Supporting information for

Effect of Substituent on C-H Activation Catalysed by a nonheme Iron-Oxo Complex: A Computational Investigation of Reactivity and Hydrogen Tunneling

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Table S1 The relative energies (in kcal mol^{-1}) for all the investigated reactions computed at different level of theory.

Reactions	Spin state	Species	B1+ZPE	B2+ZPE	B2+G^{corr}(298K)
H	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	17.3	14.6	26.9
		^{3}I	-0.2	-5.3	4.2
	S=2	^{5}R+S	5.8	1.7	-0.01
		^{5}TS	21.1	10.6	18.6
		^{5}I	5.4	-9.3	-2.3
$N(CH3)_2$	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	17.3	14.7	26.7
		^{3}I	-0.2	-5.1	4.1
	S=2	^{5}R+S	5.4	1.5	-0.6
		^{5}TS	21.0	10.7	19.1
		^{5}I	5.0	-8.8	-3.3
OMe	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	17.3	14.7	26.7
		^{3}I	-0.4	-5.2	3.9
	S=2	^{5}R+S	5.5	1.6	-0.2
		^{5}TS	20.9	10.6	18.8
		^{5}I	6.6	-7.7	-0.7
NO_2	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	16.5	13.8	25.4
		^{3}I	-0.6	-5.6	3.2
	S=2	^{5}R+S	6.6	2.4	0.6
		^{5}TS	19.3	10.3	18.5
		^{5}I	6.6	-8.8	-1.8
SO_2CF_3	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	16.5	13.9	26.1
		^{3}I	-0.8	-5.3	4.3
	S=2	^{5}R+S	6.4	2.7	1.3
		^{5}TS	20.5	10.6	18.6
		^{5}I	6.5	-7.8	0.3
N4PY	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	16.5	13.9	26.1
		^{3}I	-0.5	-5.5	3.2
	S=2	^{5}R+S	10.4	5.4	3.3
		^{5}TS	20.2	11.3	18.7
		^{5}I	4.5	-9.7	-2.7

Table S2 Transmission coefficients for hydrogen and deuterium (κ_H and κ_D), Kinetic Isotope Effect (KIE) at 298K computed using different method**.**

Reaction	Species	κ_H	κ_D	KIE_{Eyring}	KIE_{Eckart}	KIE_{Wigner}
H	S=1	154.6	11.8	5.2	68.8	7.9
	S=2	20.8	5.2	5.5	21.9**(32)***	7.5
$N(CH_3)_2$	S=1	167.6	12.3	5.2	71.2	7.9
	S=2	25.0	5.7	5.3	23.5	7.4
OMe	S=1	164.4	12.2	5.2	70.6	7.9
	S=2	23.71	5.57	5.3	22.6	7.4
NO_2	S=1	105.7	9.9	5.2	55.2	7.8
	S=2	10.1	3.8	5.0	13.3	6.6
SO_2CF_3	S=1	111.80	10.15	5.1	56.5	7.7
	S=2	10.4	3.81	5.0	13.7	6.6

*Experimental value

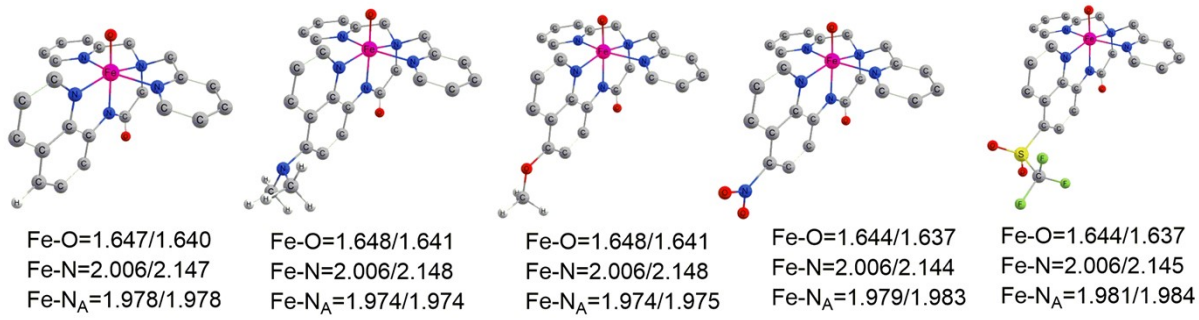

Fig. S1 Optimized geometries of the oxidants with key geometrical parameters computed at B1 level of theory (distances are in Å and angles are in degree).

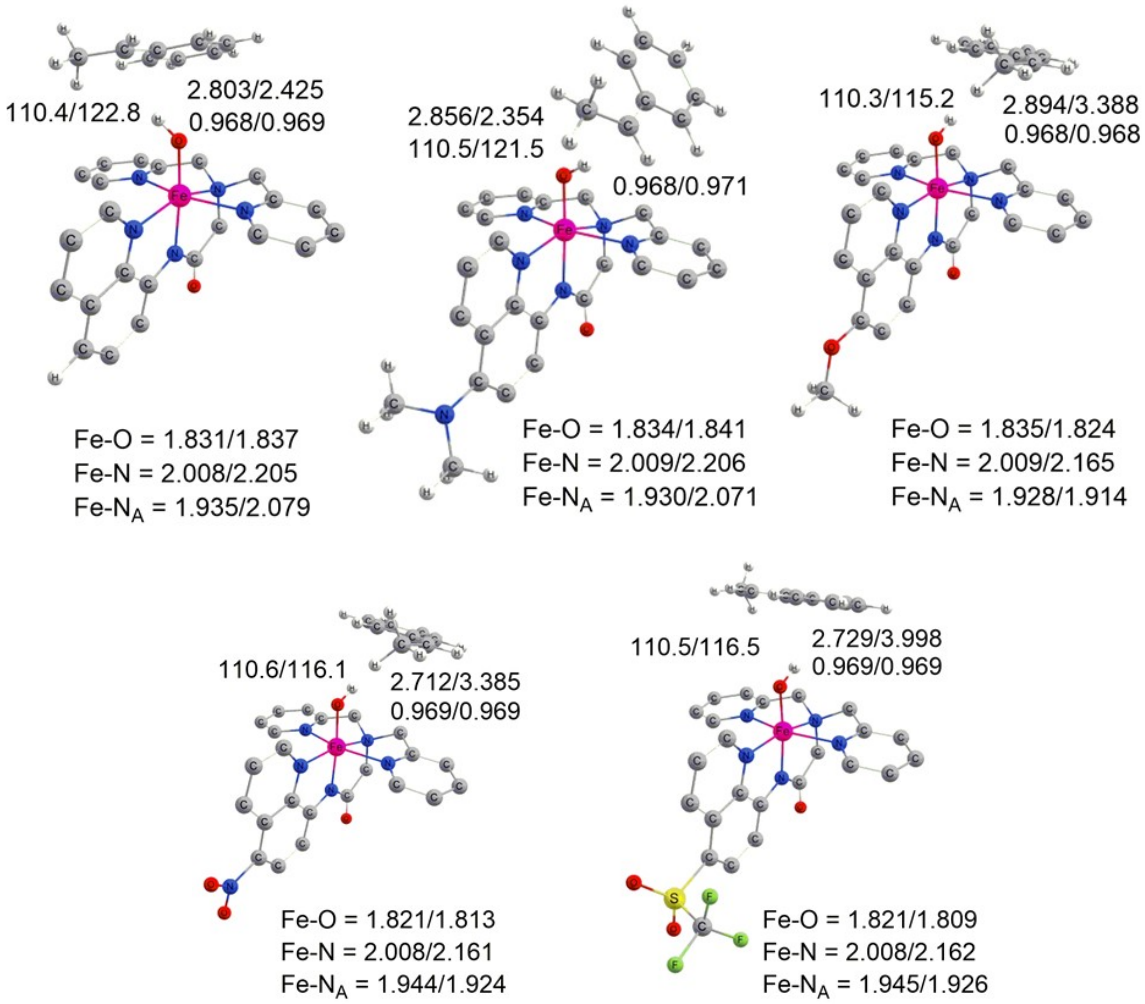

Fig. S2 Optimized geometries of the intermediates with key geometrical parameters computed at B1 level of theory (distances are in Å and angles are in degree)

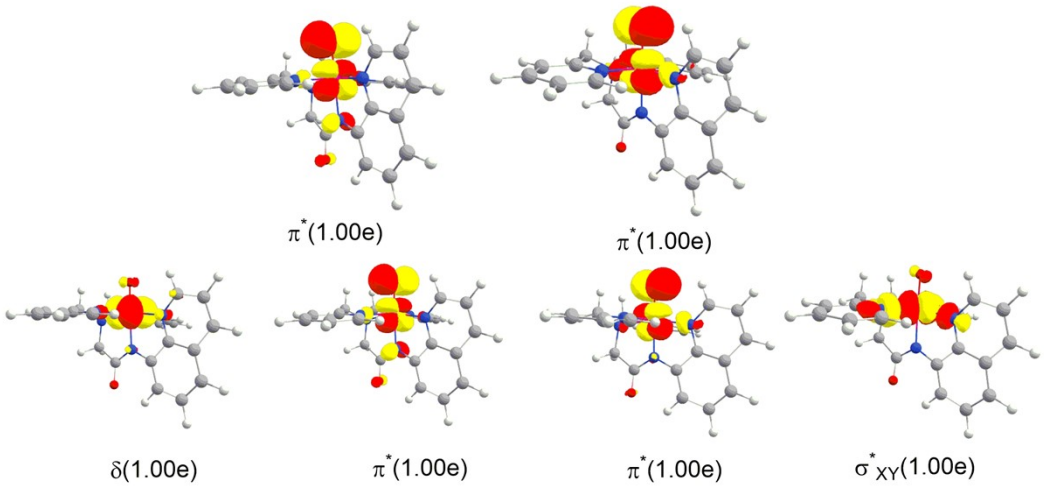

Fig. S3 Spin natural orbitals and their occupations for the oxidants of the unsubstituted parent compound (H). Upper panel represents ^{3}R while bottom panel represents ^{5}R

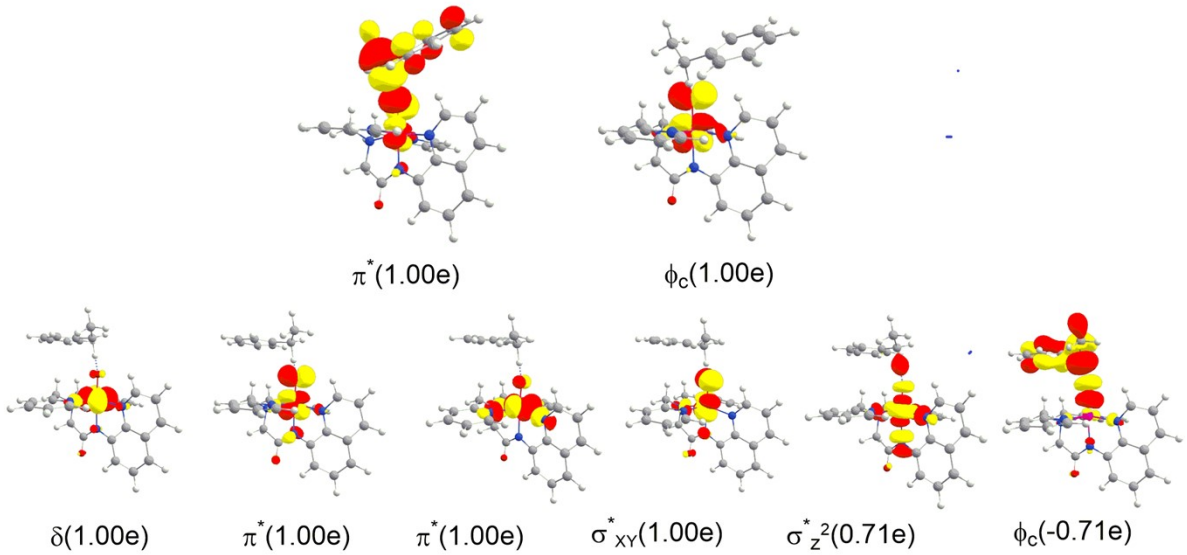

Fig. S4 Spin natural orbitals and their occupations for the transition states of the reactions between the parent compound (H) and EB. Upper panel represents ^{3}TS while bottom panel represents ^{5}TS

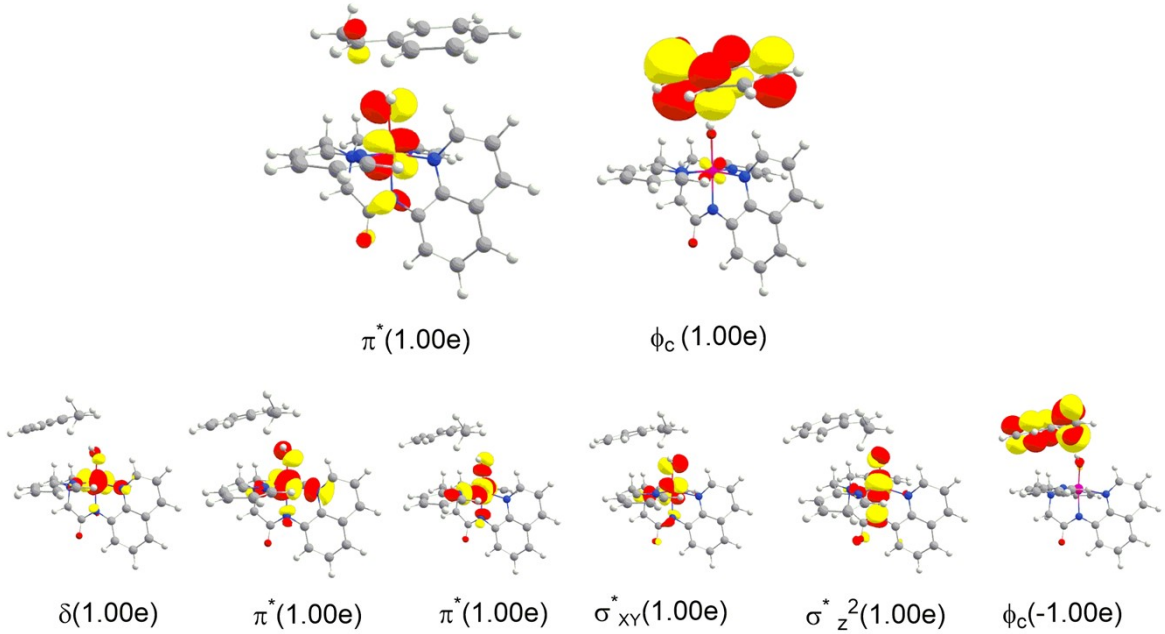

Fig. S5 Spin natural orbitals and their occupations for the intermediates for the reactions between the parent compound (H) and EB. Upper panel represents ^{3}I while bottom panel represents ^{5}I

Table S3 Mulliken spin densities and charges for oxidants

Species	Spin State	Mulliken Spin Density			Mulliken Charges		
		Fe	**O**	**Rest**	**Fe**	**O**	**Rest**
-H	S=1	1.255	0.871	-0.126	0.094	0.220	-0.314
	S=2	3.116	0.708	0.176	0.176	0.271	-0.447
$-N(CH_3)_2$	S=1	1.265	0.863	-0.128	-0.077	0.255	-0.178
	S=2	3.120	0.698	0.182	-0.065	0.297	-0.232
-OMe	S=1	1.263	0.864	-0.127	-0.131	0.241	-0.11
	S=2	3.118	0.699	0.183	0.011	0.277	-0.288
$-NO_2$	S=1	1.247	0.884	-0.131	0.027	0.278	-0.305
	S=2	3.119	0.714	0.167	0.099	0.309	-0.408
$-SO_2CF_3$	S=1	1.247	0.883	-0.13	-0.150	0.278	-0.128
	S=2	3.113	0.717	0.17	0.215	0.297	-0.512

Table S4 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**
H	**^{3}TS**	0.995	0.634	-0.031	0.359	0.043	-1.647	0.329	0.694	-0.756	1.38
	^{3}I	0.974	0.108	0.003	0.834	0.081	-1.602	0.023	0.443	-0.234	1.37
	^{5}TS	3.791	0.180	0.031	-0.294	0.292	-1.853	0.717	0.929	-0.946	1.15
	^{5}I	4.254	0.280	0.028	-0.826	0.264	-1.156	0.038	0.504	-0.396	1.01
$N(CH_3)_2$	**^{3}TS**	0.991	0.633	-0.027	0.360	0.043	-1.706	0.283	0.628	-0.697	1.49
	^{3}I	0.970	0.104	0.004	0.831	0.091	-1.511	-0.001	0.378	-0.186	1.32
	^{5}TS	3.777	0.173	0.032	-0.297	0.315	-2.044	0.718	0.934	-0.947	1.34
	^{5}I	4.212	0.276	0.049	-0.822	0.285	-1.847	0.252	0.474	-0.312	1.43
OMe	**^{3}TS**	0.995	0.632	-0.030	0.365	0.038	-1.606	0.301	0.667	-0.732	1.37
	^{3}I	0.970	0.104	0.003	0.832	0.091	-1.334	-0.012	0.383	-0.209	1.17
	^{5}TS	3.779	0.171	0.031	-0.297	0.316	-1.792	0.700	0.949	-0.940	1.08
	^{5}I	4.238	0.277	0.025	-0.821	0.281	-0.913	0.045	0.457	-0.407	0.82
NO_2	**^{3}TS**	0.977	0.648	-0.023	0.362	0.036	-1.505	0.385	0.639	-0.774	1.26
	^{3}I	0.967	0.121	0.002	0.820	0.09	-1.433	0.063	0.407	-0.137	1.1
	^{5}TS	3.774	0.203	0.026	-0.278	0.275	-1.966	0.755	0.869	-0.937	1.28
	^{5}I	4.245	0.300	0.026	-0.811	0.24	-1.160	0.128	0.539	-0.417	0.91
SO2CF3	**^{3}TS**	0.978	0.651	-0.028	0.357	0.042	-1.595	0.276	0.661	-0.730	1.39
	^{3}I	0.965	0.121	0.003	0.831	0.08	-1.384	-0.015	0.401	-0.237	1.24
	^{5}TS	3.763	0.203	0.026	-0.278	0.286	-1.853	0.723	0.904	-0.941	1.17
	^{5}I	4.234	0.303	0.026	-0.821	0.258	-1.113	0.042	0.477	-0.397	0.99

