Electronic Supporting Information

for

Unveiling the Importance of Catalyst Framework and Non Covalent Interactions in an Asymmetric Fe-Catalyzed O–H Insertion: Insights from Computational Tools

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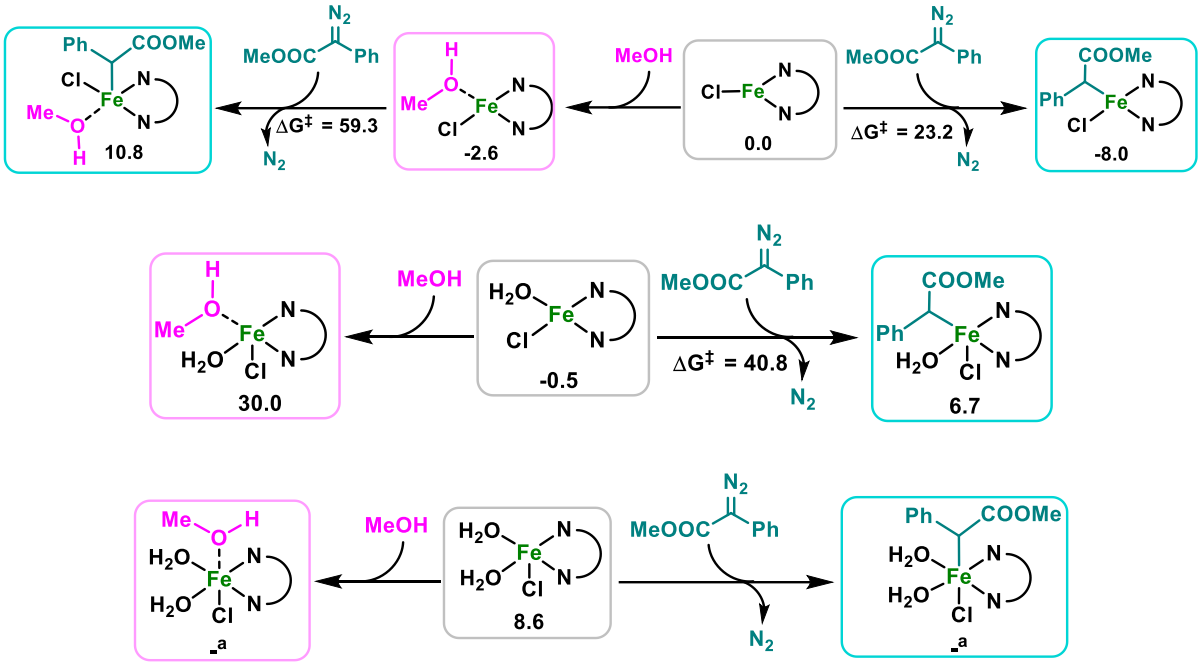
Computational Details

Geometry optimizations were performed with the (U)B3LYP[1] functional augmented with D3(BJ) empirical dispersion correction in G16 software.[2] For geometry optimization in the gas phase, the standard split valence 6-31G(d,p) basis set was used for all atoms except Fe, for which, LANL2DZ was used[3] (BS1 = (U)B3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe)). Harmonic vibrational frequency calculations were conducted for all stationary points to confirm whether they are local minima or transition state structures at the same level of theory and to determine the thermal corrections for the enthalpies, free energies and entropies.[4] Further, the transition states were characterized by intrinsic reaction coordinate (IRC) analysis, to ensure the stationary points were connected to each other.[5] For single-point energy calculations, solvent effects were taken into account using the SMD continuum solvation model in chloroform.[6] Single-point energy calculations were carried out at the 6-311+G(3df,3pd) basis set for all atoms other than Fe, for which SDD[7] basis set consisting of Stuttgart–Dresden effective core potential (ECP) was used on the (U)B3LYP-D3(BJ)/6-31G(d,p)-optimized stationary points (BS2 = (U)B3LYP-D3(BJ)/6-311++G(3df,3pd),SDD(Fe)). Further for the tautomerization step, the lowest diastereomeric TSs were optimized in the solvent phase to ensure the correct energy difference at the $SMD_{(chloroform)}$/(U)B3LYP-D3(BJ)//6-311+G(3df,3pd)//$SMD_{(chloroform)}$/(U)B3LYP-D3(BJ)/6-31G(d,p) using the G09 program.[8] Additional single point calculations were also done at the ωB97M-V/def2-QZVPP functional to ensure the trend of the free energy profile is not changing appreciably.[9] The high-Level ab initio DLPNO-CCSD(T) calculations and ωB97M-V calculations were performed using the ORCA 5.0.4 software.[10] Gibbs free energies are reported using GoodVibes package wherein Truhlar-type quasi harmonic corrections are incorporated, where entropy terms for lower frequencies (<100cm^{-1}) were calculated from free-rotor approximation.[11] The energy decomposition analysis (EDA) was performed using the Amsterdam Density Functional (ADF) software, employing the unrestricted fragment approach at the B3LYP-D3(BJ) functional with a triple-ζ basis set, excluding solvent effects.[12] Analyses of electron densities was performed using AIMAll software which operates based on Bader's AIM (Atoms-in-Molecule) framework.[13]



Scheme 1 Different possible active species for $Fe(Cl_2).4H_2O$/L1* catalyzed O–H insertion reaction and comparison of preference of attack between two reactants (diazo and methanol). The relative free energy barriers (ΔG) are given in kcal/mol. [a]Substrate is going away from the catalyst.

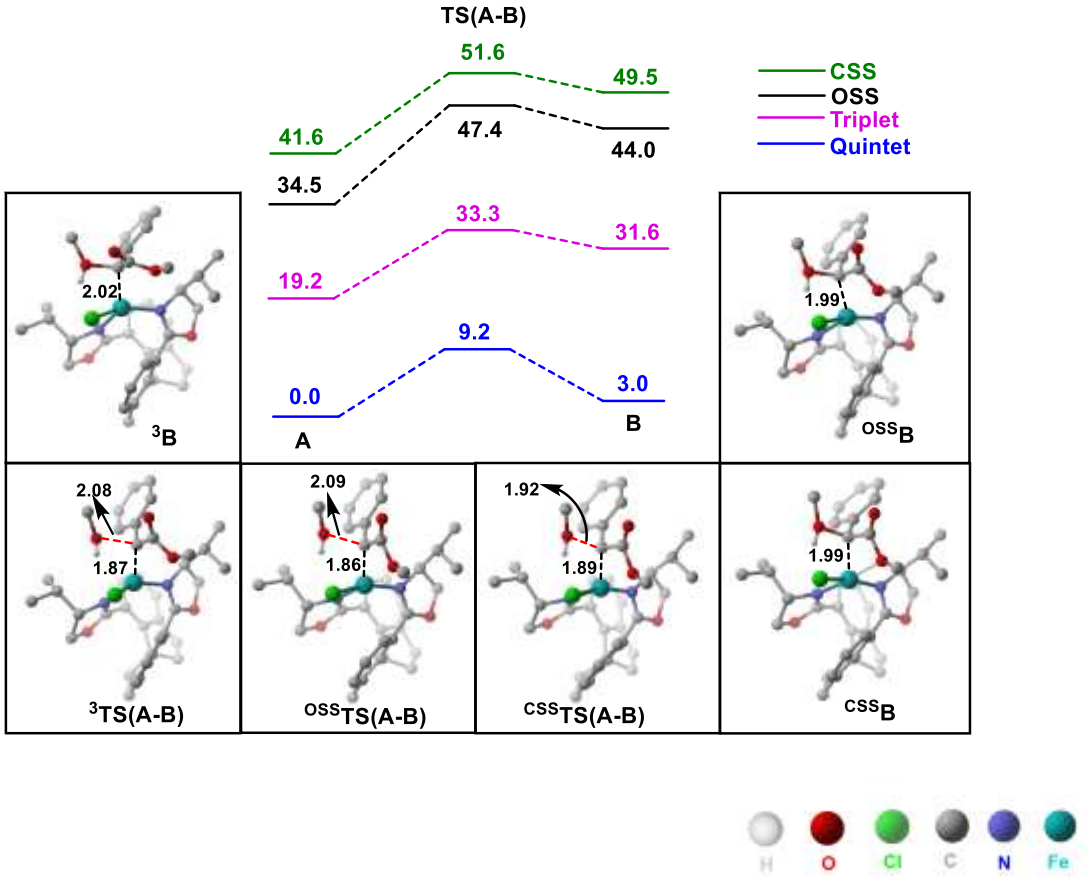


Fig. S1 Free energy profile for the metal-ylide formation at different spin states at the $SMD_{(chloroform)}$/(U)B3LYP-D3(BJ)/6-311++G(d,p),SDD(Fe)//BS1. Distances are in Å. Hydrogens are omitted for clarity. OSS = Open-shell singlet and CSS = closed-shell singlet.

The HAT (hydrogen atom transfer) pathway via **TS(A-H)** is 23.8 kcal/mol higher in energy than the nucleophilic pathway. Also, an alternative pathway where methanol first attacks Fe via **TS(A-E)**, which is then followed by a migratory insertion through **TS(E-B)** to yield **B** is 3.2 kcal/mol higher than **TS(A-B)** as seen in Fig. S2.

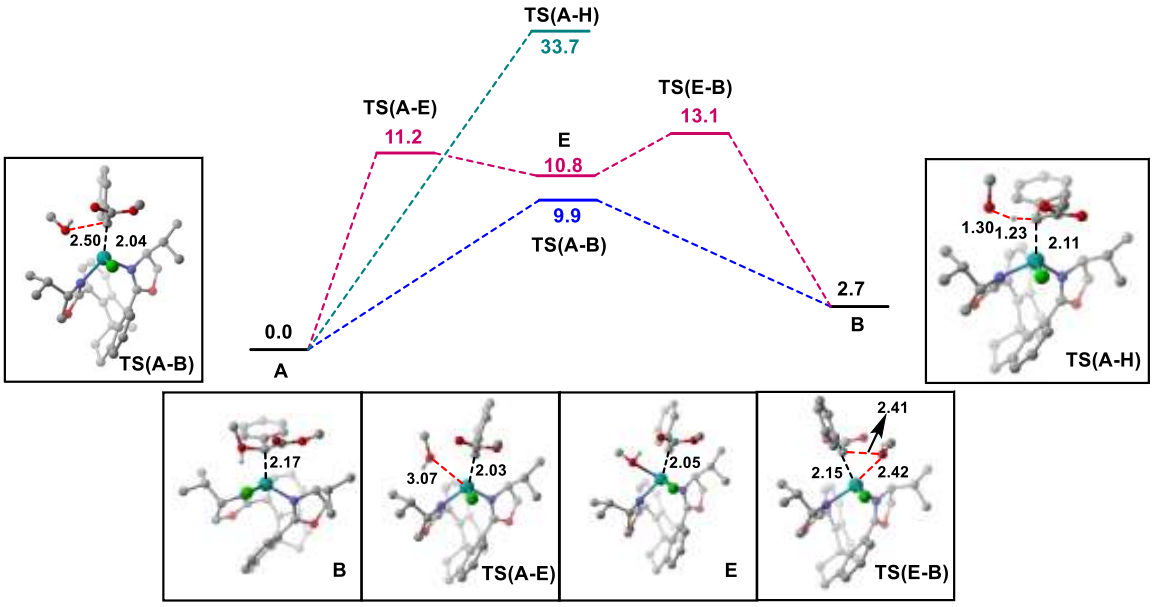


Fig. S2 Free energy profile for the different possible pathways from metallocarbene, **A** to form metal-ylide, **B** for the quintet spin state. Distances are in Å. Hydrogens are omitted for clarity.

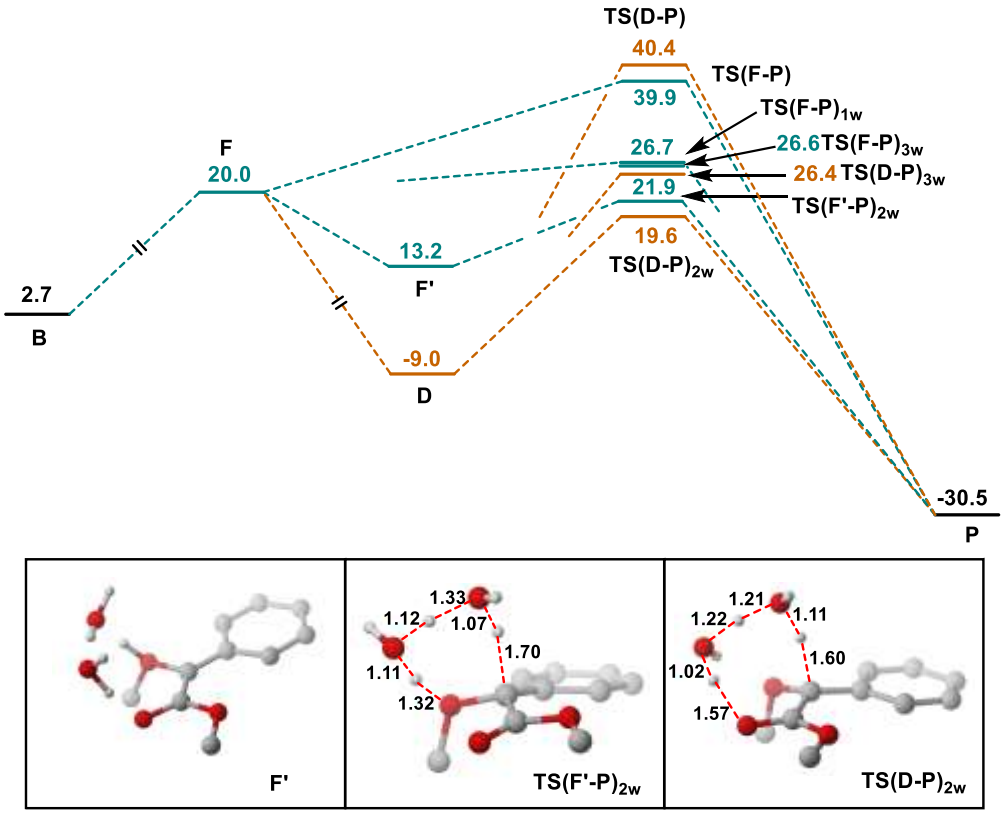


Fig. S3 Free energy profile for the metal free pathway. Distances are in Å. Hydrogens are omitted for clarity.

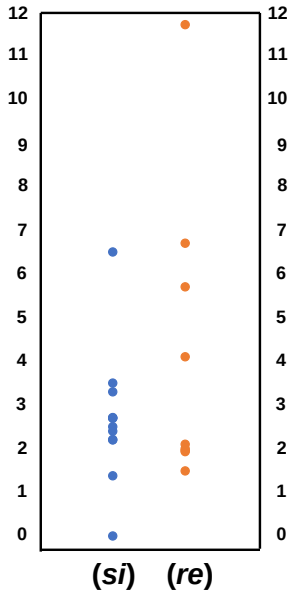


Fig. S4 Activation free energies (kcal/mol) of all possible conformers for **(*R*)-TS(D$_f$-P)$_{3w}$** (from *si*-face) and **(*S*)-TS(D$_f$-P)$_{3w}$** (from *re*-face) at the SMD$_{(chloroform)}$/UB3LYP-D3(BJ)/6-311++G(d,p),SDD(Fe)//BS1.

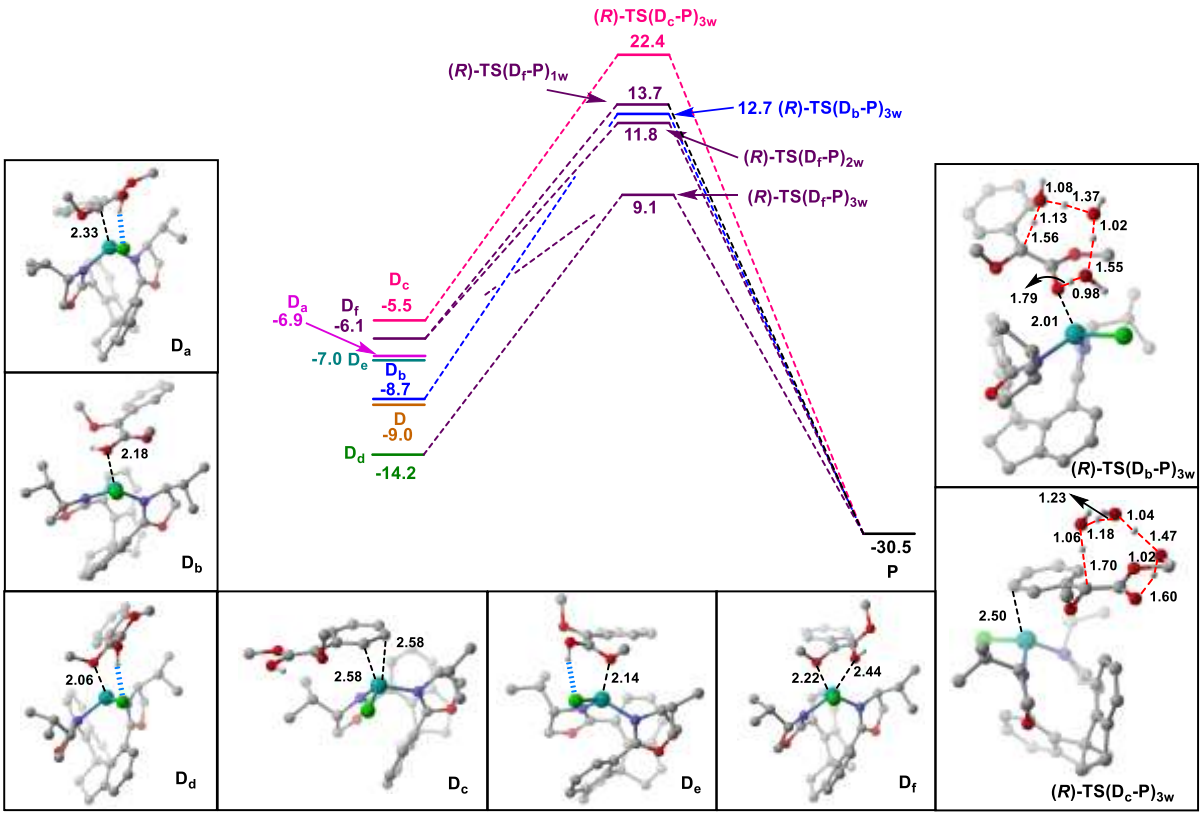
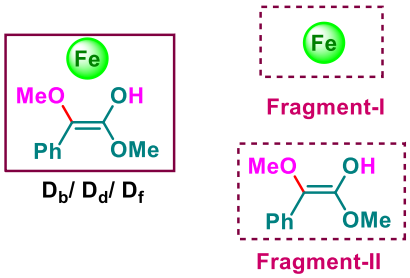


Fig. S5 Free energy profile for the [1,3]-proton transfer from all possible enols. All the free energy are reported in kcal/mol.

Table S1 Distortion-Interaction Analysis for Different Enols

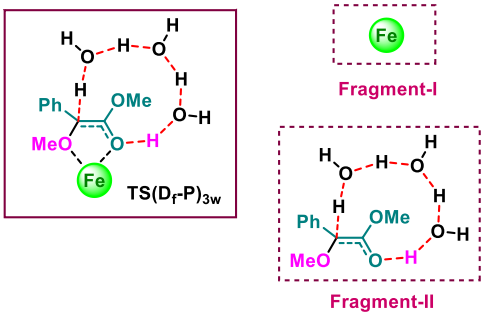


	Distortion energy		Interaction energy
	Fragment-I	**Fragment-II**	
D_b	0.9	1.5	-19.4
D_d	2.4	4.7	-29.8
D_f	3.8	8.1	-26.7

Table S2 Energy Decomposition Analysis for **D_b** and **D_d** enol

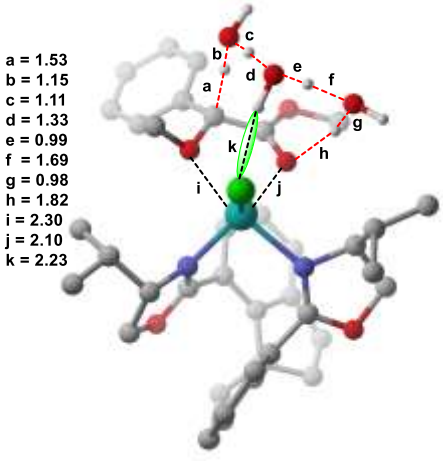
	D_b	D_d
Total Pauli Repulsion	70.58	105.13
Electrostatic Interaction	-51.99	-77.52
Orbital Interaction	-33.53	-40.4
Dispersion Energy	-17.9	-21.9
Total Bonding Energy	-32.84	-34.3

Table S3 Distortion-Interaction Analysis for two lowest diastereomeric TSs for L1*[a]

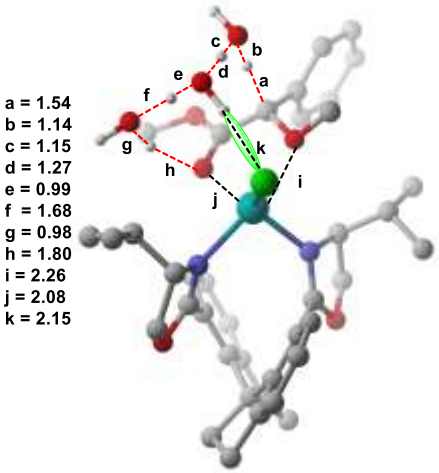


	Distortion energy		Interaction energy
	Fragment-I	**Fragment-II**	
(*R*)-TS(D_f-P)$_{3w}$	11.4	1.5	-47.4
(*S*)-TS(D_f-P)$_{3w}$	11.4	2.5	-45.0

[a]Geometry optimizations at the SMD$_{(chloroform)}$/UB3LYP-D3(BJ)/6-311++G(3df,3pd),SDD(Fe)//SMD$_{(chloroform)}$/UB3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe) level of theory.

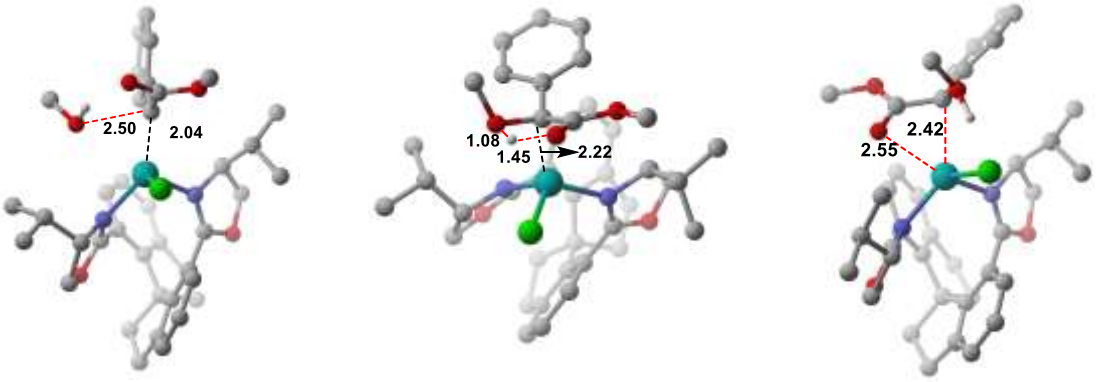


(*R*)-TS(D_f-P)$_{3w}$ (0.0, 0.0)

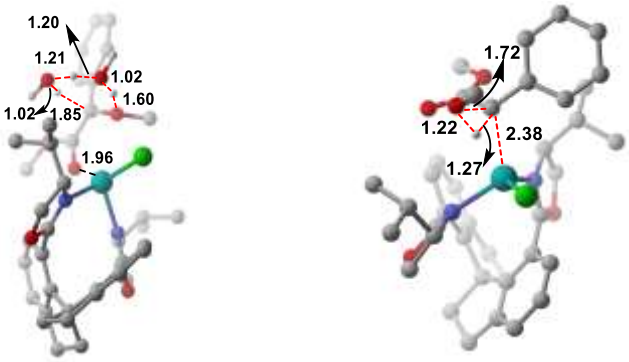


(*S*)-TS(D_f-P)$_{3w}$ (1.8, 1.7)

Fig. S6 Optimized geometries of lowest energy diastereomeric TSs for the Fe/L1* system for the quintet spin state. The H-bonding interaction of the water molecule with the chloride is shown in the green circle. All distances are in Å. Relative free energies (kcal/mol) are reported at the $SMD_{(chloroform)}$/BS2//BS1 with or without Truhlar's Quasi Harmonic correction respectively.



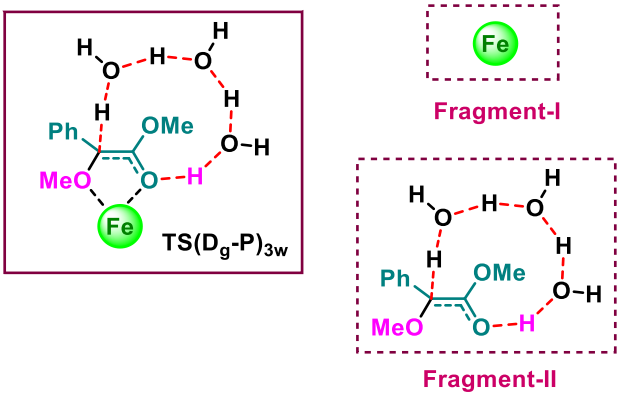
TS(A-B) **TS(B-D)** **TS(B-C)**



TS(C-P)$_{2w}$ **TS(B-P)**

Fig. S7 Optimized geometries of key TSs for the quintet spin state for the Fe/L1* system. Distances are in Å.

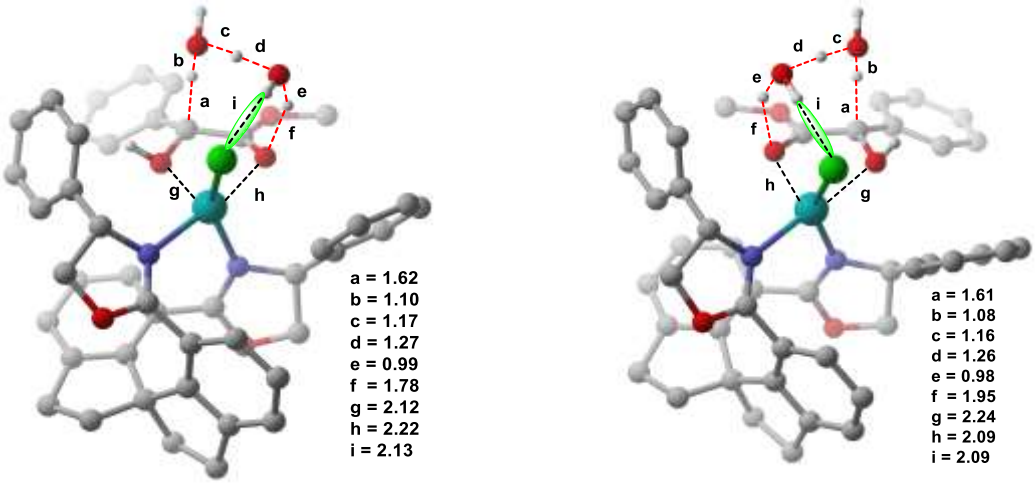
Table S4 Distortion-Interaction Analysis for two lowest diastereomeric TSs for L3*



	Distortion energy		Interaction energy
	Fragment-I	**Fragment-II**	
(*R*)-TS(D$_f$-P)$_{3w}$	5.6	2.4	-52.4
(*S*)-TS(D$_f$-P)$_{3w}$	5.7	2.6	-49.6

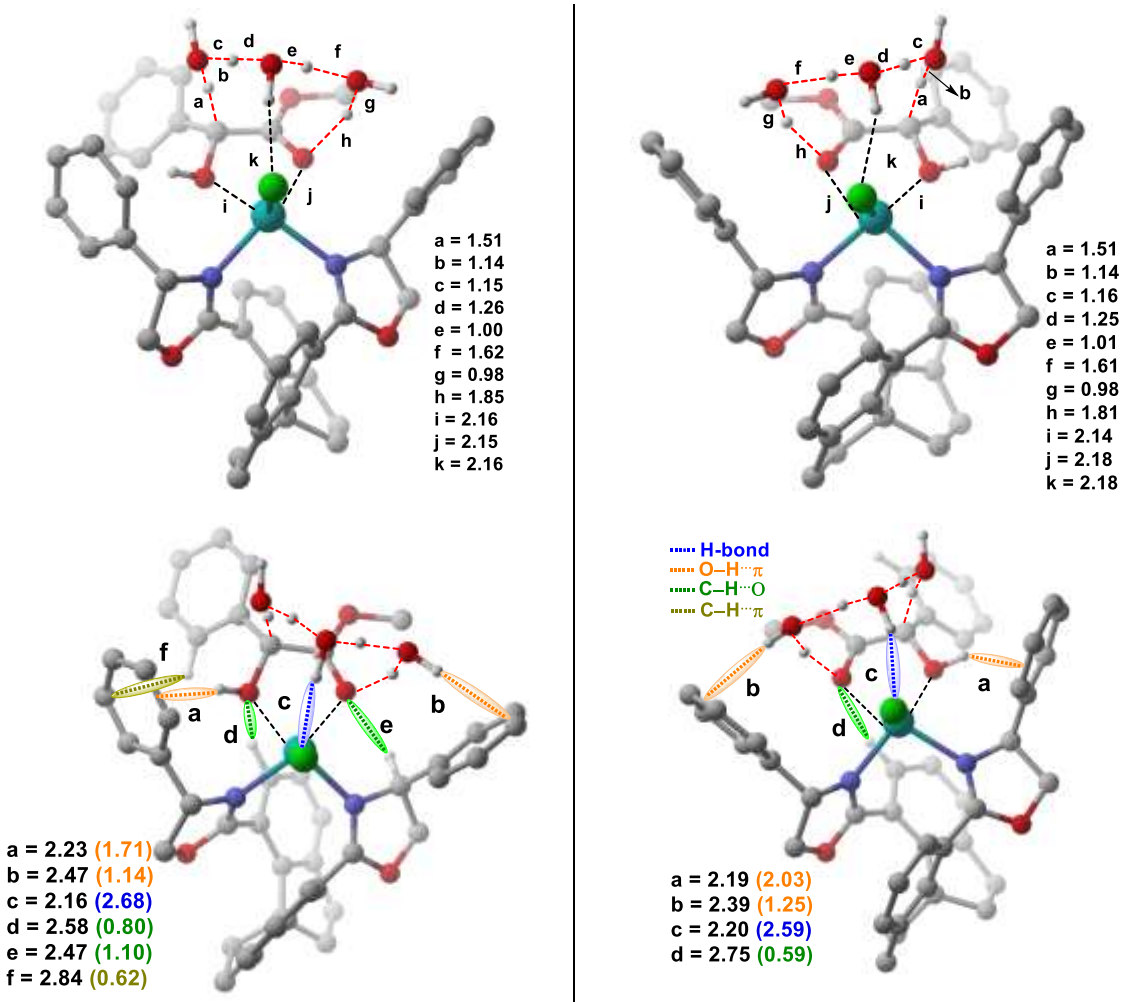
Table S5 Energy Decomposition Analysis for two lowest diastereomeric TSs for L3*

	(*R*)-TS(D$_f$-P)$_{3w}$	**(*S*)-TS(D$_f$-P)$_{3w}$**
Total Pauli Repulsion	117.07	106.31
Electrostatic Interaction	-108.96	-100.5
Orbital Interaction	-64.11	-58.14
Dispersion Energy	-26.78	-24.57
Total Bonding Energy	-82.78	-76.91



(*R*)-TS(D$_f$-P)$_{2w}$ (0.0, 0.0) **(*S*)-TS(D$_f$-P)$_{2w}$** (0.0, 0.2)

Fig. S8 Optimized geometries of two lowest diastereomeric TSs for the Fe/L2* system on the quintet surface at the SMD$_{(chloroform)}$/BS2//BS1 level of theory with or without Truhlar's Quasi Harmonic correction respectively. Distances are in Å. The H-bonding interaction of the water molecule with the chloride is shown in the green circle.

