Impact of Carboxylate Ligation on the C-H Activation Reactivity of Non-heme Fe(IV)O Complex: A Computational Investigation

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Table S1 The relative energies and free energies at 298K (kcal mol^{-1}) for all the species involved in the investigated reactions computed at different levels of theory.

Reactions	Spin state	Species	B1+ZPE	B2+ZPE	B2+G^{corr}
1-EB	S=1	^{3}RC	0.0	0.0	0.0
		^{3}TS	17.5	14.9	26.3
		^{3}IH	1.7	-4.5	5.1
	S=2	^{5}RC	9.9	6.5	3.8
		^{5}TS	21.3	12.0	21.5
		^{5}IH	7.9	-6.9	0.5
2-EB	S=1	^{3}RC	0.0	0.0	0.0
		^{3}TS	10.8	14.2	25.8
		^{3}IH	-4.3	-4.3	5.6
	S=2	^{5}RC	1.6	2.9	3.7
		^{5}TS	9.8	9.2	18.6
		^{5}IH	-10.1	-14.2	-6.4
1-DHT	S=1	^{3}RC	0.0	0.0	0.0
		^{3}TS	11.6	10.5	22.3
		^{3}IH	-11.2	-16.6	-7.2
	S=2	^{5}RC	9.9	6.5	3.8
		^{5}TS	15.4	7.5	17.1
		^{5}IH	1.6	-18.6	-10.4
2-DHT	S=1	^{3}RC	0.0	0.0	0.0
		^{3}TS	6.3	9.9	21.0
		^{3}IH	-16.7	-16.0	-6.8
	S=2	^{5}RC	1.6	2.9	3.7
		^{5}TS	5.4	3.6	13.0
		^{5}IH	-23.0	-25.3	-17.0
	S=1	^{3}RC	0.0	0.0	0.0

3-EB		^{3}TS	14.3	13.4	24.7
		^{3}IH	-2.3	-3.7	9.4
	S=2	^{5}RC	2.1	2.0	3.6
		^{5}TS	9.5	7.8	17.5
		^{5}IH	-12.1	-15.4	-3.5
4- EB	S=1	^{3}RC	0.0	0.0	0.0
		^{3}TS	14.9	11.4	22.3
		^{3}IH	-3.6	-1.5	10.3
	S=2	^{5}RC	3.9	1.5	2.7
		^{5}TS	6.0	5.7	16.1
		^{3}IH	-17.4	-12.3	-1.2
1-DMB	S=1	^{3}RC	0.0	0.0	0.0
		^{3}TS	20.4	17.6	29.6
		^{3}IH	9.5	3.4	12.3
	S=2	^{5}RC	9.9	6.5	3.8
		^{5}TS	22.0	15.3	24.4
		^{3}IH	13.7	4.4	11.5

Table S2 Calculated and experimental bond dissociation energy and enthalpy (kcal mol^{-1}) computed at B3LYP and CBS-QB3 method.

	B3LYP		CBS-QB3		Experiment
Substrate	ΔE_{BDE}	ΔH_{BDE}	ΔE_{BDE}	ΔH_{BDE}	
DHT	70.7	72.3	74.6	75.2	77.0*
EB	83.1	84.6	82.6	84.2	85.4**

*Y. R. Luo, *Comprehensive Handbook of Chemical Bond Energies*, Taylor & Francis, Boca Raton, 2007 *******J. Org. Chem*., 2019, **84**, 13549–13556.

Table S3 Calculated % volume buried and % free space for oxidants computed on the geometry optimized at B1 level of theory.

Oxidants	Spin state	% Volume buried	% Free space
1	S=1	92.4	7.6
	S=2	91.4	8.6
2	S=1	87.1	12.9
	S=2	86.9	13.1
3	S=1	86.5	13.5
	S=2	84.2	15.8
4	S=1	84.6	15.4
	S=2	81.9	18.1

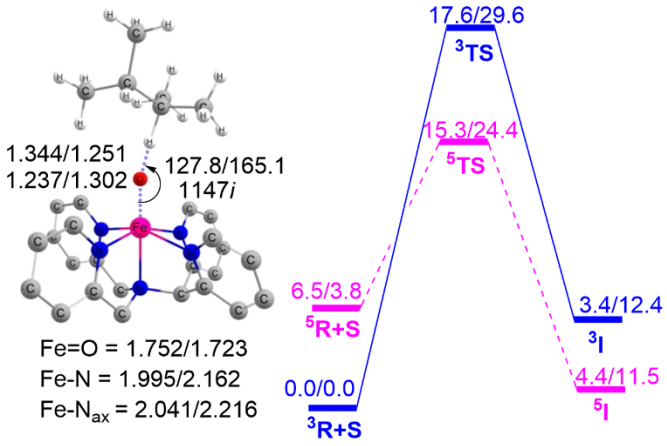

Fig. S1 The potential energy profile computed for C–H activation reactions of 1+DMB with the associated transition state. The energies are stated as ΔE (B2+ZPE)/ ΔG(B2+ G^{corr}_{298K}) in kcal mol^{-1}. Both triplet/quintet spin state geometric parameters are provided along with the lengths and angles expressed in angstroms and degrees, respectively.

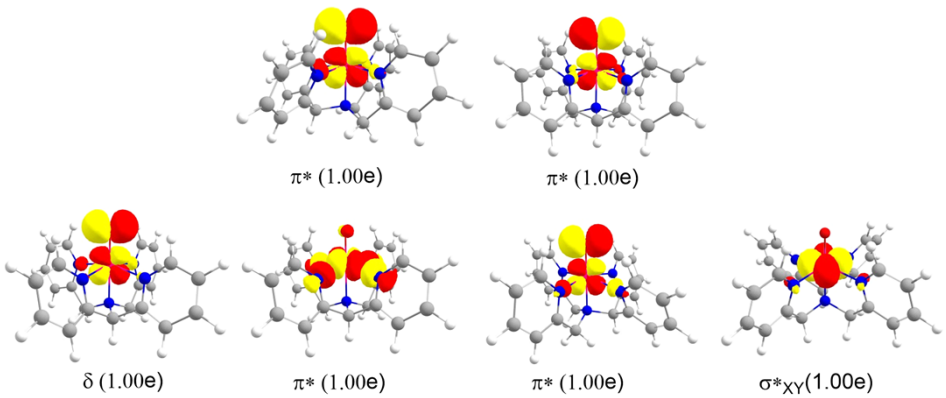

Fig. S2 Spin natural orbitals and their occupations for the oxidants of complex 1. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

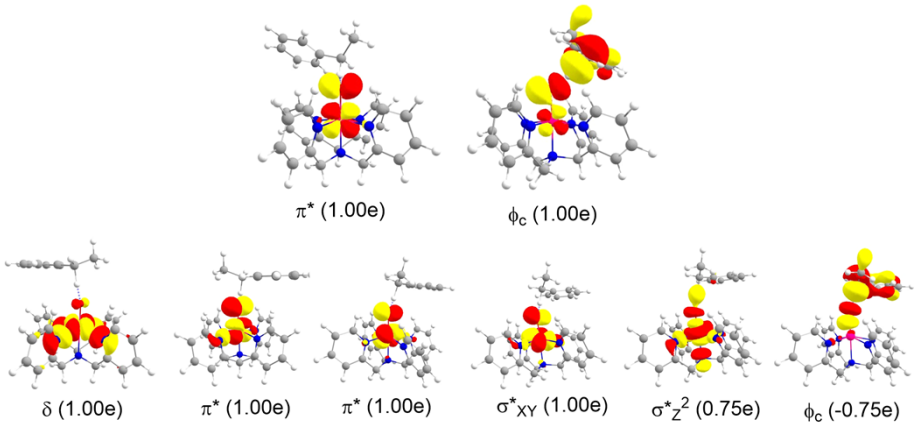

Fig. S3 Spin natural orbitals and their occupations for the transition states of the reaction between complex 1 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

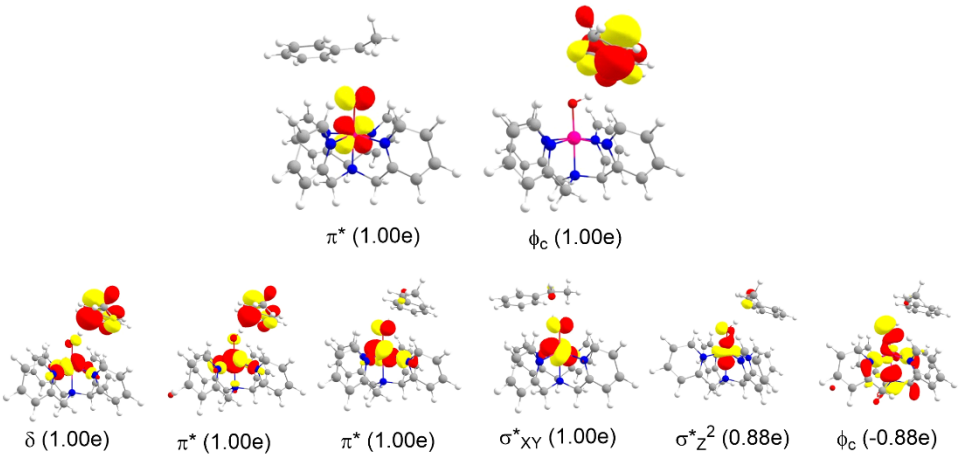

Fig. S4 Spin natural orbitals and their occupations for the intermediates of the reaction between complex 1 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

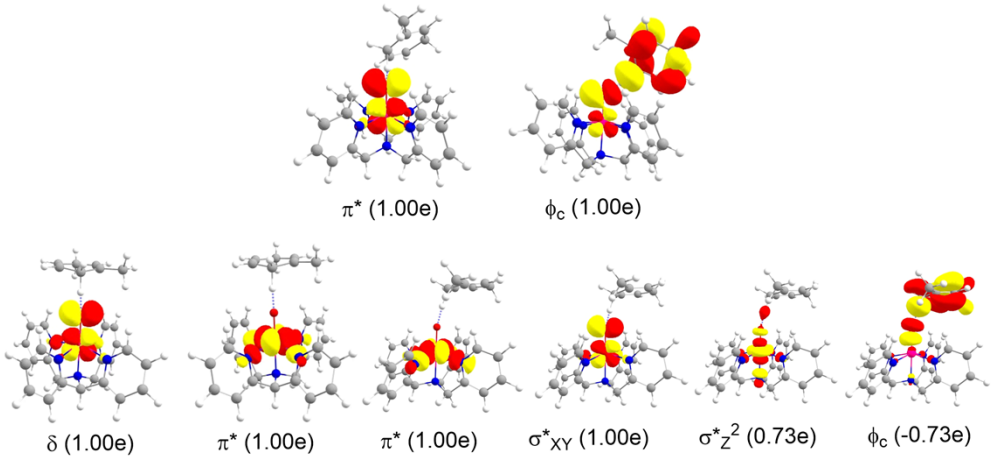

Fig. S5 Spin natural orbitals and their occupations for the transition states of the reaction between complex 1 and DHT. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

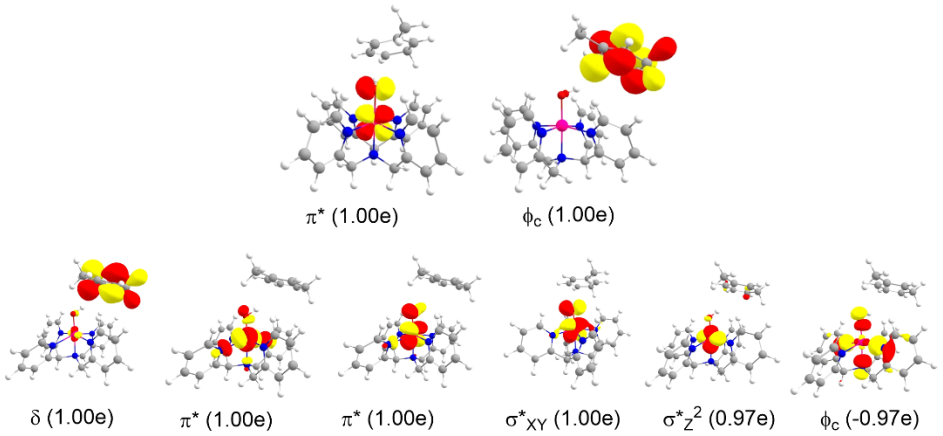

Fig. S6 Spin natural orbitals and their occupations for the intermediates of the reaction between complex 1 and DHT. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

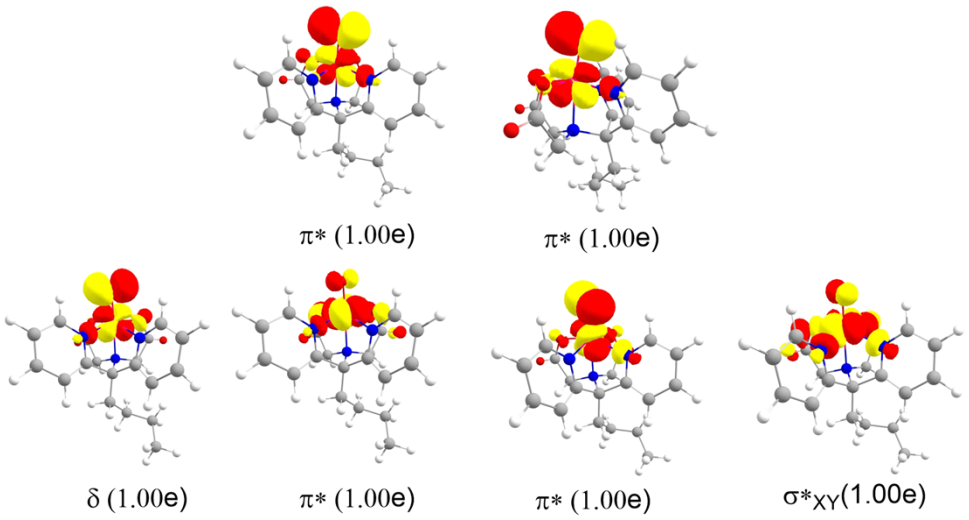

Fig. S7 Spin natural orbitals and their occupations for the oxidants of complex 2. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

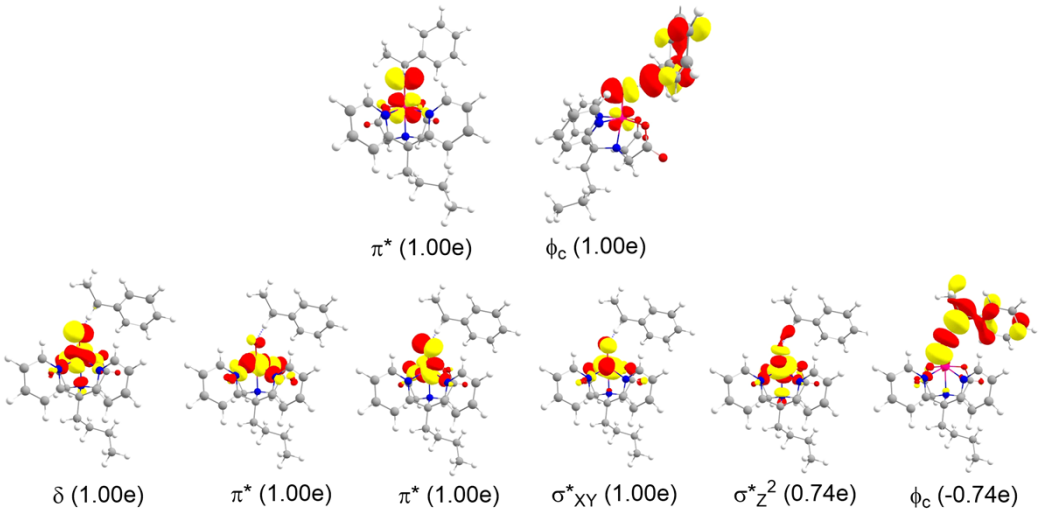

Fig. S8 Spin natural orbitals and their occupations for the transition states of the reaction between complex 2 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

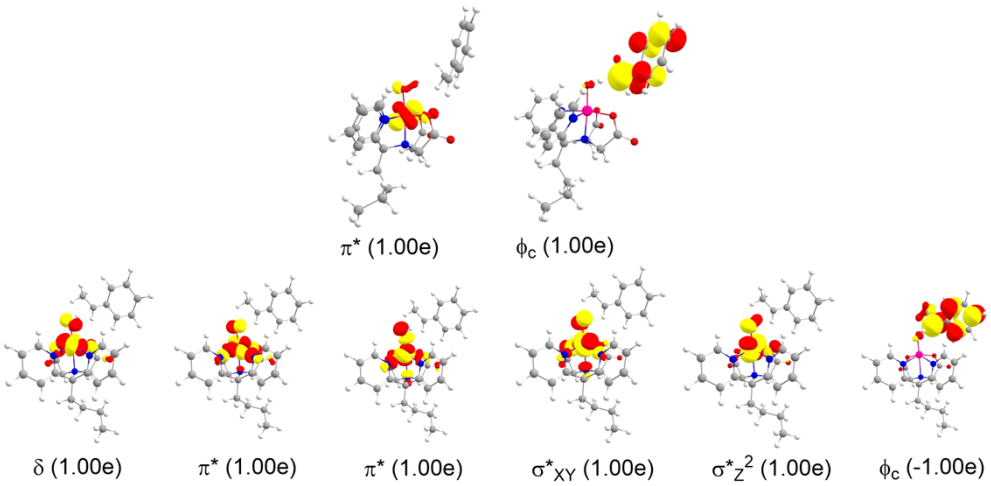

Fig. S9 Spin natural orbitals and their occupations for the intermediates of the reaction between complex 2 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

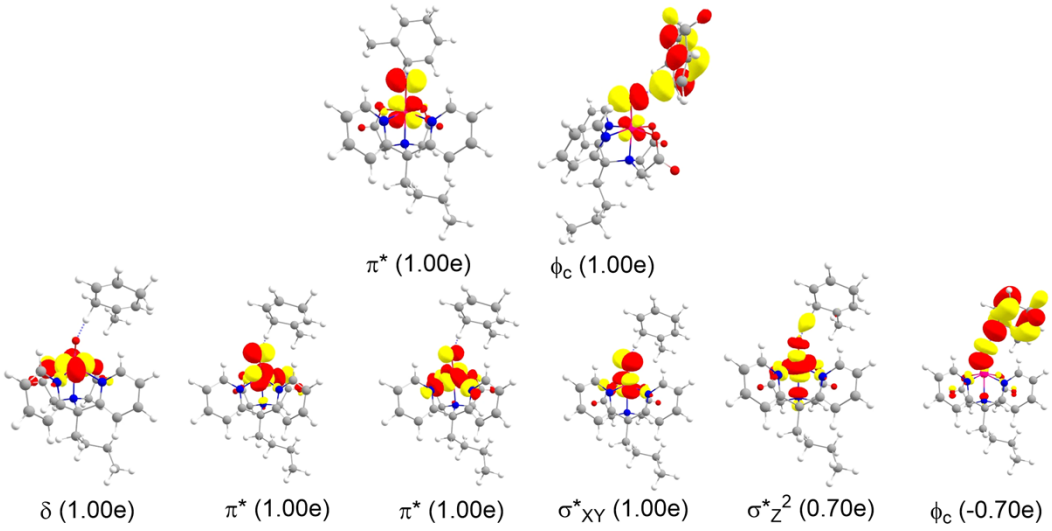

Fig. S10 Spin natural orbitals and their occupations for the transition states of the reaction between complex 2 and DHT. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