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

^{3}1 [Fe(IV)ODpaqH]ClO_4

Zero-point correction= 0.417631 (Hartree/Particle)
Thermal correction to Energy= 0.447724
Thermal correction to Enthalpy= 0.448668
Thermal correction to Gibbs Free Energy= 0.352774
Sum of electronic and zero-point Energies= -2196.566613
Sum of electronic and thermal Energies= -2196.536520
Sum of electronic and thermal Enthalpies= -2196.535576
Sum of electronic and thermal Free Energies= -2196.631470

Fe	-0.878994000	-0.287693000	-0.874977000
N	-0.878572000	0.098642000	1.064781000
C	-1.984565000	0.786245000	1.541844000
C	-2.932119000	1.091623000	0.515854000
C	-2.270223000	1.196513000	2.841076000
C	-4.136923000	1.794287000	0.793651000
C	-3.469190000	1.895524000	3.115750000
H	-1.566106000	0.973871000	3.630820000
C	-3.454324000	0.919151000	-1.758957000
C	-5.005378000	2.044107000	-0.299718000
C	-4.389342000	2.195359000	2.131355000
H	-3.663373000	2.202714000	4.139145000
C	-4.667192000	1.610257000	-1.564512000
H	-3.145306000	0.558651000	-2.733702000
H	-5.935359000	2.578428000	-0.129147000
H	-5.303362000	2.732777000	2.362450000
H	-5.314865000	1.789272000	-2.414793000
N	-2.621505000	0.671925000	-0.754121000
C	0.170270000	-0.325924000	1.801791000
O	0.354020000	-0.194133000	3.016488000
C	1.225804000	-1.050988000	0.959747000
H	2.179637000	-0.527994000	1.073986000
N	0.887787000	-1.164214000	-0.510321000
C	-0.642218000	-3.067385000	-0.482774000
C	-2.861784000	-2.455041000	-0.119275000
C	-0.922175000	-4.395760000	-0.175823000
C	-3.214677000	-3.765766000	0.184788000
H	-3.591418000	-1.655540000	-0.103606000
C	-2.228652000	-4.750943000	0.158495000
H	-0.127924000	-5.133420000	-0.200798000
H	-4.241677000	-3.998325000	0.440851000
H	-2.470405000	-5.780714000	0.399494000
N	-1.604338000	-2.117793000	-0.446244000
C	0.714003000	-2.584741000	-0.930284000
H	0.749968000	-2.613776000	-2.022915000
H	1.520297000	-3.214343000	-0.542888000
H	1.361722000	-2.052866000	1.375122000
C	-0.136549000	2.634907000	-1.138358000
C	1.563936000	1.045948000	-1.290478000
C	0.772529000	3.677260000	-1.284831000
H	-1.195625000	2.821222000	-1.014463000
C	2.531320000	2.039307000	-1.416295000
C	2.126785000	3.374067000	-1.419539000
H	0.418081000	4.701389000	-1.281429000
H	3.578280000	1.765086000	-1.489570000
H	2.861444000	4.166482000	-1.517793000
N	0.253913000	1.350461000	-1.142637000
C	1.873039000	-0.427126000	-1.358188000
H	1.730702000	-0.761441000	-2.389849000
H	2.899231000	-0.652201000	-1.053700000
O	-0.930789000	-0.588392000	-2.493022000
Cl	5.360209000	0.063438000	0.608672000
O	6.559690000	-0.172312000	1.464471000
O	4.257945000	0.657567000	1.433747000
O	4.892465000	-1.238984000	0.027663000
O	5.710556000	1.004235000	-0.504016000

^{5}1 [Fe(IV)ODpaqH]ClO_4

Zero-point correction= 0.415623 (Hartree/Particle)
Thermal correction to Energy= 0.446677
Thermal correction to Enthalpy= 0.447621
Thermal correction to Gibbs Free Energy= 0.347994
Sum of electronic and zero-point Energies= -2196.557364
Sum of electronic and thermal Energies= -2196.526310
Sum of electronic and thermal Enthalpies= -2196.525365
Sum of electronic and thermal Free Energies= -2196.624993

Fe	-1.009761000	-0.226271000	-0.964482000
N	-0.962797000	0.129987000	0.980789000
C	-2.082761000	0.761195000	1.522291000
C	-3.096830000	1.046673000	0.558797000
C	-2.321828000	1.132524000	2.843376000
C	-4.315570000	1.687259000	0.915117000
C	-3.534656000	1.770229000	3.198008000
H	-1.571110000	0.927749000	3.592524000
C	-3.735136000	0.903429000	-1.691610000
C	-5.249773000	1.919878000	-0.124614000
C	-4.518146000	2.048968000	2.272294000
H	-3.684830000	2.044941000	4.237760000
C	-4.963189000	1.531644000	-1.419166000
H	-3.462249000	0.579608000	-2.690219000
H	-6.192524000	2.406363000	0.108238000
H	-5.441892000	2.539006000	2.561994000
H	-5.664576000	1.701124000	-2.227588000
N	-2.839460000	0.671953000	-0.734833000
C	0.125725000	-0.250045000	1.704486000
O	0.298258000	-0.102861000	2.917077000
C	1.230214000	-0.931044000	0.889851000
H	2.154343000	-0.364004000	1.038350000
N	0.953685000	-1.081132000	-0.575450000
C	-0.410767000	-3.129878000	-0.524059000
C	-2.679176000	-2.783153000	-0.146720000
C	-0.526383000	-4.480596000	-0.199995000
C	-2.876211000	-4.122045000	0.176136000
H	-3.496600000	-2.070172000	-0.132875000
C	-1.778813000	-4.983396000	0.150431000
H	0.349656000	-5.119381000	-0.224228000
H	-3.865381000	-4.472786000	0.446807000
H	-1.894760000	-6.031569000	0.405608000
N	-1.472667000	-2.306645000	-0.489172000
C	0.883366000	-2.504006000	-0.989306000
H	0.907271000	-2.534886000	-2.083208000
H	1.747039000	-3.067404000	-0.619725000
H	1.398528000	-1.916396000	1.333854000
C	-0.067716000	2.770272000	-1.224771000
C	1.613360000	1.165100000	-1.332281000
C	0.854743000	3.806659000	-1.326095000
H	-1.131276000	2.963849000	-1.135117000
C	2.599357000	2.147756000	-1.413047000
C	2.210080000	3.486940000	-1.415689000
H	0.513874000	4.835581000	-1.322016000
H	3.645313000	1.862038000	-1.452609000
H	2.957017000	4.271726000	-1.477958000
N	0.310700000	1.483055000	-1.229823000

C	1.918464000	-0.312385000	-1.405477000
H	1.791561000	-0.636341000	-2.443537000
H	2.949098000	-0.524440000	-1.103326000
O	-1.127531000	-0.491923000	-2.578582000
Cl	5.375825000	0.099902000	0.691534000
O	6.580112000	-0.164889000	1.532705000
O	4.296173000	0.711671000	1.532786000
O	4.876557000	-1.189428000	0.108243000
O	5.733921000	1.039643000	-0.419800000

^{3}2 [Fe(IV)ODpaqN(CH$_3$)$_2$]ClO$_4$

Zero-point correction= 0.490607 (Hartree/Particle)
Thermal correction to Energy= 0.524902
Thermal correction to Enthalpy= 0.525846
Thermal correction to Gibbs Free Energy= 0.420998
Sum of electronic and zero-point Energies= -2330.461072
Sum of electronic and thermal Energies= -2330.426778
Sum of electronic and thermal Enthalpies= -2330.425833
Sum of electronic and thermal Free Energies= -2330.530681

Fe	-0.154727000	0.842373000	0.970839000
N	-0.491460000	0.096315000	-0.825392000
C	-1.771781000	-0.400690000	-1.038398000
C	-2.613488000	-0.288520000	0.108530000
C	-2.319971000	-0.960383000	-2.185585000
C	-3.964101000	-0.736269000	0.105501000
C	-3.648654000	-1.441708000	-2.186704000
H	-1.708978000	-1.046221000	-3.073857000
C	-2.788635000	0.499063000	2.309579000
C	-4.727757000	-0.474463000	1.269130000
C	-4.479114000	-1.371570000	-1.076217000
H	-4.016547000	-1.899384000	-3.098287000
C	-4.145281000	0.131291000	2.364673000
H	-2.281012000	0.970401000	3.143700000
H	-5.779421000	-0.737157000	1.279017000
H	-4.715641000	0.340312000	3.262170000
N	-2.058881000	0.306286000	1.216218000
C	0.507540000	0.125188000	-1.730126000
O	0.490860000	-0.270255000	-2.902058000
C	1.795511000	0.734614000	-1.165042000
H	2.596028000	-0.006384000	-1.246381000
N	1.689455000	1.203847000	0.269106000
C	0.592953000	3.362270000	-0.044716000
C	-1.733050000	3.213318000	-0.073353000
C	0.553561000	4.630485000	-0.616678000
C	-1.846607000	4.482384000	-0.631873000
H	-2.606335000	2.614581000	0.151965000
C	-0.684820000	5.200894000	-0.910207000
H	1.478404000	5.156376000	-0.825562000
H	-2.828544000	4.887798000	-0.845868000
H	-0.739844000	6.189075000	-1.354470000
N	-0.539703000	2.670128000	0.213606000
C	1.867995000	2.680103000	0.381474000
H	2.051358000	2.912065000	1.434334000
H	2.728625000	3.021527000	-0.201254000
H	2.079351000	1.579138000	-1.798132000
C	-0.000619000	-2.061418000	1.807607000
C	1.995142000	-0.908387000	1.450792000
C	0.685529000	-3.236773000	2.094630000
H	-1.082109000	-2.018466000	1.825947000
C	2.745052000	-2.054466000	1.701385000
C	2.078423000	-3.233797000	2.033606000
H	0.130599000	-4.132339000	2.348722000
H	3.826015000	-2.020175000	1.616413000
H	2.640386000	-4.139997000	2.234461000
N	0.642874000	-0.926011000	1.493627000
C	2.606805000	0.439296000	1.167013000
H	2.676238000	0.990425000	2.109387000
H	3.607182000	0.359599000	0.731885000
O	0.073178000	1.458525000	2.481789000
Cl	5.645157000	-1.199169000	-0.931675000
O	6.760171000	-1.410990000	-1.900616000
O	4.351563000	-1.648923000	-1.542223000
O	5.546585000	0.258252000	-0.587978000
O	5.905558000	-1.985587000	0.317400000
N	-5.812683000	-1.854124000	-1.059265000
C	-6.482500000	-1.942925000	-2.353789000
H	-6.119341000	-2.774408000	-2.981018000
H	-7.551727000	-2.101155000	-2.183421000
H	-6.354429000	-1.008663000	-2.905675000
C	-6.017295000	-3.077935000	-0.269546000
H	-7.088132000	-3.223148000	-0.097623000
H	-5.624764000	-3.970088000	-0.784842000
H	-5.521692000	-3.000395000	0.699145000

^{5}2 [Fe(IV)ODpaqN(CH$_3$)$_2$]ClO$_4$

Zero-point correction= 0.488544 (Hartree/Particle)
Thermal correction to Energy= 0.523857
Thermal correction to Enthalpy= 0.524801
Thermal correction to Gibbs Free Energy= 0.415607
Sum of electronic and zero-point Energies= -2330.452393
Sum of electronic and thermal Energies= -2330.417080
Sum of electronic and thermal Enthalpies= -2330.416136
Sum of electronic and thermal Free Energies= -2330.525330

Fe	-0.271817000	0.819543000	1.100113000
N	-0.572661000	0.081904000	-0.706393000
C	-1.861336000	-0.386165000	-0.976721000
C	-2.758627000	-0.262280000	0.122263000
C	-2.368670000	-0.927825000	-2.152945000
C	-4.117318000	-0.680980000	0.049921000
C	-3.704400000	-1.382197000	-2.225083000
H	-1.719512000	-1.023875000	-3.011415000
C	-3.034190000	0.530005000	2.315020000
C	-4.932853000	-0.394713000	1.168963000
C	-4.588206000	-1.305727000	-1.157096000
H	-4.031671000	-1.827822000	-3.157618000
C	-4.397296000	0.199600000	2.297977000
H	-2.558773000	0.987896000	3.175797000
H	-5.990559000	-0.628047000	1.122903000
H	-5.012859000	0.424478000	3.160945000
N	-2.252164000	0.317565000	1.258372000
C	0.448955000	0.064772000	-1.602720000
O	0.410511000	-0.352481000	-2.764310000
C	1.771959000	0.632373000	-1.077704000
H	2.537058000	-0.142377000	-1.188119000
N	1.746588000	1.125644000	0.337312000
C	0.816537000	3.373902000	-0.036705000
C	-1.506025000	3.467470000	-0.104774000
C	0.920576000	4.625860000	-0.640961000
C	-1.483415000	4.725991000	-0.697446000
H	-2.439612000	2.962808000	0.120023000
C	-0.247241000	5.312446000	-0.971132000
H	1.898124000	5.048778000	-0.845259000
H	-2.413848000	5.225093000	-0.942303000
H	-0.192594000	6.288871000	-1.441125000
N	-0.378940000	2.814459000	0.216411000
C	2.016758000	2.581288000	0.426718000
H	2.203715000	2.822077000	1.478027000
H	2.911667000	2.854293000	-0.143226000
H	2.061962000	1.449431000	-1.744771000
C	0.100480000	-2.195785000	1.936678000
C	2.059363000	-1.016226000	1.507246000
C	0.807366000	-3.370545000	2.172794000
H	-0.981789000	-2.161050000	2.002790000
C	2.835627000	-2.157812000	1.704307000

C	2.196978000	-3.349229000	2.047712000
H	0.275349000	-4.277669000	2.435536000
H	3.911447000	-2.110003000	1.570795000
H	2.777037000	-4.252417000	2.207442000
N	0.719278000	-1.050249000	1.613291000
C	2.653412000	0.341862000	1.216609000
H	2.744066000	0.883742000	2.163707000
H	3.651100000	0.257419000	0.773776000
O	-0.111948000	1.420536000	2.618717000
Cl	5.662341000	-1.215238000	-1.038230000
O	6.785013000	-1.397651000	-2.005038000
O	4.384363000	-1.704892000	-1.649968000
O	5.521958000	0.239448000	-0.698646000
O	5.944868000	-1.990197000	0.213473000
N	-5.925588000	-1.763093000	-1.210221000
C	-6.525639000	-1.859780000	-2.538006000
H	-6.146819000	-2.710017000	-3.129287000
H	-7.605580000	-1.992091000	-2.423226000
H	-6.347235000	-0.938314000	-3.097127000
C	-6.214037000	-2.961180000	-0.406410000
H	-7.296181000	-3.060086000	-0.278996000
H	-5.836234000	-3.877013000	-0.889372000
H	-5.757085000	-2.885645000	0.580795000

^{3}3 [Fe(IV)ODpaqOMe]ClO_4

Zero-point correction= 0.450233 (Hartree/Particle)
Thermal correction to Energy= 0.483033
Thermal correction to Enthalpy= 0.483977
Thermal correction to Gibbs Free Energy= 0.382089
Sum of electronic and zero-point Energies= -2311.057771
Sum of electronic and thermal Energies= -2311.024971
Sum of electronic and thermal Enthalpies= -2311.024027
Sum of electronic and thermal Free Energies= -2311.125916

Fe	0.382872000	0.724140000	-0.966146000
N	0.654471000	-0.019299000	0.842463000
C	1.898869000	-0.598370000	1.072770000
C	2.755023000	-0.546900000	-0.066320000
C	2.394853000	-1.195654000	2.224358000
C	4.071859000	-1.080330000	-0.049838000
C	3.703770000	-1.733285000	2.261921000
H	1.765800000	-1.246806000	3.102598000
C	2.985047000	0.135254000	-2.295878000
C	4.837511000	-0.976793000	-1.234101000
C	4.539928000	-1.686613000	1.159267000
H	4.041173000	-2.188210000	3.185173000
C	4.296519000	-0.372079000	-2.351898000
H	2.516065000	0.619277000	-3.145331000
H	5.845317000	-1.375787000	-1.249918000
H	4.861561000	-0.279735000	-3.271926000
N	2.246506000	0.049194000	-1.194309000
C	-0.347614000	0.083150000	1.736373000
O	-0.369011000	-0.306116000	2.910959000
C	-1.584645000	0.778082000	1.156082000
H	-2.437908000	0.098793000	1.238646000
N	-1.435186000	1.223660000	-0.281941000
C	-0.189009000	3.302346000	0.014334000
C	2.120592000	2.990824000	0.053506000
C	-0.062389000	4.570885000	0.572792000
C	2.321436000	4.254972000	0.598321000
H	2.950148000	2.329712000	-0.162304000
C	1.212103000	5.056088000	0.864974000
H	-0.948597000	5.162821000	0.772108000
H	3.328894000	4.592881000	0.810987000
H	1.335052000	6.042766000	1.298841000
N	0.892889000	2.529319000	-0.231266000
C	-1.507124000	2.707573000	-0.411385000
H	-1.668061000	2.939828000	-1.467823000
H	-2.343949000	3.116399000	0.162323000
H	-1.810243000	1.647842000	1.778428000
C	0.027305000	-2.173575000	-1.761639000
C	-1.883370000	-0.875295000	-1.440097000
C	-0.738915000	-3.300894000	-2.038635000
H	1.109201000	-2.208600000	-1.770429000
C	-2.711432000	-1.968127000	-1.682038000
C	-2.128491000	-3.196992000	-1.991549000
H	-0.247636000	-4.237653000	-2.274547000
H	-3.787783000	-1.855051000	-1.608024000
H	-2.752287000	-4.063380000	-2.185338000
N	-0.535510000	-0.990371000	-1.470295000
C	-2.398589000	0.516525000	-1.178833000
H	-2.419955000	1.059384000	-2.128308000
H	-3.405624000	0.515485000	-0.751685000
O	0.207665000	1.333524000	-2.486908000
Cl	-5.574798000	-0.866165000	0.905956000
O	-6.716430000	-0.978290000	1.860563000
O	-4.326572000	-1.397537000	1.544612000
O	-5.364953000	0.573620000	0.538694000
O	-5.873841000	-1.654384000	-0.333331000
O	5.806794000	-2.175334000	1.105062000
C	6.341580000	-2.793973000	2.275140000
H	5.750571000	-3.669846000	2.565166000
H	7.351898000	-3.106955000	2.012047000
H	6.382949000	-2.088306000	3.112351000