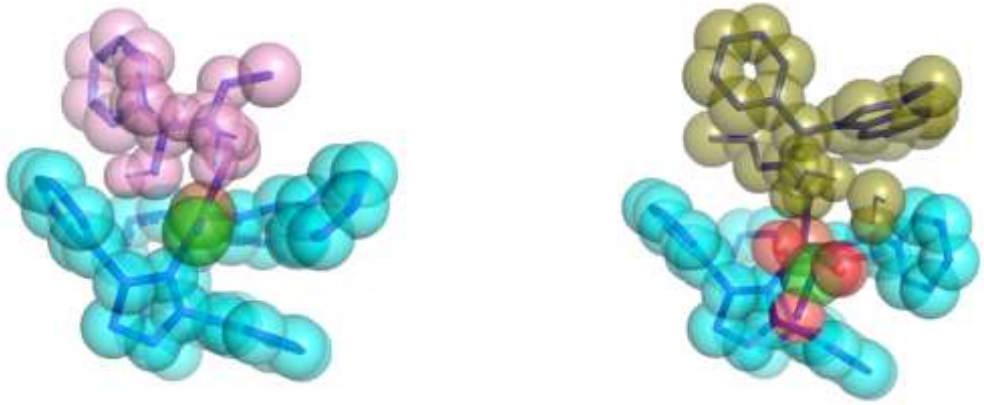


(*R*)-TS(D$_f$-P)$_{3w}$ (0.0, 0.0) **(*S*)-TS(D$_f$-P)$_{3w}$** (2.5, 1.8)

Fig. S9 Optimized geometries of two lowest diastereomeric TSs for the Fe/L3* system on the quintet surface at the SMD$_{(chloroform)}$/BS2//BS1 with or without Truhlar's Quasi Harmonic correction respectively. Distances are in Å. Given all the distances (Å) of non-covalent interactions with the electron densities (ρ x 10^{-2} au) in parenthesis at the bond critical points (*bcps*).

As can be seen from Fig. S8 and S9, the energy difference between two diastereomeric TSs for Fe/L3* and Fe/L2* is 2.0 and 0.0 kcal/mol, respectively. For Fe/L2*, an *ee* of ~30% is reported which is difficult to calculate due to calculation errors associated with computational methods. For the Fe/L3*, the energy difference is due to the stronger interaction between the substrate and the catalyst (-52.4 vs -49.6 kcal/mol) (Table S4 and S5), primarily electrostatic interactions, which can be seen from Fig. S9, where the **(*R*)-TS(D$_f$-P)$_{3w}$** has additional C–H···O (e) and C–H···π (f) interactions.

For the Fe-catalyzed O–H insertion reaction, the L2* ((*R*a,*S*,*S*)-Ph) yields low *ee*, in contrast, for the Fe/L2* catalyzed indole alkylation, the L2* showed moderate *ee* of 78%, while for L3* (L3* = (*Sa*,*S*,*S*)-Ph) very low *ee* was observed.[14] As can be seen from Fig. 4 of the main text, there is ample free space for the substrate in the case of L2*, illustrating the poor interaction of the substrate with the catalyst (Fig. S8). In the case of indole alkylation catalyzed by Fe/L2*, enol binds to Fe through its OH group only and van der Waals surface showed weaker interaction of enol with the chiral catalyst. However, in contrast to O–H insertion, the *ee* was not significantly low, possibly due to the bulky nature of the indole, which can provide moderate interactions with ligands, as seen from Fig. S10(b). Therefore, introducing strongly coordinating and slightly polarizable substituents on the substrate could be beneficial for achieving high *ee*.



(a) **(b)**

Fe(L2*)(Cl) **Fe(L2*)(ClO_4)**

Fig. S10 Space filling models for the lowest TSs for (a) O–H insertion and (b) indole alkylation catalyzed by Fe/L2*. The catalysts are in cyan and substrates along with the water molecules are in purple and olive respectively.

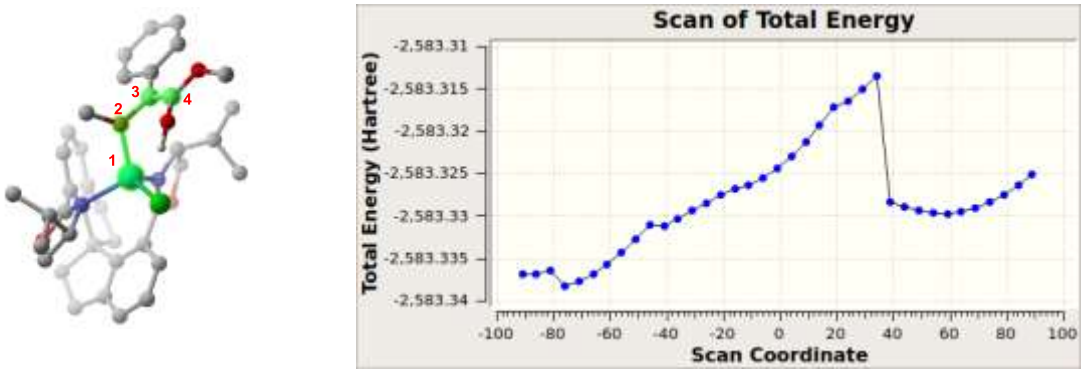


Fig. S11 Relaxed PES for the (*si*) to (*re*)-face conversion along Fe1-O2-C3-C4 dihedral angle at the $SMD_{(chloroform)}$/UB3LYP-D3(BJ)/6-311++G(d,p),SDD(Fe)//UB3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe).

Table S6 Relative Free Energies (ΔG) (kcal/mol) for Fe/L1* system at different level of theories for the quintet spin state

	X	Y	Z
A	0.0	0.0	0.0
TS(A-B)	10.2	9.9	8.6
B	3.9	2.7	-1.5
TS(B-D_a)	7.6	6.3	1.7
TS(B-D_a)$_{1w}$	9.2	8.8	-
TS(B-C)	15.1	14.1	7.3
(*R*)-TS(B-P)	35.9	35.2	33.0
C	-2.9	-1.8	-8.3
(*R*)-TS(C-P)$_{1w}$	19.6	21.3	11.9
(*R*)-TS(C-P)$_{2w}$	11.1	12.2	5.3
(*R*)-TS(C-P)$_{3w}$	12.3	13.8	7.4
D	-8.4	-9.0	-12.8
D_a	-5.9	-6.9	-11.8
D_b	-9.0	-8.7	-16.3
D_c	-5.5	-5.5	-10.8
D_d	-14.1	-14.2	-19.3
D_e	-6.5	-7.0	-13.3
D_f	-4.9	-6.1	-14.3
F	20.8	20.0	16.9

F'	12.2	13.2	11.9
(*R*)-TS(F-P)	40.6	39.9	36.4
(*R*)-TS(F-P)$_{1w}$	26.7	26.6	24.2
(*R*)-TS(F'-P)$_{2w}$	21.3	21.9	25.9
(*R*)-TS(F-P)$_{3w}$	25.9	26.6	25.9
(*R*)-TS(D-P)	41.2	40.4	35.9
(*R*)-TS(D-P)$_{1w}$	23.0	22.8	20.0
(*R*)-TS(D-P)$_{2w}$	19.1	19.5	18.4
(*R*)-TS(D-P)$_{3w}$	25.5	26.4	25.1
(*R*)-TS(D$_f$-P)$_{1w}$	13.3	13.6	3.4
(*R*)-TS(D$_f$-P)$_{2w}$	11.4	11.8	4.3
(*R*)-TS(D$_f$-P)$_{3w}$	9.1	9.9	3.6
(*S*)-TS(D$_f$-P)$_{3w}$	10.8	11.7	4.8
(*R*)-TS(D$_b$-P)$_{3w}$	11.3	12.7	8.3
(*R*)-TS(D$_c$-P)$_{3w}$	21.2	22.4	20.5
TS(A-E)	11.8	11.2	11.5
E	11.8	10.8	9.8
TS(E-B)	12.8	13.2	8.5
TS(A-H)	34.6	33.7	45.0

X = SMD$_{(chloroform)}$/UB3LYP-D3(BJ)/6-311++G(3df,3pd),SDD(Fe)//UB3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe), Y = relative free energies with Truhlar's type Quasi-Harmonic correction at 40˚C at the X level of theory and Z = SMD$_{(chloroform)}$/ωB97M-V/def2-QZVPP//B3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe).

Table S7 Relative Free Energies (ΔΔG) (kcal/mol) for Fe/L1* system for the **TS(D$_f$-P)$_{3w}$** at different level of theories[a]

X	**ΔΔG‡**
UB3LYP-D3(BJ)/6-311++G(d,p),SDD(Fe)	3.9
UB3LYP-D3(BJ)/6-311++G(3df,3pd),SDD(Fe)	4.1
UB3LYP-D3(BJ)/def2-QZVPP	0.9
DLPNO-CCSD(T)/def2-TZVP	0.4
ωB97M-V/def2-QZVPP	0.6

ΔΔG‡= (**(*S*)-TS(D$_f$-P)$_{3w}$** - **(*R*)-TS(D$_f$-P)$_{3w}$**). [a]SMD$_{(chloroform)}$/X//SMD$_{(chloroform)}$/BS1.

Table S8 Relative Free Energies (ΔΔG) (kcal/mol) for Fe/L2* system for the **TS(D_f-P)$_{3w}$** at different level of theories[a]

X	ΔΔG‡
UB3LYP-D3(BJ)/6-311++G(d,p),SDD(Fe)	0.0
UB3LYP-D3(BJ)/6-311++G(3df,3pd),SDD(Fe)	0.0
UB3LYP-D3(BJ)/def2-QZVPP	0.0
DLPNO-CCSD(T)/def2-TZVP	-0.7
ωB97M-V/def2-QZVPP	-0.6

[a]$SMD_{(chloroform)}$/X//BS1.

Table S9 Relative Free Energies (ΔΔG) (kcal/mol) for Fe/L3* system for the **TS(D_f-P)$_{3w}$** at different level of theories[a]

X	ΔΔG‡
UB3LYP-D3(BJ)/6-311++G(d,p),SDD(Fe)	2.5
UB3LYP-D3(BJ)/6-311++G(3df,3pd),SDD(Fe)	2.5
UB3LYP-D3(BJ)/def2-QZVPP	2.3
DLPNO-CCSD(T)/def2-TZVP	2.6
ωB97M-V/def2-QZVPP	2.3

[a]$SMD_{(chloroform)}$/X//BS1.

Table S10 Total Electronic Energies (a.u.) for Fe/L1* system at the $SMD_{(chloroform)}$/(U)B3LYP-D3(BJ)/6-311++G(d,p),SDD(Fe)//(U)B3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe)

	OSS	CSS	Triplet	Quintet
A	-2468.55960002	-2468.55438104	-2468.58088298	-2468.60857435
TS(A-B)	-2584.33828495	-2584.33402108	-2584.356233	-2584.38987754
B	-2584.34415141	-2584.33801518	-2584.3610567	-2584.40748532

Table S11 Total Electronic Energies (a.u.) for Fe/L1* system at the $SMD_{(chloroform)}$/UB3LYP-D3(BJ)/6-311++G(3df,3pd),SDD(Fe)//UB3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe) (**X**) and $SMD_{(chloroform)}$/ωB97M-V/def2-QZVPP//UB3LYP-D3(BJ)/6-31G(d,p),LANL2DZ(Fe) (**Y**) for the quintet spin state

	X	Y
A	-2468.7483122	-3607.71758412863
TS(A-B)	-2584.53666697	-3723.45720163005
B	-2584.55450885	-3723.48103093735
TS(B-D_a)	-2584.54665749	-3723.47397071063

TS(B-D_a)$_{1w}$	-2661.03391148	-
TS(B-C)	-2584.53469863	-3723.46504077925
(*R*)-TS(B-P)	-2584.49364072	-3723.4163200685
C	-2584.55780444	-3723.48434290164
(*R*)-TS(C-P)$_{1w}$	-2661.00985609	-3799.91490384779
(*R*)-TS(C-P)$_{2w}$	-2737.51663353	-3876.39376348508
(*R*)-TS(C-P)$_{3w}$	-2814.00550946	-3952.85599683064
D	-614.194583195	-613.974870591267
D_a	-2584.56875857	-3723.49602620879
D_b	-2584.57046795	-3723.49982052688
D_c	-2584.56626883	-3723.49265120653
D_d	-2584.57976031	-3723.5058386356
D_e	-2584.56862018	-3723.49734538962
D_f	-2584.56709013	-3723.49993027354
F	-614.147038946	-613.926626584258
F'	-767.138891884	-766.862546043662
(*R*)-TS(F-P)	-614.110335414	-766.847097538285
(*R*)-TS(F-P)$_{1w}$	-690.62385288	-690.37614750916
(*R*)-TS(F'-P)$_{2w}$	-767.122636023	-766.847097538285
(*R*)-TS(F-P)$_{3w}$	-843.606916415	-843.305084023709
(*R*)-TS(D-P)	-614.109264854	-613.891065254275
(*R*)-TS(D-P)$_{1w}$	-690.63179525	-690.384902555946
(*R*)-TS(D-P)$_{2w}$	-767.127781784	-766.852182817533
(*R*)-TS(D-P)$_{3w}$	-843.608824521	-843.307684549364
(*R*)-TS(D_f-P)$_{2w}$	-2737.51923736	-3876.39842472706
(*R*)-TS(D_f-P)$_{3w}$	-2814.01355823	-3952.86499604591
(*S*)-TS(D_f-P)$_{3w}$	-2814.01182286	-3952.86414221925
(*R*)-TS(D_b-P)$_{3w}$	-2814.00733213	-3952.8547735699
(*R*)-TS(D_c-P)$_{3w}$	-2813.99068928	-3952.83337989909
TS(A-E)	-2584.53368232	-3723.45202421803
E	-2584.53632179	-3723.45740178544
TS(E-B)	-2584.53258885	-3723.45720618624

TS(A-H)	-2584.49319987	-3723.39455679373
(*R*)-TS(D_f-P)$_{3w}$-L3*	-3001.01559286	-4139.8592477822
(*S*)-TS(D_f-P)$_{3w}$-L3*	-3001.0107181	-4139.85457273941
(*R*)-TS(D_f-P)$_{3w}$-L2*	-2924.51433925	-4063.38655919993
(*S*)-TS(D_f-P)$_{3w}$-L2*	-2924.51425746	-4063.38729615372

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Coordinates of optimized geometries

A

Number of imaginary frequencies: 0 Electronic energy: HF=-2467.5398886

Zero-point correction= 0.730978 (Hartree/Particle)
Thermal correction to Energy= 0.775585
Thermal correction to Enthalpy= 0.776529
Thermal correction to Gibbs Free Energy= 0.649239
Sum of electronic and zero-point Energies= -2466.808910
Sum of electronic and thermal Energies= -2466.764304
Sum of electronic and thermal Enthalpies= -2466.763360
Sum of electronic and thermal Free Energies= -2466.890650

Cartesian Coordinates

C	2.746151	1.266889	-1.086313
C	1.696687	0.578197	-1.712310
C	0.881960	1.259899	-2.628681
C	1.092211	2.614426	-2.889203
C	2.116568	3.309122	-2.239260
C	2.941920	2.628862	-1.344995
H	0.104473	0.715832	-3.154089
H	2.278413	4.363065	-2.445551
C	1.438162	-0.859064	-1.469829
C	3.789556	0.740026	-0.114720
C	4.397731	2.052213	0.481801
H	5.458888	1.927061	0.707741
H	3.886256	2.305441	1.409680
C	4.133712	3.150377	-0.575168
O	2.359928	-1.712938	-1.921059
C	0.541400	-2.862946	-0.925639
N	0.404549	-1.378790	-0.894143
C	3.245781	-0.219903	0.928838
C	2.050770	-0.136983	1.660661
C	1.687684	-1.196077	2.507195
C	2.515090	-2.311940	2.631257
C	3.712293	-2.388431	1.914723
C	4.068592	-1.342407	1.063068
H	0.756618	-1.149328	3.057633
H	4.355539	-3.257823	2.016112
C	1.127430	1.004290	1.532528
C	4.883617	-0.123933	-0.833726
H	5.722916	0.493922	-1.160639
H	4.453621	-0.597359	-1.716671
C	5.291432	-1.211767	0.185334
O	1.589860	2.225986	1.804081
C	-0.725792	2.280515	1.310156
H	-1.214511	2.527196	0.365168
N	-0.121422	0.932259	1.193406
C	0.517119	3.173933	1.513715
H	0.808384	3.717388	0.611877
H	0.448724	3.857176	2.359478
C	1.947749	-3.058630	-1.531198
H	2.678475	-3.419950	-0.805722
H	1.971770	-3.677560	-2.428269
H	2.217996	-3.122091	3.288447
H	4.986962	3.267535	-1.254998
H	3.952667	4.131332	-0.125742
H	6.150197	-0.893920	0.789968
H	5.574514	-2.152216	-0.296383

H	0.467849	3.124711	-3.615596
H	0.515307	-3.217940	0.106623
Fe	-1.053148	-0.731170	0.435505
Cl	-1.432429	-2.428699	1.885816
C	-2.886198	-0.129807	-0.128886
C	-3.330008	0.865960	-1.042728
C	-2.368042	1.609793	-1.775038
C	-4.707514	1.160592	-1.246183
C	-2.755201	2.595607	-2.665925
H	-1.318990	1.394110	-1.618605
C	-5.091933	2.146006	-2.141021
H	-5.458366	0.612923	-0.687474
C	-4.118701	2.862776	-2.850253
H	-2.009873	3.161006	-3.214687
H	-6.143253	2.365779	-2.291856
H	-4.425639	3.635505	-3.548362
C	-3.922898	-0.776352	0.706013
O	-4.277396	-0.233385	1.737279
O	-4.338545	-1.950686	0.244561
C	-5.158718	-2.729895	1.152880
H	-6.032337	-2.155766	1.464426
H	-5.452980	-3.611525	0.587411
H	-4.559593	-3.005577	2.022502
C	-1.785291	2.317825	2.427503
H	-2.531614	1.559252	2.162160
C	-2.485545	3.681637	2.438136
H	-3.299091	3.685085	3.167999
H	-1.799125	4.491484	2.711992
H	-2.914035	3.918943	1.457992
C	-1.212713	1.950257	3.799682
H	-0.770779	0.950054	3.793716
H	-0.450116	2.663353	4.133456
H	-2.008584	1.950916	4.548855
C	-0.633064	-3.502729	-1.688486
H	-1.535854	-3.208310	-1.136281
C	-0.528193	-5.030478	-1.626315
H	-1.401108	-5.493418	-2.094196
H	0.357602	-5.397582	-2.157739
H	-0.475081	-5.381600	-0.590989
C	-0.758791	-2.986367	-3.124749
H	-0.889149	-1.900040	-3.148309
H	0.120020	-3.237567	-3.729539
H	-1.626724	-3.436266	-3.614443

TS(A-B)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2924669
Zero-point correction= 0.785102 (Hartree/Particle)
Thermal correction to Energy= 0.832900
Thermal correction to Enthalpy= 0.833844
Thermal correction to Gibbs Free Energy= 0.700860
Sum of electronic and zero-point Energies= -2582.507365
Sum of electronic and thermal Energies= -2582.459567
Sum of electronic and thermal Enthalpies= -2582.458623
Sum of electronic and thermal Free Energies= -2582.591607
.....

Cartesian Coordinates

.....

C	-2.716576	-1.381830	-1.274648
C	-1.733375	-0.492387	-1.736544
C	-0.765635	-0.949414	-2.643328
C	-0.776600	-2.274238	-3.079654
C	-1.743140	-3.166460	-2.604888
C	-2.706035	-2.715042	-1.703237
H	-0.025598	-0.250776	-3.020113
H	-1.747471	-4.198416	-2.943571
C	-1.674051	0.910713	-1.283490
C	-3.850110	-1.135265	-0.289123
C	-4.272066	-2.587195	0.114366
H	-5.342845	-2.642901	0.322193
H	-3.739102	-2.887865	1.015145
C	-3.842781	-3.484341	-1.070165
O	-2.763864	1.653902	-1.490124
C	-1.055148	2.909100	-0.433577
N	-0.674346	1.489779	-0.705910
C	-3.471220	-0.242462	0.881966
C	-2.263562	-0.197874	1.595213
C	-2.062692	0.812498	2.548952
C	-3.074464	1.735202	2.813264
C	-4.290327	1.672822	2.124260
C	-4.474120	0.694551	1.147443
H	-1.115092	0.875445	3.070128
H	-5.074833	2.394158	2.334473
C	-1.203171	-1.199762	1.388496
C	-5.056658	-0.360833	-0.923065
H	-5.776727	-1.048774	-1.372150
H	-4.693790	0.305868	-1.705083
C	-5.655688	0.476761	0.230392
O	-1.553077	-2.479528	1.587479
C	0.754209	-2.285169	1.164395
H	1.325429	-2.433418	0.247027
N	0.034388	-0.989422	1.078573
C	-0.402505	-3.299333	1.237740
H	-0.620200	-3.768810	0.274622
H	-0.292800	-4.060331	2.009690
C	-2.542077	2.944706	-0.846060
H	-3.223338	2.999284	0.003765
H	-2.786307	3.716332	-1.575649
H	-2.909655	2.506493	3.558257
H	-4.655810	-3.604953	-1.797298
H	-3.551124	-4.490240	-0.753808
H	-6.444140	-0.074793	0.758115
H	-6.102036	1.412243	-0.118895
H	-0.038799	-2.608004	-3.802387
H	-0.948971	3.071202	0.641042
Fe	0.966096	0.771999	0.382476
Cl	1.203590	2.176135	2.157754
C	2.873405	0.144899	0.013626
C	3.431068	-0.764825	-0.933420
C	2.562208	-1.506686	-1.774518
C	4.831745	-0.969322	-1.065562
C	3.062108	-2.418807	-2.688814

H	1.494184	-1.350088	-1.686923
C	5.329501	-1.883527	-1.982180
H	5.515732	-0.400551	-0.444825
C	4.446523	-2.609116	-2.791551
H	2.386821	-2.986133	-3.320217
H	6.399405	-2.036017	-2.074366
H	4.839793	-3.325088	-3.506595
C	3.842676	0.884729	0.867286
O	4.313852	1.968739	0.547982
O	4.093162	0.256518	2.009791
C	4.805913	1.025040	3.014804
H	4.195686	1.883490	3.300010
H	4.937660	0.342496	3.851607
H	5.768206	1.357803	2.624312
C	1.735290	-2.294255	2.351055
H	2.405655	-1.442782	2.191995
C	2.582630	-3.571419	2.321688
H	3.339574	-3.546777	3.110223
H	1.974584	-4.468841	2.484518
H	3.100435	-3.685252	1.362632
C	1.040737	-2.088778	3.700768
H	0.501126	-1.138538	3.729282
H	0.334719	-2.895150	3.928767
H	1.781475	-2.069972	4.504907
C	-0.143327	3.905159	-1.168996
H	0.872437	3.689354	-0.827234
C	-0.496723	5.338063	-0.753947
H	0.192924	6.050258	-1.215464
H	-1.509082	5.617856	-1.068942
H	-0.431668	5.463515	0.331594
C	-0.172803	3.720886	-2.688501
H	0.073048	2.692544	-2.967907
H	-1.151694	3.965108	-3.116620
H	0.559565	4.379451	-3.163735
O	2.537488	2.157070	-1.444973
C	3.036146	1.958376	-2.761747
H	3.382584	2.901880	-3.198230
H	3.859681	1.233079	-2.781444
H	2.214275	1.575019	-3.369750
H	3.269969	2.428220	-0.851375

B

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3112762
Zero-point correction= 0.788017 (Hartree/Particle)
Thermal correction to Energy= 0.834385
Thermal correction to Enthalpy= 0.835329
Thermal correction to Gibbs Free Energy= 0.708609
Sum of electronic and zero-point Energies= -2582.523259
Sum of electronic and thermal Energies= -2582.476891
Sum of electronic and thermal Enthalpies= -2582.475947
Sum of electronic and thermal Free Energies= -2582.602668

.....

Cartesian Coordinates

.....

C	2.759979	-0.541835	1.551174

C	1.592871	0.235231	1.649499
C	0.600510	-0.123260	2.575781
C	0.790891	-1.217667	3.417747
C	1.962852	-1.977216	3.339369
C	2.934345	-1.643149	2.395792
H	-0.303381	0.469053	2.647435
H	2.107178	-2.829168	3.997768
C	1.353180	1.400339	0.780434
C	3.892564	-0.444554	0.537400
C	4.589604	-1.841064	0.668926
H	5.666007	-1.761327	0.501952
H	4.185367	-2.527015	-0.074264
C	4.236535	-2.345753	2.087838
O	2.298520	2.345122	0.742535
C	0.465781	2.920899	-0.632614
N	0.312397	1.601748	0.038487
C	3.406988	-0.119079	-0.868454
C	2.242787	-0.558094	-1.521373
C	1.890327	0.006027	-2.760082
C	2.717405	0.955397	-3.357919
C	3.895539	1.366202	-2.724595
C	4.223061	0.840949	-1.474398
H	0.975031	-0.306817	-3.250576
H	4.537273	2.106028	-3.194493
C	1.358037	-1.581331	-0.945835
C	4.908232	0.713948	0.820044
H	5.728004	0.373473	1.456460
H	4.401436	1.530817	1.332328
C	5.383746	1.191998	-0.572103
O	1.913629	-2.727416	-0.545685
C	-0.431343	-2.824907	-0.363289
H	-1.118779	-2.673629	0.472419
N	0.069351	-1.501196	-0.813881
C	0.865900	-3.511657	0.100797
H	1.029726	-3.438253	1.178040
H	0.979221	-4.542037	-0.232421
C	1.923052	3.295615	-0.299818
H	2.606045	3.139005	-1.136108
H	2.051973	4.296825	0.109481
H	2.440263	1.374782	-4.319207
H	5.000625	-2.051378	2.818428
H	4.153927	-3.435372	2.138317
H	6.283775	0.653244	-0.894496
H	5.628879	2.257821	-0.590044
H	0.019309	-1.472489	4.135656
H	0.335436	2.765639	-1.705105
Fe	-1.026261	0.216541	-0.730525
Cl	-1.704070	1.244468	-2.794088
C	-3.082348	0.302637	-0.037772
C	-2.953193	0.396115	1.444855
C	-2.949647	-0.747540	2.267635
C	-2.748871	1.647897	2.058666
C	-2.768807	-0.631951	3.644806
H	-3.105202	-1.722527	1.828824
C	-2.569090	1.753947	3.436308
H	-2.724043	2.544407	1.454187

C	-2.577785	0.614595	4.242149
H	-2.787313	-1.529696	4.255464
H	-2.420900	2.734571	3.877620
H	-2.441067	0.697758	5.315048
C	-3.932353	-0.707307	-0.719497
O	-4.647230	-0.456393	-1.672822
O	-3.793020	-1.957187	-0.222604
C	-4.669455	-2.939400	-0.820943
H	-4.398703	-3.104311	-1.865285
H	-4.527871	-3.846728	-0.237708
H	-5.705006	-2.601329	-0.768780
C	-1.180197	-3.544202	-1.503159
H	-2.009367	-2.881321	-1.773081
C	-1.762250	-4.867028	-0.989988
H	-2.420257	-5.314536	-1.739650
H	-0.974322	-5.597900	-0.777291
H	-2.340709	-4.723871	-0.071704
C	-0.318546	-3.754977	-2.752733
H	0.040887	-2.806172	-3.159492
H	0.548542	-4.393158	-2.550646
H	-0.906110	-4.244426	-3.534130
C	-0.601451	3.919685	-0.148621
H	-1.562390	3.417746	-0.314390
C	-0.573220	5.181813	-1.018136
H	-1.361829	5.876931	-0.716327
H	0.380141	5.714142	-0.921849
H	-0.720457	4.938702	-2.075059
C	-0.476662	4.250141	1.342840
H	-0.459534	3.347548	1.958830
H	0.429739	4.826280	1.555952
H	-1.324253	4.860923	1.668511
O	-3.477326	1.634307	-0.596343
C	-4.859564	2.137337	-0.465141
H	-4.823382	3.170690	-0.806751
H	-5.514792	1.518803	-1.071345
H	-5.096198	2.084288	0.595246
H	-3.096190	1.653837	-1.551047

TS(B-D)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.3029539
Zero-point correction= 0.786144 (Hartree/Particle)
Thermal correction to Energy= 0.832282
Thermal correction to Enthalpy= 0.833227
Thermal correction to Gibbs Free Energy= 0.706673
Sum of electronic and zero-point Energies= -2582.517249
Sum of electronic and thermal Energies= -2582.471111
Sum of electronic and thermal Enthalpies= -2582.470167
Sum of electronic and thermal Free Energies= -2582.596720

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Cartesian Coordinates

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C	2.835677	-0.592271	1.486618
C	1.660423	0.163580	1.636442
C	0.707896	-0.233723	2.588068
C	0.946575	-1.332949	3.409854

C	2.130195	-2.067794	3.282385
C	3.058004	-1.703770	2.307547
H	-0.206815	0.333092	2.691656
H	2.313467	-2.926795	3.921616
C	1.380096	1.355931	0.816241
C	3.923072	-0.471783	0.428865
C	4.616389	-1.873923	0.496702
H	5.679815	-1.801876	0.257809
H	4.153746	-2.547711	-0.223858
C	4.351653	-2.388345	1.930253
O	2.336051	2.290615	0.761307
C	0.434645	2.956967	-0.468662
N	0.299195	1.608587	0.148729
C	3.386675	-0.112345	-0.948616
C	2.193449	-0.524106	-1.567148
C	1.820197	0.050780	-2.794535
C	2.645076	0.991707	-3.408511
C	3.844443	1.383276	-2.804613
C	4.199656	0.840846	-1.569661
H	0.883184	-0.234768	-3.257752
H	4.482974	2.118995	-3.285319
C	1.295452	-1.522638	-0.965280
C	4.959237	0.670693	0.697802
H	5.794597	0.312598	1.303840
H	4.476588	1.485170	1.236754
C	5.395432	1.161668	-0.702319
O	1.832921	-2.682994	-0.572058
C	-0.505099	-2.715447	-0.331333
H	-1.171900	-2.544347	0.517591
N	0.014097	-1.407457	-0.798082
C	0.782841	-3.430959	0.112060
H	0.974338	-3.346731	1.183609
H	0.860291	-4.469200	-0.207727
C	1.919173	3.285555	-0.221582
H	2.541163	3.141063	-1.106800
H	2.101445	4.268635	0.211157
H	2.345462	1.422133	-4.358076
H	5.151048	-2.084018	2.617898
H	4.286333	-3.478951	1.982115
H	6.276215	0.614257	-1.061429
H	5.656397	2.223878	-0.713626
H	0.202523	-1.612950	4.147606
H	0.227880	2.856999	-1.536805
Fe	-1.054058	0.360430	-0.800494
Cl	-1.579571	1.130007	-2.886342
C	-3.103737	0.386324	0.043695
C	-2.924658	0.208406	1.499201
C	-2.526344	1.300779	2.294260
C	-3.079567	-1.044884	2.120689
C	-2.346325	1.159584	3.668412
H	-2.344930	2.261781	1.830415
C	-2.863890	-1.184699	3.490862
H	-3.384146	-1.901551	1.533751
C	-2.511436	-0.086046	4.276884
H	-2.058403	2.023477	4.259333
H	-2.995652	-2.159795	3.949698

H	-2.366395	-0.198424	5.346065
C	-3.951879	-0.431432	-0.825064
O	-4.569375	0.154233	-1.739341
O	-3.977075	-1.744118	-0.660731
C	-4.774597	-2.483140	-1.625282
H	-4.384146	-2.319416	-2.630494
H	-4.678315	-3.525217	-1.330617
H	-5.813274	-2.155400	-1.574949
C	-1.286410	-3.417773	-1.460343
H	-2.050097	-2.699254	-1.772706
C	-1.987966	-4.666312	-0.914181
H	-2.600717	-5.135857	-1.689067
H	-1.267195	-5.419840	-0.577207
H	-2.636373	-4.422449	-0.065593
C	-0.422633	-3.737539	-2.685242
H	0.036400	-2.836238	-3.099848
H	0.372594	-4.454188	-2.454599
H	-1.039542	-4.181200	-3.471599
C	-0.581626	3.943808	0.135615
H	-1.561699	3.468853	-0.002860
C	-0.580663	5.254753	-0.659159
H	-1.338341	5.942048	-0.272188
H	0.386155	5.766341	-0.587921
H	-0.792969	5.076671	-1.717899
C	-0.358526	4.186250	1.632996
H	-0.311614	3.249718	2.195795
H	0.569829	4.736133	1.819481
H	-1.172849	4.788222	2.047657
O	-3.595431	1.772044	-0.350837
C	-4.782113	2.288414	0.363747
H	-5.074996	3.184802	-0.180816
H	-5.570826	1.535703	0.343494
H	-4.489657	2.522812	1.381676
H	-4.005875	1.410702	-1.285834

TS(B-D)$_{1w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2659.7599847
Zero-point correction= 0.810346 (Hartree/Particle)
Thermal correction to Energy= 0.858503
Thermal correction to Enthalpy= 0.859447
Thermal correction to Gibbs Free Energy= 0.728658
Sum of electronic and zero-point Energies= -2658.949639
Sum of electronic and thermal Energies= -2658.901482
Sum of electronic and thermal Enthalpies= -2658.900538
Sum of electronic and thermal Free Energies= -2659.031327
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Cartesian Coordinates
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C	3.145988	-0.691939	1.203370
C	1.941566	-0.109349	1.629505
C	1.143532	-0.796243	2.557212
C	1.548316	-2.024599	3.072385
C	2.760012	-2.593630	2.665647