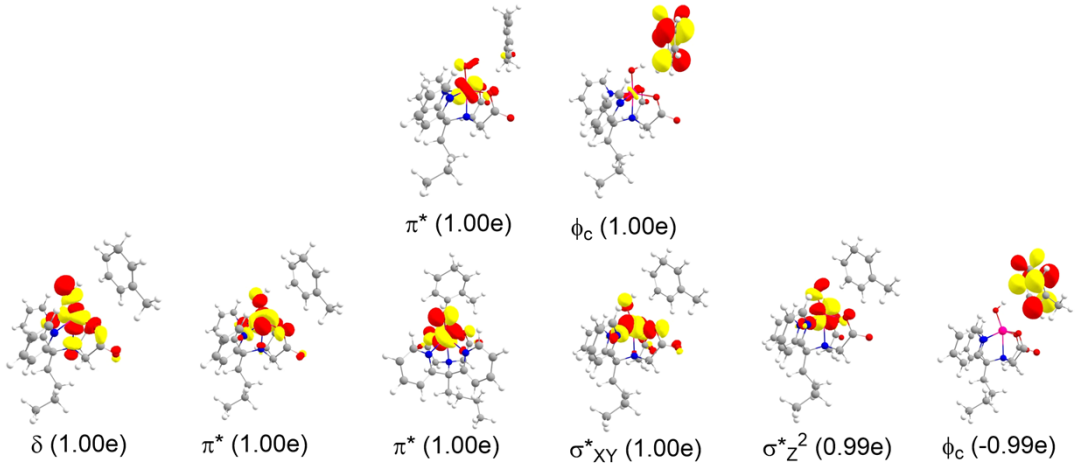

Fig. S11 Spin natural orbitals and their occupations for the intermediates of the reaction between complex 2 and DHT. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

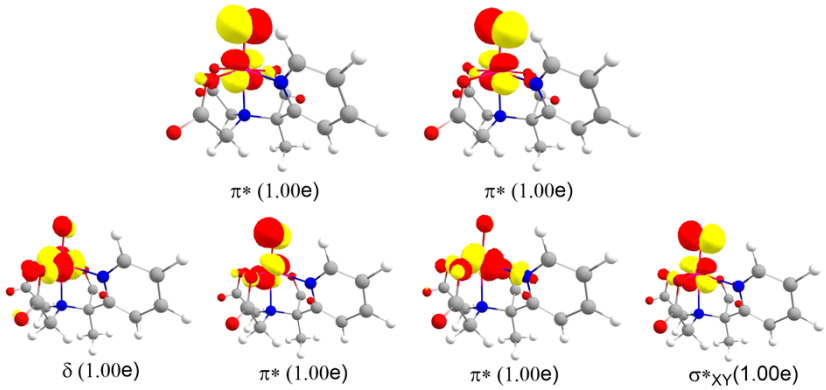

Fig. S12 Spin natural orbitals and their occupations for the oxidants of complex 3. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

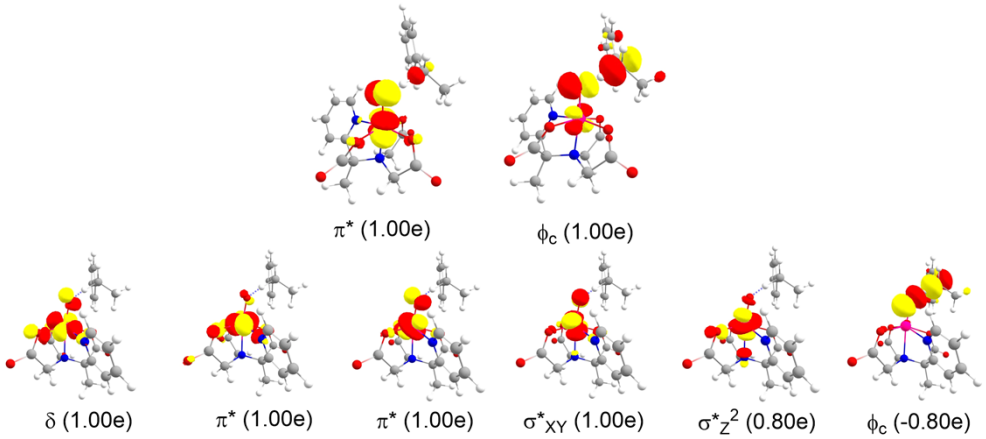

Fig. S13 Spin natural orbitals and their occupations for the transition states of the reaction between complex 3 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

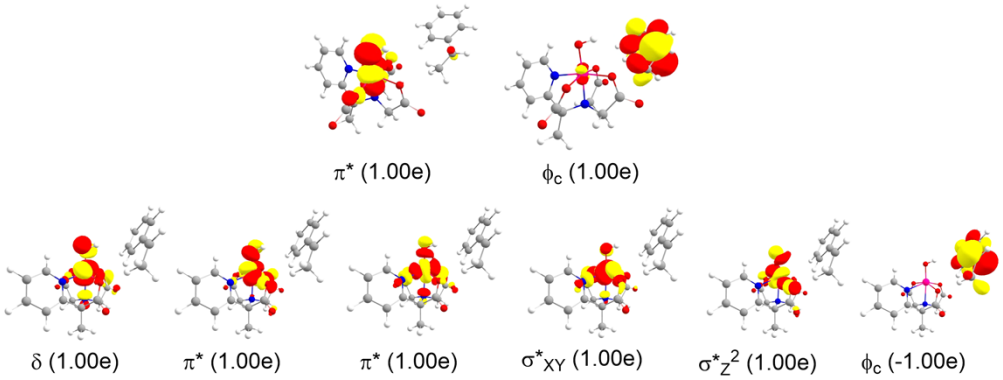

Fig. S14 Spin natural orbitals and their occupations for the intermediates of the reaction between complex 3 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

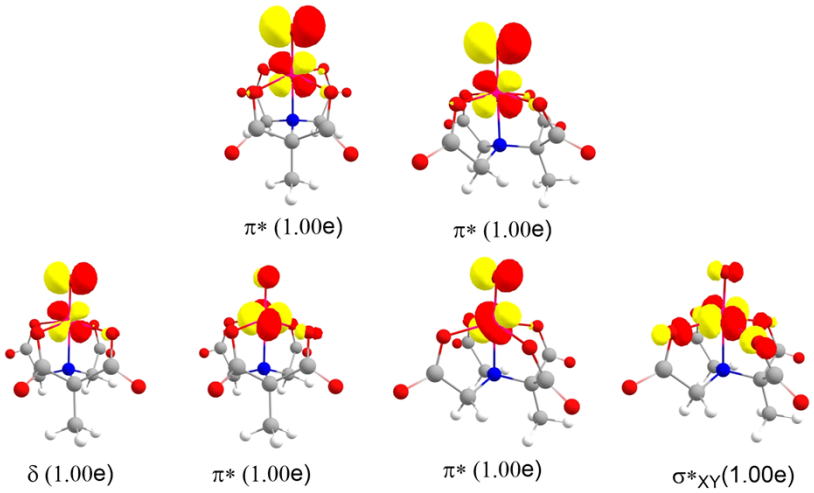

Fig. S15 Spin natural orbitals and their occupations for the oxidants of complex 4. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

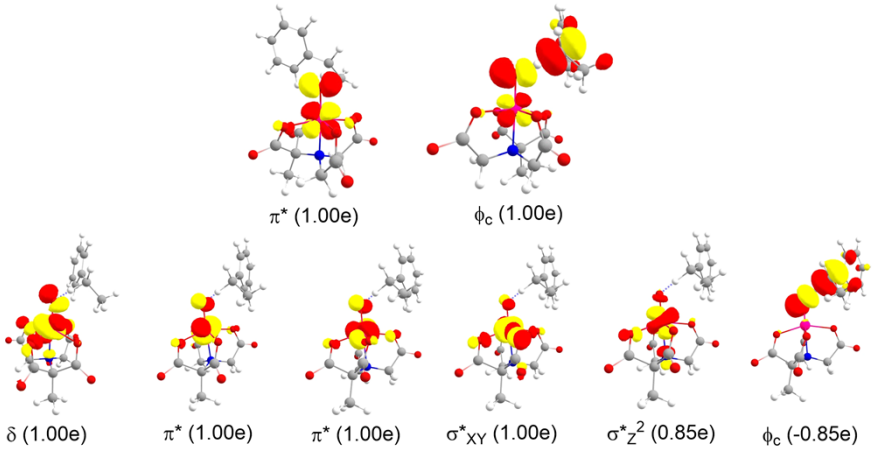

Fig. S16 Spin natural orbitals and their occupations for the transition states of the reaction between complex 4 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

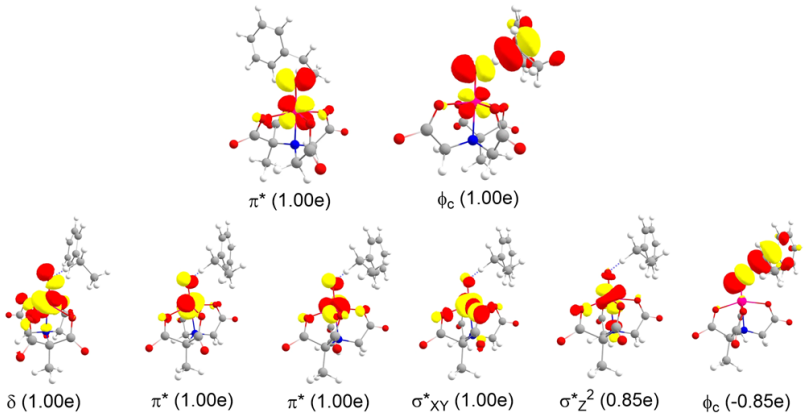

Fig. S17 Spin natural orbitals and their occupations for the intermediates of the reaction between complex 4 and EB. The upper panel represents ^{3}R while the bottom panel represents ^{5}R.

Table S4 Mulliken spin densities and charges for all the investigated oxidants

Species	Spin State	Mulliken Spin Density			Mulliken Charges		
		Fe	**O**	**Rest**	**Fe**	**O**	**Rest**
1	S=1	1.152	0.896	-0.048	0.602	-0.459	-0.143
	S=2	2.965	0.724	0.311	0.766	-0.436	-0.33
2	S=1	1.167	0.875	-0.042	0.651	-0.424	-0.227
	S=2	2.997	0.618	0.385	0.814	-0.422	-0.392
3	S=1	1.155	0.881	-0.036	0.654	-0.419	0.765
	S=2	3.014	0.634	0.352	0.794	-0.418	0.624
4	S=1	1.156	0.877	-0.033	0.629	-0.421	1.792
	S=2	3.043	0.624	0.333	0.748	-0.438	1.69

Table S5 Mulliken spin densities and charges of stationary points along S=1 and S=2

Oxidant	Species	Mulliken Spin Density					Mulliken Charges				
		Fe	**O**	**H**	**C**	**Rest**	**Fe**	**O**	H	C	**Rest**
1+EB	**^{3}TS**	0.935	0.649	-0.060	0.423	0.053	0.573	-0.630	0.335	-0.385	0.107
	^{3}I	0.933	0.145	-0.007	0.759	0.17	0.539	-0.747	0.404	-0.194	-0.002
	^{5}TS	3.764	0.212	0.017	-0.317	0.324	0.848	-0.661	0.342	-0.396	-0.133
	^{5}I	4.021	0.373	-0.009	-0.719	0.334	0.846	-0.811	0.430	-0.246	-0.219
2+EB	**^{3}TS**	0.909	0.688	-0.059	0.403	0.059	0.590	-0.583	0.349	-0.379	0.023
	^{3}I	0.906	0.161	0.002	0.737	0.194	0.570	-0.726	0.430	-0.237	-0.037
	^{5}TS	3.762	0.043	0.032	-0.264	0.427	0.897	-0.623	0.320	-0.376	-0.218
	^{5}I	4.023	0.338	-0.005	-0.729	0.373	0.902	-0.816	0.429	-0.247	-0.268
1+DHT	**^{3}TS**	0.931	0.684	-0.055	0.304	0.136	0.585	-0.613	0.309	-0.432	0.151
	^{3}I	0.929	0.152	0.003	0.568	0.348	0.530	-0.751	0.411	-0.245	0.055
	^{5}TS	3.700	0.300	0.012	-0.206	0.194	0.838	-0.633	0.320	-0.439	-0.086
	^{5}I	2.793	0.180	0.016	0.550	0.461	0.698	-0.764	0.434	-0.245	-0.123

2+DHT	^{3}**TS**	0.911	0.720	-0.055	0.294	0.13	0.590	-0.563	0.326	-0.439	0.086
	^{3}**I**	0.910	0.155	-0.002	0.572	0.365	0.562	-0.728	0.437	-0.248	-0.023
	^{5}**TS**	3.682	0.167	0.025	-0.199	0.325	0.891	-0.616	0.320	-0.428	-0.167
	^{5}**I**	4.018	0.343	0.000	-0.572	0.211	0.882	-0.823	0.429	-0.185	-0.303
3-EB	^{3}**TS**	0.952	0.634	-0.073	0.445	0.042	0.625	-0.602	0.385	-0.374	0.966
	^{3}**I**	0.892	0.144	-0.006	0.756	0.214	0.593	-0.715	0.404	-0.192	0.91
	^{5}**TS**	3.869	-0.075	0.052	-0.321	0.475	0.902	-0.635	0.339	-0.373	0.767
	^{5}**I**	4.043	0.346	0.002	-0.757	0.366	0.901	-0.804	0.410	-0.185	0.678
4-EB	^{3}**TS**	1.014	0.582	-0.078	0.445	0.037	0.621	-0.606	0.408	-0.371	1.948
	^{3}**I**	0.915	0.127	-0.005	0.763	0.2	0.596	-0.714	0.381	-0.195	1.932
	^{5}**TS**	3.941	-0.181	0.070	-0.361	0.531	0.858	-0.652	0.354	-0.368	1.808
	^{5}**I**	4.069	0.290	0.003	-0.760	0.398	0.855	-0.802	0.394	-0.195	1.748

Cartesian coordinates of all the stationary points and thermochemistry data computed at B1 Level of Theory

Complex ^{3}1

Zero-point correction= 0.442934 (Hartree/Particle)
Thermal correction to Energy= 0.477905
Thermal correction to Enthalpy= 0.478849
Thermal correction to Gibbs Free Energy= 0.371654
Sum of electronic and zero-point Energies= -2882.53907
Sum of electronic and thermal Energies= -2882.504102
Sum of electronic and thermal Enthalpies= -2882.503158
Sum of electronic and thermal Free Energies= -2882.610

Fe	-0.358296000	-1.733953000	0.141219000
N	0.060441000	0.276164000	-0.041588000
N	1.129511000	-1.869236000	-1.183164000
N	1.080662000	-1.611610000	1.518209000
N	-1.616495000	-1.370182000	-1.339579000
N	-1.674491000	-1.102638000	1.471943000
O	-0.678774000	-3.326654000	0.285674000
C	1.354458000	-2.851782000	-2.066223000
C	2.428136000	-2.787609000	-2.949820000
C	3.270552000	-1.675261000	-2.908604000
C	3.035547000	-0.654129000	-1.984065000
C	1.947550000	-0.793208000	-1.128229000
C	1.567739000	0.163069000	-0.006002000
C	1.906468000	-0.565102000	1.287521000
C	2.966745000	-0.265780000	2.136981000
C	3.165167000	-1.092778000	3.245807000
C	2.314918000	-2.177095000	3.469452000
C	1.270387000	-2.408344000	2.578844000
C	-2.529854000	-2.255041000	-1.788173000
C	-3.384322000	-1.949370000	-2.835054000
C	-3.297235000	-0.684959000	-3.426764000
C	-2.360575000	0.223409000	-2.952812000
C	-1.522855000	-0.148038000	-1.899227000
C	-0.475532000	0.786550000	-1.348451000
C	-0.516022000	1.015968000	1.131519000
C	-1.609793000	0.207452000	1.785588000
C	-2.506963000	0.773853000	2.692284000
C	-3.474894000	-0.032496000	3.277243000
C	-3.527476000	-1.390126000	2.947828000
C	-2.613834000	-1.889697000	2.033226000
H	0.662663000	-3.686268000	-2.036809000
H	2.594811000	-3.597611000	-3.651881000
H	4.111847000	-1.598760000	-3.590816000
H	3.661138000	0.229466000	-1.913924000
H	2.064202000	1.131600000	-0.088747000
H	3.599060000	0.589186000	1.921656000
H	3.983922000	-0.887816000	3.928930000
H	2.453205000	-2.838587000	4.318009000
H	0.574605000	-3.233123000	2.685516000
H	-2.539602000	-3.212920000	-1.281013000
H	-4.109646000	-2.682954000	-3.169808000
H	-3.966821000	-0.406416000	-4.234528000
H	-2.293551000	1.227742000	-3.356693000
H	-2.480935000	1.841703000	2.874431000
H	-4.195088000	0.397308000	3.966286000
H	-4.273346000	-2.049750000	3.378002000
H	-2.597921000	-2.928652000	1.724672000
H	-0.915114000	1.781176000	-1.213461000
H	0.352296000	0.884291000	-2.058299000
H	-0.910326000	1.985132000	0.808847000
H	0.283555000	1.211883000	1.853192000
Cl	-3.580301000	2.742653000	-0.185970000
O	-4.028558000	3.124220000	1.183247000
O	-2.184826000	3.287126000	-0.418531000
O	-4.500954000	3.260213000	-1.223279000
O	-3.499147000	1.236263000	-0.280046000
Cl	4.424048000	2.384882000	-0.174355000
O	3.565208000	2.402205000	-1.414647000
O	5.486618000	3.406873000	-0.255309000
O	5.011678000	1.003962000	-0.035597000
O	3.529479000	2.631251000	1.015029000