^{5}3 [Fe(IV)ODpaqOMe]ClO_4

Zero-point correction= 0.448284 (Hartree/Particle)
Thermal correction to Energy= 0.482041
Thermal correction to Enthalpy= 0.482985
Thermal correction to Gibbs Free Energy= 0.377332
Sum of electronic and zero-point Energies= -2311.049053
Sum of electronic and thermal Energies= -2311.015296
Sum of electronic and thermal Enthalpies= -2311.014351
Sum of electronic and thermal Free Energies= -2311.120004

Fe	0.502257000	0.692641000	-1.095423000
N	0.730907000	-0.031805000	0.727255000
C	1.982434000	-0.583813000	1.021618000
C	2.899431000	-0.527866000	-0.065366000
C	2.431104000	-1.161820000	2.204142000
C	4.224357000	-1.034038000	0.028207000
C	3.745807000	-1.672049000	2.320828000
H	1.759326000	-1.219931000	3.048366000
C	3.241597000	0.134923000	-2.289651000
C	5.049051000	-0.926524000	-1.112561000
C	4.641326000	-1.619310000	1.266686000
H	4.038086000	-2.110419000	3.267052000
C	4.560524000	-0.344275000	-2.269269000
H	2.809635000	0.600174000	-3.169262000
H	6.064091000	-1.304878000	-1.068417000
H	5.176073000	-0.251794000	-3.156116000
N	2.444992000	0.044705000	-1.225916000
C	-0.297706000	0.038401000	1.611345000
O	-0.300485000	-0.361429000	2.780223000
C	-1.571265000	0.690613000	1.063076000
H	-2.390985000	-0.025695000	1.175279000
N	-1.495579000	1.159281000	-0.358564000
C	-0.404978000	3.338279000	-0.009668000
C	1.917669000	3.262807000	0.075768000
C	-0.421303000	4.603679000	0.574979000
C	1.983005000	4.528692000	0.649351000
H	2.813448000	2.687916000	-0.133784000
C	0.791244000	5.208173000	0.904239000
H	-1.366774000	5.099846000	0.765124000
H	2.945747000	4.962269000	0.894148000
H	0.804925000	6.193190000	1.359029000

N	0.748049000	2.689120000	-0.244924000
C	-1.656695000	2.629079000	-0.471906000
H	-1.816815000	2.866965000	-1.528286000
H	-2.533551000	2.975948000	0.085788000
H	-1.808937000	1.536438000	1.714696000
C	-0.083957000	-2.300414000	-1.885107000
C	-1.954133000	-0.971450000	-1.499172000
C	-0.873760000	-3.422980000	-2.112071000
H	0.998509000	-2.347755000	-1.938375000
C	-2.811012000	-2.055129000	-1.688760000
C	-2.259349000	-3.296234000	-2.005602000
H	-0.407841000	-4.371380000	-2.353724000
H	-3.881651000	-1.924838000	-1.570421000
H	-2.903314000	-4.156167000	-2.158925000
N	-0.619149000	-1.106710000	-1.587456000
C	-2.448773000	0.431276000	-1.236481000
H	-2.488996000	0.963283000	-2.192639000
H	-3.454332000	0.427989000	-0.803705000
O	0.400287000	1.275751000	-2.625906000
Cl	-5.560696000	-0.893631000	1.017935000
O	-6.671185000	-0.996688000	2.010203000
O	-4.311331000	-1.489562000	1.594047000
O	-5.313151000	0.548906000	0.687793000
O	-5.932884000	-1.630357000	-0.233278000
O	5.916811000	-2.080619000	1.286745000
C	6.401865000	-2.674116000	2.492256000
H	5.814752000	-3.559200000	2.760543000
H	7.431130000	-2.967246000	2.286635000
H	6.382701000	-1.957256000	3.320428000

^{3}4 [Fe(IV)ODpaqNO$_2$]ClO$_4$

Zero-point correction= 0.419980 (Hartree/Particle)
Thermal correction to Energy= 0.452739
Thermal correction to Enthalpy= 0.453683
Thermal correction to Gibbs Free Energy= 0.350566
Sum of electronic and zero-point Energies= -2401.059279
Sum of electronic and thermal Energies= -2401.026520
Sum of electronic and thermal Enthalpies= -2401.025576
Sum of electronic and thermal Free Energies= -2401.128693

Fe	0.218691000	0.783682000	-0.976418000
N	0.537998000	0.029685000	0.826035000
C	1.780281000	-0.496532000	1.053100000
C	2.652936000	-0.415545000	-0.090368000
C	2.276628000	-1.077931000	2.222163000
C	3.990701000	-0.904777000	-0.080211000
C	3.586462000	-1.560163000	2.250734000
H	1.642247000	-1.150772000	3.093286000
C	2.820608000	0.309613000	-2.312049000
C	4.731405000	-0.739391000	-1.283551000
C	4.434708000	-1.492711000	1.151711000
H	3.967838000	-2.011178000	3.157622000
C	4.148964000	-0.140069000	-2.380476000
H	2.320442000	0.785090000	-3.147874000
H	5.751374000	-1.087485000	-1.328501000
H	4.706216000	-0.009850000	-3.300773000
N	2.106458000	0.173933000	-1.201338000
C	-0.479276000	0.096047000	1.730084000
O	-0.477104000	-0.295652000	2.895866000
C	-1.739407000	0.743313000	1.150215000
H	-2.561099000	0.025011000	1.227737000
N	-1.610211000	1.209357000	-0.282842000
C	-0.442586000	3.330227000	0.031487000
C	1.877489000	3.104086000	0.056668000
C	-0.359924000	4.598589000	0.598008000
C	2.034006000	4.371060000	0.608558000
H	2.731287000	2.478160000	-0.168626000
C	0.897226000	5.128527000	0.886922000
H	-1.266372000	5.155798000	0.805929000
H	3.029476000	4.744652000	0.817485000
H	0.985872000	6.116093000	1.326932000
N	0.665778000	2.598455000	-0.224273000
C	-1.739433000	2.691870000	-0.393996000
H	-1.916444000	2.930212000	-1.446481000
H	-2.588262000	3.059904000	0.189205000
H	-2.002180000	1.594399000	1.783160000
C	-0.035499000	-2.118515000	-1.799815000
C	-1.990202000	-0.891588000	-1.460285000
C	-0.762566000	-3.267556000	-2.090913000
H	1.046809000	-2.118229000	-1.811605000
C	-2.779870000	-2.009364000	-1.715182000
C	-2.154833000	-3.212910000	-2.040805000
H	-0.238968000	-4.183130000	-2.339787000
H	-3.859281000	-1.934747000	-1.637684000
H	-2.748226000	-4.098006000	-2.244927000
N	-0.638760000	-0.958989000	-1.491969000
C	-2.553122000	0.477859000	-1.183733000
H	-2.597411000	1.029792000	-2.127090000
H	-3.557113000	0.439325000	-0.751546000
O	0.022955000	1.397099000	-2.488723000
Cl	-5.611397000	-1.035463000	0.929463000
O	-6.716046000	-1.210091000	1.916778000
O	-4.321898000	-1.523796000	1.520507000
O	-5.471118000	0.417481000	0.580473000
O	-5.915259000	-1.815814000	-0.313265000
N	5.764001000	-2.047155000	1.327642000
O	6.091188000	-2.437798000	2.455294000
O	6.526850000	-2.121395000	0.353965000

^{5}4 [Fe(IV)ODpaqNO$_2$]ClO$_4$

Zero-point correction= 0.417957 (Hartree/Particle)
Thermal correction to Energy= 0.451707
Thermal correction to Enthalpy= 0.452652
Thermal correction to Gibbs Free Energy= 0.345534
Sum of electronic and zero-point Energies= -2401.048826
Sum of electronic and thermal Energies= -2401.015075
Sum of electronic and thermal Enthalpies= -2401.014131
Sum of electronic and thermal Free Energies= -2401.121248

Fe	0.325966000	0.762633000	-1.104720000
N	0.607771000	0.018266000	0.711851000
C	1.859101000	-0.482240000	0.995086000
C	2.791773000	-0.389537000	-0.097614000
C	2.310922000	-1.050389000	2.188397000
C	4.136011000	-0.852956000	-0.016151000
C	3.628272000	-1.507582000	2.288501000
H	1.638392000	-1.136009000	3.027813000
C	3.068598000	0.333935000	-2.312092000
C	4.937193000	-0.670881000	-1.177088000
C	4.529295000	-1.429445000	1.236586000
H	3.967109000	-1.948223000	3.217180000
C	4.406637000	-0.084892000	-2.308600000
H	2.604113000	0.796443000	-3.175978000
H	5.965650000	-0.997005000	-1.163970000
H	5.013113000	0.056202000	-3.195404000
N	2.299542000	0.184525000	-1.238547000
C	-0.431650000	0.044627000	1.607924000
O	-0.409936000	-0.362929000	2.766893000
C	-1.728380000	0.650424000	1.066391000
H	-2.515820000	-0.102299000	1.173888000
N	-1.677210000	1.138810000	-0.348564000
C	-0.663614000	3.352418000	0.015342000
C	1.662214000	3.359996000	0.082625000
C	-0.720196000	4.612894000	0.607369000
C	1.685797000	4.623777000	0.663107000
H	2.577101000	2.820680000	-0.137525000

C	0.472436000	5.258385000	0.931134000
H	-1.681320000	5.073789000	0.807102000
H	2.634330000	5.090033000	0.902835000
H	0.454277000	6.240602000	1.391616000
N	0.510818000	2.746079000	-0.231790000
C	-1.893393000	2.603913000	-0.442908000
H	-2.073502000	2.847662000	-1.494608000
H	-2.776706000	2.910657000	0.127412000
H	-1.998656000	1.476123000	1.730641000
C	-0.128566000	-2.234673000	-1.938587000
C	-2.051875000	-0.991935000	-1.519454000
C	-0.872449000	-3.383736000	-2.184902000
H	0.954302000	-2.237011000	-1.998832000
C	-2.863023000	-2.106702000	-1.726962000
C	-2.261477000	-3.317164000	-2.069984000
H	-0.368405000	-4.306509000	-2.447889000
H	-3.937461000	-2.023111000	-1.601435000
H	-2.869641000	-4.200067000	-2.237744000
N	-0.712087000	-1.070388000	-1.613992000
C	-2.604867000	0.383653000	-1.232514000
H	-2.674065000	0.927979000	-2.179864000
H	-3.605751000	0.332363000	-0.792783000
O	0.184092000	1.362229000	-2.621061000
Cl	-5.598796000	-1.065357000	1.043622000
O	-6.686099000	-1.232518000	2.052011000
O	-4.318531000	-1.632067000	1.581568000
O	-5.405228000	0.393085000	0.747680000
O	-5.967530000	-1.781359000	-0.220278000
N	5.858529000	-1.964006000	1.479502000
O	6.150773000	-2.298834000	2.633190000
O	6.649118000	-2.078110000	0.533228000

^{3}5 [Fe(IV)ODpaqSO$_2$CF$_3$]ClO$_4$

Zero-point correction= 0.431861 (Hartree/Particle)
Thermal correction to Energy= 0.469295
Thermal correction to Enthalpy= 0.470239
Thermal correction to Gibbs Free Energy= 0.355932
Sum of electronic and zero-point Energies= -3082.127891
Sum of electronic and thermal Energies= -3082.090458
Sum of electronic and thermal Enthalpies= -3082.089514
Sum of electronic and thermal Free Energies= -3082.203821

Fe	0.791582000	1.129094000	0.940325000
N	0.226253000	0.399728000	-0.812904000
C	-1.110849000	0.140684000	-0.961723000
C	-1.884416000	0.473849000	0.205912000
C	-1.776370000	-0.382377000	-2.071522000
C	-3.293144000	0.294911000	0.268213000
C	-3.163995000	-0.571109000	-2.024724000
H	-1.215412000	-0.637412000	-2.958745000
C	-1.795610000	1.316282000	2.388125000
C	-3.932311000	0.669457000	1.481167000
C	-3.917190000	-0.246399000	-0.903427000
H	-3.668924000	-0.973569000	-2.895609000
C	-3.187604000	1.172443000	2.525922000
H	-1.169767000	1.705624000	3.182897000
H	-5.004199000	0.565915000	1.582196000
H	-3.660597000	1.461401000	3.456934000
N	-1.174277000	0.978335000	1.264930000
C	1.190096000	0.177538000	-1.747514000
O	1.052970000	-0.293975000	-2.875586000
C	2.578130000	0.612943000	-1.271377000
H	3.281112000	-0.213851000	-1.400345000
N	2.634233000	1.103204000	0.158343000
C	1.980636000	3.431322000	-0.163587000
C	-0.330087000	3.738239000	-0.124481000
C	2.171086000	4.677901000	-0.751847000
C	-0.211478000	4.999600000	-0.698208000
H	-1.296632000	3.324915000	0.133329000
C	1.058962000	5.475927000	-1.018517000
H	3.173739000	5.011495000	-0.993877000
H	-1.102147000	5.585861000	-0.890998000
H	1.183585000	6.452109000	-1.474907000
N	0.743241000	2.975379000	0.137389000
C	3.110770000	2.516113000	0.232048000
H	3.380245000	2.720839000	1.271774000
H	3.997477000	2.667544000	-0.390398000
H	2.914187000	1.414283000	-1.934646000
C	0.407125000	-1.718294000	1.892364000
C	2.570603000	-1.001232000	1.400069000
C	0.861318000	-2.993044000	2.211686000
H	-0.642669000	-1.462532000	1.953426000
C	3.092311000	-2.260487000	1.684953000
C	2.223653000	-3.268996000	2.100732000
H	0.153215000	-3.748315000	2.531842000
H	4.157029000	-2.431344000	1.567241000
H	2.605293000	-4.258530000	2.329683000
N	1.245392000	-0.746765000	1.495762000
C	3.427964000	0.179738000	1.026428000
H	3.680930000	0.725588000	1.939986000
H	4.353657000	-0.130750000	0.535934000
O	1.193289000	1.726067000	2.418096000
Cl	6.260416000	-2.096788000	-0.890684000
O	7.670722000	-2.093533000	-1.379941000
O	5.491163000	-1.008314000	-1.583802000
O	6.246753000	-1.840608000	0.589939000
O	5.622286000	-3.417028000	-1.173435000
S	-5.662427000	-0.547654000	-1.014450000
O	-6.422579000	0.453375000	-0.249874000
O	-6.018249000	-0.846943000	-2.407860000
C	-5.900161000	-2.166607000	-0.090430000
F	-7.195991000	-2.473981000	-0.106722000
F	-5.487877000	-2.032057000	1.173848000
F	-5.200674000	-3.131716000	-0.685774000

^{5}5 [Fe(IV)ODpaqSO$_2$CF$_3$]ClO$_4$

Zero-point correction= 0.429799 (Hartree/Particle)
Thermal correction to Energy= 0.468170
Thermal correction to Enthalpy= 0.469114
Thermal correction to Gibbs Free Energy= 0.351666
Sum of electronic and zero-point Energies= -3082.117769
Sum of electronic and thermal Energies= -3082.079398
Sum of electronic and thermal Enthalpies= -3082.078454
Sum of electronic and thermal Free Energies= -3082.195902

Fe	0.751057000	1.144404000	1.102489000
N	0.222396000	0.365759000	-0.644088000
C	-1.121780000	0.132265000	-0.844430000
C	-1.951351000	0.505842000	0.270184000
C	-1.745507000	-0.406345000	-1.971065000
C	-3.364284000	0.351035000	0.265524000
C	-3.138358000	-0.572392000	-1.990929000
H	-1.150908000	-0.692406000	-2.825036000
C	-1.964714000	1.411008000	2.432270000
C	-4.056828000	0.768931000	1.433695000
C	-3.941314000	-0.209628000	-0.919806000
H	-3.602616000	-0.987716000	-2.878212000
C	-3.361686000	1.291758000	2.504379000
H	-1.373636000	1.815492000	3.246506000
H	-5.134166000	0.683736000	1.481257000
H	-3.879409000	1.613136000	3.400168000
N	-1.294065000	1.029841000	1.350180000
C	1.194943000	0.097469000	-1.572975000
O	1.026300000	-0.375878000	-2.694657000
C	2.618617000	0.438403000	-1.126138000
H	3.219077000	-0.473124000	-1.207524000

N	2.747526000	1.014787000	0.250330000
C	2.229010000	3.371332000	-0.236208000
C	-0.037533000	3.896282000	-0.218708000
C	2.531978000	4.546201000	-0.921922000
C	0.188878000	5.093534000	-0.889557000
H	-1.036477000	3.591974000	0.074063000
C	1.496730000	5.420934000	-1.248756000
H	3.559488000	4.765158000	-1.190738000
H	-0.644187000	5.744489000	-1.127903000
H	1.707763000	6.342237000	-1.781497000
N	0.964056000	3.060613000	0.097578000
C	3.285551000	2.397509000	0.230643000
H	3.568445000	2.659685000	1.254920000
H	4.184237000	2.463603000	-0.391972000
H	3.024553000	1.141914000	-1.858531000
C	0.572254000	-1.821056000	2.128244000
C	2.700006000	-1.067655000	1.558265000
C	1.054965000	-3.090366000	2.428568000
H	-0.480293000	-1.577794000	2.224248000
C	3.253915000	-2.320923000	1.815472000
C	2.417192000	-3.343002000	2.262648000
H	0.372861000	-3.859548000	2.771785000
H	4.312874000	-2.488039000	1.648488000
H	2.822814000	-4.327691000	2.470945000
N	1.382336000	-0.838506000	1.704243000
C	3.528209000	0.128838000	1.154584000
H	3.762579000	0.703029000	2.056817000
H	4.469970000	-0.173488000	0.686055000
O	1.098752000	1.790392000	2.565725000
Cl	6.005399000	-2.139341000	-1.095974000
O	6.970249000	-2.608308000	-2.133371000
O	4.602060000	-2.408673000	-1.551459000
O	6.177445000	-0.664635000	-0.877815000
O	6.257408000	-2.862806000	0.192188000
S	-5.686940000	-0.477807000	-1.114406000
O	-6.460635000	0.559478000	-0.414903000
O	-5.975304000	-0.804230000	-2.516886000
C	-6.006510000	-2.067028000	-0.163771000
F	-7.306968000	-2.344109000	-0.235392000
F	-5.651669000	-1.908774000	1.114961000
F	-5.302634000	-3.061929000	-0.701351000

