2.360594 | 1.894322 |
| O | -5.896352 | -0.578126 | 0.638991 |
| C | 2.099364 | -0.341792 | 3.105676 |
| C | 3.348388 | -0.150385 | 3.819999 |
| C | 4.291773 | -0.902553 | 3.153150 |
| C | 3.594329 | -1.508718 | 2.018468 |
| C | 3.530724 | 0.709633 | 5.032810 |
| C | 5.705795 | -1.100882 | 3.448595 |
| C | 6.318365 | -0.984095 | 4.638428 |
| C | 3.548301 | -2.976743 | 0.020189 |
| C | 4.209548 | -3.860873 | -0.923569 |
| C | 3.237166 | -4.278198 | -1.804711 |
| C | 1.993322 | -3.652533 | -1.358024 |
| C | 5.651039 | -4.265682 | -0.870660 |
| C | 3.339515 | -5.197762 | -2.932352 |
| C | 4.412000 | -5.401087 | -3.713897 |
| C | -0.468725 | -3.377064 | -1.494769 |
| C | -1.747364 | -3.713858 | -2.097192 |
| C | -2.705669 | -3.088858 | -1.343296 |

| | | | |
|---|---|---|---|
| C | -1.997323 | -2.368407 | -0.293350 |
| C | -1.924129 | -4.588630 | -3.301723 |
| C | -4.194265 | -3.132680 | -1.539855 |
| C | -4.894167 | -4.217308 | -0.665734 |
| C | -6.373960 | -4.241974 | -0.941390 |
| O | -6.695460 | -5.000188 | -2.001580 |
| O | -7.235638 | -3.617830 | -0.333274 |
| N | -0.607160 | -0.866229 | 1.869354 |
| N | 2.279968 | -1.152503 | 2.018815 |
| N | 2.217178 | -2.853076 | -0.277324 |
| N | -0.648821 | -2.554664 | -0.415462 |
| H | -2.731514 | 1.739770 | 4.821161 |
| H | -1.145708 | 2.392919 | 4.405491 |
| H | -1.274876 | 1.021285 | 5.504723 |
| H | 4.548488 | 1.109499 | 5.075745 |
| H | 3.363337 | 0.152585 | 5.964279 |
| H | 2.837994 | 1.556826 | 5.034687 |
| H | 5.791846 | -5.244897 | -1.337261 |
| H | 6.011991 | -4.330752 | 0.160548 |
| H | 6.305381 | -3.559612 | -1.399987 |
| H | -1.342716 | -4.220901 | -4.155213 |
| H | -2.970698 | -4.637337 | -3.614610 |
| H | -1.593509 | -5.616254 | -3.107060 |

| | | | |
|---|---|---|---|
| H | 7.387584 | -1.148472 | 4.729021 |
| H | 5.783819 | -0.754294 | 5.553233 |
| H | 4.384797 | -6.130277 | -4.517700 |
| H | 5.334431 | -4.842290 | -3.595637 |
| H | -5.865339 | -0.397235 | 3.639607 |
| H | -4.622803 | -1.600925 | 3.403526 |
| H | -4.355567 | 0.918655 | 1.766259 |
| H | -4.188093 | 1.150735 | 3.485844 |
| H | -4.740561 | -4.001926 | 0.393560 |
| H | -4.467715 | -5.197529 | -0.892101 |
| H | -4.419266 | -3.341432 | -2.590855 |
| H | -4.650008 | -2.163629 | -1.312707 |
| H | -3.683846 | -1.504956 | 0.630842 |
| H | 0.893503 | 0.843325 | 4.378024 |
| H | 5.244817 | -2.570711 | 1.215193 |
| H | 0.723326 | -4.503566 | -2.825282 |
| H | 6.328294 | -1.387397 | 2.601245 |
| H | 2.442145 | -5.775089 | -3.153031 |
| Fe | 0.798153 | -1.852718 | 0.798512 |
| H | -4.495517 | 3.958133 | 3.037682 |
| H | 6.631386 | 2.806793 | 1.082613 |
| H | 4.987681 | 0.181131 | -2.226690 |
| H | -6.831559 | -2.694234 | 1.044101 |

| | | | |
|---|---|---|---|
| H | -1.219173 | -4.053557 | 1.773480 |
| H | -7.656397 | -4.917460 | -2.129426 |
| H | -2.781704 | 4.356669 | 2.862390 |
| C | 1.077586 | 0.030938 | -0.343431 |
| C | -0.010296 | 0.389739 | -1.224866 |
| C | 2.307793 | 0.101987 | -1.246993 |
| N | 0.843919 | 5.187879 | -0.270171 |
| C | 0.548120 | 5.752892 | 0.965870 |
| H | 1.100887 | 0.660140 | 0.542612 |
| C | -0.044032 | 5.328283 | -1.339325 |
| C | 0.055495 | 4.531538 | -2.506293 |
| C | -1.094313 | 6.278678 | -1.286189 |
| C | -0.860998 | 4.666996 | -3.544484 |
| H | 0.842547 | 3.795721 | -2.608475 |
| C | -2.009213 | 6.394538 | -2.329844 |
| H | -1.154134 | 6.961006 | -0.447480 |
| C | -1.915646 | 5.586499 | -3.468487 |
| H | -0.749598 | 4.038696 | -4.423861 |
| H | -2.787823 | 7.150624 | -2.262654 |
| H | -2.613510 | 5.700682 | -4.292348 |
| C | 2.115889 | 4.468707 | -0.466336 |
| H | 1.905166 | 3.499444 | -0.929929 |
| H | -0.507060 | 5.852640 | 1.192064 |

| | | | |
|---|---|---|---|
| C | 1.537645 | 5.830179 | 2.078524 |
| H | 1.761064 | 4.859560 | 2.555338 |
| H | 2.498126 | 6.255915 | 1.762101 |
| H | 1.137395 | 6.477889 | 2.864811 |
| H | -2.047584 | 2.070239 | -1.857412 |
| H | -3.019519 | 0.280344 | -1.193783 |
| H | -4.646466 | 0.283693 | -0.576702 |
| O | 0.331471 | 0.246646 | -2.543398 |
| O | -1.149264 | 0.817538 | -0.970587 |
| C | 1.699995 | -0.214276 | -2.620730 |
| H | 2.168622 | 0.307272 | -3.461687 |
| H | 1.688519 | -1.289705 | -2.821773 |
| H | 2.749442 | 1.110355 | -1.249605 |
| H | 3.095568 | -0.605162 | -0.985863 |
| H | 2.513670 | 4.236774 | 0.520826 |
| C | 3.153056 | 5.249182 | -1.277746 |
| H | 3.384887 | 6.201553 | -0.790269 |
| H | 4.078057 | 4.669289 | -1.358372 |
| H | 2.789555 | 5.469120 | -2.285802 |

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$$\left[ {}^{3}\mathbf{TS(D\text{-}P)}^{\mathbf{A}}_{(1S,2R)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 4 Electronic energy : HF=-3384.9764879

Zero-point correction= 1.240053 (Hartree/Particle)

Thermal correction to Energy= 1.320237

Thermal correction to Enthalpy= 1.321181

Thermal correction to Gibbs Free Energy= 1.110212

Sum of electronic and zero-point Energies= -3383.736435

Sum of electronic and thermal Energies= -3383.656251

Sum of electronic and thermal Enthalpies= -3383.655307

Sum of electronic and thermal Free Energies= -3383.866276

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -4.886330 | -1.632937 | 2.286624 |
| H | -4.093467 | -2.081439 | 1.680540 |
| C | -4.444498 | -1.567856 | 3.759462 |
| H | -5.273064 | -1.171985 | 4.355933 |
| H | -4.252477 | -2.595111 | 4.120640 |
| O | -3.325552 | -0.733668 | 3.960775 |
| H | -2.653110 | -0.955710 | 3.274972 |
| C | -6.198639 | -2.343483 | 2.130360 |

| | | | |
|---|---|---|---|
| O | -7.204529 | -2.077137 | 2.789905 |
| N | -6.196584 | -3.324938 | 1.191679 |
| H | -5.358950 | -3.542682 | 0.672181 |
| C | -7.396570 | -4.067408 | 0.944271 |
| H | -7.162742 | -4.925259 | 0.308448 |
| H | -7.829661 | -4.422951 | 1.884911 |
| C | -1.189993 | 4.566693 | -2.610889 |
| H | -0.733757 | 5.160640 | -3.410636 |
| C | -2.324539 | 5.328554 | -1.916544 |
| H | -3.094461 | 5.597779 | -2.654886 |
| H | -2.816583 | 4.654512 | -1.202725 |
| C | -1.893597 | 6.602450 | -1.162304 |
| H | -1.116638 | 6.311108 | -0.438790 |
| C | -1.291124 | 7.663189 | -2.096179 |
| H | -0.998313 | 8.559647 | -1.537528 |
| H | -0.402462 | 7.293891 | -2.616574 |
| H | -2.020259 | 7.970365 | -2.857112 |
| C | -3.074411 | 7.189823 | -0.374492 |
| H | -2.774719 | 8.074733 | 0.199121 |
| H | -3.883081 | 7.493889 | -1.051203 |
| H | -3.490795 | 6.459296 | 0.328060 |
| C | 2.433400 | -2.831021 | -2.863340 |
| H | 2.714528 | -3.346423 | -1.922217 |

| | | | |
|---|---|---|---|
| H | 3.185244 | -2.028541 | -3.016616 |
| O | 1.127707 | -2.376440 | -2.878702 |
| C | 3.222522 | -1.110620 | 0.534945 |
| C | 1.712466 | 1.390774 | -3.321409 |
| C | -2.491741 | -0.991833 | -3.235102 |
| C | -0.730830 | -3.866957 | 0.230709 |
| C | 3.170404 | -0.195953 | -0.514860 |
| C | 4.244644 | 0.725303 | -0.853889 |
| C | 3.824332 | 1.423150 | -1.956058 |
| C | 2.495358 | 0.925416 | -2.271138 |
| C | 4.551561 | 2.482464 | -2.729415 |
| C | 5.583511 | 0.770201 | -0.173076 |
| C | 6.537076 | -0.324120 | -0.719056 |
| C | 7.893712 | -0.412026 | -0.047129 |
| O | 8.538589 | 0.755495 | 0.171724 |
| O | 8.452982 | -1.447919 | 0.260621 |
| C | 0.416593 | 0.976667 | -3.626235 |
| C | -0.369886 | 1.517821 | -4.714681 |
| C | -1.607082 | 0.914440 | -4.643352 |
| C | -1.520384 | -0.044324 | -3.540292 |
| C | 0.103770 | 2.557303 | -5.685751 |
| C | -2.745517 | 1.195589 | -5.512006 |
| C | -4.051523 | 1.150219 | -5.201968 |

| | | | |
|---|---|---|---|
| C | -2.383300 | -2.000728 | -2.280120 |
| C | -3.395577 | -3.012401 | -2.055685 |
| C | -2.892069 | -3.849284 | -1.079417 |
| C | -1.580437 | -3.310245 | -0.722479 |
| C | -3.492550 | -5.019685 | -0.458352 |
| C | -4.489823 | -5.793889 | -0.930385 |
| C | 0.502592 | -3.365586 | 0.622343 |
| C | 1.296935 | -3.915964 | 1.710965 |
| C | 2.402915 | -3.117972 | 1.829643 |
| C | 2.276897 | -2.100171 | 0.790740 |
| C | 0.908408 | -5.112196 | 2.526551 |
| C | 3.523762 | -3.246469 | 2.828189 |
| C | 4.815514 | -3.918227 | 2.297485 |
| C | 5.887845 | -2.940049 | 1.850787 |
| O | 5.986532 | -1.791082 | 2.251759 |
| O | 6.747025 | -3.487903 | 0.981685 |
| N | 2.128919 | -0.056477 | -1.388636 |
| N | -0.299571 | 0.037971 | -2.931494 |
| N | -1.305825 | -2.196767 | -1.456488 |
| N | 1.122224 | -2.274772 | 0.079466 |
| H | 5.498114 | 2.754348 | -2.251087 |
| H | 3.956527 | 3.399413 | -2.817307 |
| H | 4.783768 | 2.154598 | -3.750770 |

| | | | |
|---|---|---|---|
| H | 0.287654 | 3.520974 | -5.194099 |
| H | -0.631242 | 2.734059 | -6.475627 |
| H | 1.042788 | 2.256451 | -6.165412 |
| H | 1.645055 | -5.325083 | 3.306319 |
| H | 0.819751 | -6.013225 | 1.906566 |
| H | -0.060166 | -4.962905 | 3.018632 |
| H | -4.808088 | 1.387394 | -5.944189 |
| H | -4.404418 | 0.900519 | -4.206821 |
| H | -4.850284 | -6.640100 | -0.353069 |
| H | -4.942740 | -5.640818 | -1.903338 |
| H | 6.715398 | -0.146131 | -1.788528 |
| H | 6.062855 | -1.302331 | -0.640770 |
| H | 5.478568 | 0.631848 | 0.907801 |
| H | 6.022867 | 1.768410 | -0.322485 |
| H | 4.605694 | -4.613032 | 1.479964 |
| H | 5.281554 | -4.513494 | 3.095264 |
| H | 3.159042 | -3.830387 | 3.678872 |
| H | 3.800206 | -2.265063 | 3.228407 |
| H | 4.089651 | -1.078503 | 1.181953 |
| H | 2.143454 | 2.158877 | -3.955386 |
| H | -3.382503 | -0.987403 | -3.849064 |
| H | -1.074434 | -4.758251 | 0.742972 |
| H | -2.486042 | 1.511602 | -6.523544 |

| | | | |
|---|---|---|---|
| H | -3.075393 | -5.297182 | 0.509240 |
| Fe | 0.452628 | -1.193677 | -1.487804 |
| H | -8.162915 | -3.459601 | 0.445105 |
| H | -0.399517 | 4.299399 | -1.901853 |
| H | 7.420975 | -2.803806 | 0.737383 |
| H | 7.970798 | 1.493124 | -0.095078 |
| H | 2.601003 | -3.565345 | -3.676596 |
| H | -4.999571 | -0.604158 | 1.926293 |
| H | -1.555590 | 3.639363 | -3.060059 |
| C | -0.365750 | 0.581690 | 0.625925 |
| C | -0.904082 | 1.790720 | -0.079798 |
| C | -2.401314 | 1.430940 | -0.184897 |
| H | -2.641097 | 1.015791 | -1.168892 |
| O | -2.648818 | 0.415789 | 0.807540 |
| C | -1.433478 | -0.143112 | 1.205146 |
| O | -1.457806 | -1.089321 | 2.010298 |
| H | -3.074473 | 2.269637 | 0.022017 |
| H | -0.466268 | 1.962243 | -1.065804 |
| H | -0.761519 | 2.712062 | 0.511726 |
| C | -0.125124 | 1.572320 | 3.223551 |
| N | -0.910189 | 2.683038 | 3.382743 |
| C | -0.402638 | 3.994579 | 3.587459 |
| C | 0.543276 | 4.268109 | 4.592697 |

| | | | |
|---|---|---|---|
| C | -0.876780 | 5.063065 | 2.802979 |
| C | 1.017971 | 5.564852 | 4.783652 |
| H | 0.883797 | 3.464614 | 5.235286 |
| C | -0.410326 | 6.357873 | 3.011314 |
| H | -1.595174 | 4.864749 | 2.013930 |
| C | 0.546172 | 6.618652 | 3.997968 |
| H | 1.748209 | 5.753692 | 5.566277 |
| H | -0.786022 | 7.165324 | 2.388571 |
| H | 0.914506 | 7.628486 | 4.153322 |
| C | -2.369899 | 2.487690 | 3.546410 |
| H | -2.659132 | 1.580048 | 3.016876 |
| C | 1.363845 | 1.634571 | 3.160127 |
| H | 1.710268 | 2.439819 | 2.501890 |
| H | 1.840324 | 1.800664 | 4.139910 |
| H | 1.745258 | 0.687383 | 2.773533 |
| H | -2.878834 | 3.327614 | 3.065351 |
| C | -2.786341 | 2.384553 | 5.014622 |
| H | -2.477940 | 3.268810 | 5.583011 |
| H | -3.874534 | 2.289504 | 5.080101 |
| H | -2.356074 | 1.489855 | 5.471010 |
| H | -0.607553 | 0.623207 | 3.419935 |
| C | -4.724374 | -3.079765 | -2.743942 |
| H | -4.714387 | -3.772533 | -3.596677 |

H -5.505720 -3.426346 -2.058807

H -5.030998 -2.101946 -3.125186

H 0.669375 0.372376 0.819495

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$^{OSS}C^{L9}$

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Number of imaginary frequencies : 2 Electronic energy : HF=-2940.1276648

Zero-point correction= 1.012248 (Hartree/Particle)

Thermal correction to Energy= 1.079709

Thermal correction to Enthalpy= 1.080653

Thermal correction to Gibbs Free Energy= 0.896869

Sum of electronic and zero-point Energies= -2939.115416

Sum of electronic and thermal Energies= -2939.047956

Sum of electronic and thermal Enthalpies= -2939.047012

Sum of electronic and thermal Free Energies= -2939.230795

.....

Cartesian Coordinates

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C -4.216400 -3.497498 1.857649

H -3.622954 -3.066110 1.044962

| | | | |
|---|---|---|---|
| C | -3.297620 | -4.272178 | 2.829143 |
| H | -3.932989 | -4.803068 | 3.546030 |
| H | -2.741462 | -5.038191 | 2.257170 |
| O | -2.442767 | -3.436526 | 3.565814 |
| H | -1.915239 | -2.902366 | 2.937154 |
| C | -5.340821 | -4.355160 | 1.361464 |
| O | -6.180032 | -4.857308 | 2.109494 |
| N | -5.339578 | -4.545317 | 0.013396 |
| H | -4.586281 | -4.173653 | -0.547173 |
| C | -6.300812 | -5.410555 | -0.596969 |
| H | -6.949333 | -5.787568 | 0.195210 |
| H | -6.916611 | -4.884286 | -1.338324 |
| C | -3.341167 | 5.177336 | 1.604198 |
| H | -3.381903 | 6.192996 | 1.196080 |
| C | -4.721643 | 4.511790 | 1.625787 |
| H | -5.108828 | 4.448679 | 0.599306 |
| H | -4.606113 | 3.474138 | 1.966366 |
| C | -5.768658 | 5.203293 | 2.521444 |
| H | -5.341495 | 5.281559 | 3.533496 |
| C | -6.104366 | 6.624283 | 2.042774 |
| H | -6.852047 | 7.092917 | 2.693140 |
| H | -5.223518 | 7.273604 | 2.031600 |
| H | -6.515687 | 6.603711 | 1.025557 |

| | | | |
|---|---|---|---|
| C | -7.044384 | 4.352930 | 2.615808 |
| H | -7.785208 | 4.813376 | 3.279685 |
| H | -7.509747 | 4.237444 | 1.628956 |
| H | -6.827933 | 3.349514 | 2.998022 |
| C | 1.808367 | 0.916399 | -3.217319 |
| H | 2.739000 | 1.292142 | -2.744607 |
| H | 1.178806 | 1.808596 | -3.408270 |
| O | 1.171429 | -0.059340 | -2.475816 |
| C | 3.454309 | -0.384926 | 0.728430 |
| C | 1.123384 | 3.552664 | -0.836963 |
| C | -2.625372 | 0.762820 | -2.086070 |
| C | -0.039035 | -3.190209 | -1.065542 |
| C | 3.153442 | 0.936000 | 0.401349 |
| C | 4.059975 | 2.061767 | 0.608829 |
| C | 3.404308 | 3.175400 | 0.157198 |
| C | 2.106513 | 2.719936 | -0.318275 |
| C | 3.888509 | 4.593787 | 0.108891 |
| C | 5.485209 | 1.958493 | 1.077318 |
| C | 6.431678 | 1.634783 | -0.112142 |
| C | 7.911109 | 1.547920 | 0.227492 |
| O | 8.290632 | 0.509461 | 1.031394 |
| O | 8.750630 | 2.307774 | -0.194045 |
| C | -0.132699 | 3.144319 | -1.288406 |

| | | | |
|---|---|---|---|
| C | -1.159703 | 4.045074 | -1.768997 |
| C | -2.261752 | 3.266850 | -2.053090 |
| C | -1.856940 | 1.884148 | -1.791036 |
| C | -1.018531 | 5.534265 | -1.872272 |
| C | -3.552606 | 3.761240 | -2.520696 |
| C | -4.772901 | 3.252950 | -2.279259 |
| C | -2.248811 | -0.570894 | -1.932924 |
| C | -3.054986 | -1.692560 | -2.377130 |
| C | -2.312436 | -2.826411 | -2.113690 |
| C | -1.072439 | -2.359898 | -1.491923 |
| C | -2.633347 | -4.226280 | -2.343359 |
| C | -3.557633 | -4.747350 | -3.174324 |
| C | 1.128754 | -2.772482 | -0.445775 |
| C | 2.146936 | -3.676903 | 0.073235 |
| C | 3.116592 | -2.888372 | 0.628566 |
| C | 2.688341 | -1.505592 | 0.412847 |
| C | 2.073705 | -5.172488 | 0.001555 |
| C | 4.365118 | -3.344465 | 1.336141 |
| C | 5.654002 | -3.363220 | 0.474348 |
| C | 6.583111 | -2.196690 | 0.705968 |
| O | 6.506248 | -1.415738 | 1.648485 |
| O | 7.548342 | -2.104491 | -0.220568 |
| N | 1.990649 | 1.363767 | -0.170693 |

| | | | |
|---|---|---|---|
| N | -0.576040 | 1.850466 | -1.316411 |
| N | -1.071120 | -1.006677 | -1.391248 |
| N | 1.480470 | -1.476328 | -0.215187 |
| H | 4.863157 | 4.702205 | 0.593530 |
| H | 3.193146 | 5.276211 | 0.613101 |
| H | 3.994465 | 4.952561 | -0.922826 |
| H | -0.965641 | 6.009220 | -0.883885 |
| H | -1.865492 | 5.982907 | -2.398626 |
| H | -0.105936 | 5.813768 | -2.411710 |
| H | 2.921521 | -5.644058 | 0.507257 |
| H | 2.074362 | -5.528640 | -1.036537 |
| H | 1.158196 | -5.552168 | 0.470583 |
| H | -5.661268 | 3.721811 | -2.692307 |
| H | -4.925944 | 2.378112 | -1.656478 |
| H | -3.697632 | -5.822349 | -3.237117 |
| H | -4.167938 | -4.139635 | -3.832416 |
| H | 6.331112 | 2.408987 | -0.874704 |
| H | 6.112238 | 0.687329 | -0.562715 |
| H | 5.580192 | 1.189854 | 1.852269 |
| H | 5.804021 | 2.902271 | 1.534257 |
| H | 5.426492 | -3.409272 | -0.595168 |
| H | 6.254721 | -4.257681 | 0.690032 |
| H | 4.197057 | -4.359451 | 1.708633 |

| | | | |
|---|---|---|---|
| H | 4.553815 | -2.725943 | 2.219326 |
| H | 4.392962 | -0.562584 | 1.236906 |
| H | 1.345500 | 4.613543 | -0.885278 |
| H | -3.584428 | 0.949102 | -2.550833 |
| H | -0.160755 | -4.257792 | -1.208001 |
| H | -3.505936 | 4.676423 | -3.112939 |
| H | -2.045098 | -4.936607 | -1.763251 |
| Fe | 0.428929 | 0.179831 | -0.712304 |
| H | -5.821942 | -6.259608 | -1.102053 |
| H | -2.915288 | 5.242315 | 2.612982 |
| H | 8.118693 | -1.342092 | 0.007733 |
| H | 7.523302 | 0.013803 | 1.403037 |
| H | 2.101255 | 0.520890 | -4.208783 |
| H | -4.649735 | -2.667208 | 2.426987 |
| H | -2.647348 | 4.604126 | 0.981672 |
| C | -0.283861 | 0.318831 | 0.962328 |
| C | -0.302454 | 1.555572 | 1.825289 |
| C | -1.352522 | 1.269336 | 2.909011 |
| H | -2.323221 | 1.721745 | 2.667933 |
| O | -1.510360 | -0.157879 | 2.924604 |
| C | -0.948058 | -0.712580 | 1.795647 |
| O | -1.046676 | -1.923128 | 1.633531 |
| H | -1.064165 | 1.586036 | 3.916136 |

| | | | |
|---|---|---|---|
| H | -0.513194 | 2.467067 | 1.260114 |
| H | 0.695399 | 1.691996 | 2.270241 |
| C | -4.424590 | -1.597468 | -2.976560 |
| H | -4.400616 | -1.642023 | -4.074138 |
| H | -5.060944 | -2.422524 | -2.637492 |
| H | -4.922807 | -0.663691 | -2.701973 |

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$$\left[{}^{OSS}\mathbf{TS(C\text{-}D)}^{A}_{(S)}\right]^{L9}$$

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Number of imaginary frequencies : 4 Electronic energy : HF=-3384.9572674

Zero-point correction= 1.239260 (Hartree/Particle)