Complex ^{5}1

Zero-point correction= 0.440548 (Hartree/Particle)
Thermal correction to Energy= 0.476711
Thermal correction to Enthalpy= 0.477655
Thermal correction to Gibbs Free Energy= 0.365010
Sum of electronic and zero-point Energies= -2882.52326
Sum of electronic and thermal Energies= -2882.487107
Sum of electronic and thermal Enthalpies= -2882.486163
Sum of electronic and thermal Free Energies= -2882.598

Fe	0.427906000	-1.818066000	0.000019000
N	-0.119954000	0.185455000	-0.000023000
N	-1.210683000	-1.838784000	1.414822000
N	-1.210702000	-1.838878000	-1.414705000
N	1.655405000	-1.189301000	1.547713000
N	1.655377000	-1.189364000	-1.547750000
O	0.856505000	-3.387258000	0.000056000
C	-1.467874000	-2.702167000	2.406591000
C	-2.562232000	-2.530809000	3.250345000

C	-3.398903000	-1.430947000	3.049698000
C	-3.132245000	-0.530643000	2.014994000
C	-2.018267000	-0.775627000	1.215899000
C	-1.628672000	0.050315000	0.000003000
C	-2.018294000	-0.775718000	-1.215823000
C	-3.132307000	-0.530808000	-2.014890000
C	-3.398993000	-1.431187000	-3.049523000
C	-2.562310000	-2.531049000	-3.250128000
C	-1.467916000	-2.702334000	-2.406406000
C	2.624668000	-1.935375000	2.114695000
C	3.449145000	-1.427159000	3.104737000
C	3.269118000	-0.099599000	3.508984000
C	2.273910000	0.666801000	2.916837000
C	1.477694000	0.091519000	1.924611000
C	0.380361000	0.872218000	1.247794000
C	0.380316000	0.872160000	-1.247899000
C	1.477640000	0.091439000	-1.924694000
C	2.273862000	0.666711000	-2.916923000
C	3.269097000	-0.099681000	-3.509033000
C	3.449145000	-1.427225000	-3.104745000
C	2.624665000	-1.935430000	-2.114699000
H	-0.780247000	-3.536104000	2.506720000
H	-2.750052000	-3.246425000	4.043869000
H	-4.258206000	-1.270707000	3.694087000
H	-3.756413000	0.334660000	1.817801000
H	-2.100370000	1.032510000	-0.000032000
H	-3.756483000	0.334497000	-1.817726000
H	-4.258323000	-1.271005000	-3.693888000
H	-2.750150000	-3.246721000	-4.043596000
H	-0.780280000	-3.536267000	-2.506501000
H	2.710774000	-2.951712000	1.745357000
H	4.224091000	-2.050369000	3.537612000
H	3.914842000	0.338636000	4.263536000
H	2.145646000	1.713319000	3.170136000
H	2.145559000	1.713219000	-3.170257000
H	3.914826000	0.338547000	-4.263585000
H	4.224112000	-2.050430000	-3.537589000
H	2.710794000	-2.951755000	-1.745331000
H	0.762128000	1.865703000	0.993595000
H	-0.462499000	1.009316000	1.932403000
H	0.762152000	1.865650000	-0.993774000
H	-0.462568000	1.009235000	-1.932483000
Cl	3.611013000	2.468159000	-0.000018000
O	4.345272000	2.860660000	-1.229625000
O	2.243458000	3.121304000	-0.000662000
O	4.344159000	2.860763000	1.230234000
O	3.401163000	0.970880000	-0.000045000
Cl	-4.131305000	2.609012000	-0.000065000
O	-3.246345000	2.608927000	1.220294000
O	-5.033277000	3.777767000	-0.000113000
O	-4.919057000	1.320330000	-0.000019000
O	-3.246338000	2.608835000	-1.220419000

Complex ^{3}2

Zero-point correction= 0.388768 (Hartree/Particle)
Thermal correction to Energy= 0.413339
Thermal correction to Enthalpy= 0.414283
Thermal correction to Gibbs Free Energy= 0.335167
Sum of electronic and zero-point Energies= -1400.10748
Sum of electronic and thermal Energies= -1400.082916
Sum of electronic and thermal Enthalpies= -1400.081971
Sum of electronic and thermal Free Energies= -1400.161

Fe	-1.412404000	0.720542000	0.607693000
O	-2.753016000	0.839115000	-0.729806000
O	-1.044952000	2.572178000	0.451761000
C	-0.339003000	-1.799603000	-0.110096000
C	-2.466099000	-2.062735000	0.827887000
C	-0.210011000	-3.176336000	-0.285057000
C	-2.409747000	-3.446022000	0.671483000
H	-3.313103000	-1.542785000	1.262158000
C	-1.263144000	-4.005432000	0.111669000
H	0.682276000	-3.602271000	-0.726976000
H	-3.246215000	-4.061811000	0.983481000
H	-1.183980000	-5.080263000	-0.022621000
C	0.588112000	0.904515000	2.830909000
C	1.242494000	-0.271273000	0.915817000
C	1.799479000	0.629929000	3.463171000
H	-0.209734000	1.477601000	3.290811000
C	2.462959000	-0.603228000	1.497227000
C	2.742194000	-0.141002000	2.786833000
H	1.988264000	1.008452000	4.461830000
H	3.189298000	-1.200888000	0.961611000
H	3.693173000	-0.382312000	3.252640000
N	0.331615000	0.452377000	1.599454000
N	-1.449133000	-1.282230000	0.448392000
N	-0.072998000	0.450558000	-0.994855000
O	-2.344713000	0.768407000	1.938352000
C	0.637562000	1.762618000	-1.091799000
H	1.633922000	1.680727000	-0.654117000
H	0.766640000	2.054069000	-2.136724000
C	-0.081039000	2.918910000	-0.348514000
O	0.337116000	4.050271000	-0.532905000
C	-0.930855000	0.168255000	-2.180277000
H	-0.913944000	-0.900755000	-2.408571000
C	-2.417691000	0.557140000	-1.955931000
O	-3.163640000	0.528381000	-2.920320000
C	0.723510000	-0.723970000	-0.466950000
C	1.770354000	-1.316065000	-1.450157000
C	2.720312000	-0.393223000	-2.247184000
H	2.355627000	-2.074645000	-0.915505000
H	1.190988000	-1.874194000	-2.193962000
C	3.957067000	0.182443000	-1.531981000
H	3.079844000	-0.992639000	-3.094823000
H	2.142524000	0.419026000	-2.696160000
C	5.047709000	-0.856925000	-1.242230000
H	4.383609000	0.960618000	-2.177140000
H	5.905187000	-0.398187000	-0.737918000
H	4.692646000	-1.676061000	-0.603485000
H	5.411789000	-1.309870000	-2.172231000
H	3.671551000	0.692597000	-0.604232000
H	-0.555591000	0.689784000	-3.064593000

Complex ^{5}2

Zero-point correction= 0.387207 (Hartree/Particle)
Thermal correction to Energy= 0.412612
Thermal correction to Enthalpy= 0.413556
Thermal correction to Gibbs Free Energy= 0.331029
Sum of electronic and zero-point Energies= -1400.10491
Sum of electronic and thermal Energies= -1400.079509
Sum of electronic and thermal Enthalpies= -1400.078565
Sum of electronic and thermal Free Energies= -1400.161

Fe	-1.575789000	0.757179000	0.648563000
O	-2.866380000	0.756297000	-0.818565000
O	-1.026300000	2.597088000	0.710754000
C	-0.306369000	-1.805140000	-0.187825000
C	-2.379860000	-2.245639000	0.790875000
C	-0.106861000	-3.161682000	-0.447602000
C	-2.255364000	-3.613521000	0.554972000

H	-3.245318000	-1.805358000	1.275784000
C	-1.098605000	-4.071709000	-0.071294000
H	0.793119000	-3.513197000	-0.936499000
H	-3.045231000	-4.293335000	0.855631000
H	-0.962991000	-5.130592000	-0.271681000
C	0.689028000	0.651391000	2.940665000
C	1.270355000	-0.323976000	0.905734000
C	1.921608000	0.323803000	3.505292000
H	-0.082649000	1.184088000	3.487897000
C	2.515625000	-0.704114000	1.404382000
C	2.841169000	-0.369777000	2.722094000
H	2.145915000	0.604030000	4.528920000
H	3.225575000	-1.241833000	0.789352000
H	3.809777000	-0.649429000	3.126340000
N	0.384746000	0.322178000	1.682988000
N	-1.424187000	-1.385172000	0.427769000
N	-0.128104000	0.526730000	-0.928416000
O	-2.562047000	0.727149000	1.935495000
C	0.590335000	1.842905000	-0.943830000
H	1.609451000	1.715465000	-0.576925000
H	0.662014000	2.220846000	-1.966056000
C	-0.048332000	2.956497000	-0.074570000
O	0.433683000	4.072166000	-0.159506000
C	-0.918498000	0.283065000	-2.172199000
H	-0.875002000	-0.777988000	-2.431479000
C	-2.426353000	0.628079000	-2.037716000
O	-3.083805000	0.688834000	-3.062199000
C	0.707501000	-0.667179000	-0.491574000
C	1.741054000	-1.157464000	-1.548087000
C	2.658435000	-0.167330000	-2.302548000
H	2.355265000	-1.938202000	-1.083769000
H	1.157094000	-1.676587000	-2.315455000
C	3.908299000	0.373484000	-1.582025000
H	3.002670000	-0.703674000	-3.197525000
H	2.061855000	0.665743000	-2.682717000
C	5.024160000	-0.665567000	-1.410872000
H	4.301482000	1.208125000	-2.175745000
H	5.889098000	-0.233635000	-0.895773000
H	4.702082000	-1.540445000	-0.831422000
H	5.366671000	-1.034021000	-2.385316000
H	3.646114000	0.802243000	-0.607412000
H	-0.498842000	0.835930000	-3.016238000

Complex ^{3}3

Zero-point correction= 0.234387 (Hartree/Particle)
Thermal correction to Energy= 0.253195
Thermal correction to Enthalpy= 0.254139
Thermal correction to Gibbs Free Energy= 0.187681
Sum of electronic and zero-point Energies= -1223.30581
Sum of electronic and thermal Energies= -1223.287002
Sum of electronic and thermal Enthalpies= -1223.286058
Sum of electronic and thermal Free Energies= -1223.352

e	0.540685000	-0.555876000	-0.958187000
O	0.684411000	-2.170514000	0.088146000
O	2.437811000	-0.387704000	-0.970885000
C	-1.714613000	0.519591000	0.351279000
C	-2.372931000	-1.284796000	-0.981789000
C	-3.028389000	0.729100000	0.773294000
C	-3.705122000	-1.135062000	-0.600932000
H	-2.027358000	-2.043029000	-1.676668000
C	-4.031368000	-0.111782000	0.289328000
H	-3.258611000	1.532585000	1.463357000
H	-4.462094000	-1.804608000	-0.996163000
H	-5.060719000	0.032828000	0.607276000
C	-0.184414000	2.129186000	-0.663671000
N	-1.422356000	-0.475377000	-0.511062000
N	0.639971000	0.418174000	0.890695000
O	0.310089000	-1.269018000	-2.401778000
C	1.985010000	1.052150000	0.909305000
H	1.903776000	2.093926000	0.588617000
H	2.405577000	1.051418000	1.919813000
C	2.976620000	0.359448000	-0.060280000
O	4.172315000	0.592625000	0.078430000
C	0.470023000	-0.625302000	1.932897000
H	-0.528855000	-0.553121000	2.374258000
C	0.622157000	-2.065655000	1.377100000
O	0.633538000	-2.988764000	2.185886000
C	-0.506226000	1.367565000	0.705602000
H	1.186822000	-0.483039000	2.747263000
O	0.331287000	1.352668000	-1.545334000
O	-0.459832000	3.322131000	-0.753305000
C	-0.726889000	2.337283000	1.860295000
H	-1.462647000	3.092034000	1.572262000
H	-1.059696000	1.823458000	2.770351000
H	0.202607000	2.868986000	2.081218000

Complex ^{5}3

Zero-point correction= 0.232956 (Hartree/Particle)
Thermal correction to Energy= 0.252545
Thermal correction to Enthalpy= 0.253489
Thermal correction to Gibbs Free Energy= 0.183788
Sum of electronic and zero-point Energies= -1223.30909
Sum of electronic and thermal Energies= -1223.289502
Sum of electronic and thermal Enthalpies= -1223.288558
Sum of electronic and thermal Free Energies= -1223.358

Fe	0.685039000	-0.609326000	-1.025795000
O	0.542411000	-2.233121000	0.116967000
O	2.637524000	-0.386361000	-0.855516000
C	-1.739152000	0.538874000	0.313057000
C	-2.494510000	-1.235931000	-0.990885000
C	-3.033316000	0.794303000	0.774991000
C	-3.812806000	-1.043530000	-0.578457000
H	-2.204958000	-2.021917000	-1.682085000
C	-4.078499000	-0.009923000	0.319415000
H	-3.219223000	1.603037000	1.472111000
H	-4.602588000	-1.688841000	-0.949817000
H	-5.092711000	0.170250000	0.666845000
C	-0.194584000	2.119154000	-0.732569000
N	-1.502417000	-0.460249000	-0.555088000
N	0.645552000	0.410343000	0.835000000
O	0.567999000	-1.345149000	-2.467294000
C	1.969622000	1.086420000	0.924787000
H	1.892830000	2.084447000	0.485235000
H	2.284475000	1.205142000	1.966182000
C	3.070547000	0.342446000	0.126634000
O	4.239841000	0.538833000	0.435590000
C	0.447446000	-0.606895000	1.905782000
H	-0.489234000	-0.419638000	2.438763000
C	0.410575000	-2.070843000	1.394048000
O	0.248378000	-2.951096000	2.233458000
C	-0.504268000	1.364531000	0.639315000
H	1.250069000	-0.529988000	2.644862000
O	0.326232000	1.346118000	-1.613446000
O	-0.495446000	3.305599000	-0.830885000

C	-0.698636000	2.347982000	1.789681000
H	-1.425376000	3.108655000	1.495528000
H	-1.034044000	1.851516000	2.708069000
H	0.237789000	2.871043000	1.999799000

Complex ^{3}4

Zero-point correction= 0.166944 (Hartree/Particle)
Thermal correction to Energy= 0.183867
Thermal correction to Enthalpy= 0.184811
Thermal correction to Gibbs Free Energy= 0.122521
Sum of electronic and zero-point Energies= -1164.23020
Sum of electronic and thermal Energies= -1164.213279
Sum of electronic and thermal Enthalpies= -1164.212335
Sum of electronic and thermal Free Energies= -1164.274

Fe	-0.518047000	0.000283000	-1.097044000
O	-1.792781000	-1.361248000	-0.508001000
O	0.903668000	-1.382338000	-1.185469000
O	0.904463000	1.381952000	-1.186042000
O	-1.793183000	1.361004000	-0.507312000
O	-0.912790000	0.000994000	-2.676068000
N	0.084404000	-0.000252000	0.900961000
C	-1.659654000	-1.813944000	0.688722000
C	-0.467089000	-1.238850000	1.495295000
C	-1.659341000	1.814013000	0.689244000
C	-0.467274000	1.237969000	1.495922000
H	-0.779766000	-1.075526000	2.533669000
H	0.308812000	-2.010175000	1.508882000
H	-0.780643000	1.073757000	2.533924000
H	0.308743000	2.009188000	1.510621000
O	-2.355436000	2.677073000	1.235787000
O	-2.356438000	-2.676512000	1.235149000
C	1.561155000	-0.000065000	0.641159000
C	1.813353000	1.238836000	-0.282623000
C	1.813167000	-1.239098000	-0.282638000
O	2.801670000	-1.958239000	-0.105514000
O	2.801841000	1.957916000	-0.105107000
C	2.435600000	-0.000086000	1.885829000
H	2.255668000	-0.894493000	2.493760000
H	3.482030000	-0.000225000	1.577024000
H	2.255935000	0.894412000	2.493710000

Complex ^{5}4

Zero-point correction= 0.165687 (Hartree/Particle)
Thermal correction to Energy= 0.183306
Thermal correction to Enthalpy= 0.184250
Thermal correction to Gibbs Free Energy= 0.119293
Sum of electronic and zero-point Energies= -1164.23652
Sum of electronic and thermal Energies= -1164.218900
Sum of electronic and thermal Enthalpies= -1164.217956
Sum of electronic and thermal Free Energies= -1164.282

Fe	-0.545177000	-0.000088000	-1.165734000
O	-1.830238000	-1.432170000	-0.500639000
O	0.993026000	-1.410962000	-1.199234000
O	0.991338000	1.411061000	-1.198966000
O	-1.830540000	1.432648000	-0.500867000
O	-0.953014000	-0.000218000	-2.739382000
N	0.072689000	-0.000356000	0.847595000
C	-1.688037000	-1.824990000	0.715787000
C	-0.466291000	-1.236989000	1.467735000
C	-1.688858000	1.824223000	0.715953000
C	-0.467487000	1.235756000	1.468224000
H	-0.733635000	-1.066048000	2.516942000
H	0.308497000	-2.009039000	1.451986000
H	-0.735740000	1.063595000	2.516971000
H	0.307125000	2.008008000	1.453978000
O	-2.383886000	2.648390000	1.319874000
O	-2.382813000	-2.649760000	1.319082000
C	1.564563000	0.000295000	0.638777000
C	1.861508000	1.246517000	-0.265482000
C	1.862727000	-1.245557000	-0.265568000
O	2.858647000	-1.942578000	-0.040456000
O	2.856804000	1.944467000	-0.040701000
C	2.382652000	0.000603000	1.922379000
H	2.180845000	-0.894042000	2.522717000
H	3.439860000	0.001422000	1.653693000
H	2.179579000	0.894700000	2.523116000

EB

Zero-point correction= 0.157375 (Hartree/Particle)
Thermal correction to Energy= 0.164699
Thermal correction to Enthalpy= 0.165643
Thermal correction to Gibbs Free Energy= 0.125145
Sum of electronic and zero-point Energies= -310.722853
Sum of electronic and thermal Energies= -310.715528
Sum of electronic and thermal Enthalpies= -310.714584
Sum of electronic and thermal Free Energies= -310.7550

C	-0.434678000	0.000078000	-0.328435000
C	0.270520000	1.202597000	-0.184975000
C	1.637314000	1.205767000	0.096272000
C	2.326003000	-0.000079000	0.238545000
C	1.637171000	-1.205864000	0.096215000
C	0.270402000	-1.202541000	-0.185025000
H	-0.257890000	2.147093000	-0.299391000
H	2.165348000	2.150444000	0.199392000
H	3.391267000	-0.000175000	0.453709000
H	2.165153000	-2.150576000	0.199279000
H	-0.258157000	-2.146949000	-0.299482000
C	-1.926434000	0.000186000	-0.592421000
H	-2.192702000	0.879593000	-1.192454000
H	-2.192781000	-0.878908000	-1.192876000
C	-2.763059000	-0.000126000	0.700012000
H	-3.835617000	-0.000031000	0.472856000
H	-2.544056000	-0.884628000	1.308683000
H	-2.543991000	0.884029000	1.309154000