^{3}6 [Fe(IV)ON4PYH](ClO$_4$)$_2$

Zero-point correction= 0.441657 (Hartree/Particle)
Thermal correction to Energy= 0.477178
Thermal correction to Enthalpy= 0.478122
Thermal correction to Gibbs Free Energy= 0.366609
Sum of electronic and zero-point Energies= -2882.637657
Sum of electronic and thermal Energies= -2882.602135
Sum of electronic and thermal Enthalpies= -2882.601191
Sum of electronic and thermal Free Energies= -2882.712705

Fe	-0.593420000	-1.950277000	0.132451000
N	-0.064316000	0.039302000	-0.042733000
N	0.896229000	-2.154440000	-1.181282000
N	0.828546000	-1.893368000	1.530860000
N	-1.837355000	-1.513579000	-1.342770000
N	-1.929419000	-1.239328000	1.410646000
O	-0.988805000	-3.524463000	0.276677000
C	1.074961000	-3.136934000	-2.075078000
C	2.162326000	-3.124665000	-2.945374000
C	3.070028000	-2.068193000	-2.879711000
C	2.878115000	-1.045277000	-1.945904000
C	1.772435000	-1.126413000	-1.110080000
C	1.433445000	-0.154414000	0.008234000
C	1.717911000	-0.899855000	1.302807000
C	2.789613000	-0.665430000	2.153769000
C	2.931975000	-1.493608000	3.271634000
C	2.010590000	-2.515384000	3.498355000
C	0.959665000	-2.689027000	2.601082000
C	-2.793189000	-2.348563000	-1.793887000
C	-3.672253000	-1.970501000	-2.798966000
C	-3.563357000	-0.687750000	-3.339619000
C	-2.575907000	0.170858000	-2.864405000
C	-1.713117000	-0.274455000	-1.864443000
C	-0.573793000	0.571223000	-1.348240000
C	-0.623140000	0.790582000	1.126283000
C	-1.839662000	0.083709000	1.671421000
C	-2.797109000	0.728947000	2.451368000
C	-3.840360000	-0.018298000	2.993723000
C	-3.906960000	-1.388902000	2.737889000
C	-2.936838000	-1.966035000	1.929435000
H	0.337893000	-3.931281000	-2.072654000
H	2.287916000	-3.933154000	-3.655773000
H	3.922965000	-2.037059000	-3.549347000
H	3.567622000	-0.210642000	-1.860010000
H	1.992798000	0.783153000	-0.066575000
H	3.491545000	0.135386000	1.941197000
H	3.757229000	-1.339041000	3.958634000
H	2.097508000	-3.174885000	4.353655000
H	0.214247000	-3.466869000	2.717279000
H	-2.826878000	-3.324385000	-1.324726000
H	-4.427955000	-2.667723000	-3.140905000
H	-4.243229000	-0.358788000	-4.118359000
H	-2.471718000	1.177913000	-3.249907000
H	-2.729619000	1.800200000	2.604119000
H	-4.596647000	0.464630000	3.603518000
H	-4.702144000	-2.003701000	3.142724000
H	-2.940339000	-3.018792000	1.673834000
H	-0.886635000	1.612053000	-1.237682000
H	0.238180000	0.554622000	-2.080732000
H	-0.847195000	1.822353000	0.846376000
H	0.134243000	0.831789000	1.914216000
Cl	-2.848368000	3.796422000	-0.141218000
O	-3.253935000	3.992626000	1.286340000
O	-1.345916000	3.807732000	-0.233524000
O	-3.406797000	4.893815000	-0.983208000
O	-3.351936000	2.471809000	-0.628566000
Cl	4.783069000	2.288204000	-0.132564000
O	5.136836000	1.421462000	-1.303490000
O	5.526706000	3.577613000	-0.219203000
O	5.142778000	1.582373000	1.140025000
O	3.306216000	2.558654000	-0.146691000

^{5}6 [Fe(IV)ON4PYH](ClO$_4$)$_2$

Zero-point correction= 0.439491 (Hartree/Particle)
Thermal correction to Energy= 0.476058
Thermal correction to Enthalpy= 0.477002
Thermal correction to Gibbs Free Energy= 0.360929
Sum of electronic and zero-point Energies= -2882.621060
Sum of electronic and thermal Energies= -2882.584492
Sum of electronic and thermal Enthalpies= -2882.583548
Sum of electronic and thermal Free Energies= -2882.699621

Fe	0.829384000	-2.102111000	0.090846000
N	0.142626000	-0.134880000	0.006008000
N	-0.765393000	-2.172060000	1.493918000
N	-0.772313000	-2.270193000	-1.347057000
N	2.135353000	-1.246568000	1.506248000
N	2.091450000	-1.416574000	-1.418929000
O	1.361349000	-3.635903000	0.163019000
C	-0.940741000	-3.013350000	2.522778000
C	-2.045554000	-2.906214000	3.363918000
C	-2.979082000	-1.898704000	3.122469000
C	-2.794011000	-1.021767000	2.048716000
C	-1.667449000	-1.194294000	1.254143000

C	-1.352060000	-0.379246000	0.008728000
C	-1.663988000	-1.269133000	-1.185310000
C	-2.777742000	-1.132440000	-2.005032000
C	-2.960638000	-2.074504000	-3.022492000
C	-2.037392000	-3.106921000	-3.184706000
C	-0.944956000	-3.172473000	-2.322563000
C	3.230189000	-1.845347000	2.008348000
C	4.159796000	-1.145605000	2.767562000
C	3.955781000	0.218648000	2.983854000
C	2.821933000	0.837546000	2.457621000
C	1.915472000	0.066714000	1.733491000
C	0.607523000	0.615944000	1.223077000
C	0.628882000	0.525059000	-1.256691000
C	1.875236000	-0.136675000	-1.790147000
C	2.736293000	0.510945000	-2.674135000
C	3.817397000	-0.195287000	-3.198183000
C	4.019689000	-1.525148000	-2.821762000
C	3.137911000	-2.101212000	-1.917634000
H	-0.180847000	-3.774710000	2.659877000
H	-2.163859000	-3.600691000	4.187287000
H	-3.846958000	-1.791942000	3.764757000
H	-3.504817000	-0.230039000	1.831194000
H	-1.920717000	0.555599000	-0.019168000
H	-3.479375000	-0.318045000	-1.849785000
H	-3.818192000	-1.998501000	-3.682773000
H	-2.154159000	-3.851483000	-3.963394000
H	-0.192851000	-3.949843000	-2.402142000
H	3.344672000	-2.898580000	1.777389000
H	5.029147000	-1.657569000	3.163034000
H	4.676869000	0.797823000	3.551217000
H	2.647102000	1.900666000	2.580165000
H	2.563864000	1.550714000	-2.924744000
H	4.499639000	0.289186000	-3.888841000
H	4.850113000	-2.103499000	-3.209178000
H	3.248837000	-3.120704000	-1.566013000
H	0.673120000	1.684584000	1.004212000
H	-0.141346000	0.494605000	2.010502000
H	0.795441000	1.590696000	-1.082183000
H	-0.154635000	0.443647000	-2.015274000
Cl	2.143746000	4.196597000	-0.069092000
O	2.193286000	5.616481000	-0.523401000
O	0.710895000	3.736664000	-0.027982000
O	2.735430000	4.080519000	1.301440000
O	2.908648000	3.329613000	-1.021144000
Cl	-4.744767000	2.063722000	-0.053654000
O	-3.264047000	2.304630000	0.011053000
O	-5.461961000	3.370954000	-0.054505000
O	-5.165625000	1.257180000	1.137687000
O	-5.067309000	1.309895000	-1.308554000

Cartesian coordinates of the Oxidant:

EB

Zero-point correction= 0.156843 (Hartree/Particle)
Thermal correction to Energy= 0.164182
Thermal correction to Enthalpy= 0.165126
Thermal correction to Gibbs Free Energy= 0.124587
Sum of electronic and zero-point Energies= -310.740718
Sum of electronic and thermal Energies= -310.733379
Sum of electronic and thermal Enthalpies= -310.732435
Sum of electronic and thermal Free Energies= -310.772975

C	0.435602000	-0.000023000	-0.327560000
C	-0.270068000	-1.203512000	-0.184119000
C	-1.638114000	-1.206523000	0.095786000
C	-2.327546000	0.000024000	0.237287000
C	-1.638041000	1.206580000	0.095660000
C	-0.270031000	1.203532000	-0.184186000
H	0.258103000	-2.147434000	-0.297425000
H	-2.165924000	-2.150604000	0.198778000
H	-3.392347000	0.000121000	0.451502000
H	-2.165944000	2.150612000	0.198547000
H	0.258349000	2.147321000	-0.297487000
C	1.927029000	-0.000167000	-0.592033000
H	2.191512000	-0.879546000	-1.190773000
H	2.191803000	0.878753000	-1.191316000
C	2.763862000	0.000109000	0.699570000
H	3.834545000	0.000347000	0.470950000
H	2.546669000	0.884615000	1.307259000
H	2.547070000	-0.884305000	1.307533000

Cartesian coordinates of the stationary points for the reactions with substrates:

1+EB

^{3}TS

Zero-point correction= 0.568834 (Hartree/Particle)
Thermal correction to Energy= 0.607851
Thermal correction to Enthalpy= 0.608796
Thermal correction to Gibbs Free Energy= 0.491298
Sum of electronic and zero-point Energies= -2507.279724
Sum of electronic and thermal Energies= -2507.240706
Sum of electronic and thermal Enthalpies= -2507.239762
Sum of electronic and thermal Free Energies= -2507.357260

Fe	0.255601000	-0.011388000	0.020936000
O	0.813555000	-1.436950000	0.863336000
N	-0.441348000	1.628335000	-0.836277000
C	0.369762000	2.748420000	-0.739857000
C	1.566737000	2.508384000	0.004300000
C	0.162974000	4.026533000	-1.254433000
C	2.524983000	3.535086000	0.230282000
C	1.120671000	5.043428000	-1.033963000
H	-0.736642000	4.226568000	-1.819451000
C	2.821138000	0.950674000	1.215876000
C	3.670924000	3.193445000	0.993743000
C	2.276473000	4.822450000	-0.312017000
H	0.930394000	6.029089000	-1.448666000
C	3.815432000	1.913793000	1.484838000
H	2.898320000	-0.065171000	1.583523000
H	4.426134000	3.949774000	1.186639000
H	2.998170000	5.616598000	-0.149788000
H	4.680440000	1.625963000	2.070687000
N	1.741679000	1.237637000	0.496675000
C	-1.622127000	1.565758000	-1.484936000
O	-2.209166000	2.467972000	-2.095551000
C	-2.258140000	0.174564000	-1.418545000
H	-3.235987000	0.262262000	-0.936248000
N	-1.428914000	-0.856344000	-0.689894000
C	0.219243000	-1.453417000	-2.397161000
C	2.124901000	-0.115784000	-2.369750000
C	0.510083000	-1.901459000	-3.683079000
C	2.483201000	-0.528829000	-3.649194000
H	2.728561000	0.592206000	-1.816287000
C	1.661771000	-1.436293000	-4.316948000
H	-0.158368000	-2.599711000	-4.174129000
H	3.384641000	-0.137640000	-4.106313000
H	1.908558000	-1.771554000	-5.318807000
N	1.020628000	-0.571688000	-1.755569000
C	-0.965028000	-1.941867000	-1.600185000
H	-0.643039000	-2.779326000	-0.975716000
H	-1.773603000	-2.290747000	-2.249460000
H	-2.441350000	-0.165486000	-2.441231000
C	-0.692732000	1.264305000	2.600659000
C	-2.045942000	-0.354953000	1.616362000

C	-1.614165000	1.470309000	3.622700000
H	0.235454000	1.820391000	2.556178000
C	-3.024847000	-0.184508000	2.592311000
C	-2.800772000	0.738255000	3.614012000
H	-1.402516000	2.197851000	4.397705000
H	-3.948294000	-0.750915000	2.534137000
H	-3.546916000	0.888511000	4.387437000
N	-0.904817000	0.370626000	1.621958000
C	-2.144604000	-1.377839000	0.513300000
H	-1.621838000	-2.281559000	0.836917000
H	-3.181131000	-1.632893000	0.274114000
Cl	-6.147920000	-0.825864000	0.134750000
O	-7.542307000	-0.774809000	-0.395218000
O	-5.493260000	0.512340000	-0.034916000
O	-5.361061000	-1.858409000	-0.617744000
O	-6.174397000	-1.186808000	1.589234000
C	3.980638000	-2.482351000	0.603791000
C	4.378673000	-2.564129000	1.954937000
C	5.590482000	-2.020857000	2.380106000
C	6.437905000	-1.381720000	1.469054000
C	6.060340000	-1.291328000	0.125510000
C	4.847639000	-1.831054000	-0.298707000
H	3.735752000	-3.056599000	2.677816000
H	5.876580000	-2.098480000	3.425215000
H	7.382719000	-0.962476000	1.801967000
H	6.713903000	-0.803507000	-0.592099000
H	4.564151000	-1.761538000	-1.345585000
C	2.681197000	-3.011757000	0.131418000
H	1.782190000	-2.125197000	0.425603000
H	2.629092000	-3.043941000	-0.960608000
C	2.124784000	-4.273361000	0.773141000
H	1.152334000	-4.527435000	0.341948000
H	2.796398000	-5.126218000	0.609644000
H	1.987850000	-4.163085000	1.852994000

^{3}IH

Zero-point correction= 0.571934 (Hartree/Particle)
Thermal correction to Energy= 0.612361
Thermal correction to Enthalpy= 0.613305
Thermal correction to Gibbs Free Energy= 0.489888
Sum of electronic and zero-point Energies= -2507.307697
Sum of electronic and thermal Energies= -2507.267271
Sum of electronic and thermal Enthalpies= -2507.266327
Sum of electronic and thermal Free Energies= -2507.389744

Fe	-0.238503000	0.104532000	-0.031224000
O	-0.844754000	-1.409035000	-0.863903000
N	0.455135000	1.687054000	0.840815000
C	-0.353667000	2.813978000	0.772677000
C	-1.541411000	2.606885000	0.002328000
C	-0.144761000	4.070736000	1.333698000
C	-2.487611000	3.649070000	-0.200972000
C	-1.091286000	5.102989000	1.134578000
H	0.748681000	4.244515000	1.917043000
C	-2.792427000	1.102550000	-1.274995000
C	-3.625879000	3.343678000	-0.990783000
C	-2.237289000	4.915401000	0.388814000
H	-0.899583000	6.072241000	1.585482000
C	-3.775380000	2.082035000	-1.525274000
H	-2.878858000	0.101292000	-1.682237000
H	-4.371897000	4.112741000	-1.168254000
H	-2.950614000	5.720309000	0.243320000
H	-4.635410000	1.820851000	-2.130419000
N	-1.719198000	1.353954000	-0.534411000
C	1.633673000	1.591328000	1.497544000
O	2.224110000	2.474184000	2.129475000
C	2.247901000	0.189932000	1.412012000
H	3.220701000	0.268523000	0.917594000
N	1.393784000	-0.820444000	0.687274000
C	-0.314436000	-1.364437000	2.365674000
C	-2.201375000	0.001160000	2.299742000
C	-0.654510000	-1.828069000	3.633926000
C	-2.609448000	-0.430980000	3.557103000
H	-2.776444000	0.727611000	1.740039000
C	-1.820681000	-1.358272000	4.236841000
H	-0.013183000	-2.544910000	4.134392000
H	-3.522567000	-0.038402000	3.989069000
H	-2.105251000	-1.707337000	5.223926000
N	-1.080902000	-0.456725000	1.716091000
C	0.876543000	-1.881055000	1.596394000
H	0.537588000	-2.709811000	0.969497000
H	1.658871000	-2.251095000	2.266080000
H	2.441877000	-0.157845000	2.430282000
C	0.789230000	1.349282000	-2.575881000
C	2.051833000	-0.353321000	-1.608106000
C	1.713962000	1.506049000	-3.603028000
H	-0.103925000	1.959132000	-2.520241000
C	3.031752000	-0.235379000	-2.590652000
C	2.854848000	0.704040000	-3.606315000
H	1.541292000	2.249713000	-4.372295000
H	3.921831000	-0.853271000	-2.540127000
H	3.603331000	0.814568000	-4.384181000
N	0.955306000	0.437630000	-1.604280000
C	2.097001000	-1.378450000	-0.504397000
H	1.535207000	-2.256588000	-0.831590000
H	3.119631000	-1.678830000	-0.257398000
Cl	6.111149000	-0.932603000	-0.099824000
O	7.501534000	-0.904806000	0.442761000
O	5.491156000	0.426491000	0.029840000
O	5.290442000	-1.924718000	0.670537000
O	6.141701000	-1.330804000	-1.544302000
C	-4.157292000	-2.894307000	-0.479977000
C	-4.079297000	-2.815971000	-1.903701000
C	-4.922066000	-1.975668000	-2.621763000
C	-5.872631000	-1.181912000	-1.963305000
C	-5.965905000	-1.237141000	-0.563196000
C	-5.129721000	-2.070296000	0.164576000
H	-3.354004000	-3.425692000	-2.432973000
H	-4.845371000	-1.939155000	-3.705016000
H	-6.533033000	-0.533878000	-2.531405000
H	-6.699652000	-0.625584000	-0.045478000
H	-5.209636000	-2.109066000	1.247943000
C	-3.321110000	-3.745334000	0.286107000
H	-1.757917000	-1.595318000	-0.602558000
H	-3.448840000	-3.724663000	1.365651000
C	-2.269222000	-4.646880000	-0.280651000
H	-1.862405000	-5.306924000	0.489280000
H	-2.655758000	-5.276273000	-1.093125000
H	-1.431534000	-4.071050000	-0.701252000

^{5}TS

Zero-point correction= 0.565533 (Hartree/Particle)
Thermal correction to Energy= 0.606077
Thermal correction to Enthalpy= 0.607021
Thermal correction to Gibbs Free Energy= 0.481180
Sum of electronic and zero-point Energies= -2507.273648
Sum of electronic and thermal Energies= -2507.233104
Sum of electronic and thermal Enthalpies= -2507.232160
Sum of electronic and thermal Free Energies= -2507.358001