Thermal correction to Energy= 1.317904

Thermal correction to Enthalpy= 1.318849

Thermal correction to Gibbs Free Energy= 1.117347

Sum of electronic and zero-point Energies= -3383.718007

Sum of electronic and thermal Energies= -3383.639363

Sum of electronic and thermal Enthalpies= -3383.638419

Sum of electronic and thermal Free Energies= -3383.839921

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| C | -5.343439 | -1.591059 | 2.563166 |
| H | -5.016833 | -1.144319 | 1.616749 |
| C | -4.374789 | -2.731625 | 2.947305 |
| H | -4.651463 | -3.110184 | 3.935765 |
| H | -4.498727 | -3.561853 | 2.233365 |
| O | -3.021126 | -2.327527 | 3.032302 |
| H | -2.701047 | -2.131084 | 2.139041 |
| C | -6.739410 | -2.146406 | 2.460518 |
| O | -7.449049 | -2.356365 | 3.442153 |
| N | -7.093554 | -2.478266 | 1.188141 |
| H | -6.453692 | -2.317431 | 0.421560 |
| C | -8.283431 | -3.231898 | 0.921838 |
| H | -8.055484 | -4.247242 | 0.570646 |
| H | -8.844684 | -3.301645 | 1.854933 |
| C | -1.956700 | 5.955803 | -0.203949 |
| H | -1.568915 | 6.703596 | -0.904890 |
| C | -1.551858 | 6.255126 | 1.243426 |
| H | -1.931328 | 7.245220 | 1.544599 |
| H | -2.043707 | 5.521124 | 1.893726 |
| C | -0.036045 | 6.186812 | 1.514797 |
| H | 0.304954 | 5.192234 | 1.199546 |
| C | 0.752296 | 7.239730 | 0.721066 |

| | | | |
|---|---|---|---|
| H | 1.824649 | 7.170183 | 0.937199 |
| H | 0.627200 | 7.114305 | -0.359207 |
| H | 0.426099 | 8.257295 | 0.979020 |
| C | 0.248868 | 6.331150 | 3.017034 |
| H | 1.315085 | 6.201524 | 3.233602 |
| H | -0.053241 | 7.320905 | 3.387555 |
| H | -0.300622 | 5.579901 | 3.596351 |
| C | 0.799375 | -0.814814 | -4.009142 |
| H | 1.859615 | -0.600326 | -3.773643 |
| H | 0.387519 | 0.100112 | -4.475518 |
| O | 0.064757 | -1.253076 | -2.915465 |
| C | 2.351318 | -2.137886 | 0.016553 |
| C | 2.086044 | 2.124405 | -2.245981 |
| C | -2.636661 | 1.421085 | -2.926826 |
| C | -2.398670 | -2.781217 | -0.542035 |
| C | 2.701257 | -0.947068 | -0.618242 |
| C | 4.078034 | -0.497814 | -0.811443 |
| C | 4.002435 | 0.722977 | -1.426292 |
| C | 2.585682 | 0.996069 | -1.614918 |
| C | 5.114711 | 1.626965 | -1.865841 |
| C | 5.305200 | -1.315295 | -0.514302 |
| C | 5.579694 | -2.329282 | -1.659401 |
| C | 6.812010 | -3.204204 | -1.492412 |

| | | | |
|---|---|---|---|
| O | 6.793470 | -4.089555 | -0.449694 |
| O | 7.763094 | -3.188084 | -2.236723 |
| C | 0.748088 | 2.355085 | -2.552226 |
| C | 0.265599 | 3.529732 | -3.248283 |
| C | -1.090983 | 3.362651 | -3.402635 |
| C | -1.402820 | 2.052999 | -2.825271 |
| C | 1.109716 | 4.704158 | -3.638263 |
| C | -2.005799 | 4.314382 | -4.024873 |
| C | -3.293170 | 4.539834 | -3.717214 |
| C | -2.973859 | 0.166855 | -2.418950 |
| C | -4.252743 | -0.477029 | -2.630334 |
| C | -4.195655 | -1.678998 | -1.948807 |
| C | -2.867440 | -1.735379 | -1.342610 |
| C | -5.167198 | -2.757268 | -1.889009 |
| C | -6.489341 | -2.711114 | -2.153100 |
| C | -1.093193 | -2.926053 | -0.081599 |
| C | -0.611824 | -4.086199 | 0.659170 |
| C | 0.740506 | -3.920975 | 0.795861 |
| C | 1.063869 | -2.650367 | 0.148812 |
| C | -1.485887 | -5.187280 | 1.180396 |
| C | 1.702962 | -4.844652 | 1.495881 |
| C | 2.518069 | -5.784091 | 0.569946 |
| C | 3.938808 | -5.338673 | 0.317705 |

| | | | |
|---|---|---|---|
| O | 4.526485 | -4.479101 | 0.965398 |
| O | 4.526434 | -6.005701 | -0.685164 |
| N | 1.826718 | -0.031206 | -1.122296 |
| N | -0.277471 | 1.490917 | -2.290421 |
| N | -2.160013 | -0.614455 | -1.641588 |
| N | -0.066052 | -2.062768 | -0.338360 |
| H | 6.093255 | 1.221277 | -1.593294 |
| H | 5.027126 | 2.618158 | -1.405219 |
| H | 5.112801 | 1.774333 | -2.952891 |
| H | 1.461477 | 5.249686 | -2.753793 |
| H | 0.551716 | 5.412199 | -4.256846 |
| H | 1.997681 | 4.395639 | -4.202687 |
| H | -0.897748 | -5.997321 | 1.620952 |
| H | -2.103455 | -5.627831 | 0.388439 |
| H | -2.163101 | -4.810789 | 1.956999 |
| H | -3.870825 | 5.285245 | -4.255918 |
| H | -3.795469 | 4.021823 | -2.907410 |
| H | -7.090264 | -3.614709 | -2.115358 |
| H | -7.006232 | -1.795535 | -2.416961 |
| H | 5.705424 | -1.788969 | -2.599257 |
| H | 4.700972 | -2.976491 | -1.769796 |
| H | 5.190728 | -1.844932 | 0.438277 |
| H | 6.177550 | -0.662251 | -0.402761 |

| | | | |
|---|---|---|---|
| H | 2.028538 | -5.926752 | -0.398282 |
| H | 2.603351 | -6.786236 | 1.012225 |
| H | 1.135740 | -5.468394 | 2.192757 |
| H | 2.408381 | -4.272477 | 2.106816 |
| H | 3.156351 | -2.719633 | 0.444875 |
| H | 2.800507 | 2.882147 | -2.547739 |
| H | -3.398837 | 1.947792 | -3.486029 |
| H | -3.088263 | -3.587127 | -0.315082 |
| H | -1.565339 | 4.929635 | -4.810639 |
| H | -4.758595 | -3.729987 | -1.615233 |
| Fe | -0.167747 | -0.276074 | -1.300396 |
| H | -8.909154 | -2.744429 | 0.164971 |
| H | -1.586117 | 4.974174 | -0.507585 |
| H | 5.442941 | -5.672231 | -0.777902 |
| H | 6.025799 | -3.955021 | 0.153138 |
| H | 0.801519 | -1.595195 | -4.791911 |
| H | -5.312828 | -0.818785 | 3.336023 |
| H | -3.047795 | 5.949253 | -0.311398 |
| C | -0.598910 | 0.688593 | 0.506628 |
| C | -0.419733 | 2.156082 | 0.583736 |
| C | -1.961952 | 0.469879 | 1.176530 |
| C | 1.102517 | 0.099361 | 2.576117 |
| H | 0.329407 | 0.320274 | 1.437432 |

| | | | |
|---|---|---|---|
| N | 1.341219 | 1.294628 | 3.317198 |
| C | 2.506805 | 2.058153 | 3.167563 |
| C | 3.486981 | 1.752881 | 2.196608 |
| C | 2.763511 | 3.165768 | 4.009838 |
| C | 4.659844 | 2.495186 | 2.103165 |
| H | 3.325653 | 0.962208 | 1.478124 |
| C | 3.940148 | 3.903983 | 3.897903 |
| H | 2.050055 | 3.456633 | 4.769632 |
| C | 4.909866 | 3.575834 | 2.951403 |
| H | 5.382615 | 2.225217 | 1.337247 |
| H | 4.095437 | 4.743576 | 4.571577 |
| H | 5.827559 | 4.150843 | 2.868964 |
| C | 0.236038 | 1.837316 | 4.112917 |
| H | -0.695411 | 1.447090 | 3.698299 |
| C | 0.423879 | -1.032952 | 3.330250 |
| H | -0.553465 | -0.768240 | 3.742417 |
| H | 0.267448 | -1.875191 | 2.652821 |
| H | 1.050732 | -1.382250 | 4.164169 |
| H | 0.194477 | 2.920145 | 3.960215 |
| C | 0.302215 | 1.508181 | 5.612011 |
| H | 1.234052 | 1.860893 | 6.062753 |
| H | -0.533209 | 1.985317 | 6.138006 |
| H | 0.238009 | 0.430035 | 5.781386 |

| | | | |
|---|---|---|---|
| H | 2.013440 | -0.251831 | 2.101891 |
| C | -5.367309 | 0.051940 | -3.479741 |
| H | -5.840159 | -0.757933 | -4.046425 |
| H | -6.157137 | 0.528336 | -2.882372 |
| H | -5.010375 | 0.794644 | -4.197690 |
| H | -3.351682 | 2.099838 | 1.770630 |
| H | -3.226363 | 1.827226 | 0.013559 |
| C | -2.672493 | 1.814296 | 0.959920 |
| O | 0.579148 | 2.842377 | 0.460804 |
| O | -1.622458 | 2.790205 | 0.898608 |
| H | -1.869601 | 0.274872 | 2.254015 |
| H | -2.535452 | -0.351732 | 0.749104 |

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$$\left[{}^{\mathbf{OSS}}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(\boldsymbol{R})}\right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 4 Electronic energy : HF=-3384.9572674

Zero-point correction= 1.239260 (Hartree/Particle)

Thermal correction to Energy= 1.317904

Thermal correction to Enthalpy= 1.318849

Thermal correction to Gibbs Free Energy= 1.117347

Sum of electronic and zero-point Energies= -3383.718007

Sum of electronic and thermal Energies= -3383.639363

Sum of electronic and thermal Enthalpies= -3383.638419

Sum of electronic and thermal Free Energies= -3383.839921

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| C | -5.343439 | -1.591059 | 2.563166 |
| H | -5.016833 | -1.144319 | 1.616749 |
| C | -4.374789 | -2.731625 | 2.947305 |
| H | -4.651463 | -3.110184 | 3.935765 |
| H | -4.498727 | -3.561853 | 2.233365 |
| O | -3.021126 | -2.327527 | 3.032302 |
| H | -2.701047 | -2.131084 | 2.139041 |
| C | -6.739410 | -2.146406 | 2.460518 |
| O | -7.449049 | -2.356365 | 3.442153 |
| N | -7.093554 | -2.478266 | 1.188141 |
| H | -6.453692 | -2.317431 | 0.421560 |
| C | -8.283431 | -3.231898 | 0.921838 |
| H | -8.055484 | -4.247242 | 0.570646 |
| H | -8.844684 | -3.301645 | 1.854933 |
| C | -1.956700 | 5.955803 | -0.203949 |
| H | -1.568915 | 6.703596 | -0.904890 |

| | | | |
|---|---|---|---|
| C | -1.551858 | 6.255126 | 1.243426 |
| H | -1.931328 | 7.245220 | 1.544599 |
| H | -2.043707 | 5.521124 | 1.893726 |
| C | -0.036045 | 6.186812 | 1.514797 |
| H | 0.304954 | 5.192234 | 1.199546 |
| C | 0.752296 | 7.239730 | 0.721066 |
| H | 1.824649 | 7.170183 | 0.937199 |
| H | 0.627200 | 7.114305 | -0.359207 |
| H | 0.426099 | 8.257295 | 0.979020 |
| C | 0.248868 | 6.331150 | 3.017034 |
| H | 1.315085 | 6.201524 | 3.233602 |
| H | -0.053241 | 7.320905 | 3.387555 |
| H | -0.300622 | 5.579901 | 3.596351 |
| C | 0.799375 | -0.814814 | -4.009142 |
| H | 1.859615 | -0.600326 | -3.773643 |
| H | 0.387519 | 0.100112 | -4.475518 |
| O | 0.064757 | -1.253076 | -2.915465 |
| C | 2.351318 | -2.137886 | 0.016553 |
| C | 2.086044 | 2.124405 | -2.245981 |
| C | -2.636661 | 1.421085 | -2.926826 |
| C | -2.398670 | -2.781217 | -0.542035 |
| C | 2.701257 | -0.947068 | -0.618242 |
| C | 4.078034 | -0.497814 | -0.811443 |

| | | | |
|---|---|---|---|
| C | 4.002435 | 0.722977 | -1.426292 |
| C | 2.585682 | 0.996069 | -1.614918 |
| C | 5.114711 | 1.626965 | -1.865841 |
| C | 5.305200 | -1.315295 | -0.514302 |
| C | 5.579694 | -2.329282 | -1.659401 |
| C | 6.812010 | -3.204204 | -1.492412 |
| O | 6.793470 | -4.089555 | -0.449694 |
| O | 7.763094 | -3.188084 | -2.236723 |
| C | 0.748088 | 2.355085 | -2.552226 |
| C | 0.265599 | 3.529732 | -3.248283 |
| C | -1.090983 | 3.362651 | -3.402635 |
| C | -1.402820 | 2.052999 | -2.825271 |
| C | 1.109716 | 4.704158 | -3.638263 |
| C | -2.005799 | 4.314382 | -4.024873 |
| C | -3.293170 | 4.539834 | -3.717214 |
| C | -2.973859 | 0.166855 | -2.418950 |
| C | -4.252743 | -0.477029 | -2.630334 |
| C | -4.195655 | -1.678998 | -1.948807 |
| C | -2.867440 | -1.735379 | -1.342610 |
| C | -5.167198 | -2.757268 | -1.889009 |
| C | -6.489341 | -2.711114 | -2.153100 |
| C | -1.093193 | -2.926053 | -0.081599 |
| C | -0.611824 | -4.086199 | 0.659170 |

| | | | |
|---|---|---|---|
| C | 0.740506 | -3.920975 | 0.795861 |
| C | 1.063869 | -2.650367 | 0.148812 |
| C | -1.485887 | -5.187280 | 1.180396 |
| C | 1.702962 | -4.844652 | 1.495881 |
| C | 2.518069 | -5.784091 | 0.569946 |
| C | 3.938808 | -5.338673 | 0.317705 |
| O | 4.526485 | -4.479101 | 0.965398 |
| O | 4.526434 | -6.005701 | -0.685164 |
| N | 1.826718 | -0.031206 | -1.122296 |
| N | -0.277471 | 1.490917 | -2.290421 |
| N | -2.160013 | -0.614455 | -1.641588 |
| N | -0.066052 | -2.062768 | -0.338360 |
| H | 6.093255 | 1.221277 | -1.593294 |
| H | 5.027126 | 2.618158 | -1.405219 |
| H | 5.112801 | 1.774333 | -2.952891 |
| H | 1.461477 | 5.249686 | -2.753793 |
| H | 0.551716 | 5.412199 | -4.256846 |
| H | 1.997681 | 4.395639 | -4.202687 |
| H | -0.897748 | -5.997321 | 1.620952 |
| H | -2.103455 | -5.627831 | 0.388439 |
| H | -2.163101 | -4.810789 | 1.956999 |
| H | -3.870825 | 5.285245 | -4.255918 |
| H | -3.795469 | 4.021823 | -2.907410 |

| | | | |
|---|---|---|---|
| H | -7.090264 | -3.614709 | -2.115358 |
| H | -7.006232 | -1.795535 | -2.416961 |
| H | 5.705424 | -1.788969 | -2.599257 |
| H | 4.700972 | -2.976491 | -1.769796 |
| H | 5.190728 | -1.844932 | 0.438277 |
| H | 6.177550 | -0.662251 | -0.402761 |
| H | 2.028538 | -5.926752 | -0.398282 |
| H | 2.603351 | -6.786236 | 1.012225 |
| H | 1.135740 | -5.468394 | 2.192757 |
| H | 2.408381 | -4.272477 | 2.106816 |
| H | 3.156351 | -2.719633 | 0.444875 |
| H | 2.800507 | 2.882147 | -2.547739 |
| H | -3.398837 | 1.947792 | -3.486029 |
| H | -3.088263 | -3.587127 | -0.315082 |
| H | -1.565339 | 4.929635 | -4.810639 |
| H | -4.758595 | -3.729987 | -1.615233 |
| Fe | -0.167747 | -0.276074 | -1.300396 |
| H | -8.909154 | -2.744429 | 0.164971 |
| H | -1.586117 | 4.974174 | -0.507585 |
| H | 5.442941 | -5.672231 | -0.777902 |
| H | 6.025799 | -3.955021 | 0.153138 |
| H | 0.801519 | -1.595195 | -4.791911 |
| H | -5.312828 | -0.818785 | 3.336023 |

| | | | |
|---|---|---|---|
| H | -3.047795 | 5.949253 | -0.311398 |
| C | -0.598910 | 0.688593 | 0.506628 |
| C | -0.419733 | 2.156082 | 0.583736 |
| C | -1.961952 | 0.469879 | 1.176530 |
| C | 1.102517 | 0.099361 | 2.576117 |
| H | 0.329407 | 0.320274 | 1.437432 |
| N | 1.341219 | 1.294628 | 3.317198 |
| C | 2.506805 | 2.058153 | 3.167563 |
| C | 3.486981 | 1.752881 | 2.196608 |
| C | 2.763511 | 3.165768 | 4.009838 |
| C | 4.659844 | 2.495186 | 2.103165 |
| H | 3.325653 | 0.962208 | 1.478124 |
| C | 3.940148 | 3.903983 | 3.897903 |
| H | 2.050055 | 3.456633 | 4.769632 |
| C | 4.909866 | 3.575834 | 2.951403 |
| H | 5.382615 | 2.225217 | 1.337247 |
| H | 4.095437 | 4.743576 | 4.571577 |
| H | 5.827559 | 4.150843 | 2.868964 |
| C | 0.236038 | 1.837316 | 4.112917 |
| H | -0.695411 | 1.447090 | 3.698299 |
| C | 0.423879 | -1.032952 | 3.330250 |
| H | -0.553465 | -0.768240 | 3.742417 |
| H | 0.267448 | -1.875191 | 2.652821 |

| | | | |
|---|---|---|---|
| H | 1.050732 | -1.382250 | 4.164169 |
| H | 0.194477 | 2.920145 | 3.960215 |
| C | 0.302215 | 1.508181 | 5.612011 |
| H | 1.234052 | 1.860893 | 6.062753 |
| H | -0.533209 | 1.985317 | 6.138006 |
| H | 0.238009 | 0.430035 | 5.781386 |
| H | 2.013440 | -0.251831 | 2.101891 |
| C | -5.367309 | 0.051940 | -3.479741 |
| H | -5.840159 | -0.757933 | -4.046425 |
| H | -6.157137 | 0.528336 | -2.882372 |
| H | -5.010375 | 0.794644 | -4.197690 |
| H | -3.351682 | 2.099838 | 1.770630 |
| H | -3.226363 | 1.827226 | 0.013559 |
| C | -2.672493 | 1.814296 | 0.959920 |
| O | 0.579148 | 2.842377 | 0.460804 |
| O | -1.622458 | 2.790205 | 0.898608 |
| H | -1.869601 | 0.274872 | 2.254015 |
| H | -2.535452 | -0.351732 | 0.749104 |

**QM Cluster 2**

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**C** **L9**

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Number of imaginary frequencies : 4 Electronic energy : HF=-3591.3175661

Zero-point correction= 1.275613 (Hartree/Particle)

Thermal correction to Energy= 1.357275

Thermal correction to Enthalpy= 1.358220

Thermal correction to Gibbs Free Energy= 1.145138

Sum of electronic and zero-point Energies= -3590.041953

Sum of electronic and thermal Energies= -3589.960291

Sum of electronic and thermal Enthalpies= -3589.959346

Sum of electronic and thermal Free Energies= -3590.172429

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 6.437088 | 2.314315 | -3.200074 |
| C | 6.851705 | 1.319554 | -4.181483 |
| C | 4.992683 | 2.471703 | -3.329793 |
| C | 4.458682 | 1.349537 | -4.241636 |
| C | 5.670325 | 1.058218 | -5.141879 |
| H | 4.812764 | 3.465942 | -3.776795 |
| H | 4.515649 | 2.499438 | -2.343454 |
| H | 3.558265 | 1.638001 | -4.789776 |

| | | | |
|---|---|---|---|
| H | 4.205304 | 0.472888 | -3.635263 |
| H | 5.704633 | 1.766853 | -5.979547 |
| H | 5.674800 | 0.047492 | -5.562398 |
| H | 7.115196 | 0.399320 | -3.631617 |
| H | 7.775854 | 1.646585 | -4.678680 |
| C | -0.413020 | 5.546183 | -1.373517 |
| C | 1.072674 | 5.765588 | -1.669266 |
| O | 1.935909 | 5.057467 | -0.800656 |
| H | -0.632872 | 5.783966 | -0.327583 |
| H | 1.272797 | 5.508186 | -2.724211 |
| H | 1.322531 | 6.829841 | -1.551374 |
| H | 1.787028 | 4.099017 | -0.952425 |
| H | -1.038151 | 6.180741 | -2.014561 |
| H | -0.692380 | 4.504559 | -1.557632 |
| C | -5.073330 | 5.183592 | -2.728820 |
| C | -4.400120 | 3.913083 | -2.187816 |
| C | -5.251282 | 2.611117 | -2.299817 |
| O | -4.787080 | 1.603078 | -1.670201 |
| O | -6.296141 | 2.668207 | -2.989895 |
| H | -5.972918 | 5.426329 | -2.152092 |
| H | -3.455831 | 3.734421 | -2.721129 |
| H | -4.114766 | 4.037434 | -1.136014 |
| H | -5.394977 | 5.029000 | -3.762684 |

| | | | |
|---|---|---|---|
| H | -4.396037 | 6.046923 | -2.688946 |
| N | -7.242343 | -0.560427 | 0.051384 |
| C | -7.691381 | -0.985792 | -1.271582 |
| C | -6.673257 | -1.843586 | -2.005121 |
| O | -7.025602 | -2.824781 | -2.668879 |
| C | -7.443919 | 0.875536 | 0.127077 |
| C | -8.485000 | 1.268946 | -0.940811 |
| C | -8.164195 | 0.268952 | -2.061045 |
| H | -6.473467 | 1.340852 | -0.128071 |
| H | -7.696739 | 1.169836 | 1.154878 |
| H | -8.361934 | 2.299204 | -1.282940 |
| H | -9.505056 | 1.132554 | -0.552359 |
| H | -7.357907 | 0.700187 | -2.663724 |
| H | -9.014609 | 0.044791 | -2.713522 |
| H | -8.544080 | -1.665939 | -1.111654 |
| N | -5.395122 | -1.451845 | -1.809850 |
| C | 1.641548 | -1.866950 | 3.393811 |
| O | 1.605917 | -0.535355 | 3.002883 |
| H | 2.215210 | -2.516291 | 2.708743 |
| H | 0.636831 | -2.316778 | 3.497178 |
| H | 2.124554 | -1.950723 | 4.386230 |
| C | 3.437717 | -1.439216 | -0.402494 |
| C | -0.884201 | -2.914236 | 1.186618 |

| | | | |
|---|---|---|---|
| C | -1.645962 | 1.431856 | 3.156425 |
| C | 2.668808 | 2.897908 | 1.599946 |
| C | 2.275879 | -2.196512 | -0.244695 |
| C | 2.075963 | -3.552330 | -0.748623 |
| C | 0.849868 | -3.957984 | -0.291670 |
| C | 0.311598 | -2.853575 | 0.478838 |
| C | 0.163240 | -5.272425 | -0.511478 |
| C | 3.005124 | -4.372985 | -1.597774 |
| C | 3.843876 | -5.434487 | -0.814853 |
| C | 5.039287 | -4.794053 | -0.159236 |
| O | 5.996860 | -4.511858 | -1.036681 |
| O | 5.106224 | -4.518774 | 1.037220 |
| C | -1.435287 | -1.891738 | 1.959084 |
| C | -2.633929 | -2.016305 | 2.764317 |
| C | -2.866836 | -0.768116 | 3.302602 |
| C | -1.785727 | 0.087673 | 2.825309 |
| C | -3.435127 | -3.264857 | 2.961683 |
| C | -3.955238 | -0.314859 | 4.157094 |
| C | -4.703068 | -1.048066 | 4.998989 |
| C | -0.568224 | 2.247822 | 2.831203 |
| C | -0.474604 | 3.657065 | 3.181981 |
| C | 0.747229 | 4.085108 | 2.719546 |
| C | 1.377019 | 2.916701 | 2.107886 |

| | | | |
|---|---|---|---|
| C | -1.553748 | 4.457224 | 3.844230 |
| C | 1.319613 | 5.427448 | 2.688452 |
| C | 1.194656 | 6.375644 | 3.631213 |
| C | 3.290285 | 1.807691 | 1.006089 |
| C | 4.655437 | 1.834104 | 0.522287 |
| C | 4.894736 | 0.601562 | -0.028489 |
| C | 3.652766 | -0.156297 | 0.103359 |
| C | 5.579478 | 3.012198 | 0.616329 |
| C | 6.203789 | 0.154230 | -0.609747 |
| C | 7.246795 | -0.366335 | 0.442864 |
| C | 7.040927 | -1.838693 | 0.657072 |
| O | 7.560604 | -2.673384 | -0.094482 |
| O | 6.206275 | -2.146100 | 1.630487 |
| N | 1.180999 | -1.796435 | 0.468844 |
| N | -0.931207 | -0.621166 | 2.033468 |
| N | 0.555280 | 1.837490 | 2.171388 |
| N | 2.716888 | 0.594891 | 0.754931 |
| H | 0.676198 | -5.872878 | -1.269800 |
| H | -0.870870 | -5.134842 | -0.845193 |
| H | 0.122890 | -5.873945 | 0.406776 |
| H | -3.291491 | -3.976531 | 2.145524 |
| H | -4.503865 | -3.035090 | 3.019362 |
| H | -3.160742 | -3.781161 | 3.892791 |

| | | | |
|---|---|---|---|
| H | -1.546369 | 4.341370 | 4.937344 |
| H | -2.546814 | 4.155766 | 3.494442 |
| H | -1.426525 | 5.522660 | 3.629614 |
| H | 6.431885 | 2.907949 | -0.061748 |
| H | 5.973679 | 3.149343 | 1.632593 |
| H | 5.059489 | 3.937289 | 0.344296 |
| H | -5.510924 | -0.590409 | 5.562738 |
| H | -4.536276 | -2.107199 | 5.161057 |
| H | 1.625477 | 7.363574 | 3.490939 |
| H | 0.678821 | 6.196230 | 4.570158 |
| H | 4.207210 | -6.192191 | -1.517794 |
| H | 3.230090 | -5.911840 | -0.049421 |
| H | 3.690597 | -3.739695 | -2.169794 |
| H | 2.413242 | -4.921474 | -2.340158 |
| H | 7.136379 | 0.186213 | 1.377876 |
| H | 8.257609 | -0.231125 | 0.048574 |
| H | 6.666369 | 1.000847 | -1.128283 |
| H | 6.065958 | -0.623633 | -1.369778 |
| H | 4.254935 | -1.896972 | -0.951760 |
| H | -1.416374 | -3.858285 | 1.164677 |
| H | -2.433371 | 1.878944 | 3.751944 |
| H | 3.238126 | 3.816866 | 1.666721 |
| H | -4.185058 | 0.748184 | 4.090807 |

| | | | |
|---|---|---|---|
| H | 1.872249 | 5.660803 | 1.777757 |
| Fe | 0.884600 | 0.012281 | 1.345357 |
| C | -4.271484 | -2.195027 | -2.333197 |
| C | -4.284236 | -3.725449 | -2.153791 |
| C | -4.261297 | -4.300811 | -0.722516 |
| C | -5.565900 | -4.082408 | 0.062601 |
| C | -3.946230 | -5.806124 | -0.789456 |
| C | 0.025234 | 0.714351 | -0.343858 |
| C | -1.382198 | 0.367599 | -0.749062 |
| C | 0.480497 | 1.685782 | -1.320625 |
| H | -5.141146 | -4.135405 | -2.694148 |
| H | -3.377678 | -4.077219 | -2.668503 |
| H | -3.443819 | -3.807501 | -0.177199 |
| H | -5.534765 | -4.624811 | 1.015809 |
| H | -5.743056 | -3.027452 | 0.281745 |
| H | -6.423768 | -4.451560 | -0.510175 |
| H | -3.868773 | -6.243953 | 0.213245 |
| H | -4.742330 | -6.342256 | -1.322655 |
| H | -3.005634 | -6.005221 | -1.316851 |
| H | -4.157490 | -2.004275 | -3.413173 |
| H | -3.376378 | -1.784530 | -1.853563 |
| H | 5.913242 | -3.096842 | 1.544308 |
| H | 6.690084 | -3.927075 | -0.604280 |

| | | | |
|---|---|---|---|
| H | -5.224326 | -0.469569 | -1.560968 |
| H | -1.579915 | -0.708563 | -0.692396 |
| H | -2.114313 | 0.843254 | -0.079562 |
| O | -0.463469 | 1.880944 | -2.320665 |
| O | 1.515370 | 2.364126 | -1.382322 |
| C | -1.535987 | 0.927197 | -2.171785 |
| H | -1.401771 | 0.148124 | -2.936140 |
| H | -2.495929 | 1.424093 | -2.326561 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(\boldsymbol{R})} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 6 Electronic energy : HF=-4036.1391135