C	3.543799	-1.929328	1.723644
H	0.207636	-0.355640	2.868695
H	3.076335	-3.552640	3.065905
C	1.462477	1.194470	1.138968
C	4.099839	-0.227040	0.115773
C	4.908522	-1.529695	-0.203011
H	5.931078	-1.296618	-0.508346
H	4.427405	-2.068740	-1.018777
C	4.839896	-2.376811	1.087916
O	2.325138	2.218644	1.193394
C	0.204900	2.946168	0.486437
N	0.275952	1.473253	0.697774
C	3.403879	0.368988	-1.097307
C	2.199988	-0.021964	-1.709487
C	1.700271	0.733388	-2.781890
C	2.396184	1.850804	-3.240878
C	3.594414	2.237610	-2.634043
C	4.085840	1.499346	-1.557607
H	0.763029	0.452987	-3.244024
H	4.130808	3.112251	-2.990941
C	1.436664	-1.200115	-1.256804
C	5.060548	0.926649	0.557304
H	5.974058	0.531195	1.007532
H	4.564142	1.554335	1.296588
C	5.324211	1.746979	-0.726497
O	2.094513	-2.363518	-1.215548
C	-0.172811	-2.653810	-0.628601
H	-0.636437	-2.706507	0.359190
N	0.189709	-1.239547	-0.902434
C	1.201634	-3.351580	-0.623854
H	1.573308	-3.560563	0.380905
H	1.254945	-4.248189	-1.240407
C	1.688038	3.346509	0.520480
H	2.131857	3.418236	-0.475335
H	1.908975	4.241957	1.100195
H	1.992863	2.422985	-4.069400
H	5.680816	-2.154787	1.757336
H	4.867292	-3.452162	0.889614
H	6.212071	1.382494	-1.258817
H	5.492466	2.808026	-0.520081
H	0.913831	-2.540026	3.785568
H	-0.228244	3.130300	-0.499318
Fe	-1.040979	0.377820	-0.506169
Cl	-1.519236	1.623280	-2.400812
C	-1.173678	-3.176858	-1.676797
H	-2.056916	-2.538913	-1.579659
C	-1.584490	-4.616315	-1.345412
H	-2.387952	-4.947714	-2.009395
H	-0.751987	-5.316987	-1.474825
H	-1.939902	-4.702697	-0.314289
C	-0.654163	-3.046166	-3.112501
H	-0.446971	-2.003808	-3.368976
H	0.260152	-3.628211	-3.274146
H	-1.400875	-3.419651	-3.819406
C	-0.690671	3.596657	1.559824
H	-1.639194	3.049517	1.515603

C	-0.962543	5.061834	1.200921
H	-1.639389	5.520299	1.928252
H	-0.040820	5.654507	1.202935
H	-1.414892	5.146548	0.207622
C	-0.139996	3.444427	2.982143
H	0.023591	2.394266	3.241690
H	0.807951	3.976308	3.114071
H	-0.845635	3.859035	3.707933
C	-3.115557	0.213965	0.305279
C	-2.911690	-0.928819	1.241592
C	-2.301075	-0.662781	2.484359
C	-3.310424	-2.252447	0.975684
C	-2.095633	-1.675249	3.419054
H	-2.002816	0.354387	2.714739
C	-3.084069	-3.263467	1.908368
H	-3.804391	-2.488129	0.043867
C	-2.474473	-2.986899	3.133481
H	-1.637918	-1.435119	4.374296
H	-3.411351	-4.273518	1.681620
H	-2.316026	-3.776970	3.860022
C	-3.921809	0.145862	-0.912815
O	-4.599479	1.086654	-1.367202
O	-3.791828	-0.993418	-1.600450
C	-4.253809	-0.966520	-2.972874
H	-3.704859	-0.197919	-3.519301
H	-4.031039	-1.958557	-3.362154
H	-5.324704	-0.765728	-3.009259
C	-4.727243	1.364915	1.781024
H	-5.543653	1.211577	1.072451
H	-4.678039	0.549828	2.500937
O	-3.459512	1.428480	1.062714
H	-3.482977	2.453808	0.331778
O	-3.651597	3.226305	-0.515075
H	-4.060964	2.509908	-1.133791
H	-4.336538	3.876460	-0.298463
H	-4.833483	2.316705	2.303962

TS(B-C)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2957598
Zero-point correction= 0.786270 (Hartree/Particle)
Thermal correction to Energy= 0.832366
Thermal correction to Enthalpy= 0.833310
Thermal correction to Gibbs Free Energy= 0.706680
Sum of electronic and zero-point Energies= -2582.509490
Sum of electronic and thermal Energies= -2582.463394
Sum of electronic and thermal Enthalpies= -2582.462450
Sum of electronic and thermal Free Energies= -2582.589080

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Cartesian Coordinates

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C	2.100497	-1.649503	1.554092
C	1.475954	-0.409454	1.764085
C	0.259155	-0.363219	2.463614
C	-0.312887	-1.530654	2.969172
C	0.316242	-2.763324	2.773273

C	1.516835	-2.815068	2.064061
H	-0.209837	0.599152	2.627039
H	-0.129887	-3.672513	3.165527
C	1.979780	0.845659	1.175452
C	3.325653	-1.967700	0.705833
C	3.235222	-3.523304	0.541088
H	4.228573	-3.976478	0.538743
H	2.757748	-3.765623	-0.407503
C	2.351721	-4.023070	1.708812
O	3.256902	1.168268	1.365751
C	2.145785	2.757455	-0.021681
N	1.267114	1.652975	0.458282
C	3.311393	-1.197371	-0.605996
C	2.213187	-0.931604	-1.436418
C	2.361268	-0.039149	-2.509621
C	3.605403	0.537876	-2.769678
C	4.709384	0.243018	-1.962387
C	4.550913	-0.610800	-0.870892
H	1.506684	0.194215	-3.135078
H	5.675458	0.692118	-2.174635
C	0.905424	-1.589340	-1.235798
C	4.684706	-1.525543	1.349556
H	5.147834	-2.350375	1.895305
H	4.511848	-0.714046	2.055652
C	5.560335	-1.014112	0.179038
O	0.870179	-2.913256	-1.430604
C	-1.294634	-2.050391	-1.061942
H	-1.920933	-2.008940	-0.170800
N	-0.220967	-1.028466	-0.943630
C	-0.480859	-3.357060	-1.101722
H	-0.429246	-3.856935	-0.131125
H	-0.789706	-4.062385	-1.871648
C	3.498160	2.419269	0.657228
H	4.313479	2.244823	-0.044540
H	3.796633	3.151425	1.409060
H	3.712520	1.216924	-3.609228
H	2.958762	-4.317526	2.574217
H	1.747097	-4.893584	1.437480
H	6.209387	-1.807713	-0.211758
H	6.213843	-0.189187	0.477330
H	-1.243054	-1.474341	3.524826
H	2.219567	2.648331	-1.109531
C	-2.879288	0.963643	0.253672
C	-2.411730	1.662554	1.447103
O	-1.538452	2.546539	1.371404
O	-2.898775	1.242892	2.620701
C	-2.407589	1.909328	3.803112
H	-1.327726	1.786844	3.905758
H	-2.642713	2.973979	3.760594
Fe	-0.522479	0.905838	-0.289117
Cl	-0.941373	1.939871	-2.428698
C	-2.176661	-1.783754	-2.297897
H	-2.621627	-0.795713	-2.136494
C	-1.380143	-1.734871	-3.605244
H	-0.646399	-0.925792	-3.595425
H	-0.860646	-2.678951	-3.805238

H	-2.054649	-1.551797	-4.446096
C	-3.311615	-2.812754	-2.357130
H	-3.863779	-2.858747	-1.415588
H	-4.019914	-2.548643	-3.146919
H	-2.933792	-3.815970	-2.586246
C	1.657714	4.180713	0.301054
H	1.525879	4.239811	1.390857
C	2.731711	5.194173	-0.129593
H	2.397751	6.210911	0.092690
H	3.691840	5.051077	0.375365
H	2.905818	5.133270	-1.210157
C	0.331812	4.521375	-0.382149
H	0.425273	4.448085	-1.469920
H	-0.469873	3.860278	-0.060720
H	0.043970	5.548307	-0.135579
C	-3.934327	3.182421	-0.464522
H	-4.174408	3.656723	-1.415322
H	-4.838646	2.886897	0.064959
H	-3.290428	3.814297	0.146572
O	-3.226165	1.948173	-0.797785
H	-2.926730	1.433434	4.633109
C	-3.901520	-0.102906	0.306523
C	-4.995640	-0.136186	-0.573876
C	-3.775921	-1.146676	1.243575
C	-5.945887	-1.154908	-0.495924
H	-5.104033	0.630864	-1.331334
C	-4.727281	-2.159226	1.318754
H	-2.929087	-1.155124	1.918620
C	-5.824380	-2.167889	0.453512
H	-6.783952	-1.153057	-1.185824
H	-4.610925	-2.946880	2.057168
H	-6.566194	-2.957160	0.514138
H	-2.453872	2.067749	-1.492533

TS(B-P)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2537803
Zero-point correction= 0.781669 (Hartree/Particle)
Thermal correction to Energy= 0.829299
Thermal correction to Enthalpy= 0.830243
Thermal correction to Gibbs Free Energy= 0.698908
Sum of electronic and zero-point Energies= -2582.469095
Sum of electronic and thermal Energies= -2582.421465
Sum of electronic and thermal Enthalpies= -2582.420521
Sum of electronic and thermal Free Energies= -2582.551856

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Cartesian Coordinates

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C	3.027093	-1.183834	1.041136
C	2.034190	-0.351354	1.582008
C	1.231556	-0.826556	2.630420
C	1.447795	-2.105367	3.147619
C	2.444076	-2.931936	2.618420
C	3.220129	-2.469868	1.556694
H	0.455800	-0.190449	3.041969
H	2.609075	-3.922974	3.031335

C	1.848472	1.039078	1.111635
C	3.950120	-0.923275	-0.140923
C	4.471065	-2.357937	-0.490713
H	5.497827	-2.324519	-0.861384
H	3.848884	-2.796446	-1.270275
C	4.326876	-3.179875	0.811516
O	2.872200	1.869686	1.333218
C	1.074314	2.996924	0.280483
N	0.817056	1.547692	0.524254
C	3.261977	-0.219163	-1.300879
C	1.977042	-0.436374	-1.828155
C	1.492652	0.412519	-2.836296
C	2.284732	1.453825	-3.320600
C	3.567669	1.660529	-2.808367
C	4.047904	0.824138	-1.799249
H	0.499455	0.257100	-3.241367
H	4.182608	2.471286	-3.188202
C	1.074856	-1.461402	-1.275609
C	5.135124	0.046098	0.195745
H	6.017666	-0.510059	0.519005
H	4.845596	0.712396	1.007237
C	5.380954	0.870325	-1.089402
O	1.498734	-2.720638	-1.221209
C	-0.679404	-2.506985	-0.300379
H	-0.866278	-2.386979	0.768495
N	-0.110281	-1.229437	-0.798763
C	0.479783	-3.504964	-0.530723
H	0.928638	-3.867542	0.394716
H	0.224191	-4.342503	-1.179748
C	2.548442	3.147978	0.711261
H	3.230284	3.278341	-0.131377
H	2.720874	3.924546	1.455887
H	1.892360	2.103516	-4.095202
H	5.249180	-3.154285	1.405417
H	4.103402	-4.233606	0.620480
H	6.151291	0.410045	-1.720905
H	5.715820	1.889967	-0.876922
H	0.849095	-2.452222	3.983893
H	0.965146	3.174701	-0.791429
C	-2.805995	0.628422	0.620650
O	-3.131467	2.239289	1.120212
C	-4.145549	2.900420	0.335806
H	-2.284917	1.766295	0.386607
C	-2.370220	0.026373	1.919948
O	-1.726817	0.606576	2.770697
O	-2.718394	-1.274298	1.998353
C	-2.345124	-1.959502	3.211716
H	-2.578546	-1.345123	4.081997
H	-2.926609	-2.880144	3.214260
C	0.066071	3.886970	1.029741
H	-0.918907	3.624572	0.627391
C	0.045800	3.626690	2.538277
H	-0.264030	2.603641	2.760318
H	1.023455	3.811285	2.998941
H	-0.669287	4.297259	3.022885
C	0.324400	5.359866	0.690157

H	0.310407	5.529822	-0.391490
H	-0.444480	5.993513	1.140208
H	1.290919	5.703384	1.076642
C	-2.007639	-2.861758	-0.987934
H	-2.697662	-2.055656	-0.731639
C	-1.893448	-2.917248	-2.513178
H	-1.227275	-3.719567	-2.850290
H	-2.875890	-3.103224	-2.955402
H	-1.520398	-1.972584	-2.919947
C	-2.578691	-4.156087	-0.398436
H	-2.681448	-4.084397	0.689331
H	-3.569927	-4.356020	-0.813784
H	-1.949879	-5.024880	-0.624663
H	-1.277376	-2.183712	3.198942
C	-3.958603	0.069792	-0.112266
C	-5.080622	-0.414254	0.588526
C	-3.969929	0.030675	-1.516506
C	-6.168275	-0.942127	-0.097818
H	-5.094017	-0.379238	1.671840
C	-5.056261	-0.509749	-2.201690
H	-3.128002	0.427022	-2.070193
C	-6.155015	-0.998764	-1.495022
H	-7.027055	-1.310666	0.453633
H	-5.045112	-0.540741	-3.286248
H	-7.002904	-1.416857	-2.028325
H	-4.165726	3.919208	0.727858
H	-3.881866	2.915846	-0.724313
H	-5.114505	2.420579	0.482677
Fe	-0.727647	0.705864	-0.540877
Cl	-1.357201	2.258907	-2.088255

C

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3162651
Zero-point correction= 0.786155 (Hartree/Particle)
Thermal correction to Energy= 0.833474
Thermal correction to Enthalpy= 0.834418
Thermal correction to Gibbs Free Energy= 0.701089
Sum of electronic and zero-point Energies= -2582.530110
Sum of electronic and thermal Energies= -2582.482791
Sum of electronic and thermal Enthalpies= -2582.481847
Sum of electronic and thermal Free Energies= -2582.615176
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Cartesian Coordinates
.....

C	-3.283589	0.710338	-1.449400
C	-1.905338	0.683090	-1.714625
C	-1.413376	-0.217023	-2.672147
C	-2.281719	-1.050847	-3.375614
C	-3.657488	-1.005610	-3.128538
C	-4.148250	-0.129835	-2.161140
H	-0.349604	-0.248005	-2.866964
H	-4.333829	-1.652685	-3.679544
C	-0.937560	1.507835	-0.961992
C	-4.026937	1.472006	-0.361771
C	-5.414889	0.745945	-0.320270

H	-6.220558	1.448897	-0.098460
H	-5.410073	-0.012194	0.462508
C	-5.573475	0.063944	-1.698881
O	-1.113951	2.830336	-0.949729
C	0.775854	2.196079	0.345551
N	0.073589	1.055626	-0.296181
C	-3.290961	1.451889	0.969395
C	-2.601061	0.387807	1.573095
C	-1.887853	0.616119	2.759656
C	-1.881780	1.883919	3.341634
C	-2.580195	2.939777	2.748576
C	-3.275979	2.718634	1.560128
H	-1.338008	-0.195597	3.220067
H	-2.572525	3.924824	3.206317
C	-2.562134	-0.959748	0.969640
C	-4.182679	3.003888	-0.647823
H	-5.126893	3.215610	-1.154284
H	-3.373676	3.341223	-1.294702
C	-4.069061	3.700649	0.729019
O	-3.716131	-1.615279	0.831749
C	-1.893855	-2.905917	0.023849
H	-1.622383	-2.929855	-1.036718
N	-1.504606	-1.579841	0.556047
C	-3.433495	-2.887816	0.175094
H	-3.958592	-2.881468	-0.780803
H	-3.830179	-3.676465	0.815014
C	-0.080077	3.407528	-0.090217
H	-0.591530	3.895839	0.740006
H	0.458836	4.145065	-0.685878
H	-1.327186	2.044344	4.260038
H	-6.106398	0.710750	-2.407186
H	-6.134590	-0.873482	-1.643196
H	-5.056216	3.857820	1.181543
H	-3.592347	4.683033	0.662391
H	-1.885412	-1.731323	-4.122474
H	0.706285	2.046783	1.426586
C	3.935745	-0.957475	-0.096985
O	3.719702	-1.443154	1.248425
C	2.930101	-1.279953	-0.976917
O	1.794888	-1.831151	-0.633793
O	3.171866	-1.022316	-2.281299
C	2.136864	-1.213606	-3.246918
H	1.409637	-1.950339	-2.906047
H	1.644720	-0.256807	-3.449657
C	-1.148178	-4.041830	0.748921
H	-0.081722	-3.872674	0.540467
C	-1.347446	-4.002547	2.267279
H	-0.997376	-3.057624	2.691713
H	-2.399328	-4.136440	2.544094
H	-0.785157	-4.811082	2.742451
C	-1.534911	-5.397637	0.146508
H	-1.374749	-5.417816	-0.936754
H	-0.936991	-6.198567	0.589180
H	-2.587208	-5.636983	0.337288
C	2.263916	2.230209	-0.041890
H	2.670242	1.267212	0.284598

C	2.491238	2.343038	-1.551122
H	1.949158	1.564407	-2.094800
H	2.172539	3.315878	-1.942291
H	3.553687	2.225837	-1.777257
C	3.003528	3.324709	0.733726
H	2.852196	3.218754	1.813021
H	4.077307	3.262393	0.537957
H	2.669431	4.326823	0.439602
Fe	0.397879	-0.881349	0.326050
Cl	1.351690	-0.589678	2.527962
H	2.627531	-1.559854	-4.157184
C	3.895255	-2.881412	1.459073
H	3.174159	-3.415608	0.841201
H	4.921508	-3.108283	1.179162
H	3.723849	-3.054249	2.520989
C	5.129612	-0.128891	-0.226324
C	5.652239	0.253487	-1.479371
C	5.760872	0.366295	0.933615
C	6.745454	1.112479	-1.557095
H	5.201735	-0.125000	-2.385315
C	6.856442	1.220856	0.842541
H	5.385569	0.089675	1.911783
C	7.354383	1.605796	-0.402299
H	7.129390	1.390208	-2.534077
H	7.319863	1.588249	1.753066
H	8.207605	2.272452	-0.471568
H	2.864517	-1.089082	1.733780

TS(C-P)$_{1w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2659.728481
Zero-point correction= 0.808619 (Hartree/Particle)
Thermal correction to Energy= 0.857952
Thermal correction to Enthalpy= 0.858896
Thermal correction to Gibbs Free Energy= 0.721128
Sum of electronic and zero-point Energies= -2658.919862
Sum of electronic and thermal Energies= -2658.870529
Sum of electronic and thermal Enthalpies= -2658.869585
Sum of electronic and thermal Free Energies= -2659.007353

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Cartesian Coordinates

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C	-2.502661	-0.878739	-1.983610
C	-1.273853	-0.253546	-1.722867
C	-0.086112	-0.976681	-1.910729
C	-0.123920	-2.279063	-2.404553
C	-1.346928	-2.890459	-2.700647
C	-2.530071	-2.191130	-2.470462
H	0.856481	-0.520599	-1.640520
H	-1.373290	-3.906462	-3.083932
C	-1.174319	1.120645	-1.194508
C	-3.905244	-0.378200	-1.674155
C	-4.755391	-1.692006	-1.736370
H	-5.762593	-1.494415	-2.109582
H	-4.844862	-2.116876	-0.736796
C	-3.956403	-2.661209	-2.637757

O	-1.781265	2.098277	-1.877833
C	-0.597675	2.953323	-0.011632
N	-0.519638	1.480418	-0.141836
C	-3.989282	0.342683	-0.336675
C	-3.353143	0.024277	0.875037
C	-3.473159	0.901594	1.963365
C	-4.237101	2.063205	1.847807
C	-4.885591	2.370639	0.648306
C	-4.749118	1.511447	-0.441866
H	-2.954373	0.683371	2.888608
H	-5.479626	3.276250	0.564000
C	-2.511653	-1.181404	1.024075
C	-4.436917	0.697952	-2.679056
H	-4.982013	0.233441	-3.503986
H	-3.598587	1.251983	-3.100559
C	-5.315191	1.652408	-1.836351
O	-3.093422	-2.372655	0.829082
C	-0.789508	-2.604029	1.351881
H	-0.050623	-2.716420	0.550989
N	-1.256706	-1.202605	1.322275
C	-2.071250	-3.397629	1.002643
H	-1.995707	-3.944801	0.062084
H	-2.412523	-4.064867	1.795451
C	-1.622876	3.328438	-1.104347
H	-2.604121	3.578472	-0.696882
H	-1.291936	4.105146	-1.793728
H	-4.319373	2.730257	2.699372
H	-4.257004	-2.569999	-3.689332
H	-4.094933	-3.709462	-2.357684
H	-6.367301	1.340649	-1.845702
H	-5.287389	2.682008	-2.205176
H	0.802422	-2.822925	-2.559167
H	-0.987894	3.180816	0.983887
C	-0.112936	-2.948016	2.691093
H	0.758571	-2.281653	2.758861
C	0.399991	-4.392675	2.667388
H	0.971345	-4.613366	3.572849
H	-0.425250	-5.112425	2.621512
H	1.051876	-4.575410	1.805263
C	-1.014003	-2.668061	3.897333
H	-1.925468	-3.276410	3.875452
H	-0.487481	-2.907931	4.825162
H	-1.301036	-1.614178	3.940091
C	0.804116	3.580072	-0.141698
H	1.403403	3.122243	0.656588
C	1.479008	3.252984	-1.477670
H	0.950175	3.703495	-2.324775
H	2.501476	3.642118	-1.490450
H	1.521339	2.172899	-1.646467
C	0.744113	5.088577	0.119719
H	0.293780	5.304793	1.093518
H	1.747667	5.522736	0.108593
H	0.157496	5.606349	-0.647816
Fe	0.080832	0.367652	1.501182
Cl	-0.357217	1.514577	3.417434
C	3.805287	-0.294935	-0.366021

C	3.061696	0.178597	0.733932
O	3.640207	1.146012	1.456698
C	3.058113	1.513180	2.724317
H	2.170375	2.131522	2.587609
H	2.789088	0.626115	3.299381
H	3.832857	2.080801	3.237688
C	3.150235	-2.656633	-0.501158
H	4.179309	-2.937791	-0.267513
H	2.536302	-2.644061	0.400674
O	3.125357	-1.337630	-1.085393
H	3.433979	0.634114	-1.854626
C	5.263975	-0.238219	-0.607531
C	5.831439	-1.064169	-1.604629
C	6.122289	0.668219	0.048571
C	7.189430	-0.996504	-1.917798
H	5.219421	-1.797922	-2.119398
C	7.476042	0.725433	-0.270412
H	5.724649	1.327001	0.806429
C	8.023433	-0.099769	-1.254759
H	7.592232	-1.657593	-2.679291
H	8.110317	1.430406	0.258414
H	9.079305	-0.045084	-1.497021
O	1.902408	-0.265317	1.022998
O	3.215279	0.248923	-2.809076
H	3.092979	-0.725406	-2.348487
H	4.065079	0.254816	-3.286741
H	2.729243	-3.341639	-1.238060

TS(C-P)$_{2w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2736.2031161
Zero-point correction= 0.833999 (Hartree/Particle)
Thermal correction to Energy= 0.885105
Thermal correction to Enthalpy= 0.886049
Thermal correction to Gibbs Free Energy= 0.746670
Sum of electronic and zero-point Energies= -2735.369117
Sum of electronic and thermal Energies= -2735.318011
Sum of electronic and thermal Enthalpies= -2735.317067
Sum of electronic and thermal Free Energies= -2735.456446

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Cartesian Coordinates

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C	-3.444296	-0.943265	-1.388865
C	-2.224851	-0.327218	-1.711398
C	-1.265190	-1.046973	-2.437265
C	-1.531980	-2.347555	-2.863146
C	-2.753419	-2.956362	-2.556816
C	-3.697500	-2.253513	-1.810063
H	-0.309862	-0.583356	-2.645738
H	-2.957350	-3.970479	-2.888247
C	-1.898691	1.043831	-1.271224
C	-4.568905	-0.422645	-0.506161
C	-5.374802	-1.724637	-0.177490
H	-6.442620	-1.514548	-0.084669
H	-5.030860	-2.139566	0.769188
C	-5.052505	-2.712668	-1.322750

O	-2.741872	2.017109	-1.645638
C	-0.949130	2.867648	-0.349931
N	-0.876700	1.405067	-0.572404
C	-4.066424	0.318771	0.724237
C	-2.972929	0.010230	1.550724
C	-2.611098	0.901558	2.570770
C	-3.343677	2.071489	2.773515
C	-4.441333	2.371788	1.961572
C	-4.791185	1.495811	0.934337
H	-1.748127	0.686861	3.188301
H	-5.009043	3.283642	2.124259
C	-2.163939	-1.207384	1.336472
C	-5.477551	0.645604	-1.203563
H	-6.327498	0.174930	-1.702976
H	-4.901710	1.182334	-1.956687
C	-5.901979	1.623389	-0.082905
O	-2.804900	-2.383766	1.417525
C	-0.522535	-2.673890	0.850815
H	-0.251368	-2.777718	-0.204813
N	-0.906117	-1.259794	1.060148
C	-1.836882	-3.434643	1.140017
H	-2.203564	-4.001010	0.283170
H	-1.794507	-4.078534	2.020398
C	-2.270504	3.259794	-1.050261
H	-3.037316	3.597298	-0.351560
H	-2.158383	3.985205	-1.857869
H	-3.050235	2.750511	3.567172
H	-5.785166	-2.636194	-2.136250
H	-5.054576	-3.755534	-0.992155
H	-6.856876	1.324812	0.368054
H	-6.031103	2.647123	-0.446798
H	-0.787430	-2.888853	-3.438157
H	-1.022171	3.029364	0.728539
C	3.836128	-0.197979	-0.164713
O	3.323697	0.381873	1.030518
H	3.303705	1.973706	1.142735
C	2.841395	-0.772428	-0.953946
O	1.574462	-0.662350	-0.747276
O	3.246704	-1.422386	-2.067517
C	2.243274	-1.846950	-2.994497
H	1.474217	-2.440815	-2.497777
H	1.775727	-0.987975	-3.486675
O	3.432258	2.928220	0.811404
H	3.820345	1.294476	-1.260939
H	3.650013	2.750377	-0.350982
O	3.779764	2.293884	-1.468155
C	0.695296	-3.071718	1.700837
H	1.520866	-2.458292	1.318388
C	0.510968	-2.752445	3.186991
H	0.322895	-1.686503	3.343375
H	-0.323279	-3.313653	3.622724
H	1.409443	-3.024537	3.748792
C	1.059603	-4.540737	1.458177
H	1.197150	-4.748979	0.391505
H	1.989770	-4.797194	1.972665
H	0.284091	-5.216140	1.836553

C	0.325817	3.571657	-0.845649
H	1.129218	3.181831	-0.209778
C	0.650716	3.239724	-2.306755
H	0.803391	2.162814	-2.445522
H	-0.152126	3.539552	-2.988992
H	1.542209	3.786777	-2.640157
C	0.238774	5.081711	-0.601030
H	0.018878	5.296665	0.449114
H	1.184760	5.570744	-0.851731
H	-0.539473	5.548717	-1.214875
Fe	0.465112	0.256286	0.587892
Cl	0.765170	1.613470	2.423626
H	2.770796	-2.448331	-3.734111
C	3.541645	-0.404891	2.227699
H	3.179218	-1.421470	2.061291
H	4.605630	-0.432016	2.472316
H	2.962208	0.077319	3.013485
C	5.300293	-0.371157	-0.232402
C	5.932911	-1.379508	-0.983265
C	6.119751	0.521949	0.487123
C	7.322209	-1.476714	-1.013003
H	5.334482	-2.086559	-1.540711
C	7.507115	0.414298	0.461883
H	5.661626	1.310491	1.075544
C	8.119324	-0.586207	-0.292970
H	7.784598	-2.265621	-1.598423
H	8.110126	1.115458	1.030749
H	9.200594	-0.671861	-0.317407
H	2.997277	2.458498	-2.018802
H	4.135940	3.359634	1.315956

TS(C-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2812.6589068
Zero-point correction= 0.858853 (Hartree/Particle)
Thermal correction to Energy= 0.912190
Thermal correction to Enthalpy= 0.913134
Thermal correction to Gibbs Free Energy= 0.769589
Sum of electronic and zero-point Energies= -2811.800053
Sum of electronic and thermal Energies= -2811.746717
Sum of electronic and thermal Enthalpies= -2811.745772
Sum of electronic and thermal Free Energies= -2811.889318
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Cartesian Coordinates
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C	-3.469241	-0.634598	-1.553607
C	-2.160749	-0.161813	-1.748303
C	-1.245097	-0.955189	-2.455162
C	-1.635333	-2.181936	-2.987588
C	-2.942590	-2.645953	-2.809378
C	-3.847169	-1.874663	-2.082025
H	-0.226415	-0.606837	-2.562288
H	-3.244136	-3.604066	-3.222818
C	-1.697138	1.124354	-1.196989
C	-4.589725	-0.034992	-0.716959
C	-5.554909	-1.252679	-0.521616
H	-6.595873	-0.926799	-0.464599
H	-5.311600	-1.766785	0.407673

C	-5.279585	-2.190682	-1.718557
O	-2.435726	2.207085	-1.482238
C	-0.543532	2.774659	-0.189722
N	-0.637347	1.324477	-0.483711
C	-4.113434	0.579447	0.589932
C	-3.117203	0.120279	1.466954
C	-2.772902	0.900316	2.580366
C	-3.427698	2.108076	2.821799
C	-4.428061	2.559574	1.955423
C	-4.757467	1.795950	0.836140
H	-1.986985	0.565309	3.244833
H	-4.935616	3.500493	2.148538
C	-2.417556	-1.162119	1.240520
C	-5.331078	1.159238	-1.406195
H	-6.171235	0.807721	-2.009591
H	-4.642953	1.688673	-2.064306
C	-5.765629	2.091517	-0.251049
O	-3.184027	-2.264982	1.230816
C	-0.903361	-2.790494	0.870528
H	-0.463744	-2.923348	-0.121715
N	-1.156171	-1.342411	1.049786
C	-2.324071	-3.396805	0.918890
H	-2.649468	-3.798578	-0.042354
H	-2.468195	-4.142448	1.701758
C	-1.883124	3.321083	-0.724679
H	-2.591924	3.552524	0.072396
H	-1.795198	4.168948	-1.404898
H	-3.151462	2.697601	3.689714
H	-5.937772	-1.962508	-2.566655
H	-5.433495	-3.245413	-1.472640
H	-6.776551	1.848173	0.099893
H	-5.778641	3.145353	-0.544842
H	-0.921180	-2.779218	-3.544840
H	-0.486987	2.888817	0.894579
C	3.613669	-0.494913	-0.219382
O	3.080825	0.031047	0.999058
H	3.235651	1.671600	1.437523
C	2.635837	-1.234765	-0.907342
O	1.387139	-1.202997	-0.616175
O	3.031629	-1.919436	-1.992702
C	2.026905	-2.506339	-2.829879
H	1.284605	-3.042193	-2.237183
H	1.529796	-1.738086	-3.429847
O	3.271109	2.639240	1.627994
H	3.576207	0.784452	-1.283537
O	3.628238	1.657192	-1.899728
C	0.095799	-3.316327	1.917028
H	1.024635	-2.758933	1.735601
C	-0.349770	-3.036857	3.355123
H	-0.479704	-1.965099	3.528088
H	-1.293119	-3.540914	3.593735
H	0.399511	-3.402999	4.062689
C	0.390553	-4.800579	1.674046
H	0.724432	-4.980010	0.646157
H	1.174944	-5.153495	2.349088
H	-0.494271	-5.421515	1.854085
C	0.734102	3.371414	-0.804954
H	1.557823	2.790811	-0.372221
C	0.777953	3.224759	-2.329858
H	0.677716	2.176075	-2.635497

H	-0.032208	3.774534	-2.819135
H	1.709834	3.631614	-2.739031
C	0.918185	4.827046	-0.365259
H	0.923455	4.913671	0.725709
H	1.864047	5.230452	-0.740452
H	0.121412	5.472120	-0.750637
Fe	0.470735	-0.041046	0.718419
Cl	0.617759	1.227250	2.673056
H	2.562467	-3.191223	-3.486034
C	3.370601	-0.794359	2.158714
H	3.034648	-1.818174	1.968667
H	4.443548	-0.792273	2.357746
H	2.816017	-0.359279	2.988592
C	5.088641	-0.651623	-0.263966
C	5.742394	-1.699289	-0.934312
C	5.879066	0.318114	0.383808
C	7.134389	-1.766538	-0.956265
H	5.162408	-2.460971	-1.437388
C	7.268763	0.238606	0.367980
H	5.405058	1.138484	0.912602
C	7.906107	-0.803242	-0.306584
H	7.617351	-2.586882	-1.478479
H	7.853085	0.996259	0.880856
H	8.989366	-0.864097	-0.324057
H	2.757157	1.802607	-2.297151
H	2.430713	2.803893	2.083607
H	3.953427	2.573677	-1.283900
O	4.297125	3.483899	-0.485744
H	3.848227	3.314424	0.422296
H	4.235062	4.408899	-0.749661