DHT

Zero-point correction= 0.150555 (Hartree/Particle)
Thermal correction to Energy= 0.157305
Thermal correction to Enthalpy= 0.158249
Thermal correction to Gibbs Free Energy= 0.120110
Sum of electronic and zero-point Energies= -272.587920
Sum of electronic and thermal Energies= -272.581171
Sum of electronic and thermal Enthalpies= -272.580227
Sum of electronic and thermal Free Energies= -272.6183

C	1.277370000	-1.253007000	-0.000742000
C	1.908645000	0.112883000	0.000698000
C	1.201662000	1.244063000	0.000708000
C	-0.303255000	1.283307000	-0.001263000
C	-0.953285000	-0.083078000	0.000003000
C	-0.227648000	-1.207244000	0.000140000
H	1.633920000	-1.828132000	-0.872404000
H	-0.663014000	1.861820000	0.867422000
H	1.635014000	-1.830311000	0.868996000

H	-0.660787000	1.858785000	-0.872946000
C	-2.459558000	-0.095094000	0.000690000
H	-2.861809000	0.426144000	-0.879767000
H	-2.857322000	-1.115074000	0.001281000
H	-2.861348000	0.427112000	0.880713000
H	2.996940000	0.153312000	0.002124000
H	1.715049000	2.204641000	0.002252000
H	-0.740226000	-2.169271000	0.000928000

1+EB

^{3}TS

Zero-point correction= 0.594602 (Hartree/Particle)
Thermal correction to Energy= 0.638480
Thermal correction to Enthalpy= 0.639424
Thermal correction to Gibbs Free Energy= 0.509356
Sum of electronic and zero-point Energies= -3193.23398
Sum of electronic and thermal Energies= -3193.190104
Sum of electronic and thermal Enthalpies= -3193.189160
Sum of electronic and thermal Free Energies= -3193.319

Fe	-0.375615000	-0.897355000	0.394900000
N	1.095244000	0.456784000	-0.005622000
N	-0.862759000	0.466600000	1.778694000
N	-1.384822000	0.240092000	-0.901548000
N	0.982724000	-1.671560000	1.624449000
N	0.445122000	-1.908669000	-1.102684000
O	-1.568286000	-2.123075000	0.724249000
C	-1.463024000	0.281992000	2.963566000
C	-1.665398000	1.339341000	3.845462000
C	-1.215842000	2.611087000	3.485658000
C	-0.572079000	2.801319000	2.260889000
C	-0.414634000	1.694968000	1.430598000
C	0.239030000	1.706478000	0.055888000
C	-0.874981000	1.493228000	-0.957630000
C	-1.356119000	2.447293000	-1.847693000
C	-2.400195000	2.074718000	-2.699025000
C	-2.919311000	0.781543000	-2.639094000
C	-2.379772000	-0.119594000	-1.724721000
C	0.859070000	-2.856903000	2.252711000
C	1.857827000	-3.349654000	3.078616000
C	3.025015000	-2.597376000	3.244872000
C	3.149715000	-1.381371000	2.585266000
C	2.100239000	-0.934940000	1.779888000
C	2.151163000	0.390812000	1.062651000
C	1.670430000	0.179198000	-1.366869000
C	1.420831000	-1.255569000	-1.766533000
C	2.135644000	-1.876009000	-2.792078000
C	1.812885000	-3.182209000	-3.140905000
C	0.788202000	-3.842926000	-2.457216000
C	0.132197000	-3.175852000	-1.433265000
H	-1.772295000	-0.732421000	3.187560000
H	-2.159947000	1.161600000	4.794668000
H	-1.354336000	3.453366000	4.156843000
H	-0.185171000	3.765146000	1.946433000
H	0.807809000	2.620499000	-0.129418000
H	-0.907552000	3.435293000	-1.867692000
H	-2.798284000	2.795056000	-3.407470000
H	-3.734222000	0.465014000	-3.280591000
H	-2.738561000	-1.137180000	-1.628774000
H	-0.070753000	-3.382223000	2.066089000
H	1.728756000	-4.309133000	3.567980000
H	3.836079000	-2.966561000	3.864927000
H	4.056769000	-0.791399000	2.654768000
H	2.971829000	-1.360955000	-3.250985000
H	2.370838000	-3.687477000	-3.923186000
H	0.514019000	-4.864745000	-2.697324000
H	-0.661030000	-3.623014000	-0.844826000
H	3.144208000	0.537431000	0.622977000
H	1.982180000	1.204711000	1.775075000
H	2.742276000	0.401706000	-1.375695000
H	1.192975000	0.847386000	-2.090610000
Cl	5.163363000	-1.122727000	-0.852810000
O	5.263467000	-1.407826000	-2.314312000
O	4.823636000	0.341304000	-0.659725000
O	6.427644000	-1.443802000	-0.153086000
O	4.030705000	-1.931081000	-0.265440000
Cl	0.545420000	5.345002000	-0.304251000
O	1.375801000	4.783512000	0.823239000
O	0.783602000	6.794503000	-0.460287000
O	-0.903519000	5.067487000	0.002091000
O	0.907254000	4.602337000	-1.565436000
C	-6.000324000	-2.493359000	-1.735158000
C	-6.563283000	-1.233550000	-1.966114000
C	-6.290211000	-0.184188000	-1.083482000
C	-5.459633000	-0.393462000	0.015126000
C	-4.891103000	-1.658546000	0.271234000
C	-5.176775000	-2.704773000	-0.631530000
H	-6.210281000	-3.314674000	-2.415089000
H	-7.213127000	-1.074143000	-2.822040000
H	-6.728991000	0.796058000	-1.248712000
H	-5.253944000	0.426956000	0.698755000
H	-4.751327000	-3.690157000	-0.465601000
C	-4.002129000	-1.846512000	1.436095000
H	-2.762945000	-1.849733000	1.001934000
H	-4.011172000	-0.973790000	2.096869000
C	-4.056807000	-3.157972000	2.203957000
H	-3.852492000	-4.019974000	1.560921000
H	-3.312928000	-3.166773000	3.007434000
H	-5.046476000	-3.306186000	2.657063000

^{3}IH

Zero-point correction= 0.597783 (Hartree/Particle)
Thermal correction to Energy= 0.642956
Thermal correction to Enthalpy= 0.643900
Thermal correction to Gibbs Free Energy= 0.509541
Sum of electronic and zero-point Energies= -3193.25929
Sum of electronic and thermal Energies= -3193.214124
Sum of electronic and thermal Enthalpies= -3193.213179
Sum of electronic and thermal Free Energies= -3193.347

Fe	-0.486895000	-0.764971000	0.331001000
N	1.165734000	0.348626000	0.013802000
N	-0.856126000	0.644910000	1.696212000
N	-1.290343000	0.518159000	-0.974867000
N	0.665521000	-1.754691000	1.603446000
N	0.230580000	-1.888140000	-1.129528000
O	-1.935701000	-1.801504000	0.628598000
C	-1.573697000	0.546520000	2.824422000
C	-1.674570000	1.617163000	3.708010000
C	-1.001383000	2.803090000	3.408844000
C	-0.248362000	2.902874000	2.236069000
C	-0.204875000	1.792901000	1.397937000
C	0.507256000	1.714109000	0.054214000
C	-0.591575000	1.678466000	-0.999716000
C	-0.903931000	2.709673000	-1.878926000
C	-1.983298000	2.520245000	-2.746622000

C	-2.703864000	1.326366000	-2.711277000
C	-2.323114000	0.335237000	-1.810336000
C	0.331456000	-2.911193000	2.206205000
C	1.206284000	-3.559819000	3.065024000
C	2.467145000	-2.998434000	3.290570000
C	2.807149000	-1.809462000	2.656949000
C	1.874293000	-1.199040000	1.816996000
C	2.152859000	0.113331000	1.126291000
C	1.753425000	-0.003827000	-1.327450000
C	1.320853000	-1.388616000	-1.746258000
C	1.980990000	-2.112470000	-2.739643000
C	1.481030000	-3.357377000	-3.105365000
C	0.338815000	-3.855035000	-2.471340000
C	-0.256187000	-3.094373000	-1.475336000
H	-2.062799000	-0.406568000	2.994432000
H	-2.266738000	1.515798000	4.611403000
H	-1.056616000	3.650983000	4.084958000
H	0.300368000	3.799445000	1.966330000
H	1.214418000	2.532037000	-0.100245000
H	-0.307799000	3.616451000	-1.873690000
H	-2.254451000	3.305903000	-3.445490000
H	-3.552700000	1.153669000	-3.363390000
H	-2.842051000	-0.614579000	-1.739652000
H	-0.660795000	-3.281694000	1.975134000
H	0.910395000	-4.491857000	3.534584000
H	3.183884000	-3.494345000	3.937855000
H	3.790160000	-1.367555000	2.774772000
H	2.904861000	-1.730660000	-3.159106000
H	1.991432000	-3.943733000	-3.863172000
H	-0.073635000	-4.825075000	-2.727937000
H	-1.134625000	-3.411256000	-0.924534000
H	3.174749000	0.119300000	0.730625000
H	2.071017000	0.935233000	1.844811000
H	2.845160000	0.069363000	-1.289729000
H	1.400947000	0.726486000	-2.062679000
Cl	5.011516000	-1.766647000	-0.691961000
O	5.125036000	-2.057975000	-2.151402000
O	4.858178000	-0.271118000	-0.500050000
O	6.197668000	-2.251567000	0.048446000
O	3.762945000	-2.421729000	-0.150379000
Cl	1.373138000	5.259532000	-0.231907000
O	2.048221000	4.576750000	0.931598000
O	1.848907000	6.650677000	-0.372941000
O	-0.114336000	5.219933000	0.003939000
O	1.669952000	4.461644000	-1.476962000
C	-5.497550000	-2.044493000	-1.960719000
C	-6.001266000	-0.812580000	-2.403672000
C	-6.247168000	0.207347000	-1.471154000
C	-5.999572000	-0.000011000	-0.122730000
C	-5.497913000	-1.246927000	0.357435000
C	-5.247537000	-2.264303000	-0.611892000
H	-5.311943000	-2.841041000	-2.676904000
H	-6.211634000	-0.654501000	-3.457710000
H	-6.642808000	1.163207000	-1.804314000
H	-6.202361000	0.792122000	0.594228000
H	-4.864729000	-3.226573000	-0.286606000
C	-5.280925000	-1.445477000	1.744831000
H	-2.755274000	-1.277359000	0.642434000
H	-5.518073000	-0.614880000	2.406212000
C	-4.813857000	-2.728243000	2.362755000
H	-3.813501000	-3.013402000	2.005481000
H	-4.769010000	-2.645317000	3.452613000
H	-5.485659000	-3.566165000	2.124069000

^{5}TS

Zero-point correction= 0.591621 (Hartree/Particle)
Thermal correction to Energy= 0.637039
Thermal correction to Enthalpy= 0.637983
Thermal correction to Gibbs Free Energy= 0.503242
Sum of electronic and zero-point Energies= -3193.22792
Sum of electronic and thermal Energies= -3193.182507
Sum of electronic and thermal Enthalpies= -3193.181563
Sum of electronic and thermal Free Energies= -3193.316

Fe	0.572266000	-0.650402000	-0.507012000
N	-1.144971000	0.601735000	0.095136000
N	0.641207000	1.039798000	-1.920805000
N	1.475621000	0.866432000	0.816979000
N	-0.950579000	-1.486089000	-1.701572000
N	-0.085292000	-1.678357000	1.225998000
O	1.899610000	-1.624999000	-0.984901000
C	1.186452000	1.076079000	-3.144766000
C	1.126565000	2.218836000	-3.937483000
C	0.478323000	3.348971000	-3.434469000
C	-0.092413000	3.313419000	-2.160599000
C	0.011080000	2.128427000	-1.433726000
C	-0.505982000	1.958096000	-0.011904000
C	0.717221000	1.979847000	0.894442000
C	1.072078000	3.066585000	1.691072000
C	2.255726000	2.976139000	2.427245000
C	3.037644000	1.822740000	2.345263000
C	2.611052000	0.781783000	1.524360000
C	-0.804653000	-2.638053000	-2.385240000
C	-1.861247000	-3.231688000	-3.056538000
C	-3.116262000	-2.621722000	-2.997614000
C	-3.263570000	-1.435540000	-2.288548000
C	-2.155704000	-0.886948000	-1.643656000
C	-2.265180000	0.412276000	-0.877636000
C	-1.551224000	0.265266000	1.494110000
C	-1.099096000	-1.116175000	1.910973000
C	-1.696627000	-1.775373000	2.984631000
C	-1.236203000	-3.035792000	3.346306000
C	-0.180614000	-3.608359000	2.633197000
C	0.360494000	-2.901477000	1.571544000
H	1.675655000	0.165554000	-3.477200000
H	1.577147000	2.217898000	-4.924592000
H	0.412897000	4.255198000	-4.029423000
H	-0.604992000	4.166365000	-1.727712000
H	-1.209068000	2.747311000	0.251426000
H	0.432466000	3.942661000	1.720954000
H	2.560792000	3.803962000	3.060715000
H	3.963818000	1.723601000	2.901219000
H	3.179379000	-0.136956000	1.418820000
H	0.190085000	-3.069571000	-2.366882000
H	-1.710825000	-4.166746000	-3.585111000
H	-3.977474000	-3.080573000	-3.471870000
H	-4.234391000	-0.966027000	-2.180945000
H	-2.547196000	-1.326784000	3.484476000
H	-1.716804000	-3.577747000	4.154038000
H	0.193104000	-4.597873000	2.873272000
H	1.162119000	-3.297618000	0.957744000
H	-3.224903000	0.427643000	-0.357451000
H	-2.265958000	1.252126000	-1.579892000
H	-2.636460000	0.323925000	1.598594000
H	-1.121839000	1.009809000	2.172115000

Cl	-4.001961000	-3.020783000	0.707797000
O	-4.301696000	-3.605223000	2.044169000
O	-4.023350000	-1.509782000	0.815615000
O	-5.004745000	-3.447393000	-0.306949000
O	-2.627591000	-3.444090000	0.268375000
Cl	-2.030521000	5.165994000	0.645702000
O	-2.674647000	4.401365000	-0.481441000
O	-2.788427000	6.397543000	0.949449000
O	-0.615177000	5.495257000	0.234147000
O	-1.964713000	4.263299000	1.850153000
C	5.974073000	-1.630517000	2.015127000
C	5.233616000	-2.290585000	1.038245000
C	5.124615000	-1.772900000	-0.271103000
C	5.778420000	-0.556505000	-0.557229000
C	6.521615000	0.102673000	0.419178000
C	6.623220000	-0.429354000	1.708844000
H	6.054492000	-2.055132000	3.011961000
H	4.738295000	-3.228720000	1.277851000
H	5.712014000	-0.129209000	-1.552796000
H	7.026889000	1.032754000	0.174063000
H	7.209073000	0.083519000	2.466529000
C	4.297292000	-2.485584000	-1.268368000
H	3.136839000	-2.057909000	-1.099952000
H	4.163199000	-3.540784000	-1.004677000
C	4.566265000	-2.292149000	-2.751710000
H	3.843962000	-2.860545000	-3.345554000
H	4.490774000	-1.241739000	-3.052279000
H	5.572316000	-2.643480000	-3.017386000

^{5}IH

Zero-point correction= 0.593665 (Hartree/Particle)
Thermal correction to Energy= 0.640541
Thermal correction to Enthalpy= 0.641485
Thermal correction to Gibbs Free Energy= 0.501927
Sum of electronic and zero-point Energies= -3193.24930
Sum of electronic and thermal Energies= -3193.202429
Sum of electronic and thermal Enthalpies= -3193.201485
Sum of electronic and thermal Free Energies= -3193.341

Fe	-0.347644000	-0.875832000	0.526218000
N	1.035441000	0.774096000	-0.095510000
N	-0.809043000	0.780512000	1.918355000
N	-1.569440000	0.391876000	-0.827383000
N	1.353404000	-1.288248000	1.715070000
N	0.558353000	-1.710192000	-1.202464000
O	-1.470673000	-2.192735000	1.055549000
C	-1.342713000	0.692620000	3.145605000
C	-1.554456000	1.821148000	3.932264000
C	-1.196484000	3.070309000	3.420255000
C	-0.637420000	3.164152000	2.144290000
C	-0.457131000	1.984460000	1.423520000
C	0.088247000	1.934479000	0.002704000
C	-1.099260000	1.654569000	-0.907463000
C	-1.693254000	2.619192000	-1.718649000
C	-2.809273000	2.243662000	-2.469708000
C	-3.291709000	0.936670000	-2.388081000
C	-2.640527000	0.034000000	-1.551571000
C	1.487991000	-2.438562000	2.404567000
C	2.657967000	-2.757006000	3.074921000
C	3.729062000	-1.862839000	3.008455000
C	3.585887000	-0.679463000	2.293424000
C	2.377468000	-0.417383000	1.649386000
C	2.166669000	0.866152000	0.876564000
C	1.510308000	0.529259000	-1.490417000
C	1.406631000	-0.925634000	-1.892596000
C	2.148243000	-1.431162000	-2.959586000
C	2.008055000	-2.769456000	-3.307655000
C	1.121876000	-3.574434000	-2.588117000
C	0.422635000	-3.009603000	-1.533857000
H	-1.597974000	-0.306394000	3.485755000
H	-1.987443000	1.718473000	4.921895000
H	-1.346863000	3.969566000	4.010338000
H	-0.342665000	4.111920000	1.705678000
H	0.578019000	2.869882000	-0.265442000
H	-1.281176000	3.622603000	-1.748680000
H	-3.294225000	2.970448000	-3.114850000
H	-4.158924000	0.612379000	-2.952644000
H	-2.976957000	-0.993037000	-1.450467000
H	0.625240000	-3.096632000	2.393301000
H	2.738349000	-3.697710000	3.608651000
H	4.676403000	-2.098627000	3.481860000
H	4.415326000	0.008905000	2.180917000
H	2.865855000	-0.795028000	-3.464426000
H	2.607538000	-3.186684000	-4.109947000
H	1.000037000	-4.627395000	-2.817773000
H	-0.260954000	-3.582197000	-0.915841000
H	3.094388000	1.112692000	0.356361000
H	1.963333000	1.683516000	1.575972000
H	2.549363000	0.846584000	-1.599339000
H	0.914282000	1.139438000	-2.176593000
Cl	4.693637000	-2.046413000	-0.690920000
O	5.129141000	-2.548800000	-2.023241000
O	4.340386000	-0.577916000	-0.810479000
O	5.770276000	-2.203365000	0.325654000
O	3.466556000	-2.793147000	-0.246225000
Cl	0.785149000	5.419159000	-0.664699000
O	1.589940000	4.846056000	0.472744000
O	1.214451000	6.798861000	-0.973238000
O	-0.671098000	5.387394000	-0.265054000
O	0.956201000	4.521136000	-1.862255000
C	-5.560034000	-2.752607000	-2.030928000
C	-4.957632000	-3.225407000	-0.874659000
C	-5.085487000	-2.531473000	0.366831000
C	-5.856324000	-1.331808000	0.365300000
C	-6.458233000	-0.869825000	-0.797312000
C	-6.317768000	-1.571437000	-2.003155000
H	-5.453464000	-3.307175000	-2.959394000
H	-4.383216000	-4.148582000	-0.899771000
H	-5.988797000	-0.778868000	1.289883000
H	-7.050097000	0.041115000	-0.767854000
H	-6.802206000	-1.210865000	-2.906079000
C	-4.460276000	-3.048892000	1.532128000
H	-2.441677000	-2.289272000	1.042644000
H	-3.977567000	-4.020628000	1.440180000
C	-4.559302000	-2.470077000	2.909715000
H	-3.717361000	-2.797260000	3.528873000
H	-4.574160000	-1.373911000	2.908341000
H	-5.477995000	-2.800126000	3.421126000