Zero-point correction= 1.503487 (Hartree/Particle)

Thermal correction to Energy= 1.596484

Thermal correction to Enthalpy= 1.597428

Thermal correction to Gibbs Free Energy= 1.360179

Sum of electronic and zero-point Energies= -4034.635626

Sum of electronic and thermal Energies= -4034.542629

Sum of electronic and thermal Enthalpies= -4034.541685

Sum of electronic and thermal Free Energies= -4034.778934

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 8.280009 | 1.979022 | -3.561593 |
| C | 7.287497 | 1.636453 | -2.549540 |
| C | 7.757911 | 1.513732 | -4.839302 |
| C | 6.268098 | 1.154316 | -4.661870 |
| C | 6.223039 | 0.719460 | -3.189011 |
| H | 8.341029 | 0.619254 | -5.125641 |
| H | 7.954641 | 2.261719 | -5.619505 |
| H | 5.923733 | 0.382872 | -5.357051 |
| H | 5.644786 | 2.042864 | -4.817019 |
| H | 6.526650 | -0.328020 | -3.083136 |
| H | 5.233051 | 0.826329 | -2.736772 |
| H | 6.836627 | 2.583347 | -2.202644 |
| H | 7.779784 | 1.197866 | -1.671848 |
| C | 0.146796 | 5.186282 | 1.314526 |
| C | 1.314396 | 5.320465 | 2.280916 |
| O | 1.138814 | 4.560339 | 3.477757 |
| H | 0.036555 | 4.152093 | 0.975483 |
| H | 2.251136 | 5.035731 | 1.775387 |
| H | 1.429284 | 6.360898 | 2.609336 |
| H | 0.955961 | 3.645069 | 3.213150 |

| | | | |
|---|---|---|---|
| H | -0.790121 | 5.488475 | 1.793946 |
| H | 0.302403 | 5.801497 | 0.423486 |
| C | -4.399261 | 5.836909 | -0.301430 |
| C | -5.331820 | 4.883969 | -1.052982 |
| C | -4.546740 | 3.654703 | -1.592527 |
| O | -4.954275 | 2.510571 | -1.243884 |
| O | -3.558422 | 3.930325 | -2.322070 |
| H | -3.562833 | 6.107980 | -0.951149 |
| H | -6.153644 | 4.550628 | -0.409144 |
| H | -5.772856 | 5.412314 | -1.910356 |
| H | -3.981538 | 5.353577 | 0.589881 |
| H | -4.907859 | 6.754656 | 0.025386 |
| N | -7.102556 | -0.016591 | -0.095596 |
| C | -7.578685 | -0.126597 | -1.468191 |
| C | -6.553402 | -0.680975 | -2.455642 |
| O | -6.864766 | -0.831086 | -3.640532 |
| C | -7.346261 | 1.345481 | 0.329708 |
| C | -8.452301 | 1.926144 | -0.573211 |
| C | -8.097490 | 1.270112 | -1.913674 |
| H | -6.410723 | 1.907538 | 0.117421 |
| H | -7.547396 | 1.386907 | 1.408385 |
| H | -8.433134 | 3.020154 | -0.612124 |
| H | -9.447766 | 1.612255 | -0.226384 |

| | | | |
|---|---|---|---|
| H | -7.272200 | 1.821334 | -2.373576 |
| H | -8.923531 | 1.204570 | -2.626626 |
| H | -8.411132 | -0.852673 | -1.467406 |
| N | -5.349602 | -0.952672 | -1.922696 |
| C | 1.240536 | -3.648937 | 2.944575 |
| O | 1.302474 | -2.266639 | 2.971106 |
| H | 1.641024 | -4.099618 | 2.018446 |
| H | 0.219706 | -4.052448 | 3.081952 |
| H | 1.847763 | -4.061841 | 3.774775 |
| C | 3.517680 | -0.868416 | 0.045583 |
| C | -0.149480 | -4.026684 | -0.176695 |
| C | -2.467044 | -1.590513 | 3.282598 |
| C | 1.341707 | 1.339231 | 3.764896 |
| C | 2.709697 | -1.941032 | -0.345049 |
| C | 3.058585 | -2.933676 | -1.361979 |
| C | 2.011708 | -3.816333 | -1.414164 |
| C | 1.038945 | -3.359524 | -0.445001 |
| C | 1.848349 | -5.020379 | -2.293091 |
| C | 4.277780 | -2.988210 | -2.238219 |
| C | 5.400940 | -3.969987 | -1.765409 |
| C | 6.308984 | -3.300302 | -0.770219 |
| O | 7.108736 | -2.406186 | -1.345482 |
| O | 6.287693 | -3.513560 | 0.440604 |

| | | | |
|---|---|---|---|
| C | -1.118289 | -3.631630 | 0.735686 |
| C | -2.342280 | -4.362440 | 0.992170 |
| C | -3.053577 | -3.619346 | 1.902537 |
| C | -2.200627 | -2.479559 | 2.246585 |
| C | -2.728052 | -5.656869 | 0.343047 |
| C | -4.390357 | -3.917618 | 2.413215 |
| C | -5.375090 | -3.034596 | 2.639463 |
| C | -1.625550 | -0.577180 | 3.734313 |
| C | -1.914674 | 0.263034 | 4.883893 |
| C | -0.831744 | 1.101873 | 5.029279 |
| C | 0.093053 | 0.750781 | 3.952310 |
| C | -3.179614 | 0.229331 | 5.685432 |
| C | -0.613116 | 2.185823 | 5.979409 |
| C | -1.080187 | 2.269981 | 7.236714 |
| C | 2.259243 | 1.016245 | 2.767480 |
| C | 3.546756 | 1.670583 | 2.619433 |
| C | 4.158126 | 1.077457 | 1.547284 |
| C | 3.241362 | 0.043753 | 1.066282 |
| C | 4.071659 | 2.766111 | 3.500670 |
| C | 5.501555 | 1.466635 | 1.001601 |
| C | 6.734687 | 0.952085 | 1.821824 |
| C | 7.088149 | -0.436141 | 1.372388 |
| O | 7.818870 | -0.623868 | 0.390146 |

| | | | |
|---|---|---|---|
| O | 6.498541 | -1.402102 | 2.045802 |
| N | 1.475841 | -2.219607 | 0.172394 |
| N | -1.054461 | -2.503804 | 1.506568 |
| N | -0.417544 | -0.246320 | 3.183471 |
| N | 2.094266 | 0.057961 | 1.810044 |
| H | 2.626944 | -5.067990 | -3.061148 |
| H | 0.879990 | -5.010999 | -2.806232 |
| H | 1.899072 | -5.956520 | -1.720874 |
| H | -1.976910 | -6.436546 | 0.524382 |
| H | -2.828531 | -5.550673 | -0.743192 |
| H | -3.687167 | -6.020467 | 0.721867 |
| H | -3.135288 | -0.504091 | 6.502885 |
| H | -4.040937 | -0.034276 | 5.063518 |
| H | -3.374287 | 1.206900 | 6.137883 |
| H | 4.926849 | 3.273039 | 3.040594 |
| H | 4.411140 | 2.376744 | 4.470771 |
| H | 3.306468 | 3.522184 | 3.705777 |
| H | -6.343782 | -3.362554 | 3.006487 |
| H | -5.267873 | -1.977635 | 2.418248 |
| H | -0.881266 | 3.147244 | 7.846036 |
| H | -1.651346 | 1.472132 | 7.700546 |
| H | 6.006681 | -4.261446 | -2.630557 |
| H | 4.963902 | -4.860076 | -1.310691 |

| | | | |
|---|---|---|---|
| H | 4.716055 | -1.995224 | -2.375247 |
| H | 3.971019 | -3.316140 | -3.237902 |
| H | 6.502756 | 0.968366 | 2.888333 |
| H | 7.598085 | 1.592034 | 1.620375 |
| H | 5.571545 | 2.560694 | 0.989482 |
| H | 5.617669 | 1.150791 | -0.040075 |
| H | 4.474086 | -0.767144 | -0.459038 |
| H | -0.340588 | -4.937413 | -0.733978 |
| H | -3.393128 | -1.744507 | 3.822166 |
| H | 1.653803 | 2.078124 | 4.494718 |
| H | -4.606069 | -4.974170 | 2.583467 |
| H | -0.015559 | 3.020064 | 5.610294 |
| Fe | 0.507268 | -1.191124 | 1.620378 |
| C | -4.181027 | -1.178868 | -2.746291 |
| C | -4.211746 | -2.451710 | -3.613568 |
| C | -4.096852 | -3.795828 | -2.865725 |
| C | -5.374895 | -4.167873 | -2.096395 |
| C | -3.730057 | -4.918306 | -3.851334 |
| C | -0.430114 | 0.089449 | 0.273663 |
| C | -1.477342 | -0.601906 | -0.494903 |
| C | -1.121791 | 1.384046 | 0.710919 |
| C | 0.940079 | 1.090518 | -1.880018 |
| N | 0.127043 | 2.162217 | -2.347005 |

| | | | |
|---|---|---|---|
| H | -5.108337 | -2.446661 | -4.243666 |
| H | -3.347749 | -2.368979 | -4.288331 |
| H | -3.274779 | -3.695430 | -2.143465 |
| H | -5.275730 | -5.151874 | -1.619811 |
| H | -5.602445 | -3.434915 | -1.320256 |
| H | -6.235454 | -4.210867 | -2.776963 |
| H | -3.625830 | -5.885324 | -3.342038 |
| H | -4.507752 | -5.033147 | -4.618672 |
| H | -2.785728 | -4.706217 | -4.366310 |
| H | 0.388800 | 0.492345 | -0.757671 |
| H | 1.853092 | 1.460382 | -1.417974 |
| H | -4.054987 | -0.316844 | -3.416217 |
| H | -3.314355 | -1.221051 | -2.095046 |
| C | 1.194398 | -0.034004 | -2.870678 |
| H | 1.856835 | -0.776391 | -2.425512 |
| H | 0.273117 | -0.552315 | -3.144010 |
| H | 1.666117 | 0.353627 | -3.786766 |
| C | 0.543221 | 3.495169 | -2.321231 |
| C | -0.397088 | 4.551153 | -2.443048 |
| C | 1.909943 | 3.851484 | -2.207497 |
| C | 0.028919 | 5.876186 | -2.455517 |
| H | -1.463095 | 4.345200 | -2.495852 |
| C | 2.311203 | 5.185500 | -2.206895 |

| | | | |
|---|---|---|---|
| H | 2.669048 | 3.079840 | -2.149279 |
| C | 1.380616 | 6.218296 | -2.336737 |
| H | -0.723655 | 6.656404 | -2.547173 |
| H | 3.372159 | 5.413801 | -2.121656 |
| H | 1.698403 | 7.257803 | -2.345090 |
| C | -1.186868 | 1.823790 | -2.938391 |
| H | -1.388035 | 0.782680 | -2.690199 |
| H | -1.990042 | 2.416647 | -2.487555 |
| C | -1.230982 | 2.009693 | -4.459301 |
| H | -1.018918 | 3.046844 | -4.736772 |
| H | -0.510228 | 1.361252 | -4.970258 |
| H | -2.236239 | 1.769248 | -4.820415 |
| H | 6.558770 | -2.264108 | 1.541505 |
| H | 7.530559 | -1.827563 | -0.641163 |
| H | -5.192699 | -0.634188 | -0.973081 |
| O | -2.728378 | -0.137756 | -0.163461 |
| O | -1.372367 | -1.464697 | -1.360485 |
| C | -2.621478 | 1.017589 | 0.702750 |
| H | -2.972225 | 0.723964 | 1.696701 |
| H | -3.281711 | 1.779460 | 0.282902 |
| H | -0.802987 | 1.749003 | 1.688547 |
| H | -0.940363 | 2.186357 | -0.017445 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(S)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 4 Electronic energy : HF=-4036.1421873

Zero-point correction= 1.503423 (Hartree/Particle)

Thermal correction to Energy= 1.598010

Thermal correction to Enthalpy= 1.598954

Thermal correction to Gibbs Free Energy= 1.357003

Sum of electronic and zero-point Energies= -4034.638765

Sum of electronic and thermal Energies= -4034.544177

Sum of electronic and thermal Enthalpies= -4034.543233

Sum of electronic and thermal Free Energies= -4034.785185

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 6.661333 | 4.203655 | -2.560784 |
| C | 6.201572 | 3.086919 | -3.377945 |
| C | 5.466119 | 4.898362 | -2.094642 |
| C | 4.237514 | 4.009238 | -2.368329 |
| C | 4.684689 | 3.247438 | -3.626402 |

| | | | |
|---|---|---|---|
| H | 5.398777 | 5.843624 | -2.665299 |
| H | 5.589554 | 5.193886 | -1.045538 |
| H | 3.311156 | 4.576677 | -2.487306 |
| H | 4.077038 | 3.311626 | -1.540392 |
| H | 4.513432 | 3.851912 | -4.526781 |
| H | 4.169062 | 2.292730 | -3.761018 |
| H | 6.400277 | 2.160800 | -2.812119 |
| H | 6.810109 | 3.016581 | -4.290659 |
| C | -1.263942 | 5.676179 | 0.632538 |
| C | -0.170044 | 5.926271 | -0.409239 |
| O | 1.097841 | 5.418535 | -0.030874 |
| H | -1.420448 | 4.604341 | 0.764883 |
| H | -0.490393 | 5.499713 | -1.373918 |
| H | -0.042695 | 7.008149 | -0.565046 |
| H | 1.045387 | 4.439535 | -0.120330 |
| H | -0.977089 | 6.112764 | 1.596572 |
| H | -2.213388 | 6.127184 | 0.315700 |
| C | -5.942586 | 5.041913 | -0.554074 |
| C | -5.221104 | 3.745719 | -0.144914 |
| C | -5.721425 | 2.429702 | -0.819315 |
| O | -5.337964 | 1.353832 | -0.246026 |
| O | -6.418310 | 2.526187 | -1.856388 |
| H | -6.987813 | 5.036581 | -0.222012 |

| | | | |
|---|---|---|---|
| H | -4.152957 | 3.831461 | -0.388069 |
| H | -5.259871 | 3.602678 | 0.941672 |
| H | -5.955589 | 5.132995 | -1.643901 |
| H | -5.452717 | 5.925547 | -0.125894 |
| N | -7.282758 | -1.425994 | 0.985198 |
| C | -7.750721 | -1.572012 | -0.390730 |
| C | -6.699031 | -2.146959 | -1.325112 |
| O | -6.986690 | -3.020793 | -2.149494 |
| C | -7.601645 | -0.073905 | 1.405805 |
| C | -8.699032 | 0.470236 | 0.468554 |
| C | -8.333116 | -0.204261 | -0.862265 |
| H | -6.686065 | 0.531040 | 1.261497 |
| H | -7.853899 | -0.058514 | 2.474918 |
| H | -8.688468 | 1.561537 | 0.396035 |
| H | -9.693636 | 0.154267 | 0.815289 |
| H | -7.576000 | 0.399903 | -1.374620 |
| H | -9.185194 | -0.336281 | -1.536974 |
| H | -8.548840 | -2.331545 | -0.378878 |
| N | -5.464474 | -1.636388 | -1.119760 |
| C | 1.935030 | -2.280057 | 3.526991 |
| O | 2.239565 | -1.070418 | 2.921225 |
| H | 1.864056 | -3.126696 | 2.821274 |
| H | 0.994144 | -2.262791 | 4.107680 |

| | | | |
|---|---|---|---|
| H | 2.736443 | -2.541875 | 4.244801 |
| C | 3.695564 | -1.739580 | -0.498087 |
| C | -0.540640 | -3.314973 | 1.230695 |
| C | -0.927865 | 0.728489 | 3.849135 |
| C | 3.081323 | 2.462466 | 1.825383 |
| C | 2.537715 | -2.500109 | -0.328794 |
| C | 2.311214 | -3.824469 | -0.899070 |
| C | 1.103430 | -4.255253 | -0.413596 |
| C | 0.603460 | -3.199202 | 0.443684 |
| C | 0.423463 | -5.568491 | -0.659046 |
| C | 3.195475 | -4.601316 | -1.833641 |
| C | 4.040895 | -5.728006 | -1.155995 |
| C | 5.275791 | -5.151361 | -0.515439 |
| O | 6.198632 | -4.828459 | -1.415613 |
| O | 5.399535 | -4.952913 | 0.691666 |
| C | -0.998644 | -2.376836 | 2.151723 |
| C | -2.103995 | -2.590928 | 3.063956 |
| C | -2.247134 | -1.425990 | 3.782038 |
| C | -1.184551 | -0.532947 | 3.320293 |
| C | -2.938570 | -3.831623 | 3.155809 |
| C | -3.267387 | -1.176361 | 4.796308 |
| C | -3.902588 | -0.024836 | 5.063219 |
| C | 0.084430 | 1.595616 | 3.451667 |

| | | | |
|---|---|---|---|
| C | 0.262106 | 2.934551 | 3.996274 |
| C | 1.364880 | 3.458133 | 3.368843 |
| C | 1.863645 | 2.407341 | 2.485567 |
| C | -0.656677 | 3.597528 | 4.975631 |
| C | 1.904805 | 4.816930 | 3.420218 |
| C | 2.078466 | 5.558386 | 4.524494 |
| C | 3.647092 | 1.432344 | 1.079703 |
| C | 5.003171 | 1.459203 | 0.566297 |
| C | 5.196139 | 0.263439 | -0.078312 |
| C | 3.942511 | -0.476014 | 0.044252 |
| C | 5.998188 | 2.560434 | 0.787529 |
| C | 6.484470 | -0.170523 | -0.715005 |
| C | 7.540313 | -0.778950 | 0.275773 |
| C | 7.323339 | -2.261287 | 0.393033 |
| O | 7.799424 | -3.042180 | -0.440327 |
| O | 6.535355 | -2.629560 | 1.382584 |
| N | 1.468784 | -2.139810 | 0.447353 |
| N | -0.458810 | -1.131123 | 2.330702 |
| N | 1.045030 | 1.319523 | 2.520426 |
| N | 3.033880 | 0.258986 | 0.751655 |
| H | 0.831350 | -6.073395 | -1.541329 |
| H | -0.651173 | -5.443636 | -0.820447 |
| H | 0.540379 | -6.256563 | 0.189785 |

| | | | |
|---|---|---|---|
| H | -2.334815 | -4.734571 | 3.014397 |
| H | -3.733382 | -3.845016 | 2.401619 |
| H | -3.426513 | -3.909983 | 4.132735 |
| H | -0.492119 | 3.242345 | 6.002386 |
| H | -1.707088 | 3.402918 | 4.732889 |
| H | -0.500875 | 4.680045 | 4.973175 |
| H | 6.736771 | 2.614691 | -0.019888 |
| H | 6.551800 | 2.428548 | 1.727672 |
| H | 5.511402 | 3.538569 | 0.842677 |
| H | -4.657998 | 0.024568 | 5.842379 |
| H | -3.727413 | 0.881542 | 4.493854 |
| H | 2.438270 | 6.582151 | 4.462390 |
| H | 1.879829 | 5.167259 | 5.518694 |
| H | 4.357297 | -6.445868 | -1.920605 |
| H | 3.449899 | -6.241589 | -0.396215 |
| H | 3.872398 | -3.943264 | -2.387398 |
| H | 2.566713 | -5.088705 | -2.588554 |
| H | 7.457434 | -0.292801 | 1.249557 |
| H | 8.544725 | -0.628719 | -0.129594 |
| H | 6.962803 | 0.702974 | -1.172734 |
| H | 6.320835 | -0.884453 | -1.530085 |
| H | 4.486281 | -2.179801 | -1.098631 |
| H | -1.085557 | -4.250313 | 1.168529 |

| | | | |
|---|---|---|---|
| H | -1.569822 | 1.059343 | 4.654960 |
| H | 3.663870 | 3.367703 | 1.953839 |
| H | -3.566665 | -2.055343 | 5.370453 |
| H | 2.132759 | 5.255176 | 2.447314 |
| Fe | 1.245782 | -0.403537 | 1.455869 |
| C | -4.302932 | -2.090846 | -1.851398 |
| C | -4.128649 | -3.610431 | -2.043033 |
| C | -3.928168 | -4.501979 | -0.799529 |
| C | -5.165097 | -4.610115 | 0.108087 |
| C | -3.510453 | -5.910115 | -1.260524 |
| C | 0.130789 | 0.436178 | -0.118663 |
| C | -1.351930 | 0.075962 | -0.258471 |
| C | 0.093018 | 1.910175 | -0.157649 |
| C | 0.874122 | 0.474935 | -2.731086 |
| N | -0.333251 | 0.341411 | -3.488012 |
| H | -4.972928 | -3.988953 | -2.623979 |
| H | -3.230529 | -3.714068 | -2.669867 |
| H | -3.102322 | -4.078221 | -0.209333 |
| H | -4.990035 | -5.343955 | 0.905499 |
| H | -5.422667 | -3.656487 | 0.574305 |
| H | -6.036734 | -4.938363 | -0.468273 |
| H | -3.289541 | -6.562372 | -0.406906 |
| H | -4.319023 | -6.380674 | -1.834999 |

| | | | |
|---|---|---|---|
| H | -2.623418 | -5.884250 | -1.904192 |
| H | 0.669268 | 0.205067 | -1.383566 |
| H | 1.114559 | 1.526351 | -2.592627 |
| H | -4.294610 | -1.646323 | -2.861030 |
| H | -3.428835 | -1.690727 | -1.327734 |
| C | 2.071283 | -0.313301 | -3.230774 |
| H | 2.935092 | -0.096565 | -2.598782 |
| H | 1.919459 | -1.396819 | -3.197352 |
| H | 2.315498 | -0.041737 | -4.269933 |
| C | -1.165312 | 1.465881 | -3.706175 |
| C | -2.566589 | 1.404066 | -3.566915 |
| C | -0.596683 | 2.703554 | -4.070675 |
| C | -3.361450 | 2.539121 | -3.734002 |
| H | -3.048949 | 0.480554 | -3.269766 |
| C | -1.394672 | 3.830506 | -4.248482 |
| H | 0.476645 | 2.776429 | -4.212692 |
| C | -2.780020 | 3.761137 | -4.077449 |
| H | -4.429131 | 2.471233 | -3.536102 |
| H | -0.924364 | 4.772388 | -4.522154 |
| H | -3.396556 | 4.647937 | -4.192953 |
| C | -0.868574 | -1.000300 | -3.719855 |
| H | -0.176298 | -1.713232 | -3.268303 |
| H | -1.820161 | -1.144703 | -3.195743 |

| | | | |
|---|---|---|---|
| C | -1.052326 | -1.315198 | -5.208440 |
| H | -1.735943 | -0.598774 | -5.674141 |
| H | -0.095355 | -1.265379 | -5.738518 |
| H | -1.472478 | -2.319384 | -5.339313 |
| H | 6.231133 | -3.571766 | 1.249026 |
| H | 6.913540 | -4.272348 | -0.981283 |
| H | -5.397786 | -0.706738 | -0.685358 |
| O | 0.991066 | 2.704776 | -0.449127 |
| O | -1.150577 | 2.392876 | 0.130871 |
| C | -2.059746 | 1.282969 | 0.369855 |
| H | -1.640136 | 0.014390 | -1.313968 |
| H | -1.636943 | -0.859783 | 0.218968 |
| H | -3.031379 | 1.523749 | -0.064810 |
| H | -2.172661 | 1.170243 | 1.450784 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{C}}_{(\boldsymbol{R})} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 5 Electronic energy : HF=-4036.1430714

Zero-point correction= 1.503578 (Hartree/Particle)