D

Number of imaginary frequencies: 0 Electronic energy: HF=-613.9663991
Zero-point correction= 0.204667 (Hartree/Particle)
Thermal correction to Energy= 0.217456
Thermal correction to Enthalpy= 0.218400
Thermal correction to Gibbs Free Energy= 0.164793
Sum of electronic and zero-point Energies= -613.761732
Sum of electronic and thermal Energies= -613.748943
Sum of electronic and thermal Enthalpies= -613.747999
Sum of electronic and thermal Free Energies= -613.801606

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Cartesian Coordinates

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C	-0.810794	0.042725	-0.055649
C	-1.144303	-1.205995	0.505042
C	-2.464452	-1.648190	0.511747
C	-3.485876	-0.859350	-0.021838
C	-3.168123	0.383212	-0.571949
C	-1.849310	0.829076	-0.591728
H	-0.364803	-1.821654	0.934717
H	-2.698332	-2.615079	0.948658
H	-4.514170	-1.207556	-0.006919
H	-3.950031	1.007856	-0.994769
H	-1.603103	1.785607	-1.039316
C	0.557089	0.556353	-0.099232
C	1.728415	-0.116596	0.011891

O	2.920178	0.512282	-0.136599
O	1.814356	-1.430590	0.278621
C	2.872263	-2.148797	-0.374188
H	2.745051	-3.189139	-0.074700
H	2.784609	-2.063108	-1.462618
H	3.850980	-1.783180	-0.056683
O	0.736381	1.928476	-0.351460
H	2.682578	1.414933	-0.416057
C	0.455360	2.748368	0.789819
H	1.122874	2.499132	1.624024
H	-0.582979	2.622367	1.113825
H	0.618388	3.783646	0.481856

D_a

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3305337
Zero-point correction= 0.787951 (Hartree/Particle)
Thermal correction to Energy= 0.834878
Thermal correction to Enthalpy= 0.835822
Thermal correction to Gibbs Free Energy= 0.707212
Sum of electronic and zero-point Energies= -2582.542583
Sum of electronic and thermal Energies= -2582.495656
Sum of electronic and thermal Enthalpies= -2582.494711
Sum of electronic and thermal Free Energies= -2582.623322

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Cartesian Coordinates

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C	2.835147	-0.850088	1.330346
C	1.691781	-0.075666	1.592081
C	0.730413	-0.553687	2.497003
C	0.930886	-1.759896	3.164976
C	2.082892	-2.517180	2.928586
C	3.019610	-2.064996	1.999928
H	-0.162147	0.028974	2.684275
H	2.236549	-3.457591	3.450302
C	1.442314	1.213783	0.927373
C	3.914287	-0.637989	0.278445
C	4.563963	-2.059251	0.169784
H	5.628440	-1.990722	-0.064988
H	4.080090	-2.624119	-0.626699
C	4.286595	-2.740838	1.528992
O	2.426701	2.116161	0.948765
C	0.501530	3.006219	-0.080676
N	0.348312	1.583845	0.335744
C	3.373111	-0.113558	-1.043053
C	2.171684	-0.437765	-1.696189
C	1.817823	0.250690	-2.867363
C	2.662921	1.230565	-3.387459
C	3.864611	1.544653	-2.745132
C	4.206898	0.878203	-1.568663
H	0.883171	0.020887	-3.363570
H	4.518123	2.310426	-3.153154
C	1.257825	-1.469724	-1.169358
C	4.986830	0.436867	0.658398
H	5.821317	-0.012481	1.201485
H	4.537859	1.194555	1.299359

C	5.415484	1.077704	-0.682725
O	1.757071	-2.698852	-1.012351
C	-0.520753	-2.615413	-0.379884
H	-0.896190	-2.486078	0.639129
N	0.017226	-1.311311	-0.832164
C	0.731360	-3.518973	-0.380929
H	1.084587	-3.761294	0.622430
H	0.630827	-4.427615	-0.974584
C	2.014369	3.229031	0.097622
H	2.574528	3.140952	-0.835572
H	2.279605	4.150202	0.614523
H	2.377264	1.750673	-4.295580
H	5.097827	-2.552853	2.243791
H	4.184197	-3.826546	1.443872
H	6.283111	0.561751	-1.113174
H	5.694757	2.129920	-0.575451
H	0.181789	-2.104411	3.868949
H	0.215701	3.085791	-1.132812
Fe	-1.019292	0.469275	-0.700404
Cl	-1.500744	1.238404	-2.842603
C	-3.204533	0.580303	0.116294
C	-2.944750	0.097259	1.491902
C	-2.590917	1.038434	2.479059
C	-3.015487	-1.260649	1.865338
C	-2.355027	0.643370	3.794255
H	-2.503759	2.081638	2.208081
C	-2.765303	-1.647823	3.179440
H	-3.296521	-2.006437	1.135417
C	-2.442443	-0.702047	4.155264
H	-2.101166	1.392639	4.537601
H	-2.838909	-2.698135	3.444892
H	-2.265763	-1.008403	5.181054
C	-3.991185	-0.054868	-0.848019
O	-4.286895	0.497812	-2.010877
O	-4.508461	-1.254166	-0.633701
C	-5.154434	-1.933360	-1.739364
H	-4.468523	-2.022808	-2.583316
H	-5.415812	-2.913211	-1.344883
H	-6.049015	-1.389408	-2.043474
C	-1.678412	-3.075238	-1.282998
H	-2.436246	-2.290063	-1.197470
C	-2.289782	-4.374831	-0.747955
H	-3.173059	-4.653639	-1.329435
H	-1.585154	-5.211093	-0.815410
H	-2.592578	-4.276376	0.300201
C	-1.277404	-3.181905	-2.757321
H	-0.926192	-2.221086	-3.142686
H	-0.490185	-3.927350	-2.915210
H	-2.135044	-3.489930	-3.362582
C	-0.409905	3.925909	0.754276
H	-1.421505	3.537930	0.599805
C	-0.355553	5.357651	0.208369
H	-1.059733	5.999737	0.744942
H	0.639653	5.800877	0.328624
H	-0.612680	5.389726	-0.855454
C	-0.097417	3.873302	2.253952

H	-0.164063	2.854259	2.645226
H	0.902811	4.259172	2.478738
H	-0.810474	4.489637	2.809421
O	-3.034781	1.960837	-0.092816
C	-4.209634	2.764094	0.136812
H	-3.886689	3.803579	0.067730
H	-4.966313	2.563996	-0.627054
H	-4.620174	2.564708	1.131253
H	-3.544279	1.089777	-2.299441

D_b

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3256158
Zero-point correction= 0.787934 (Hartree/Particle)
Thermal correction to Energy= 0.835248
Thermal correction to Enthalpy= 0.836192
Thermal correction to Gibbs Free Energy= 0.703937
Sum of electronic and zero-point Energies= -2582.537682
Sum of electronic and thermal Energies= -2582.490368
Sum of electronic and thermal Enthalpies= -2582.489423
Sum of electronic and thermal Free Energies= -2582.621679

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Cartesian Coordinates

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C	-1.584446	-1.783002	-1.710817
C	-0.868005	-0.575150	-1.726160
C	0.509039	-0.595278	-1.998019
C	1.152485	-1.801355	-2.277525
C	0.433622	-3.000739	-2.289203
C	-0.930238	-2.985261	-1.996916
H	1.068028	0.332156	-2.020093
H	0.937729	-3.937404	-2.509753
C	-1.509330	0.720572	-1.424328
C	-3.028775	-2.025107	-1.294247
C	-3.066761	-3.574902	-1.071208
H	-4.033724	-3.991350	-1.361324
H	-2.910366	-3.797928	-0.016163
C	-1.891442	-4.147058	-1.898679
O	-2.499382	1.124835	-2.225263
C	-2.056811	2.730019	-0.536969
N	-1.199416	1.521823	-0.456968
C	-3.413359	-1.213439	-0.065905
C	-2.653510	-0.962926	1.088142
C	-3.127638	-0.042507	2.039372
C	-4.357910	0.589210	1.852532
C	-5.127300	0.317264	0.717322
C	-4.646044	-0.576987	-0.239976
H	-2.536298	0.173462	2.923216
H	-6.086297	0.808058	0.577839
C	-1.314397	-1.543758	1.296087
C	-4.082302	-1.561832	-2.357992
H	-4.372619	-2.388515	-3.009737
H	-3.653505	-0.780039	-2.984188
C	-5.271793	-0.986018	-1.553052
O	-1.162974	-2.867700	1.275221
C	0.877984	-1.776771	1.785909

H	1.712851	-1.513392	1.134164
N	-0.243250	-0.848967	1.511658
C	0.272298	-3.138237	1.383219
H	0.604655	-3.479884	0.401707
H	0.398232	-3.927254	2.123354
C	-3.031140	2.370962	-1.681399
H	-4.043119	2.163127	-1.330443
H	-3.058347	3.095232	-2.495475
H	-4.713955	1.291662	2.598685
H	-2.216603	-4.446258	-2.903091
H	-1.443477	-5.030663	-1.434850
H	-6.041299	-1.747477	-1.374436
H	-5.763977	-0.155270	-2.067412
H	2.217985	-1.800247	-2.481760
H	-2.594719	2.821408	0.411199
Fe	-0.218240	1.182887	1.319373
Cl	-0.467217	2.398617	3.175047
C	3.358744	1.057529	-0.706913
C	2.750798	1.219795	0.482892
O	1.638152	2.050870	0.568999
O	3.021959	0.571892	1.619347
C	3.323441	1.423289	2.760023
H	2.435973	1.984069	3.061099
H	3.629786	0.744265	3.554090
H	4.142768	2.101403	2.505176
C	1.333189	-1.653573	3.252908
H	1.543139	-0.589087	3.401526
C	2.635282	-2.434091	3.461446
H	3.002561	-2.305276	4.483470
H	2.491446	-3.509482	3.303938
H	3.413255	-2.091985	2.771168
C	0.245805	-2.053032	4.255298
H	-0.664968	-1.463816	4.115650
H	-0.015079	-3.114477	4.182725
H	0.594810	-1.875919	5.276097
C	-1.203651	3.997640	-0.735703
H	-0.534884	4.039588	0.135603
C	-2.090897	5.247017	-0.698658
H	-1.481894	6.152725	-0.760005
H	-2.791449	5.268019	-1.541341
H	-2.670928	5.295228	0.228163
C	-0.347335	3.944600	-2.006681
H	0.283430	3.050019	-2.046738
H	-0.963991	3.948158	-2.912103
H	0.304410	4.821301	-2.060244
O	2.729279	1.757339	-1.743576
C	3.537008	2.801524	-2.325658
H	2.923901	3.263458	-3.099903
H	3.807437	3.542265	-1.565650
H	4.444898	2.384837	-2.767895
H	1.526217	2.420445	-0.329854
C	4.452379	0.140208	-1.044579
C	4.573643	-0.307650	-2.372685
C	5.368393	-0.327918	-0.086730
C	5.577263	-1.205878	-2.729545
H	3.870120	0.045422	-3.118960

C	6.366834	-1.227378	-0.450307
H	5.297760	0.013398	0.938168
C	6.477109	-1.671080	-1.770048
H	5.656005	-1.540706	-3.759131
H	7.068971	-1.577055	0.300026
H	7.261060	-2.367841	-2.048155

D_c

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3208071
Zero-point correction= 0.788397 (Hartree/Particle)
Thermal correction to Energy= 0.835559
Thermal correction to Enthalpy= 0.836503
Thermal correction to Gibbs Free Energy= 0.705495
Sum of electronic and zero-point Energies= -2582.532410
Sum of electronic and thermal Energies= -2582.485248
Sum of electronic and thermal Enthalpies= -2582.484304
Sum of electronic and thermal Free Energies= -2582.615312

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Cartesian Coordinates

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C	-3.250467	-0.725542	1.390222
C	-1.876619	-0.786952	1.677317
C	-1.372764	-0.072323	2.774414
C	-2.225126	0.679192	3.580974
C	-3.594052	0.737345	3.299075
C	-4.096542	0.040052	2.201330
H	-0.313592	-0.123040	2.988563
H	-4.257133	1.324374	3.928005
C	-0.930285	-1.550555	0.843251
C	-4.013154	-1.324004	0.217611
C	-5.356395	-0.519403	0.236680
H	-6.191826	-1.139139	-0.096238
H	-5.283373	0.334210	-0.436086
C	-5.518014	-0.021951	1.691734
O	-1.197769	-2.841893	0.641871
C	0.806702	-2.212334	-0.448538
N	0.145093	-1.094858	0.282161
C	-3.260741	-1.238471	-1.100962
C	-2.451294	-0.197778	-1.585173
C	-1.735846	-0.381627	-2.779829
C	-1.855766	-1.574720	-3.491836
C	-2.679676	-2.602260	-3.021526
C	-3.366303	-2.433236	-1.819286
H	-1.082082	0.402889	-3.140538
H	-2.769731	-3.529440	-3.580350
C	-2.322818	1.088381	-0.875775
C	-4.279330	-2.861261	0.356466
H	-5.222556	-3.054293	0.872487
H	-3.479153	-3.321883	0.935082
C	-4.256225	-3.412357	-1.088361
O	-3.452863	1.762393	-0.632478
C	-1.564873	3.003561	0.035542
H	-1.109445	3.120679	1.021918
N	-1.226741	1.657473	-0.484032
C	-3.098664	2.929260	0.165725

H	-3.431069	2.733370	1.187706
H	-3.632334	3.784041	-0.247900
C	-0.225006	-3.351902	-0.320621
H	-0.766551	-3.545408	-1.247674
H	0.175672	-4.280687	0.084568
H	-1.300821	-1.699682	-4.415577
H	-6.097521	-0.731613	2.295717
H	-6.034151	0.940589	1.753355
H	-5.259316	-3.410214	-1.533398
H	-3.889305	-4.441582	-1.139553
H	-1.823512	1.215266	4.435053
H	0.914455	-1.904496	-1.491722
Fe	0.645752	0.773818	-0.406027
Cl	1.581689	0.722489	-2.457865
C	-1.027750	4.101080	-0.906097
H	0.052240	3.921212	-0.992341
C	-1.237055	5.485005	-0.280592
H	-0.784019	6.260379	-0.903765
H	-2.301646	5.726829	-0.185309
H	-0.788852	5.550714	0.717178
C	-1.614360	4.011285	-2.318850
H	-1.398327	3.044115	-2.779816
H	-2.699058	4.164082	-2.323153
H	-1.175476	4.783783	-2.955702
C	2.205421	-2.497407	0.121414
H	2.750583	-1.550823	0.046809
C	2.930432	-3.521802	-0.757682
H	3.949729	-3.679897	-0.396751
H	2.428261	-4.496205	-0.745936
H	2.989652	-3.181756	-1.796385
C	2.172562	-2.918239	1.592566
H	1.657061	-2.175917	2.207937
H	1.676535	-3.885076	1.732428
H	3.191036	-3.014325	1.975941
C	2.735500	2.060264	0.378568
C	3.544040	0.977037	0.821599
C	1.677747	2.542979	1.164734
H	2.972247	2.535266	-0.564754
C	3.225153	0.395906	2.070609
C	1.367515	1.935127	2.388931
H	1.139587	3.425648	0.838334
C	2.155827	0.865139	2.827014
H	3.826881	-0.420367	2.444226
H	0.550466	2.308512	2.995723
H	1.945949	0.397622	3.784633
C	4.634778	0.539403	-0.019609
C	5.404782	-0.585825	0.091476
O	4.932386	1.290185	-1.162260
O	6.326754	-0.878567	-0.835232
H	6.196613	-0.218409	-1.543457
O	5.283929	-1.471878	1.083198
C	6.246909	-2.543636	1.150649
H	6.214611	-3.152204	0.245409
H	7.254168	-2.144692	1.288623
H	5.951816	-3.133062	2.017294
C	5.775715	2.424583	-0.892372

H	6.735734	2.106457	-0.469401
H	5.936518	2.924606	-1.848580
H	5.291028	3.115678	-0.194629

D_d

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3369244
Zero-point correction= 0.787856 (Hartree/Particle)
Thermal correction to Energy= 0.835000
Thermal correction to Enthalpy= 0.835945
Thermal correction to Gibbs Free Energy= 0.705185
Sum of electronic and zero-point Energies= -2582.549068
Sum of electronic and thermal Energies= -2582.501924
Sum of electronic and thermal Enthalpies= -2582.500980
Sum of electronic and thermal Free Energies= -2582.631739

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Cartesian Coordinates

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C	-2.659929	-1.689358	-1.058632
C	-1.874380	-0.679863	-1.639267
C	-0.852825	-1.032492	-2.534523
C	-0.636714	-2.369319	-2.865662
C	-1.422028	-3.374567	-2.293484
C	-2.424771	-3.028924	-1.387682
H	-0.249395	-0.251577	-2.985473
H	-1.249577	-4.415111	-2.552488
C	-2.048525	0.743786	-1.297848
C	-3.747329	-1.564572	0.000535
C	-3.908018	-3.039073	0.504234
H	-4.946906	-3.254254	0.762771
H	-3.304251	-3.191884	1.397653
C	-3.377362	-3.933652	-0.641028
O	-3.250521	1.290199	-1.485063
C	-1.718605	2.869631	-0.598901
N	-1.132009	1.519661	-0.815976
C	-3.393216	-0.567721	1.094558
C	-2.151921	-0.354612	1.715722
C	-1.994762	0.733520	2.590347
C	-3.076739	1.568796	2.869693
C	-4.322408	1.335549	2.278564
C	-4.469552	0.276200	1.382270
H	-1.031377	0.918728	3.052110
H	-5.163364	1.984992	2.504381
C	-0.988786	-1.224368	1.462617
C	-5.100181	-0.998250	-0.553122
H	-5.768921	-1.805864	-0.858337
H	-4.909109	-0.375297	-1.426198
C	-5.686980	-0.128493	0.583925
O	-1.113226	-2.522462	1.734630
C	1.091832	-2.007664	1.038332
H	1.537735	-2.112401	0.048688
N	0.168335	-0.843051	1.020548
C	0.126397	-3.177030	1.322031
H	-0.104414	-3.765116	0.431261
H	0.433496	-3.831234	2.136845
C	-3.204459	2.654063	-0.962586

H	-3.867411	2.687097	-0.097380
H	-3.576228	3.313285	-1.746623
H	-2.944545	2.400324	3.553773
H	-4.186816	-4.249858	-1.310891
H	-2.897594	-4.845732	-0.273963
H	-6.371735	-0.705879	1.217691
H	-6.252319	0.728629	0.206682
H	0.139370	-2.625003	-3.578581
H	-1.610489	3.105892	0.462443
Fe	0.547443	1.001720	0.264831
Cl	0.990473	2.723975	1.737830
C	3.457585	0.658522	-0.499568
C	3.764103	-0.678465	-1.003297
C	4.949732	-1.371097	-0.678378
C	2.837956	-1.326867	-1.847292
C	5.182626	-2.651697	-1.171412
H	5.685343	-0.902829	-0.041368
C	3.080414	-2.610177	-2.333401
H	1.915230	-0.826220	-2.111758
C	4.252985	-3.285573	-1.998714
H	6.104465	-3.159108	-0.904091
H	2.346373	-3.083968	-2.977570
H	4.444086	-4.282910	-2.380614
C	4.218956	1.510569	0.253450
O	3.841837	2.737547	0.624524
O	5.459071	1.169433	0.612279
C	6.136933	1.991357	1.584666
H	5.552152	2.066413	2.504082
H	7.078486	1.477947	1.773297
H	6.321804	2.989562	1.185165
C	2.222286	-1.805519	2.065492
H	2.778793	-0.924892	1.720795
C	3.175840	-3.006076	2.033399
H	4.050695	-2.810662	2.659426
H	2.696947	-3.911415	2.423874
H	3.528742	-3.210728	1.019391
C	1.700469	-1.521929	3.477584
H	1.095327	-0.611593	3.508022
H	1.096096	-2.350724	3.864024
H	2.537192	-1.384321	4.167835
C	-0.976686	3.944721	-1.411948
H	0.072155	3.873935	-1.096061
C	-1.483492	5.339094	-1.026267
H	-0.921792	6.112781	-1.556517
H	-2.540437	5.468908	-1.286792
H	-1.371895	5.517675	0.047590
C	-1.055021	3.708100	-2.923976
H	-0.752465	2.691876	-3.197309
H	-2.068668	3.864609	-3.307961
H	-0.402193	4.407479	-3.453645
O	2.215921	1.198931	-0.935057
C	2.316942	2.042913	-2.109947
H	1.299237	2.273745	-2.420935
H	2.856275	2.956443	-1.852016
H	2.842297	1.492096	-2.892266
H	2.886896	2.781632	0.866940

D_e

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3250947
Zero-point correction= 0.787983 (Hartree/Particle)
Thermal correction to Energy= 0.834949
Thermal correction to Enthalpy= 0.835893
Thermal correction to Gibbs Free Energy= 0.706234
Sum of electronic and zero-point Energies= -2582.537112
Sum of electronic and thermal Energies= -2582.490146
Sum of electronic and thermal Enthalpies= -2582.489202
Sum of electronic and thermal Free Energies= -2582.618860

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Cartesian Coordinates

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C	-2.415078	-0.152855	-1.921308
C	-1.053790	0.155986	-1.751059
C	-0.080152	-0.691111	-2.306923
C	-0.465896	-1.799579	-3.060409
C	-1.819714	-2.090028	-3.255772
C	-2.786855	-1.274572	-2.669199
H	0.970859	-0.464660	-2.172820
H	-2.113744	-2.953766	-3.845391
C	-0.609318	1.345977	-1.003791
C	-3.633675	0.511274	-1.294011
C	-4.744045	-0.578086	-1.473816
H	-5.725844	-0.121627	-1.617197
H	-4.792715	-1.205309	-0.584022
C	-4.290064	-1.428921	-2.682124
O	-1.100477	2.526147	-1.386542
C	0.457135	2.799058	0.369100
7	0.226399	1.374983	-0.013016
C	-3.409754	0.930184	0.151290
C	-2.703330	0.260534	1.165238
C	-2.487212	0.904787	2.397271
C	-3.003118	2.179683	2.623157
C	-3.731558	2.833747	1.624334
C	-3.919347	2.210504	0.390382
H	-1.923498	0.401732	3.175143
H	-4.132849	3.826955	1.804185
C	-2.113876	-1.072741	0.972153
C	-4.051700	1.856316	-1.979649
H	-4.776302	1.682538	-2.778108
H	-3.176569	2.332997	-2.419186
C	-4.610708	2.743817	-0.842928
O	-2.881521	-2.056155	0.503783
C	-0.727468	-2.852648	1.040517
H	0.157983	-3.030077	0.422361
7	-0.882353	-1.391935	1.236035
C	-2.011715	-3.207292	0.265852
H	-1.858791	-3.272223	-0.812779
H	-2.533527	-4.090285	0.631395
C	-0.649792	3.524380	-0.419285
H	-1.514313	3.785071	0.194259
H	-0.308232	4.391702	-0.982015
H	-2.834515	2.660936	3.580500

H	-4.697507	-1.037049	-3.622679
H	-4.611462	-2.471752	-2.607561
H	-5.696829	2.626184	-0.739898
H	-4.422284	3.808453	-1.008707
H	0.299705	-2.429952	-3.496121
H	0.292459	2.890641	1.445514
Fe	0.600835	-0.012212	1.425388
Cl	1.071917	0.926869	3.466619
C	3.878042	0.157650	-0.239809
C	3.467549	-0.022779	1.031343
O	3.926717	0.678588	2.079572
O	2.500510	-0.992707	1.327299
C	2.919875	-1.962178	2.333062
H	2.810760	-1.534853	3.330428
H	2.267760	-2.824951	2.209787
H	3.957277	-2.239694	2.140216
C	-0.560144	-3.569155	2.397172
H	0.284167	-3.075563	2.894603
C	-0.196996	-5.042166	2.176130
H	-0.006139	-5.539018	3.130849
H	-1.010493	-5.587135	1.684205
H	0.699096	-5.149188	1.554617
C	-1.778525	-3.409923	3.313590
H	-2.009206	-2.357361	3.499478
H	-2.670965	-3.889531	2.898202
H	-1.580986	-3.878024	4.281420
C	1.897885	3.235398	0.046304
H	2.557814	2.535331	0.569197
C	2.159861	4.634886	0.614666
H	3.201907	4.920588	0.449465
H	1.533347	5.394134	0.131815
H	1.967591	4.671352	1.691945
C	2.217656	3.156057	-1.448903
H	2.016076	2.159825	-1.850926
H	1.642360	3.885388	-2.030002
H	3.277554	3.361440	-1.609891
O	4.618259	1.292051	-0.483000
C	6.032337	1.066282	-0.570677
H	6.481215	2.028103	-0.820880
H	6.423802	0.716577	0.390232
H	6.266251	0.336358	-1.354020
H	3.182668	0.917677	2.674058
C	3.564934	-0.692745	-1.403919
C	3.649040	-0.114978	-2.683860
C	3.227848	-2.055784	-1.308824
C	3.386772	-0.867246	-3.827055
H	3.926024	0.928807	-2.766495
C	2.974572	-2.805855	-2.454255
H	3.189915	-2.539361	-0.341800
C	3.049753	-2.217110	-3.719251
H	3.455427	-0.399303	-4.803974
H	2.735233	-3.860933	-2.359997
H	2.862437	-2.807798	-4.610434

D_e

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.3270359
Zero-point correction= 0.788080 (Hartree/Particle)
Thermal correction to Energy= 0.835232
Thermal correction to Enthalpy= 0.836176
Thermal correction to Gibbs Free Energy= 0.707245
Sum of electronic and zero-point Energies= -2582.538956
Sum of electronic and thermal Energies= -2582.491804
Sum of electronic and thermal Enthalpies= -2582.490860
Sum of electronic and thermal Free Energies= -2582.619791
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Cartesian Coordinates
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C	1.717056	-1.979038	1.354116
C	1.057625	-0.773630	1.648872
C	-0.243937	-0.813110	2.172974
C	-0.862661	-2.034293	2.435753
C	-0.194339	-3.233909	2.169376
C	1.085448	-3.199245	1.616197
H	-0.764637	0.115356	2.370083
H	-0.678150	-4.184892	2.373969
C	1.675438	0.538375	1.379976
C	3.044013	-2.189933	0.637515
C	2.966334	-3.694294	0.207759
H	3.952613	-4.162700	0.234920
H	2.588113	-3.768405	-0.810707
C	1.962161	-4.351899	1.183962
O	2.880309	0.767421	1.910881
C	2.125771	2.633153	0.660231
N	1.168419	1.495113	0.673578
C	3.247159	-1.216198	-0.515873
C	2.298066	-0.721681	-1.427352
C	2.660083	0.314242	-2.305727
C	3.961507	0.813955	-2.302193
C	4.915128	0.298382	-1.418168
C	4.546916	-0.701509	-0.517667
H	1.920138	0.726125	-2.982663
H	5.928258	0.690417	-1.419277
C	0.921283	-1.235910	-1.490559
C	4.305098	-1.928058	1.529124
H	4.633401	-2.843447	2.026431
H	4.066496	-1.194902	2.298505
C	5.372127	-1.345909	0.572440
O	0.765747	-2.561356	-1.584017
C	-1.296996	-1.458848	-1.796593
H	-2.104125	-1.252085	-1.092128
N	-0.169135	-0.532432	-1.511959
C	-0.665108	-2.829302	-1.501695
H	-0.868469	-3.184595	-0.489003
H	-0.895452	-3.604423	-2.231102
C	3.347299	2.054639	1.406795
H	4.194522	1.853954	0.749833
H	3.670045	2.641562	2.266621
H	4.228591	1.608850	-2.990400
H	2.473677	-4.778735	2.056028
H	1.395962	-5.165036	0.720225
H	6.001733	-2.137303	0.146284

H	6.043797	-0.640740	1.070645
H	-1.866465	-2.045863	2.844443
H	2.369013	2.842863	-0.383807
Fe	-0.314752	1.406675	-0.789351
Cl	0.196616	3.103493	-2.233444
C	-3.099634	0.901674	0.329696
C	-3.664851	0.021208	1.351928
C	-4.261315	-1.202993	0.997856
C	-3.557688	0.347157	2.715017
C	-4.763371	-2.057972	1.976472
H	-4.309717	-1.493498	-0.046748
C	-4.054179	-0.513678	3.690604
H	-3.076084	1.272175	3.011837
C	-4.665185	-1.716542	3.326772
H	-5.219103	-2.998732	1.684226
H	-3.965649	-0.244289	4.738174
H	-5.054117	-2.383617	4.088904
C	-3.454126	1.033422	-0.968849
O	-2.526832	1.588985	-1.794593
O	-4.559317	0.626657	-1.607785
C	-5.839529	0.820551	-0.964640
H	-6.051714	0.004984	-0.271649
H	-5.845330	1.771553	-0.426348
H	-6.571834	0.831731	-1.770698
C	-1.817024	-1.279055	-3.238428
H	-2.070227	-0.218776	-3.330926
C	-3.100150	-2.094816	-3.438212
H	-3.496962	-1.942951	-4.445741
H	-2.921507	-3.169758	-3.319934
H	-3.875520	-1.794701	-2.726203
C	-0.760778	-1.601118	-4.301363
H	0.136199	-0.988157	-4.177451
H	-0.461755	-2.654472	-4.280812
H	-1.160770	-1.398011	-5.298453
C	1.509806	3.901563	1.274636
H	0.628232	4.119126	0.659055
C	2.474494	5.083491	1.125141
H	2.015111	6.004002	1.495646
H	3.396449	4.927859	1.697438
H	2.745332	5.240981	0.076677
C	1.070023	3.701101	2.728910
H	0.402420	2.839965	2.836323
H	1.925676	3.540668	3.393678
H	0.543985	4.587319	3.096186
O	-1.941777	1.628183	0.701543
C	-2.200746	3.039766	0.937919
H	-1.323670	3.430689	1.449342
H	-2.343340	3.557409	-0.013817
H	-3.084330	3.142450	1.570029
H	-2.917086	2.050772	-2.551858

F

Number of imaginary frequencies: 0 Electronic energy: HF=-613.9050605
Zero-point correction= 0.203690 (Hartree/Particle)
Thermal correction to Energy= 0.216695

Thermal correction to Enthalpy= 0.217639
Thermal correction to Gibbs Free Energy= 0.163712
Sum of electronic and zero-point Energies= -613.701371
Sum of electronic and thermal Energies= -613.688365
Sum of electronic and thermal Enthalpies= -613.687421
Sum of electronic and thermal Free Energies= -613.741348
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Cartesian Coordinates
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C	0.852994	0.031250	-0.120474
C	1.223688	-1.339778	-0.072305
C	2.552253	-1.716061	0.045486
C	3.581645	-0.767360	0.112569
C	3.241363	0.580641	0.076264
C	1.907743	0.977671	-0.028118
H	0.445148	-2.087747	-0.136533
H	2.793794	-2.775257	0.076951
H	4.618080	-1.076546	0.197331
H	4.013639	1.342065	0.144828
H	1.708735	2.048765	0.021600
C	-0.510793	0.427758	-0.292763
C	-1.789727	-0.150783	-0.157270
O	-2.858656	0.474516	-0.169447
O	-1.746504	-1.509996	0.027184
C	-3.021498	-2.117939	0.241260
H	-2.819520	-3.181149	0.378666
H	-3.511069	-1.707329	1.129020
H	-3.680697	-1.964676	-0.617475
O	-0.674997	1.884333	-0.539640
H	0.149801	2.197766	-0.955755
C	-1.046610	2.706827	0.631190
H	-0.323064	2.526664	1.425904
H	-2.043479	2.348122	0.877749
H	-1.056475	3.745137	0.297892

F'

Number of imaginary frequencies: 0 Electronic energy: HF=-766.8288898
Zero-point correction= 0.252446 (Hartree/Particle)
Thermal correction to Energy= 0.269699
Thermal correction to Enthalpy= 0.270643
Thermal correction to Gibbs Free Energy= 0.206227
Sum of electronic and zero-point Energies= -766.576444
Sum of electronic and thermal Energies= -766.559191
Sum of electronic and thermal Enthalpies= -766.558247
Sum of electronic and thermal Free Energies= -766.622663
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Cartesian Coordinates
.....