2+EB

^{3}TS

Zero-point correction= 0.540629 (Hartree/Particle)
Thermal correction to Energy= 0.573992
Thermal correction to Enthalpy= 0.574936
Thermal correction to Gibbs Free Energy= 0.473316

Sum of electronic and zero-point Energies= -1710.81314
Sum of electronic and thermal Energies= -1710.779778
Sum of electronic and thermal Enthalpies= -1710.778834
Sum of electronic and thermal Free Energies= -1710.880

Fe	-0.258009000	-0.623172000	-0.078868000
O	-0.498926000	-2.069743000	-1.301108000
O	-1.107354000	0.570846000	-1.310499000
C	2.242385000	-1.321231000	0.976563000
C	0.603974000	-2.789097000	1.774428000
C	3.237855000	-1.996668000	1.680088000
C	1.548642000	-3.515876000	2.496352000
H	-0.455013000	-3.022887000	1.760538000
C	2.880453000	-3.109434000	2.447279000
H	4.271404000	-1.676341000	1.632942000
H	1.240925000	-4.376581000	3.080242000
H	3.642776000	-3.652715000	2.998043000
C	-0.326630000	1.761543000	1.723671000
C	1.768745000	1.052949000	0.955194000
C	0.250736000	2.788996000	2.468022000
H	-1.393754000	1.569564000	1.691052000
C	2.411940000	2.042761000	1.692633000
C	1.637493000	2.922599000	2.455190000
H	-0.377211000	3.458575000	3.045697000
H	3.490049000	2.138043000	1.673903000
H	2.120635000	3.706882000	3.030628000
N	0.426162000	0.923183000	1.003852000
N	0.958711000	-1.724271000	1.047866000
N	1.502415000	-0.247860000	-1.082587000
O	-1.638387000	-0.908365000	0.917468000
C	1.200374000	0.959056000	-1.918199000
H	1.626889000	1.848546000	-1.451194000
H	1.652662000	0.863309000	-2.907869000
C	-0.317691000	1.234514000	-2.096473000
O	-0.643850000	2.079996000	-2.916162000
C	1.760145000	-1.464331000	-1.908651000
H	2.503825000	-2.095551000	-1.414648000
C	0.488600000	-2.338356000	-2.102701000
O	0.531991000	-3.227299000	-2.937769000
C	2.433054000	-0.050527000	0.103075000
C	3.933058000	0.137220000	-0.249517000
C	4.368580000	1.098707000	-1.379038000
H	4.475182000	0.382678000	0.672322000
H	4.293682000	-0.856543000	-0.537600000
C	4.415360000	2.609088000	-1.081054000
H	5.383360000	0.788030000	-1.663335000
H	3.754996000	0.917056000	-2.265348000
C	5.559615000	3.023208000	-0.146691000
H	4.541726000	3.133957000	-2.036232000
H	5.552523000	4.104315000	0.030082000
H	5.504636000	2.531340000	0.833124000
H	6.532046000	2.763443000	-0.582124000
H	3.457892000	2.958768000	-0.676802000
H	2.165988000	-1.192517000	-2.886390000
C	-5.139868000	2.462331000	-0.256110000
C	-4.355757000	1.369247000	-0.614675000
C	-4.637735000	0.079043000	-0.113114000
C	-5.726973000	-0.063965000	0.768268000
C	-6.511519000	1.032799000	1.124429000
C	-6.223252000	2.301149000	0.614766000
H	-4.909394000	3.444511000	-0.661958000
H	-3.505825000	1.496266000	-1.280209000
H	-5.969912000	-1.043783000	1.168943000
H	-7.353705000	0.895913000	1.798741000
H	-6.837638000	3.154635000	0.890558000
C	-3.765543000	-1.052330000	-0.501750000
H	-2.723766000	-0.948416000	0.217944000
H	-3.297535000	-0.898701000	-1.476933000
C	-4.233710000	-2.481075000	-0.293990000
H	-3.447946000	-3.173769000	-0.610165000
H	-4.469384000	-2.693650000	0.755660000
H	-5.134651000	-2.696679000	-0.886368000

^{3}IH

Zero-point correction= 0.544020 (Hartree/Particle)
Thermal correction to Energy= 0.578640
Thermal correction to Enthalpy= 0.579584
Thermal correction to Gibbs Free Energy= 0.473864
Sum of electronic and zero-point Energies= -1710.83722
Sum of electronic and thermal Energies= -1710.802606
Sum of electronic and thermal Enthalpies= -1710.801662
Sum of electronic and thermal Free Energies= -1710.907

Fe	-0.201974000	0.485900000	-0.143171000
O	-0.751947000	1.845347000	1.082857000
O	-1.133998000	-0.823642000	0.894246000
C	2.345711000	1.437237000	-0.790397000
C	0.715678000	2.791538000	-1.785167000
C	3.368940000	2.228679000	-1.307915000
C	1.687595000	3.629203000	-2.329704000
H	-0.350898000	2.926472000	-1.929560000
C	3.028541000	3.340208000	-2.085276000
H	4.408936000	1.997717000	-1.112304000
H	1.393670000	4.483914000	-2.929301000
H	3.811221000	3.973144000	-2.493247000
C	0.192920000	-1.761747000	-2.069449000
C	2.082229000	-0.961225000	-0.940189000
C	0.958201000	-2.695784000	-2.766371000
H	-0.876441000	-1.637051000	-2.201665000
C	2.907704000	-1.855069000	-1.615573000
C	2.331737000	-2.736160000	-2.536509000
H	0.483258000	-3.365881000	-3.474738000
H	3.974289000	-1.875434000	-1.431826000
H	2.958155000	-3.447129000	-3.067321000
N	0.756605000	-0.925624000	-1.192169000
N	1.055806000	1.732162000	-1.044627000
N	1.404431000	0.199806000	1.088888000
O	-1.504524000	0.712971000	-1.343461000
C	1.084742000	-1.070178000	1.820287000
H	1.633257000	-1.900806000	1.372378000
H	1.394482000	-0.999944000	2.865177000
C	-0.420490000	-1.453352000	1.776782000
O	-0.798752000	-2.339850000	2.526574000
C	1.434364000	1.385384000	1.997616000
H	2.178995000	2.102578000	1.641739000
C	0.074479000	2.138161000	2.043466000
O	-0.088776000	2.969047000	2.921626000
C	2.516343000	0.141141000	0.050475000
C	3.957214000	0.054106000	0.619097000
C	4.301266000	-0.931041000	1.759654000
H	4.648359000	-0.097178000	-0.219551000
H	4.184648000	1.056016000	1.000125000
C	4.516151000	-2.415200000	1.408576000
H	5.233971000	-0.559951000	2.206177000
H	3.551495000	-0.844660000	2.550492000
C	5.816474000	-2.690873000	0.642419000

H	4.542386000	-2.980177000	2.348728000
H	5.924408000	-3.758183000	0.420492000
H	5.867566000	-2.151587000	-0.312351000
H	6.688819000	-2.383527000	1.231660000
H	3.661207000	-2.813291000	0.849064000
H	1.723924000	1.092823000	3.009964000
C	-5.386974000	-2.469425000	-0.140587000
C	-4.581055000	-1.466982000	0.376892000
C	-4.942273000	-0.090512000	0.246960000
C	-6.158952000	0.203000000	-0.436361000
C	-6.955479000	-0.811862000	-0.949813000
C	-6.580758000	-2.154851000	-0.808269000
H	-5.090317000	-3.509194000	-0.023265000
H	-3.652404000	-1.712333000	0.885733000
H	-6.471019000	1.237364000	-0.548367000
H	-7.880954000	-0.560084000	-1.462962000
H	-7.210385000	-2.944494000	-1.209836000
C	-4.098341000	0.909964000	0.793459000
H	-2.352315000	0.688889000	-0.857917000
H	-3.222098000	0.574995000	1.341476000
C	-4.352799000	2.384784000	0.756422000
H	-3.420746000	2.927148000	0.941722000
H	-4.765906000	2.720514000	-0.204185000
H	-5.071169000	2.695697000	1.533374000

^{5}TS

Zero-point correction= 0.539097 (Hartree/Particle)
Thermal correction to Energy= 0.573667
Thermal correction to Enthalpy= 0.574612
Thermal correction to Gibbs Free Energy= 0.468304
Sum of electronic and zero-point Energies= -1710.81441
Sum of electronic and thermal Energies= -1710.779843
Sum of electronic and thermal Enthalpies= -1710.778899
Sum of electronic and thermal Free Energies= -1710.885

Fe	0.327158000	-1.144446000	0.497723000
O	-0.387168000	-2.645563000	1.502298000
O	0.901316000	0.008465000	1.967943000
C	-2.156182000	-1.038372000	-1.263021000
C	-0.776179000	-2.803395000	-1.916533000
C	-3.101987000	-1.387018000	-2.229871000
C	-1.678487000	-3.216656000	-2.894578000
H	0.167224000	-3.308183000	-1.735832000
C	-2.856792000	-2.491087000	-3.049931000
H	-4.017635000	-0.821800000	-2.347658000
H	-1.457273000	-4.080651000	-3.512000000
H	-3.586801000	-2.777848000	-3.801505000
C	1.074354000	1.497450000	-1.186949000
C	-1.214289000	1.165229000	-0.903512000
C	0.864504000	2.643164000	-1.954302000
H	2.069633000	1.130752000	-0.957478000
C	-1.503542000	2.286116000	-1.680993000
C	-0.447068000	3.034439000	-2.207544000
H	1.711010000	3.201907000	-2.338598000
H	-2.526179000	2.583311000	-1.873077000
H	-0.655564000	3.916043000	-2.807082000
N	0.058807000	0.786149000	-0.688577000
N	-1.020695000	-1.744937000	-1.136607000
N	-1.727852000	-0.256050000	1.025452000
O	1.764333000	-1.721700000	-0.254837000
C	-1.389096000	0.829062000	1.989951000
H	-1.563491000	1.805444000	1.535449000
H	-2.037968000	0.772022000	2.868671000
C	0.075349000	0.856844000	2.504933000
O	0.344631000	1.694073000	3.352506000
C	-2.463838000	-1.389518000	1.640430000
H	-3.212230000	-1.771192000	0.939681000
C	-1.582288000	-2.610230000	2.023074000
O	-2.086771000	-3.466597000	2.729863000
C	-2.258770000	0.190243000	-0.310218000
C	-3.732725000	0.700243000	-0.285242000
C	-4.222950000	1.677016000	0.808257000
H	-3.979908000	1.105895000	-1.273621000
H	-4.351692000	-0.197921000	-0.185165000
C	-3.893808000	3.174800000	0.660429000
H	-5.317717000	1.582925000	0.825430000
H	-3.891041000	1.321084000	1.786880000
C	-4.691107000	3.879456000	-0.444920000
H	-4.121820000	3.663700000	1.615956000
H	-4.424188000	4.940098000	-0.508917000
H	-4.519515000	3.438926000	-1.435498000
H	-5.768354000	3.818307000	-0.248318000
H	-2.820009000	3.327071000	0.499527000
H	-3.008307000	-1.067134000	2.532953000
C	4.302168000	2.197267000	0.948945000
C	4.061275000	0.825947000	0.995408000
C	4.618172000	-0.040246000	0.030110000
C	5.408236000	0.521128000	-0.989697000
C	5.653205000	1.894540000	-1.031579000
C	5.103087000	2.738119000	-0.062947000
H	3.860554000	2.841977000	1.704064000
H	3.406468000	0.421342000	1.763000000
H	5.850359000	-0.120511000	-1.745960000
H	6.280203000	2.305241000	-1.819226000
H	5.298025000	3.807099000	-0.094853000
C	4.315015000	-1.498366000	0.108395000
H	3.145866000	-1.604589000	-0.136532000
H	4.314307000	-1.842464000	1.149545000
C	5.063300000	-2.459201000	-0.801840000
H	4.709178000	-3.482164000	-0.641551000
H	4.917799000	-2.218937000	-1.861076000
H	6.143076000	-2.441569000	-0.599603000

^{5}IH

Zero-point correction= 0.540975 (Hartree/Particle)
Thermal correction to Energy= 0.576946
Thermal correction to Enthalpy= 0.577890
Thermal correction to Gibbs Free Energy= 0.467619
Sum of electronic and zero-point Energies= -1710.84645
Sum of electronic and thermal Energies= -1710.810487
Sum of electronic and thermal Enthalpies= -1710.809543
Sum of electronic and thermal Free Energies= -1710.919

Fe	0.352791000	-1.191681000	0.108952000
O	-0.221800000	-2.775728000	1.077734000
O	1.107533000	-0.203493000	1.590774000
C	-2.396089000	-0.913668000	-1.233388000
C	-1.112743000	-2.546910000	-2.298245000
C	-3.470952000	-1.164284000	-2.089204000
C	-2.144464000	-2.857126000	-3.182406000
H	-0.146772000	-3.041976000	-2.323847000
C	-3.339279000	-2.150915000	-3.069941000
H	-4.398238000	-0.612611000	-2.002050000
H	-2.008288000	-3.628250000	-3.933015000
H	-4.169326000	-2.360902000	-3.738519000
C	0.795843000	1.673633000	-1.333737000

C	-1.422867000	1.253981000	-0.762241000
C	0.465062000	2.887565000	-1.935413000
H	1.818244000	1.312095000	-1.289461000
C	-1.834030000	2.443038000	-1.364121000
C	-0.873562000	3.269240000	-1.953802000
H	1.239672000	3.505501000	-2.376735000
H	-2.876813000	2.732260000	-1.374064000
H	-1.176112000	4.203070000	-2.419130000
N	-0.128846000	0.886869000	-0.774099000
N	-1.251293000	-1.603458000	-1.361077000
N	-1.638748000	-0.385400000	1.043480000
O	1.718501000	-1.628781000	-1.027184000
C	-1.146795000	0.589211000	2.056612000
H	-1.433587000	1.605488000	1.783675000
H	-1.610049000	0.385902000	3.027291000
C	0.385859000	0.629261000	2.288003000
O	0.812504000	1.443113000	3.091318000
C	-2.265330000	-1.592928000	1.632527000
H	-3.068643000	-1.946335000	0.978801000
C	-1.304274000	-2.800608000	1.806525000
O	-1.654592000	-3.701927000	2.549179000
C	-2.362117000	0.194680000	-0.136517000
C	-3.818820000	0.664267000	0.165148000
C	-4.140275000	1.500318000	1.425104000
H	-4.216399000	1.172811000	-0.721195000
H	-4.409333000	-0.254218000	0.253793000
C	-3.846388000	3.012469000	1.398943000
H	-5.218425000	1.379378000	1.599813000
H	-3.658411000	1.045065000	2.294494000
C	-4.807979000	3.816352000	0.514036000
H	-3.927342000	3.387789000	2.426893000
H	-4.560645000	4.883493000	0.530970000
H	-4.786836000	3.492578000	-0.534467000
H	-5.842037000	3.708407000	0.863183000
H	-2.811127000	3.206132000	1.093910000
H	-2.723561000	-1.373861000	2.602086000
C	4.478512000	2.484898000	0.178886000
C	4.114993000	1.243894000	0.681684000
C	4.775714000	0.051751000	0.249513000
C	5.816928000	0.196253000	-0.714230000
C	6.166755000	1.444885000	-1.210349000
C	5.504381000	2.599657000	-0.772016000
H	3.967678000	3.375997000	0.536293000
H	3.319777000	1.162062000	1.418095000
H	6.350790000	-0.682985000	-1.061812000
H	6.966992000	1.525434000	-1.942197000
H	5.788867000	3.574394000	-1.159191000
C	4.379006000	-1.199806000	0.789257000
H	2.615933000	-1.507063000	-0.665654000
H	3.598711000	-1.177127000	1.546762000
C	5.015692000	-2.525150000	0.505054000
H	4.286065000	-3.335479000	0.614510000
H	5.441996000	-2.589586000	-0.502364000
H	5.833011000	-2.739040000	1.213594000

1+DHT

^{3}TS

Zero-point correction= 0.588224 (Hartree/Particle)