Thermal correction to Energy= 1.597188

Thermal correction to Enthalpy= 1.598132

Thermal correction to Gibbs Free Energy= 1.359413

Sum of electronic and zero-point Energies= -4034.639493

Sum of electronic and thermal Energies= -4034.545884

Sum of electronic and thermal Enthalpies= -4034.544939

Sum of electronic and thermal Free Energies= -4034.783659

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | -5.708246 | -3.484218 | -2.379909 |
| C | -6.116290 | -2.765823 | -3.577594 |
| C | -4.310301 | -3.856959 | -2.561763 |
| C | -3.822775 | -3.329427 | -3.931189 |
| C | -5.134656 | -3.132840 | -4.708025 |
| H | -4.252863 | -4.957038 | -2.491871 |
| H | -3.707104 | -3.469306 | -1.727325 |
| H | -3.125294 | -4.008665 | -4.429450 |
| H | -3.305150 | -2.377467 | -3.782700 |
| H | -5.452333 | -4.069627 | -5.185328 |
| H | -5.072809 | -2.366847 | -5.488218 |
| H | -6.049591 | -1.684980 | -3.355558 |
| H | -7.171837 | -2.969094 | -3.803606 |
| C | 0.982550 | -5.184277 | 1.142774 |

| | | | |
|---|---|---|---|
| C | -0.396274 | -5.373454 | 0.505103 |
| O | -1.391080 | -4.538934 | 1.075708 |
| H | 1.344016 | -4.163334 | 1.018973 |
| H | -0.324716 | -5.218498 | -0.581155 |
| H | -0.724058 | -6.412808 | 0.653644 |
| H | -1.435824 | -3.699381 | 0.578495 |
| H | 0.938064 | -5.392834 | 2.217349 |
| H | 1.717853 | -5.860923 | 0.690689 |
| C | 5.745695 | -4.853969 | 0.192389 |
| C | 7.132686 | -4.633467 | 0.794055 |
| C | 7.542066 | -3.146841 | 1.031117 |
| O | 8.724038 | -2.979954 | 1.418520 |
| O | 6.648343 | -2.269470 | 0.828359 |
| H | 5.669754 | -4.399542 | -0.799831 |
| H | 7.212621 | -5.142732 | 1.765315 |
| H | 7.910060 | -5.087635 | 0.165054 |
| H | 4.979050 | -4.384465 | 0.815023 |
| H | 5.507263 | -5.922786 | 0.095763 |
| N | 7.170740 | 1.566634 | 1.075172 |
| C | 7.826340 | 1.668082 | -0.224102 |
| C | 6.837039 | 1.773101 | -1.381629 |
| O | 7.171189 | 1.593988 | -2.554096 |
| C | 7.779463 | 0.453275 | 1.763049 |

| | | | |
|---|---|---|---|
| C | 9.147250 | 0.172155 | 1.116004 |
| C | 8.825390 | 0.489006 | -0.350998 |
| H | 7.160910 | -0.462408 | 1.566994 |
| H | 7.785397 | 0.620496 | 2.848371 |
| H | 9.428635 | -0.874710 | 1.271070 |
| H | 9.921802 | 0.849235 | 1.507503 |
| H | 8.319173 | -0.371595 | -0.798440 |
| H | 9.692048 | 0.738053 | -0.969711 |
| H | 8.384613 | 2.624149 | -0.233257 |
| N | 5.583769 | 2.106018 | -0.995489 |
| C | -2.032348 | 3.148701 | 2.981909 |
| O | -2.045998 | 1.777507 | 2.752754 |
| H | -2.537690 | 3.732886 | 2.191700 |
| H | -1.013139 | 3.563256 | 3.089895 |
| H | -2.564445 | 3.363423 | 3.926443 |
| C | -4.570999 | 0.769215 | -0.066816 |
| C | -0.971802 | 4.002629 | -0.315028 |
| C | 1.657105 | 1.278056 | 2.682313 |
| C | -1.881233 | -1.999173 | 2.840256 |
| C | -3.825989 | 1.901074 | -0.397373 |
| C | -4.306812 | 3.009092 | -1.214460 |
| C | -3.277447 | 3.913572 | -1.286641 |
| C | -2.185935 | 3.355739 | -0.517467 |

| | | | |
|---|---|---|---|
| C | -3.243347 | 5.236242 | -1.993590 |
| C | -5.655236 | 3.169543 | -1.857712 |
| C | -6.688665 | 3.996056 | -1.024255 |
| C | -7.407498 | 3.121495 | -0.028010 |
| O | -8.276388 | 2.309492 | -0.620530 |
| O | -7.189831 | 3.126727 | 1.181524 |
| C | 0.085977 | 3.526686 | 0.453196 |
| C | 1.281121 | 4.288188 | 0.738153 |
| C | 2.070353 | 3.493342 | 1.540871 |
| C | 1.301278 | 2.268839 | 1.772332 |
| C | 1.536548 | 5.688917 | 0.266160 |
| C | 3.387865 | 3.851675 | 2.059447 |
| C | 4.412952 | 3.036704 | 2.359371 |
| C | 0.911105 | 0.150254 | 3.009763 |
| C | 1.332921 | -0.842268 | 3.985016 |
| C | 0.342954 | -1.799674 | 4.007619 |
| C | -0.668886 | -1.354802 | 3.052215 |
| C | 2.630117 | -0.827462 | 4.733641 |
| C | 0.265350 | -3.051923 | 4.749550 |
| C | 0.808277 | -3.324322 | 5.947565 |
| C | -2.919887 | -1.533070 | 2.047597 |
| C | -4.171466 | -2.247151 | 1.870371 |
| C | -4.951666 | -1.463073 | 1.067538 |

| | | | |
|---|---|---|---|
| C | -4.151893 | -0.281068 | 0.747197 |
| C | -4.461107 | -3.607872 | 2.428656 |
| C | -6.342119 | -1.791697 | 0.605904 |
| C | -7.459850 | -1.548280 | 1.679206 |
| C | -7.878623 | -0.106753 | 1.633748 |
| O | -8.795514 | 0.278237 | 0.897966 |
| O | -7.130804 | 0.705797 | 2.357890 |
| N | -2.534156 | 2.134128 | -0.004259 |
| N | 0.125083 | 2.307452 | 1.076612 |
| N | -0.290734 | -0.193558 | 2.457098 |
| N | -2.928438 | -0.361916 | 1.349031 |
| H | -4.109291 | 5.364316 | -2.650814 |
| H | -2.344003 | 5.340455 | -2.612051 |
| H | -3.243587 | 6.078353 | -1.288515 |
| H | 1.408590 | 5.785996 | -0.818396 |
| H | 2.553170 | 6.013567 | 0.501260 |
| H | 0.841894 | 6.400341 | 0.732840 |
| H | 2.562375 | -0.253817 | 5.668413 |
| H | 3.434043 | -0.384393 | 4.138530 |
| H | 2.933754 | -1.845016 | 4.996581 |
| H | -5.419673 | -3.991859 | 2.066289 |
| H | -4.501320 | -3.602642 | 3.526141 |
| H | -3.676408 | -4.312446 | 2.129197 |

| | | | |
|---|---|---|---|
| H | 5.359839 | 3.429342 | 2.712963 |
| H | 4.372605 | 1.961349 | 2.228316 |
| H | 0.711842 | -4.311765 | 6.390069 |
| H | 1.347171 | -2.581068 | 6.525945 |
| H | -7.439574 | 4.414262 | -1.703767 |
| H | -6.189045 | 4.807367 | -0.492588 |
| H | -6.101186 | 2.200658 | -2.103134 |
| H | -5.526112 | 3.689369 | -2.813901 |
| H | -7.085441 | -1.814589 | 2.669999 |
| H | -8.337380 | -2.153667 | 1.438220 |
| H | -6.385470 | -2.844408 | 0.311366 |
| H | -6.604066 | -1.241478 | -0.303299 |
| H | -5.573880 | 0.704642 | -0.476215 |
| H | -0.856016 | 4.985574 | -0.758870 |
| H | 2.580441 | 1.426981 | 3.225183 |
| H | -2.040086 | -2.941641 | 3.347441 |
| H | 3.555497 | 4.923280 | 2.175375 |
| H | -0.291062 | -3.847018 | 4.253309 |
| Fe | -1.394247 | 0.947456 | 1.197681 |
| C | 4.495350 | 2.154429 | -1.944716 |
| C | 4.520162 | 3.356110 | -2.911878 |
| C | 4.187209 | 4.742377 | -2.327850 |
| C | 5.280468 | 5.294744 | -1.399360 |

| | | | |
|---|---|---|---|
| C | 3.907611 | 5.739365 | -3.464856 |
| C | -0.646484 | -0.135205 | -0.588905 |
| C | -1.537919 | -1.173023 | -1.110760 |
| C | -0.342472 | 0.713016 | -1.829260 |
| C | 1.486122 | -1.881462 | -0.597634 |
| N | 2.110908 | -1.895191 | -1.888025 |
| H | 5.500607 | 3.375524 | -3.402062 |
| H | 3.784513 | 3.133314 | -3.698074 |
| H | 3.264894 | 4.639502 | -1.739541 |
| H | 5.013755 | 6.296503 | -1.038572 |
| H | 5.440150 | 4.652060 | -0.531824 |
| H | 6.236016 | 5.376812 | -1.933043 |
| H | 3.640171 | 6.728169 | -3.072650 |
| H | 4.794293 | 5.863958 | -4.100059 |
| H | 3.086700 | 5.398135 | -4.106086 |
| H | 0.522908 | -0.924740 | -0.441498 |
| H | 0.854452 | -2.758542 | -0.487483 |
| H | 4.532286 | 1.252737 | -2.560991 |
| H | 3.555799 | 2.145322 | -1.383253 |
| C | 2.425400 | -1.729189 | 0.586800 |
| H | 3.237360 | -2.466048 | 0.565998 |
| H | 2.882856 | -0.738212 | 0.647719 |
| H | 1.855670 | -1.871646 | 1.505836 |

| | | | |
|---|---|---|---|
| C | 3.253339 | -1.000915 | -2.108357 |
| H | 3.158602 | -0.186487 | -1.391234 |
| H | -7.277393 | 1.650358 | 2.074792 |
| H | -8.601015 | 1.619832 | 0.034984 |
| H | 5.422430 | 2.132846 | 0.005534 |
| C | -1.544033 | 0.450133 | -2.753061 |
| O | -2.073094 | -0.825977 | -2.341866 |
| O | -1.824941 | -2.293213 | -0.674982 |
| H | 0.579817 | 0.366655 | -2.319858 |
| H | -0.219040 | 1.775663 | -1.619846 |
| H | -1.284525 | 0.370041 | -3.814600 |
| H | -2.326338 | 1.206909 | -2.633957 |
| H | 3.135118 | -0.543521 | -3.097844 |
| C | 4.646580 | -1.640525 | -1.981573 |
| H | 4.712395 | -2.564248 | -2.564048 |
| H | 5.404109 | -0.949145 | -2.368907 |
| H | 4.924742 | -1.874024 | -0.950378 |
| C | 1.658463 | -2.683060 | -2.946402 |
| C | 0.447108 | -3.416074 | -2.881050 |
| C | 2.400111 | -2.784734 | -4.151997 |
| C | 0.042860 | -4.228231 | -3.936636 |
| H | -0.214452 | -3.317631 | -2.031464 |
| C | 1.972186 | -3.595171 | -5.200286 |

| | | | |
|---|---|---|---|
| H | 3.333582 | -2.250988 | -4.267811 |
| C | 0.795148 | -4.338747 | -5.108135 |
| H | -0.892616 | -4.773101 | -3.836584 |
| H | 2.583070 | -3.647755 | -6.099217 |
| H | 0.468568 | -4.975014 | -5.926096 |

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**C** **L10**

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Number of imaginary frequencies : 3 Electronic energy : HF=-3756.8096966

Zero-point correction= 1.317972 (Hartree/Particle)

Thermal correction to Energy= 1.403842

Thermal correction to Enthalpy= 1.404786

Thermal correction to Gibbs Free Energy= 1.175349

Sum of electronic and zero-point Energies= -3755.491724

Sum of electronic and thermal Energies= -3755.405855

Sum of electronic and thermal Enthalpies= -3755.404910

Sum of electronic and thermal Free Energies= -3755.634347

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | -9.678984 | -4.927967 | 0.235993 |
| C | -9.313300 | -4.169984 | -0.952937 |
| C | -9.093742 | -4.234348 | 1.375127 |
| C | -8.600354 | -2.848351 | 0.909380 |
| C | -8.254675 | -3.116246 | -0.563881 |
| H | -8.247938 | -4.847741 | 1.733777 |
| H | -9.812195 | -4.204943 | 2.204758 |
| H | -7.248386 | -3.543599 | -0.645285 |
| H | -8.285449 | -2.220830 | -1.191093 |
| H | -10.231880 | -3.682691 | -1.326132 |
| H | -8.997268 | -4.855892 | -1.750077 |
| C | -3.801173 | -1.261828 | 5.565587 |
| C | -2.650818 | -0.735966 | 4.712979 |
| O | -2.606777 | -1.475454 | 3.501089 |
| H | -4.754990 | -1.126979 | 5.045345 |
| H | -2.799291 | 0.336744 | 4.519826 |
| H | -1.705128 | -0.838650 | 5.270913 |
| H | -1.933247 | -1.083496 | 2.916708 |
| H | -3.848669 | -0.727047 | 6.520076 |
| H | -3.670291 | -2.329590 | 5.768681 |
| C | 3.644148 | -2.931549 | 7.083509 |
| C | 4.674319 | -2.753213 | 5.963269 |
| C | 4.324425 | -3.410695 | 4.608044 |

| | | | |
|---|---|---|---|
| O | 5.166165 | -3.357870 | 3.693727 |
| O | 3.170286 | -3.978992 | 4.532883 |
| H | 2.679600 | -2.500590 | 6.800224 |
| H | 4.846689 | -1.687149 | 5.764206 |
| H | 5.651491 | -3.150620 | 6.266239 |
| H | 3.977683 | -2.448434 | 8.010453 |
| H | 3.470888 | -3.991978 | 7.289367 |
| N | 7.500897 | -2.715301 | -1.248026 |
| C | 6.540853 | -2.249845 | -0.251375 |
| C | 5.785946 | -0.995437 | -0.767750 |
| O | 5.853041 | 0.065658 | -0.154750 |
| C | 8.756423 | -2.933323 | -0.544530 |
| C | 8.457812 | -2.990890 | 0.966384 |
| C | 7.252696 | -2.047226 | 1.100361 |
| H | 9.415186 | -2.076817 | -0.778156 |
| H | 9.260138 | -3.820740 | -0.950053 |
| H | 9.311339 | -2.692929 | 1.582743 |
| H | 8.180380 | -4.010824 | 1.256961 |
| H | 7.568176 | -1.002953 | 1.180780 |
| H | 6.611222 | -2.282779 | 1.954627 |
| H | 5.781328 | -3.047056 | -0.155220 |
| N | 5.040069 | -1.078411 | -1.916110 |
| C | 4.645892 | -2.217763 | -2.755607 |

| | | | |
|---|---|---|---|
| C | 3.641439 | -3.202193 | -2.096722 |
| C | 2.685722 | -2.556999 | -1.081410 |
| C | 1.602512 | -3.530440 | -0.573464 |
| N | 1.019723 | -3.155661 | 0.706821 |
| C | 1.532166 | -3.524840 | 1.903431 |
| N | 2.550531 | -4.385040 | 2.024629 |
| N | 0.941914 | -3.083298 | 3.023799 |
| H | 4.538508 | -0.213723 | -2.078568 |
| H | 5.545656 | -2.756636 | -3.065305 |
| H | 3.074281 | -3.692112 | -2.900057 |
| H | 4.196236 | -4.005615 | -1.593798 |
| H | 3.258627 | -2.200019 | -0.219233 |
| H | 2.197919 | -1.673146 | -1.509176 |
| H | 0.787850 | -3.599152 | -1.302032 |
| H | 2.006468 | -4.544854 | -0.476831 |
| H | 0.357599 | -2.382110 | 0.739612 |
| H | 1.513754 | -3.190587 | 3.866086 |
| H | 4.195377 | -1.777520 | -3.648684 |
| C | -2.573782 | 2.653765 | -2.523055 |
| O | -1.817152 | 3.220473 | -1.499914 |
| H | -1.966406 | 2.079616 | -3.245432 |
| H | -3.078863 | 3.453091 | -3.093042 |
| H | -3.361523 | 1.972285 | -2.155411 |

| | | | |
|---|---|---|---|
| C | -0.577229 | -0.534657 | -2.369543 |
| C | 1.858101 | 3.652721 | -2.120936 |
| C | -0.766905 | 5.026764 | 1.685188 |
| C | -3.352058 | 0.965335 | 1.300764 |
| C | 0.339965 | 0.485621 | -2.643473 |
| C | 1.315916 | 0.482278 | -3.729267 |
| C | 2.000919 | 1.668460 | -3.636222 |
| C | 1.436434 | 2.384911 | -2.510445 |
| C | 3.091949 | 2.187918 | -4.526223 |
| C | 1.521464 | -0.557190 | -4.795741 |
| C | 0.742298 | -0.291315 | -6.124975 |
| C | -0.662191 | -0.831673 | -6.038320 |
| O | -0.682536 | -2.158123 | -6.083346 |
| O | -1.663094 | -0.132785 | -5.893642 |
| C | 1.349651 | 4.412683 | -1.072412 |
| C | 1.824795 | 5.739373 | -0.720371 |
| C | 1.091791 | 6.128798 | 0.378275 |
| C | 0.169489 | 5.027116 | 0.656844 |
| C | 2.866199 | 6.514929 | -1.466963 |
| C | 1.127819 | 7.380208 | 1.123675 |
| C | 2.175882 | 8.205621 | 1.282499 |
| C | -1.707580 | 4.031118 | 1.928097 |
| C | -2.738686 | 4.117552 | 2.945506 |

| | | | |
|---|---|---|---|
| C | -3.490898 | 2.969035 | 2.830276 |
| C | -2.894693 | 2.204387 | 1.735888 |
| C | -2.950282 | 5.275793 | 3.871384 |
| C | -4.680144 | 2.559522 | 3.566208 |
| C | -5.024301 | 2.901446 | 4.819644 |
| C | -2.816962 | 0.204258 | 0.267814 |
| C | -3.312001 | -1.115098 | -0.081244 |
| C | -2.536199 | -1.557426 | -1.117112 |
| C | -1.564449 | -0.497059 | -1.384863 |
| C | -4.423414 | -1.824479 | 0.631966 |
| C | -2.694369 | -2.880102 | -1.813205 |
| C | -3.868657 | -2.938075 | -2.847764 |
| C | -3.408684 | -2.350734 | -4.153033 |
| O | -3.557781 | -1.043754 | -4.250273 |
| O | -2.857164 | -3.050603 | -5.008676 |
| N | 0.443414 | 1.646110 | -1.926374 |
| N | 0.358893 | 4.008000 | -0.223492 |
| N | -1.820661 | 2.863198 | 1.222901 |
| N | -1.765211 | 0.550882 | -0.527857 |
| Fe | -0.692558 | 2.251171 | -0.356041 |
| H | 3.463399 | 1.414385 | -5.205004 |
| H | 3.947770 | 2.554814 | -3.947965 |
| H | 2.745339 | 3.024094 | -5.147055 |

| | | | |
|---|---|---|---|
| H | 3.881932 | 6.305616 | -1.104259 |
| H | 2.699279 | 7.590835 | -1.355661 |
| H | 2.850423 | 6.280512 | -2.536059 |
| H | -4.008098 | 5.368971 | 4.136656 |
| H | -2.633884 | 6.218483 | 3.414566 |
| H | -2.389938 | 5.166297 | 4.810011 |
| H | -4.202156 | -1.892977 | 1.703604 |
| H | -4.562211 | -2.840305 | 0.249458 |
| H | -5.380604 | -1.298432 | 0.519229 |
| H | 2.076061 | 9.128643 | 1.845951 |
| H | 3.160121 | 7.982590 | 0.884582 |
| H | -5.953304 | 2.547140 | 5.256146 |
| H | -4.391733 | 3.513822 | 5.453162 |
| H | 1.251305 | -0.809102 | -6.944769 |
| H | 0.704017 | 0.777661 | -6.338908 |
| H | 1.268007 | -1.561317 | -4.440665 |
| H | 2.586228 | -0.589200 | -5.053134 |
| H | -4.731330 | -2.394103 | -2.457441 |
| H | -4.140164 | -3.980360 | -3.033131 |
| H | -2.893959 | -3.653837 | -1.063652 |
| H | -1.772215 | -3.187405 | -2.319188 |
| H | -0.541381 | -1.414201 | -3.005147 |
| H | 2.663073 | 4.092739 | -2.698875 |

| | | | |
|---|---|---|---|
| H | -0.783187 | 5.888876 | 2.341294 |
| H | -4.183864 | 0.528335 | 1.838956 |
| H | 0.190865 | 7.667268 | 1.600864 |
| H | -5.359219 | 1.900600 | 3.025877 |
| H | -1.596060 | -2.495340 | -5.836579 |
| H | -2.999721 | -0.688947 | -5.000001 |
| H | -7.756801 | -2.471596 | 1.494105 |
| H | -9.412583 | -2.115066 | 0.983584 |
| H | 0.337261 | -2.270295 | 2.925711 |
| C | 0.610602 | 1.382292 | 0.914178 |
| C | 0.561276 | 0.142105 | 1.663368 |
| C | 2.704628 | 0.917607 | 2.055023 |
| H | 3.505992 | 0.467602 | 1.458673 |
| C | 1.933611 | 2.005816 | 1.287706 |
| H | 3.130743 | 1.252165 | 3.005214 |
| H | 1.759696 | 2.894449 | 1.912218 |
| H | 2.485228 | 2.360883 | 0.411856 |
| O | -0.337709 | -0.718538 | 1.784957 |
| O | 1.727503 | -0.101108 | 2.350337 |
| H | 3.185876 | -4.480837 | 1.249036 |
| H | 2.971544 | -4.385592 | 3.013715 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(R)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 3 Electronic energy : HF=-4201.5517378

Zero-point correction= 1.545329 (Hartree/Particle)

Thermal correction to Energy= 1.644108

Thermal correction to Enthalpy= 1.645053

Thermal correction to Gibbs Free Energy= 1.389227

Sum of electronic and zero-point Energies= -4200.006409

Sum of electronic and thermal Energies= -4199.907629

Sum of electronic and thermal Enthalpies= -4199.906685

Sum of electronic and thermal Free Energies= -4200.162510

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 7.200624 | 2.495276 | -1.831402 |
| C | 7.493100 | 2.220815 | -3.230318 |
| C | 6.580744 | 3.812462 | -1.770062 |
| C | 6.283008 | 4.282041 | -3.209790 |
| C | 7.354572 | 3.537654 | -4.022164 |
| H | 7.299817 | 4.487958 | -1.273734 |
| H | 5.699890 | 3.782373 | -1.117045 |

| | | | |
|---|---|---|---|
| H | 8.302955 | 4.088656 | -4.002462 |
| H | 7.081525 | 3.382353 | -5.070054 |
| H | 6.754074 | 1.478219 | -3.580110 |
| H | 8.473626 | 1.735590 | -3.321314 |
| C | 0.838293 | 6.056293 | 1.494665 |
| C | 2.359183 | 5.931643 | 1.496270 |
| O | 2.827859 | 4.687761 | 0.976920 |
| H | 0.426961 | 5.920202 | 0.491531 |
| H | 2.804529 | 6.700179 | 0.853762 |
| H | 2.743602 | 6.094194 | 2.515396 |
| H | 2.428005 | 3.973764 | 1.495227 |
| H | 0.532920 | 7.042174 | 1.864450 |
| H | 0.388717 | 5.303345 | 2.152011 |
| C | -6.879473 | 5.850465 | 0.546513 |
| C | -7.235062 | 5.126283 | -0.755865 |
| C | -6.062296 | 5.155464 | -1.788699 |
| O | -5.853137 | 4.083239 | -2.419233 |
| O | -5.455722 | 6.257298 | -1.881361 |
| H | -7.736637 | 5.944486 | 1.228517 |
| H | -7.522540 | 4.084692 | -0.571914 |
| H | -8.102678 | 5.622622 | -1.217756 |
| H | -6.500388 | 6.846085 | 0.301030 |
| H | -6.083401 | 5.321012 | 1.084374 |

| | | | |
|---|---|---|---|
| N | -8.200807 | -3.237317 | -0.216202 |
| C | -7.727846 | -1.927563 | -0.652525 |
| C | -6.258339 | -1.687070 | -0.169468 |
| O | -6.021465 | -0.788683 | 0.625334 |
| C | -9.466562 | -3.025160 | 0.467965 |
| C | -10.004487 | -1.643812 | 0.048621 |
| C | -8.708168 | -0.846512 | -0.158640 |
| H | -9.263342 | -3.047110 | 1.554089 |
| H | -10.144129 | -3.864732 | 0.267702 |
| H | -10.670065 | -1.198959 | 0.793946 |
| H | -10.566374 | -1.731864 | -0.889097 |
| H | -8.333352 | -0.435750 | 0.782167 |
| H | -8.805732 | -0.015968 | -0.861241 |
| H | -7.684959 | -1.954427 | -1.755869 |
| N | -5.230660 | -2.452681 | -0.674183 |
| C | -5.265485 | -3.747149 | -1.353892 |
| C | -4.814406 | -3.714833 | -2.822824 |
| C | -3.299925 | -3.560464 | -2.973791 |
| C | -2.815947 | -3.639424 | -4.427653 |
| N | -1.347030 | -3.685930 | -4.528800 |
| C | -0.580921 | -2.670945 | -4.048507 |
| N | -0.948435 | -1.403879 | -4.154728 |
| N | 0.619629 | -2.945213 | -3.498987 |

| | | | |
|---|---|---|---|
| H | -4.342876 | -2.167043 | -0.274913 |
| H | -6.287906 | -4.126350 | -1.284071 |
| H | -5.131341 | -4.656325 | -3.293921 |
| H | -5.340658 | -2.905158 | -3.343362 |
| H | -2.966535 | -2.615333 | -2.528522 |
| H | -2.805344 | -4.362569 | -2.408604 |
| H | -3.189109 | -4.544576 | -4.916553 |
| H | -3.194565 | -2.801026 | -5.022550 |
| H | -0.939182 | -4.602395 | -4.400732 |
| H | -1.842092 | -1.160267 | -4.551072 |
| H | -0.503267 | -0.789779 | -3.419067 |
| H | 1.008272 | -2.149827 | -2.980542 |
| H | -4.634852 | -4.448834 | -0.792179 |
| C | 2.103716 | -2.795573 | 3.152489 |
| O | 1.327855 | -1.640332 | 3.157322 |
| H | 1.588174 | -3.668046 | 2.710453 |
| H | 2.350808 | -3.068900 | 4.193435 |
| H | 3.063065 | -2.681663 | 2.618284 |
| C | 3.301756 | -2.125867 | -0.262554 |
| C | -1.247003 | -3.322470 | 0.930790 |
| C | -1.565236 | 0.528892 | 3.822396 |
| C | 2.932418 | 1.756292 | 2.609930 |
| C | 2.084524 | -2.813147 | -0.194255 |

| | | | |
|---|---|---|---|
| C | 1.831221 | -4.135833 | -0.755044 |
| C | 0.533096 | -4.452824 | -0.419598 |
| C | 0.020158 | -3.333630 | 0.343531 |
| C | -0.201863 | -5.737420 | -0.677228 |
| C | 2.784392 | -5.040228 | -1.491339 |
| C | 3.495967 | -6.107602 | -0.599043 |
| C | 4.748827 | -5.542431 | 0.023019 |
| O | 5.699911 | -5.347275 | -0.880722 |
| O | 4.858137 | -5.259381 | 1.213509 |
| C | -1.751684 | -2.365043 | 1.801985 |
| C | -3.012077 | -2.498894 | 2.521898 |
| C | -3.102417 | -1.396437 | 3.335925 |
| C | -1.882845 | -0.625259 | 3.114607 |
| C | -3.933467 | -3.680638 | 2.472059 |
| C | -4.138787 | -1.055507 | 4.309332 |
| C | -5.459490 | -1.174281 | 4.113686 |
| C | -0.368399 | 1.229332 | 3.734267 |
| C | -0.038567 | 2.383596 | 4.554619 |
| C | 1.245329 | 2.740423 | 4.212293 |
| C | 1.667404 | 1.781589 | 3.186329 |
| C | -0.925322 | 2.986185 | 5.599717 |
| C | 2.098432 | 3.785114 | 4.765720 |
| C | 1.710191 | 4.954563 | 5.302782 |

| | | | |
|---|---|---|---|
| C | 3.416516 | 0.807044 | 1.712159 |
| C | 4.780624 | 0.818072 | 1.215740 |
| C | 4.904745 | -0.271412 | 0.396950 |
| C | 3.603326 | -0.937827 | 0.398857 |
| C | 5.807466 | 1.860077 | 1.549012 |
| C | 6.155280 | -0.650085 | -0.345485 |
| C | 7.274773 | -1.284867 | 0.545616 |
| C | 6.979818 | -2.742635 | 0.752991 |
| O | 6.180158 | -3.001861 | 1.770950 |
| O | 7.392756 | -3.600744 | -0.035094 |
| N | 0.970841 | -2.358267 | 0.459613 |
| N | -1.105078 | -1.212958 | 2.163017 |
| N | 0.667192 | 0.908382 | 2.900836 |
| N | 2.722204 | -0.244618 | 1.191079 |
| Fe | 0.802812 | -0.683689 | 1.623173 |
| C | 0.016990 | 0.534412 | 0.055036 |
| C | -1.246222 | 1.357439 | 0.364039 |
| C | -0.320634 | -0.104309 | -1.186776 |
| N | 0.619871 | 2.741413 | -2.459342 |
| C | 1.407835 | 2.499838 | -1.309807 |
| C | -0.418124 | 3.727914 | -2.438709 |
| C | -0.120494 | 5.063868 | -2.134624 |
| C | -1.744998 | 3.374078 | -2.733025 |