C	0.041163	-0.127604	-0.270170
C	1.066609	0.807008	-0.356133
O	2.273479	0.540401	-0.652400
O	0.710455	2.107111	-0.103022
C	1.755539	3.066292	-0.246625
H	2.550919	2.908524	0.489622
H	1.285823	4.036511	-0.078445

H	2.199872	3.026944	-1.244470
C	0.867921	-1.766855	-1.913392
H	1.686015	-1.107489	-2.202654
H	-0.019239	-1.606038	-2.525273
O	0.495787	-1.474582	-0.539861
C	-1.383869	-0.035327	-0.025054
C	-2.036020	1.192308	0.241008
C	-2.186434	-1.200204	-0.040418
C	-3.406495	1.237909	0.472892
H	-1.455657	2.103849	0.260696
C	-3.557790	-1.139565	0.191659
H	-1.724443	-2.161428	-0.234733
C	-4.185483	0.078495	0.451394
H	-3.872795	2.199305	0.672680
H	-4.138890	-2.057950	0.169095
H	-5.254804	0.124515	0.632683
H	1.216652	-1.844222	0.238068
O	1.988217	-2.254000	1.186123
H	2.736559	-1.548596	1.303641
H	3.653131	0.210769	1.971626
O	3.704162	-0.408193	1.232929
H	1.169714	-2.815481	-1.937724
H	1.484671	-2.290855	2.009731
H	3.254831	0.060991	0.454336

(R)-TS(F-P)

Number of imaginary frequencies: 1 Electronic energy: HF=-613.8800451
Zero-point correction= 0.198472 (Hartree/Particle)
Thermal correction to Energy= 0.211320
Thermal correction to Enthalpy= 0.212264
Thermal correction to Gibbs Free Energy= 0.158550
Sum of electronic and zero-point Energies= -613.681573
Sum of electronic and thermal Energies= -613.668726
Sum of electronic and thermal Enthalpies= -613.667781
Sum of electronic and thermal Free Energies= -613.721495

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Cartesian Coordinates

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C	0.514200	0.446425	-0.516124
C	1.732361	-0.232180	-0.120406
O	2.852810	0.274034	-0.072883
O	1.534906	-1.557007	0.108614
C	2.730890	-2.314545	0.333028
H	3.412393	-2.227134	-0.516984
H	2.402075	-3.346555	0.456097
H	3.246783	-1.968104	1.231726
C	1.456346	2.635200	0.563034
H	2.492082	2.306391	0.537970
H	0.979924	2.339596	1.499998
O	0.696738	1.993514	-0.507429
C	-0.881183	0.086381	-0.247399
C	-1.312461	-1.255374	-0.300345
C	-1.843555	1.075827	0.031402
C	-2.642910	-1.583581	-0.057610
H	-0.598002	-2.034655	-0.526397

C	-3.171692	0.735078	0.279134
H	-1.548560	2.117729	0.046282
C	-3.583966	-0.596006	0.239084
H	-2.945641	-2.626011	-0.103698
H	-3.888317	1.521518	0.499141
H	-4.620307	-0.859303	0.426553
H	1.054277	1.402333	-1.390124
H	1.349477	3.706520	0.390233

(R)-TS(F-P)$_{1w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-690.3558277
Zero-point correction= 0.224070 (Hartree/Particle)
Thermal correction to Energy= 0.238506
Thermal correction to Enthalpy= 0.239450
Thermal correction to Gibbs Free Energy= 0.182135
Sum of electronic and zero-point Energies= -690.131758
Sum of electronic and thermal Energies= -690.117322
Sum of electronic and thermal Enthalpies= -690.116377
Sum of electronic and thermal Free Energies= -690.173692

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Cartesian Coordinates

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C	0.460983	-0.347287	0.196920
C	1.607061	0.478176	-0.146787
O	2.711299	0.045631	-0.469423
O	1.385457	1.812251	0.023746
C	2.533399	2.642010	-0.184614
H	3.334218	2.382593	0.512888
H	2.191603	3.662769	-0.010606
H	2.912957	2.535120	-1.203882
C	1.067808	-2.078801	-1.544492
H	2.021935	-1.617788	-1.794104
H	0.265784	-1.714456	-2.188727
O	0.712388	-1.747296	-0.181633
C	-0.967494	0.000029	0.080949
C	-1.448525	1.308084	0.301794
C	-1.921363	-1.000385	-0.199429
C	-2.808899	1.592540	0.225088
H	-0.747124	2.098193	0.530045
C	-3.281431	-0.705572	-0.275615
H	-1.592016	-2.021268	-0.353759
C	-3.740092	0.593920	-0.066864
H	-3.143659	2.611998	0.397436
H	-3.984927	-1.502960	-0.500179
H	-4.799374	0.824084	-0.125792
H	1.261992	-2.104936	0.820578
H	1.009601	-0.890337	1.655245
O	1.479623	-1.825532	1.998863
H	0.828518	-2.272042	2.559858
H	1.121677	-3.167702	-1.593124

(R)-TS(F'-P)$_{2w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-766.8153541
Zero-point correction= 0.249096 (Hartree/Particle)

Thermal correction to Energy= 0.265559
Thermal correction to Enthalpy= 0.266503
Thermal correction to Gibbs Free Energy= 0.204377
Sum of electronic and zero-point Energies= -766.566259
Sum of electronic and thermal Energies= -766.549796
Sum of electronic and thermal Enthalpies= -766.548851
Sum of electronic and thermal Free Energies= -766.610977
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Cartesian Coordinates
.....

C	-0.305908	0.187831	-0.055743
C	-1.292614	-0.812891	-0.395701
O	-2.399125	-0.571319	-0.880411
O	-0.960656	-2.081759	0.005946
C	-1.963651	-3.069233	-0.245005
H	-2.889875	-2.836332	0.288492
H	-1.545436	-4.010625	0.113635
H	-2.191883	-3.136254	-1.311908
C	-0.680860	1.556764	-2.057504
H	-1.419221	0.870404	-2.473687
H	0.326943	1.313078	-2.399533
O	-0.702746	1.474090	-0.614544
C	1.157700	0.035635	0.012880
C	1.800768	-1.201599	0.233342
C	1.980187	1.178229	-0.094633
C	3.187480	-1.281555	0.326722
H	1.204770	-2.098505	0.327405
C	3.367213	1.087237	-0.004891
H	1.518138	2.147645	-0.241653
C	3.987450	-0.143729	0.205509
H	3.648034	-2.252000	0.492996
H	3.965069	1.990282	-0.097369
H	5.068358	-0.215392	0.277293
H	-1.776509	1.914963	0.016758
O	-2.531342	2.215961	0.779811
H	-2.212309	1.527079	1.598981
H	-0.896068	0.364374	1.529022
O	-1.522223	0.664265	2.337717
H	-0.922339	2.589614	-2.319814
H	-2.333643	3.121526	1.057587
H	-2.041886	-0.119894	2.563786

(R)-TS(D-P)

Number of imaginary frequencies: 1 Electronic energy: HF=-613.8786122
Zero-point correction= 0.198372 (Hartree/Particle)
Thermal correction to Energy= 0.211081
Thermal correction to Enthalpy= 0.212025
Thermal correction to Gibbs Free Energy= 0.158377
Sum of electronic and zero-point Energies= -613.680241
Sum of electronic and thermal Energies= -613.667531
Sum of electronic and thermal Enthalpies= -613.666587
Sum of electronic and thermal Free Energies= -613.720235
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Cartesian Coordinates
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C	0.813209	0.106039	0.118361
C	1.144214	-1.088044	0.784051
C	2.428547	-1.617825	0.708419
C	3.423618	-0.952346	-0.012956
C	3.111110	0.240922	-0.665665
C	1.819558	0.762470	-0.607776
H	0.385357	-1.598350	1.372760
H	2.659612	-2.545029	1.225528
H	4.429637	-1.358059	-0.060991
H	3.875580	0.764772	-1.233093
H	1.568015	1.673456	-1.138918
C	-0.549637	0.664358	0.226514
C	-1.706037	-0.206019	0.037761
O	-2.670744	0.152319	0.817965
O	-1.781943	-1.268051	-0.716622
C	-2.951348	-2.110187	-0.576104
H	-2.690076	-3.055445	-1.049484
H	-3.187936	-2.245428	0.480809
H	-3.797490	-1.645675	-1.085394
O	-0.760150	1.879110	-0.494147
C	-0.569943	3.040209	0.299264
H	0.422502	3.051014	0.768636
H	-1.330875	3.116979	1.089119
H	-1.751212	0.798086	1.273963
H	-0.660153	3.899194	-0.371714

(*R*)-TS(D-P)$_{1w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-690.3697589
Zero-point correction= 0.225097 (Hartree/Particle)
Thermal correction to Energy= 0.239096
Thermal correction to Enthalpy= 0.240040
Thermal correction to Gibbs Free Energy= 0.184113
Sum of electronic and zero-point Energies= -690.144661
Sum of electronic and thermal Energies= -690.130663
Sum of electronic and thermal Enthalpies= -690.129719
Sum of electronic and thermal Free Energies= -690.185646

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Cartesian Coordinates

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C	-1.021382	-0.067562	0.103677
C	-1.470604	1.248165	0.333876
C	-2.829328	1.550515	0.332514
C	-3.784490	0.556537	0.109799
C	-3.355300	-0.752867	-0.102013
C	-1.996444	-1.062054	-0.100641
H	-0.751378	2.037125	0.509085
H	-3.143867	2.575542	0.509173
H	-4.842838	0.798882	0.107820
H	-4.081252	-1.544452	-0.266847
H	-1.675725	-2.087185	-0.241372
C	0.404857	-0.456996	0.150133
C	1.518161	0.391270	-0.161345
O	2.720165	-0.002815	-0.011557
O	1.284714	1.669975	-0.489611
C	2.425681	2.543926	-0.498361

H	2.027769	3.533111	-0.723306
H	2.923383	2.541256	0.474405
H	3.141277	2.235360	-1.263015
O	0.657390	-1.830981	-0.154768
C	0.828754	-2.087224	-1.548755
H	1.751083	-1.624701	-1.920056
H	-0.026655	-1.712288	-2.122370
H	1.129343	-0.733902	1.544667
O	2.068614	-1.222303	1.973047
H	2.602733	-0.800587	1.099653
H	1.882960	-2.139609	1.709291
H	0.896684	-3.171828	-1.667327

(*R*)-TS(D-P)$_{2w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-766.8291268
Zero-point correction= 0.249880 (Hartree/Particle)
Thermal correction to Energy= 0.266052
Thermal correction to Enthalpy= 0.266996
Thermal correction to Gibbs Free Energy= 0.206103
Sum of electronic and zero-point Energies= -766.579247
Sum of electronic and thermal Energies= -766.563075
Sum of electronic and thermal Enthalpies= -766.562131
Sum of electronic and thermal Free Energies= -766.623024

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Cartesian Coordinates

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C	-1.195799	-0.043485	0.001552
C	-1.810844	1.213184	0.173812
C	-3.196137	1.323784	0.278181
C	-4.015870	0.196701	0.217146
C	-3.421327	-1.054843	0.056791
C	-2.037837	-1.174351	-0.043842
H	-1.203143	2.105175	0.218777
H	-3.637403	2.308976	0.404499
H	-5.094555	0.291691	0.296233
H	-4.036528	-1.949595	0.013494
H	-1.588290	-2.154558	-0.148528
C	0.270586	-0.262007	-0.066120
C	1.283761	0.718614	-0.345841
O	2.483703	0.449828	-0.606319
O	0.926372	2.015564	-0.179118
C	1.987986	2.972981	-0.276515
H	1.519188	3.942467	-0.106610
H	2.757922	2.784052	0.476596
H	2.452992	2.940808	-1.264179
O	0.631232	-1.557761	-0.566546
C	0.557677	-1.652624	-1.994289
H	1.301138	-0.997940	-2.461803
H	-0.445250	-1.384984	-2.342094
H	0.755084	-0.518152	1.434486
O	1.347079	-0.913778	2.287340
H	1.600765	-0.163408	2.842834
H	2.250271	-2.153053	0.181266
O	2.963039	-1.696395	0.685430
H	2.987149	-0.841492	0.122619

H	2.269095	-1.324540	1.617875
H	0.766976	-2.692845	-2.257005

(*R*)-TS(D-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-843.2689692
Zero-point correction= 0.276244 (Hartree/Particle)
Thermal correction to Energy= 0.294770
Thermal correction to Enthalpy= 0.295714
Thermal correction to Gibbs Free Energy= 0.229494
Sum of electronic and zero-point Energies= -842.992725
Sum of electronic and thermal Energies= -842.974199
Sum of electronic and thermal Enthalpies= -842.973255
Sum of electronic and thermal Free Energies= -843.039475

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Cartesian Coordinates

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C	0.032185	-0.272916	0.085848
C	1.509105	-0.099741	0.024953
C	2.112121	0.569517	-1.051048
C	2.340005	-0.601017	1.041668
C	3.492965	0.745273	-1.103374
H	1.484476	0.958333	-1.846493
C	3.723849	-0.444435	0.978831
H	1.884621	-1.102286	1.890081
C	4.308691	0.231846	-0.092788
H	3.935751	1.271665	-1.944420
H	4.345995	-0.841786	1.776237
H	5.386407	0.355858	-0.141423
C	-0.788402	0.848067	0.439448
O	-1.887304	0.782978	1.029312
O	-0.314675	2.040656	-0.015441
C	-1.152412	3.170560	0.225672
H	-2.093317	3.094895	-0.330585
H	-1.383667	3.272039	1.289054
H	-0.586040	4.034782	-0.122816
C	0.064289	-2.677130	0.279776
H	-0.436603	-3.473186	0.835582
H	-0.169763	-2.766443	-0.787824
O	-0.414433	-1.442960	0.823920
H	-3.446009	0.808989	0.503570
H	-0.682097	-0.580473	-1.359368
O	-4.278660	0.396722	0.147304
H	-4.887401	0.358176	0.895926
H	-2.286541	-1.412025	-1.168268
O	-1.385767	-0.998819	-2.079317
H	-1.702404	-0.267906	-2.627916
O	-2.817568	-1.686311	-0.232441
H	-2.071399	-1.543294	0.429951
H	-3.505148	-0.954228	-0.060064
H	1.146017	-2.771392	0.408168

(*R*)-TS(D$_f$-P)$_{2w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2736.2143707
Zero-point correction= 0.834086 (Hartree/Particle)

Thermal correction to Energy= 0.884396
Thermal correction to Enthalpy= 0.885340
Thermal correction to Gibbs Free Energy= 0.749724
Sum of electronic and zero-point Energies= -2735.380285
Sum of electronic and thermal Energies= -2735.329974
Sum of electronic and thermal Enthalpies= -2735.329030
Sum of electronic and thermal Free Energies= -2735.464646

Cartesian Coordinates

C	-2.639587	-1.808070	-1.158969
C	-1.711098	-0.861357	-1.623926
C	-0.597991	-1.302467	-2.357214
C	-0.429394	-2.655766	-2.645173
C	-1.356652	-3.596894	-2.185335
C	-2.447411	-3.167843	-1.431679
H	0.117369	-0.578233	-2.723718
H	-1.219847	-4.651755	-2.404870
C	-1.892410	0.586906	-1.394713
C	-3.862606	-1.601835	-0.275383
C	-4.133039	-3.043184	0.270914
H	-5.199547	-3.207447	0.440278
H	-3.615450	-3.182023	1.219075
C	-3.537724	-3.996041	-0.791529
O	-3.063684	1.090874	-1.806827
C	-1.676284	2.779554	-0.926900
N	-1.056924	1.422013	-0.866320
C	-3.670385	-0.546432	0.803024
C	-2.523622	-0.258959	1.562641
C	-2.512917	0.876334	2.392276
C	-3.644834	1.682005	2.494510
C	-4.798045	1.376577	1.763449
C	-4.797560	0.274558	0.908514
H	-1.617283	1.119934	2.952397
H	-5.678486	2.007588	1.844949
C	-1.310053	-1.082034	1.497571
C	-5.115955	-1.068445	-1.050266
H	-5.715748	-1.891548	-1.445237
H	-4.794887	-0.452001	-1.888822
C	-5.884308	-0.196555	-0.030272
O	-1.450069	-2.411673	1.569753
C	0.817048	-1.809290	1.572271
H	1.594367	-1.765207	0.804990
N	-0.092927	-0.644329	1.409355
C	-0.134305	-2.987387	1.310373
H	-0.128543	-3.323192	0.270969
H	-0.007740	-3.834065	1.983270
C	-3.120791	2.477866	-1.361489
H	-3.831609	2.519864	-0.534332
H	-3.481453	3.076169	-2.197510
H	-3.623996	2.551220	3.143058
H	-4.286444	-4.273301	-1.544509
H	-3.162860	-4.928388	-0.359442
H	-6.626410	-0.787005	0.522038
H	-6.424299	0.628244	-0.504136
H	0.424850	-2.974352	-3.233525

H	-1.653372	3.195457	0.079444
Fe	0.561332	1.129902	0.548346
Cl	0.291064	3.194238	1.692216
C	3.326321	0.311792	-0.556766
C	3.926766	-0.789828	-1.356866
C	5.309177	-0.860127	-1.567448
C	3.108141	-1.795830	-1.894972
C	5.863922	-1.918312	-2.285737
H	5.951970	-0.087975	-1.156046
C	3.662232	-2.844353	-2.626523
H	2.037349	-1.750628	-1.730384
C	5.042767	-2.910861	-2.823356
H	6.938054	-1.961719	-2.435979
H	3.017833	-3.617531	-3.035247
H	5.475304	-3.727791	-3.391767
C	3.407948	0.317896	0.859307
O	2.562621	0.917844	1.592076
O	4.506946	-0.239452	1.383306
C	4.803692	0.042364	2.763856
H	5.035318	1.103474	2.896776
H	3.971237	-0.233444	3.410633
H	5.680743	-0.559653	2.994475
C	1.478260	-1.802525	2.965644
H	1.921229	-0.807736	3.064715
C	2.597994	-2.849522	3.013305
H	3.113864	-2.819269	3.977438
H	2.206289	-3.865947	2.891306
H	3.338757	-2.677628	2.225407
C	0.477009	-1.978959	4.112743
H	-0.302531	-1.212121	4.090941
H	-0.007867	-2.960620	4.094210
H	0.993043	-1.892211	5.073003
C	-0.880023	3.717261	-1.852715
H	0.162877	3.637748	-1.519646
C	-1.327240	5.167639	-1.636427
H	-0.746890	5.850275	-2.263665
H	-2.383025	5.302569	-1.899784
H	-1.195161	5.466683	-0.592440
C	-0.959971	3.321406	-3.332493
H	-0.766626	2.256189	-3.494472
H	-1.946592	3.539954	-3.753901
H	-0.230214	3.886262	-3.919536
O	1.983765	0.677254	-0.970211
C	1.950943	1.306175	-2.268701
H	0.906888	1.511498	-2.482110
H	2.522965	2.236308	-2.250378
H	2.367053	0.623427	-3.012689
H	3.088950	2.539517	1.955064
O	3.299172	3.456268	1.641162
H	3.760886	3.239309	0.518998
O	4.180950	2.869083	-0.530859
H	4.015078	1.781789	-0.601074
H	5.117398	3.078080	-0.659016
H	2.387721	3.833628	1.594400

(*R*)-TS(D_f-P)$_{1w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2659.6742271
Zero-point correction= 0.812716 (Hartree/Particle)
Thermal correction to Energy= 0.861086
Thermal correction to Enthalpy= 0.862030
Thermal correction to Gibbs Free Energy= 0.729658
Sum of electronic and zero-point Energies= -2658.861511
Sum of electronic and thermal Energies= -2658.813141
Sum of electronic and thermal Enthalpies= -2658.812197
Sum of electronic and thermal Free Energies= -2658.944569

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Cartesian Coordinates

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C	-1.798133	-0.063318	2.303102
C	-0.745806	-0.761257	1.692782
C	0.581326	-0.463418	2.043164
C	0.850900	0.510911	3.005542
C	-0.197085	1.205864	3.615727
C	-1.515595	0.916171	3.260515
H	1.394451	-1.007603	1.574902
H	0.014816	1.964152	4.364138
C	-0.990145	-1.704730	0.588626
C	-3.297062	-0.196366	2.074856
C	-3.845239	1.116034	2.725025
H	-4.843380	0.965852	3.142544
H	-3.918725	1.895109	1.964870
C	-2.797137	1.520878	3.787636
O	-1.774757	-2.761273	0.782494
C	-1.014682	-2.628582	-1.471504
N	-0.513213	-1.539679	-0.600696
C	-3.713922	-0.388665	0.623110
C	-3.242334	0.268184	-0.521213
C	-3.686898	-0.145966	-1.786130
C	-4.621076	-1.176265	-1.900763
C	-5.126776	-1.801818	-0.756527
C	-4.658597	-1.413596	0.497841
H	-3.316080	0.358406	-2.672546
H	-5.869031	-2.589589	-0.847093
C	-2.389163	1.476042	-0.444200
C	-3.879821	-1.478451	2.764460
H	-4.199009	-1.268198	3.787789
H	-3.108264	-2.248490	2.806827
C	-5.032723	-1.959586	1.855561
O	-3.050417	2.593987	-0.086961
C	-0.800485	3.052780	-0.639331
H	0.048200	3.152305	0.036298
N	-1.142467	1.607074	-0.728708
C	-2.073625	3.668942	-0.023722
H	-1.953359	3.942654	1.027504
H	-2.478885	4.516145	-0.577392
C	-1.933418	-3.426324	-0.511108
H	-2.988827	-3.365974	-0.773534
H	-1.636621	-4.466118	-0.375018
H	-4.965615	-1.479727	-2.884003
H	-3.033007	1.088678	4.768370
H	-2.734008	2.604136	3.927821

H	-5.995977	-1.539943	2.171999
H	-5.143683	-3.047720	1.861473
H	1.881230	0.724924	3.268293
H	-1.606948	-2.166571	-2.267038
Fe	0.492073	0.226527	-1.005643
Cl	0.988808	0.333985	-3.400544
C	-0.392383	3.607591	-2.018148
H	0.460974	2.999992	-2.342444
C	0.072817	5.062116	-1.884309
H	0.452373	5.434962	-2.839585
H	-0.746896	5.723886	-1.583066
H	0.871399	5.162378	-1.140052
C	-1.485845	3.442364	-3.076805
H	-1.733458	2.387735	-3.220237
H	-2.400269	3.984524	-2.811017
H	-1.143085	3.832693	-4.038736
C	0.125490	-3.438415	-2.110451
H	0.684081	-2.718987	-2.720540
C	-0.445430	-4.503781	-3.054148
H	0.362000	-5.025061	-3.575247
H	-1.021215	-5.260834	-2.509501
H	-1.099952	-4.059068	-3.810712
C	1.070585	-4.041953	-1.066501
H	1.469771	-3.272624	-0.400133
H	0.569006	-4.798255	-0.452985
H	1.913307	-4.536759	-1.557177
C	3.449669	0.055374	-0.021010
C	4.532742	-0.576828	0.755520
C	5.714492	0.117939	1.054605
C	4.387861	-1.894474	1.222564
C	6.715729	-0.482963	1.813238
H	5.841335	1.133420	0.694859
C	5.397521	-2.497691	1.969943
H	3.476126	-2.442216	1.004066
C	6.564544	-1.793967	2.269967
H	7.622730	0.069440	2.038025
H	5.269935	-3.516516	2.322702
H	7.351224	-2.263569	2.851476
C	2.801936	1.227945	0.338976
O	1.721396	1.643737	-0.258212
O	3.352437	1.999797	1.294200
C	2.735149	3.268977	1.543628
H	2.741153	3.898011	0.648310
H	1.706542	3.136813	1.887998
H	3.338272	3.731456	2.323858
C	3.293378	-1.576872	-1.778202
H	2.538893	-1.943495	-2.467739
H	4.012239	-0.955927	-2.322762
O	2.602949	-0.803633	-0.777435
H	3.687659	1.092179	-1.622647
H	2.760511	2.292837	-1.932482
O	3.321345	1.646944	-2.416521
H	3.830812	-2.404124	-1.312739
H	2.575181	1.072038	-2.910315

TS(A-E)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2864235
Zero-point correction= 0.784716 (Hartree/Particle)
Thermal correction to Energy= 0.832892
Thermal correction to Enthalpy= 0.833836
Thermal correction to Gibbs Free Energy= 0.700336
Sum of electronic and zero-point Energies= -2582.501708
Sum of electronic and thermal Energies= -2582.453531
Sum of electronic and thermal Enthalpies= -2582.452587
Sum of electronic and thermal Free Energies= -2582.586088

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Cartesian Coordinates

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C	-2.626202	-1.492250	-1.221937
C	-1.691389	-0.564779	-1.710624
C	-0.686587	-0.992177	-2.592615
C	-0.628288	-2.329357	-2.987788
C	-1.550985	-3.257850	-2.496510
C	-2.541848	-2.834289	-1.611501
H	0.036796	-0.270786	-2.960347
H	-1.498182	-4.297963	-2.805218
C	-1.707046	0.849619	-1.293648
C	-3.768183	-1.281428	-0.237560
C	-4.109924	-2.743448	0.203950
H	-5.174791	-2.851187	0.421684
H	-3.556545	-2.992404	1.108617
C	-3.638414	-3.645577	-0.960014
O	-2.830849	1.539277	-1.500214
C	-1.177606	2.888123	-0.471978
N	-0.732328	1.489928	-0.733452
C	-3.429890	-0.346284	0.912892
C	-2.229094	-0.236607	1.630689
C	-2.076555	0.798892	2.566177
C	-3.127680	1.683116	2.808229
C	-4.336905	1.554521	2.117056
C	-4.474181	0.550320	1.159057
H	-1.136332	0.910957	3.092244
H	-5.153764	2.243425	2.312408
C	-1.126432	-1.201998	1.461479
C	-5.014820	-0.583988	-0.882272
H	-5.704478	-1.318204	-1.304864
H	-4.690087	0.074710	-1.687554
C	-5.645954	0.258665	0.250082
O	-1.407066	-2.477549	1.759271
C	0.878868	-2.206176	1.248725
H	1.407454	-2.397494	0.314600
N	0.092698	-0.956403	1.105679
C	-0.220740	-3.265909	1.454319
H	-0.437066	-3.836461	0.547540
H	-0.050964	-3.942713	2.291261
C	-2.666412	2.849218	-0.875208
H	-3.340792	2.880242	-0.018991
H	-2.956756	3.598772	-1.610762
H	-2.999477	2.474181	3.539574
H	-4.445449	-3.822609	-1.682272
H	-3.297856	-4.628416	-0.620788

H	-6.409745	-0.310625	0.794874
H	-6.131935	1.164979	-0.122613
H	0.137274	-2.645057	-3.689805
H	-1.072150	3.065469	0.599515
Fe	0.917792	0.808300	0.354951
Cl	1.080258	2.314473	2.058363
C	2.846387	0.280033	0.017567
C	3.451177	-0.738988	-0.771306
C	2.638626	-1.551802	-1.604787
C	4.848103	-1.002026	-0.727390
C	3.189697	-2.581358	-2.348060
H	1.580170	-1.338028	-1.662216
C	5.395624	-2.037810	-1.468298
H	5.485494	-0.393742	-0.095065
C	4.568282	-2.825992	-2.278679
H	2.559373	-3.195782	-2.982016
H	6.460774	-2.237439	-1.423977
H	5.001018	-3.634090	-2.860503
C	3.758522	1.226225	0.690381
O	4.057801	2.250122	0.100127
O	4.140326	0.879745	1.915549
C	4.797448	1.917118	2.689181
H	4.088781	2.728182	2.865024
H	5.081200	1.439298	3.624496
H	5.674305	2.288941	2.157735
C	1.920091	-2.074422	2.374969
H	2.523024	-1.192812	2.123666
C	2.849154	-3.293180	2.374992
H	3.636377	-3.175159	3.124333
H	2.308623	-4.216347	2.614326
H	3.329861	-3.427216	1.399412
C	1.287864	-1.817625	3.745949
H	0.684948	-0.905753	3.740019
H	0.654505	-2.650993	4.070087
H	2.068133	-1.690071	4.501039
C	-0.302507	3.912874	-1.216551
H	0.733306	3.670613	-0.935601
C	-0.592204	5.325351	-0.696062
H	0.053302	6.058170	-1.187564
H	-1.629967	5.617335	-0.896167
H	-0.419417	5.389947	0.382174
C	-0.445255	3.838680	-2.743636
H	-0.342579	2.819993	-3.132247
H	-1.419397	4.213705	-3.073147
H	0.312596	4.461958	-3.227202
O	1.716910	1.262646	-2.570258
C	2.989955	1.568186	-3.152354
H	2.881638	2.219337	-4.027362
H	3.658437	2.033879	-2.420963
H	3.422005	0.619821	-3.476971
H	1.293601	2.093282	-2.324193

E

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.2938146
Zero-point correction= 0.786076 (Hartree/Particle)

Thermal correction to Energy= 0.834123
Thermal correction to Enthalpy= 0.835067
Thermal correction to Gibbs Free Energy= 0.703105
Sum of electronic and zero-point Energies= -2582.507738
Sum of electronic and thermal Energies= -2582.459692
Sum of electronic and thermal Enthalpies= -2582.458748
Sum of electronic and thermal Free Energies= -2582.590710

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Cartesian Coordinates

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C	-2.634869	-1.536663	-1.192266
C	-1.746131	-0.556680	-1.664675
C	-0.768692	-0.912646	-2.607691
C	-0.678230	-2.222442	-3.074753
C	-1.554855	-3.202331	-2.596648
C	-2.523748	-2.854137	-1.656848
H	-0.105709	-0.142721	-2.989215
H	-1.482179	-4.223975	-2.958093
C	-1.780212	0.833328	-1.182248
C	-3.730543	-1.423693	-0.139762
C	-3.988477	-2.920492	0.241335
H	-5.033177	-3.083255	0.515166
H	-3.370344	-3.193724	1.095199
C	-3.557892	-3.737503	-0.998162
O	-2.972603	1.436362	-1.173313
C	-1.276868	2.912589	-0.476546
N	-0.769812	1.531420	-0.773615
C	-3.378227	-0.535264	1.043218
C	-2.134410	-0.359097	1.667514
C	-1.995831	0.616131	2.667401
C	-3.101980	1.366248	3.066789
C	-4.348564	1.174757	2.460042
C	-4.473099	0.241882	1.431083
H	-1.026466	0.780763	3.122131
H	-5.203459	1.768371	2.770859
C	-0.993212	-1.234524	1.345229
C	-5.049240	-0.762977	-0.666750
H	-5.708985	-1.503564	-1.125000
H	-4.808547	-0.011466	-1.418085
C	-5.675001	-0.076134	0.570308
O	-1.217827	-2.544591	1.554209
C	1.006335	-2.158294	0.921784
H	1.504840	-2.249332	-0.043007
N	0.186105	-0.916559	0.925155
C	-0.053969	-3.262086	1.066928
H	-0.326745	-3.717960	0.111268
H	0.189809	-4.034998	1.795255
C	-2.799764	2.698390	-0.460154
H	-3.209465	2.560314	0.540821
H	-3.366713	3.455352	-0.999435
H	-2.987165	2.108271	3.849942
H	-4.398802	-3.896461	-1.685221
H	-3.169917	-4.727156	-0.739507
H	-6.353423	-0.754402	1.103378
H	-6.256265	0.812205	0.307187
H	0.065794	-2.478527	-3.822558

H	-0.907468	3.196478	0.510413
Fe	1.040123	0.951277	0.208603
Cl	1.149282	2.205161	2.106303
C	2.959427	0.265284	-0.010230
C	3.563899	-0.646902	-0.920960
C	2.758032	-1.277186	-1.908150
C	4.945232	-0.985455	-0.864215
C	3.300524	-2.194318	-2.791846
H	1.704741	-1.026956	-1.956155
C	5.481261	-1.914486	-1.741783
H	5.575175	-0.525336	-0.110774
C	4.662194	-2.515654	-2.706792
H	2.676719	-2.666869	-3.542962
H	6.532747	-2.174553	-1.685786
H	5.087724	-3.238992	-3.395423
C	3.869820	1.088204	0.814656
O	4.190129	2.202261	0.411414
O	4.246427	0.560004	1.969195
C	4.904624	1.465855	2.896540
H	4.217011	2.274908	3.147434
H	5.131408	0.858925	3.770293
H	5.814872	1.866933	2.449590
C	2.077347	-2.120453	2.025867
H	2.651385	-1.202597	1.861522
C	3.038187	-3.303643	1.870002
H	3.845372	-3.240836	2.604781
H	2.531758	-4.263327	2.024931
H	3.491461	-3.320527	0.872298
C	1.484631	-2.025022	3.434975
H	0.862725	-1.132584	3.542145
H	0.880036	-2.902567	3.689193
H	2.287195	-1.957513	4.174484
C	-0.804481	3.957782	-1.506508
H	0.285474	3.936082	-1.470081
C	-1.257299	5.357151	-1.068372
H	-0.854373	6.115783	-1.745266
H	-2.348410	5.461259	-1.081003
H	-0.906978	5.589674	-0.057559
C	-1.260236	3.640507	-2.935434
H	-0.951051	2.638642	-3.249988
H	-2.348694	3.700779	-3.044141
H	-0.826796	4.357016	-3.639058
O	1.988425	2.621983	-1.139944
C	2.259705	2.397022	-2.524838
H	2.648808	3.305543	-2.994510
H	2.974644	1.579625	-2.671005
H	1.312613	2.135168	-2.998848
H	2.835050	2.772718	-0.667956