Fe	-1.111903000	-0.331698000	-0.197343000
O	-0.896731000	-1.878363000	-0.917929000
N	-1.532443000	1.527859000	0.611682000
C	-2.805684000	2.035705000	0.383761000
C	-3.648786000	1.170276000	-0.389226000
C	-3.345376000	3.251263000	0.804142000

C	-4.987226000	1.530237000	-0.718033000
C	-4.674695000	3.604954000	0.474506000
H	-2.729539000	3.920035000	1.387871000
C	-3.844038000	-0.871018000	-1.519290000
C	-5.738177000	0.604787000	-1.484601000
C	-5.491231000	2.777867000	-0.267222000
H	-5.054426000	4.561306000	0.822395000
C	-5.173041000	-0.589670000	-1.884064000
H	-3.352847000	-1.794290000	-1.807436000
H	-6.762415000	0.847791000	-1.752579000
H	-6.509710000	3.061575000	-0.512531000
H	-5.730198000	-1.311085000	-2.470425000
N	-3.114089000	-0.022083000	-0.800551000
C	-0.578868000	2.172496000	1.324932000
O	-0.658430000	3.275592000	1.881780000
C	0.757883000	1.424283000	1.447853000
H	1.540958000	2.084632000	1.062444000
N	0.845395000	0.090223000	0.774431000
C	-0.191557000	-1.305923000	2.519387000
C	-2.510977000	-1.446456000	2.435001000
C	-0.178086000	-1.758754000	3.838173000
C	-2.577442000	-1.915501000	3.743265000
H	-3.406430000	-1.296789000	1.840618000
C	-1.388142000	-2.072159000	4.456019000
H	0.764305000	-1.860976000	4.365109000
H	-3.539030000	-2.143396000	4.188611000
H	-1.402504000	-2.426992000	5.481369000
N	-1.343719000	-1.152843000	1.841517000
C	1.070572000	-1.010263000	1.742026000
H	1.341301000	-1.907472000	1.175179000
H	1.901656000	-0.783210000	2.419881000
H	0.958021000	1.305902000	2.517077000
C	-0.513362000	1.305423000	-2.844758000
C	1.340775000	0.836266000	-1.520081000
C	0.257360000	2.032290000	-3.746532000
H	-1.582928000	1.183759000	-2.981674000
C	2.175371000	1.567912000	-2.365033000
C	1.623502000	2.168098000	-3.496621000
H	-0.208589000	2.486777000	-4.613362000
H	3.228048000	1.675297000	-2.124292000
H	2.251235000	2.742515000	-4.170330000
N	0.021121000	0.722104000	-1.760793000
C	1.854524000	0.081127000	-0.316299000
H	2.014671000	-0.961336000	-0.612590000
H	2.812029000	0.486110000	0.028259000
Cl	4.740726000	2.878260000	0.499652000
O	5.797162000	3.707182000	1.152541000
O	3.444581000	3.630442000	0.487309000
O	4.564046000	1.598282000	1.261658000
O	5.148073000	2.563308000	-0.908496000
C	1.324982000	-4.265379000	-1.163105000
C	1.641878000	-4.790221000	0.107227000
C	2.959810000	-4.816489000	0.561916000
C	3.992953000	-4.313210000	-0.235160000
C	3.697087000	-3.783950000	-1.496228000
C	2.381104000	-3.758814000	-1.951626000
H	0.854366000	-5.187906000	0.739140000
H	3.182521000	-5.232729000	1.540131000
H	5.018272000	-4.334897000	0.121597000
H	4.493618000	-3.396282000	-2.124583000
H	2.157391000	-3.351430000	-2.934381000
C	-0.065328000	-4.176117000	-1.662989000
H	-0.459088000	-3.042763000	-1.307550000
H	-0.096845000	-4.073878000	-2.752654000
C	-1.117332000	-5.140152000	-1.139902000
H	-2.091617000	-4.916673000	-1.583414000
H	-0.862355000	-6.176541000	-1.395934000
H	-1.226951000	-5.085114000	-0.052658000

^{5}IH

Zero-point correction= 0.567938 (Hartree/Particle)
Thermal correction to Energy= 0.609952
Thermal correction to Enthalpy= 0.610896
Thermal correction to Gibbs Free Energy= 0.481901
Sum of electronic and zero-point Energies= -2507.298722
Sum of electronic and thermal Energies= -2507.256708
Sum of electronic and thermal Enthalpies= -2507.255764
Sum of electronic and thermal Free Energies= -2507.384759

Fe	0.899791000	-0.305463000	-0.487057000
O	1.355927000	1.020623000	-1.673784000
N	0.581810000	-1.858382000	0.857603000
C	1.533886000	-2.871757000	0.905697000
C	2.611637000	-2.709090000	-0.027868000
C	1.560653000	-3.998899000	1.726850000
C	3.669225000	-3.658850000	-0.119014000
C	2.612922000	-4.939681000	1.632211000
H	0.761689000	-4.144040000	2.439059000
C	3.553589000	-1.388875000	-1.712307000
C	4.686623000	-3.406718000	-1.072586000
C	3.650505000	-4.790657000	0.737119000
H	2.592435000	-5.803127000	2.290787000
C	4.632104000	-2.278812000	-1.866825000
H	3.464528000	-0.486996000	-2.309066000
H	5.508108000	-4.110907000	-1.168928000
H	4.451819000	-5.520079000	0.674881000
H	5.400330000	-2.066998000	-2.601466000
N	2.582889000	-1.600417000	-0.827451000
C	-0.510036000	-1.820830000	1.663541000
O	-0.833738000	-2.626775000	2.544721000
C	-1.464746000	-0.643942000	1.416334000
H	-2.414380000	-1.067701000	1.074676000
N	-1.006609000	0.397739000	0.447061000
C	0.603002000	1.621650000	1.864849000
C	2.788621000	0.828291000	1.842261000
C	0.829536000	2.311654000	3.055182000
C	3.095891000	1.502629000	3.020135000
H	3.525777000	0.217990000	1.330660000
C	2.095183000	2.253902000	3.637742000
H	0.027693000	2.881637000	3.511537000
H	4.091437000	1.429360000	3.442460000
H	2.295334000	2.783178000	4.563643000
N	1.570947000	0.891439000	1.279938000
C	-0.706168000	1.688893000	1.114585000
H	-0.613297000	2.457241000	0.340065000
H	-1.522879000	1.989737000	1.780669000
H	-1.670820000	-0.182862000	2.386895000
C	-0.467713000	-2.097104000	-2.704655000
C	-1.880544000	-0.584984000	-1.638097000
C	-1.514675000	-2.611717000	-3.461801000
H	0.543442000	-2.479215000	-2.800162000
C	-2.984406000	-1.065026000	-2.342134000
C	-2.794110000	-2.088363000	-3.270612000
H	-1.328385000	-3.408898000	-4.172243000
H	-3.969827000	-0.654766000	-2.147686000
H	-3.637041000	-2.478831000	-3.831729000
N	-0.650507000	-1.105704000	-1.817178000
C	-1.967417000	0.575462000	-0.674752000
H	-1.682691000	1.486198000	-1.212346000
H	-2.988425000	0.707316000	-0.301361000
Cl	-5.674637000	-0.543825000	0.602148000
O	-6.925070000	-0.741724000	1.393599000
O	-4.790929000	-1.745925000	0.745872000
O	-4.947909000	0.668587000	1.104416000
O	-6.020081000	-0.349305000	-0.843656000

C	1.667735000	4.479405000	-1.130778000
C	1.422903000	4.998052000	0.175258000
C	0.168156000	5.477025000	0.531137000
C	-0.891463000	5.460216000	-0.387438000
C	-0.675876000	4.957029000	-1.680402000
C	0.573210000	4.478446000	-2.047859000
H	2.229911000	5.023460000	0.900233000
H	0.009045000	5.870425000	1.531293000
H	-1.869075000	5.836451000	-0.102346000
H	-1.489774000	4.945925000	-2.399913000
H	0.733495000	4.092776000	-3.051232000
C	2.933036000	3.977165000	-1.532586000
H	1.886727000	1.792062000	-1.421052000
H	3.034769000	3.667372000	-2.570524000
C	4.161866000	3.956013000	-0.678101000
H	4.934369000	3.321975000	-1.120678000
H	4.594813000	4.961814000	-0.563463000
H	3.961062000	3.586836000	0.334632000

2+EB

^{3}TS

Zero-point correction= 0.641492 (Hartree/Particle)
Thermal correction to Energy= 0.684808
Thermal correction to Enthalpy= 0.685753
Thermal correction to Gibbs Free Energy= 0.558776
Sum of electronic and zero-point Energies= -2641.174191
Sum of electronic and thermal Energies= -2641.130874
Sum of electronic and thermal Enthalpies= -2641.129930
Sum of electronic and thermal Free Energies= -2641.256907

Fe	0.058482000	-0.430023000	-0.017453000
N	0.344991000	1.311513000	0.866369000
C	-0.712729000	2.207860000	0.781963000
C	-1.814247000	1.710227000	0.022595000
C	-0.832075000	3.479417000	1.330898000
C	-2.992490000	2.478479000	-0.194401000
C	-1.986686000	4.259114000	1.095803000
H	-0.017597000	3.875904000	1.921434000
C	-2.679673000	-0.112323000	-1.166592000
C	-4.051346000	1.846065000	-0.891520000
C	-3.057342000	3.812302000	0.333932000
H	-2.015516000	5.256097000	1.521725000
C	-3.893840000	0.566381000	-1.382302000
H	-2.510967000	-1.114734000	-1.540433000
H	-4.989251000	2.375204000	-1.016402000
H	-4.691476000	0.063260000	-1.916125000
N	-1.686762000	0.434035000	-0.472927000
C	1.505573000	1.525474000	1.514128000
O	1.861910000	2.535876000	2.136275000
C	2.453505000	0.325021000	1.437430000
H	3.389950000	0.646997000	0.972899000
N	1.897808000	-0.858819000	0.681497000
C	0.447108000	-1.865576000	2.373848000
C	-1.720417000	-1.015181000	2.374372000
C	0.278180000	-2.392004000	3.651782000
C	-1.963236000	-1.523443000	3.646782000
H	-2.477276000	-0.459817000	1.835120000
C	-0.946969000	-2.223188000	4.296141000
H	1.095356000	-2.921351000	4.128899000
H	-2.928536000	-1.364246000	4.113017000
H	-1.101476000	-2.625003000	5.291960000
N	-0.543740000	-1.187257000	1.749796000
C	1.708925000	-2.043435000	1.566050000
H	1.590048000	-2.918791000	0.922231000
H	2.580548000	-2.205164000	2.207411000
H	2.696456000	0.018333000	2.458267000
C	0.661674000	1.078265000	-2.573218000
C	2.371730000	-0.176894000	-1.612713000
C	1.503607000	1.523057000	-3.587790000
H	-0.374649000	1.388400000	-2.521618000
C	3.278401000	0.247059000	-2.581324000
C	2.833841000	1.105273000	-3.587087000
H	1.119011000	2.190325000	-4.350440000
H	4.312657000	-0.076543000	-2.530290000
H	3.519750000	1.448765000	-4.354608000
N	1.087570000	0.246676000	-1.609768000
C	2.718180000	-1.165803000	-0.528698000
H	2.432193000	-2.163366000	-0.872139000
H	3.785822000	-1.165033000	-0.290464000
O	-0.141979000	-1.934218000	-0.884896000
Cl	6.479098000	0.304997000	-0.149186000
O	7.818362000	0.681613000	0.391562000
O	5.514671000	1.434452000	0.056267000
O	5.972136000	-0.912517000	0.566388000
O	6.592116000	0.007139000	-1.613784000
C	-2.937131000	-3.747874000	-0.634430000
C	-3.305801000	-3.910335000	-1.986634000
C	-4.616038000	-3.681850000	-2.405509000
C	-5.593832000	-3.285367000	-1.487130000
C	-5.247182000	-3.119719000	-0.142376000
C	-3.937061000	-3.344871000	0.275594000
H	-2.562175000	-4.217615000	-2.715356000
H	-4.876426000	-3.815821000	-3.451641000
H	-6.614276000	-3.111374000	-1.815318000
H	-5.999818000	-2.818991000	0.580934000
H	-3.676953000	-3.218861000	1.323277000
C	-1.545165000	-3.938949000	-0.168063000
H	-0.899741000	-2.849160000	-0.452870000
H	-1.483984000	-3.969828000	0.923500000
C	-0.689786000	-5.011418000	-0.824651000
H	0.316190000	-5.017172000	-0.395261000
H	-1.123886000	-6.008244000	-0.672655000
H	-0.586985000	-4.856907000	-1.902881000
N	-4.221415000	4.585641000	0.079336000
C	-4.532784000	5.619799000	1.062060000
H	-3.859166000	6.492040000	1.013060000
H	-5.550355000	5.979400000	0.880868000
H	-4.487675000	5.202043000	2.070729000
C	-4.321114000	5.107827000	-1.291648000
H	-5.339442000	5.466994000	-1.469504000
H	-3.623346000	5.943614000	-1.466778000
H	-4.101773000	4.324675000	-2.018991000

^{3}IH

Zero-point correction= 0.644748 (Hartree/Particle)
Thermal correction to Energy= 0.689426
Thermal correction to Enthalpy= 0.690370
Thermal correction to Gibbs Free Energy= 0.557607
Sum of electronic and zero-point Energies= -2641.202180
Sum of electronic and thermal Energies= -2641.157502
Sum of electronic and thermal Enthalpies= -2641.156557
Sum of electronic and thermal Free Energies= -2641.289321

Fe	0.058245000	-0.311553000	-0.056740000
N	0.281765000	1.373835000	0.856996000
C	-0.807196000	2.238017000	0.796103000
C	-1.879162000	1.744114000	-0.008665000
C	-0.973532000	3.476599000	1.402395000
C	-3.074525000	2.489396000	-0.211083000
C	-2.145251000	4.234903000	1.181735000
H	-0.181233000	3.868119000	2.025611000
C	-2.673052000	-0.043600000	-1.292758000
C	-4.104030000	1.860343000	-0.953467000
C	-3.187211000	3.795622000	0.377044000
H	-2.209983000	5.209280000	1.653233000

C	-3.902988000	0.608736000	-1.498255000
H	-2.476544000	-1.023561000	-1.713426000
H	-5.055082000	2.367445000	-1.069526000
H	-4.678170000	0.107922000	-2.066064000
N	-1.705660000	0.495754000	-0.559534000
C	1.432646000	1.591616000	1.529305000
O	1.751594000	2.590414000	2.185919000
C	2.407501000	0.412691000	1.433909000
H	3.332790000	0.762660000	0.966538000
N	1.873056000	-0.773553000	0.670437000
C	0.360668000	-1.805709000	2.306574000
C	-1.824831000	-1.000109000	2.241633000
C	0.147603000	-2.375612000	3.559130000
C	-2.111301000	-1.556723000	3.483686000
H	-2.570166000	-0.442629000	1.688927000
C	-1.107153000	-2.253370000	4.154824000
H	0.954403000	-2.904864000	4.053803000
H	-3.099895000	-1.436055000	3.910933000
H	-1.294791000	-2.690691000	5.129839000
N	-0.617445000	-1.123911000	1.664934000
C	1.655367000	-1.958227000	1.546306000
H	1.561985000	-2.831143000	0.895378000
H	2.501769000	-2.117636000	2.221517000
H	2.666664000	0.105155000	2.450702000
C	0.731943000	1.228666000	-2.555434000
C	2.404502000	-0.083776000	-1.601310000
C	1.589164000	1.660971000	-3.561907000
H	-0.295639000	1.566454000	-2.502350000
C	3.325233000	0.325783000	-2.562712000
C	2.907343000	1.205642000	-3.561071000
H	1.226483000	2.347395000	-4.318193000
H	4.350922000	-0.023208000	-2.509415000
H	3.605265000	1.538526000	-4.322430000
N	1.132271000	0.373731000	-1.600827000
C	2.717464000	-1.085274000	-0.519305000
H	2.424456000	-2.075588000	-0.876160000
H	3.780282000	-1.098890000	-0.260018000
O	-0.099088000	-1.916416000	-0.930513000
Cl	6.464846000	0.395307000	-0.061409000
O	7.789923000	0.783247000	0.506014000
O	5.492172000	1.523586000	0.109332000
O	5.946238000	-0.816145000	0.655833000
O	6.613244000	0.081779000	-1.519430000
C	-2.846891000	-4.311309000	-0.486381000
C	-2.798827000	-4.175700000	-1.907118000
C	-3.854004000	-3.603082000	-2.607915000
C	-4.994891000	-3.143036000	-1.934371000
C	-5.064633000	-3.261133000	-0.536759000
C	-4.018145000	-3.829459000	0.173762000
H	-1.927610000	-4.531100000	-2.448110000
H	-3.794201000	-3.517392000	-3.689468000
H	-5.818560000	-2.703968000	-2.488981000
H	-5.945201000	-2.907743000	-0.007458000
H	-4.080854000	-3.919261000	1.255240000
C	-1.794187000	-4.896720000	0.261446000
H	-0.933338000	-2.347902000	-0.697636000
H	-1.920116000	-4.946280000	1.340198000
C	-0.522256000	-5.425169000	-0.324421000
H	0.077010000	-5.934762000	0.433905000
H	-0.705449000	-6.136162000	-1.141180000
H	0.091215000	-4.615088000	-0.745734000
N	-4.366478000	4.547602000	0.136073000
C	-4.718791000	5.535083000	1.152474000
H	-4.068574000	6.426094000	1.145084000
H	-5.743352000	5.873560000	0.970406000
H	-4.675511000	5.080933000	2.145325000
C	-4.467613000	5.117142000	-1.216077000
H	-5.495199000	5.448851000	-1.393582000
H	-3.796282000	5.981532000	-1.349892000
H	-4.213248000	4.370325000	-1.969514000

^{5}TS

Zero-point correction= 0.638378 (Hartree/Particle)
Thermal correction to Energy= 0.683144
Thermal correction to Enthalpy= 0.684089
Thermal correction to Gibbs Free Energy= 0.549856
Sum of electronic and zero-point Energies= -2641.168281
Sum of electronic and thermal Energies= -2641.123514
Sum of electronic and thermal Enthalpies= -2641.122570
Sum of electronic and thermal Free Energies= -2641.256802