| | | | |
|---|---|---|---|
| C | -1.144555 | 6.016045 | -2.091527 |
| C | -2.764222 | 4.325446 | -2.692137 |
| C | -2.465148 | 5.653374 | -2.361481 |
| C | 0.850794 | 2.049238 | -3.725128 |
| C | 2.863083 | 2.138166 | -1.539753 |
| C | -2.358895 | 0.641437 | -0.414655 |
| O | -1.665099 | -0.085571 | -1.473248 |
| O | 0.424632 | -0.578400 | -2.082447 |
| H | 0.299554 | -6.348516 | -1.435894 |
| H | -1.230628 | -5.565297 | -1.016684 |
| H | -0.273623 | -6.352970 | 0.228879 |
| H | -4.612124 | -3.657666 | 1.611130 |
| H | -4.561921 | -3.703221 | 3.366992 |
| H | -3.372732 | -4.621187 | 2.425579 |
| H | -0.329030 | 3.460993 | 6.384915 |
| H | -1.562153 | 2.230568 | 6.069604 |
| H | -1.589378 | 3.755356 | 5.183799 |
| H | 5.371762 | 2.865349 | 1.513490 |
| H | 6.639219 | 1.839470 | 0.839719 |
| H | 6.218812 | 1.722406 | 2.558166 |
| H | -6.165107 | -0.914106 | 4.897796 |
| H | -5.869408 | -1.471466 | 3.153942 |
| H | 2.440043 | 5.646369 | 5.712515 |

| | | | |
|---|---|---|---|
| H | 0.672056 | 5.267373 | 5.332578 |
| H | 3.789383 | -6.955967 | -1.226752 |
| H | 2.830015 | -6.456136 | 0.191438 |
| H | 3.548855 | -4.471153 | -2.029277 |
| H | 2.231231 | -5.593425 | -2.261361 |
| H | 7.329640 | -0.759466 | 1.501219 |
| H | 8.234622 | -1.209822 | 0.029019 |
| H | 6.583218 | 0.255325 | -0.791137 |
| H | 5.941564 | -1.331732 | -1.176320 |
| H | 4.100480 | -2.589301 | -0.833578 |
| H | -1.871312 | -4.192143 | 0.752819 |
| H | -2.309946 | 0.898705 | 4.516934 |
| H | 3.636330 | 2.516918 | 2.927143 |
| H | -3.788476 | -0.668952 | 5.266933 |
| H | 3.168397 | 3.579106 | 4.739882 |
| H | 6.448754 | -4.805285 | -0.481413 |
| H | 5.821520 | -3.930341 | 1.698888 |
| H | 0.908158 | 1.493675 | -0.544616 |
| H | 0.910471 | 5.344041 | -1.934032 |
| H | -1.976366 | 2.333528 | -2.948532 |
| H | -0.900420 | 7.047215 | -1.843540 |
| H | -3.815756 | 4.065289 | -2.852435 |
| H | 1.426423 | 1.145122 | -3.526878 |

| | | | |
|---|---|---|---|
| H | 1.303360 | 3.329566 | -0.609627 |
| H | 2.981980 | 1.167771 | -2.029051 |
| H | 3.364151 | 2.901926 | -2.151107 |
| H | 3.377003 | 2.083715 | -0.581162 |
| H | -2.895971 | -0.085695 | 0.201362 |
| H | -3.076339 | 1.309528 | -0.895316 |
| H | -1.488783 | 1.419236 | 1.421428 |
| H | -1.144345 | 2.384829 | -0.006458 |
| H | 6.322513 | 5.368977 | -3.323455 |
| H | 5.281059 | 3.953705 | -3.509374 |
| H | -0.112771 | 1.718297 | -4.131208 |
| C | 1.549162 | 2.925018 | -4.775835 |
| H | 0.975573 | 3.838750 | -4.957598 |
| H | 2.552163 | 3.214969 | -4.446499 |
| H | 1.642687 | 2.384369 | -5.725861 |
| H | -3.305543 | 6.342015 | -2.291357 |
| H | 0.682623 | -3.794080 | -2.947213 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(S)} \right]^{\mathbf{L10}}$$

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Number of imaginary frequencies : 3 Electronic energy : HF=-4201.536019

Zero-point correction= 1.546794 (Hartree/Particle)

Thermal correction to Energy= 1.644636

Thermal correction to Enthalpy= 1.645581

Thermal correction to Gibbs Free Energy= 1.395167

Sum of electronic and zero-point Energies= -4199.989225

Sum of electronic and thermal Energies= -4199.891383

Sum of electronic and thermal Enthalpies= -4199.890438

Sum of electronic and thermal Free Energies= -4200.140852

.....

Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | 7.611009 | 1.675634 | -2.126661 |
| C | 8.060443 | 1.346423 | -3.472084 |
| C | 6.930772 | 2.961106 | -2.200086 |
| C | 6.728664 | 3.322705 | -3.686610 |
| C | 7.909905 | 2.602290 | -4.356592 |
| H | 7.578054 | 3.702376 | -1.698707 |
| H | 6.005500 | 2.929288 | -1.611623 |
| H | 8.816694 | 3.216186 | -4.294313 |
| H | 7.739963 | 2.367163 | -5.411440 |
| H | 7.418135 | 0.527828 | -3.842082 |
| H | 9.077728 | 0.935147 | -3.436848 |

| | | | |
|---|---|---|---|
| C | 1.446149 | 5.932482 | 0.595100 |
| C | 2.646834 | 5.296432 | 1.294892 |
| O | 2.896423 | 3.969788 | 0.856147 |
| H | 1.616089 | 5.979018 | -0.486528 |
| H | 3.558958 | 5.871413 | 1.083486 |
| H | 2.495842 | 5.327068 | 2.385936 |
| H | 2.086091 | 3.458524 | 1.066603 |
| H | 1.280818 | 6.956091 | 0.955435 |
| H | 0.544985 | 5.344308 | 0.782088 |
| C | -6.232038 | 6.010923 | -0.647700 |
| C | -6.673098 | 4.541672 | -0.738098 |
| C | -6.077253 | 3.768847 | -1.960654 |
| O | -5.937631 | 2.520630 | -1.829897 |
| O | -5.797320 | 4.467980 | -2.974772 |
| H | -6.766181 | 6.557360 | 0.141696 |
| H | -6.419579 | 3.991739 | 0.175375 |
| H | -7.769897 | 4.496901 | -0.826488 |
| H | -6.407933 | 6.499457 | -1.609751 |
| H | -5.158706 | 6.084475 | -0.436517 |
| N | -8.372658 | -2.918078 | -1.121418 |
| C | -7.439940 | -1.795781 | -1.149143 |
| C | -6.265018 | -2.016826 | -0.163535 |
| O | -6.292703 | -1.515851 | 0.953439 |

| | | | |
|---|---|---|---|
| C | -9.709464 | -2.337461 | -1.077418 |
| C | -9.600199 | -0.837362 | -1.421900 |
| C | -8.208778 | -0.488137 | -0.876816 |
| H | -10.085492 | -2.470938 | -0.047116 |
| H | -10.385663 | -2.913726 | -1.722990 |
| H | -10.401790 | -0.238733 | -0.979503 |
| H | -9.641632 | -0.695779 | -2.508790 |
| H | -8.242542 | -0.330459 | 0.205130 |
| H | -7.732135 | 0.390838 | -1.323868 |
| H | -7.011705 | -1.773907 | -2.167872 |
| N | -5.155364 | -2.723604 | -0.577877 |
| C | -5.051704 | -3.790982 | -1.575193 |
| C | -4.311839 | -3.417679 | -2.865661 |
| C | -2.928331 | -2.808121 | -2.597314 |
| C | -1.870360 | -3.209065 | -3.631254 |
| N | -0.572360 | -2.591486 | -3.342146 |
| C | -0.327843 | -1.284469 | -3.566726 |
| N | -0.980252 | -0.637669 | -4.562707 |
| N | 0.607328 | -0.633066 | -2.893277 |
| H | -4.428649 | -2.702119 | 0.127904 |
| H | -6.061753 | -4.141425 | -1.810708 |
| H | -4.218266 | -4.338011 | -3.460662 |
| H | -4.919789 | -2.725484 | -3.459483 |

| | | | |
|---|---|---|---|
| H | -3.001356 | -1.716917 | -2.543530 |
| H | -2.555314 | -3.121509 | -1.615596 |
| H | -1.717368 | -4.292537 | -3.620791 |
| H | -2.176031 | -2.967926 | -4.656063 |
| H | -0.117130 | -2.965508 | -2.506328 |
| H | -1.831813 | -1.026846 | -4.932088 |
| H | -0.923462 | 0.371880 | -4.577901 |
| H | 0.572162 | 0.425322 | -2.899704 |
| H | -4.532821 | -4.632617 | -1.098904 |
| C | 2.187426 | -2.771810 | 3.123192 |
| O | 1.236313 | -1.765291 | 3.247076 |
| H | 1.894837 | -3.566676 | 2.413456 |
| H | 2.328371 | -3.257234 | 4.104218 |
| H | 3.177167 | -2.404672 | 2.801338 |
| C | 2.853939 | -2.098603 | -0.419033 |
| C | -1.576361 | -3.088827 | 1.313892 |
| C | -1.411805 | 0.804097 | 4.154197 |
| C | 3.178038 | 1.457872 | 2.850767 |
| C | 1.588004 | -2.684702 | -0.268844 |
| C | 1.162729 | -3.938005 | -0.879706 |
| C | -0.078221 | -4.224560 | -0.342673 |
| C | -0.402912 | -3.139371 | 0.554859 |
| C | -0.895094 | -5.468432 | -0.546971 |

| | | | |
|---|---|---|---|
| C | 1.919062 | -4.828301 | -1.831734 |
| C | 2.599923 | -6.068030 | -1.170461 |
| C | 3.948987 | -5.700255 | -0.605230 |
| O | 4.843881 | -5.497164 | -1.562547 |
| O | 4.175358 | -5.561014 | 0.594441 |
| C | -1.934197 | -2.103995 | 2.225773 |
| C | -3.160653 | -2.123936 | 3.012190 |
| C | -3.142155 | -0.980740 | 3.772549 |
| C | -1.874025 | -0.317658 | 3.477298 |
| C | -4.182226 | -3.219811 | 3.033833 |
| C | -4.131525 | -0.510451 | 4.738066 |
| C | -5.460710 | -0.639389 | 4.611452 |
| C | -0.127226 | 1.323650 | 4.063955 |
| C | 0.374224 | 2.403414 | 4.900086 |
| C | 1.692215 | 2.571350 | 4.553994 |
| C | 1.960931 | 1.588326 | 3.501751 |
| C | -0.414954 | 3.122231 | 5.948929 |
| C | 2.689495 | 3.482314 | 5.101289 |
| C | 2.472325 | 4.691398 | 5.644963 |
| C | 3.478465 | 0.563252 | 1.828293 |
| C | 4.786430 | 0.483699 | 1.205297 |
| C | 4.718430 | -0.524923 | 0.282320 |
| C | 3.351683 | -1.040570 | 0.340344 |

| | | | |
|---|---|---|---|
| C | 5.936099 | 1.394648 | 1.517266 |
| C | 5.851557 | -0.968125 | -0.599425 |
| C | 6.956575 | -1.802824 | 0.131474 |
| C | 6.521054 | -3.236966 | 0.215767 |
| O | 5.775191 | -3.524384 | 1.266519 |
| O | 6.777569 | -4.040848 | -0.687700 |
| N | 0.604523 | -2.211146 | 0.565230 |
| N | -1.186357 | -0.993338 | 2.515966 |
| N | 0.846412 | 0.862325 | 3.226243 |
| N | 2.626032 | -0.347829 | 1.275973 |
| Fe | 0.714062 | -0.625683 | 1.858302 |
| C | -0.091370 | 0.813081 | 0.375415 |
| C | -0.424006 | 2.138089 | 0.945742 |
| C | -1.415087 | 0.383973 | -0.275153 |
| N | 0.659226 | 2.162576 | -2.846975 |
| C | 1.404629 | 2.140749 | -1.573614 |
| C | -0.520356 | 3.025397 | -2.820201 |
| C | -0.413639 | 4.386413 | -2.505130 |
| C | -1.784015 | 2.507642 | -3.131838 |
| C | -1.544719 | 5.205301 | -2.526828 |
| C | -2.920017 | 3.319711 | -3.137777 |
| C | -2.796598 | 4.680768 | -2.847509 |
| C | 1.450235 | 2.342368 | -4.100194 |

| | | | |
|---|---|---|---|
| C | 2.842059 | 1.684278 | -1.645207 |
| H | -0.596198 | -6.004830 | -1.453768 |
| H | -1.966898 | -5.256734 | -0.627722 |
| H | -0.777005 | -6.166776 | 0.291701 |
| H | -5.000347 | -3.029704 | 2.330430 |
| H | -4.637183 | -3.284688 | 4.027802 |
| H | -3.737511 | -4.193712 | 2.802678 |
| H | 0.243952 | 3.505536 | 6.734061 |
| H | -1.153665 | 2.465496 | 6.418784 |
| H | -0.961167 | 3.978232 | 5.531511 |
| H | 5.607442 | 2.440096 | 1.491658 |
| H | 6.747120 | 1.280830 | 0.792437 |
| H | 6.351529 | 1.207581 | 2.516137 |
| H | -6.130869 | -0.271392 | 5.383183 |
| H | -5.915223 | -1.063669 | 3.721677 |
| H | 3.295931 | 5.277798 | 6.041416 |
| H | 1.487391 | 5.143501 | 5.685882 |
| H | 2.753232 | -6.837325 | -1.934572 |
| H | 1.976202 | -6.471621 | -0.371800 |
| H | 2.677962 | -4.270501 | -2.388962 |
| H | 1.221867 | -5.213322 | -2.586476 |
| H | 7.134210 | -1.390063 | 1.126468 |
| H | 7.879452 | -1.766783 | -0.452027 |

| | | | |
|---|---|---|---|
| H | 6.357116 | -0.086685 | -1.010268 |
| H | 5.493199 | -1.543547 | -1.460591 |
| H | 3.538819 | -2.575448 | -1.113533 |
| H | -2.257309 | -3.927041 | 1.209679 |
| H | -2.092278 | 1.275384 | 4.852584 |
| H | 3.969009 | 2.136383 | 3.143055 |
| H | -3.741844 | -0.008239 | 5.623483 |
| H | 3.720290 | 3.131424 | 5.056782 |
| H | 5.675213 | -5.081326 | -1.174666 |
| H | 5.312014 | -4.397811 | 1.130365 |
| H | 0.760360 | 1.283311 | -0.632088 |
| H | 0.547897 | 4.802534 | -2.226118 |
| H | -1.899630 | 1.442470 | -3.306137 |
| H | -1.441036 | 6.257372 | -2.273163 |
| H | -3.919405 | 2.922016 | -3.302520 |
| H | 2.219331 | 1.563834 | -4.114537 |
| H | 1.307029 | 3.071151 | -1.017119 |
| H | 2.957244 | 0.658361 | -2.011165 |
| H | 3.464959 | 2.333624 | -2.276931 |
| H | 3.259638 | 1.728524 | -0.640683 |
| H | 6.712952 | 4.401044 | -3.867913 |
| H | 5.777188 | 2.912476 | -4.045029 |
| H | 0.768371 | 2.124121 | -4.932485 |

| | | | |
|---|---|---|---|
| C | 2.101756 | 3.707628 | -4.356539 |
| H | 1.351363 | 4.488110 | -4.497340 |
| H | 2.754202 | 4.007629 | -3.531783 |
| H | 2.709503 | 3.651493 | -5.267654 |
| H | -3.708048 | 5.271050 | -2.844389 |
| H | 1.006587 | -1.071195 | -2.066968 |
| C | -2.489806 | 1.266639 | 0.398061 |
| H | -1.407973 | 0.585544 | -1.352528 |
| H | -1.636104 | -0.677301 | -0.145535 |
| H | -3.227993 | 1.690179 | -0.289311 |
| H | -3.016583 | 0.735509 | 1.195420 |
| O | -1.765434 | 2.365111 | 0.994625 |
| O | 0.332599 | 3.030450 | 1.329779 |

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**$C^{S264A}$**

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Number of imaginary frequencies : 3 Electronic energy : HF=-3681.588917

Zero-point correction= 1.311326 (Hartree/Particle)

Thermal correction to Energy= 1.397153

Thermal correction to Enthalpy= 1.398097

Thermal correction to Gibbs Free Energy= 1.162960

Sum of electronic and zero-point Energies= -3680.277591

Sum of electronic and thermal Energies= -3680.191764

Sum of electronic and thermal Enthalpies= -3680.190820

Sum of electronic and thermal Free Energies= -3680.425957

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 7 | 10.254548 | -4.141866 | -0.472014 |
| 6 | 9.225926 | -4.687003 | 0.403152 |
| 6 | 9.775096 | -2.845222 | -0.930652 |
| 6 | 8.540468 | -2.449673 | -0.093441 |
| 6 | 7.953786 | -3.822733 | 0.270549 |
| 1 | 9.505513 | -2.953874 | -1.996434 |
| 1 | 10.593108 | -2.113484 | -0.904498 |
| 1 | 7.326452 | -4.197885 | -0.546738 |
| 1 | 7.343808 | -3.811190 | 1.178405 |
| 1 | 9.618971 | -4.647793 | 1.434920 |
| 1 | 9.074568 | -5.752088 | 0.183330 |
| 6 | 3.255672 | -2.163520 | -5.867236 |
| 1 | 3.989242 | -2.586202 | -5.170411 |
| 1 | 3.294712 | -2.762520 | -6.784548 |
| 6 | -4.377484 | -3.528585 | -6.497374 |

| | | | |
|---|---|---|---|
| 6 | -5.381400 | -3.238808 | -5.376678 |
| 6 | -4.981155 | -3.730126 | -3.965810 |
| 8 | -5.779551 | -3.552500 | -3.031124 |
| 8 | -3.831004 | -4.308070 | -3.879506 |
| 1 | -3.419929 | -3.036134 | -6.304148 |
| 1 | -5.573763 | -2.160900 | -5.297399 |
| 1 | -6.356441 | -3.689196 | -5.604051 |
| 1 | -4.752346 | -3.177527 | -7.467094 |
| 1 | -4.175241 | -4.600971 | -6.571226 |
| 7 | -7.346013 | -2.284593 | 2.074079 |
| 6 | -6.503124 | -1.888629 | 0.948993 |
| 6 | -5.703928 | -0.607942 | 1.302604 |
| 8 | -5.854099 | 0.420934 | 0.649247 |
| 6 | -8.672699 | -2.536152 | 1.530979 |
| 6 | -8.545994 | -2.692338 | 0.003210 |
| 6 | -7.360178 | -1.772378 | -0.326622 |
| 1 | -9.299583 | -1.660705 | 1.781894 |
| 1 | -9.129000 | -3.391520 | 2.046642 |
| 1 | -9.462339 | -2.424838 | -0.531489 |
| 1 | -8.305256 | -3.730489 | -0.252523 |
| 1 | -7.677786 | -0.732877 | -0.448544 |
| 1 | -6.819682 | -2.081971 | -1.225612 |
| 1 | -5.755970 | -2.691762 | 0.819611 |

| | | | |
|---|---|---|---|
| 7 | -4.818648 | -0.631985 | 2.348209 |
| 6 | -4.372662 | -1.703963 | 3.249004 |
| 6 | -3.525449 | -2.816607 | 2.583853 |
| 6 | -2.614043 | -2.334502 | 1.447005 |
| 6 | -1.664168 | -3.437254 | 0.935938 |
| 7 | -1.198288 | -3.233893 | -0.427645 |
| 6 | -1.885955 | -3.642025 | -1.523625 |
| 7 | -2.892010 | -4.517142 | -1.477182 |
| 7 | -1.471662 | -3.209558 | -2.726447 |
| 1 | -4.320493 | 0.246358 | 2.415771 |
| 1 | -5.245691 | -2.147936 | 3.736289 |
| 1 | -2.932952 | -3.298588 | 3.374037 |
| 1 | -4.191430 | -3.598175 | 2.194860 |
| 1 | -3.224337 | -1.988788 | 0.606753 |
| 1 | -2.018076 | -1.470152 | 1.764387 |
| 1 | -0.782538 | -3.502902 | 1.582779 |
| 1 | -2.144607 | -4.420707 | 0.994801 |
| 1 | -0.586992 | -2.434399 | -0.604639 |
| 1 | -2.136911 | -3.390854 | -3.481795 |
| 1 | -3.776817 | -1.203659 | 4.017451 |
| 6 | 3.026562 | 2.664455 | 1.807445 |
| 8 | 2.345751 | 3.057523 | 0.659853 |
| 1 | 2.395306 | 2.673751 | 2.714184 |

| | | | |
|---|---|---|---|
| 1 | 3.867535 | 3.355177 | 1.993609 |
| 1 | 3.454559 | 1.649079 | 1.729455 |
| 6 | 0.834891 | -0.360922 | 2.308149 |
| 6 | -1.089655 | 4.078657 | 2.053182 |
| 6 | 0.655228 | 4.634891 | -2.413376 |
| 6 | 3.012329 | 0.454377 | -1.941734 |
| 6 | 0.105928 | 0.787424 | 2.627491 |
| 6 | -0.649970 | 1.000035 | 3.858706 |
| 6 | -1.170691 | 2.266212 | 3.777340 |
| 6 | -0.739357 | 2.810043 | 2.504631 |
| 6 | -2.011639 | 2.993962 | 4.784199 |
| 6 | -0.828819 | 0.060298 | 5.018622 |
| 6 | 0.136877 | 0.312750 | 6.221390 |
| 6 | 1.467187 | -0.351379 | 5.977288 |
| 8 | 1.399113 | -1.667176 | 6.137962 |
| 8 | 2.479560 | 0.246112 | 5.617097 |
| 6 | -0.772908 | 4.634892 | 0.818287 |
| 6 | -1.209615 | 5.947641 | 0.380502 |
| 6 | -0.745301 | 6.097167 | -0.907883 |
| 6 | -0.008900 | 4.871738 | -1.215098 |
| 6 | -1.967581 | 6.932776 | 1.216337 |
| 6 | -0.869449 | 7.232101 | -1.813299 |
| 6 | -1.856541 | 8.142677 | -1.848936 |

| | | | |
|---|---|---|---|
| 6 | 1.454138 | 3.531350 | -2.693001 |
| 6 | 2.264947 | 3.396229 | -3.890896 |
| 6 | 2.968312 | 2.221524 | -3.746561 |
| 6 | 2.554307 | 1.659954 | -2.459414 |
| 6 | 2.347659 | 4.396890 | -5.001986 |
| 6 | 3.981639 | 1.635990 | -4.612519 |
| 6 | 4.124069 | 1.802100 | -5.939312 |
| 6 | 2.621743 | -0.129964 | -0.742300 |
| 6 | 3.081238 | -1.434841 | -0.310329 |
| 6 | 2.460775 | -1.693033 | 0.882562 |
| 6 | 1.626625 | -0.528537 | 1.170548 |
| 6 | 4.040061 | -2.303554 | -1.067833 |
| 6 | 2.649149 | -2.936653 | 1.704843 |
| 6 | 3.971698 | -2.975329 | 2.543670 |
| 6 | 3.761883 | -2.239635 | 3.838228 |
| 8 | 4.001929 | -0.944151 | 3.779783 |
| 8 | 3.315236 | -2.817920 | 4.834147 |
| 7 | 0.023972 | 1.897376 | 1.830064 |
| 7 | -0.053459 | 4.009687 | -0.162286 |
| 7 | 1.639320 | 2.464849 | -1.858448 |
| 7 | 1.748549 | 0.392509 | 0.166365 |
| 26 | 0.834098 | 2.173737 | -0.011877 |
| 1 | -2.346060 | 2.329773 | 5.586795 |

| | | | |
|---|---|---|---|
| 1 | -2.906528 | 3.430385 | 4.325620 |
| 1 | -1.460416 | 3.818679 | 5.254236 |
| 1 | -3.055058 | 6.798898 | 1.135240 |
| 1 | -1.744643 | 7.957057 | 0.901789 |
| 1 | -1.708676 | 6.841725 | 2.275954 |
| 1 | 3.345698 | 4.392332 | -5.451935 |
| 1 | 2.144611 | 5.411528 | -4.646517 |
| 1 | 1.629829 | 4.184952 | -5.806125 |
| 1 | 3.719478 | -2.441362 | -2.106669 |
| 1 | 4.125220 | -3.297222 | -0.618304 |
| 1 | 5.048564 | -1.870029 | -1.096997 |
| 1 | -1.830402 | 8.962996 | -2.560099 |
| 1 | -2.723770 | 8.089404 | -1.199457 |
| 1 | 4.947547 | 1.334433 | -6.470739 |
| 1 | 3.425610 | 2.378707 | -6.535667 |
| 1 | -0.299415 | -0.122191 | 7.126489 |
| 1 | 0.290405 | 1.382730 | 6.368618 |
| 1 | -0.732718 | -0.985799 | 4.710339 |
| 1 | -1.849988 | 0.167204 | 5.403170 |
| 1 | 4.786952 | -2.529791 | 1.969561 |
| 1 | 4.215394 | -4.011635 | 2.791176 |
| 1 | 2.672696 | -3.803616 | 1.035187 |
| 1 | 1.804946 | -3.108616 | 2.381774 |

| | | | |
|---|---|---|---|
| 1 | 0.826366 | -1.169955 | 3.032055 |
| 1 | -1.694798 | 4.681252 | 2.721230 |
| 1 | 0.577681 | 5.395085 | -3.181308 |
| 1 | 3.718114 | -0.105161 | -2.544582 |
| 1 | -0.063234 | 7.342871 | -2.538203 |
| 1 | 4.709459 | 0.997590 | -4.112330 |
| 1 | 2.236497 | -2.097307 | 5.788637 |
| 1 | 3.598992 | -0.483839 | 4.571192 |
| 1 | 7.841997 | -1.803676 | -0.632587 |
| 1 | 8.853732 | -1.916179 | 0.811772 |
| 1 | -0.942907 | -2.334353 | -2.713736 |
| 6 | -0.799287 | 1.323997 | -0.813688 |
| 6 | -0.964929 | 0.052428 | -1.473556 |
| 6 | -3.075402 | 0.989649 | -1.575069 |
| 1 | -4.010348 | 0.682126 | -1.100980 |
| 6 | -2.191376 | 1.896189 | -0.699321 |
| 1 | -3.307068 | 1.452946 | -2.542521 |
| 1 | -2.239635 | 2.944422 | -1.009590 |
| 1 | -2.523922 | 1.880935 | 0.350222 |
| 8 | -0.146895 | -0.851958 | -1.734118 |
| 8 | -2.281940 | -0.186134 | -1.826278 |
| 1 | -3.339270 | -4.701957 | -0.595211 |
| 1 | -3.457797 | -4.571746 | -2.397859 |

| | | | |
|---|---|---|---|
| 1 | 3.582147 | -1.148327 | -6.113843 |
| 6 | 1.848924 | -2.155823 | -5.260920 |
| 1 | 1.802975 | -1.542693 | -4.355156 |
| 1 | 1.117721 | -1.747270 | -5.966560 |
| 1 | 1.518185 | -3.165343 | -4.994081 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(R)} \right]^{\mathbf{S264A}}$$