TS(E-B)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2941833
Zero-point correction= 0.785384 (Hartree/Particle)
Thermal correction to Energy= 0.832925
Thermal correction to Enthalpy= 0.833869
Thermal correction to Gibbs Free Energy= 0.702379

Sum of electronic and zero-point Energies= -2582.508799
Sum of electronic and thermal Energies= -2582.461258
Sum of electronic and thermal Enthalpies= -2582.460314
Sum of electronic and thermal Free Energies= -2582.591804

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Cartesian Coordinates

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C	-2.961013	0.073800	1.587290
C	-1.621815	-0.311945	1.751387
C	-0.810904	0.397023	2.651592
C	-1.341698	1.451131	3.394709
C	-2.678696	1.831347	3.235628
C	-3.476502	1.149160	2.319927
H	0.223155	0.098479	2.778324
H	-3.084691	2.656576	3.813475
C	-1.042345	-1.455871	1.017797
C	-3.993734	-0.462731	0.608903
C	-5.059840	0.682888	0.579346
H	-6.063442	0.285055	0.413011
H	-4.832677	1.375678	-0.229856
C	-4.916225	1.406640	1.938710
O	-1.659307	-2.635805	1.189463
C	0.253992	-2.854342	-0.174641
N	-0.001214	-1.454473	0.257404
C	-3.412893	-0.814717	-0.751637
C	-2.405325	-0.156476	-1.477267
C	-1.921164	-0.738255	-2.660354
C	-2.453176	-1.940839	-3.122322
C	-3.467221	-2.587149	-2.408664
C	-3.931355	-2.026199	-1.218989
H	-1.122600	-0.251637	-3.206217
H	-3.876896	-3.526253	-2.769766
C	-1.819608	1.119840	-1.037725
C	-4.647035	-1.813727	1.057668
H	-5.532234	-1.640200	1.673975
H	-3.933013	-2.388696	1.646380
C	-4.961562	-2.568179	-0.254687
O	-2.674486	2.104022	-0.721368
C	-0.462749	2.880667	-0.704626
H	0.283475	3.053515	0.074222
N	-0.559934	1.418171	-0.965971
C	-1.875068	3.201489	-0.191465
H	-1.956347	3.164563	0.897703
H	-2.298638	4.129924	-0.571778
C	-1.019776	-3.587398	0.290739
H	-1.718805	-3.781910	-0.525195
H	-0.838405	-4.500783	0.856973
H	-2.068240	-2.375074	-4.038859
H	-5.584977	0.975017	2.694368
H	-5.154211	2.472534	1.876735
H	-5.971860	-2.337758	-0.616249
H	-4.906488	-3.654530	-0.138645
H	-0.718017	1.974100	4.111448
H	0.332361	-2.858313	-1.263725
C	-0.048686	3.646173	-1.980276
H	0.884767	3.180206	-2.308390

C	0.238561	5.113109	-1.636561
H	0.606081	5.648905	-2.516145
H	-0.662619	5.635045	-1.294365
H	0.994162	5.200190	-0.847837
C	-1.064313	3.516740	-3.120784
H	-1.233646	2.471577	-3.393806
H	-2.030908	3.965741	-2.868417
H	-0.691336	4.030433	-4.011233
C	1.576284	-3.379827	0.414655
H	2.353525	-2.711010	0.032105
C	1.874402	-4.786594	-0.115637
H	2.859669	-5.122700	0.220077
H	1.143807	-5.519679	0.244337
H	1.864013	-4.808632	-1.210201
C	1.618889	-3.314920	1.944221
H	1.485505	-2.290068	2.302741
H	0.843759	-3.938885	2.402787
H	2.584044	-3.674664	2.312722
Fe	1.059220	0.102446	-0.776599
C	2.726903	0.389503	0.554879
C	4.013882	-0.195548	0.433999
C	4.260939	-1.148759	-0.596686
C	5.089955	0.145468	1.309199
C	5.506724	-1.740411	-0.727941
H	3.468889	-1.368359	-1.304904
C	6.323937	-0.465538	1.183279
H	4.927680	0.868989	2.099971
C	6.532596	-1.408268	0.164729
H	5.686010	-2.456505	-1.522564
H	7.131014	-0.213898	1.862714
H	7.505802	-1.879386	0.064626
C	2.560455	1.475640	1.541063
O	2.455971	2.663538	1.243107
O	2.469348	1.017885	2.793387
C	2.238762	2.018285	3.818048
H	1.402176	2.657369	3.536517
H	2.021190	1.454534	4.723015
H	3.135144	2.627460	3.947558
O	2.559074	1.927997	-1.292683
C	3.690828	1.879527	-2.167727
H	3.837890	2.854836	-2.641678
H	4.600103	1.595704	-1.625308
H	3.464116	1.128078	-2.922770
H	2.672213	2.579970	-0.571036
Cl	1.556857	-0.914149	-2.789954

(*R*)-TS(D_f-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2812.6676872
Zero-point correction= 0.859867 (Hartree/Particle)
Thermal correction to Energy= 0.912872
Thermal correction to Enthalpy= 0.913816
Thermal correction to Gibbs Free Energy= 0.772550
Sum of electronic and zero-point Energies= -2811.807820

Sum of electronic and thermal Energies= -2811.754815
Sum of electronic and thermal Enthalpies= -2811.753871
Sum of electronic and thermal Free Energies= -2811.895138

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Cartesian Coordinates

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C	2.075218	-0.930431	-2.073977
C	1.018972	-1.383188	-1.268887
C	-0.288587	-1.385703	-1.776863
C	-0.537831	-0.948123	-3.078006
C	0.511025	-0.484945	-3.878165
C	1.811537	-0.478161	-3.371548
H	-1.099552	-1.762374	-1.164808
H	0.315495	-0.142478	-4.890416
C	1.239685	-1.746221	0.141029
C	3.560373	-0.840715	-1.752790
C	4.083001	0.115993	-2.874431
H	5.114549	-0.118346	-3.147099
H	4.059449	1.145052	-2.515232
C	3.093040	-0.050623	-4.050875
O	2.117627	-2.707362	0.428941
C	1.240811	-1.698614	2.396774
N	0.678732	-1.148508	1.138108
C	3.896721	-0.385576	-0.339242
C	3.285646	0.610208	0.434446
C	3.682579	0.787757	1.769198
C	4.706900	0.008003	2.307221
C	5.343438	-0.960803	1.524011
C	4.920477	-1.164802	0.211529
H	3.203148	1.554245	2.369102
H	6.148508	-1.558318	1.941751
C	2.341528	1.588679	-0.146406
C	4.264622	-2.239193	-1.824840
H	4.605272	-2.461239	-2.838794
H	3.557903	-3.015738	-1.529377
C	5.415232	-2.176121	-0.796066
O	2.925470	2.454949	-0.998429
C	0.678104	3.023123	-0.594478
H	-0.207421	2.803195	-1.190459
N	1.090918	1.771547	0.099114
C	1.881971	3.324074	-1.507903
H	1.705770	3.052689	-2.552437
H	2.249681	4.348631	-1.452364
C	2.257155	-2.748233	1.882738
H	3.291352	-2.497334	2.113468
H	2.038227	-3.768335	2.198258
H	5.014674	0.164036	3.336026
H	3.422846	-0.834537	-4.744412
H	2.980611	0.864125	-4.640674
H	6.345968	-1.820561	-1.256129
H	5.633345	-3.150645	-0.350013

H	-1.553371	-0.974686	-3.458909
H	1.764668	-0.879094	2.898060
Fe	-0.518365	0.552082	0.949090
Cl	-1.071462	1.662306	2.930226
C	0.331711	4.126117	0.427597
H	-0.512425	3.741443	1.011997
C	-0.110248	5.402967	-0.301794
H	-0.520596	6.129912	0.406059
H	0.728244	5.895147	-0.805376
H	-0.866124	5.200701	-1.071581
C	1.468389	4.404535	1.414740
H	1.677712	3.521051	2.021588
H	2.389425	4.708638	0.904454
H	1.188641	5.212307	2.096401
C	0.165343	-2.243224	3.348696
H	-0.491146	-1.390966	3.561267
C	0.804926	-2.677882	4.672933
H	0.037112	-2.999952	5.381506
H	1.491509	-3.520855	4.532455
H	1.363950	-1.857676	5.134619
C	-0.658926	-3.367930	2.714809
H	-1.069185	-3.058715	1.750357
H	-0.060580	-4.271290	2.556352
H	-1.492251	-3.648302	3.365118
C	-3.291287	-0.460472	-0.134299
C	-3.888153	-1.675073	-0.767046
C	-4.957024	-1.570735	-1.672171
C	-3.404746	-2.953862	-0.448659
C	-5.500925	-2.708684	-2.262697
H	-5.355363	-0.594200	-1.923809
C	-3.958654	-4.091968	-1.034601
H	-2.592286	-3.055459	0.260962
C	-5.005946	-3.975718	-1.947145
H	-6.322984	-2.605742	-2.964305
H	-3.567967	-5.071140	-0.774906
H	-5.438101	-4.860996	-2.401979
C	-2.734832	0.585988	-0.923385
O	-1.800837	1.347999	-0.508979
O	-3.295171	0.808775	-2.112561
C	-2.781431	1.899964	-2.901401
H	-2.987684	2.853317	-2.410909
H	-1.708360	1.775856	-3.061717
H	-3.316102	1.838903	-3.847936
C	-3.125548	-1.029604	2.199723
H	-2.378717	-1.358566	2.914199
H	-3.625375	-0.144352	2.592393
O	-2.424826	-0.727484	0.976949
H	-2.416232	3.036017	-0.219737
H	-4.458932	0.339522	0.440001
O	-3.046666	3.762750	-0.039247
H	-2.526825	4.574495	0.008323

H	-4.717786	1.713402	1.594747
O	-5.249088	0.904114	1.049716
H	-5.949612	1.259104	0.483776
O	-3.989699	2.655508	2.179613
H	-3.177243	2.307646	2.608347
H	-3.657593	3.233396	1.443936
H	-3.853536	-1.824333	2.022477

(*S*)-TS(D_f-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2812.6724125
Zero-point correction= 0.860019 (Hartree/Particle)
Thermal correction to Energy= 0.912522
Thermal correction to Enthalpy= 0.913466
Thermal correction to Gibbs Free Energy= 0.773535
Sum of electronic and zero-point Energies= -2811.812394
Sum of electronic and thermal Energies= -2811.759891
Sum of electronic and thermal Enthalpies= -2811.758947
Sum of electronic and thermal Free Energies= -2811.898878

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Cartesian Coordinates

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C	2.829273	-1.465265	1.581709
C	1.972362	-0.364686	1.745018
C	0.855429	-0.483130	2.587756
C	0.623731	-1.664534	3.289345
C	1.493319	-2.752476	3.148237
C	2.579979	-2.651773	2.281078
H	0.177270	0.356816	2.673324
H	1.308688	-3.673660	3.693402
C	2.189851	0.906707	1.029941
C	3.992126	-1.635891	0.613212
C	4.171854	-3.191008	0.568635
H	5.219983	-3.462814	0.425297
H	3.599879	-3.605295	-0.260100
C	3.595103	-3.707551	1.907968
O	3.407890	1.455423	1.139657
C	1.979756	2.783240	-0.194122
N	1.330349	1.543981	0.307531
C	3.738719	-0.989075	-0.742504
C	2.535738	-0.893495	-1.463119
C	2.482267	-0.084271	-2.611767
C	3.626290	0.571926	-3.061359
C	4.833504	0.446486	-2.364484
C	4.876438	-0.314978	-1.196709
H	1.544030	0.021270	-3.145132
H	5.722821	0.960776	-2.717562
C	1.318236	-1.613093	-1.066364
C	5.319877	-0.943511	1.072257
H	5.926493	-1.616764	1.682180
H	5.088362	-0.062550	1.669552

C	6.025529	-0.511801	-0.234539
O	1.451667	-2.911145	-0.764046
C	-0.808000	-2.301985	-0.829262
H	-1.568922	-2.033073	-0.096841
N	0.109347	-1.142983	-1.030599
C	0.152302	-3.365119	-0.280078
H	0.202848	-3.381104	0.811308
H	-0.009165	-4.369531	-0.668160
C	3.448946	2.599656	0.237342
H	4.107739	2.334251	-0.590583
H	3.867706	3.438670	0.792935
H	3.574453	1.183851	-3.955661
H	4.372290	-3.768248	2.680446
H	3.156175	-4.705655	1.820812
H	6.695505	-1.297919	-0.605438
H	6.632889	0.388927	-0.107370
H	-0.235661	-1.739885	3.948387
H	1.885749	2.788252	-1.281062
Fe	-0.485314	0.808518	-0.558148
Cl	-0.550350	2.342508	-2.377732
C	-1.506359	-2.694406	-2.147991
H	-1.997292	-1.786560	-2.501952
C	-2.591903	-3.743296	-1.876118
H	-3.131081	-3.979929	-2.797670
H	-2.163995	-4.681823	-1.504309
H	-3.317956	-3.386854	-1.140070
C	-0.533018	-3.151027	-3.241198
H	0.215444	-2.386034	-3.466847
H	-0.007422	-4.072415	-2.969331
H	-1.082083	-3.352946	-4.165064
C	1.289001	4.044638	0.351880
H	0.244446	3.963360	0.033296
C	1.879862	5.297833	-0.303391
H	1.345457	6.194910	0.022636
H	2.934511	5.435198	-0.038573
H	1.806497	5.240649	-1.393514
C	1.329953	4.123482	1.882553
H	0.863159	3.249031	2.347106
H	2.354498	4.190704	2.262728
H	0.818767	5.025507	2.239929
C	-3.483121	0.303745	0.168009
C	-4.469733	-0.810927	0.320080
C	-5.694595	-0.775457	-0.360714
C	-4.167760	-1.939096	1.100233
C	-6.584131	-1.847534	-0.283873
H	-5.953638	0.100109	-0.948045
C	-5.060940	-3.004448	1.190807
H	-3.231510	-1.971559	1.650344
C	-6.268766	-2.964250	0.490396
H	-7.526406	-1.806042	-0.820895
H	-4.815594	-3.866457	1.803524

H	-6.963265	-3.795697	0.555505
C	-2.726096	0.754172	1.275090
O	-1.548097	1.253783	1.169025
O	-3.337844	0.725984	2.459633
C	-2.696803	1.360182	3.581369
H	-2.598939	2.433984	3.407755
H	-1.715008	0.920465	3.768897
H	-3.357664	1.173673	4.426147
C	-3.250638	0.348663	-2.258320
H	-2.452290	0.357091	-2.997271
H	-3.797860	1.291784	-2.313732
O	-2.613996	0.188795	-0.978828
H	-1.565197	3.023004	1.477528
H	-4.252440	1.611462	-0.090817
O	-1.924930	3.934494	1.471065
H	-1.236447	4.504680	1.833993
H	-3.849380	3.264812	-0.776538
O	-4.718806	2.561242	-0.502205
H	-5.313276	2.961157	0.149192
O	-2.830099	3.980928	-1.010826
H	-2.163091	3.519355	-1.574345
H	-2.399551	4.125571	-0.126434
H	-3.936052	-0.483487	-2.437943

(*R*)-TS(D_b-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2812.658333
Zero-point correction= 0.859348 (Hartree/Particle)
Thermal correction to Energy= 0.912665
Thermal correction to Enthalpy= 0.913609
Thermal correction to Gibbs Free Energy= 0.769772
Sum of electronic and zero-point Energies= -2811.798985
Sum of electronic and thermal Energies= -2811.745668
Sum of electronic and thermal Enthalpies= -2811.744724
Sum of electronic and thermal Free Energies= -2811.888562

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Cartesian Coordinates

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C	2.313226	1.839801	-1.425415
C	1.314948	0.872185	-1.617113
C	-0.018572	1.278056	-1.782088
C	-0.340682	2.636376	-1.780209
C	0.657152	3.602596	-1.615190
C	1.979389	3.197429	-1.430598
H	-0.793145	0.535369	-1.937530
H	0.401496	4.658564	-1.618059
C	1.614324	-0.575142	-1.599156
C	3.781484	1.629858	-1.085387
C	4.226527	3.046607	-0.587364
H	5.255767	3.262449	-0.882232
H	4.176079	3.086298	0.500218

C	3.207514	4.044566	-1.188920
O	2.418622	-1.062887	-2.548700
C	1.668761	-2.776980	-1.081763
N	1.161814	-1.428027	-0.743425
C	3.977869	0.518264	-0.063600
C	3.203848	0.227550	1.071533
C	3.444950	-0.958944	1.785094
C	4.469978	-1.818840	1.391023
C	5.259573	-1.514894	0.277633
C	5.001641	-0.352528	-0.449470
H	2.825447	-1.206051	2.640718
H	6.057093	-2.187143	-0.025843
C	2.078113	1.073326	1.502746
C	4.645432	1.137365	-2.296319
H	5.110029	1.977522	-2.816941
H	4.010498	0.612796	-3.010024
C	5.677900	0.149691	-1.703980
O	2.295956	2.372078	1.727093
C	0.086041	1.769511	2.297316
H	-0.858263	1.852940	1.752892
N	0.871431	0.654135	1.717717
C	0.996514	2.979628	2.010583
H	0.701231	3.532148	1.116574
H	1.131048	3.658003	2.851814
C	2.601097	-2.487821	-2.282388
H	3.656470	-2.640022	-2.051706
H	2.336605	-3.023006	-3.194745
H	4.649366	-2.727887	1.955465
H	3.566506	4.459100	-2.139412
H	3.013628	4.894061	-0.527265
H	6.614803	0.657674	-1.442529
H	5.937372	-0.654073	-2.399307
H	-1.376174	2.935041	-1.908988
H	2.247747	-3.136824	-0.226119
Fe	0.120658	-1.105661	0.985785
Cl	0.133016	-2.717680	2.639096
C	-0.212456	1.506414	3.787915
H	-0.707000	0.529387	3.824501
C	-1.186633	2.562952	4.321888
H	-1.473327	2.336653	5.352527
H	-0.736200	3.562142	4.323821
H	-2.098599	2.610965	3.716646
C	1.053220	1.405568	4.645872
H	1.718210	0.615220	4.287599
H	1.614078	2.346098	4.666253
H	0.786429	1.164691	5.678375
C	0.510740	-3.759574	-1.337508
H	-0.037004	-3.827592	-0.389129
C	1.059693	-5.155062	-1.654432
H	0.242357	-5.876774	-1.733246
H	1.600556	-5.171314	-2.607794

H	1.740943	-5.504776	-0.871700
C	-0.463707	-3.257762	-2.408004
H	-0.912022	-2.302979	-2.122627
H	0.026383	-3.134671	-3.381213
H	-1.271224	-3.983289	-2.544124
C	-3.363329	0.037200	-0.969575
C	-4.186631	1.271271	-1.157804
C	-5.150604	1.691980	-0.223975
C	-4.040487	2.010942	-2.342800
C	-5.923387	2.826968	-0.461413
H	-5.274196	1.148973	0.706661
C	-4.817560	3.145167	-2.576658
H	-3.309737	1.689007	-3.075598
C	-5.762692	3.560005	-1.638604
H	-6.656347	3.138454	0.276702
H	-4.684151	3.703328	-3.498410
H	-6.369628	4.440371	-1.822795
C	-2.678032	-0.266219	0.224232
O	-1.770725	-1.167810	0.296697
O	-3.081131	0.363408	1.345522
C	-3.033079	-0.385842	2.581360
H	-3.808398	-1.157082	2.570602
H	-2.061591	-0.854763	2.738229
H	-3.234806	0.339927	3.366954
C	-3.460678	-1.188698	-3.017761
H	-2.837222	-1.359334	-3.896677
H	-3.731832	-2.154420	-2.575074
O	-2.680572	-0.407855	-2.113247
H	-2.166327	-2.907301	0.465130
H	-4.508516	-0.964754	-0.615057
O	-2.426575	-3.740892	0.908111
H	-1.791217	-3.784701	1.647160
H	-5.225946	-2.290625	0.405107
O	-5.416950	-1.613761	-0.419866
H	-6.159060	-1.019904	-0.230808
O	-4.846080	-3.098247	1.448834
H	-5.406304	-3.870747	1.600758
H	-3.891495	-3.433056	1.307101
H	-4.372076	-0.658724	-3.317623

(*R*)-TS(D_c-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2812.6352195
Zero-point correction= 0.858594 (Hartree/Particle)
Thermal correction to Energy= 0.912151
Thermal correction to Enthalpy= 0.913096
Thermal correction to Gibbs Free Energy= 0.767846
Sum of electronic and zero-point Energies= -2811.776626
Sum of electronic and thermal Energies= -2811.723068
Sum of electronic and thermal Enthalpies= -2811.722124
Sum of electronic and thermal Free Energies= -2811.867374

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Cartesian Coordinates
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C	-1.710971	-1.986136	-1.586200
C	-0.920438	-0.822968	-1.556890
C	0.478195	-0.943694	-1.530778
C	1.082154	-2.200173	-1.571922
C	0.293877	-3.353246	-1.633119
C	-1.095174	-3.241440	-1.626180
H	1.084763	-0.046934	-1.483344
H	0.764358	-4.332198	-1.663108
C	-1.516683	0.521880	-1.507397
C	-3.220396	-2.126119	-1.442596
C	-3.385074	-3.633503	-1.050114
H	-4.319361	-4.043945	-1.439916
H	-3.402482	-3.729400	0.035198
C	-2.131134	-4.341304	-1.609891
O	-2.443630	0.808011	-2.424432
C	-2.067583	2.660722	-1.003664
N	-1.238829	1.468874	-0.665068
C	-3.819877	-1.168365	-0.425331
C	-3.292394	-0.750396	0.808166
C	-3.968540	0.235548	1.544408
C	-5.163092	0.773798	1.066398
C	-5.697093	0.344681	-0.152465
C	-5.014390	-0.616401	-0.897791
H	-3.551759	0.586743	2.480045
H	-6.627567	0.767518	-0.520751
C	-2.032490	-1.299483	1.348376
C	-4.029380	-1.797791	-2.741636
H	-4.166610	-2.689886	-3.357146
H	-3.489940	-1.060614	-3.334846
C	-5.366110	-1.193572	-2.250223
O	-1.971967	-2.622512	1.534390
C	0.018290	-1.567553	2.254682
H	0.958876	-1.455078	1.709882
N	-0.973766	-0.630406	1.675453
C	-0.610519	-2.942820	1.950551
H	-0.130171	-3.450598	1.112274
H	-0.681688	-3.611169	2.808354
C	-3.009997	2.110243	-2.093338
H	-4.025157	1.935137	-1.733306
H	-3.030563	2.697886	-3.010697
H	-5.673350	1.533340	1.649150
H	-2.301252	-4.710077	-2.629601
H	-1.828109	-5.202503	-1.007215
H	-6.136748	-1.966717	-2.137370
H	-5.768069	-0.445582	-2.940138
H	2.162081	-2.276888	-1.540680
H	-2.630949	2.936287	-0.108269
Fe	-0.606309	1.357822	1.279187

Cl	-1.793623	2.682962	2.689927
C	0.250270	-1.255975	3.746703
H	0.576356	-0.208088	3.786385
C	1.385440	-2.126947	4.296877
H	1.611187	-1.858308	5.332427
H	1.116685	-3.189550	4.288516
H	2.300717	-2.007868	3.707592
C	-1.025510	-1.367765	4.587275
H	-1.802498	-0.691393	4.221731
H	-1.426234	-2.387464	4.589195
H	-0.817375	-1.099420	5.626603
C	-1.196105	3.857907	-1.419092
H	-0.559641	4.068130	-0.552633
C	-2.074526	5.089999	-1.666196
H	-1.454605	5.967072	-1.871843
H	-2.735059	4.951860	-2.529890
H	-2.698034	5.315626	-0.795127
C	-0.289756	3.543415	-2.612606
H	0.367517	2.696065	-2.399865
H	-0.867452	3.312591	-3.514703
H	0.341075	4.405754	-2.848099
C	3.446762	-0.015620	-0.002223
C	3.948526	-0.330155	-1.303245
O	4.254558	-1.485481	-1.675296
O	4.215307	0.744909	-2.100474
C	4.732831	0.451541	-3.411149
H	5.741453	0.035892	-3.349665
H	4.084424	-0.256585	-3.930904
H	4.750601	1.406953	-3.934610
C	4.264524	-1.786960	1.366073
H	3.893987	-2.676809	1.880446
H	4.989068	-2.097017	0.604239
O	3.140046	-1.152880	0.774382
H	5.798098	-1.816831	-1.937085
H	4.954727	0.641692	0.436592
O	6.799760	-1.847598	-1.941671
H	7.076100	-2.750864	-2.135136
H	6.757379	0.313568	0.334708
O	5.903092	1.055026	0.664844
H	5.962828	1.902981	0.200865
O	7.627560	-0.477693	-0.014077
H	7.975639	-1.005585	0.715591
H	7.343219	-1.098619	-0.794062
H	4.754697	-1.130151	2.099172
C	1.492544	2.353737	2.189079
C	1.402065	3.517172	1.406480
C	2.109061	1.200528	1.685478
H	1.110030	2.357408	3.205563
C	1.960879	3.498947	0.127200
H	0.907330	4.398252	1.797449
C	2.702861	1.179631	0.395151

H	2.214634	0.328776	2.315443
C	2.593868	2.362893	-0.374442
H	1.903449	4.384161	-0.498322
H	3.019895	2.389638	-1.367197

Cartesian coordinates of solvent optimization geometries

(*R*)-TS(D_f-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2812.7531036
Zero-point correction= 0.859689 (Hartree/Particle)
Thermal correction to Energy= 0.912231
Thermal correction to Enthalpy= 0.913175
Thermal correction to Gibbs Free Energy= 0.773984
Sum of electronic and zero-point Energies= -2811.893415
Sum of electronic and thermal Energies= -2811.840872
Sum of electronic and thermal Enthalpies= -2811.839928
Sum of electronic and thermal Free Energies= -2811.979120
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Cartesian Coordinates
.....

C	2.035306	-0.919153	-2.096736
C	0.993764	-1.398520	-1.287597
C	-0.316669	-1.424875	-1.789287
C	-0.583199	-0.975514	-3.083216
C	0.451636	-0.487764	-3.887413
C	1.755002	-0.462606	-3.389772
H	-1.116747	-1.812280	-1.169654
H	0.241191	-0.135784	-4.893478
C	1.235222	-1.792068	0.112295
C	3.524040	-0.817446	-1.792865
C	4.017898	0.163113	-2.904754
H	5.053109	-0.044838	-3.185445
H	3.971336	1.187161	-2.532469
C	3.023445	-0.008754	-4.075407
O	2.109145	-2.767049	0.356781
C	1.248275	-1.834097	2.369193
N	0.690440	-1.224193	1.136461
C	3.878120	-0.388781	-0.374955
C	3.291896	0.607361	0.417830
C	3.691362	0.749208	1.756119
C	4.697917	-0.063564	2.278721
C	5.318111	-1.025617	1.474997
C	4.892069	-1.193374	0.158210
H	3.223157	1.510264	2.372488
H	6.109758	-1.649235	1.880598
C	2.368695	1.623054	-0.135562
C	4.230368	-2.212865	-1.906192
H	4.578259	-2.395868	-2.925575
H	3.520054	-2.999035	-1.646769
C	5.371998	-2.193163	-0.867293

O	2.974728	2.525321	-0.933479
C	0.728732	3.101817	-0.525082
H	-0.162434	2.935093	-1.130517
N	1.118743	1.809320	0.103830
C	1.939952	3.426597	-1.418305
H	1.768235	3.197025	-2.473225
H	2.318752	4.443895	-1.321226
C	2.256240	-2.866315	1.809571
H	3.293002	-2.631760	2.045415
H	2.035652	-3.898120	2.082106
H	5.002648	0.059842	3.313188
H	3.361224	-0.782461	-4.776634
H	2.889364	0.910228	-4.654062
H	6.314133	-1.849495	-1.312794
H	5.563636	-3.180483	-0.436743
H	-1.600763	-1.005727	-3.458130
H	1.775211	-1.043907	2.911337
Fe	-0.476320	0.500774	0.910420
Cl	-1.010981	1.560863	2.999997
C	0.404858	4.156562	0.553514
H	-0.431491	3.747837	1.132683
C	-0.043161	5.466125	-0.107755
H	-0.459620	6.152811	0.636148
H	0.795927	5.982714	-0.586731
H	-0.796720	5.299840	-0.887780
C	1.562297	4.395032	1.526243
H	1.843148	3.474531	2.044592
H	2.448668	4.787713	1.015412
H	1.270966	5.126972	2.285762
C	0.162308	-2.418421	3.286316
H	-0.482457	-1.572414	3.551406
C	0.796165	-2.945991	4.578208
H	0.022267	-3.284148	5.274030
H	1.456680	-3.799357	4.384166
H	1.383482	-2.169491	5.080134
C	-0.682674	-3.486399	2.586401
H	-1.100166	-3.107723	1.649807
H	-0.096440	-4.383299	2.357626
H	-1.514060	-3.799663	3.225343
C	-3.296802	-0.415878	-0.118042
C	-3.934110	-1.596022	-0.770010
C	-4.968761	-1.442026	-1.710618
C	-3.532459	-2.899175	-0.431091
C	-5.553970	-2.553525	-2.313112
H	-5.309157	-0.448337	-1.977663
C	-4.128055	-4.009462	-1.030456
H	-2.750274	-3.042197	0.304466
C	-5.138294	-3.844509	-1.977820
H	-6.346718	-2.409589	-3.041711
H	-3.797415	-5.006560	-0.753753
H	-5.601798	-4.708507	-2.443998

C	-2.725110	0.641928	-0.881460
O	-1.786732	1.384568	-0.439286
O	-3.270880	0.898604	-2.068071
C	-2.713011	1.973975	-2.852979
H	-2.910746	2.936692	-2.377445
H	-1.641057	1.826638	-2.995404
H	-3.229982	1.918768	-3.810245
C	-3.133973	-1.000513	2.212839
H	-2.410585	-1.426221	2.901473
H	-3.535625	-0.085611	2.650491
O	-2.436522	-0.728745	0.982247
H	-2.374255	3.124146	-0.201859
H	-4.459384	0.411119	0.476709
O	-3.018767	3.832673	-0.002664
H	-2.509787	4.652788	0.063676
H	-4.676785	1.755235	1.614115
O	-5.235512	0.990884	1.069979
H	-5.867765	1.410752	0.461806
O	-3.878203	2.684237	2.218478
H	-3.056501	2.286414	2.584110
H	-3.563436	3.264389	1.473517
H	-3.941626	-1.715655	2.039880

(*S*)-TS(D_f-P)$_{3w}$

Number of imaginary frequencies: 1 Electronic energy: HF=-2812.7534417
Zero-point correction= 0.860468 (Hartree/Particle)
Thermal correction to Energy= 0.912705
Thermal correction to Enthalpy= 0.913649
Thermal correction to Gibbs Free Energy= 0.773197
Sum of electronic and zero-point Energies= -2811.892974
Sum of electronic and thermal Energies= -2811.840737
Sum of electronic and thermal Enthalpies= -2811.839793
Sum of electronic and thermal Free Energies= -2811.980245

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Cartesian Coordinates

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C	2.951271	-1.258074	1.680439
C	1.996166	-0.234856	1.790826
C	0.867082	-0.432293	2.602404
C	0.721030	-1.612701	3.329510
C	1.688546	-2.620673	3.242758
C	2.788734	-2.443972	2.404795
H	0.112842	0.344328	2.648914
H	1.566644	-3.543417	3.803012
C	2.125323	1.031764	1.044918
C	4.148985	-1.344763	0.744457
C	4.485068	-2.874955	0.759271
H	5.561469	-3.038853	0.673399
H	4.000286	-3.368472	-0.081352
C	3.900593	-3.415859	2.085839