Thermal correction to Energy= 0.631440

Thermal correction to Enthalpy= 0.632385

Thermal correction to Gibbs Free Energy= 0.505275

Sum of electronic and zero-point Energies= -3155.10786

Sum of electronic and thermal Energies= -3155.064646

Sum of electronic and thermal Enthalpies= -3155.063702

Sum of electronic and thermal Free Energies= -3155.190

Fe	0.414503000	-0.977867000	0.265958000
N	-0.926351000	0.530891000	-0.052934000
N	1.492534000	0.081043000	-1.041153000
N	1.080526000	0.294565000	1.656345000
N	-0.551638000	-1.853000000	-1.235168000
N	-0.975080000	-1.647338000	1.516791000
O	1.488977000	-2.305557000	0.526264000
C	2.418154000	-0.360721000	-1.904164000
C	3.002118000	0.496238000	-2.833092000
C	2.610204000	1.835285000	-2.857012000
C	1.645220000	2.295202000	-1.957452000
C	1.106656000	1.377819000	-1.060623000
C	0.057744000	1.682602000	-0.000326000
C	0.754325000	1.570996000	1.348971000
C	1.055027000	2.634056000	2.196094000
C	1.712991000	2.346582000	3.394130000
C	2.037810000	1.026125000	3.711038000
C	1.697900000	0.017655000	2.813949000
C	-0.374201000	-3.132078000	-1.618733000
C	-1.102059000	-3.687812000	-2.659754000
C	-2.053055000	-2.896809000	-3.312158000
C	-2.237391000	-1.581662000	-2.905217000
C	-1.460339000	-1.078483000	-1.859933000
C	-1.581248000	0.351132000	-1.393721000
C	-1.938339000	0.541266000	1.058252000
C	-2.019567000	-0.816953000	1.713672000
C	-3.101356000	-1.194882000	2.510305000
C	-3.081505000	-2.442694000	3.122407000
C	-1.986340000	-3.288355000	2.923663000
C	-0.953795000	-2.859567000	2.102831000
H	2.681385000	-1.409717000	-1.827166000
H	3.746754000	0.113420000	-3.523135000
H	3.046227000	2.523182000	-3.575284000
H	1.296836000	3.323063000	-1.946622000
H	-0.417157000	2.655640000	-0.145653000
H	0.763002000	3.640821000	1.915302000
H	1.960435000	3.152572000	4.078409000
H	2.541182000	0.774448000	4.638647000
H	1.910801000	-1.029022000	3.000339000
H	0.375250000	-3.680716000	-1.059816000
H	-0.936618000	-4.722061000	-2.942067000
H	-2.657120000	-3.308713000	-4.114691000
H	-2.994324000	-0.951196000	-3.358219000
H	-3.966679000	-0.546102000	2.583399000
H	-3.923041000	-2.761513000	3.729629000
H	-1.940136000	-4.272080000	3.378738000
H	-0.078843000	-3.461597000	1.884677000
H	-2.637963000	0.636313000	-1.340264000
H	-1.096321000	1.017231000	-2.114638000
H	-2.918195000	0.842973000	0.674128000
H	-1.635791000	1.286908000	1.800447000
Cl	-5.215654000	-0.579096000	-0.424005000
O	-5.820757000	-0.611413000	0.939893000
O	-4.650751000	0.803779000	-0.678548000
O	-6.213341000	-0.915796000	-1.464391000
O	-4.064457000	-1.555224000	-0.480208000
Cl	0.155394000	5.343858000	-0.288859000
O	-0.336708000	4.682804000	-1.551737000
O	0.087812000	6.814936000	-0.404973000

O	1.570327000	4.887781000	-0.043692000
O	-0.696615000	4.856367000	0.856315000
C	5.996026000	-1.502523000	-1.090076000
C	5.550246000	-0.549656000	-0.020133000
C	4.674984000	-0.900356000	0.939450000
C	4.042559000	-2.229914000	0.990422000
C	4.553562000	-3.237594000	0.028779000
C	5.422847000	-2.883640000	-0.940515000
H	5.748360000	-1.091026000	-2.085475000
H	3.922019000	-2.624711000	2.008546000
H	7.098477000	-1.557818000	-1.100944000
H	2.799403000	-2.126406000	0.722456000
C	4.040229000	-4.647076000	0.176572000
H	2.944049000	-4.664067000	0.146829000
H	4.421827000	-5.302571000	-0.612363000
H	4.338415000	-5.072399000	1.144574000
H	5.985136000	0.447444000	-0.025116000
H	4.404694000	-0.181547000	1.709700000
H	5.773027000	-3.636820000	-1.644882000

^{3}IH

Zero-point correction= 0.591455 (Hartree/Particle)
Thermal correction to Energy= 0.635835
Thermal correction to Enthalpy= 0.636779
Thermal correction to Gibbs Free Energy= 0.504719
Sum of electronic and zero-point Energies= -3155.14477
Sum of electronic and thermal Energies= -3155.100398
Sum of electronic and thermal Enthalpies= -3155.099454
Sum of electronic and thermal Free Energies= -3155.231

Fe	0.342401000	-1.004329000	0.237151000
N	-0.984541000	0.491558000	-0.048494000
N	1.418893000	0.048475000	-1.077711000
N	1.066830000	0.256121000	1.605452000
N	-0.649655000	-1.894805000	-1.228191000
N	-1.008209000	-1.693617000	1.507775000
O	1.490410000	-2.372309000	0.494005000
C	2.349253000	-0.387713000	-1.938796000
C	2.935319000	0.474293000	-2.861993000
C	2.533981000	1.810767000	-2.886997000
C	1.564086000	2.265065000	-1.989519000
C	1.029718000	1.344986000	-1.093112000
C	-0.003142000	1.647915000	-0.015466000
C	0.727136000	1.533871000	1.316367000
C	1.056451000	2.592176000	2.157677000
C	1.762785000	2.298343000	3.326903000
C	2.109408000	0.978217000	3.619788000
C	1.736935000	-0.026563000	2.731541000
C	-0.481356000	-3.177571000	-1.600882000
C	-1.238873000	-3.741850000	-2.616486000
C	-2.206819000	-2.955872000	-3.249801000
C	-2.379831000	-1.635599000	-2.852443000
C	-1.573118000	-1.123547000	-1.834966000
C	-1.669870000	0.310845000	-1.377097000
C	-1.975756000	0.497055000	1.085023000
C	-2.052376000	-0.868407000	1.726657000
C	-3.121928000	-1.258603000	2.533053000
C	-3.085068000	-2.512254000	3.133874000
C	-1.987961000	-3.350216000	2.914165000
C	-0.968730000	-2.910187000	2.081870000
H	2.619438000	-1.435178000	-1.863560000
H	3.686172000	0.096164000	-3.547739000
H	2.968912000	2.502011000	-3.602672000
H	1.212353000	3.291792000	-1.976847000
H	-0.484143000	2.619343000	-0.150523000
H	0.752317000	3.600063000	1.894305000
H	2.034130000	3.100807000	4.006244000
H	2.654706000	0.723906000	4.522606000
H	1.964268000	-1.073672000	2.898997000
H	0.284288000	-3.718597000	-1.056523000
H	-1.082866000	-4.778899000	-2.893814000
H	-2.832997000	-3.375384000	-4.031170000
H	-3.148298000	-1.009498000	-3.291541000
H	-3.990040000	-0.615470000	2.623266000
H	-3.916080000	-2.841028000	3.750271000
H	-1.930410000	-4.336667000	3.361980000
H	-0.091389000	-3.502401000	1.846753000
H	-2.720946000	0.612059000	-1.302855000
H	-1.188518000	0.966368000	-2.109903000
H	-2.958972000	0.814336000	0.722742000
H	-1.648406000	1.231027000	1.828217000
Cl	-5.306273000	-0.521083000	-0.329990000
O	-5.864272000	-0.543274000	1.054354000
O	-4.706825000	0.845264000	-0.595810000
O	-6.349597000	-0.819277000	-1.336245000
O	-4.188418000	-1.531761000	-0.431292000
Cl	0.093739000	5.303445000	-0.298764000
O	-0.421227000	4.637981000	-1.550556000
O	0.015011000	6.773755000	-0.414705000
O	1.516055000	4.855446000	-0.083561000
O	-0.731200000	4.811578000	0.864255000
C	6.192224000	-0.981860000	-0.952242000
C	5.976468000	-0.446376000	0.432871000
C	5.310779000	-1.169578000	1.383796000
C	4.777162000	-2.453371000	1.100942000
C	4.921489000	-3.033171000	-0.199560000
C	5.582157000	-2.337415000	-1.176148000
H	5.807254000	-0.260573000	-1.698535000
H	4.291626000	-3.025706000	1.887358000
H	7.276441000	-1.017420000	-1.175906000
H	2.410995000	-2.061945000	0.575010000
C	4.335713000	-4.403102000	-0.457169000
H	3.252827000	-4.399502000	-0.281401000
H	4.517081000	-4.731705000	-1.485274000
H	4.771126000	-5.151156000	0.217079000
H	6.381124000	0.534499000	0.667778000
H	5.191630000	-0.758440000	2.383980000
H	5.706902000	-2.781769000	-2.161910000

^{5}TS

Zero-point correction= 0.585789 (Hartree/Particle)
Thermal correction to Energy= 0.630525
Thermal correction to Enthalpy= 0.631469
Thermal correction to Gibbs Free Energy= 0.499388
Sum of electronic and zero-point Energies= -3155.10240
Sum of electronic and thermal Energies= -3155.057666
Sum of electronic and thermal Enthalpies= -3155.056722
Sum of electronic and thermal Free Energies= -3155.188

Fe	0.437714000	-0.958011000	0.154512000
N	-1.171353000	0.536456000	-0.037948000
N	-1.059884000	-1.642152000	1.608297000
N	-0.978718000	-1.912028000	-1.233920000
N	1.055163000	0.480971000	1.591827000
N	1.158247000	0.193466000	-1.475707000

O	1.674863000	-2.114460000	0.300054000
C	-0.874584000	-2.400819000	2.697368000
C	-1.927432000	-2.725042000	3.548667000
C	-3.202832000	-2.240636000	3.250956000
C	-3.398671000	-1.449648000	2.116823000
C	-2.290671000	-1.171995000	1.318266000
C	-2.358626000	-0.384913000	0.016995000
C	-2.222342000	-1.405272000	-1.104098000
C	-3.287464000	-1.839002000	-1.891478000
C	-3.034156000	-2.829976000	-2.842176000
C	-1.745805000	-3.351821000	-2.975104000
C	-0.738890000	-2.863008000	-2.147249000
C	2.262476000	0.465675000	2.187330000
C	2.682464000	1.487841000	3.023679000
C	1.831169000	2.575331000	3.229526000
C	0.587576000	2.590098000	2.609617000
C	0.224288000	1.521725000	1.790347000
C	-1.128813000	1.485508000	1.116971000
C	-1.051636000	1.242631000	-1.350634000
C	0.346373000	1.170800000	-1.921876000
C	0.770493000	2.072630000	-2.897109000
C	2.055671000	1.956875000	-3.413047000
C	2.887592000	0.936219000	-2.948325000
C	2.405867000	0.082078000	-1.969114000
H	0.139485000	-2.747162000	2.870994000
H	-1.746996000	-3.342765000	4.422273000
H	-4.043947000	-2.474529000	3.896960000
H	-4.370938000	-1.052446000	1.843805000
H	-3.291542000	0.171080000	-0.063503000
H	-4.272256000	-1.405933000	-1.748764000
H	-3.840643000	-3.189529000	-3.474465000
H	-1.520681000	-4.123173000	-3.704266000
H	0.281577000	-3.229397000	-2.198876000
H	2.889531000	-0.391503000	1.964923000
H	3.667348000	1.447340000	3.476448000
H	2.143392000	3.415874000	3.840461000
H	-0.075951000	3.441390000	2.708170000
H	0.118262000	2.883976000	-3.198610000
H	2.413434000	2.673443000	-4.144961000
H	3.902956000	0.824537000	-3.313253000
H	3.013611000	-0.710536000	-1.544816000
H	-1.378984000	2.495248000	0.785684000
H	-1.891763000	1.188027000	1.843676000
H	-1.331859000	2.292363000	-1.243029000
H	-1.757915000	0.793077000	-2.056010000
Cl	1.795801000	4.124485000	-0.278472000
O	2.200650000	4.766022000	-1.560083000
O	0.305120000	3.858946000	-0.309945000
O	2.107820000	4.999373000	0.885494000
O	2.508256000	2.808799000	-0.126037000
Cl	-5.838908000	0.540682000	-0.169770000
O	-5.122901000	1.107759000	1.028565000
O	-7.214790000	1.071357000	-0.262836000
O	-5.852106000	-0.963332000	-0.033999000
O	-5.043397000	0.887710000	-1.401381000
C	6.195881000	-1.399413000	0.334597000
C	5.631019000	-1.845645000	1.650293000
C	4.643440000	-2.755564000	1.738258000
C	3.996338000	-3.335587000	0.543430000
C	4.664083000	-3.071852000	-0.756160000
C	5.652294000	-2.155477000	-0.842706000
H	6.018887000	-0.316874000	0.200555000
H	3.689078000	-4.381741000	0.673358000
H	7.295715000	-1.483460000	0.354880000
H	2.905369000	-2.804702000	0.454532000
C	4.153737000	-3.828708000	-1.954180000
H	3.079090000	-3.649847000	-2.093361000
H	4.672385000	-3.535904000	-2.872116000
H	4.280211000	-4.911153000	-1.820184000
H	6.070646000	-1.423699000	2.551504000
H	4.273405000	-3.067458000	2.712704000
H	6.115984000	-1.956702000	-1.807640000

^{5}IH

Zero-point correction= 0.588205 (Hartree/Particle)
Thermal correction to Energy= 0.634036
Thermal correction to Enthalpy= 0.634980
Thermal correction to Gibbs Free Energy= 0.499609
Sum of electronic and zero-point Energies= -3155.12441
Sum of electronic and thermal Energies= -3155.078584
Sum of electronic and thermal Enthalpies= -3155.077640
Sum of electronic and thermal Free Energies= -3155.213

Fe	0.297845000	-1.041786000	0.016502000
N	-1.162466000	0.434918000	-0.095481000
N	-1.034771000	-1.780154000	1.350124000
N	-1.199066000	-1.877928000	-1.562545000
N	1.044389000	0.403959000	1.575077000
N	1.161646000	0.034030000	-1.427715000
O	1.460652000	-2.379590000	0.111473000
C	-0.783158000	-2.634915000	2.352190000
C	-1.797967000	-3.071015000	3.197808000
C	-3.097114000	-2.603376000	2.988835000
C	-3.358800000	-1.716937000	1.942387000
C	-2.291666000	-1.325231000	1.137987000
C	-2.406326000	-0.427793000	-0.080721000
C	-2.400460000	-1.333312000	-1.301398000
C	-3.542700000	-1.616319000	-2.048013000
C	-3.411599000	-2.513005000	-3.111239000
C	-2.166302000	-3.081086000	-3.386009000
C	-1.078742000	-2.732191000	-2.585657000
C	2.245280000	0.423981000	2.176920000
C	2.652071000	1.465373000	2.999097000
C	1.787960000	2.545491000	3.183521000
C	0.548004000	2.531515000	2.555946000
C	0.209601000	1.437601000	1.758824000
C	-1.146165000	1.352811000	1.099595000
C	-0.984008000	1.198887000	-1.380612000
C	0.409355000	1.039605000	-1.925681000
C	0.907126000	1.891209000	-2.909275000
C	2.199077000	1.699806000	-3.383020000
C	2.962308000	0.652236000	-2.867148000
C	2.414122000	-0.154683000	-1.882253000
H	0.244260000	-2.967557000	2.444681000
H	-1.568267000	-3.764116000	4.000112000
H	-3.906875000	-2.925258000	3.636858000
H	-4.353590000	-1.332518000	1.735178000
H	-3.295904000	0.199057000	-0.057042000
H	-4.485890000	-1.142796000	-1.793967000
H	-4.276075000	-2.761345000	-3.719930000
H	-2.034198000	-3.780308000	-4.205330000
H	-0.086899000	-3.141953000	-2.755060000
H	2.901343000	-0.419593000	1.983232000
H	3.635745000	1.443240000	3.455977000
H	2.086369000	3.399985000	3.781896000

H	-0.130760000	3.372725000	2.637427000
H	0.305262000	2.726408000	-3.247264000
H	2.613100000	2.378511000	-4.120988000
H	3.979323000	0.474701000	-3.199425000
H	2.969409000	-0.972069000	-1.438151000
H	-1.470217000	2.348846000	0.793307000
H	-1.886817000	0.985483000	1.816082000
H	-1.171686000	2.260133000	-1.210651000
H	-1.718593000	0.840116000	-2.106931000
Cl	1.825566000	4.020611000	-0.372470000
O	2.204573000	4.595526000	-1.694812000
O	0.331866000	3.766182000	-0.360250000
O	2.169668000	4.946953000	0.738458000
O	2.531768000	2.707407000	-0.176389000
Cl	-5.738522000	0.794499000	0.271153000
O	-4.822912000	1.176250000	1.404658000
O	-7.047963000	1.464706000	0.398538000
O	-5.900390000	-0.707933000	0.288458000
O	-5.063154000	1.169673000	-1.023269000
C	6.109815000	-0.929669000	0.261989000
C	5.762015000	-1.255729000	1.684108000
C	4.998054000	-2.345203000	2.003475000
C	4.497143000	-3.218005000	1.001898000
C	4.810056000	-3.002089000	-0.378070000
C	5.571412000	-1.919742000	-0.731549000
H	5.756555000	0.089610000	0.012723000
H	3.922587000	-4.095464000	1.286134000
H	7.207957000	-0.847601000	0.153180000
H	2.331440000	-2.196381000	0.511260000
C	4.287717000	-3.978938000	-1.406747000
H	3.190919000	-3.996661000	-1.398206000
H	4.620419000	-3.716554000	-2.415859000
H	4.631799000	-4.998207000	-1.192251000
H	6.146106000	-0.602390000	2.463159000
H	4.774844000	-2.560260000	3.046440000
H	5.826992000	-1.761011000	-1.777537000

2+DHT

^{3}TS

Zero-point correction= 0.534173 (Hartree/Particle)
Thermal correction to Energy= 0.567019
Thermal correction to Enthalpy= 0.567963
Thermal correction to Gibbs Free Energy= 0.467770
Sum of electronic and zero-point Energies= -1672.68525
Sum of electronic and thermal Energies= -1672.652412
Sum of electronic and thermal Enthalpies= -1672.651468
Sum of electronic and thermal Free Energies= -1672.751