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Number of imaginary frequencies : 4 Electronic energy : HF=-4126.336545

Zero-point correction= 1.539292 (Hartree/Particle)

Thermal correction to Energy= 1.636781

Thermal correction to Enthalpy= 1.637725

Thermal correction to Gibbs Free Energy= 1.385405

Sum of electronic and zero-point Energies= -4124.797825

Sum of electronic and thermal Energies= -4124.700336

Sum of electronic and thermal Enthalpies= -4124.699392

Sum of electronic and thermal Free Energies= -4124.951712

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 7 | 7.301997 | 2.494873 | -1.799335 |
| 6 | 7.508650 | 2.363652 | -3.233285 |
| 6 | 6.769142 | 3.829725 | -1.562647 |
| 6 | 6.433326 | 4.475067 | -2.923873 |
| 6 | 7.416642 | 3.766333 | -3.868702 |
| 1 | 7.548416 | 4.404253 | -1.031541 |
| 1 | 5.917803 | 3.771339 | -0.873282 |
| 1 | 8.397581 | 4.256482 | -3.840327 |
| 1 | 7.084712 | 3.745160 | -4.910739 |
| 1 | 6.708005 | 1.709039 | -3.621332 |
| 1 | 8.450526 | 1.835389 | -3.430468 |
| 6 | 0.791398 | 6.109139 | 1.475384 |
| 1 | 0.227864 | 6.040947 | 0.540880 |
| 1 | 0.382799 | 6.950134 | 2.047112 |
| 1 | 0.596426 | 5.198093 | 2.049499 |
| 6 | -6.920535 | 5.800751 | 0.507630 |
| 6 | -7.217417 | 4.892440 | -0.690203 |
| 6 | -6.088069 | 4.933436 | -1.770754 |
| 8 | -5.809182 | 3.832710 | -2.320217 |
| 8 | -5.586271 | 6.070965 | -1.983035 |
| 1 | -7.767548 | 5.874209 | 1.204576 |
| 1 | -7.372476 | 3.852975 | -0.379040 |
| 1 | -8.151325 | 5.224037 | -1.170500 |

| | | | |
|---|---|---|---|
| 1 | -6.666972 | 6.797743 | 0.137662 |
| 1 | -6.055441 | 5.433328 | 1.073123 |
| 7 | -8.125648 | -3.305506 | -0.273003 |
| 6 | -7.662170 | -1.987631 | -0.694927 |
| 6 | -6.200790 | -1.739672 | -0.190539 |
| 8 | -5.981836 | -0.855601 | 0.625007 |
| 6 | -9.399780 | -3.111219 | 0.400925 |
| 6 | -9.948192 | -1.732668 | -0.014111 |
| 6 | -8.658404 | -0.920336 | -0.203494 |
| 1 | -9.206129 | -3.138303 | 1.488673 |
| 1 | -10.066673 | -3.956424 | 0.188836 |
| 1 | -10.625486 | -1.300033 | 0.727861 |
| 1 | -10.500208 | -1.820083 | -0.957745 |
| 1 | -8.297152 | -0.512429 | 0.743828 |
| 1 | -8.757450 | -0.085978 | -0.901313 |
| 1 | -7.605742 | -2.005556 | -1.797696 |
| 7 | -5.159430 | -2.484511 | -0.700050 |
| 6 | -5.174016 | -3.774105 | -1.390349 |
| 6 | -4.722030 | -3.709973 | -2.858099 |
| 6 | -3.216380 | -3.478994 | -3.001171 |
| 6 | -2.722867 | -3.494869 | -4.453681 |
| 7 | -1.252311 | -3.505201 | -4.543886 |
| 6 | -0.508718 | -2.484387 | -4.038458 |

| | | | |
|---|---|---|---|
| 7 | -0.885620 | -1.220085 | -4.149712 |
| 7 | 0.679473 | -2.751440 | -3.462094 |
| 1 | -4.278410 | -2.194888 | -0.288959 |
| 1 | -6.189091 | -4.173126 | -1.324899 |
| 1 | -4.991266 | -4.661234 | -3.339117 |
| 1 | -5.285448 | -2.921592 | -3.372494 |
| 1 | -2.929092 | -2.530567 | -2.531277 |
| 1 | -2.684826 | -4.270590 | -2.455505 |
| 1 | -3.071219 | -4.390441 | -4.977514 |
| 1 | -3.116238 | -2.644257 | -5.020591 |
| 1 | -0.828783 | -4.414621 | -4.414738 |
| 1 | -1.770922 | -0.979429 | -4.565947 |
| 1 | -0.449286 | -0.597488 | -3.422826 |
| 1 | 1.053130 | -1.952249 | -2.935684 |
| 1 | -4.527750 | -4.467683 | -0.836477 |
| 6 | 2.170403 | -2.725394 | 3.134916 |
| 8 | 1.361883 | -1.593979 | 3.160061 |
| 1 | 1.686109 | -3.600046 | 2.662969 |
| 1 | 2.412601 | -3.019542 | 4.171314 |
| 1 | 3.132118 | -2.570393 | 2.615463 |
| 6 | 3.216468 | -2.153135 | -0.326545 |
| 6 | -1.326621 | -3.177313 | 1.039117 |
| 6 | -1.433175 | 0.729848 | 3.870755 |

| | | | |
|---|---|---|---|
| 6 | 3.110789 | 1.703295 | 2.602282 |
| 6 | 1.979747 | -2.796535 | -0.208405 |
| 6 | 1.660836 | -4.116484 | -0.742643 |
| 6 | 0.365451 | -4.384384 | -0.356099 |
| 6 | -0.081158 | -3.239961 | 0.409779 |
| 6 | -0.415791 | -5.649765 | -0.565077 |
| 6 | 2.554428 | -5.069238 | -1.493852 |
| 6 | 3.243682 | -6.157561 | -0.609135 |
| 6 | 4.542829 | -5.645183 | -0.039448 |
| 8 | 5.467817 | -5.501982 | -0.979259 |
| 8 | 4.708859 | -5.357121 | 1.143309 |
| 6 | -1.769959 | -2.190914 | 1.910858 |
| 6 | -3.023236 | -2.260814 | 2.651376 |
| 6 | -3.059685 | -1.138756 | 3.441607 |
| 6 | -1.810619 | -0.424121 | 3.192675 |
| 6 | -3.992060 | -3.404459 | 2.630572 |
| 6 | -4.082724 | -0.725524 | 4.400907 |
| 6 | -5.405962 | -0.793711 | 4.196647 |
| 6 | -0.207388 | 1.374665 | 3.749731 |
| 6 | 0.188334 | 2.528354 | 4.542047 |
| 6 | 1.485890 | 2.810648 | 4.183420 |
| 6 | 1.851278 | 1.809873 | 3.177076 |
| 6 | -0.659346 | 3.200284 | 5.577314 |

| | | | |
|---|---|---|---|
| 6 | 2.392908 | 3.826572 | 4.703372 |
| 6 | 2.065995 | 5.031264 | 5.200393 |
| 6 | 3.533164 | 0.733838 | 1.695950 |
| 6 | 4.885649 | 0.674346 | 1.172165 |
| 6 | 4.923502 | -0.387910 | 0.310055 |
| 6 | 3.588582 | -0.982165 | 0.330883 |
| 6 | 6.003989 | 1.606397 | 1.534649 |
| 6 | 6.130812 | -0.807022 | -0.481900 |
| 6 | 7.259422 | -1.493138 | 0.357198 |
| 6 | 6.910524 | -2.936564 | 0.580420 |
| 8 | 6.142160 | -3.158456 | 1.630372 |
| 8 | 7.256233 | -3.812924 | -0.219766 |
| 7 | 0.905002 | -2.295010 | 0.477486 |
| 7 | -1.071883 | -1.060208 | 2.241102 |
| 7 | 0.802544 | 0.986277 | 2.914323 |
| 7 | 2.767350 | -0.261173 | 1.161362 |
| 26 | 0.838221 | -0.610104 | 1.645919 |
| 6 | 0.054199 | 0.652777 | 0.102066 |
| 6 | -1.228311 | 1.445547 | 0.411970 |
| 6 | -0.254226 | 0.044451 | -1.163226 |
| 7 | 0.734281 | 2.974480 | -2.308587 |
| 6 | 1.393781 | 2.757251 | -1.075836 |
| 6 | -0.381412 | 3.871504 | -2.386862 |

| | | | |
|---|---|---|---|
| 6 | -0.199056 | 5.240561 | -2.147270 |
| 6 | -1.665937 | 3.397366 | -2.697474 |
| 6 | -1.294683 | 6.109818 | -2.177452 |
| 6 | -2.758193 | 4.265109 | -2.724729 |
| 6 | -2.574661 | 5.627489 | -2.454968 |
| 6 | 1.137498 | 2.291961 | -3.534842 |
| 6 | 2.905173 | 2.617838 | -1.125186 |
| 6 | -2.317780 | 0.715403 | -0.385084 |
| 8 | -1.597641 | 0.033828 | -1.456904 |
| 8 | 0.507848 | -0.385926 | -2.065812 |
| 1 | 0.012279 | -6.265653 | -1.363813 |
| 1 | -1.462313 | -5.451994 | -0.824423 |
| 1 | -0.431968 | -6.270704 | 0.340231 |
| 1 | -4.658145 | -3.383600 | 1.760259 |
| 1 | -4.630031 | -3.371544 | 3.518128 |
| 1 | -3.468747 | -4.367696 | 2.622444 |
| 1 | -0.033967 | 3.673571 | 6.340412 |
| 1 | -1.322136 | 2.487600 | 6.077779 |
| 1 | -1.295176 | 3.983691 | 5.144250 |
| 1 | 5.650878 | 2.637793 | 1.643292 |
| 1 | 6.782784 | 1.609926 | 0.766816 |
| 1 | 6.471056 | 1.330983 | 2.490062 |
| 1 | -6.106160 | -0.479245 | 4.965630 |

| | | | |
|---|---|---|---|
| 1 | -5.819856 | -1.106776 | 3.243147 |
| 1 | 2.830635 | 5.699166 | 5.585883 |
| 1 | 1.045499 | 5.398194 | 5.216105 |
| 1 | 3.474074 | -7.028207 | -1.232657 |
| 1 | 2.589250 | -6.461865 | 0.208643 |
| 1 | 3.327708 | -4.540731 | -2.059970 |
| 1 | 1.955893 | -5.607637 | -2.240564 |
| 1 | 7.381982 | -0.972915 | 1.309225 |
| 1 | 8.197370 | -1.460139 | -0.202268 |
| 1 | 6.577181 | 0.086681 | -0.933781 |
| 1 | 5.859884 | -1.469514 | -1.311440 |
| 1 | 3.977137 | -2.647229 | -0.923533 |
| 1 | -1.986659 | -4.026459 | 0.894140 |
| 1 | -2.150027 | 1.146715 | 4.568014 |
| 1 | 3.852038 | 2.432488 | 2.907036 |
| 1 | -3.721849 | -0.324009 | 5.348423 |
| 1 | 3.450798 | 3.564778 | 4.684264 |
| 1 | 6.252429 | -4.986874 | -0.614801 |
| 1 | 5.740747 | -4.071112 | 1.577386 |
| 1 | 0.939808 | 1.655263 | -0.422985 |
| 1 | 0.800869 | 5.611331 | -1.935832 |
| 1 | -1.806402 | 2.332022 | -2.863830 |
| 1 | -1.140307 | 7.167818 | -1.975271 |

| | | | |
|---|---|---|---|
| 1 | -3.783142 | 3.914245 | -2.878914 |
| 1 | 1.714776 | 1.405714 | -3.267069 |
| 1 | 1.071538 | 3.515534 | -0.359187 |
| 1 | 3.227798 | 1.728386 | -1.673748 |
| 1 | 3.363886 | 3.498553 | -1.598750 |
| 1 | 3.293431 | 2.527750 | -0.110805 |
| 1 | -2.833650 | -0.041955 | 0.211969 |
| 1 | -3.053695 | 1.372138 | -0.853664 |
| 1 | -1.480021 | 1.493901 | 1.467433 |
| 1 | -1.147767 | 2.478230 | 0.050898 |
| 1 | 6.535896 | 5.563846 | -2.920164 |
| 1 | 5.399940 | 4.239957 | -3.203651 |
| 1 | 0.238479 | 1.928084 | -4.047322 |
| 6 | 1.921762 | 3.191562 | -4.501372 |
| 1 | 1.342550 | 4.086404 | -4.748816 |
| 1 | 2.870697 | 3.514579 | -4.060705 |
| 1 | 2.141071 | 2.656787 | -5.433900 |
| 1 | -3.469807 | 6.247502 | -2.429043 |
| 1 | 0.730897 | -3.600773 | -2.908536 |
| 6 | 2.290407 | 6.289342 | 1.224247 |
| 1 | 2.697242 | 5.458063 | 0.637804 |
| 1 | 2.498448 | 7.214237 | 0.673604 |
| 1 | 2.846877 | 6.327639 | 2.167073 |

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$$\left[ {}^{3}\mathbf{TS(C\text{-}D)}^{\mathbf{A}}_{(S)} \right]^{\mathbf{S264A}}$$

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Number of imaginary frequencies : 5 Electronic energy : HF=-4126.3115209

Zero-point correction= 1.539772 (Hartree/Particle)

Thermal correction to Energy= 1.635601

Thermal correction to Enthalpy= 1.636545

Thermal correction to Gibbs Free Energy= 1.393457

Sum of electronic and zero-point Energies= -4124.772152

Sum of electronic and thermal Energies= -4124.676323

Sum of electronic and thermal Enthalpies= -4124.675379

Sum of electronic and thermal Free Energies= -4124.918467

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| 7 | 7.525545 | 1.341428 | -2.437384 |
| 6 | 8.053552 | 1.112515 | -3.773131 |
| 6 | 6.839235 | 2.625315 | -2.457851 |
| 6 | 6.720742 | 3.093102 | -3.923500 |
| 6 | 7.945234 | 2.428201 | -4.572704 |

| | | | |
|---|---|---|---|
| 1 | 7.447974 | 3.331682 | -1.866300 |
| 1 | 5.881598 | 2.543119 | -1.929751 |
| 1 | 8.841570 | 3.039636 | -4.412819 |
| 1 | 7.839415 | 2.269170 | -5.649838 |
| 1 | 7.439346 | 0.321112 | -4.238354 |
| 1 | 9.069888 | 0.702301 | -3.709274 |
| 6 | 1.479740 | 6.026762 | -0.037151 |
| 1 | 1.277072 | 6.290537 | -1.082935 |
| 1 | 0.786839 | 5.244204 | 0.274329 |
| 6 | -6.220496 | 5.939216 | -1.134175 |
| 6 | -7.038488 | 4.646076 | -0.986089 |
| 6 | -6.656590 | 3.466070 | -1.949007 |
| 8 | -7.149361 | 2.348162 | -1.657509 |
| 8 | -5.920576 | 3.760694 | -2.935688 |
| 1 | -6.616385 | 6.749277 | -0.505958 |
| 1 | -6.982643 | 4.265181 | 0.041310 |
| 1 | -8.103732 | 4.862413 | -1.158819 |
| 1 | -6.224893 | 6.265787 | -2.178314 |
| 1 | -5.174605 | 5.777636 | -0.849950 |
| 7 | -8.105129 | -3.137541 | -1.043980 |
| 6 | -7.375859 | -1.886822 | -0.863175 |
| 6 | -6.228670 | -2.057124 | 0.163262 |
| 8 | -6.271268 | -1.487733 | 1.245783 |

| | | | |
|---|---|---|---|
| 6 | -9.520683 | -2.789737 | -1.036172 |
| 6 | -9.645269 | -1.260860 | -1.195681 |
| 6 | -8.362918 | -0.754734 | -0.518460 |
| 1 | -9.927489 | -3.113646 | -0.060914 |
| 1 | -10.051186 | -3.381422 | -1.794534 |
| 1 | -10.559016 | -0.858847 | -0.748327 |
| 1 | -9.651676 | -0.991449 | -2.258477 |
| 1 | -8.482975 | -0.708413 | 0.568089 |
| 1 | -8.021446 | 0.226901 | -0.868335 |
| 1 | -6.893766 | -1.654220 | -1.828884 |
| 7 | -5.117619 | -2.805717 | -0.174891 |
| 6 | -4.980262 | -3.899105 | -1.142154 |
| 6 | -4.785770 | -3.450369 | -2.602164 |
| 6 | -3.558383 | -2.552960 | -2.810036 |
| 6 | -2.259941 | -3.364679 | -2.994083 |
| 7 | -1.044441 | -2.638025 | -2.627100 |
| 6 | -0.545551 | -1.585606 | -3.280460 |
| 7 | -1.068362 | -1.236124 | -4.486829 |
| 7 | 0.506966 | -0.909917 | -2.826668 |
| 1 | -4.435274 | -2.783809 | 0.572803 |
| 1 | -5.863739 | -4.544400 | -1.096708 |
| 1 | -4.718720 | -4.349679 | -3.230889 |
| 1 | -5.685269 | -2.925628 | -2.932493 |

| | | | |
|---|---|---|---|
| 1 | -3.732248 | -1.900676 | -3.674770 |
| 1 | -3.452642 | -1.888456 | -1.945928 |
| 1 | -2.277907 | -4.245691 | -2.348360 |
| 1 | -2.168269 | -3.734522 | -4.023191 |
| 1 | -0.653879 | -2.837927 | -1.706715 |
| 1 | -2.042870 | -1.426048 | -4.663343 |
| 1 | -0.720949 | -0.379464 | -4.893324 |
| 1 | 0.517482 | 0.139873 | -2.991447 |
| 1 | -4.121510 | -4.493628 | -0.814570 |
| 6 | 2.336374 | -2.390551 | 3.297373 |
| 8 | 1.604038 | -1.213040 | 3.383889 |
| 1 | 1.753390 | -3.244302 | 2.906959 |
| 1 | 2.677912 | -2.678261 | 4.307170 |
| 1 | 3.239577 | -2.303508 | 2.669636 |
| 6 | 2.741890 | -2.231130 | -0.326312 |
| 6 | -1.537081 | -2.597127 | 1.945139 |
| 6 | -0.819731 | 1.643502 | 4.123654 |
| 6 | 3.653232 | 1.706513 | 2.346291 |
| 6 | 1.461652 | -2.683240 | 0.028977 |
| 6 | 0.880326 | -3.961028 | -0.362246 |
| 6 | -0.309212 | -4.070356 | 0.330808 |
| 6 | -0.450840 | -2.857176 | 1.105046 |
| 6 | -1.235554 | -5.251398 | 0.374018 |

| | | | |
|---|---|---|---|
| 6 | 1.435059 | -5.004775 | -1.294755 |
| 6 | 2.063620 | -6.248737 | -0.592085 |
| 6 | 3.484652 | -5.961611 | -0.178359 |
| 8 | 4.306975 | -5.944944 | -1.218540 |
| 8 | 3.826342 | -5.720844 | 0.977305 |
| 6 | -1.735440 | -1.461949 | 2.719104 |
| 6 | -2.895069 | -1.249190 | 3.573439 |
| 6 | -2.712442 | -0.020682 | 4.161764 |
| 6 | -1.421854 | 0.471693 | 3.680674 |
| 6 | -4.021586 | -2.214145 | 3.776179 |
| 6 | -3.561627 | 0.677454 | 5.121454 |
| 6 | -4.901175 | 0.627082 | 5.180413 |
| 6 | 0.475139 | 2.045274 | 3.825063 |
| 6 | 1.121075 | 3.208735 | 4.416096 |
| 6 | 2.404067 | 3.217013 | 3.930480 |
| 6 | 2.505794 | 2.055129 | 3.042424 |
| 6 | 0.484389 | 4.148233 | 5.391191 |
| 6 | 3.503946 | 4.127199 | 4.224779 |
| 6 | 3.414493 | 5.430641 | 4.536802 |
| 6 | 3.797231 | 0.633226 | 1.471676 |
| 6 | 5.045354 | 0.310659 | 0.806988 |
| 6 | 4.798744 | -0.784983 | 0.021509 |
| 6 | 3.395087 | -1.130906 | 0.230067 |

| | | | |
|---|---|---|---|
| 6 | 6.341799 | 1.043650 | 0.990893 |
| 6 | 5.815123 | -1.452798 | -0.862259 |
| 6 | 6.879651 | -2.314472 | -0.103440 |
| 6 | 6.316331 | -3.679705 | 0.167998 |
| 8 | 5.631124 | -3.778616 | 1.291446 |
| 8 | 6.427092 | -4.594304 | -0.656122 |
| 7 | 0.615563 | -2.026610 | 0.888071 |
| 7 | -0.875257 | -0.397942 | 2.788655 |
| 7 | 1.327798 | 1.384095 | 2.990332 |
| 7 | 2.815889 | -0.241155 | 1.100176 |
| 26 | 0.957521 | -0.279777 | 1.896437 |
| 6 | 0.022086 | 0.892780 | 0.319326 |
| 6 | -0.296059 | 2.286389 | 0.719790 |
| 6 | -1.316456 | 0.383142 | -0.232087 |
| 7 | 0.631356 | 1.891770 | -3.012737 |
| 6 | 1.466015 | 1.937616 | -1.799230 |
| 6 | -0.595728 | 2.682562 | -2.926866 |
| 6 | -0.592018 | 3.992589 | -2.435110 |
| 6 | -1.806360 | 2.133363 | -3.372179 |
| 6 | -1.778398 | 4.727177 | -2.375333 |
| 6 | -2.992995 | 2.864505 | -3.302612 |
| 6 | -2.981619 | 4.169156 | -2.802354 |
| 6 | 1.328973 | 2.122482 | -4.312254 |

| | | | |
|---|---|---|---|
| 6 | 2.873395 | 1.415178 | -1.958220 |
| 1 | -1.121496 | -5.890666 | -0.508311 |
| 1 | -2.286983 | -4.951237 | 0.432807 |
| 1 | -1.043385 | -5.882078 | 1.251897 |
| 1 | -4.820811 | -2.066894 | 3.038484 |
| 1 | -4.466358 | -2.074190 | 4.766540 |
| 1 | -3.679275 | -3.252947 | 3.707896 |
| 1 | 1.242167 | 4.629424 | 6.016859 |
| 1 | -0.218970 | 3.629447 | 6.050259 |
| 1 | -0.075382 | 4.943291 | 4.881568 |
| 1 | 6.187713 | 2.127608 | 1.031432 |
| 1 | 7.035190 | 0.843996 | 0.169384 |
| 1 | 6.837318 | 0.760167 | 1.929246 |
| 1 | -5.444450 | 1.176170 | 5.943815 |
| 1 | -5.494238 | 0.079393 | 4.455605 |
| 1 | 4.304367 | 6.011464 | 4.761110 |
| 1 | 2.468448 | 5.960931 | 4.550869 |
| 1 | 2.077609 | -7.085637 | -1.297964 |
| 1 | 1.484841 | -6.528479 | 0.289160 |
| 1 | 2.176040 | -4.579820 | -1.978848 |
| 1 | 0.622151 | -5.375605 | -1.931737 |
| 1 | 7.164497 | -1.818977 | 0.826670 |
| 1 | 7.760718 | -2.439583 | -0.737385 |

| | | | |
|---|---|---|---|
| 1 | 6.371065 | -0.677206 | -1.401606 |
| 1 | 5.339418 | -2.078763 | -1.625590 |
| 1 | 3.314698 | -2.856054 | -1.004696 |
| 1 | -2.290292 | -3.374133 | 2.021180 |
| 1 | -1.393099 | 2.272608 | 4.793132 |
| 1 | 4.526932 | 2.330014 | 2.493618 |
| 1 | -3.043134 | 1.300510 | 5.849860 |
| 1 | 4.501476 | 3.688946 | 4.184728 |
| 1 | 5.201187 | -5.572960 | -0.943444 |
| 1 | 5.084033 | -4.614182 | 1.288466 |
| 1 | 0.844686 | 1.198192 | -0.748302 |
| 1 | 0.326784 | 4.437236 | -2.074536 |
| 1 | -1.822884 | 1.112038 | -3.740659 |
| 1 | -1.754422 | 5.735659 | -1.971135 |
| 1 | -3.959948 | 2.455606 | -3.583571 |
| 1 | 2.127738 | 1.378707 | -4.399358 |
| 1 | 1.437673 | 2.894934 | -1.279662 |
| 1 | 2.916437 | 0.381932 | -2.319490 |
| 1 | 3.482086 | 2.024571 | -2.643856 |
| 1 | 3.360467 | 1.438412 | -0.983869 |
| 1 | 6.706279 | 4.181611 | -4.026818 |
| 1 | 5.795557 | 2.705569 | -4.366305 |
| 1 | 0.597575 | 1.899137 | -5.099451 |

| | | | |
|---|---|---|---|
| 6 | 1.897454 | 3.525536 | -4.554431 |
| 1 | 1.104630 | 4.276900 | -4.557157 |
| 1 | 2.624536 | 3.803637 | -3.785885 |
| 1 | 2.402334 | 3.556192 | -5.527042 |
| 1 | -3.939286 | 4.677673 | -2.739192 |
| 1 | 0.890474 | -1.197568 | -1.929237 |
| 6 | -2.369273 | 1.325585 | 0.394392 |
| 1 | -1.364831 | 0.478542 | -1.323349 |
| 1 | -1.523936 | -0.659654 | 0.016373 |
| 1 | -3.144272 | 1.647417 | -0.306177 |
| 1 | -2.848533 | 0.883299 | 1.272239 |
| 8 | -1.646594 | 2.498543 | 0.811239 |
| 8 | 0.471367 | 3.214277 | 0.929428 |
| 1 | 1.274605 | 6.923971 | 0.559991 |
| 6 | 2.929170 | 5.569946 | 0.148418 |
| 1 | 3.129399 | 5.321951 | 1.195263 |
| 1 | 3.138104 | 4.668777 | -0.438833 |
| 1 | 3.645621 | 6.342816 | -0.158639 |

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$$\left[ {}^{3}\mathbf{TS(D\text{-}P)}^{\mathbf{A}}_{(1S,2R)} \right]^{\mathbf{L9}}$$

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Number of imaginary frequencies : 6 Electronic energy : HF=-4036.1586765

Zero-point correction= 1.503347 (Hartree/Particle)

Thermal correction to Energy= 1.597821

Thermal correction to Enthalpy= 1.598766

Thermal correction to Gibbs Free Energy= 1.357036

Sum of electronic and zero-point Energies= -4034.655329

Sum of electronic and thermal Energies= -4034.560855

Sum of electronic and thermal Enthalpies= -4034.559911

Sum of electronic and thermal Free Energies= -4034.801641

.....