Fe	0.467975000	0.707314000	-0.161013000
N	1.351095000	-0.969825000	0.657795000
C	2.717784000	-1.124937000	0.442518000
C	3.317705000	-0.065868000	-0.310459000
C	3.552518000	-2.163366000	0.845873000
C	4.707228000	-0.056629000	-0.629135000
C	4.937097000	-2.141913000	0.566271000
H	3.128249000	-2.985227000	1.404891000
C	2.958035000	1.923734000	-1.498422000
C	5.165486000	0.982450000	-1.472386000
C	5.547779000	-1.112093000	-0.133475000
H	5.537502000	-2.965112000	0.937692000
C	4.301593000	1.972540000	-1.901538000
H	2.237763000	2.678142000	-1.796574000
H	6.200816000	0.978082000	-1.794198000
H	4.639141000	2.773300000	-2.549250000
N	2.486125000	0.934172000	-0.743672000
C	0.594001000	-1.849141000	1.352720000
O	0.955232000	-2.900414000	1.900643000
C	-0.891971000	-1.475504000	1.472552000
H	-1.477334000	-2.321080000	1.098025000
N	-1.323843000	-0.216922000	0.786642000
C	-0.724609000	1.411082000	2.535026000
C	1.475316000	2.162188000	2.482212000
C	-0.878367000	1.848862000	3.850129000
C	1.394567000	2.636984000	3.787627000
H	2.387623000	2.253108000	1.901597000
C	0.195452000	2.474539000	4.482398000
H	-1.821899000	1.699320000	4.363730000
H	2.253994000	3.113888000	4.244658000
H	0.099272000	2.823971000	5.505202000
N	0.437404000	1.566762000	1.874852000
C	-1.849937000	0.787352000	1.741460000
H	-2.340267000	1.578111000	1.163513000
H	-2.601962000	0.350096000	2.408585000
H	-1.114174000	-1.400189000	2.541475000
C	0.359305000	-1.041602000	-2.807096000
C	-1.568534000	-1.082031000	-1.506248000
C	-0.173502000	-1.958643000	-3.707684000
H	1.357430000	-0.635500000	-2.935243000
C	-2.162410000	-2.020768000	-2.350102000
C	-1.454112000	-2.458758000	-3.469059000
H	0.409365000	-2.276750000	-4.564534000
H	-3.149596000	-2.407903000	-2.119159000
H	-1.893460000	-3.188439000	-4.141683000
N	-0.326527000	-0.615785000	-1.735257000
C	-2.282389000	-0.483683000	-0.316547000
H	-2.709906000	0.476565000	-0.625480000
H	-3.103024000	-1.126441000	0.019631000
O	-0.131549000	2.145231000	-0.894354000
Cl	-4.371458000	-3.930292000	0.497931000
O	-5.190718000	-4.985556000	1.164947000
O	-2.920911000	-4.301129000	0.563399000
O	-4.579896000	-2.617944000	1.193877000

O	-4.789017000	-3.801507000	-0.936235000
C	-2.922114000	3.811003000	-1.239217000
C	-3.403516000	4.245234000	0.013497000
C	-4.687611000	3.910247000	0.441815000
C	-5.520535000	3.128048000	-0.364590000
C	-5.058531000	2.684177000	-1.608529000
C	-3.776556000	3.019626000	-2.037559000
H	-2.773246000	4.855376000	0.652384000
H	-5.040992000	4.262112000	1.406767000
H	-6.519933000	2.868735000	-0.028396000
H	-5.700387000	2.081354000	-2.244327000
H	-3.424823000	2.676745000	-3.007415000
C	-1.549739000	4.104427000	-1.709580000
H	-0.864088000	3.129812000	-1.320076000
H	-1.463541000	3.997644000	-2.795808000
C	-0.820804000	5.331352000	-1.187256000
H	0.187890000	5.381452000	-1.606721000
H	-1.347440000	6.251858000	-1.470235000
H	-0.727000000	5.325508000	-0.097140000
N	6.936294000	-1.067575000	-0.419141000
C	7.693313000	-0.062931000	0.342877000
H	7.848138000	-0.372206000	1.389811000
H	8.673490000	0.081557000	-0.121678000
H	7.170344000	0.894329000	0.345911000
C	7.631779000	-2.351366000	-0.436269000
H	8.619187000	-2.207711000	-0.885482000
H	7.783047000	-2.783279000	0.567345000
H	7.075942000	-3.069358000	-1.044008000

^{5}IH

Zero-point correction= 0.640737 (Hartree/Particle)
Thermal correction to Energy= 0.687098
Thermal correction to Enthalpy= 0.688042
Thermal correction to Gibbs Free Energy= 0.547600
Sum of electronic and zero-point Energies= -2641.193861
Sum of electronic and thermal Energies= -2641.147500
Sum of electronic and thermal Enthalpies= -2641.146556
Sum of electronic and thermal Free Energies= -2641.286998

Fe	0.443675000	0.613766000	0.572622000
N	1.324944000	-1.240515000	0.302989000
C	2.646641000	-1.268069000	-0.135331000
C	3.242545000	0.024315000	-0.298292000
C	3.440307000	-2.370806000	-0.440802000
C	4.589449000	0.185919000	-0.736329000
C	4.786428000	-2.219366000	-0.839149000
H	3.018213000	-3.360515000	-0.342395000
C	2.907088000	2.340641000	-0.232643000
C	5.031996000	1.508256000	-0.973033000
C	5.398302000	-0.980926000	-0.967763000
H	5.359035000	-3.120715000	-1.027326000
C	4.201737000	2.583728000	-0.717237000
H	2.215338000	3.145529000	-0.006597000
H	6.024763000	1.665203000	-1.379538000
H	4.527355000	3.601941000	-0.896115000
N	2.445325000	1.106573000	-0.044565000
C	0.595407000	-2.359441000	0.541201000
O	0.948956000	-3.539192000	0.416361000
C	-0.832226000	-2.116042000	1.053782000
H	-1.514707000	-2.697002000	0.425766000
N	-1.285758000	-0.692838000	1.122011000
C	-0.469077000	-0.099212000	3.373430000
C	1.726669000	0.662712000	3.472361000
C	-0.476173000	-0.358468000	4.743232000
C	1.790676000	0.444418000	4.844674000
H	2.574218000	1.055741000	2.920288000
C	0.668480000	-0.077854000	5.488699000
H	-1.362663000	-0.771710000	5.211742000
H	2.700560000	0.672411000	5.387741000
H	0.685647000	-0.270698000	6.556388000
N	0.620456000	0.398967000	2.758165000
C	-1.683646000	-0.297583000	2.495964000
H	-2.214383000	0.657747000	2.428401000
H	-2.371828000	-1.026845000	2.938738000
H	-0.883081000	-2.559615000	2.053080000
C	-0.051997000	0.432715000	-2.587370000
C	-1.807427000	-0.321982000	-1.262063000
C	-0.706065000	0.047901000	-3.753903000
H	0.930538000	0.892856000	-2.614839000
C	-2.515240000	-0.758288000	-2.382217000
C	-1.956012000	-0.562808000	-3.645572000
H	-0.237722000	0.213893000	-4.717322000
H	-3.473282000	-1.253031000	-2.258115000
H	-2.486190000	-0.891851000	-4.533557000
N	-0.594906000	0.254371000	-1.372514000
C	-2.364209000	-0.403990000	0.139461000
H	-2.787400000	0.575510000	0.387731000
H	-3.167158000	-1.145546000	0.207934000
O	-0.196435000	2.334656000	0.706436000
Cl	-4.493820000	-3.843245000	-0.550834000
O	-5.308108000	-5.085543000	-0.399273000
O	-3.075054000	-4.204979000	-0.869475000
O	-4.530788000	-3.059354000	0.727563000
O	-5.056256000	-3.006232000	-1.660572000
C	-2.641417000	4.221659000	-1.014057000
C	-3.028733000	5.148123000	-0.000677000
C	-4.258415000	5.039314000	0.635727000
C	-5.152549000	4.014035000	0.296131000
C	-4.798310000	3.092420000	-0.701575000
C	-3.573561000	3.191341000	-1.345272000
H	-2.354778000	5.952785000	0.274793000
H	-4.529282000	5.759167000	1.403162000
H	-6.111945000	3.935600000	0.798144000
H	-5.488018000	2.299183000	-0.976119000
H	-3.309020000	2.477387000	-2.120977000
C	-1.392095000	4.288570000	-1.684579000
H	-0.588180000	2.790158000	-0.056139000
H	-1.221977000	3.567088000	-2.480990000
C	-0.350681000	5.343892000	-1.479320000
H	0.626462000	5.000474000	-1.830661000
H	-0.588033000	6.260637000	-2.041496000
H	-0.248706000	5.637223000	-0.428931000
N	6.749201000	-0.809149000	-1.354677000
C	7.648946000	-0.327290000	-0.295401000
H	7.905040000	-1.127480000	0.418230000
H	8.575320000	0.041506000	-0.746064000
H	7.188830000	0.489242000	0.262017000
C	7.353846000	-1.908068000	-2.102016000
H	8.297554000	-1.559500000	-2.532239000
H	7.577612000	-2.790956000	-1.480122000
H	6.693815000	-2.213898000	-2.917168000

3+EB

^{3}TS

Zero-point correction= 0.601171 (Hartree/Particle)
Thermal correction to Energy= 0.642995
Thermal correction to Enthalpy= 0.643939
Thermal correction to Gibbs Free Energy= 0.519857
Sum of electronic and zero-point Energies= -2621.770907
Sum of electronic and thermal Energies= -2621.729082
Sum of electronic and thermal Enthalpies= -2621.728138
Sum of electronic and thermal Free Energies= -2621.852221

Fe	-0.067205000	-0.319731000	-0.014858000
N	0.370412000	1.430395000	0.784779000
C	-0.603921000	2.413549000	0.644431000

C	-1.743413000	1.972282000	-0.091105000
C	-0.603871000	3.724048000	1.106646000
C	-2.845885000	2.827290000	-0.362579000
C	-1.695941000	4.588100000	0.853542000
H	0.248824000	4.082622000	1.666619000
C	-2.742512000	0.201353000	-1.251048000
C	-3.919642000	2.297264000	-1.115514000
C	-2.801964000	4.167966000	0.134952000
H	-1.644655000	5.599610000	1.237687000
C	-3.865932000	0.991909000	-1.560425000
H	-2.661652000	-0.827198000	-1.580865000
H	-4.773497000	2.927381000	-1.337023000
H	-4.672650000	0.557964000	-2.139137000
N	-1.724865000	0.672611000	-0.537641000
C	1.540679000	1.572944000	1.431693000
O	1.982501000	2.578658000	2.006262000
C	2.378015000	0.290700000	1.424743000
H	3.340744000	0.503309000	0.951339000
N	1.721494000	-0.876215000	0.724839000
C	0.173487000	-1.663356000	2.447889000
C	-1.911357000	-0.629072000	2.379986000
C	-0.052391000	-2.110933000	3.746951000
C	-2.209095000	-1.052261000	3.671678000
H	-2.612302000	-0.037340000	1.805096000
C	-1.263603000	-1.805345000	4.366721000
H	0.711250000	-2.685747000	4.258781000
H	-3.160987000	-0.787585000	4.117081000
H	-1.461455000	-2.143546000	5.378382000
N	-0.748585000	-0.932119000	1.779736000
C	1.421333000	-1.991974000	1.666185000
H	1.231079000	-2.885738000	1.066221000
H	2.269980000	-2.196512000	2.325974000
H	2.589548000	0.016233000	2.461668000
C	0.689845000	0.997023000	-2.636122000
C	2.270125000	-0.359753000	-1.595554000
C	1.575057000	1.308783000	-3.663336000
H	-0.313288000	1.404158000	-2.612034000
C	3.217616000	-0.072616000	-2.575244000
C	2.860433000	0.769643000	-3.628141000
H	1.258398000	1.968490000	-4.462937000
H	4.216540000	-0.488456000	-2.497115000
H	3.579272000	1.007385000	-4.405487000
N	1.030800000	0.180069000	-1.627319000
C	2.517440000	-1.318785000	-0.459190000
H	2.142591000	-2.302229000	-0.754380000
H	3.579141000	-1.403209000	-0.209870000
O	-0.393446000	-1.844279000	-0.806002000
Cl	6.387431000	-0.161132000	-0.120980000
O	7.750339000	0.144757000	0.405365000
O	5.525259000	1.062257000	-0.033468000
O	5.768844000	-1.259878000	0.692478000
O	6.485729000	-0.599429000	-1.550980000
O	-3.891068000	4.928209000	-0.159394000
C	-3.912688000	6.279107000	0.299550000
H	-3.082728000	6.855476000	-0.124586000
H	-4.859012000	6.696648000	-0.044374000
H	-3.867693000	6.327274000	1.393426000
C	-3.376439000	-3.340167000	-0.540163000
C	-3.732233000	-3.532844000	-1.891855000
C	-5.004054000	-3.196445000	-2.354090000
C	-5.955452000	-2.659232000	-1.480649000
C	-5.621048000	-2.461203000	-0.137230000
C	-4.348822000	-2.793969000	0.323901000
H	-3.008670000	-3.948788000	-2.586036000
H	-5.255365000	-3.356286000	-3.398805000
H	-6.946410000	-2.401412000	-1.842331000
H	-6.354032000	-2.051041000	0.551672000
H	-4.098945000	-2.641985000	1.370642000
C	-2.020833000	-3.647303000	-0.030425000
H	-1.257766000	-2.648890000	-0.353177000
H	-1.983891000	-3.625258000	1.062489000
C	-1.270058000	-4.836665000	-0.609177000
H	-0.277317000	-4.921122000	-0.157952000
H	-1.807319000	-5.773801000	-0.413358000
H	-1.134022000	-4.753953000	-1.691619000

^{3}IH

Zero-point correction= 0.604316 (Hartree/Particle)
Thermal correction to Energy= 0.647523
Thermal correction to Enthalpy= 0.648467
Thermal correction to Gibbs Free Energy= 0.518561
Sum of electronic and zero-point Energies= -2621.799082
Sum of electronic and thermal Energies= -2621.755875
Sum of electronic and thermal Enthalpies= -2621.754931
Sum of electronic and thermal Free Energies= -2621.884836

Fe	-0.063422000	-0.195125000	-0.069304000
N	0.320736000	1.489486000	0.786845000
C	-0.677075000	2.456712000	0.681169000
C	-1.786471000	2.037183000	-0.113117000
C	-0.717222000	3.734563000	1.223066000
C	-2.898462000	2.886435000	-0.361269000
C	-1.819927000	4.591691000	0.993160000
H	0.112908000	4.075196000	1.826607000
C	-2.719028000	0.322840000	-1.401973000
C	-3.941471000	2.383544000	-1.173515000
C	-2.896453000	4.194909000	0.218861000
H	-1.800240000	5.578237000	1.439846000
C	-3.850266000	1.108406000	-1.694042000
H	-2.615608000	-0.682714000	-1.794734000
H	-4.802188000	3.009643000	-1.379185000
H	-4.633571000	0.694987000	-2.318072000
N	-1.728502000	0.766857000	-0.635788000
C	1.479441000	1.614514000	1.467015000
O	1.890207000	2.599849000	2.093214000
C	2.332128000	0.341458000	1.424973000
H	3.289232000	0.578916000	0.951108000
N	1.685088000	-0.813751000	0.701832000
C	0.055499000	-1.619159000	2.352604000
C	-2.036933000	-0.602611000	2.218704000
C	-0.230414000	-2.113784000	3.622492000
C	-2.394747000	-1.077676000	3.476045000
H	-2.715055000	0.003286000	1.631527000
C	-1.474442000	-1.842950000	4.191186000
H	0.512689000	-2.700578000	4.150799000
H	-3.372161000	-0.842184000	3.880651000
H	-1.718080000	-2.219477000	5.179098000
N	-0.840299000	-0.868714000	1.668728000
C	1.336846000	-1.933356000	1.620021000
H	1.162107000	-2.817857000	1.002225000
H	2.154280000	-2.151825000	2.314171000
H	2.556150000	0.048782000	2.454466000
C	0.798547000	1.173390000	-2.611716000
C	2.309664000	-0.274173000	-1.586734000
C	1.707103000	1.471398000	-3.621825000
H	-0.186683000	1.622138000	-2.585926000
C	3.278273000	-0.004354000	-2.550437000
C	2.967747000	0.875962000	-3.586738000
H	1.428369000	2.163383000	-4.408078000
H	4.259138000	-0.460493000	-2.470227000
H	3.704585000	1.101134000	-4.350872000
N	1.094376000	0.317127000	-1.620758000
C	2.503007000	-1.259800000	-0.463123000
H	2.108685000	-2.226491000	-0.785497000
H	3.555767000	-1.376036000	-0.189174000

O	-0.375864000	-1.808571000	-0.884874000
Cl	6.376234000	-0.153071000	-0.023440000
O	7.730153000	0.147811000	0.528748000
O	5.518494000	1.074759000	0.045910000
O	5.737231000	-1.247757000	0.779142000
O	6.500698000	-0.593617000	-1.450634000
O	-3.992372000	4.949728000	-0.059041000
C	-4.057542000	6.268446000	0.483117000
H	-3.229261000	6.887364000	0.120366000
H	-5.003091000	6.686745000	0.138188000
H	-4.044449000	6.247519000	1.578612000
C	-3.385871000	-3.864460000	-0.382008000
C	-3.255765000	-3.812412000	-1.803067000
C	-4.204336000	-3.164207000	-2.585852000
C	-5.315414000	-2.543536000	-1.996832000
C	-5.464253000	-2.577603000	-0.600832000
C	-4.524381000	-3.220095000	0.190894000
H	-2.406759000	-4.292352000	-2.279325000
H	-4.084267000	-3.144717000	-3.665620000
H	-6.055987000	-2.045187000	-2.614873000
H	-6.322604000	-2.099839000	-0.136688000
H	-4.648045000	-3.243781000	1.270576000
C	-2.442625000	-4.521396000	0.447973000
H	-1.264519000	-2.126675000	-0.671616000
H	-2.624793000	-4.499839000	1.519585000
C	-1.211232000	-5.215526000	-0.044055000
H	-0.699374000	-5.732101000	0.771377000
H	-1.435968000	-5.957441000	-0.822262000
H	-0.499932000	-4.503080000	-0.487256000