O	3.273036	1.707201	1.202576
C	1.788855	2.848543	-0.237320
N	1.250259	1.554132	0.255021
C	3.862475	-0.769394	-0.639095
C	2.675617	-0.823659	-1.393024
C	2.572590	-0.065254	-2.571037
C	3.652292	0.696703	-3.013422
C	4.843750	0.726534	-2.280716
C	4.934964	0.007678	-1.088883
H	1.646847	-0.083403	-3.134637
H	5.681240	1.327090	-2.624520
C	1.529914	-1.655618	-0.996300
C	5.388376	-0.506145	1.206750
H	6.047518	-1.098160	1.845776
H	5.053002	0.360542	1.774741
C	6.073159	-0.034318	-0.096068
O	1.810908	-2.914996	-0.646527
C	-0.509087	-2.569984	-0.718406
H	-1.264761	-2.354296	0.039153
N	0.273347	-1.326949	-0.992152
C	0.570662	-3.513815	-0.167653
H	0.615670	-3.531196	0.923021
H	0.531898	-4.529252	-0.557130
C	3.244037	2.829209	0.268894
H	3.968730	2.616508	-0.518229
H	3.546054	3.719874	0.819534
H	3.561375	1.271677	-3.929259
H	4.650558	-3.403728	2.887137
H	3.544604	-4.446712	1.998653
H	6.835202	-0.750695	-0.428625
H	6.571006	0.933335	0.016419
H	-0.151432	-1.751240	3.960464
H	1.752640	2.832547	-1.327174
Fe	-0.478760	0.613986	-0.599544
Cl	-0.633834	2.107350	-2.512726
C	-1.213361	-3.094989	-1.987959
H	-1.947163	-2.333043	-2.260559
C	-1.967722	-4.395913	-1.675602
H	-2.654973	-4.642028	-2.490809
H	-1.281983	-5.242873	-1.564018
H	-2.552832	-4.320106	-0.753461
C	-0.264308	-3.279761	-3.175945
H	0.208566	-2.337346	-3.466429
H	0.526880	-4.006189	-2.958295
H	-0.817768	-3.652141	-4.043545
C	0.945918	4.036931	0.258022
H	-0.067573	3.854341	-0.113655
C	1.449425	5.336194	-0.378677
H	0.809352	6.178842	-0.098086
H	2.468519	5.577624	-0.055066
H	1.449978	5.264989	-1.471449

C	0.899531	4.131658	1.786688
H	0.439292	3.245626	2.234544
H	1.899896	4.242935	2.219316
H	0.329817	5.012313	2.103749
C	-3.513811	0.150273	0.064752
C	-4.571196	-0.873719	0.312191
C	-4.476050	-2.149355	-0.264244
C	-5.707879	-0.572117	1.081345
C	-5.473602	-3.103078	-0.062533
H	-3.615203	-2.389273	-0.872395
C	-6.697835	-1.530302	1.291496
H	-5.813073	0.414131	1.520540
C	-6.588620	-2.800574	0.719776
H	-5.375719	-4.083549	-0.520001
H	-7.565961	-1.278645	1.893869
H	-7.367177	-3.540872	0.876369
C	-2.794964	0.746402	1.138304
O	-1.631484	1.260719	0.998296
O	-3.423503	0.820987	2.308644
C	-2.779777	1.505563	3.403249
H	-2.724560	2.576727	3.200025
H	-1.782743	1.100460	3.584998
H	-3.420267	1.321224	4.264832
C	-3.171347	-0.010031	-2.323444
H	-2.414006	-0.356069	-3.024649
H	-3.406096	1.030781	-2.546809
O	-2.608382	-0.151343	-1.003473
H	-1.810633	3.108336	1.220095
H	-4.310797	1.388596	-0.392599
O	-2.332094	3.933059	1.158622
H	-1.770464	4.637339	1.510980
H	-4.077457	2.979930	-1.151226
O	-4.856538	2.253805	-0.888423
H	-5.478151	2.650390	-0.254433
O	-3.024568	3.798813	-1.389800
H	-2.296671	3.294754	-1.823471
H	-2.690978	4.006207	-0.476599
H	-4.071580	-0.622398	-2.414116

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^{1CSS}**A**

Number of imaginary frequencies: 0 Electronic energy: HF=-2467.5092782
Zero-point correction= 0.735285 (Hartree/Particle)
Thermal correction to Energy= 0.777647
Thermal correction to Enthalpy= 0.778591
Thermal correction to Gibbs Free Energy= 0.661413
Sum of electronic and zero-point Energies= -2466.773993
Sum of electronic and thermal Energies= -2466.731632
Sum of electronic and thermal Enthalpies= -2466.730688
Sum of electronic and thermal Free Energies= -2466.847865
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Cartesian Coordinates

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C	-2.815935	-0.925920	-1.184163
C	-1.625483	-0.307502	-1.597170
C	-0.868583	-0.900945	-2.619100
C	-1.308116	-2.075345	-3.231586
C	-2.500816	-2.684066	-2.826391
C	-3.236930	-2.115681	-1.787821
H	0.051315	-0.432490	-2.948044
H	-2.838523	-3.598009	-3.306174
C	-1.252598	1.034785	-1.089822
C	-3.754592	-0.530789	-0.049789
C	-4.521027	-1.866908	0.218208
H	-5.529252	-1.680033	0.594728
H	-3.984043	-2.453193	0.964792
C	-4.505314	-2.616296	-1.134297
O	-2.121889	1.979013	-1.487929
C	-0.328811	2.949325	-0.344477
N	-0.243977	1.444257	-0.383562
C	-3.043410	0.039817	1.167095
C	-1.834919	-0.371392	1.749125
C	-1.260475	0.395969	2.777427
C	-1.906084	1.546492	3.235367
C	-3.125060	1.939853	2.678489
C	-3.685450	1.186554	1.644568
H	-0.323861	0.083731	3.230257
H	-3.622602	2.836618	3.035875
C	-1.042637	-1.452729	1.149082
C	-4.747636	0.621421	-0.431692
H	-5.681256	0.221129	-0.832955
H	-4.297961	1.251644	-1.198156
C	-4.953263	1.442209	0.863517
O	-1.582755	-2.653219	0.947678
C	0.621660	-2.520480	0.054271
H	0.836320	-2.270207	-0.988736
N	0.158418	-1.272399	0.709864
C	-0.636379	-3.421005	0.143660
H	-1.105798	-3.600186	-0.822616
H	-0.467218	-4.364541	0.660880
C	-1.763963	3.209981	-0.800036
H	-2.459266	3.327159	0.035667
H	-1.881250	4.032238	-1.504227
H	-1.444177	2.137728	4.017908
H	-5.374453	-2.349877	-1.749097
H	-4.521761	-3.703287	-1.014676
H	-5.817813	1.080586	1.434532
H	-5.127227	2.504178	0.666830
H	-0.719082	-2.514075	-4.030478
H	-0.184590	3.261245	0.684609
Fe	0.981657	0.508847	0.950392
Cl	1.603908	2.445474	1.987521

C	2.550163	0.140043	0.209705
C	3.173979	0.099350	-1.071669
C	2.462408	0.589256	-2.193109
C	4.471912	-0.439464	-1.273643
C	3.019463	0.555628	-3.460577
H	1.480769	1.002098	-2.021846
C	5.018393	-0.482300	-2.548886
H	5.034502	-0.813940	-0.428553
C	4.299145	0.015329	-3.641466
H	2.468619	0.950233	-4.308081
H	6.009730	-0.897166	-2.697213
H	4.737875	-0.014738	-4.633879
C	3.152635	-0.240691	1.516400
O	2.289365	-0.383558	2.400700
O	4.446827	-0.318690	1.724362
C	4.865443	-0.512690	3.106929
H	4.513541	-1.481979	3.463092
H	5.951725	-0.473539	3.080972
H	4.452058	0.287052	3.722174
C	1.881410	-3.149556	0.675768
H	2.681343	-2.408396	0.577966
C	2.309687	-4.366219	-0.156937
H	3.248251	-4.777494	0.224069
H	1.565392	-5.169010	-0.115660
H	2.460584	-4.099211	-1.208244
C	1.716209	-3.494377	2.157832
H	1.425205	-2.619067	2.741570
H	0.967474	-4.278779	2.310838
H	2.659173	-3.872965	2.563408
C	0.770862	3.592110	-1.210587
H	1.699706	3.084390	-0.930628
C	0.920312	5.070895	-0.833637
H	1.709405	5.542392	-1.426251
H	-0.005556	5.627934	-1.021782
H	1.178029	5.176713	0.223629
C	0.541983	3.426896	-2.719752
H	0.284779	2.401599	-3.003997
H	-0.266505	4.072676	-3.077589
H	1.444334	3.707060	-3.270564

1OSSA

Number of imaginary frequencies: 0 Electronic energy: HF=-2467.507816
Zero-point correction= 0.732672 (Hartree/Particle)
Thermal correction to Energy= 0.776392
Thermal correction to Enthalpy= 0.777336
Thermal correction to Gibbs Free Energy= 0.655265
Sum of electronic and zero-point Energies= -2466.775144
Sum of electronic and thermal Energies= -2466.731424
Sum of electronic and thermal Enthalpies= -2466.730480
Sum of electronic and thermal Free Energies= -2466.852551

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Cartesian Coordinates
.....

C	-2.992324	-0.925888	-0.925457
C	-1.839145	-0.440272	-1.557455
C	-1.220685	-1.230886	-2.539290
C	-1.749687	-2.473512	-2.887344
C	-2.906130	-2.950679	-2.261957
C	-3.513225	-2.177514	-1.274559
H	-0.345096	-0.857893	-3.055571
H	-3.319715	-3.915823	-2.539156
C	-1.343914	0.941434	-1.333727
C	-3.802953	-0.292297	0.195038
C	-4.620847	-1.508503	0.741996
H	-5.588866	-1.192790	1.137439
H	-4.065854	-1.985104	1.551408
C	-4.738539	-2.489174	-0.446511
O	-2.127709	1.882252	-1.884384
C	-0.166496	2.835132	-1.008218
N	-0.261520	1.360169	-0.759668
C	-2.966586	0.397617	1.257870
C	-1.758263	-0.023611	1.834346
C	-1.092418	0.821549	2.740589
C	-1.637444	2.064551	3.072453
C	-2.847015	2.475107	2.511317
C	-3.506134	1.638419	1.607305
H	-0.169664	0.494232	3.210561
H	-3.266290	3.443046	2.769368
C	-1.056394	-1.226136	1.364196
C	-4.740509	0.862572	-0.297349
H	-5.722354	0.480483	-0.585303
H	-4.299797	1.340587	-1.172707
C	-4.803649	1.874739	0.870167
O	-1.653747	-2.411946	1.347725
C	0.556756	-2.531480	0.464759
H	0.831283	-2.476980	-0.592819
N	0.148147	-1.173355	0.892106
C	-0.758207	-3.330948	0.639686
H	-1.243249	-3.579269	-0.303767
H	-0.656855	-4.220071	1.260165
C	-1.578384	3.177187	-1.500821
H	-2.217711	3.577745	-0.709535
H	-1.616675	3.825426	-2.375362
H	-1.102844	2.710364	3.759331
H	-5.644619	-2.298637	-1.035537
H	-4.781294	-3.534277	-0.127098
H	-5.649419	1.666251	1.537594
H	-4.919312	2.907297	0.527927
H	-1.263735	-3.065381	-3.656153
H	0.043152	3.322264	-0.058785
Fe	0.950506	0.627186	0.771137

Cl	1.665935	2.583721	1.649120
C	2.589878	0.101848	0.242409
C	3.076396	-0.436108	-0.988220
C	2.248235	-0.402911	-2.135796
C	4.357261	-1.040428	-1.090670
C	2.677072	-0.944077	-3.336325
H	1.284817	0.075135	-2.042055
C	4.773098	-1.599479	-2.290044
H	5.011081	-1.061238	-0.227200
C	3.937854	-1.549751	-3.412684
H	2.043638	-0.896847	-4.216304
H	5.749237	-2.067008	-2.361049
H	4.273773	-1.979218	-4.351379
C	3.473933	0.172412	1.449824
O	3.132433	-0.354794	2.495923
O	4.576552	0.891304	1.266431
C	5.314299	1.228880	2.469199
H	5.664696	0.321489	2.963392
H	6.149132	1.838132	2.129722
H	4.664830	1.793558	3.140025
C	1.751145	-3.078487	1.266302
H	2.569378	-2.368876	1.122627
C	2.192023	-4.426383	0.682714
H	3.083675	-4.791324	1.199328
H	1.417586	-5.193800	0.794851
H	2.431027	-4.342087	-0.383222
C	1.473203	-3.152872	2.769481
H	1.209732	-2.171789	3.170082
H	0.670513	-3.860029	3.006557
H	2.368703	-3.488929	3.298277
C	0.987007	3.144993	-1.980645
H	1.861791	2.628480	-1.567715
C	1.282392	4.649402	-1.970904
H	2.124524	4.881299	-2.628808
H	0.422371	5.229593	-2.326132
H	1.534114	4.991984	-0.963050
C	0.740446	2.631601	-3.404475
H	0.455577	1.575489	-3.425644
H	-0.051037	3.196559	-3.907994
H	1.646776	2.739342	-4.006732

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^{3}A

Number of imaginary frequencies: 0 Electronic energy: HF=-2467.5256443
Zero-point correction= 0.731985 (Hartree/Particle)
Thermal correction to Energy= 0.775740
Thermal correction to Enthalpy= 0.776684
Thermal correction to Gibbs Free Energy= 0.652125
Sum of electronic and zero-point Energies= -2466.793659
Sum of electronic and thermal Energies= -2466.749904
Sum of electronic and thermal Enthalpies= -2466.748960

Sum of electronic and thermal Free Energies= -2466.873519

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Cartesian Coordinates

.....

C	-2.836974	-1.161496	-1.027198
C	-1.812976	-0.369891	-1.565705
C	-1.051298	-0.870789	-2.633002
C	-1.343063	-2.121191	-3.178998
C	-2.387582	-2.895823	-2.661263
C	-3.114007	-2.420158	-1.570409
H	-0.248399	-0.271278	-3.045909
H	-2.613852	-3.866131	-3.093624
C	-1.600456	1.025780	-1.118686
C	-3.700385	-0.888564	0.196617
C	-4.248034	-2.313833	0.540072
H	-5.243187	-2.260012	0.986978
H	-3.584268	-2.799738	1.255792
C	-4.224678	-3.093097	-0.796285
O	-2.609759	1.854366	-1.434394
C	-0.813404	3.031849	-0.482319
N	-0.580672	1.554329	-0.527861
C	-2.941774	-0.221924	1.335717
C	-1.640421	-0.476850	1.800311
C	-1.076629	0.354775	2.786128
C	-1.812570	1.419305	3.308785
C	-3.112920	1.662579	2.861213
C	-3.670018	0.841327	1.878619
H	-0.078023	0.149967	3.161792
H	-3.682588	2.492339	3.269222
C	-0.771840	-1.470054	1.157647
C	-4.867449	0.122692	-0.073443
H	-5.780428	-0.399262	-0.367859
H	-4.589656	0.792546	-0.886515
C	-5.032822	0.932761	1.233490
O	-1.197920	-2.710501	0.965947
C	0.990403	-2.409754	0.083960
H	1.248381	-2.163027	-0.949706
N	0.411814	-1.189431	0.702786
C	-0.208491	-3.386633	0.126035
H	-0.674291	-3.544690	-0.845531
H	0.013801	-4.340621	0.600950
C	-2.304162	3.144917	-0.832037
H	-2.940684	3.249708	0.050657
H	-2.547242	3.916967	-1.561074
H	-1.362560	2.057451	4.060962
H	-5.173976	-2.988417	-1.336656
H	-4.056406	-4.164503	-0.655139
H	-5.783464	0.481067	1.894303
H	-5.351246	1.963714	1.053293
H	-0.757518	-2.489387	-4.015159
H	-0.624936	3.374789	0.532951

Fe	0.976372	0.722922	0.759679
Cl	1.495114	2.661054	1.722942
C	2.707356	0.349384	0.263118
C	3.147927	0.134088	-1.075521
C	2.348004	0.582953	-2.158455
C	4.341712	-0.578797	-1.368832
C	2.722955	0.333791	-3.469332
H	1.445860	1.138949	-1.939717
C	4.698856	-0.835086	-2.685040
H	4.971948	-0.917040	-0.556483
C	3.896162	-0.381904	-3.738583
H	2.111408	0.703355	-4.286513
H	5.610785	-1.383769	-2.896430
H	4.188944	-0.578010	-4.765002
C	3.473867	0.162711	1.516258
O	2.902315	-0.153152	2.552067
O	4.781842	0.409863	1.421320
C	5.521636	0.346667	2.664873
H	5.472963	-0.661952	3.079755
H	6.543674	0.613180	2.403580
H	5.101557	1.056135	3.379592
C	2.245982	-2.935597	0.803824
H	2.989835	-2.138292	0.752475
C	2.816954	-4.131157	0.029992
H	3.749955	-4.468426	0.489215
H	2.131672	-4.986098	0.028874
H	3.030577	-3.866399	-1.011209
C	1.998579	-3.251898	2.280498
H	1.657046	-2.366689	2.820660
H	1.264091	-4.054129	2.412066
H	2.926682	-3.586058	2.751944
C	0.154366	3.762365	-1.433525
H	1.157412	3.429220	-1.142226
C	0.078597	5.274694	-1.193598
H	0.799224	5.800858	-1.825557
H	-0.914832	5.672241	-1.432755
H	0.302606	5.518727	-0.150863
C	-0.068334	3.414521	-2.910251
H	-0.048501	2.335004	-3.090411
H	-1.027794	3.792757	-3.278754
H	0.714586	3.866169	-3.525706

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^{1CSS}(A-B)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2582425
Zero-point correction= 0.787897 (Hartree/Particle)
Thermal correction to Energy= 0.833586
Thermal correction to Enthalpy= 0.834530
Thermal correction to Gibbs Free Energy= 0.712525
Sum of electronic and zero-point Energies= -2582.470345
Sum of electronic and thermal Energies= -2582.424656

Sum of electronic and thermal Enthalpies= -2582.423712
Sum of electronic and thermal Free Energies= -2582.545717
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Cartesian Coordinates
.....

C	-3.013231	-0.982752	-1.007064
C	-1.811272	-0.503150	-1.547294
C	-1.126113	-1.295586	-2.480677
C	-1.644150	-2.528097	-2.879166
C	-2.847659	-2.999766	-2.344005
C	-3.514271	-2.230931	-1.391517
H	-0.198532	-0.938762	-2.906611
H	-3.245952	-3.961013	-2.655189
C	-1.351555	0.884600	-1.290863
C	-3.888110	-0.354495	0.068096
C	-4.704986	-1.583862	0.582469
H	-5.687009	-1.284764	0.956114
H	-4.163621	-2.065588	1.397984
C	-4.778680	-2.547552	-0.624823
O	-2.172248	1.793152	-1.853825
C	-0.280047	2.833708	-0.976564
N	-0.305995	1.357157	-0.685726
C	-3.101226	0.371520	1.145498
C	-1.893128	-0.005592	1.749135
C	-1.249182	0.892763	2.619846
C	-1.812671	2.141709	2.891344
C	-3.027405	2.505831	2.307404
C	-3.664968	1.618094	1.438674
H	-0.328655	0.599095	3.113207
H	-3.462726	3.478469	2.516386
C	-1.162560	-1.208339	1.320999
C	-4.833869	0.771024	-0.476640
H	-5.801057	0.363657	-0.778944
H	-4.378936	1.236545	-1.350682
C	-4.948129	1.808492	0.664758
O	-1.753486	-2.404296	1.329982
C	0.465140	-2.521783	0.486356
H	0.798033	-2.496887	-0.554170
N	0.040869	-1.149718	0.856961
C	-0.855144	-3.316792	0.622727
H	-1.320916	-3.546024	-0.334815
H	-0.771000	-4.219151	1.226349
C	-1.717640	3.102614	-1.414230
H	-2.362370	3.411402	-0.586078
H	-1.823667	3.792264	-2.250353
H	-1.291919	2.828468	3.548847
H	-5.658403	-2.341472	-1.247732
H	-4.841486	-3.596811	-0.322877
H	-5.805408	1.596004	1.316192
H	-5.077032	2.830448	0.296595
H	-1.105391	-3.121252	-3.611021

H	-0.045604	3.356277	-0.054246
Fe	0.859699	0.668255	0.825306
Cl	1.577723	2.807639	1.608078
C	2.538774	0.154801	0.123831
C	2.921820	-0.669410	-1.018226
C	2.272193	-0.455305	-2.247757
C	3.911589	-1.668798	-0.935051
C	2.585544	-1.227313	-3.358821
H	1.534721	0.333169	-2.301198
C	4.203729	-2.460476	-2.044421
H	4.448458	-1.821661	-0.006367
C	3.543075	-2.242771	-3.255028
H	2.088151	-1.043695	-4.306257
H	4.958149	-3.236579	-1.967876
H	3.781237	-2.854095	-4.119683
C	3.239164	-0.033206	1.456195
O	4.400514	-0.102569	1.762372
O	2.200445	-0.022340	2.360476
C	2.495068	0.236702	3.756116
H	2.516392	1.318050	3.898264
H	1.690555	-0.222185	4.328185
H	3.454210	-0.214649	4.004523
C	1.608726	-3.061385	1.367289
H	2.436861	-2.357398	1.268228
C	2.096486	-4.408157	0.820452
H	2.943967	-4.774601	1.406352
H	1.314595	-5.174282	0.867872
H	2.420163	-4.316542	-0.221217
C	1.234861	-3.139728	2.850157
H	0.849637	-2.184161	3.214233
H	0.476570	-3.905578	3.042752
H	2.112838	-3.399074	3.448338
C	0.798580	3.166400	-2.026226
H	1.712943	2.676376	-1.680664
C	1.050562	4.679325	-2.040908
H	1.841988	4.932403	-2.752257
H	0.154258	5.234139	-2.342587
H	1.352923	5.036600	-1.051804
C	0.476726	2.643571	-3.432593
H	0.227301	1.578184	-3.439137
H	-0.364962	3.178218	-3.884698
H	1.339070	2.783200	-4.090734
O	3.428576	1.783234	-0.384703
C	4.864403	1.881514	-0.423436
H	5.123965	2.819043	-0.922076
H	5.293022	1.839667	0.578526
H	5.222552	1.038850	-1.015686
H	3.011434	2.397159	0.281460

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^{1OSS}(A-B)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2599403
Zero-point correction= 0.787138 (Hartree/Particle)
Thermal correction to Energy= 0.833447
Thermal correction to Enthalpy= 0.834391
Thermal correction to Gibbs Free Energy= 0.710134
Sum of electronic and zero-point Energies= -2582.472802
Sum of electronic and thermal Energies= -2582.426493
Sum of electronic and thermal Enthalpies= -2582.425549
Sum of electronic and thermal Free Energies= -2582.549806
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Cartesian Coordinates
.....

C	-3.047987	-0.913461	-1.031186
C	-1.853668	-0.418675	-1.574522
C	-1.178628	-1.187091	-2.535351
C	-1.700328	-2.409355	-2.959338
C	-2.898842	-2.893753	-2.424370
C	-3.555064	-2.149773	-1.445427
H	-0.256951	-0.817841	-2.963892
H	-3.301793	-3.845820	-2.757114
C	-1.379409	0.956546	-1.281794
C	-3.905283	-0.317485	0.075789
C	-4.729563	-1.556417	0.555625
H	-5.708441	-1.261053	0.940163
H	-4.190785	-2.065310	1.356089
C	-4.813834	-2.485172	-0.677878
O	-2.196284	1.899775	-1.787774
C	-0.259338	2.869557	-0.910682
N	-0.309949	1.384367	-0.688522
C	-3.097694	0.356057	1.171849
C	-1.892298	-0.062810	1.754545
C	-1.232228	0.788746	2.659654
C	-1.776865	2.033290	2.984781
C	-2.987595	2.438784	2.420912
C	-3.641501	1.597290	1.518637
H	-0.313340	0.461981	3.135727
H	-3.408207	3.407888	2.672192
C	-1.181385	-1.261866	1.284979
C	-4.843215	0.838997	-0.414665
H	-5.819770	0.454757	-0.717111
H	-4.394904	1.329716	-1.278189
C	-4.927902	1.836823	0.764085
O	-1.792537	-2.445180	1.245397
C	0.430541	-2.572431	0.410696
H	0.753727	-2.511522	-0.631804
N	0.029367	-1.211068	0.837243
C	-0.900069	-3.354744	0.525868
H	-1.364358	-3.560368	-0.437855
H	-0.829915	-4.268883	1.113552
C	-1.698956	3.184732	-1.318514
H	-2.322806	3.485590	-0.471808

H	-1.801108	3.899995	-2.133387
H	-1.243085	2.684639	3.667161
H	-5.697421	-2.259701	-1.288441
H	-4.876990	-3.542437	-0.405342
H	-5.782774	1.616869	1.416169
H	-5.041867	2.873267	0.433349
H	-1.170000	-2.983326	-3.712334
H	-0.006252	3.344215	0.033368
Fe	0.867655	0.617338	0.827194
Cl	1.569517	2.694860	1.739741
C	2.508525	0.069109	0.155654
C	2.896904	-0.654689	-1.037106
C	2.226444	-0.377316	-2.244754
C	3.912726	-1.635254	-1.029410
C	2.545942	-1.066023	-3.406380
H	1.471760	0.395859	-2.237720
C	4.210471	-2.343108	-2.190725
H	4.461416	-1.835333	-0.117210
C	3.530389	-2.060974	-3.378148
H	2.035357	-0.832717	-4.335597
H	4.983204	-3.104546	-2.174370
H	3.774341	-2.607323	-4.283798
C	3.264242	-0.137754	1.451013
O	4.444748	-0.203624	1.682718
O	2.285817	-0.167579	2.409050
C	2.670642	0.034511	3.790609
H	2.750018	1.108723	3.964832
H	1.875166	-0.401990	4.392134
H	3.619794	-0.465599	3.977634
C	1.578061	-3.155531	1.257102
H	2.413408	-2.458058	1.167398
C	2.040432	-4.489901	0.660300
H	2.890410	-4.886442	1.222355
H	1.249015	-5.247049	0.692671
H	2.352156	-4.368433	-0.382221
C	1.223925	-3.272744	2.742011
H	0.871966	-2.318488	3.141714
H	0.447961	-4.024113	2.921598
H	2.103277	-3.575032	3.317538
C	0.819159	3.229046	-1.951236
H	1.731318	2.720846	-1.623949
C	1.084633	4.739293	-1.915042
H	1.879245	5.008091	-2.616894
H	0.194040	5.312903	-2.198113
H	1.390438	5.060533	-0.914629
C	0.486153	2.757431	-3.372736
H	0.231371	1.693934	-3.414479
H	-0.355642	3.311794	-3.800575
H	1.345062	2.915121	-4.031206
O	3.486371	1.844866	-0.341099
C	4.915413	1.941279	-0.358362

H	5.201668	2.904174	-0.793540
H	5.338671	1.832744	0.642157
H	5.280560	1.134309	-0.995913
H	3.081701	2.409856	0.360759

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^{3}(A-B)

Number of imaginary frequencies: 1 Electronic energy: HF=-2583.2721148
Zero-point correction= 0.786232 (Hartree/Particle)
Thermal correction to Energy= 0.833205
Thermal correction to Enthalpy= 0.834149
Thermal correction to Gibbs Free Energy= 0.705567
Sum of electronic and zero-point Energies= -2582.485883
Sum of electronic and thermal Energies= -2582.438910
Sum of electronic and thermal Enthalpies= -2582.437966
Sum of electronic and thermal Free Energies= -2582.566548

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Cartesian Coordinates

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C	-3.055300	-1.040446	-1.025047
C	-2.002053	-0.320611	-1.605813
C	-1.291864	-0.894895	-2.670916
C	-1.644420	-2.152408	-3.159908
C	-2.708116	-2.860968	-2.590318
C	-3.397827	-2.305785	-1.513672
H	-0.484581	-0.339832	-3.132104
H	-2.982876	-3.838247	-2.976454
C	-1.687527	1.069444	-1.200230
C	-3.900687	-0.671811	0.183996
C	-4.524492	-2.048586	0.589339
H	-5.518104	-1.921424	1.024820
H	-3.890893	-2.533311	1.332228
C	-4.535750	-2.890635	-0.708383
O	-2.637130	1.963805	-1.520882
C	-0.736770	3.024947	-0.633032
N	-0.620563	1.535523	-0.640296
C	-3.110271	0.002812	1.294503
C	-1.819129	-0.292612	1.763409
C	-1.225777	0.544336	2.724104
C	-1.916339	1.651867	3.216791
C	-3.205182	1.937235	2.761181
C	-3.793995	1.112144	1.801134
H	-0.228738	0.322472	3.089159
H	-3.739774	2.801780	3.143811
C	-1.005100	-1.367598	1.178946
C	-5.011614	0.386964	-0.133114
H	-5.945831	-0.096502	-0.427115
H	-4.687911	1.019013	-0.959772
C	-5.150473	1.241000	1.148213
O	-1.515667	-2.594627	1.086331
C	0.699869	-2.525792	0.256116

H	1.058569	-2.413412	-0.769222
N	0.196134	-1.205193	0.716834
C	-0.580471	-3.386669	0.291390
H	-1.034240	-3.525877	-0.690128
H	-0.462051	-4.345857	0.792873
C	-2.221228	3.243753	-0.961695
H	-2.831556	3.422236	-0.072370
H	-2.417697	4.010624	-1.710196
H	-1.437989	2.294395	3.947431
H	-5.479800	-2.770752	-1.254871
H	-4.414502	-3.960615	-0.516327
H	-5.922443	0.839444	1.816906
H	-5.425287	2.278320	0.935693
H	-1.092346	-2.577486	-3.991846
H	-0.501195	3.379322	0.369454
Fe	0.896981	0.675497	0.584701
Cl	1.462482	2.562286	1.790348
C	2.666278	0.226800	0.157279
C	3.011026	-0.495410	-1.053776
C	2.206228	-0.310886	-2.198946
C	4.083402	-1.410181	-1.112723
C	2.445866	-1.039728	-3.355327
H	1.411051	0.424030	-2.154683
C	4.306754	-2.153185	-2.268760
H	4.730945	-1.535874	-0.253240
C	3.489892	-1.972171	-3.387754
H	1.830359	-0.884042	-4.235694
H	5.125542	-2.864174	-2.302698
H	3.674131	-2.547038	-4.289799
C	3.597436	0.137662	1.345464
O	4.781052	0.401152	1.344817
O	2.916147	-0.278627	2.424426
C	3.664273	-0.340227	3.658741
H	3.950424	0.668837	3.960338
H	2.986175	-0.784308	4.384630
H	4.557473	-0.953782	3.530546
C	1.845155	-3.064674	1.133889
H	2.640064	-2.318927	1.093524
C	2.398197	-4.361364	0.530867
H	3.257992	-4.713711	1.107412
H	1.654900	-5.166330	0.536261
H	2.725373	-4.208544	-0.502791
C	1.443954	-3.226585	2.602610
H	1.088362	-2.281222	3.020261
H	0.660143	-3.979625	2.737153
H	2.305258	-3.549936	3.193978
C	0.268081	3.646835	-1.622349
H	1.249698	3.259479	-1.328703
C	0.288372	5.170842	-1.456757
H	1.046839	5.618725	-2.105016
H	-0.674072	5.620961	-1.726786

H	0.516201	5.452607	-0.423898
C	0.017051	3.236463	-3.077596
H	0.028099	2.149029	-3.200910
H	-0.943997	3.606410	-3.450978
H	0.796025	3.648050	-3.725496
O	3.267922	2.106877	-0.511582
C	4.631290	2.365895	-0.880777
H	4.688028	3.351104	-1.353927
H	5.293927	2.305800	-0.017201
H	4.909158	1.600247	-1.606850
H	2.987432	2.620587	0.277310

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^{1CSS}B

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.2627798
Zero-point correction= 0.788620 (Hartree/Particle)
Thermal correction to Energy= 0.834343
Thermal correction to Enthalpy= 0.835288
Thermal correction to Gibbs Free Energy= 0.713174
Sum of electronic and zero-point Energies= -2582.474160
Sum of electronic and thermal Energies= -2582.428436
Sum of electronic and thermal Enthalpies= -2582.427492
Sum of electronic and thermal Free Energies= -2582.549606

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Cartesian Coordinates

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C	-2.989185	1.020542	0.985951
C	-1.816291	0.484735	1.536963
C	-1.122341	1.227565	2.503184
C	-1.605447	2.466518	2.924562
C	-2.780691	2.994354	2.378642
C	-3.453799	2.275453	1.392055
H	-0.214839	0.827081	2.932945
H	-3.150485	3.961383	2.706676
C	-1.401368	-0.909753	1.248691
C	-3.857920	0.453305	-0.127638
C	-4.616471	1.724871	-0.628218
H	-5.598990	1.471947	-1.033420
H	-4.037582	2.208161	-1.416280
C	-4.686354	2.658154	0.603555
O	-2.276957	-1.803401	1.753916
C	-0.403924	-2.887346	0.895894
N	-0.357598	-1.402585	0.657665
C	-3.062539	-0.273473	-1.198837
C	-1.823580	0.077010	-1.753386
C	-1.176205	-0.828111	-2.616170
C	-1.765529	-2.056241	-2.926443
C	-3.010840	-2.392236	-2.391479
C	-3.652323	-1.498048	-1.532345
H	-0.235850	-0.550394	-3.081136
H	-3.467635	-3.347734	-2.631529