Cartesian Coordinates

.....

| | | | |
|---|---|---|---|
| N | 5.750640 | 4.679187 | -1.787403 |
| C | 6.082134 | 3.579345 | -2.685703 |
| C | 4.317270 | 4.918921 | -1.918112 |
| C | 3.696940 | 3.782017 | -2.754355 |
| C | 4.882469 | 3.338335 | -3.627391 |
| H | 4.200484 | 5.897070 | -2.420440 |
| H | 3.852845 | 5.036441 | -0.931051 |
| H | 2.828939 | 4.110716 | -3.332838 |
| H | 3.357435 | 2.981872 | -2.089562 |
| H | 4.969638 | 3.976981 | -4.516740 |

| | | | |
|---|---|---|---|
| H | 4.810307 | 2.301166 | -3.969055 |
| H | 6.252777 | 2.688915 | -2.057266 |
| H | 7.033575 | 3.782590 | -3.196754 |
| C | -1.468762 | 5.242064 | 1.643423 |
| C | -0.468854 | 5.636486 | 0.548776 |
| O | 0.859628 | 5.218480 | 0.817146 |
| H | -1.519792 | 4.154386 | 1.723041 |
| H | -0.817194 | 5.234897 | -0.412640 |
| H | -0.450327 | 6.734014 | 0.453176 |
| H | 0.980831 | 4.323990 | 0.426856 |
| H | -1.158064 | 5.650510 | 2.612177 |
| H | -2.471282 | 5.622364 | 1.408145 |
| C | -6.120857 | 4.563010 | 0.379634 |
| C | -6.200450 | 3.086030 | 0.792897 |
| C | -5.561895 | 2.059960 | -0.194560 |
| O | -5.612170 | 0.846893 | 0.188058 |
| O | -5.064688 | 2.504356 | -1.254765 |
| H | -6.620542 | 4.724478 | -0.581055 |
| H | -5.716893 | 2.935575 | 1.766768 |
| H | -7.248170 | 2.788185 | 0.941995 |
| H | -5.078703 | 4.871291 | 0.254407 |
| H | -6.588971 | 5.214637 | 1.129367 |
| N | -7.147636 | -2.155435 | 1.003920 |

| | | | |
|---|---|---|---|
| C | -7.623999 | -2.086063 | -0.374770 |
| C | -6.561813 | -2.422789 | -1.408607 |
| O | -6.837683 | -3.107232 | -2.399268 |
| C | -7.606365 | -0.953645 | 1.673920 |
| C | -8.769807 | -0.368500 | 0.847715 |
| C | -8.320613 | -0.710427 | -0.580336 |
| H | -6.768945 | -0.229564 | 1.635963 |
| H | -7.839158 | -1.164480 | 2.726008 |
| H | -8.901260 | 0.705998 | 1.009191 |
| H | -9.715951 | -0.871494 | 1.094288 |
| H | -7.583387 | 0.026751 | -0.908005 |
| H | -9.134657 | -0.762244 | -1.309964 |
| H | -8.371538 | -2.888428 | -0.491561 |
| N | -5.335760 | -1.951438 | -1.094384 |
| C | 2.108233 | -2.882042 | 3.408726 |
| O | 2.386789 | -1.567796 | 3.078531 |
| H | 2.259879 | -3.594490 | 2.573411 |
| H | 1.073048 | -3.041646 | 3.773793 |
| H | 2.775039 | -3.227609 | 4.226336 |
| C | 3.841272 | -1.720821 | -0.590006 |
| C | -0.412429 | -3.463541 | 0.942936 |
| C | -0.941754 | 0.387185 | 3.815859 |
| C | 3.218197 | 2.197912 | 2.179618 |

| | | | |
|---|---|---|---|
| C | 2.694229 | -2.511624 | -0.483915 |
| C | 2.465129 | -3.763831 | -1.195687 |
| C | 1.265777 | -4.253249 | -0.745032 |
| C | 0.766843 | -3.295650 | 0.220477 |
| C | 0.582562 | -5.529891 | -1.132789 |
| C | 3.334715 | -4.422803 | -2.229257 |
| C | 4.206926 | -5.607236 | -1.700028 |
| C | 5.455340 | -5.090661 | -1.035199 |
| O | 6.345787 | -4.652999 | -1.919977 |
| O | 5.616360 | -5.031520 | 0.182112 |
| C | -0.927208 | -2.584827 | 1.891805 |
| C | -2.131373 | -2.817264 | 2.664344 |
| C | -2.317781 | -1.695946 | 3.439831 |
| C | -1.184542 | -0.817492 | 3.163885 |
| C | -3.032247 | -4.011619 | 2.578451 |
| C | -3.444013 | -1.475105 | 4.341651 |
| C | -4.069091 | -0.318481 | 4.610809 |
| C | 0.131410 | 1.241101 | 3.586369 |
| C | 0.296461 | 2.526612 | 4.246651 |
| C | 1.448106 | 3.072885 | 3.737519 |
| C | 1.982319 | 2.089040 | 2.800115 |
| C | -0.671741 | 3.130765 | 5.216575 |
| C | 2.009203 | 4.406688 | 3.952799 |

| | | | |
|---|---|---|---|
| C | 2.147919 | 5.022429 | 5.136276 |
| C | 3.794077 | 1.247396 | 1.343111 |
| C | 5.132528 | 1.360067 | 0.796377 |
| C | 5.326357 | 0.246097 | 0.020582 |
| C | 4.092557 | -0.532774 | 0.099971 |
| C | 6.088476 | 2.484524 | 1.071397 |
| C | 6.599390 | -0.095689 | -0.700901 |
| C | 7.688515 | -0.801540 | 0.184182 |
| C | 7.490742 | -2.290389 | 0.135769 |
| O | 7.952082 | -2.963659 | -0.794675 |
| O | 6.736532 | -2.780266 | 1.097770 |
| N | 1.635889 | -2.245214 | 0.345744 |
| N | -0.369533 | -1.373067 | 2.216894 |
| N | 1.156194 | 1.006624 | 2.711499 |
| N | 3.197804 | 0.091406 | 0.926137 |
| H | 1.009202 | -5.953702 | -2.048308 |
| H | -0.486817 | -5.378963 | -1.309367 |
| H | 0.669881 | -6.296458 | -0.350346 |
| H | -2.504480 | -4.895999 | 2.209459 |
| H | -3.885871 | -3.829754 | 1.915381 |
| H | -3.445791 | -4.265258 | 3.561682 |
| H | -0.600587 | 2.669416 | 6.211252 |
| H | -1.706375 | 3.005783 | 4.878330 |

| | | | |
|---|---|---|---|
| H | -0.478349 | 4.200574 | 5.333911 |
| H | 7.107535 | 2.231318 | 0.761324 |
| H | 6.125169 | 2.723021 | 2.140401 |
| H | 5.815189 | 3.406674 | 0.541957 |
| H | -4.912930 | -0.289073 | 5.294374 |
| H | -3.796123 | 0.614433 | 4.129717 |
| H | 2.529866 | 6.038173 | 5.199814 |
| H | 1.896229 | 4.532891 | 6.073327 |
| H | 4.507122 | -6.235745 | -2.545763 |
| H | 3.641347 | -6.205259 | -0.983981 |
| H | 3.992530 | -3.699550 | -2.721454 |
| H | 2.693372 | -4.831275 | -3.019649 |
| H | 7.626870 | -0.431981 | 1.209328 |
| H | 8.680067 | -0.593277 | -0.227649 |
| H | 7.056634 | 0.826097 | -1.076179 |
| H | 6.414702 | -0.715897 | -1.585123 |
| H | 4.619579 | -2.075085 | -1.260098 |
| H | -0.964467 | -4.380652 | 0.770288 |
| H | -1.651354 | 0.680682 | 4.578674 |
| H | 3.792448 | 3.094836 | 2.384629 |
| H | -3.840115 | -2.378961 | 4.808727 |
| H | 2.286095 | 4.939921 | 3.043341 |
| Fe | 1.448096 | -0.670456 | 1.618915 |

| | | | |
|---|---|---|---|
| C | -4.165218 | -2.238394 | -1.892587 |
| C | -3.966236 | -3.689988 | -2.371453 |
| C | -3.752113 | -4.797906 | -1.318462 |
| C | -5.002983 | -5.131236 | -0.488530 |
| C | -3.256343 | -6.072224 | -2.025544 |
| C | 0.299930 | 0.544415 | -0.648599 |
| C | -1.146042 | 0.131218 | -0.620875 |
| C | 0.383644 | 1.942614 | -0.369171 |
| C | 0.320492 | 1.384190 | -3.318329 |
| N | -0.964396 | 1.618284 | -3.760094 |
| H | -4.801715 | -3.965422 | -3.019697 |
| H | -3.065166 | -3.655749 | -3.001238 |
| H | -2.962373 | -4.461527 | -0.630754 |
| H | -4.801112 | -5.974649 | 0.184150 |
| H | -5.334117 | -4.287308 | 0.119603 |
| H | -5.835210 | -5.410645 | -1.144246 |
| H | -3.040650 | -6.871104 | -1.305895 |
| H | -4.020893 | -6.448432 | -2.717861 |
| H | -2.346211 | -5.889452 | -2.608276 |
| H | 0.812624 | 2.241273 | -2.881776 |
| H | -4.156670 | -1.603349 | -2.794012 |
| H | -3.298308 | -1.934140 | -1.296527 |
| C | 1.143904 | 0.244016 | -3.825005 |

| | | | |
|---|---|---|---|
| H | 2.116152 | 0.258168 | -3.326519 |
| H | 0.700350 | -0.738513 | -3.619105 |
| H | 1.321953 | 0.290585 | -4.915373 |
| C | -1.513285 | 2.932084 | -3.691819 |
| C | -2.786700 | 3.154957 | -3.147133 |
| C | -0.765335 | 4.026604 | -4.160860 |
| C | -3.294171 | 4.450856 | -3.070666 |
| H | -3.388886 | 2.360225 | -2.716617 |
| C | -1.281779 | 5.318271 | -4.079670 |
| H | 0.216943 | 3.852717 | -4.590396 |
| C | -2.551035 | 5.538337 | -3.537049 |
| H | -4.260753 | 4.575927 | -2.593758 |
| H | -0.688617 | 6.154252 | -4.443426 |
| H | -2.946347 | 6.548268 | -3.462308 |
| C | -1.792789 | 0.559301 | -4.345626 |
| H | -1.404682 | -0.405605 | -4.014886 |
| H | -2.805829 | 0.641099 | -3.943171 |
| C | -1.842141 | 0.619004 | -5.878097 |
| H | -2.227396 | 1.587466 | -6.211966 |
| H | -0.846753 | 0.479215 | -6.312645 |
| H | -2.502155 | -0.164660 | -6.267749 |
| H | 6.439758 | -3.706083 | 0.867779 |
| H | 7.066482 | -4.138335 | -1.445628 |

| | | | |
|---|---|---|---|
| H | -5.288998 | -1.118499 | -0.496113 |
| O | 1.324041 | 2.750655 | -0.449665 |
| O | -0.850843 | 2.415647 | 0.009650 |
| C | -1.799286 | 1.324224 | 0.107498 |
| H | -1.567559 | 0.027230 | -1.631655 |
| H | -1.330136 | -0.806042 | -0.092230 |
| H | -2.740031 | 1.658766 | -0.332819 |
| H | -1.951154 | 1.106657 | 1.168625 |
| H | 1.119203 | -0.025080 | -1.049760 |

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**$B^{L9}$**

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Number of imaginary frequencies : 1 Electronic energy : HF=-3700.828767

Zero-point correction= 1.285143 (Hartree/Particle)

Thermal correction to Energy= 1.371602

Thermal correction to Enthalpy= 1.372546

Thermal correction to Gibbs Free Energy= 1.145232

Sum of electronic and zero-point Energies= -3699.543623

Sum of electronic and thermal Energies= -3699.457165

Sum of electronic and thermal Enthalpies= -3699.456221

Sum of electronic and thermal Free Energies= -3699.683535

.....

Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | -5.437426 | 2.927578 | 3.254686 |
| C | -5.792733 | 2.169938 | 4.445024 |
| C | -3.994527 | 3.137565 | 3.293340 |
| C | -3.417609 | 2.421529 | 4.534329 |
| C | -4.640343 | 2.312559 | 5.460467 |
| H | -3.821070 | 4.226880 | 3.323577 |
| H | -3.537295 | 2.793537 | 2.356287 |
| H | -2.579783 | 2.962539 | 4.983590 |
| H | -3.054750 | 1.431380 | 4.243659 |
| H | -4.772624 | 3.233339 | 6.044300 |
| H | -4.584799 | 1.476566 | 6.165585 |
| H | -5.904725 | 1.112256 | 4.144724 |
| H | -6.775081 | 2.488310 | 4.820310 |
| C | 1.412016 | 5.541952 | 0.541543 |
| C | 0.089347 | 5.893952 | 1.225580 |
| O | -1.039158 | 5.286111 | 0.623309 |
| H | 1.379020 | 5.814735 | -0.518470 |
| H | 0.152906 | 5.632456 | 2.295843 |
| H | -0.080573 | 6.979140 | 1.176203 |

| | | | |
|---|---|---|---|
| H | -0.988340 | 4.323814 | 0.806858 |
| H | 2.247561 | 6.076464 | 1.011834 |
| H | 1.608723 | 4.469389 | 0.618550 |
| C | 6.153897 | 4.793280 | 1.341916 |
| C | 5.356174 | 3.494279 | 1.464858 |
| C | 6.204429 | 2.202359 | 1.339069 |
| O | 5.523737 | 1.119751 | 1.295817 |
| O | 7.448750 | 2.314772 | 1.295226 |
| H | 6.626244 | 4.868198 | 0.356780 |
| H | 4.837068 | 3.452256 | 2.432348 |
| H | 4.560576 | 3.450323 | 0.711310 |
| H | 6.961925 | 4.817518 | 2.079173 |
| H | 5.515307 | 5.674918 | 1.484730 |
| N | 6.804762 | -1.583270 | -0.900307 |
| C | 7.999917 | -1.660413 | -0.064218 |
| C | 7.652257 | -2.062005 | 1.389926 |
| O | 8.221633 | -3.011922 | 1.940193 |
| C | 6.751227 | -0.240773 | -1.449978 |
| C | 8.185391 | 0.322927 | -1.446775 |
| C | 8.765649 | -0.307899 | -0.170943 |
| H | 6.117062 | 0.356285 | -0.768030 |
| H | 6.257453 | -0.253365 | -2.428809 |
| H | 8.203855 | 1.415077 | -1.402739 |

| | | | |
|---|---|---|---|
| H | 8.727545 | -0.005738 | -2.345076 |
| H | 8.523805 | 0.351320 | 0.669116 |
| H | 9.850936 | -0.453427 | -0.205502 |
| H | 8.608855 | -2.498810 | -0.431509 |
| N | 6.714238 | -1.296306 | 1.987735 |
| C | -1.886217 | -1.848546 | -3.508285 |
| O | -2.006503 | -0.640178 | -2.828215 |
| H | -2.092618 | -2.729716 | -2.877434 |
| H | -0.887559 | -1.995334 | -3.957108 |
| H | -2.618599 | -1.866170 | -4.334914 |
| C | -4.057910 | -1.255638 | 0.292392 |
| C | 0.117401 | -3.454636 | -0.797177 |
| C | 1.558572 | 0.536547 | -3.102424 |
| C | -2.326857 | 2.893394 | -1.492861 |
| C | -3.065016 | -2.225537 | 0.170523 |
| C | -3.167935 | -3.596807 | 0.652712 |
| C | -1.963931 | -4.195424 | 0.382315 |
| C | -1.149790 | -3.199344 | -0.280963 |
| C | -1.528600 | -5.600420 | 0.675809 |
| C | -4.341708 | -4.255194 | 1.319516 |
| C | -5.304331 | -5.019847 | 0.351798 |
| C | -6.317058 | -4.084406 | -0.257895 |
| O | -7.237396 | -3.707728 | 0.624208 |

| | | | |
|---|---|---|---|
| O | -6.278186 | -3.680883 | -1.418422 |
| C | 0.867408 | -2.573703 | -1.567547 |
| C | 2.102861 | -2.918620 | -2.244420 |
| C | 2.475471 | -1.799742 | -2.954408 |
| C | 1.473859 | -0.779730 | -2.665518 |
| C | 2.775940 | -4.255693 | -2.202379 |
| C | 3.585119 | -1.631007 | -3.888822 |
| C | 4.817065 | -2.150274 | -3.769978 |
| C | 0.670053 | 1.560819 | -2.788056 |
| C | 0.813051 | 2.931236 | -3.246850 |
| C | -0.278700 | 3.614458 | -2.762448 |
| C | -1.073245 | 2.636129 | -2.028448 |
| C | 1.975323 | 3.464443 | -4.027004 |
| C | -0.600079 | 5.037373 | -2.832149 |
| C | -0.360682 | 5.861943 | -3.864612 |
| C | -3.152175 | 1.959783 | -0.878874 |
| C | -4.490997 | 2.258782 | -0.408573 |
| C | -5.002169 | 1.082872 | 0.072755 |
| C | -3.952990 | 0.080699 | -0.089475 |
| C | -5.141017 | 3.610011 | -0.446089 |
| C | -6.372318 | 0.910174 | 0.659796 |
| C | -7.523431 | 0.743218 | -0.393569 |
| C | -7.638771 | -0.705848 | -0.772053 |

| | | | |
|---|---|---|---|
| O | -8.346632 | -1.486720 | -0.124115 |
| O | -6.860831 | -1.078861 | -1.771001 |
| N | -1.831118 | -2.017866 | -0.385549 |
| N | 0.511372 | -1.277004 | -1.832249 |
| N | -0.460257 | 1.419119 | -2.030519 |
| N | -2.845991 | 0.649448 | -0.654536 |
| H | -2.247588 | -6.119210 | 1.317666 |
| H | -0.558465 | -5.621647 | 1.185939 |
| H | -1.420587 | -6.197124 | -0.239891 |
| H | 2.047132 | -5.072994 | -2.164120 |
| H | 3.428163 | -4.355067 | -1.325627 |
| H | 3.403496 | -4.396405 | -3.087900 |
| H | 1.876405 | 3.272300 | -5.104652 |
| H | 2.917006 | 3.009704 | -3.702334 |
| H | 2.059042 | 4.547294 | -3.895866 |
| H | -5.929301 | 3.686908 | 0.308757 |
| H | -5.587533 | 3.830361 | -1.425949 |
| H | -4.414402 | 4.401603 | -0.236239 |
| H | 5.560884 | -1.989035 | -4.546350 |
| H | 5.147359 | -2.676117 | -2.879868 |
| H | -0.601000 | 6.919930 | -3.801200 |
| H | 0.062378 | 5.512390 | -4.801948 |
| H | -5.851562 | -5.779167 | 0.921502 |

| | | | |
|---|---|---|---|
| H | -4.737767 | -5.502843 | -0.445913 |
| H | -4.928873 | -3.536199 | 1.899370 |
| H | -3.967389 | -4.987654 | 2.043243 |
| H | -7.315819 | 1.361350 | -1.269559 |
| H | -8.474563 | 1.042612 | 0.054639 |
| H | -6.599682 | 1.793446 | 1.265754 |
| H | -6.409270 | 0.060476 | 1.350838 |
| H | -4.988684 | -1.561706 | 0.758686 |
| H | 0.525844 | -4.446226 | -0.637513 |
| H | 2.411159 | 0.793908 | -3.720452 |
| H | -2.703539 | 3.904622 | -1.585570 |
| H | 3.365610 | -1.027983 | -4.771477 |
| H | -1.048238 | 5.446159 | -1.925968 |
| Fe | -1.159180 | -0.301038 | -1.212143 |
| C | 6.359770 | -1.511671 | 3.380627 |
| C | 5.475812 | -2.741169 | 3.661943 |
| C | 4.069663 | -2.736466 | 3.020557 |
| C | 4.079310 | -3.217967 | 1.560207 |
| C | 3.096347 | -3.590738 | 3.850050 |
| C | -0.159070 | 0.259393 | 0.812740 |
| C | 1.308533 | -0.195576 | 0.898586 |
| C | -0.092042 | 1.727321 | 1.086989 |
| H | 6.024292 | -3.640745 | 3.357712 |

| | | | |
|---|---|---|---|
| H | 5.366281 | -2.797275 | 4.755920 |
| H | 3.696442 | -1.701811 | 3.031837 |
| H | 3.070916 | -3.177400 | 1.131788 |
| H | 4.739207 | -2.614824 | 0.933880 |
| H | 4.425711 | -4.259553 | 1.507461 |
| H | 2.092697 | -3.590639 | 3.409691 |
| H | 3.438283 | -4.633638 | 3.898950 |
| H | 3.011391 | -3.221623 | 4.879435 |
| H | 7.277852 | -1.612482 | 3.975418 |
| H | 5.843535 | -0.602171 | 3.706125 |
| H | -6.774985 | -2.072626 | -1.786434 |
| H | -7.777890 | -2.949140 | 0.248346 |
| H | 6.348227 | -0.416334 | 1.563688 |
| H | 1.406413 | -1.129686 | 1.457939 |
| H | 1.732389 | -0.354811 | -0.090505 |
| O | 1.196687 | 2.131538 | 1.287163 |
| O | -1.000953 | 2.539437 | 1.204212 |
| C | 2.031677 | 0.973972 | 1.574663 |
| H | 2.069310 | 0.870913 | 2.667845 |
| H | 3.043685 | 1.168027 | 1.212134 |
| N | -0.963746 | -0.413966 | 1.862515 |
| N | -1.913725 | -0.028368 | 2.454064 |

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**TS(B-C)$^{L9}$**

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Number of imaginary frequencies : 2 Electronic energy : HF=-3700.8252996

Zero-point correction= 1.283370 (Hartree/Particle)

Thermal correction to Energy= 1.369702

Thermal correction to Enthalpy= 1.370647

Thermal correction to Gibbs Free Energy= 1.143594

Sum of electronic and zero-point Energies= -3699.541930

Sum of electronic and thermal Energies= -3699.455597

Sum of electronic and thermal Enthalpies= -3699.454653

Sum of electronic and thermal Free Energies= -3699.681706

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | -5.676974 | 2.776995 | 3.484344 |
| C | -5.940721 | 1.795126 | 4.526692 |
| C | -4.239512 | 3.027412 | 3.484398 |
| C | -3.564506 | 2.074332 | 4.493727 |
| C | -4.714026 | 1.746287 | 5.461277 |

| | | | |
|---|---|---|---|
| H | -4.093821 | 4.086732 | 3.759422 |
| H | -3.840075 | 2.928029 | 2.467135 |
| H | -2.698043 | 2.524839 | 4.985861 |
| H | -3.214269 | 1.175322 | 3.977923 |
| H | -4.805699 | 2.520248 | 6.235008 |
| H | -4.599082 | 0.782244 | 5.966984 |
| H | -6.082450 | 0.817534 | 4.031703 |
| H | -6.890745 | 2.022334 | 5.029704 |
| C | 1.180307 | 5.490569 | 0.764983 |
| C | -0.205919 | 5.833351 | 1.314770 |
| O | -1.259972 | 5.158320 | 0.651234 |
| H | 1.229630 | 5.698547 | -0.308728 |
| H | -0.227963 | 5.629794 | 2.399276 |
| H | -0.403008 | 6.907677 | 1.191291 |
| H | -1.173908 | 4.203414 | 0.855195 |
| H | 1.955580 | 6.081738 | 1.269190 |
| H | 1.405937 | 4.432354 | 0.924907 |
| C | 5.938798 | 4.835413 | 1.548862 |
| C | 5.193420 | 3.507492 | 1.681093 |
| C | 6.080899 | 2.249873 | 1.495567 |
| O | 5.436451 | 1.145216 | 1.455241 |
| O | 7.317778 | 2.406996 | 1.406874 |
| H | 6.364791 | 4.944456 | 0.545960 |

| | | | |
|---|---|---|---|
| H | 4.717738 | 3.430103 | 2.668566 |
| H | 4.368942 | 3.448207 | 0.960318 |
| H | 6.776908 | 4.875575 | 2.251021 |
| H | 5.276867 | 5.691274 | 1.735515 |
| N | 6.722530 | -1.471350 | -0.873033 |
| C | 7.952381 | -1.513478 | -0.085937 |
| C | 7.672880 | -1.965963 | 1.368335 |
| O | 8.287196 | -2.915364 | 1.868726 |
| C | 6.586026 | -0.119724 | -1.384918 |
| C | 7.992966 | 0.507996 | -1.424386 |
| C | 8.653434 | -0.126471 | -0.189716 |
| H | 5.955109 | 0.432353 | -0.663322 |
| H | 6.054415 | -0.132698 | -2.343613 |
| H | 7.965436 | 1.598519 | -1.353112 |
| H | 8.511171 | 0.225788 | -2.352050 |
| H | 8.421253 | 0.501988 | 0.676247 |
| H | 9.741468 | -0.223434 | -0.273847 |
| H | 8.582060 | -2.316054 | -0.495619 |
| N | 6.735587 | -1.246314 | 2.022023 |
| C | -1.920740 | -1.830361 | -3.557867 |
| O | -1.957320 | -0.603958 | -2.906063 |
| H | -2.272370 | -2.670645 | -2.933173 |
| H | -0.912598 | -2.099852 | -3.922802 |

| | | | |
|---|---|---|---|
| H | -2.581995 | -1.792147 | -4.442691 |
| C | -4.006971 | -1.198444 | 0.255750 |
| C | 0.120066 | -3.460659 | -0.889227 |
| C | 1.619402 | 0.523360 | -3.170501 |
| C | -2.226677 | 2.927026 | -1.534127 |
| C | -3.035270 | -2.187421 | 0.109009 |
| C | -3.157050 | -3.560892 | 0.583960 |
| C | -1.967602 | -4.178653 | 0.294491 |
| C | -1.142946 | -3.191003 | -0.370200 |
| C | -1.553911 | -5.593272 | 0.572530 |
| C | -4.334165 | -4.203556 | 1.260118 |
| C | -5.321855 | -4.943478 | 0.298642 |
| C | -6.323459 | -3.985578 | -0.294217 |
| O | -7.224074 | -3.593305 | 0.601556 |
| O | -6.292586 | -3.579414 | -1.453969 |
| C | 0.885474 | -2.584086 | -1.650492 |
| C | 2.122100 | -2.940260 | -2.321448 |
| C | 2.509335 | -1.823866 | -3.026288 |
| C | 1.515610 | -0.794527 | -2.740238 |
| C | 2.782850 | -4.283328 | -2.274636 |
| C | 3.631379 | -1.661177 | -3.947786 |
| C | 4.865919 | -2.165833 | -3.798196 |
| C | 0.746636 | 1.560568 | -2.850282 |