^{5}TS

Zero-point correction= 0.598047 (Hartree/Particle)
Thermal correction to Energy= 0.641320
Thermal correction to Enthalpy= 0.642264
Thermal correction to Gibbs Free Energy= 0.510732
Sum of electronic and zero-point Energies= -2621.765128
Sum of electronic and thermal Energies= -2621.721855
Sum of electronic and thermal Enthalpies= -2621.720911
Sum of electronic and thermal Free Energies= -2621.852443

Fe	0.647230000	0.692856000	-0.162106000
N	1.512305000	-0.991838000	0.659219000
C	2.880240000	-1.159176000	0.448370000
C	3.485597000	-0.111391000	-0.313580000
C	3.710567000	-2.191293000	0.875271000
C	4.874053000	-0.110680000	-0.628337000
C	5.092572000	-2.208000000	0.571685000
H	3.281660000	-2.997359000	1.453320000
C	3.170764000	1.913658000	-1.450573000
C	5.377341000	0.969325000	-1.386497000
C	5.682781000	-1.196872000	-0.164376000
H	5.683466000	-3.040724000	0.933435000
C	4.529543000	1.981207000	-1.798081000
H	2.462365000	2.679727000	-1.747661000
H	6.431640000	0.991072000	-1.638351000
H	4.893056000	2.819592000	-2.380645000
N	2.671820000	0.906462000	-0.736961000
C	0.747268000	-1.862277000	1.354446000
O	1.099472000	-2.914939000	1.906892000
C	-0.736495000	-1.477998000	1.467691000
H	-1.326217000	-2.318508000	1.088578000
N	-1.155487000	-0.215098000	0.781343000
C	-0.544976000	1.405842000	2.532375000
C	1.661622000	2.137135000	2.485181000
C	-0.697533000	1.843130000	3.847776000
C	1.582471000	2.610843000	3.791108000
H	2.575987000	2.220791000	1.906736000
C	0.380533000	2.458242000	4.483190000
H	-1.643474000	1.701409000	4.359158000
H	2.445232000	3.079341000	4.250548000
H	0.285372000	2.807091000	5.506289000
N	0.619728000	1.551934000	1.874747000
C	-1.674209000	0.793563000	1.735534000
H	-2.155304000	1.589509000	1.156945000
H	-2.432142000	0.363203000	2.400466000
H	-0.963927000	-1.402615000	2.535520000
C	0.526595000	-1.047105000	-2.811447000
C	-1.403591000	-1.074243000	-1.513584000
C	-0.012755000	-1.957039000	-3.715317000
H	1.528400000	-0.649217000	-2.936809000
C	-2.004240000	-2.005538000	-2.360894000
C	-1.298023000	-2.446671000	-3.479920000
H	0.568605000	-2.277859000	-4.572178000
H	-2.995135000	-2.384688000	-2.132615000
H	-1.742667000	-3.170703000	-4.155165000
N	-0.157202000	-0.618361000	-1.739472000
C	-2.114363000	-0.472468000	-0.323738000
H	-2.534012000	0.491608000	-0.631622000
H	-2.940572000	-1.109387000	0.009940000
O	0.064765000	2.137435000	-0.896199000
Cl	-4.232990000	-3.906171000	0.474798000
O	-5.059374000	-4.957715000	1.138908000
O	-2.784413000	-4.283813000	0.544974000
O	-4.437574000	-2.593006000	1.170308000
O	-4.645168000	-3.775223000	-0.960731000
C	-2.702525000	3.843633000	-1.225033000
C	-3.178969000	4.276634000	0.029950000
C	-4.467047000	3.954539000	0.456263000
C	-5.308993000	3.186687000	-0.354519000
C	-4.852029000	2.744231000	-1.600835000
C	-3.566114000	3.066880000	-2.027863000
H	-2.541633000	4.875775000	0.672222000
H	-4.816429000	4.305293000	1.423075000
H	-6.311462000	2.937380000	-0.019900000
H	-5.500858000	2.152555000	-2.240022000
H	-3.218248000	2.725206000	-2.999541000
C	-1.326569000	4.123221000	-1.693638000
H	-0.653795000	3.137008000	-1.312496000
H	-1.242257000	4.024076000	-2.780745000
C	-0.582016000	5.336687000	-1.161971000
H	0.426794000	5.377822000	-1.582144000
H	-1.097501000	6.265967000	-1.436673000
H	-0.487185000	5.320578000	-0.072038000
O	6.996826000	-1.126391000	-0.504480000
C	7.860318000	-2.179624000	-0.077236000
H	7.546388000	-3.142903000	-0.494603000
H	8.850985000	-1.924919000	-0.453691000
H	7.890404000	-2.248434000	1.015913000

^{5}IH

Zero-point correction= 0.602093 (Hartree/Particle)
Thermal correction to Energy= 0.646346
Thermal correction to Enthalpy= 0.647290
Thermal correction to Gibbs Free Energy= 0.512893
Sum of electronic and zero-point Energies= -2621.789536
Sum of electronic and thermal Energies= -2621.745283
Sum of electronic and thermal Enthalpies= -2621.744339
Sum of electronic and thermal Free Energies= -2621.878736

Fe	0.762640000	0.668257000	0.091080000
N	1.558641000	-1.007965000	0.558639000
C	2.922762000	-1.143849000	0.259209000
C	3.490184000	0.018723000	-0.336259000
C	3.760749000	-2.231551000	0.464231000
C	4.857028000	0.089828000	-0.714123000
C	5.127255000	-2.183955000	0.094326000

H	3.359961000	-3.128615000	0.914319000
C	3.096398000	2.207432000	-1.079414000
C	5.312187000	1.295056000	-1.294865000
C	5.683840000	-1.056745000	-0.484258000
H	5.733640000	-3.062349000	0.277864000
C	4.436850000	2.350844000	-1.476955000
H	2.360533000	2.996167000	-1.197507000
H	6.351199000	1.378285000	-1.593298000
H	4.766161000	3.283078000	-1.920560000
N	2.647491000	1.083070000	-0.531331000
C	0.794389000	-1.967753000	1.144008000
O	1.164196000	-3.091067000	1.497766000
C	-0.665144000	-1.565819000	1.374675000
H	-1.301505000	-2.315284000	0.894296000
N	-1.045137000	-0.190036000	0.900930000
C	-0.349070000	1.088157000	2.892343000
C	1.894150000	1.683846000	2.933919000
C	-0.481980000	1.348325000	4.256125000
C	1.840184000	1.978444000	4.292947000
H	2.813725000	1.792220000	2.367586000
C	0.629065000	1.804822000	4.964171000
H	-1.436630000	1.194717000	4.747655000
H	2.727859000	2.327447000	4.808030000
H	0.551837000	2.015509000	6.025844000
N	0.821721000	1.251600000	2.253735000
C	-1.512029000	0.658055000	2.026174000
H	-1.986690000	1.551795000	1.606727000
H	-2.271572000	0.139292000	2.622236000
H	-0.854344000	-1.646197000	2.449069000
C	0.458266000	-0.647932000	-2.825894000
C	-1.429622000	-0.726176000	-1.475523000
C	-0.172467000	-1.377281000	-3.829359000
H	1.483936000	-0.308779000	-2.931961000
C	-2.123686000	-1.481724000	-2.420870000
C	-1.483919000	-1.804751000	-3.617438000
H	0.359070000	-1.611694000	-4.744659000
H	-3.131945000	-1.821882000	-2.208189000
H	-1.999626000	-2.391279000	-4.371057000
N	-0.160996000	-0.330296000	-1.679019000
C	-2.060419000	-0.256086000	-0.184983000
H	-2.455117000	0.753671000	-0.341824000
H	-2.899072000	-0.897550000	0.105319000
O	0.207566000	2.327656000	-0.424233000
Cl	-4.235244000	-3.679550000	0.289100000
O	-5.064477000	-4.783643000	0.856797000
O	-2.811849000	-4.131688000	0.161561000
O	-4.296021000	-2.487131000	1.198136000
O	-4.760816000	-3.298845000	-1.061975000
C	-3.319383000	3.358530000	-1.582741000
C	-2.700123000	4.099982000	-0.530578000
C	-3.274203000	4.165085000	0.735264000
C	-4.479492000	3.502974000	1.009060000
C	-5.111421000	2.773486000	-0.010912000
C	-4.549695000	2.701579000	-1.277249000
H	-1.777519000	4.637169000	-0.727336000
H	-2.785553000	4.742628000	1.515250000
H	-4.922917000	3.559161000	1.998269000
H	-6.047823000	2.261207000	0.191607000
H	-5.046397000	2.134592000	-2.060406000
C	-2.754033000	3.257585000	-2.878196000
H	-0.728790000	2.516071000	-0.265536000
H	-3.307461000	2.686418000	-3.619402000
C	-1.445462000	3.861957000	-3.279340000
H	-1.192611000	3.604693000	-4.310587000
H	-1.456374000	4.959266000	-3.204773000
H	-0.629855000	3.513243000	-2.629963000
O	6.978021000	-0.920883000	-0.869826000
C	7.860491000	-2.026793000	-0.675040000
H	7.523472000	-2.904774000	-1.237071000
H	8.831034000	-1.703365000	-1.050782000
H	7.944984000	-2.282764000	0.386840000

4+EB

^{3}TS

Zero-point correction= 0.571011 (Hartree/Particle)
Thermal correction to Energy= 0.612815
Thermal correction to Enthalpy= 0.613760
Thermal correction to Gibbs Free Energy= 0.487692
Sum of electronic and zero-point Energies= -2711.773670
Sum of electronic and thermal Energies= -2711.731865
Sum of electronic and thermal Enthalpies= -2711.730921
Sum of electronic and thermal Free Energies= -2711.856989

Fe	0.024371000	-0.402322000	-0.022183000
N	0.371575000	1.364660000	0.796508000
C	-0.621756000	2.295902000	0.681467000
C	-1.771196000	1.822617000	-0.047419000
C	-0.643697000	3.606284000	1.170108000
C	-2.919219000	2.630419000	-0.291133000
C	-1.761453000	4.408889000	0.943288000
H	0.205175000	3.984409000	1.720194000
C	-2.671478000	0.000846000	-1.209432000
C	-3.963620000	2.029593000	-1.047506000
C	-2.877167000	3.962563000	0.242740000
H	-1.775658000	5.421495000	1.324995000
C	-3.833493000	0.734121000	-1.500024000
H	-2.532382000	-1.018818000	-1.546313000
H	-4.854052000	2.598455000	-1.264214000
H	-4.621830000	0.266467000	-2.078005000
N	-1.680887000	0.531790000	-0.502249000
C	1.558515000	1.548335000	1.438761000
O	1.955744000	2.563143000	2.011565000
C	2.444496000	0.302515000	1.407914000
H	3.397802000	0.568733000	0.942060000
N	1.841629000	-0.880240000	0.688380000
C	0.359315000	-1.782461000	2.410845000
C	-1.773974000	-0.850169000	2.385932000
C	0.169371000	-2.270090000	3.700950000
C	-2.037115000	-1.317258000	3.669706000
H	-2.510502000	-0.281301000	1.833024000
C	-1.048910000	-2.038626000	4.338493000
H	0.965475000	-2.818114000	4.192163000
H	-2.996364000	-1.110279000	4.129441000
H	-1.219673000	-2.409285000	5.343632000
N	-0.603521000	-1.081605000	1.767698000
C	1.612716000	-2.030318000	1.610005000
H	1.464281000	-2.920655000	0.993527000
H	2.479612000	-2.201556000	2.254942000
H	2.664749000	0.023070000	2.441354000
C	0.681474000	0.991185000	-2.635712000
C	2.341723000	-0.293286000	-1.628235000
C	1.538660000	1.362269000	-3.666648000
H	-0.341438000	1.344546000	-2.599516000
C	3.262942000	0.056765000	-2.612289000
C	2.851398000	0.892649000	-3.650104000
H	1.179039000	2.013970000	-4.454440000
H	4.283286000	-0.305825000	-2.548164000
H	3.548975000	1.178858000	-4.430397000
N	1.075259000	0.181107000	-1.640131000
C	2.650526000	-1.256703000	-0.511552000
H	2.327687000	-2.254108000	-0.821020000
H	3.716668000	-1.288045000	-0.269564000
O	-0.253901000	-1.911605000	-0.847575000
Cl	6.410376000	0.140859000	-0.122913000
O	7.739452000	0.527441000	0.434561000

O	5.462235000	1.298713000	-0.021094000
O	5.856246000	-1.017527000	0.654111000
O	6.560282000	-0.253825000	-1.560577000
N	-3.966502000	4.906569000	0.096523000
O	-3.802159000	6.061931000	0.510989000
O	-5.028167000	4.538175000	-0.427564000
C	-3.090483000	-3.606623000	-0.549367000
C	-3.445572000	-3.784034000	-1.903274000
C	-4.737631000	-3.506138000	-2.347706000
C	-5.709263000	-3.043855000	-1.453809000
C	-5.375419000	-2.861659000	-0.107990000
C	-4.083237000	-3.135992000	0.335631000
H	-2.706056000	-4.141859000	-2.612781000
H	-4.988770000	-3.652740000	-3.394326000
H	-6.715633000	-2.831159000	-1.801941000
H	-6.123951000	-2.509470000	0.595984000
H	-3.832802000	-2.996896000	1.383974000
C	-1.714968000	-3.848539000	-0.057478000
H	-1.030291000	-2.798481000	-0.367924000
H	-1.668757000	-3.850033000	1.035245000
C	-0.899440000	-4.975305000	-0.672490000
H	0.100021000	-5.013153000	-0.229839000
H	-1.379782000	-5.946605000	-0.497071000
H	-0.777838000	-4.856789000	-1.753194000

^{3}IH

Zero-point correction= 0.574048 (Hartree/Particle)
Thermal correction to Energy= 0.617296
Thermal correction to Enthalpy= 0.618240
Thermal correction to Gibbs Free Energy= 0.486429
Sum of electronic and zero-point Energies= -2711.800973
Sum of electronic and thermal Energies= -2711.757725
Sum of electronic and thermal Enthalpies= -2711.756781
Sum of electronic and thermal Free Energies= -2711.888592

Fe	0.028130000	-0.304186000	-0.046639000
N	0.333517000	1.427900000	0.782020000
C	-0.685847000	2.336467000	0.683014000
C	-1.815732000	1.856634000	-0.072425000
C	-0.741833000	3.630780000	1.206548000
C	-2.978242000	2.646062000	-0.306654000
C	-1.875174000	4.415464000	0.988774000
H	0.092735000	4.012487000	1.775867000
C	-2.663147000	0.049974000	-1.294703000
C	-3.998769000	2.046514000	-1.095934000
C	-2.971890000	3.962968000	0.264529000
H	-1.916150000	5.416504000	1.398094000
C	-3.835875000	0.767289000	-1.582606000
H	-2.503219000	-0.957529000	-1.661065000
H	-4.897640000	2.603075000	-1.310082000
H	-4.606047000	0.300169000	-2.184689000
N	-1.691943000	0.580530000	-0.561895000
C	1.514839000	1.618953000	1.437324000
O	1.888727000	2.633126000	2.024836000
C	2.417123000	0.383304000	1.404066000
H	3.363865000	0.661558000	0.931430000
N	1.824486000	-0.807287000	0.691672000
C	0.287045000	-1.705035000	2.380225000
C	-1.861674000	-0.807959000	2.294870000
C	0.061015000	-2.209986000	3.657818000
C	-2.160764000	-1.297254000	3.561675000
H	-2.588936000	-0.244899000	1.724364000
C	-1.181844000	-2.007013000	4.256073000
H	0.848769000	-2.751733000	4.169115000
H	-3.139608000	-1.115482000	3.989536000
H	-1.379784000	-2.392658000	5.250576000
N	-0.665416000	-1.008661000	1.715234000
C	1.565695000	-1.946675000	1.617617000
H	1.430157000	-2.840285000	1.003039000
H	2.412318000	-2.114249000	2.290018000
H	2.649457000	0.112107000	2.437206000
C	0.745716000	1.084218000	-2.626239000
C	2.369549000	-0.244608000	-1.614136000
C	1.612833000	1.428200000	-3.657693000
H	-0.266531000	1.466949000	-2.589259000
C	3.299855000	0.076823000	-2.599305000
C	2.911567000	0.920475000	-3.639699000
H	1.272585000	2.088599000	-4.446791000
H	4.310365000	-0.311513000	-2.532210000
H	3.617027000	1.184861000	-4.420613000
N	1.116904000	0.264101000	-1.629627000
C	2.649124000	-1.205173000	-0.488125000
H	2.316058000	-2.199005000	-0.796400000
H	3.711049000	-1.248408000	-0.229554000
O	-0.219655000	-1.915453000	-0.857360000
Cl	6.403794000	0.195496000	-0.063025000
O	7.728134000	0.590676000	0.499983000
O	5.459418000	1.359192000	0.000670000
O	5.836805000	-0.941935000	0.735122000
O	6.568590000	-0.233957000	-1.489000000
N	-4.083336000	4.885306000	0.133670000
O	-3.937443000	6.041983000	0.549629000
O	-5.142975000	4.494501000	-0.376920000
C	-3.069991000	-4.095615000	-0.413682000
C	-3.090952000	-4.058887000	-1.841078000
C	-4.133557000	-3.446343000	-2.526073000
C	-5.193976000	-2.847851000	-1.829718000
C	-5.193871000	-2.865468000	-0.425575000
C	-4.158291000	-3.471706000	0.269550000
H	-2.282244000	-4.520162000	-2.398879000
H	-4.127678000	-3.436974000	-3.612555000
H	-6.009511000	-2.378915000	-2.371739000
H	-6.011439000	-2.404010000	0.121223000
H	-4.166663000	-3.483284000	1.356403000
C	-2.029067000	-4.719107000	0.320218000
H	-1.019522000	-2.346465000	-0.521258000
H	-2.096573000	-4.682393000	1.404761000
C	-0.847250000	-5.408991000	-0.286910000
H	-0.277464000	-5.949973000	0.472443000
H	-1.140233000	-6.127476000	-1.063510000
H	-0.162996000	-4.692495000	-0.765122000