C	-1.072937	1.253705	-1.288136
C	-4.858086	-0.651286	0.360718
H	-5.822004	-0.218214	0.636410
H	-4.450282	-1.147942	1.240654
C	-4.965449	-1.663015	-0.804433
O	-1.637925	2.463914	-1.287371
C	0.580037	2.524190	-0.448553
H	0.951189	2.494435	0.578146
N	0.122801	1.158936	-0.811432
C	-0.730816	3.337591	-0.543261
H	-1.191594	3.527805	0.425397
H	-0.641311	4.265136	-1.106274
C	-1.865172	-3.111713	1.276709
H	-2.493307	-3.360685	0.416387
H	-2.027179	-3.828747	2.080289
H	-1.244938	-2.746824	-3.580490
H	-5.588881	2.467815	1.198257
H	-4.703649	3.716601	0.328873
H	-5.793547	-1.411663	-1.479367
H	-5.137603	-2.687403	-0.461463
H	-1.060224	3.022050	3.680724
H	-0.157853	-3.391154	-0.034104
Fe	0.872864	-0.697020	-0.807801
Cl	1.661204	-2.873704	-1.546664
C	2.666585	-0.377303	-0.019994
C	2.953282	0.607811	1.054556
C	2.297655	0.456939	2.286791
C	3.861782	1.664057	0.894829
C	2.523771	1.354619	3.325039
H	1.612561	-0.373061	2.407144
C	4.068669	2.579875	1.928746
H	4.415913	1.768516	-0.031439
C	3.399534	2.430029	3.143133
H	2.016695	1.221808	4.276120
H	4.767971	3.397915	1.788877
H	3.569256	3.136534	3.949193
C	3.338709	-0.169471	-1.370130
O	4.492539	-0.247297	-1.705845
O	2.300133	0.012647	-2.253419
C	2.584751	-0.159506	-3.664393
H	2.689480	-1.226643	-3.866000
H	1.733556	0.260888	-4.195817
H	3.499787	0.375654	-3.913383
C	1.695303	3.046816	-1.376987
H	2.514143	2.328988	-1.309533
C	2.216775	4.393325	-0.861568
H	3.057242	4.736686	-1.471414
H	1.446877	5.171613	-0.906007
H	2.559790	4.313762	0.174191
C	1.261651	3.128145	-2.843992
H	0.851653	2.177644	-3.194067

H	0.503048	3.900700	-3.006068
H	2.116731	3.379578	-3.477865
C	0.615422	-3.303922	1.975449
H	1.568872	-2.865724	1.670200
C	0.771568	-4.829690	1.976057
H	1.526736	-5.141250	2.703517
H	-0.164756	-5.329953	2.249028
H	1.075146	-5.195102	0.990176
C	0.284862	-2.773576	3.376435
H	0.140722	-1.689218	3.386854
H	-0.622412	-3.230443	3.784396
H	1.101102	-3.003899	4.067155
O	3.221859	-1.733742	0.481860
C	4.647791	-1.928426	0.766554
H	4.720428	-2.903527	1.246502
H	5.220410	-1.876324	-0.156966
H	4.934166	-1.134488	1.452967
H	2.817630	-2.407224	-0.190407

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^{1OSS}B

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.2657474
Zero-point correction= 0.787879 (Hartree/Particle)
Thermal correction to Energy= 0.834191
Thermal correction to Enthalpy= 0.835135
Thermal correction to Gibbs Free Energy= 0.710601
Sum of electronic and zero-point Energies= -2582.477868
Sum of electronic and thermal Energies= -2582.431557
Sum of electronic and thermal Enthalpies= -2582.430612
Sum of electronic and thermal Free Energies= -2582.555146

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Cartesian Coordinates

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C	3.034257	-0.979460	0.974636
C	1.908203	-0.381820	1.557645
C	1.238271	-1.059913	2.586667
C	1.702382	-2.294990	3.039087
C	2.835556	-2.881544	2.464807
C	3.483202	-2.227352	1.418054
H	0.367328	-0.609130	3.042637
H	3.192871	-3.843792	2.819717
C	1.506028	1.004945	1.221407
C	3.858306	-0.490339	-0.207010
C	4.579302	-1.798469	-0.669875
H	5.553477	-1.581802	-1.114166
H	3.970554	-2.305704	-1.419179
C	4.671146	-2.679078	0.598746
O	2.408340	1.919781	1.630014
C	0.486423	2.958162	0.802302
N	0.432230	1.465665	0.665138
C	3.018977	0.178953	-1.282557

C	1.761362	-0.202185	-1.773347
C	1.087003	0.648455	-2.671568
C	1.665371	1.855557	-3.073272
C	2.925622	2.222424	-2.598023
C	3.596430	1.379930	-1.709156
H	0.135556	0.340364	-3.095032
H	3.374034	3.160885	-2.910279
C	1.022085	-1.352086	-1.227551
C	4.887923	0.630419	0.170564
H	5.862978	0.204167	0.415946
H	4.531148	1.173600	1.045070
C	4.938749	1.582739	-1.047310
O	1.589290	-2.557671	-1.159700
C	-0.626949	-2.575318	-0.311663
H	-0.991167	-2.488569	0.714352
N	-0.174026	-1.233811	-0.755597
C	0.684207	-3.392470	-0.367899
H	1.149578	-3.530543	0.607697
H	0.594743	-4.348211	-0.881749
C	1.963184	3.205733	1.118655
H	2.555494	3.426918	0.226122
H	2.150647	3.954205	1.887460
H	1.123802	2.504930	-3.751809
H	5.601268	-2.490375	1.149755
H	4.648207	-3.748379	0.370308
H	5.737556	1.300779	-1.745023
H	5.121248	2.623308	-0.763254
H	1.177590	-2.800355	3.843330
H	0.209008	3.400669	-0.151435
Fe	-0.868909	0.673065	-0.782820
Cl	-1.632469	2.788496	-1.684013
C	-2.688937	0.432264	-0.020308
C	-2.944674	-0.516299	1.095650
C	-2.219906	-0.356729	2.287937
C	-3.877683	-1.558983	1.003241
C	-2.405975	-1.232592	3.352458
H	-1.510894	0.459563	2.354565
C	-4.045200	-2.452834	2.063047
H	-4.480748	-1.670008	0.108618
C	-3.309580	-2.294126	3.237294
H	-1.846490	-1.093909	4.272826
H	-4.764656	-3.260561	1.975365
H	-3.448282	-2.983349	4.063998
C	-3.444940	0.193137	-1.318642
O	-4.613051	0.376963	-1.566625
O	-2.528751	-0.185630	-2.251602
C	-2.977874	-0.201398	-3.627487
H	-3.203915	0.819756	-3.938506
H	-2.149746	-0.611344	-4.201748
H	-3.863342	-0.830156	-3.720430
C	-1.751064	-3.142253	-1.201918

H	-2.566073	-2.417851	-1.160115
C	-2.266830	-4.462529	-0.618061
H	-3.114910	-4.833139	-1.200836
H	-1.498394	-5.243493	-0.635073
H	-2.597541	-4.334181	0.416936
C	-1.330749	-3.290575	-2.667484
H	-0.944403	-2.350147	-3.068793
H	-0.558966	-4.056047	-2.799501
H	-2.187230	-3.589822	-3.278315
C	-0.502579	3.443898	1.880891
H	-1.469172	3.007235	1.613336
C	-0.634192	4.970444	1.814511
H	-1.374910	5.326768	2.536205
H	0.313197	5.467186	2.053364
H	-0.944583	5.297300	0.817120
C	-0.150626	2.969604	3.296089
H	-0.047022	1.881978	3.352559
H	0.784457	3.411030	3.655744
H	-0.936976	3.262043	3.997799
O	-3.163921	1.820480	0.464277
C	-4.558974	2.082006	0.842742
H	-4.555482	3.069272	1.302876
H	-5.194818	2.030774	-0.037645
H	-4.825758	1.315935	1.567565
H	-2.781868	2.451735	-0.254335

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^{3}B

Number of imaginary frequencies: 0 Electronic energy: HF=-2583.277967
Zero-point correction= 0.787701 (Hartree/Particle)
Thermal correction to Energy= 0.834407
Thermal correction to Enthalpy= 0.835351
Thermal correction to Gibbs Free Energy= 0.707703
Sum of electronic and zero-point Energies= -2582.490266
Sum of electronic and thermal Energies= -2582.443560
Sum of electronic and thermal Enthalpies= -2582.442616
Sum of electronic and thermal Free Energies= -2582.570264

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Cartesian Coordinates

.....

C	3.036972	-1.110308	0.961027
C	2.017801	-0.356793	1.558838
C	1.313093	-0.900207	2.643208
C	1.648371	-2.159142	3.140931
C	2.682636	-2.899969	2.557389
C	3.357824	-2.378577	1.454631
H	0.523768	-0.322172	3.108367
H	2.940907	-3.879322	2.949571
C	1.753026	1.040489	1.149509
C	3.855089	-0.777934	-0.276865
C	4.419742	-2.178081	-0.689057

H	5.401598	-2.086999	-1.158984
H	3.745878	-2.650052	-1.403559
C	4.450459	-3.005895	0.618535
O	2.753131	1.890033	1.442085
C	0.898212	3.035329	0.575344
N	0.701509	1.553951	0.602098
C	3.052845	-0.075188	-1.364080
C	1.733835	-0.314425	-1.787233
C	1.144695	0.548381	-2.727520
C	1.861675	1.628071	-3.242910
C	3.176488	1.858823	-2.831526
C	3.763409	1.006840	-1.894596
H	0.129343	0.363808	-3.062195
H	3.733585	2.700793	-3.232075
C	0.899695	-1.363320	-1.182448
C	5.016388	0.237985	-0.001089
H	5.940095	-0.281097	0.263922
H	4.746173	0.885114	0.832836
C	5.146318	1.080279	-1.290610
O	1.405290	-2.593298	-1.078781
C	-0.801114	-2.506910	-0.244437
H	-1.187755	-2.387395	0.769012
N	-0.295371	-1.182219	-0.710537
C	0.483651	-3.357894	-0.245426
H	0.943369	-3.453142	0.738338
H	0.370645	-4.337954	-0.705371
C	2.399055	3.177284	0.862939
H	2.994213	3.299981	-0.045900
H	2.658012	3.949124	1.586869
H	1.387526	2.289217	-3.959824
H	5.416182	-2.908838	1.130626
H	4.290579	-4.073690	0.443398
H	5.876204	0.642978	-1.983736
H	5.472918	2.105741	-1.094062
H	1.103549	-2.562537	3.988262
H	0.654559	3.394742	-0.422819
Fe	-0.907279	0.747533	-0.520111
Cl	-1.481785	2.727056	-1.640767
C	-2.851359	0.584340	-0.010826
C	-3.063077	-0.391320	1.091476
C	-2.269647	-0.280052	2.248148
C	-3.996483	-1.433781	1.008418
C	-2.394011	-1.201189	3.283792
H	-1.556809	0.535270	2.318031
C	-4.108402	-2.365208	2.041396
H	-4.629808	-1.526309	0.132786
C	-3.307336	-2.254466	3.178727
H	-1.780238	-1.100844	4.173645
H	-4.831964	-3.169949	1.961472
H	-3.401775	-2.976372	3.983323
C	-3.745991	0.521446	-1.225110

O	-4.633120	1.309776	-1.480412
O	-3.393669	-0.487153	-2.035970
C	-4.144389	-0.587045	-3.267439
H	-3.994331	0.313987	-3.864291
H	-3.744679	-1.462686	-3.774884
H	-5.207986	-0.708986	-3.055612
C	-1.911495	-3.079233	-1.146365
H	-2.733385	-2.367325	-1.106600
C	-2.412553	-4.412681	-0.577440
H	-3.279188	-4.764291	-1.144707
H	-1.653064	-5.200280	-0.633649
H	-2.715271	-4.308851	0.469169
C	-1.481618	-3.204409	-2.611494
H	-1.201992	-2.231975	-3.026236
H	-0.634771	-3.887162	-2.741175
H	-2.305407	-3.600518	-3.212817
C	-0.037287	3.724531	1.588518
H	-1.048424	3.398797	1.320856
C	0.030067	5.246070	1.414247
H	-0.680852	5.743276	2.080322
H	1.025119	5.636505	1.656140
H	-0.207415	5.536544	0.386131
C	0.223328	3.302640	3.038666
H	0.139801	2.219050	3.166538
H	1.218397	3.605025	3.381635
H	-0.504489	3.771850	3.706836
O	-3.084835	1.989461	0.581674
C	-4.370572	2.372419	1.194575
H	-4.190617	3.340251	1.660301
H	-5.132953	2.408505	0.422037
H	-4.579116	1.613945	1.945597
H	-2.763922	2.600339	-0.164375

(*R*)-TS(D_f-P)$_{3w}$-L3*

Number of imaginary frequencies: 1 Electronic energy: HF=-2999.6073214
Zero-point correction= 0.823660 (Hartree/Particle)
Thermal correction to Energy= 0.875680
Thermal correction to Enthalpy= 0.876624
Thermal correction to Gibbs Free Energy= 0.735913
Sum of electronic and zero-point Energies= -2998.783661
Sum of electronic and thermal Energies= -2998.731642
Sum of electronic and thermal Enthalpies= -2998.730697
Sum of electronic and thermal Free Energies= -2998.871408

Cartesian Coordinates

C	-2.960954	-0.991296	1.895356
C	-1.683216	-1.380120	1.467714
C	-0.568886	-1.098279	2.275930
C	-0.739496	-0.470110	3.509760
C	-2.017200	-0.104740	3.948036
C	-3.120514	-0.359897	3.133392

H	0.421586	-1.377468	1.931319
H	-2.145461	0.383122	4.910171
C	-1.444238	-1.980013	0.142272
C	-4.271151	-1.040818	1.123402
C	-5.192436	-0.079461	1.949262
H	-6.226376	-0.431199	1.953148
H	-5.179910	0.914136	1.502782
C	-4.574371	-0.019018	3.367063
O	-2.065995	-3.128264	-0.175419
C	-0.569005	-2.454902	-1.877717
N	-0.651080	-1.490188	-0.744556
C	-4.096490	-0.639419	-0.335644
C	-3.268703	0.358477	-0.874265
C	-3.119250	0.451491	-2.266005
C	-3.825606	-0.410358	-3.105159
C	-4.676195	-1.383453	-2.570178
C	-4.791613	-1.504727	-1.185302
H	-2.443659	1.187780	-2.685174
H	-5.224270	-2.051474	-3.228530
C	-2.547086	1.316548	-0.014244
C	-4.890733	-2.473817	1.005342
H	-5.578318	-2.677569	1.829286
H	-4.096443	-3.219543	1.037935
C	-5.576702	-2.515169	-0.380515
O	-3.308719	2.098586	0.766648
C	-1.023591	2.655215	0.955867
H	-0.292383	2.346975	1.704914
N	-1.271558	1.512055	0.048824
C	-2.412259	2.876708	1.605346
H	-2.472628	2.465730	2.615818
H	-2.750670	3.912043	1.588337
C	-1.753853	-3.394820	-1.578052
H	-2.641393	-3.138883	-2.159324
H	-1.525058	-4.455172	-1.673667
H	-3.707669	-0.322369	-4.180136
H	-5.026935	-0.764611	4.032985
H	-4.712609	0.955547	3.844803
H	-6.627979	-2.206951	-0.315908
H	-5.565681	-3.514690	-0.824730
H	0.126896	-0.270102	4.132098
H	-0.718719	-1.902640	-2.806646
Fe	0.363424	0.374812	-0.681347
Cl	0.437586	0.874727	-2.971938
C	3.161844	-0.255881	0.506595
C	3.980975	-1.143449	1.378199
C	5.247427	-0.741930	1.835189
C	3.524792	-2.429402	1.705959
C	6.019491	-1.595085	2.619688
H	5.621219	0.244722	1.584563
C	4.306864	-3.283039	2.483758
H	2.560157	-2.762384	1.343267
C	5.555604	-2.871179	2.947133
H	6.992800	-1.264692	2.969554
H	3.934688	-4.273407	2.729398
H	6.163712	-3.536126	3.551825
C	2.776647	1.064679	0.883392

O	1.705514	1.604540	0.453777
O	3.623972	1.744290	1.649597
C	3.292090	3.103840	1.997717
H	3.347123	3.744550	1.116322
H	2.290699	3.151478	2.429585
H	4.038229	3.395499	2.734875
O	1.999168	-0.892384	-0.049155
H	2.116368	3.076552	-0.596505
H	4.000744	0.010644	-0.720897
O	2.688194	3.624521	-1.169355
H	2.132405	4.369043	-1.444917
H	3.993355	0.930794	-2.347638
O	4.481320	0.068914	-1.755996
H	5.436821	0.189906	-1.664279
O	3.379612	1.847842	-2.958647
H	2.494336	1.505391	-3.213166
H	3.174787	2.609525	-2.337290
H	2.253058	-1.528155	-0.741407
C	0.807113	-3.090291	-1.864821
C	1.820472	-2.557255	-2.673007
C	1.123120	-4.110307	-0.957375
C	3.133301	-3.028312	-2.564440
H	1.582445	-1.754805	-3.364261
C	2.428422	-4.591159	-0.862147
H	0.354937	-4.518707	-0.306994
C	3.438489	-4.044309	-1.657050
H	3.912414	-2.590169	-3.178563
H	2.662845	-5.379100	-0.153867
H	4.457050	-4.406250	-1.565655
C	-0.490402	3.865940	0.215499
C	-0.655808	4.019012	-1.163598
C	0.160618	4.872364	0.941832
C	-0.178159	5.164404	-1.807888
H	-1.127203	3.234246	-1.742224
C	0.634833	6.016122	0.303373
H	0.297287	4.757732	2.014286
C	0.466659	6.165906	-1.077766
H	-0.311340	5.270437	-2.879944
H	1.137618	6.788128	0.876992
H	0.832000	7.057423	-1.577455

(*S*)-TS(D_f-P)$_{3w}$-L3*

Number of imaginary frequencies: 1 Electronic energy: HF=-2999.6018285
Zero-point correction= 0.823135 (Hartree/Particle)
Thermal correction to Energy= 0.875463
Thermal correction to Enthalpy= 0.876407
Thermal correction to Gibbs Free Energy= 0.733973
Sum of electronic and zero-point Energies= -2998.778693
Sum of electronic and thermal Energies= -2998.726365
Sum of electronic and thermal Enthalpies= -2998.725421
Sum of electronic and thermal Free Energies= -2998.867856

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Cartesian Coordinates

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C	-2.606584	-1.737313	-1.662042

C	-1.713290	-0.667954	-1.828701
C	-0.432490	-0.914045	-2.346808
C	-0.059830	-2.204579	-2.724048
C	-0.956750	-3.267092	-2.575998
C	-2.223320	-3.028129	-2.041060
H	0.263650	-0.088714	-2.452135
H	-0.664781	-4.271897	-2.867945
C	-2.023929	0.681644	-1.324288
C	-3.976140	-1.736073	-0.995621
C	-4.241224	-3.262260	-0.758417
H	-5.300106	-3.501089	-0.878748
H	-3.954489	-3.530725	0.257772
C	-3.338172	-4.011104	-1.767261
O	-3.135393	1.297032	-1.748097
C	-1.976976	2.579070	-0.108353
N	-1.305890	1.305995	-0.457415
C	-4.011747	-0.897437	0.276053
C	-3.036072	-0.789956	1.278414
C	-3.198901	0.153256	2.302759
C	-4.344243	0.950560	2.341277
C	-5.333922	0.821611	1.361162
C	-5.153375	-0.092248	0.323219
H	-2.426252	0.265363	3.054875
H	-6.226724	1.439140	1.401943
C	-1.863096	-1.691580	1.306572
C	-5.101487	-1.080091	-1.865637
H	-5.613804	-1.826786	-2.476465
H	-4.662245	-0.342716	-2.537180
C	-6.044201	-0.368737	-0.866038
O	-2.147213	-2.976586	1.582495
C	0.167843	-2.651169	1.224198
H	0.564031	-2.865999	0.228117
N	-0.623406	-1.397963	1.116249
C	-0.894168	-3.708484	1.617799
H	-0.967294	-4.534139	0.908589
H	-0.760701	-4.094119	2.630259
C	-3.236655	2.555576	-1.019068
H	-4.168718	2.532503	-0.454443
H	-3.254077	3.361501	-1.753738
H	-4.464243	1.671837	3.143158
H	-3.874230	-4.230239	-2.699379
H	-2.977743	-4.968706	-1.379273
H	-6.875112	-1.019754	-0.566146
H	-6.488601	0.539185	-1.284344
H	0.934106	-2.377732	-3.122432
H	-2.261426	2.509783	0.944261
Fe	0.330488	0.485359	0.586585
Cl	0.164753	1.603533	2.631642
C	-1.101615	3.795577	-0.300751
C	-0.903320	4.686658	0.756643
C	-0.526129	4.073658	-1.546865
C	-0.158211	5.855487	0.568205
H	-1.329473	4.464257	1.729847
C	0.220692	5.234219	-1.737720
H	-0.662611	3.375629	-2.368063
C	0.402618	6.132201	-0.681412

H	-0.028331	6.551505	1.391387
H	0.655230	5.445605	-2.709739
H	0.975195	7.041695	-0.832520
C	1.317066	-2.528834	2.201089
C	1.196297	-1.750665	3.359185
C	2.531543	-3.178164	1.933940
C	2.276341	-1.619515	4.231359
H	0.273354	-1.218260	3.557631
C	3.610731	-3.046816	2.810309
H	2.638273	-3.775111	1.032446
C	3.484338	-2.264671	3.958819
H	2.175050	-1.004051	5.119508
H	4.546885	-3.549244	2.589618
H	4.324521	-2.154997	4.636785
C	3.119896	-0.114178	-0.667234
C	3.890373	-1.085809	-1.490383
C	5.100950	-0.717094	-2.099749
C	3.443912	-2.408957	-1.636594
C	5.825393	-1.639493	-2.851179
H	5.467677	0.297443	-1.991747
C	4.177616	-3.331563	-2.382435
H	2.509892	-2.706681	-1.176067
C	5.371113	-2.952089	-2.995596
H	6.755856	-1.332881	-3.319161
H	3.812425	-4.349339	-2.485708
H	5.943234	-3.669399	-3.574825
C	2.644584	1.129294	-1.181309
O	1.569127	1.661058	-0.764247
O	3.416095	1.742810	-2.073275
C	2.989975	3.032103	-2.561099
H	3.043921	3.773542	-1.762276
H	1.969462	2.974216	-2.942575
H	3.686406	3.274630	-3.361901
O	2.037971	-0.708513	0.077782
H	1.913930	3.221111	0.083661
H	3.980345	0.323396	0.498028
O	2.446600	3.857200	0.603873
H	1.841900	4.589104	0.797138
H	3.833356	1.363869	2.056318
O	4.389237	0.475199	1.548584
H	5.346365	0.610368	1.519344
O	3.181960	2.301706	2.556688
H	2.303889	1.982812	2.859485
H	2.954468	2.989843	1.855938
H	2.399458	-1.229504	0.817302

(*R*)-TS(D_f-P)$_{3w}$-L2*

Number of imaginary frequencies: 1 Electronic energy: HF=-2923.1410912
Zero-point correction= 0.798109 (Hartree/Particle)
Thermal correction to Energy= 0.847861
Thermal correction to Enthalpy= 0.848805
Thermal correction to Gibbs Free Energy= 0.712018
Sum of electronic and zero-point Energies= -2922.342982
Sum of electronic and thermal Energies= -2922.293230
Sum of electronic and thermal Enthalpies= -2922.292286

Sum of electronic and thermal Free Energies= -2922.429073

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Cartesian Coordinates

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C	2.466828	-2.111784	-1.174257
C	1.334577	-1.361979	-1.516989
C	0.118366	-2.021369	-1.755820
C	0.052373	-3.412297	-1.692518
C	1.180495	-4.161462	-1.344219
C	2.377985	-3.503772	-1.063396
H	-0.763743	-1.444599	-2.006282
H	1.121166	-5.244639	-1.286346
C	1.369076	0.099447	-1.682555
C	3.875654	-1.633096	-0.873781
C	4.467295	-2.852705	-0.096293
H	5.551137	-2.918658	-0.216461
H	4.255139	-2.740822	0.969209
C	3.712915	-4.083215	-0.650256
O	2.235650	0.597866	-2.577170
C	0.767910	2.255556	-1.819180
N	0.581523	0.954287	-1.112206
C	3.973200	-0.320365	-0.118829
C	3.224973	0.120791	0.978426
C	3.482504	1.389370	1.521211
C	4.461955	2.210669	0.963329
C	5.207479	1.771950	-0.134380
C	4.958519	0.508568	-0.668416
H	2.913689	1.722184	2.383961
H	5.975253	2.409026	-0.563560
C	2.232803	-0.718945	1.688843
C	4.688701	-1.336049	-2.181079
H	5.209298	-2.228374	-2.536105
H	4.004891	-1.012389	-2.966137
C	5.648073	-0.178780	-1.823372
O	2.765361	-1.632695	2.521688
C	0.435207	-1.461654	2.806153
N	0.950111	-0.599600	1.693637
C	1.657714	-2.334508	3.148757
H	1.609720	-3.337082	2.717291
H	1.863392	-2.402628	4.216375
C	2.149230	2.051808	-2.459072
H	2.963470	2.379057	-1.805766
H	2.256205	2.476782	-3.455457
H	4.642550	3.192461	1.388037
H	4.224847	-4.506070	-1.524014
H	3.621212	-4.889255	0.083636
H	6.627110	-0.553860	-1.499390
H	5.830571	0.490655	-2.669160
H	-0.886968	-3.908893	-1.910328
Fe	-0.436954	0.800726	0.730447
Cl	-0.768309	1.726847	2.895539
H	0.209750	-0.773643	3.625853
H	-0.002314	2.296864	-2.599440
C	0.635344	3.478914	-0.953367
C	1.044485	3.466152	0.380578
C	0.081856	4.647497	-1.486220

C	0.875110	4.591807	1.186157
H	1.506471	2.577308	0.792894
C	-0.070563	5.782138	-0.690262
H	-0.235846	4.667596	-2.525902
C	0.317618	5.753327	0.651580
H	1.168274	4.552670	2.229990
H	-0.500048	6.684811	-1.113316
H	0.185591	6.631666	1.275135
C	-0.821214	-2.225015	2.467821
C	-0.801665	-3.311813	1.586948
C	-2.042193	-1.822396	3.027678
C	-1.977149	-3.996828	1.284054
H	0.126614	-3.612536	1.115100
C	-3.225055	-2.497802	2.708457
H	-2.064246	-0.966876	3.695519
C	-3.192568	-3.590664	1.839245
H	-1.947853	-4.838135	0.599002
H	-4.164488	-2.169798	3.141106
H	-4.108455	-4.114097	1.586826
C	-3.169325	0.066565	-0.459238
C	-3.933817	-0.911676	-1.266565
C	-5.144143	-0.568669	-1.896756
C	-3.489392	-2.240959	-1.361146
C	-5.862087	-1.519202	-2.617493
H	-5.515281	0.446963	-1.832047
C	-4.218596	-3.190441	-2.075715
H	-2.573457	-2.528487	-0.864781
C	-5.406822	-2.836367	-2.712577
H	-6.789488	-1.229963	-3.102478
H	-3.853918	-4.212398	-2.133686
H	-5.974548	-3.574118	-3.270055
C	-2.868431	1.398109	-0.836605
O	-1.953146	2.082643	-0.272326
O	-3.682205	1.978071	-1.730367
C	-3.529486	3.394454	-1.934206
H	-3.912432	3.949241	-1.071695
H	-2.483307	3.657414	-2.089847
H	-4.126771	3.623622	-2.815319
O	-2.048013	-0.488917	0.249311
H	-4.093139	0.611100	0.750558
H	-3.953694	2.054133	1.813116
O	-4.513734	1.042729	1.666201
H	-5.467806	1.165753	1.554524
O	-3.232303	3.092205	1.861541
H	-2.518682	2.879725	2.512792
H	-2.724620	3.048209	1.012929
H	-2.351938	-1.043092	0.988877

(*S*)-TS(D_h-P)$_{3w}$-L2*

Number of imaginary frequencies: 1 Electronic energy: HF=-2923.137764
Zero-point correction= 0.798014 (Hartree/Particle)
Thermal correction to Energy= 0.847886
Thermal correction to Enthalpy= 0.848830
Thermal correction to Gibbs Free Energy= 0.712329
Sum of electronic and zero-point Energies= -2922.339750

Sum of electronic and thermal Energies= -2922.289878
Sum of electronic and thermal Enthalpies= -2922.288934
Sum of electronic and thermal Free Energies= -2922.425435

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Cartesian Coordinates

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C	-2.908060	0.220213	-1.801656
C	-1.515287	0.124884	-1.897041
C	-0.791286	1.181198	-2.471427
C	-1.460337	2.297514	-2.972428
C	-2.850184	2.401293	-2.861810
C	-3.566076	1.369331	-2.255766
H	0.287079	1.106384	-2.548801
H	-3.364679	3.279128	-3.241714
C	-0.776098	-1.078956	-1.476463
C	-3.906020	-0.807344	-1.299581
C	-5.157782	0.081325	-1.014477
H	-6.085093	-0.489398	-1.103132
H	-5.102031	0.469812	0.005110
C	-5.056227	1.247561	-2.024595
O	-1.050715	-2.217764	-2.127080
C	0.814543	-2.469843	-0.724100
N	0.169535	-1.129992	-0.596569
C	-3.473132	-1.658267	-0.118645
C	-2.856087	-1.269136	1.076709
C	-2.558243	-2.240064	2.045130
C	-2.848514	-3.583990	1.815210
C	-3.465598	-3.974226	0.624698
C	-3.778358	-3.008929	-0.331025
H	-2.101391	-1.934012	2.980845
H	-3.706463	-5.018634	0.449612
C	-2.593188	0.139850	1.453845
C	-4.201734	-1.881176	-2.405631
H	-5.028104	-1.570230	-3.048795
H	-3.318133	-2.003974	-3.032803
C	-4.483915	-3.198237	-1.652174
O	-3.661317	0.794374	1.939558
C	-1.679300	2.057329	2.194997
N	-1.464048	0.762244	1.480970
C	-3.219620	2.131498	2.303411
H	-3.658980	2.834395	1.591879
H	-3.583307	2.343171	3.308521
C	-0.278783	-3.264006	-1.459406
H	-0.953278	-3.779548	-0.769702
H	0.092124	-3.945965	-2.222499
H	-2.596440	-4.322498	2.568638
H	-5.563077	1.005667	-2.967232
H	-5.507115	2.171701	-1.651253
H	-5.557959	-3.341726	-1.479136
H	-4.132184	-4.077242	-2.200319
H	-0.893983	3.092414	-3.445989
Fe	0.560887	0.221709	0.978702
Cl	1.241280	0.451349	3.258737
H	-1.217030	1.940412	3.179335
H	1.688935	-2.330401	-1.371211
C	1.273939	-3.102503	0.562404

C	0.699753	-2.776184	1.790721
C	2.299944	-4.054061	0.522303
C	1.156315	-3.364137	2.969903
H	-0.118486	-2.068198	1.831280
C	2.746584	-4.659370	1.696443
H	2.759016	-4.310420	-0.428761
C	2.180329	-4.309967	2.924859
H	0.717849	-3.073920	3.919103
H	3.543658	-5.394839	1.653957
H	2.538422	-4.770072	3.840103
C	-1.071149	3.250165	1.503509
C	-1.430928	3.563248	0.188975
C	-0.185444	4.083878	2.189791
C	-0.921441	4.703287	-0.425776
H	-2.108094	2.914071	-0.354222
C	0.336120	5.222977	1.570853
H	0.092201	3.846311	3.212588
C	-0.036031	5.537051	0.263463
H	-1.218217	4.943254	-1.442040
H	1.020017	5.866158	2.115284
H	0.352781	6.431830	-0.213011
C	3.292985	0.408710	-0.435725
C	4.184781	-0.314883	-1.373359
C	4.808505	0.302409	-2.474244
C	4.468642	-1.670871	-1.125202
C	5.655823	-0.425175	-3.306968
H	4.623978	1.347246	-2.684101
C	5.320072	-2.389690	-1.962624
H	4.016019	-2.161933	-0.273216
C	5.916879	-1.774436	-3.062055
H	6.118841	0.071279	-4.154540
H	5.519734	-3.435661	-1.747952
H	6.580742	-2.333041	-3.713737
C	2.454754	1.507249	-0.732267
O	1.453379	1.840583	-0.002542
O	2.791273	2.292448	-1.766028
C	2.082036	3.539141	-1.895229
H	2.359996	4.223525	-1.089039
H	1.005994	3.380911	-1.857884
H	2.392364	3.945587	-2.856870
O	2.659044	-0.430975	0.535818
H	4.250814	1.274558	0.534262
H	3.788434	2.353438	1.863682
O	4.667284	1.728467	1.427179
H	5.462070	2.239242	1.216529
O	2.723907	2.893069	2.255402
H	2.279266	2.219556	2.836375
H	2.118204	2.924125	1.481572
H	3.180324	-0.495162	1.349951