Fe	-0.467331000	0.210678000	0.072577000
O	-1.104001000	1.368351000	1.452891000
O	-0.991477000	-1.316931000	1.098703000
C	1.783068000	1.671144000	-0.748219000
C	-0.166977000	2.755448000	-1.451035000
C	2.579234000	2.668829000	-1.307760000
C	0.566706000	3.791667000	-2.025170000
H	-1.250014000	2.702816000	-1.469335000
C	1.957165000	3.742388000	-1.951833000
H	3.659439000	2.624053000	-1.242878000
H	0.054622000	4.612134000	-2.516158000
H	2.560334000	4.532883000	-2.388808000
C	0.141672000	-1.841137000	-2.016763000
C	1.955798000	-0.724767000	-1.046059000
C	0.986671000	-2.573584000	-2.848760000
H	-0.938835000	-1.935406000	-2.024039000
C	2.854657000	-1.405039000	-1.862763000
C	2.358803000	-2.344395000	-2.771983000
H	0.571760000	-3.297868000	-3.541353000
H	3.918777000	-1.218836000	-1.794201000
H	3.045417000	-2.891539000	-3.411396000
N	0.628191000	-0.942702000	-1.154614000
N	0.440148000	1.732818000	-0.840181000
N	1.313381000	0.177749000	1.118789000
O	-1.850017000	0.253345000	-0.940258000
C	1.323424000	-1.165757000	1.781587000
H	1.976475000	-1.845147000	1.230850000
H	1.717098000	-1.089529000	2.797656000
C	-0.072469000	-1.844618000	1.846111000
O	-0.179108000	-2.839871000	2.546764000
C	1.222814000	1.297379000	2.101100000
H	1.779776000	2.161651000	1.729029000
C	-0.238818000	1.773765000	2.334180000
O	-0.449677000	2.521441000	3.275728000
C	2.285876000	0.389056000	-0.028583000
C	3.774909000	0.552522000	0.379159000
C	4.425377000	-0.404153000	1.404587000
H	4.381615000	0.581783000	-0.534651000
H	3.853567000	1.558275000	0.806819000
C	4.874855000	-1.797976000	0.927703000
H	5.316115000	0.118110000	1.780073000
H	3.766849000	-0.506350000	2.271092000
C	6.108383000	-1.775307000	0.015742000
H	5.113331000	-2.394297000	1.817285000
H	6.389978000	-2.788335000	-0.291839000
H	5.947685000	-1.188902000	-0.898146000
H	6.968233000	-1.333486000	0.533586000
H	4.052472000	-2.325990000	0.430485000
H	1.668720000	1.013903000	3.057977000
C	-6.262638000	-1.576692000	-0.963312000
C	-5.187806000	-2.399609000	-0.308643000
C	-4.155813000	-1.847904000	0.352427000
C	-3.967599000	-0.387969000	0.448687000
C	-5.077988000	0.452594000	-0.060878000
C	-6.111611000	-0.098960000	-0.726995000
H	-6.285690000	-1.782838000	-2.049711000
H	-3.556351000	-0.056169000	1.408968000
H	-7.255370000	-1.910663000	-0.611974000
H	-2.976652000	-0.110170000	-0.241858000
C	-4.966345000	1.936989000	0.171587000
H	-4.022442000	2.317792000	-0.239016000
H	-5.796370000	2.485576000	-0.286707000
H	-4.949485000	2.167190000	1.245042000
H	-5.284427000	-3.482539000	-0.369666000
H	-3.395693000	-2.466172000	0.822571000
H	-6.906231000	0.541211000	-1.109960000

^{3}IH

Zero-point correction= 0.537518 (Hartree/Particle)
Thermal correction to Energy= 0.571449
Thermal correction to Enthalpy= 0.572393
Thermal correction to Gibbs Free Energy= 0.468198
Sum of electronic and zero-point Energies= -1672.72209
Sum of electronic and thermal Energies= -1672.688164
Sum of electronic and thermal Enthalpies= -1672.687220
Sum of electronic and thermal Free Energies= -1672.791

Fe	-0.384715000	0.013774000	-0.207284000

O	-1.359977000	1.104127000	1.024526000
O	-0.917839000	-1.547419000	0.756789000
C	1.783498000	1.709675000	-0.714315000
C	-0.142426000	2.551447000	-1.745105000
C	2.539289000	2.790249000	-1.164177000
C	0.551259000	3.662073000	-2.222805000
H	-1.194364000	2.365579000	-1.933717000
C	1.907773000	3.778240000	-1.926258000
H	3.593169000	2.873487000	-0.928365000
H	0.035100000	4.412411000	-2.811896000
H	2.477746000	4.631695000	-2.281806000
C	0.734657000	-1.933788000	-2.174654000
C	2.254198000	-0.650711000	-0.938124000
C	1.769232000	-2.567789000	-2.861147000
H	-0.317421000	-2.128289000	-2.353023000
C	3.333489000	-1.229264000	-1.599380000
C	3.082330000	-2.204941000	-2.569376000
H	1.543300000	-3.320208000	-3.608983000
H	4.349686000	-0.936888000	-1.367830000
H	3.911992000	-2.674306000	-3.089958000
N	0.988736000	-1.003338000	-1.249549000
N	0.474645000	1.614826000	-1.018291000
N	1.189468000	0.179182000	1.088151000
O	-1.651640000	-0.101814000	-1.459740000
C	1.239506000	-1.153603000	1.773604000
H	2.024397000	-1.767061000	1.327380000
H	1.480903000	-1.032886000	2.831794000
C	-0.081731000	-1.964066000	1.658211000
O	-0.201176000	-2.943722000	2.376879000
C	0.828916000	1.284787000	2.025970000
H	1.333087000	2.205668000	1.720404000
C	-0.695791000	1.589602000	2.030380000
O	-1.137004000	2.293735000	2.924675000
C	2.303810000	0.492393000	0.099683000
C	3.683951000	0.816997000	0.729764000
C	4.268290000	-0.064278000	1.857478000
H	4.417267000	0.912921000	-0.080772000
H	3.586602000	1.825190000	1.147966000
C	4.928333000	-1.402713000	1.476749000
H	5.031937000	0.550132000	2.353909000
H	3.500776000	-0.235426000	2.616818000
C	6.277335000	-1.249623000	0.762201000
H	5.089489000	-1.970497000	2.401645000
H	6.706370000	-2.227162000	0.516372000
H	6.198116000	-0.682441000	-0.174290000
H	6.997411000	-0.720419000	1.397894000
H	4.250895000	-2.014670000	0.869303000
H	1.158573000	1.056310000	3.042560000
C	-6.594631000	-0.684022000	-1.214961000
C	-5.633009000	-1.837052000	-1.253580000
C	-4.567328000	-1.907649000	-0.397421000
C	-4.314429000	-0.896331000	0.563636000
C	-5.185234000	0.234216000	0.673434000
C	-6.258578000	0.341848000	-0.167902000
H	-6.652106000	-0.203958000	-2.212355000
H	-3.453823000	-0.982156000	1.218999000
H	-7.626712000	-1.057803000	-1.058144000
H	-2.488056000	-0.330438000	-1.010560000
C	-4.896715000	1.274802000	1.731051000
H	-3.853298000	1.605775000	1.686583000
H	-5.550326000	2.147449000	1.624200000
H	-5.053491000	0.860627000	2.736046000
H	-5.811083000	-2.624212000	-1.982831000
H	-3.886717000	-2.755244000	-0.445203000
H	-6.921670000	1.201762000	-0.087671000

^{5}TS

Zero-point correction= 0.532791 (Hartree/Particle)
Thermal correction to Energy= 0.566677
Thermal correction to Enthalpy= 0.567621
Thermal correction to Gibbs Free Energy= 0.463773
Sum of electronic and zero-point Energies= -1672.68676
Sum of electronic and thermal Energies= -1672.652882
Sum of electronic and thermal Enthalpies= -1672.651937
Sum of electronic and thermal Free Energies= -1672.755

Fe	-0.479659000	-0.982007000	-0.609203000
O	0.094321000	-2.690717000	-1.333962000
O	-0.665832000	0.068207000	-2.247513000
C	1.705488000	-1.012981000	1.509948000
C	-0.022080000	-2.458370000	2.117874000
C	2.432793000	-1.360177000	2.650666000
C	0.650200000	-2.862447000	3.269719000
H	-0.998758000	-2.841842000	1.840840000
C	1.895528000	-2.298551000	3.535345000
H	3.401045000	-0.920735000	2.853835000
H	0.205329000	-3.595928000	3.933620000
H	2.452658000	-2.584000000	4.423124000
C	-1.017613000	1.939341000	0.644310000
C	1.200710000	1.238240000	0.767288000
C	-0.728570000	3.135006000	1.301711000
H	-2.020549000	1.692983000	0.306168000
C	1.561944000	2.399091000	1.450858000
C	0.581838000	3.359238000	1.715292000
H	-1.513416000	3.861329000	1.484312000
H	2.582876000	2.564948000	1.769012000
H	0.847971000	4.273656000	2.237874000
N	-0.075044000	1.025361000	0.397971000
N	0.501284000	-1.560073000	1.277570000
N	1.729498000	-0.489423000	-0.889468000
O	-2.077686000	-1.228843000	-0.079498000
C	1.718765000	0.494707000	-2.010477000
H	1.988470000	1.485998000	-1.642876000
H	2.466774000	0.223108000	-2.760419000
C	0.367333000	0.672954000	-2.755173000
O	0.375922000	1.396303000	-3.738620000
C	2.349633000	-1.790029000	-1.251693000
H	2.905066000	-2.186999000	-0.397026000
C	1.340853000	-2.901663000	-1.652794000
O	1.792383000	-3.905276000	-2.178321000
C	2.140211000	0.048960000	0.456553000
C	3.667797000	0.326509000	0.606031000
C	4.460541000	1.066817000	-0.495716000
H	3.840484000	0.818150000	1.570915000
H	4.135976000	-0.659021000	0.703057000
C	4.367455000	2.603085000	-0.564750000
H	5.515984000	0.810229000	-0.328815000
H	4.213690000	0.638047000	-1.470183000
C	5.109375000	3.321659000	0.569837000
H	4.803912000	2.922486000	-1.519459000
H	5.015774000	4.409177000	0.475772000
H	4.731595000	3.045764000	1.562821000
H	6.178282000	3.076703000	0.553424000
H	3.322037000	2.932363000	-0.593164000
H	3.070833000	-1.669117000	-2.065298000

C	-5.577109000	1.738739000	1.263904000
C	-5.679060000	0.347537000	1.820965000
C	-5.268013000	-0.732458000	1.139046000
C	-4.631914000	-0.644454000	-0.195830000
C	-4.645050000	0.700320000	-0.838066000
C	-5.052967000	1.784076000	-0.145327000
H	-6.565233000	2.229539000	1.307851000
H	-3.475450000	-0.936620000	-0.078636000
H	-4.946891000	2.360944000	1.925934000
H	-4.950360000	-1.444097000	-0.878623000
C	-4.153662000	0.786019000	-2.259609000
H	-4.737805000	0.123171000	-2.912267000
H	-4.234513000	1.805382000	-2.651271000
H	-3.105750000	0.469467000	-2.340030000
H	-6.125804000	0.236793000	2.807389000
H	-5.374795000	-1.724077000	1.574809000
H	-5.047887000	2.758938000	-0.632093000

^{5}IH

Zero-point correction= 0.534827 (Hartree/Particle)
Thermal correction to Energy= 0.569863
Thermal correction to Enthalpy= 0.570807
Thermal correction to Gibbs Free Energy= 0.463958
Sum of electronic and zero-point Energies= -1672.73207
Sum of electronic and thermal Energies= -1672.697039
Sum of electronic and thermal Enthalpies= -1672.696095
Sum of electronic and thermal Free Energies= -1672.802

Fe	-0.769933000	-0.446150000	0.144623000
O	-1.234190000	-1.153604000	-1.607981000
O	-1.279984000	1.397535000	-0.166366000
C	2.044340000	-1.732464000	0.012927000
C	0.443351000	-3.323157000	0.599027000
C	3.053684000	-2.697241000	0.044610000
C	1.393511000	-4.342314000	0.640839000
H	-0.606062000	-3.484832000	0.824177000
C	2.717374000	-4.017018000	0.357528000
H	4.082990000	-2.440907000	-0.171474000
H	1.098353000	-5.355793000	0.890853000
H	3.490278000	-4.780072000	0.379495000
C	0.473419000	0.819698000	2.801401000
C	2.068824000	0.402907000	1.153829000
C	1.438936000	1.288169000	3.692010000
H	-0.580044000	0.763345000	3.057594000
C	3.092503000	0.836858000	1.995997000
C	2.768141000	1.290424000	3.277448000
H	1.151191000	1.632172000	4.679764000
H	4.124136000	0.829635000	1.669720000
H	3.553432000	1.640227000	3.941550000
N	0.791858000	0.392187000	1.576308000
N	0.774064000	-2.065637000	0.290204000
N	1.107812000	0.244386000	-1.094638000
O	-1.827291000	-1.199792000	1.438551000
C	0.895200000	1.712318000	-1.198900000
H	1.564303000	2.233920000	-0.510649000
H	1.131566000	2.072123000	-2.204337000
C	-0.533488000	2.208998000	-0.857937000
O	-0.839365000	3.337612000	-1.211901000
C	0.954832000	-0.456751000	-2.391314000
H	1.634763000	-1.312952000	-2.431819000
C	-0.463290000	-1.031572000	-2.654731000
O	-0.734287000	-1.376498000	-3.792388000
C	2.263866000	-0.211683000	-0.254519000
C	3.665934000	-0.000293000	-0.903890000
C	4.038659000	1.338753000	-1.580546000
H	4.437672000	-0.265713000	-0.171392000
H	3.742670000	-0.763786000	-1.686004000
C	4.453371000	2.526116000	-0.690815000
H	4.886225000	1.114551000	-2.243196000
H	3.228866000	1.644264000	-2.247584000
C	5.841702000	2.371461000	-0.056220000
H	4.458594000	3.427683000	-1.316300000
H	6.090325000	3.238308000	0.565958000
H	5.918914000	1.479834000	0.579231000
H	6.615338000	2.282983000	-0.828529000
H	3.705378000	2.711966000	0.089044000
H	1.221101000	0.194861000	-3.229835000
C	-5.944739000	-0.160064000	1.528573000
C	-5.304363000	-1.285351000	0.766302000
C	-4.574890000	-1.052451000	-0.370489000
C	-4.351444000	0.260839000	-0.853759000
C	-4.880240000	1.393398000	-0.160468000
C	-5.630974000	1.198943000	0.966843000
H	-7.043574000	-0.309421000	1.559387000
H	-2.783974000	-1.160583000	1.253106000
H	-5.656148000	-0.206441000	2.596030000
H	-3.737427000	0.405777000	-1.735818000
C	-4.582517000	2.777012000	-0.688623000
H	-4.949872000	2.890898000	-1.716971000
H	-5.057157000	3.550073000	-0.074798000
H	-3.502160000	2.963039000	-0.708350000
H	-5.472460000	-2.300869000	1.117971000
H	-4.136516000	-1.884204000	-0.917457000
H	-6.037868000	2.058050000	1.497249000

3+EB

^{3}TS

Zero-point correction= 0.385783 (Hartree/Particle)
Thermal correction to Energy= 0.413379
Thermal correction to Enthalpy= 0.414323
Thermal correction to Gibbs Free Energy= 0.326238
Sum of electronic and zero-point Energies= -1534.00917
Sum of electronic and thermal Energies= -1533.981584
Sum of electronic and thermal Enthalpies= -1533.980640
Sum of electronic and thermal Free Energies= -1534.068

Fe	0.472507000	-0.468289000	-0.501214000
O	-0.517987000	-0.559233000	1.169300000
O	0.581008000	-2.379632000	-0.516238000
C	2.009981000	1.814547000	0.033570000
C	-0.200017000	2.458112000	-0.383608000
C	2.392884000	3.139402000	0.243985000
C	0.112265000	3.802359000	-0.185581000
H	-1.189850000	2.098265000	-0.644706000
C	1.427394000	4.141660000	0.132387000
H	3.421585000	3.379711000	0.487009000
H	-0.660158000	4.558475000	-0.281388000
H	1.703412000	5.180619000	0.293681000
C	2.976451000	0.189814000	-1.510488000
N	0.732356000	1.509338000	-0.274383000
N	2.140533000	-0.511084000	0.689485000
O	-0.908468000	-0.228023000	-1.518925000
C	2.706678000	-1.877293000	0.498273000
H	3.485353000	-1.843209000	-0.268049000
H	3.167359000	-2.241294000	1.421587000
C	1.642918000	-2.897987000	0.012184000

O	1.901856000	-4.091528000	0.122422000
C	1.689762000	-0.264367000	2.085216000
H	1.911708000	0.769759000	2.365991000
C	0.162376000	-0.465391000	2.266681000
O	-0.288440000	-0.471949000	3.408143000
C	2.918838000	0.597961000	0.034571000
H	2.224385000	-0.908890000	2.789165000
O	1.875242000	-0.328348000	-1.917594000
O	4.005825000	0.412669000	-2.140948000
C	4.305356000	0.835990000	0.618628000
H	4.856708000	1.533145000	-0.016865000
H	4.258907000	1.226063000	1.642708000
H	4.871464000	-0.099449000	0.627591000
C	-3.946504000	-0.529155000	-0.500115000
C	-4.968429000	-0.012974000	-1.322006000
C	-5.846278000	0.968284000	-0.862664000
C	-5.720563000	1.469009000	0.435652000
C	-4.700345000	0.981581000	1.259871000
C	-3.822408000	0.000368000	0.803229000
H	-5.073673000	-0.399954000	-2.333762000
H	-6.631244000	1.340519000	-1.518285000
H	-6.403877000	2.233733000	0.798739000
H	-4.581917000	1.374586000	2.267470000
H	-3.006925000	-0.335259000	1.436766000
C	-3.015816000	-1.559269000	-1.012820000
H	-3.273730000	-1.871036000	-2.031394000
H	-1.885129000	-0.904620000	-1.241891000
C	-2.647097000	-2.731794000	-0.119877000
H	-1.856444000	-3.328231000	-0.581752000
H	-2.265222000	-2.397073000	0.847105000
H	-3.525080000	-3.374927000	0.054332000

^{3}IH

Zero-point correction= 0.389150 (Hartree/Particle)
Thermal correction to Energy= 0.418200
Thermal correction to Enthalpy= 0.419144
Thermal correction to Gibbs Free Energy= 0.325512
Sum of electronic and zero-point Energies= -1534.03562
Sum of electronic and thermal Energies= -1534.006575
Sum of electronic and thermal Enthalpies= -1534.005631
Sum of electronic and thermal Free Energies= -1534.099