| | | | |
|---|---|---|---|
| C | 0.913993 | 2.934434 | -3.291343 |
| C | -0.167690 | 3.630116 | -2.799780 |
| C | -0.979193 | 2.655417 | -2.078271 |
| C | 2.085030 | 3.458602 | -4.064484 |
| C | -0.472302 | 5.055979 | -2.853374 |
| C | -0.173244 | 5.908777 | -3.847420 |
| C | -3.063066 | 2.002574 | -0.922002 |
| C | -4.386799 | 2.327488 | -0.427304 |
| C | -4.914981 | 1.159779 | 0.056471 |
| C | -3.886700 | 0.137171 | -0.127595 |
| C | -4.995291 | 3.698599 | -0.445468 |
| C | -6.284028 | 1.003282 | 0.651778 |
| C | -7.443971 | 0.863200 | -0.396499 |
| C | -7.588453 | -0.581700 | -0.781032 |
| O | -8.304669 | -1.352640 | -0.130312 |
| O | -6.826000 | -0.963793 | -1.788241 |
| N | -1.805913 | -1.998310 | -0.461314 |
| N | 0.545670 | -1.284227 | -1.913020 |
| N | -0.387440 | 1.429465 | -2.096860 |
| N | -2.781785 | 0.685656 | -0.712267 |
| H | -2.274939 | -6.104766 | 1.218025 |
| H | -0.578940 | -5.635388 | 1.072115 |
| H | -1.465888 | -6.184389 | -0.348916 |

| | | | |
|---|---|---|---|
| H | 2.046593 | -5.095116 | -2.271585 |
| H | 3.403504 | -4.399734 | -1.377091 |
| H | 3.439141 | -4.417958 | -3.139859 |
| H | 1.962056 | 3.325398 | -5.148651 |
| H | 3.012485 | 2.951793 | -3.779077 |
| H | 2.215472 | 4.529669 | -3.882106 |
| H | -5.864855 | 3.756930 | 0.216240 |
| H | -5.322263 | 3.993204 | -1.452208 |
| H | -4.272377 | 4.449830 | -0.107914 |
| H | 5.622870 | -2.010701 | -4.563090 |
| H | 5.183239 | -2.672817 | -2.892456 |
| H | -0.413445 | 6.965459 | -3.765821 |
| H | 0.298499 | 5.585567 | -4.770488 |
| H | -5.877109 | -5.695968 | 0.869745 |
| H | -4.773436 | -5.431955 | -0.508333 |
| H | -4.901785 | -3.478938 | 1.852409 |
| H | -3.964304 | -4.948171 | 1.973715 |
| H | -7.229140 | 1.481681 | -1.270401 |
| H | -8.386634 | 1.178065 | 0.058842 |
| H | -6.502885 | 1.878791 | 1.272536 |
| H | -6.329459 | 0.145416 | 1.332293 |
| H | -4.935388 | -1.490410 | 0.736038 |
| H | 0.515130 | -4.458675 | -0.735253 |

| | | | |
|---|---|---|---|
| H | 2.477408 | 0.770761 | -3.785253 |
| H | -2.585859 | 3.945771 | -1.606991 |
| H | 3.421020 | -1.074694 | -4.843910 |
| H | -0.972743 | 5.445285 | -1.966405 |
| Fe | -1.103570 | -0.282643 | -1.274021 |
| C | 6.428812 | -1.520570 | 3.415519 |
| C | 5.569180 | -2.772447 | 3.672648 |
| C | 4.150745 | -2.765419 | 3.057104 |
| C | 4.136896 | -3.234694 | 1.592648 |
| C | 3.193491 | -3.628834 | 3.895640 |
| C | -0.080250 | 0.265936 | 0.573820 |
| C | 1.408534 | -0.066783 | 0.642877 |
| C | -0.132384 | 1.650121 | 1.147866 |
| H | 6.124141 | -3.652771 | 3.326575 |
| H | 5.482820 | -2.867766 | 4.765968 |
| H | 3.775833 | -1.731761 | 3.083174 |
| H | 3.119980 | -3.201062 | 1.183596 |
| H | 4.778673 | -2.620384 | 0.958234 |
| H | 4.490959 | -4.272808 | 1.524144 |
| H | 2.182395 | -3.625904 | 3.472811 |
| H | 3.537544 | -4.671680 | 3.929299 |
| H | 3.126346 | -3.269083 | 4.929690 |
| H | 7.366475 | -1.631608 | 3.976691 |

| | | | |
|---|---|---|---|
| H | 5.910460 | -0.632434 | 3.792554 |
| H | -6.759237 | -1.958899 | -1.809810 |
| H | -7.755805 | -2.824625 | 0.233837 |
| H | 6.325935 | -0.367124 | 1.638853 |
| H | 1.589224 | -1.119230 | 0.873668 |
| H | 1.875257 | 0.144754 | -0.321275 |
| O | 1.082795 | 2.028351 | 1.656382 |
| O | -1.083285 | 2.413554 | 1.266202 |
| C | 1.978975 | 0.884514 | 1.695494 |
| H | 1.924881 | 0.463604 | 2.708679 |
| H | 3.002137 | 1.219348 | 1.507483 |
| N | -0.754606 | -0.674085 | 1.865773 |
| N | -1.660513 | -0.390063 | 2.523598 |

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**$B^{L10}$**

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Number of imaginary frequencies : 5 Electronic energy : HF=-3866.2991432

Zero-point correction= 1.328639 (Hartree/Particle)

Thermal correction to Energy= 1.414502

Thermal correction to Enthalpy= 1.415447

Thermal correction to Gibbs Free Energy= 1.189787

Sum of electronic and zero-point Energies= -3864.970504

Sum of electronic and thermal Energies= -3864.884641

Sum of electronic and thermal Enthalpies= -3864.883697

Sum of electronic and thermal Free Energies= -3865.109356

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | -9.643319 | -5.516930 | -0.517602 |
| C | -8.837407 | -5.152166 | -1.674735 |
| C | -9.094052 | -4.796824 | 0.623213 |
| C | -8.095638 | -3.739325 | 0.106792 |
| C | -7.584835 | -4.393725 | -1.186504 |
| H | -8.581509 | -5.537578 | 1.262672 |
| H | -9.909024 | -4.389419 | 1.235735 |
| H | -6.779154 | -5.102619 | -0.961358 |
| H | -7.201720 | -3.676672 | -1.918090 |
| H | -9.460446 | -4.504309 | -2.317061 |
| H | -8.620631 | -6.045364 | -2.275464 |
| C | -3.991282 | -1.927622 | 5.213456 |
| C | -2.845326 | -1.063482 | 4.704270 |
| O | -2.397503 | -1.580957 | 3.458880 |
| H | -4.836841 | -1.895067 | 4.518045 |

| | | | |
|---|---|---|---|
| H | -3.180197 | -0.023250 | 4.600341 |
| H | -2.028434 | -1.061666 | 5.444783 |
| H | -1.796108 | -0.924737 | 3.062718 |
| H | -4.335396 | -1.574624 | 6.191888 |
| H | -3.673892 | -2.971064 | 5.313460 |
| C | 3.492530 | -2.910672 | 7.097826 |
| C | 4.639095 | -2.723798 | 6.099568 |
| C | 4.423569 | -3.360197 | 4.707911 |
| O | 5.277896 | -3.162563 | 3.826375 |
| O | 3.361328 | -4.080563 | 4.577861 |
| H | 2.576336 | -2.430244 | 6.740545 |
| H | 4.854498 | -1.659901 | 5.940551 |
| H | 5.569007 | -3.150166 | 6.499992 |
| H | 3.741474 | -2.478807 | 8.075297 |
| H | 3.266001 | -3.971798 | 7.231221 |
| N | 7.726315 | -2.147929 | -0.980832 |
| C | 6.689585 | -1.718952 | -0.044685 |
| C | 5.931240 | -0.497266 | -0.623678 |
| O | 5.986204 | 0.593818 | -0.062884 |
| C | 8.949328 | -2.298068 | -0.206317 |
| C | 8.569103 | -2.363858 | 1.285409 |
| C | 7.312032 | -1.481951 | 1.345143 |
| H | 9.575265 | -1.409524 | -0.408878 |

| | | | |
|---|---|---|---|
| H | 9.519917 | -3.160203 | -0.576229 |
| H | 9.370207 | -2.019979 | 1.946610 |
| H | 8.326262 | -3.394422 | 1.568606 |
| H | 7.567666 | -0.423023 | 1.443033 |
| H | 6.637339 | -1.757286 | 2.160853 |
| H | 5.958359 | -2.543801 | 0.010738 |
| N | 5.184401 | -0.647193 | -1.762147 |
| C | 4.934853 | -1.792674 | -2.648381 |
| C | 4.097435 | -2.946978 | -2.040081 |
| C | 3.051872 | -2.487057 | -1.018610 |
| C | 2.079750 | -3.600885 | -0.590236 |
| N | 1.376581 | -3.316571 | 0.654241 |
| C | 1.852751 | -3.669073 | 1.869750 |
| N | 2.897386 | -4.491424 | 2.039756 |
| N | 1.198810 | -3.255845 | 2.965164 |
| H | 4.687945 | 0.206280 | -1.983328 |
| H | 5.892050 | -2.185518 | -3.005067 |
| H | 3.619501 | -3.481452 | -2.873024 |
| H | 4.767770 | -3.676263 | -1.566673 |
| H | 3.552870 | -2.105347 | -0.124928 |
| H | 2.472680 | -1.641910 | -1.404415 |
| H | 1.328481 | -3.765241 | -1.371162 |
| H | 2.600597 | -4.558189 | -0.477649 |

| | | | |
|---|---|---|---|
| H | 0.764223 | -2.496197 | 0.681368 |
| H | 1.710915 | -3.374143 | 3.843589 |
| H | 4.404261 | -1.377063 | -3.507819 |
| C | -2.407860 | 2.317574 | -2.819013 |
| O | -2.091808 | 2.945388 | -1.609841 |
| H | -1.532697 | 2.155217 | -3.467903 |
| H | -3.107283 | 2.968265 | -3.367873 |
| H | -2.900083 | 1.342448 | -2.680826 |
| C | -0.154393 | -0.443439 | -2.324577 |
| C | 1.491977 | 4.087797 | -1.798058 |
| C | -1.797011 | 4.954196 | 1.621953 |
| C | -3.509267 | 0.487071 | 1.035357 |
| C | 0.584003 | 0.728910 | -2.503768 |
| C | 1.603952 | 0.938259 | -3.523359 |
| C | 2.065121 | 2.220753 | -3.352937 |
| C | 1.317766 | 2.785334 | -2.250306 |
| C | 3.102096 | 2.954595 | -4.151721 |
| C | 2.037703 | -0.002208 | -4.612999 |
| C | 1.274297 | 0.173133 | -5.966468 |
| C | -0.003300 | -0.627203 | -5.968865 |
| O | 0.233084 | -1.929945 | -6.058003 |
| O | -1.125184 | -0.137547 | -5.853450 |
| C | 0.770356 | 4.716841 | -0.790166 |

| | | | |
|---|---|---|---|
| C | 0.982870 | 6.088494 | -0.371103 |
| C | 0.059316 | 6.333570 | 0.621290 |
| C | -0.710216 | 5.101418 | 0.768930 |
| C | 1.980274 | 7.033914 | -0.966656 |
| C | -0.195490 | 7.558518 | 1.368990 |
| C | 0.687759 | 8.522635 | 1.675733 |
| C | -2.597302 | 3.824599 | 1.721906 |
| C | -3.762681 | 3.729240 | 2.581504 |
| C | -4.262785 | 2.459594 | 2.409527 |
| C | -3.385967 | 1.810145 | 1.437386 |
| C | -4.302273 | 4.834764 | 3.435123 |
| C | -5.438642 | 1.832778 | 3.000086 |
| C | -5.993320 | 2.106441 | 4.192530 |
| C | -2.697052 | -0.170632 | 0.121309 |
| C | -2.879953 | -1.562155 | -0.237471 |
| C | -1.960431 | -1.835841 | -1.212898 |
| C | -1.195762 | -0.609176 | -1.414533 |
| C | -3.860029 | -2.483471 | 0.422562 |
| C | -1.810301 | -3.155896 | -1.914754 |
| C | -2.889402 | -3.429400 | -3.015681 |
| C | -2.493319 | -2.720395 | -4.281023 |
| O | -2.894206 | -1.464857 | -4.356488 |
| O | -1.772422 | -3.266936 | -5.121667 |

| | | | |
|---|---|---|---|
| N | 0.438379 | 1.861535 | -1.744157 |
| N | -0.240288 | 4.135997 | -0.070386 |
| N | -2.397378 | 2.655248 | 1.040030 |
| N | -1.659382 | 0.376267 | -0.579873 |
| Fe | -0.974454 | 2.251064 | -0.344652 |
| H | 3.628204 | 2.288201 | -4.841380 |
| H | 3.856446 | 3.418741 | -3.506054 |
| H | 2.657435 | 3.758127 | -4.752434 |
| H | 2.960179 | 6.968939 | -0.474564 |
| H | 1.637054 | 8.068272 | -0.867876 |
| H | 2.139643 | 6.832368 | -2.030685 |
| H | -5.382730 | 4.724886 | 3.570437 |
| H | -4.116889 | 5.816141 | 2.987410 |
| H | -3.848427 | 4.842239 | 4.435206 |
| H | -3.691419 | -2.484429 | 1.506096 |
| H | -3.755897 | -3.510064 | 0.059292 |
| H | -4.898501 | -2.175487 | 0.242952 |
| H | 0.377045 | 9.406513 | 2.224774 |
| H | 1.739645 | 8.453668 | 1.419850 |
| H | -6.886095 | 1.583825 | 4.522633 |
| H | -5.567109 | 2.826421 | 4.882671 |
| H | 1.904978 | -0.200429 | -6.779977 |
| H | 1.041259 | 1.224235 | -6.142008 |

| | | | |
|---|---|---|---|
| H | 1.957266 | -1.049191 | -4.303795 |
| H | 3.099237 | 0.170179 | -4.822115 |
| H | -3.866635 | -3.089004 | -2.666747 |
| H | -2.926040 | -4.499507 | -3.233966 |
| H | -1.892520 | -3.962505 | -1.178153 |
| H | -0.819219 | -3.265946 | -2.368263 |
| H | 0.085709 | -1.284008 | -2.967639 |
| H | 2.259057 | 4.673606 | -2.291323 |
| H | -2.051081 | 5.795904 | 2.254562 |
| H | -4.288043 | -0.102867 | 1.501172 |
| H | -1.220827 | 7.694216 | 1.712099 |
| H | -5.908286 | 1.056834 | 2.396232 |
| H | -0.607744 | -2.445857 | -5.869408 |
| H | -2.377785 | -0.982457 | -5.063350 |
| H | -7.302246 | -3.508275 | 0.822844 |
| H | -8.621450 | -2.804429 | -0.121083 |
| H | 0.498942 | -2.529362 | 2.863791 |
| C | 0.463004 | 1.511212 | 1.498423 |
| C | 0.722361 | 0.084072 | 1.312987 |
| C | 2.651707 | 1.148119 | 0.616497 |
| H | 2.651376 | 1.388783 | -0.447867 |
| C | 1.847284 | 2.165687 | 1.433372 |
| H | 3.681040 | 1.006113 | 0.949249 |

| | | | |
|---|---|---|---|
| H | 2.268104 | 2.267446 | 2.442861 |
| H | 1.858242 | 3.151283 | 0.969191 |
| O | 0.020160 | -0.896198 | 1.584371 |
| O | 1.958770 | -0.119649 | 0.780824 |
| H | 3.588256 | -4.522749 | 1.307061 |
| H | 3.262371 | -4.480033 | 3.049503 |
| N | -0.224498 | 1.822179 | 2.734834 |
| N | -1.016388 | 1.178247 | 3.341304 |

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**TS(B-C)$^{L10}$**

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Number of imaginary frequencies : 4 Electronic energy : HF=-3866.2917166

Zero-point correction= 1.325937 (Hartree/Particle)

Thermal correction to Energy= 1.413713

Thermal correction to Enthalpy= 1.414658

Thermal correction to Gibbs Free Energy= 1.180826

Sum of electronic and zero-point Energies= -3864.965779

Sum of electronic and thermal Energies= -3864.878003

Sum of electronic and thermal Enthalpies= -3864.877059

Sum of electronic and thermal Free Energies= -3865.110890

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Cartesian Coordinates

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| | | | |
|---|---|---|---|
| N | -9.840233 | -5.191691 | 0.166919 |
| C | -8.940928 | -5.053016 | -0.970489 |
| C | -9.390700 | -4.244564 | 1.178149 |
| C | -8.356821 | -3.292996 | 0.539875 |
| C | -7.736860 | -4.185221 | -0.546959 |
| H | -8.930089 | -4.830025 | 1.993892 |
| H | -10.255493 | -3.738759 | 1.627263 |
| H | -6.949786 | -4.816195 | -0.117329 |
| H | -7.296789 | -3.623326 | -1.375639 |
| H | -9.510167 | -4.562607 | -1.780387 |
| H | -8.671001 | -6.045012 | -1.356160 |
| C | -3.842270 | -1.347098 | 5.479279 |
| C | -2.784419 | -0.574491 | 4.701596 |
| O | -2.404694 | -1.342972 | 3.566101 |
| H | -4.732396 | -1.510518 | 4.862420 |
| H | -3.183821 | 0.404138 | 4.402438 |
| H | -1.916485 | -0.378487 | 5.350214 |
| H | -1.805261 | -0.810565 | 3.016167 |
| H | -4.140294 | -0.793316 | 6.376103 |
| H | -3.457954 | -2.325502 | 5.785920 |

| | | | |
|---|---|---|---|
| C | 3.669361 | -2.329707 | 7.249813 |
| C | 4.753698 | -2.142572 | 6.183997 |
| C | 4.531083 | -2.899206 | 4.854522 |
| O | 5.404274 | -2.815410 | 3.973903 |
| O | 3.439731 | -3.581160 | 4.768873 |
| H | 2.699979 | -1.971638 | 6.891068 |
| H | 4.871258 | -1.080364 | 5.932363 |
| H | 5.733133 | -2.456971 | 6.567245 |
| H | 3.916911 | -1.783194 | 8.168447 |
| H | 3.546062 | -3.387729 | 7.498371 |
| N | 7.681772 | -2.347270 | -0.996043 |
| C | 6.691251 | -1.841207 | -0.049898 |
| C | 5.889689 | -0.672408 | -0.680218 |
| O | 5.913639 | 0.443882 | -0.167768 |
| C | 8.937890 | -2.449105 | -0.267860 |
| C | 8.626559 | -2.388630 | 1.240250 |
| C | 7.379090 | -1.492538 | 1.284381 |
| H | 9.561914 | -1.588380 | -0.571077 |
| H | 9.483103 | -3.345611 | -0.591504 |
| H | 9.459536 | -1.999831 | 1.833647 |
| H | 8.391205 | -3.390403 | 1.617704 |
| H | 7.645738 | -0.431765 | 1.279882 |
| H | 6.740327 | -1.688497 | 2.150387 |

| | | | |
|---|---|---|---|
| H | 5.965832 | -2.658665 | 0.110838 |
| N | 5.141244 | -0.893482 | -1.805473 |
| C | 4.864488 | -2.103470 | -2.590997 |
| C | 3.991884 | -3.170341 | -1.881153 |
| C | 2.944148 | -2.597402 | -0.917367 |
| C | 1.978740 | -3.669696 | -0.375507 |
| N | 1.300806 | -3.292033 | 0.857426 |
| C | 1.836951 | -3.482836 | 2.086529 |
| N | 2.918095 | -4.237948 | 2.304971 |
| N | 1.202189 | -2.971772 | 3.152295 |
| H | 4.607841 | -0.069119 | -2.052057 |
| H | 5.812990 | -2.552205 | -2.900058 |
| H | 3.509363 | -3.776304 | -2.660689 |
| H | 4.641055 | -3.862552 | -1.328681 |
| H | 3.442358 | -2.120231 | -0.068642 |
| H | 2.360837 | -1.804734 | -1.400134 |
| H | 1.209449 | -3.896721 | -1.121960 |
| H | 2.504479 | -4.614959 | -0.198506 |
| H | 0.637823 | -2.517556 | 0.816554 |
| H | 1.750964 | -2.972839 | 4.016153 |
| H | 4.351036 | -1.752519 | -3.489139 |
| C | -2.467535 | 2.168409 | -2.923397 |
| O | -2.034046 | 2.866614 | -1.795729 |

| | | | |
|---|---|---|---|
| H | -1.643845 | 1.860813 | -3.590040 |
| H | -3.132991 | 2.822546 | -3.511159 |
| H | -3.038153 | 1.257994 | -2.675223 |
| C | -0.334907 | -0.723466 | -2.270343 |
| C | 1.583498 | 3.730362 | -2.258525 |
| C | -1.466185 | 5.111184 | 1.213763 |
| C | -3.499705 | 0.738386 | 1.087305 |
| C | 0.468678 | 0.375835 | -2.587816 |
| C | 1.459655 | 0.421875 | -3.657993 |
| C | 1.994697 | 1.685965 | -3.634972 |
| C | 1.323685 | 2.399726 | -2.568662 |
| C | 3.034199 | 2.276615 | -4.541965 |
| C | 1.804952 | -0.647264 | -4.657039 |
| C | 1.017724 | -0.560029 | -6.005271 |
| C | -0.305900 | -1.273628 | -5.901095 |
| O | -0.152233 | -2.591206 | -5.857325 |
| O | -1.392474 | -0.704503 | -5.818479 |
| C | 0.952753 | 4.494253 | -1.281768 |
| C | 1.260784 | 5.886407 | -1.012476 |
| C | 0.409265 | 6.278937 | -0.003380 |
| C | -0.416250 | 5.112111 | 0.302775 |
| C | 2.270301 | 6.711379 | -1.749795 |
| C | 0.261828 | 7.582234 | 0.631579 |

| | | | |
|---|---|---|---|
| C | 1.208596 | 8.521374 | 0.793110 |
| C | -2.330521 | 4.049990 | 1.452341 |
| C | -3.462605 | 4.111769 | 2.358319 |
| C | -4.053049 | 2.869044 | 2.320332 |
| C | -3.262710 | 2.076638 | 1.379299 |
| C | -3.896366 | 5.324476 | 3.122392 |
| C | -5.245691 | 2.383842 | 3.003070 |
| C | -5.736970 | 2.802434 | 4.181523 |
| C | -2.782586 | -0.049790 | 0.195335 |
| C | -3.079491 | -1.450016 | -0.038008 |
| C | -2.205392 | -1.876508 | -0.999721 |
| C | -1.362419 | -0.729241 | -1.328121 |
| C | -4.111762 | -2.235367 | 0.712432 |
| C | -2.162018 | -3.264251 | -1.575046 |
| C | -3.284589 | -3.568790 | -2.623133 |
| C | -2.875641 | -3.016419 | -3.960247 |
| O | -3.194563 | -1.750479 | -4.152181 |
| O | -2.215267 | -3.692011 | -4.755962 |
| N | 0.417670 | 1.582814 | -1.942437 |
| N | -0.043742 | 4.046644 | -0.458544 |
| N | -2.236267 | 2.812320 | 0.877039 |
| N | -1.734404 | 0.355878 | -0.579039 |
| Fe | -0.893931 | 2.183202 | -0.507699 |

| | | | |
|---|---|---|---|
| H | 3.499403 | 1.515075 | -5.174766 |
| H | 3.835176 | 2.766023 | -3.975921 |
| H | 2.605997 | 3.035374 | -5.209341 |
| H | 3.272050 | 6.639319 | -1.304640 |
| H | 1.986933 | 7.768350 | -1.737963 |
| H | 2.358692 | 6.398437 | -2.794991 |
| H | -4.976139 | 5.302591 | 3.299892 |
| H | -3.662756 | 6.245913 | 2.580022 |
| H | -3.407437 | 5.392003 | 4.103663 |
| H | -3.902848 | -2.187377 | 1.787858 |
| H | -4.114885 | -3.287537 | 0.412831 |
| H | -5.124180 | -1.844372 | 0.546990 |
| H | 0.975165 | 9.469863 | 1.267656 |
| H | 2.238580 | 8.370501 | 0.488000 |
| H | -6.651118 | 2.376961 | 4.584651 |
| H | -5.238812 | 3.550392 | 4.788811 |
| H | 1.602474 | -1.052114 | -6.789641 |
| H | 0.844530 | 0.480934 | -6.281475 |
| H | 1.671633 | -1.651730 | -4.242701 |
| H | 2.868703 | -0.562615 | -4.905716 |
| H | -4.227390 | -3.128834 | -2.291165 |
| H | -3.398546 | -4.650063 | -2.733099 |
| H | -2.279213 | -3.990072 | -0.762879 |

| | | | |
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| H | -1.191810 | -3.485025 | -2.033847 |
| H | -0.171006 | -1.635864 | -2.835240 |
| H | 2.354428 | 4.220975 | -2.841702 |
| H | -1.640562 | 6.022749 | 1.772536 |
| H | -4.306892 | 0.250737 | 1.619574 |
| H | -0.733191 | 7.807220 | 1.014896 |
| H | -5.789556 | 1.592177 | 2.488292 |
| H | -1.019223 | -3.029533 | -5.602015 |
| H | -2.668283 | -1.375494 | -4.915025 |
| H | -7.626786 | -2.905301 | 1.255616 |
| H | -8.865342 | -2.434851 | 0.084419 |
| H | 0.513754 | -2.245772 | 2.981907 |
| C | 0.507184 | 1.548904 | 1.055352 |
| C | 0.728544 | 0.114169 | 1.344118 |
| C | 2.842290 | 1.021564 | 1.483697 |
| H | 3.763264 | 0.870747 | 0.918173 |
| C | 1.922060 | 2.117195 | 0.929350 |
| H | 3.095878 | 1.167961 | 2.540387 |
| H | 2.025722 | 3.063837 | 1.465645 |
| H | 2.159995 | 2.303617 | -0.117468 |
| O | -0.093490 | -0.774031 | 1.595088 |
| O | 2.056923 | -0.198594 | 1.400383 |
| H | 3.558750 | -4.385900 | 1.542607 |

| | | | |
|---|---|---|---|
| H | 3.320990 | -4.112743 | 3.296282 |
| N | -0.034733 | 2.132768 | 2.575895 |
| N | -0.718456 | 1.577759 | 3.320355 |

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