Fe	1.121814000	-0.251762000	-0.987544000
O	-0.478253000	0.471961000	-0.168026000
O	0.222174000	-1.951604000	-1.095362000
C	3.049449000	1.178123000	0.413381000
C	2.060575000	2.585920000	-1.172862000
C	3.871355000	2.209427000	0.867065000
C	2.852803000	3.661161000	-0.770966000
H	1.330755000	2.635744000	-1.974775000
C	3.766087000	3.465278000	0.264835000
H	4.578857000	2.033451000	1.669356000
H	2.752323000	4.624100000	-1.261323000
H	4.396167000	4.283453000	0.604150000
C	3.706911000	-1.030767000	-0.376387000
N	2.168050000	1.391762000	-0.587831000
N	1.646491000	-0.736971000	0.913670000
O	0.727737000	0.272693000	-2.652481000
C	1.440528000	-2.215604000	0.976666000
H	2.388373000	-2.721303000	0.776347000
H	1.107625000	-2.517851000	1.973953000
C	0.420394000	-2.732152000	-0.083417000
O	-0.073042000	-3.840165000	0.105713000
C	0.747350000	0.002734000	1.836493000
H	1.258128000	0.897376000	2.206013000
C	-0.541096000	0.474328000	1.120326000
O	-1.489101000	0.847623000	1.812278000
C	3.078532000	-0.272353000	0.876942000
H	0.486659000	-0.604752000	2.708187000
O	2.875160000	-1.106079000	-1.352599000
O	4.862514000	-1.437295000	-0.312606000
C	3.864178000	-0.522423000	2.157154000
H	4.924199000	-0.323043000	1.981872000
H	3.504185000	0.094239000	2.989513000
H	3.782256000	-1.574965000	2.442740000
C	-5.317456000	-0.371446000	-0.018456000
C	-6.686066000	-0.262341000	-0.409475000
C	-7.378145000	0.934440000	-0.304356000
C	-6.739011000	2.080164000	0.192878000
C	-5.393369000	1.999387000	0.579365000
C	-4.685402000	0.808328000	0.481608000
H	-7.187759000	-1.147396000	-0.797122000
H	-8.421485000	0.983437000	-0.610895000
H	-7.280775000	3.019628000	0.274229000
H	-4.886517000	2.882940000	0.961250000
H	-3.641005000	0.783022000	0.783595000
C	-4.642321000	-1.611772000	-0.132021000
H	-5.208457000	-2.437187000	-0.563077000
H	0.001829000	-0.311143000	-2.933578000
C	-3.218646000	-1.865369000	0.243455000
H	-2.512721000	-1.479891000	-0.507781000
H	-2.947630000	-1.369646000	1.183420000
H	-3.011363000	-2.935389000	0.340484000

^{5}TS

Zero-point correction= 0.384318 (Hartree/Particle)
Thermal correction to Energy= 0.412983
Thermal correction to Enthalpy= 0.413928
Thermal correction to Gibbs Free Energy= 0.321492
Sum of electronic and zero-point Energies= -1534.01679
Sum of electronic and thermal Energies= -1533.988130
Sum of electronic and thermal Enthalpies= -1533.987186
Sum of electronic and thermal Free Energies= -1534.079

Fe	-0.212024000	-0.375235000	-0.863203000
O	-1.577076000	-0.687432000	-2.253661000
O	0.387385000	-2.243742000	-0.736579000
C	-2.328765000	1.172558000	0.762535000
C	-1.725380000	2.511700000	-1.042676000
C	-3.234608000	2.137824000	1.214055000
C	-2.607700000	3.520876000	-0.658195000
H	-1.096206000	2.589152000	-1.924667000
C	-3.371982000	3.323013000	0.491347000
H	-3.818688000	1.966315000	2.110500000
H	-2.691432000	4.429569000	-1.246042000
H	-4.073326000	4.083921000	0.824651000
C	-0.543504000	0.107837000	2.050675000
N	-1.597815000	1.381426000	-0.346058000
N	-1.881843000	-1.205876000	0.443998000
O	0.979997000	0.563004000	-1.744866000
C	-1.323130000	-2.480172000	0.949853000
H	-0.840744000	-2.304482000	1.916001000
H	-2.107572000	-3.228298000	1.110808000
C	-0.230524000	-3.088478000	0.031580000
O	0.005415000	-4.286218000	0.138971000
C	-3.046710000	-1.389364000	-0.450193000

H	-3.869141000	-0.732492000	-0.149114000
C	-2.767370000	-1.104104000	-1.950901000
O	-3.695706000	-1.276408000	-2.733788000
C	-2.012457000	-0.136341000	1.478151000
H	-3.427080000	-2.413422000	-0.374270000
O	0.361778000	0.055646000	1.141332000
O	-0.409083000	0.347514000	3.247880000
C	-2.993119000	-0.473543000	2.601681000
H	-2.924945000	0.273814000	3.395230000
H	-4.026090000	-0.532814000	2.237764000
H	-2.728798000	-1.435089000	3.049531000
C	4.014881000	0.942283000	-0.329960000
C	5.300160000	0.902786000	-0.897983000
C	6.281048000	0.043316000	-0.403396000
C	5.988292000	-0.807374000	0.664818000
C	4.708164000	-0.792350000	1.227027000
C	3.728433000	0.070355000	0.738863000
H	5.529937000	1.561000000	-1.733783000
H	7.271046000	0.034779000	-0.854511000
H	6.747268000	-1.485429000	1.048428000
H	4.464863000	-1.467145000	2.043909000
H	2.726133000	0.048513000	1.159316000
C	2.979899000	1.873264000	-0.864255000
H	3.357670000	2.435435000	-1.726649000
H	2.086026000	1.189483000	-1.326167000
C	2.279594000	2.781108000	0.143211000
H	1.531835000	3.402996000	-0.361857000
H	1.764701000	2.194795000	0.909057000
H	3.001767000	3.446582000	0.637836000

^{5}IH

Zero-point correction= 0.386660 (Hartree/Particle)
Thermal correction to Energy= 0.416823
Thermal correction to Enthalpy= 0.417767
Thermal correction to Gibbs Free Energy= 0.320898
Sum of electronic and zero-point Energies= -1534.05124
Sum of electronic and thermal Energies= -1534.021077
Sum of electronic and thermal Enthalpies= -1534.020133
Sum of electronic and thermal Free Energies= -1534.117

Fe	-0.313929000	-0.679153000	-0.747308000
O	-1.733305000	-1.779658000	-1.573878000
O	0.520490000	-2.121675000	0.305087000
C	-2.474135000	1.357996000	0.057442000
C	-2.102703000	1.579270000	-2.230684000
C	-3.445770000	2.362980000	0.026375000
C	-3.058934000	2.588151000	-2.342391000
H	-1.528777000	1.221082000	-3.080408000
C	-3.738770000	2.980233000	-1.189979000
H	-3.960775000	2.657323000	0.933107000
H	-3.261119000	3.047322000	-3.304897000
H	-4.493481000	3.761502000	-1.234129000
C	-0.516239000	1.231655000	1.514563000
N	-1.829798000	0.991844000	-1.064504000
N	-1.819811000	-0.799618000	0.999148000
O	0.806272000	-0.241058000	-2.137617000
C	-1.090525000	-1.575022000	2.026817000
H	-0.613963000	-0.886863000	2.731703000
H	-1.769485000	-2.208182000	2.609101000
C	0.051585000	-2.464300000	1.469076000
O	0.463196000	-3.375775000	2.175904000
C	-3.012983000	-1.490626000	0.465817000
H	-3.874108000	-0.814405000	0.452886000
C	-2.853432000	-2.042922000	-0.977316000
O	-3.801644000	-2.665274000	-1.444702000
C	-1.986935000	0.648433000	1.318216000
H	-3.291511000	-2.329373000	1.112815000
O	0.330354000	0.747867000	0.678860000
O	-0.323610000	2.078612000	2.383486000
C	-2.856262000	0.919214000	2.547011000
H	-2.812926000	1.977492000	2.813666000
H	-3.899022000	0.622741000	2.380896000
H	-2.471347000	0.360954000	3.404529000
C	4.584563000	1.064094000	0.013463000
C	5.786542000	0.692496000	-0.661854000
C	5.966820000	-0.586875000	-1.165767000
C	4.962753000	-1.555859000	-1.020619000
C	3.771125000	-1.222198000	-0.359054000
C	3.580130000	0.057466000	0.149862000
H	6.570154000	1.439176000	-0.779961000
H	6.894137000	-0.837812000	-1.677467000
H	5.105221000	-2.557502000	-1.417795000
H	2.978659000	-1.955985000	-0.233945000
H	2.647111000	0.287466000	0.653707000
C	4.433735000	2.380605000	0.511786000
H	5.279721000	3.053887000	0.368440000
H	1.711117000	-0.035872000	-1.849331000
C	3.258993000	2.925181000	1.260659000
H	3.058010000	3.963715000	0.963507000
H	2.339678000	2.350870000	1.116536000
H	3.450781000	2.950730000	2.346887000

4+EB

^{3}TS

Zero-point correction= 0.317690 (Hartree/Particle)
Thermal correction to Energy= 0.343433
Thermal correction to Enthalpy= 0.344377
Thermal correction to Gibbs Free Energy= 0.260498
Sum of electronic and zero-point Energies= -1474.93555
Sum of electronic and thermal Energies= -1474.909809
Sum of electronic and thermal Enthalpies= -1474.908865
Sum of electronic and thermal Free Energies= -1474.992

Fe	0.642104000	-0.514590000	-0.546499000
O	1.935667000	-1.325887000	-1.773111000
O	0.742958000	1.181179000	-1.573956000
O	-0.298407000	0.474521000	0.901814000
O	0.924989000	-2.003814000	0.677202000
O	-0.752121000	-1.130866000	-1.364115000
N	2.278756000	0.312687000	0.361930000
C	3.151193000	-0.919635000	-1.665973000
C	3.397720000	0.186585000	-0.605409000
C	1.802062000	-1.833705000	1.606111000
C	2.493140000	-0.447762000	1.617783000
H	4.343991000	-0.010490000	-0.088726000
H	3.513001000	1.129208000	-1.147834000
H	3.561922000	-0.578032000	1.821642000
H	2.069783000	0.112553000	2.456643000
O	2.110466000	-2.639461000	2.488270000
O	4.121487000	-1.289250000	-2.335377000
C	1.716987000	1.696976000	0.535729000
C	0.368472000	1.506443000	1.306361000
C	1.290871000	2.138888000	-0.907508000
O	1.495701000	3.293984000	-1.289156000
O	0.030704000	2.299045000	2.188393000
C	2.650594000	2.689939000	1.209529000

H	3.571684000	2.818461000	0.629701000
H	2.145311000	3.655074000	1.267730000
H	2.903338000	2.370537000	2.227250000
C	-3.790286000	-0.716132000	-0.092848000
C	-4.948179000	-0.922915000	-0.873689000
C	-5.919163000	0.067232000	-1.020338000
C	-5.760250000	1.305668000	-0.392888000
C	-4.606899000	1.538334000	0.366815000
C	-3.635220000	0.552197000	0.514718000
H	-5.082412000	-1.886366000	-1.363429000
H	-6.803951000	-0.129597000	-1.625391000
H	-6.513744000	2.083367000	-0.506644000
H	-4.453141000	2.508163000	0.836358000
H	-2.717832000	0.765453000	1.056593000
C	-2.777912000	-1.774182000	0.056163000
H	-3.046935000	-2.681770000	-0.496937000
H	-1.669855000	-1.366457000	-0.683461000
C	-2.223124000	-2.072467000	1.438309000
H	-1.392704000	-2.780027000	1.370367000
H	-1.822573000	-1.171675000	1.908734000
H	-3.003478000	-2.496271000	2.095963000

^{3}IH

Zero-point correction= 0.321549 (Hartree/Particle)
Thermal correction to Energy= 0.348617
Thermal correction to Enthalpy= 0.349561
Thermal correction to Gibbs Free Energy= 0.261727
Sum of electronic and zero-point Energies= -1474.96514
Sum of electronic and thermal Energies= -1474.938077
Sum of electronic and thermal Enthalpies= -1474.937133
Sum of electronic and thermal Free Energies= -1475.024

Fe	1.277816000	-0.522378000	-0.924526000
O	2.737315000	-1.802908000	-0.681629000
O	2.552081000	0.860762000	-1.528907000
O	-0.112563000	0.907121000	-0.806399000
O	0.140609000	-1.752890000	0.091906000
O	0.816863000	-1.139876000	-2.550503000
N	1.789918000	0.225370000	0.894843000
C	3.486491000	-1.585926000	0.342314000
C	3.152918000	-0.305757000	1.161735000
C	0.017773000	-1.512089000	1.348414000
C	0.774397000	-0.261719000	1.861079000
H	3.289976000	-0.516134000	2.228449000
H	3.891702000	0.450301000	0.881018000
H	1.226707000	-0.478896000	2.835418000
H	0.023519000	0.518107000	2.018871000
O	-0.675584000	-2.141770000	2.158030000
O	4.457001000	-2.255268000	0.710733000
C	1.700733000	1.684157000	0.534504000
C	0.251764000	1.870062000	-0.035100000
C	2.641295000	1.850434000	-0.707627000
O	3.360385000	2.847891000	-0.813933000
O	-0.414284000	2.866746000	0.276769000
C	2.029682000	2.646695000	1.664510000
H	3.052096000	2.489921000	2.028054000
H	1.955325000	3.667224000	1.285889000
H	1.326276000	2.536018000	2.497684000
C	-4.487350000	-0.673188000	-0.108373000
C	-5.776116000	-0.078678000	0.045468000
C	-5.932623000	1.298350000	0.104371000
C	-4.814213000	2.142471000	0.016031000
C	-3.534758000	1.588230000	-0.140149000
C	-3.369753000	0.209136000	-0.206680000
H	-6.646246000	-0.730929000	0.120902000
H	-6.929216000	1.723607000	0.223985000
H	-4.939485000	3.222243000	0.069886000
H	-2.648210000	2.218328000	-0.195391000
H	-2.365715000	-0.184247000	-0.334343000
C	-4.351481000	-2.083559000	-0.152357000
H	-5.268377000	-2.664832000	-0.041086000
H	1.105514000	-2.068791000	-2.517880000
C	-3.059098000	-2.825758000	-0.273109000
H	-3.238125000	-3.883830000	-0.502009000
H	-2.406671000	-2.412208000	-1.052083000
H	-2.454273000	-2.777264000	0.647718000

^{5}TS

Zero-point correction= 0.316084 (Hartree/Particle)
Thermal correction to Energy= 0.342795
Thermal correction to Enthalpy= 0.343739
Thermal correction to Gibbs Free Energy= 0.256605
Sum of electronic and zero-point Energies= -1474.94986
Sum of electronic and thermal Energies= -1474.923159
Sum of electronic and thermal Enthalpies= -1474.922214
Sum of electronic and thermal Free Energies= -1475.009

Fe	0.440588000	-0.064440000	-0.715816000
O	-0.520769000	0.499188000	1.043590000
O	1.026563000	-1.812549000	0.302510000
O	2.067161000	-0.448915000	-1.906808000
O	0.550176000	1.885218000	-1.227435000
O	-0.955032000	-0.657558000	-1.667107000
N	2.193072000	0.585501000	0.567693000
C	0.165524000	0.831106000	2.082927000
C	1.703743000	0.674738000	1.954526000
C	1.530508000	2.613353000	-0.814121000
C	2.624305000	1.879788000	0.008258000
H	2.181396000	1.501875000	2.495539000
H	1.961910000	-0.245380000	2.488785000
H	2.981764000	2.557110000	0.794595000
H	3.463320000	1.716271000	-0.675924000
O	1.705308000	3.813206000	-1.045700000
O	-0.280299000	1.208406000	3.171157000
C	3.076714000	-0.582020000	0.263882000
C	3.188573000	-0.651577000	-1.299183000
C	2.259574000	-1.862620000	0.667256000
O	2.821091000	-2.784047000	1.269434000
O	4.277451000	-0.890315000	-1.828890000
C	4.443860000	-0.534247000	0.936712000
H	4.342783000	-0.526298000	2.028168000
H	5.010891000	-1.421538000	0.652281000
H	5.007362000	0.350774000	0.618720000
C	-4.011730000	-0.765144000	-0.310364000
C	-5.296457000	-0.936575000	-0.854223000
C	-6.314789000	-0.010769000	-0.617242000
C	-6.061904000	1.117257000	0.165743000
C	-4.782389000	1.309063000	0.699229000
C	-3.764495000	0.385238000	0.466866000
H	-5.496916000	-1.814418000	-1.467061000
H	-7.303397000	-0.170400000	-1.046132000
H	-6.850044000	1.845613000	0.350163000
H	-4.568053000	2.193908000	1.294614000
H	-2.762348000	0.559154000	0.858041000
C	-2.932856000	-1.766468000	-0.556363000
H	-3.251511000	-2.525770000	-1.281793000

H	-2.009570000	-1.181722000	-1.126799000
C	-2.281533000	-2.389678000	0.674794000
H	-1.425439000	-3.005446000	0.385553000
H	-1.895874000	-1.616500000	1.343715000
H	-3.006153000	-3.010055000	1.226709000

^{5}IH

Zero-point correction= 0.319443 (Hartree/Particle)
Thermal correction to Energy= 0.347232
Thermal correction to Enthalpy= 0.348176
Thermal correction to Gibbs Free Energy= 0.258448
Sum of electronic and zero-point Energies= -1474.98707
Sum of electronic and thermal Energies= -1474.959283
Sum of electronic and thermal Enthalpies= -1474.958339
Sum of electronic and thermal Free Energies= -1475.048

Fe	0.790182000	0.026039000	-1.082049000
O	-0.363449000	1.413340000	-0.088752000
O	0.132415000	-1.337239000	0.391002000
O	2.341328000	-1.268249000	-1.302851000
O	1.937688000	1.549894000	-1.786431000
O	-0.464837000	-0.248092000	-2.443594000
N	2.090274000	0.465776000	0.744585000
C	-0.055765000	1.790553000	1.100713000
C	1.236061000	1.181187000	1.708138000
C	2.922295000	2.008309000	-1.093918000
C	3.219383000	1.263762000	0.236608000
H	1.790349000	1.983879000	2.211387000
H	0.905820000	0.489873000	2.490225000
H	3.561017000	1.997393000	0.978515000
H	4.066335000	0.600173000	0.032811000
O	3.675105000	2.937393000	-1.402769000
O	-0.711310000	2.554908000	1.821848000
C	2.393553000	-0.960452000	1.075646000
C	2.981424000	-1.603500000	-0.230081000
C	1.004952000	-1.668275000	1.279656000
O	0.848310000	-2.454760000	2.217961000
O	3.956007000	-2.355750000	-0.162831000
C	3.316870000	-1.149237000	2.274147000
H	2.872749000	-0.721764000	3.180524000
H	3.472139000	-2.215908000	2.440780000
H	4.292488000	-0.682916000	2.094461000
C	-4.397706000	-0.801250000	-0.307520000
C	-5.766516000	-0.429026000	-0.150730000
C	-6.121525000	0.780990000	0.427863000
C	-5.131930000	1.671959000	0.873807000
C	-3.777556000	1.333595000	0.732856000
C	-3.413629000	0.121514000	0.157063000
H	-6.538499000	-1.115761000	-0.497962000
H	-7.175160000	1.039345000	0.534433000
H	-5.415361000	2.620591000	1.325800000
H	-2.987921000	2.003028000	1.070292000
H	-2.359271000	-0.117201000	0.065997000
C	-4.046493000	-2.036649000	-0.907887000
H	-4.870563000	-2.670609000	-1.239165000
H	-1.133695000	0.448102000	-2.336957000
C	-2.647187000	-2.509974000	-1.139253000
H	-2.079391000	-1.847962000	-1.814681000
H	-2.043457000	-2.520365000	-0.220810000
H	-2.641658000	-3.519962000	-1.565792000