^{5}TS

Zero-point correction= 0.568007 (Hartree/Particle)
Thermal correction to Energy= 0.611242
Thermal correction to Enthalpy= 0.612186
Thermal correction to Gibbs Free Energy= 0.479493
Sum of electronic and zero-point Energies= -2711.766945
Sum of electronic and thermal Energies= -2711.723711
Sum of electronic and thermal Enthalpies= -2711.722767
Sum of electronic and thermal Free Energies= -2711.855460

Fe	0.488718000	0.718903000	-0.142357000
N	1.407244000	-0.948638000	0.705133000
C	2.757275000	-1.086876000	0.519535000
C	3.369246000	-0.031044000	-0.258318000
C	3.591014000	-2.109595000	0.987155000
C	4.762121000	-0.004052000	-0.564723000
C	4.956099000	-2.094042000	0.698172000
H	3.165666000	-2.912036000	1.570149000
C	2.984064000	1.979604000	-1.398844000
C	5.222782000	1.109241000	-1.319783000
C	5.549617000	-1.090892000	-0.056629000
H	5.585961000	-2.894457000	1.064480000
C	4.341917000	2.088424000	-1.730404000
H	2.250325000	2.718745000	-1.700959000

H	6.270380000	1.178988000	-1.568348000
H	4.687647000	2.939412000	-2.305614000
N	2.525648000	0.955458000	-0.686667000
C	0.641271000	-1.831641000	1.411277000
O	1.012376000	-2.858148000	1.984536000
C	-0.851174000	-1.481461000	1.486131000
H	-1.406864000	-2.339592000	1.094737000
N	-1.288160000	-0.232392000	0.787465000
C	-0.732487000	1.413602000	2.533127000
C	1.458905000	2.193147000	2.500621000
C	-0.908397000	1.861821000	3.841612000
C	1.354881000	2.678668000	3.800106000
H	2.377418000	2.292494000	1.931698000
C	0.149314000	2.506987000	4.481251000
H	-1.856500000	1.705186000	4.344401000
H	2.202177000	3.171122000	4.263069000
H	0.035724000	2.864700000	5.499326000
N	0.436381000	1.577698000	1.886116000
C	-1.840270000	0.769778000	1.731517000
H	-2.336024000	1.549611000	1.143685000
H	-2.592734000	0.323773000	2.391753000
H	-1.104544000	-1.412589000	2.548236000
C	0.462848000	-1.037826000	-2.776250000
C	-1.486797000	-1.105146000	-1.506890000
C	-0.045442000	-1.956176000	-3.688922000
H	1.457811000	-0.619850000	-2.887883000
C	-2.056032000	-2.045923000	-2.364900000
C	-1.324441000	-2.470875000	-3.473636000
H	0.554710000	-2.263778000	-4.537522000
H	-3.042570000	-2.444848000	-2.152981000
H	-1.744818000	-3.201849000	-4.156792000
N	-0.245559000	-0.625165000	-1.713288000
C	-2.228108000	-0.518514000	-0.328439000
H	-2.669137000	0.433350000	-0.643808000
H	-3.040221000	-1.175792000	-0.000647000
O	-0.124170000	2.136028000	-0.885401000
Cl	-4.183004000	-4.019384000	0.421827000
O	-4.906840000	-5.135264000	1.099364000
O	-2.707990000	-4.287795000	0.442579000
O	-4.460869000	-2.730950000	1.138157000
O	-4.647744000	-3.906522000	-0.998741000
N	6.973362000	-1.218858000	-0.296400000
O	7.593482000	-2.099398000	0.314300000
O	7.527423000	-0.460775000	-1.106112000
C	-2.921035000	3.800106000	-1.245708000
C	-3.409225000	4.230865000	0.005654000
C	-4.692721000	3.887947000	0.428465000
C	-5.517168000	3.100595000	-0.382022000
C	-5.047863000	2.659441000	-1.624284000
C	-3.766451000	3.002851000	-2.047994000
H	-2.784943000	4.844279000	0.647180000
H	-5.052525000	4.237041000	1.391952000
H	-6.516158000	2.834808000	-0.049775000
H	-5.683547000	2.052655000	-2.262361000
H	-3.408213000	2.662296000	-3.016209000
C	-1.548540000	4.103078000	-1.711474000
H	-0.866699000	3.143252000	-1.324549000
H	-1.459772000	3.998131000	-2.797816000
C	-0.831313000	5.337420000	-1.188804000
H	0.178810000	5.393970000	-1.603762000
H	-1.364735000	6.251609000	-1.478641000
H	-0.743347000	5.336215000	-0.098338000

^{5}IH

Zero-point correction= 0.571817 (Hartree/Particle)
Thermal correction to Energy= 0.616043
Thermal correction to Enthalpy= 0.616987
Thermal correction to Gibbs Free Energy= 0.481325
Sum of electronic and zero-point Energies= -2711.789494
Sum of electronic and thermal Energies= -2711.745269
Sum of electronic and thermal Enthalpies= -2711.744325
Sum of electronic and thermal Free Energies= -2711.879987

Fe	0.600983000	0.665390000	0.135416000
N	1.415888000	-1.010908000	0.611319000
C	2.763274000	-1.141755000	0.337194000
C	3.356431000	0.026286000	-0.258574000
C	3.584420000	-2.244991000	0.570495000
C	4.729966000	0.100306000	-0.623613000
C	4.938414000	-2.190135000	0.221753000
H	3.170300000	-3.136733000	1.015675000
C	2.935566000	2.217762000	-0.978649000
C	5.167548000	1.335237000	-1.178293000
C	5.514174000	-1.071930000	-0.362579000
H	5.568139000	-3.051526000	0.403299000
C	4.279545000	2.377670000	-1.351167000
H	2.188907000	2.996086000	-1.096189000
H	6.202303000	1.448322000	-1.462993000
H	4.609630000	3.319805000	-1.772861000
N	2.504187000	1.080444000	-0.450322000
C	0.638348000	-1.980467000	1.195223000
O	1.010401000	-3.094760000	1.553487000
C	-0.823409000	-1.581532000	1.403184000
H	-1.446521000	-2.336327000	0.913109000
N	-1.206290000	-0.208786000	0.925968000
C	-0.536728000	1.076467000	2.920946000
C	1.703718000	1.684292000	2.980336000
C	-0.684721000	1.348300000	4.280648000
C	1.633576000	1.990887000	4.335598000
H	2.628801000	1.793928000	2.423762000
C	0.416545000	1.816718000	4.995873000
H	-1.643742000	1.194498000	4.763357000
H	2.514015000	2.349551000	4.856259000
H	0.327236000	2.036569000	6.054673000
N	0.640411000	1.239284000	2.293035000
C	-1.689928000	0.634952000	2.047935000
H	-2.171570000	1.523120000	1.625566000
H	-2.447843000	0.108176000	2.638628000
H	-1.025035000	-1.665748000	2.474860000
C	0.352386000	-0.635039000	-2.780884000
C	-1.555610000	-0.735692000	-1.458139000
C	-0.262898000	-1.350410000	-3.803107000
H	1.378147000	-0.291744000	-2.869021000
C	-2.234132000	-1.478395000	-2.424518000
C	-1.576556000	-1.782899000	-3.615976000
H	0.282033000	-1.570253000	-4.714039000
H	-3.244833000	-1.823011000	-2.232405000
H	-2.080450000	-2.359017000	-4.385362000
N	-0.284242000	-0.335920000	-1.637805000
C	-2.208297000	-0.282763000	-0.172537000
H	-2.616819000	0.721667000	-0.327341000
H	-3.040344000	-0.938182000	0.104789000
O	0.053410000	2.313422000	-0.386632000
Cl	-4.301871000	-3.726302000	0.192416000
O	-5.035374000	-4.902061000	0.746584000
O	-2.849687000	-4.065697000	0.033396000
O	-4.435592000	-2.561848000	1.129449000
O	-4.874962000	-3.356648000	-1.141878000
N	6.926122000	-1.166866000	-0.693851000
O	7.561941000	-2.137111000	-0.266421000
O	7.443051000	-0.289162000	-1.397831000
C	-3.352660000	3.404952000	-1.622408000
C	-2.726039000	4.190599000	-0.607337000
C	-3.276747000	4.287279000	0.666813000
C	-4.465272000	3.614861000	0.985506000

C	-5.104816000	2.843022000	0.001926000
C	-4.566202000	2.738985000	-1.272336000
H	-1.815596000	4.734340000	-0.838887000
H	-2.782864000	4.897243000	1.418255000
H	-4.890884000	3.696453000	1.980747000
H	-6.028804000	2.323142000	0.239018000
H	-5.068692000	2.139655000	-2.027202000
C	-2.809128000	3.270252000	-2.924024000
H	-0.883392000	2.515998000	-0.244795000
H	-3.366542000	2.667606000	-3.636701000
C	-1.517480000	3.881036000	-3.367742000
H	-1.274929000	3.589261000	-4.392175000
H	-1.545978000	4.979983000	-3.334004000
H	-0.686189000	3.571183000	-2.718827000

5+EB

^{3}TS

Zero-point correction= 0.582918 (Hartree/Particle)
Thermal correction to Energy= 0.629322
Thermal correction to Enthalpy= 0.630266
Thermal correction to Gibbs Free Energy= 0.494243
Sum of electronic and zero-point Energies= -3392.842262
Sum of electronic and thermal Energies= -3392.795859
Sum of electronic and thermal Enthalpies= -3392.794914
Sum of electronic and thermal Free Energies= -3392.930937

Fe	-0.810042000	0.683873000	0.025499000
N	-0.393299000	-0.938453000	1.081605000
C	0.914361000	-1.342275000	1.089764000
C	1.777376000	-0.488747000	0.315065000
C	1.479211000	-2.443163000	1.739484000
C	3.172871000	-0.726945000	0.185121000
C	2.851639000	-2.692087000	1.620636000
H	0.850148000	-3.094868000	2.327715000
C	1.872890000	1.405857000	-1.052741000
C	3.907031000	0.189924000	-0.615210000
C	3.690756000	-1.871763000	0.875414000
H	3.276859000	-3.547261000	2.133752000
C	3.258677000	1.239733000	-1.227232000
H	1.328056000	2.215654000	-1.521829000
H	4.974167000	0.065421000	-0.740054000
H	3.801129000	1.948320000	-1.841646000
N	1.164019000	0.572329000	-0.300900000
C	-1.418132000	-1.566191000	1.718242000
O	-1.371279000	-2.597304000	2.390474000
C	-2.747914000	-0.827954000	1.558947000
H	-3.510449000	-1.524730000	1.202081000
N	-2.695148000	0.374623000	0.646878000
C	-1.912722000	2.081609000	2.208429000
C	0.407777000	2.197369000	2.361372000
C	-2.061698000	2.779468000	3.403809000
C	0.334032000	2.907023000	3.555803000
H	1.361433000	1.941941000	1.917325000
C	-0.921360000	3.203670000	4.085201000
H	-3.054661000	2.980586000	3.789905000
H	1.246077000	3.211570000	4.055618000
H	-1.012590000	3.749142000	5.018471000
N	-0.691020000	1.798655000	1.698825000
C	-3.077549000	1.624277000	1.366704000
H	-3.288954000	2.386844000	0.612799000
H	-3.979986000	1.476533000	1.967418000
H	-3.062858000	-0.506824000	2.555606000
C	-0.572974000	-1.162610000	-2.369590000
C	-2.701742000	-0.678588000	-1.562479000
C	-1.091399000	-2.006594000	-3.346248000
H	0.493054000	-0.997207000	-2.277262000
C	-3.291041000	-1.523595000	-2.500163000
C	-2.471850000	-2.193695000	-3.408206000
H	-0.419319000	-2.507771000	-4.033130000
H	-4.368520000	-1.650059000	-2.497199000
H	-2.905413000	-2.856437000	-4.149981000
N	-1.361520000	-0.513059000	-1.498163000
C	-3.500143000	0.156302000	-0.594440000
H	-3.671097000	1.135848000	-1.048395000
H	-4.465896000	-0.300727000	-0.365025000
O	-1.176762000	2.036731000	-1.010030000
Cl	-6.630896000	-2.518848000	-0.256714000
O	-8.068316000	-2.601614000	0.138363000
O	-5.826854000	-1.999945000	0.901527000
O	-6.487591000	-1.575272000	-1.416670000
O	-6.128091000	-3.869933000	-0.647262000
C	0.583054000	4.854646000	-0.926048000
C	0.938471000	5.008027000	-2.282827000
C	2.253374000	5.289051000	-2.652067000
C	3.248335000	5.424103000	-1.678117000
C	2.914622000	5.275748000	-0.328075000
C	1.601278000	4.991715000	0.040916000
H	0.181068000	4.907322000	-3.053826000
H	2.502945000	5.405604000	-3.702829000
H	4.271023000	5.645845000	-1.968181000
H	3.677966000	5.385686000	0.436869000
H	1.348732000	4.883642000	1.092352000
C	-0.794378000	4.509684000	-0.506592000
H	-0.913886000	3.232311000	-0.663597000
H	-0.933041000	4.630523000	0.571517000
C	-1.967340000	5.056731000	-1.305095000
H	-2.914345000	4.698162000	-0.891832000
H	-1.983452000	6.153893000	-1.274924000
H	-1.930190000	4.755172000	-2.356049000
S	5.399544000	-2.338213000	0.821134000
O	6.272807000	-1.156802000	0.737272000
O	5.654909000	-3.380031000	1.825233000
C	5.577594000	-3.205906000	-0.835707000
F	6.843523000	-3.597113000	-0.974146000
F	5.258510000	-2.365873000	-1.825344000
F	4.771875000	-4.266710000	-0.876739000

^{3}IH

Zero-point correction= 0.585997 (Hartree/Particle)
Thermal correction to Energy= 0.633823
Thermal correction to Enthalpy= 0.634767
Thermal correction to Gibbs Free Energy= 0.493086
Sum of electronic and zero-point Energies= -3392.869831
Sum of electronic and thermal Energies= -3392.822005
Sum of electronic and thermal Enthalpies= -3392.821061
Sum of electronic and thermal Free Energies= -3392.962742

Fe	-0.843294000	0.585229000	-0.008227000
N	-0.361668000	-0.994384000	1.019191000
C	0.970644000	-1.316996000	1.048533000
C	1.789594000	-0.436022000	0.256068000
C	1.589497000	-2.368740000	1.727056000
C	3.195683000	-0.606044000	0.133479000
C	2.974127000	-2.548763000	1.617099000
H	0.993195000	-3.038046000	2.329543000
C	1.792665000	1.432197000	-1.149590000
C	3.883650000	0.327432000	-0.688549000
C	3.770364000	-1.705396000	0.852189000
H	3.441660000	-3.367171000	2.152791000
C	3.184709000	1.330312000	-1.323150000
H	1.213047000	2.207589000	-1.637160000
H	4.955653000	0.253360000	-0.811469000
H	3.691866000	2.051180000	-1.952961000
N	1.124289000	0.580714000	-0.381966000
C	-1.357400000	-1.654470000	1.675056000
O	-1.251984000	-2.654406000	2.384950000

C	-2.731585000	-1.016210000	1.460019000
H	-3.383232000	-1.758941000	0.989797000
N	-2.714852000	0.241670000	0.626580000
C	-1.909208000	1.919757000	2.227642000
C	0.407943000	2.156299000	2.288398000
C	-2.042849000	2.595178000	3.437798000
C	0.346793000	2.851480000	3.491131000
H	1.354752000	1.957613000	1.803029000
C	-0.899137000	3.071382000	4.077285000
H	-3.028121000	2.742532000	3.865665000
H	1.261190000	3.203197000	3.954242000
H	-0.980083000	3.601032000	5.020619000
N	-0.695048000	1.701653000	1.668727000
C	-3.091390000	1.447083000	1.418866000
H	-3.351831000	2.235605000	0.708159000
H	-3.962159000	1.251454000	2.051840000
H	-3.159595000	-0.798654000	2.442073000
C	-0.628853000	-1.213124000	-2.418879000
C	-2.757887000	-0.722184000	-1.609743000
C	-1.152830000	-2.017689000	-3.424826000
H	0.438775000	-1.067161000	-2.312115000
C	-3.351508000	-1.532098000	-2.574680000
C	-2.535597000	-2.182782000	-3.499614000
H	-0.484224000	-2.507929000	-4.122810000
H	-4.428162000	-1.662561000	-2.580811000
H	-2.973894000	-2.817711000	-4.262601000
N	-1.415618000	-0.578261000	-1.534687000
C	-3.539319000	0.089016000	-0.609351000
H	-3.691705000	1.088218000	-1.023972000
H	-4.512332000	-0.355842000	-0.381887000
O	-1.323315000	2.035229000	-1.000028000
Cl	-6.195938000	-2.914396000	-0.165496000
O	-6.343350000	-1.575102000	0.494744000
O	-4.797411000	-3.414821000	0.045407000
O	-6.457003000	-2.774590000	-1.634181000
O	-7.169143000	-3.876388000	0.429942000
C	0.120530000	5.338531000	-0.743620000
C	0.245247000	5.176584000	-2.156941000
C	1.493783000	5.065715000	-2.757327000
C	2.665278000	5.110794000	-1.987127000
C	2.569313000	5.263444000	-0.594451000
C	1.329323000	5.373055000	0.016743000
H	-0.648756000	5.144045000	-2.771445000
H	1.560740000	4.948558000	-3.835455000
H	3.637522000	5.032727000	-2.464062000
H	3.471882000	5.299135000	0.009239000
H	1.263413000	5.493303000	1.095014000
C	-1.134601000	5.464846000	-0.096031000
H	-0.839930000	2.822148000	-0.707665000
H	-1.125434000	5.570413000	0.986040000
C	-2.461217000	5.451438000	-0.789490000
H	-2.696617000	4.455091000	-1.192117000
H	-3.264924000	5.725974000	-0.102039000
H	-2.492237000	6.146665000	-1.638605000
S	5.503040000	-2.082323000	0.814428000
O	6.311722000	-0.858316000	0.701701000
O	5.808524000	-3.082003000	1.846756000
C	5.731922000	-2.982765000	-0.818698000
F	7.019408000	-3.298492000	-0.949467000
F	5.360420000	-2.191306000	-1.829724000
F	4.993211000	-4.091757000	-0.828075000

^{5}TS

Zero-point correction= 0.579813 (Hartree/Particle)
Thermal correction to Energy= 0.627722
Thermal correction to Enthalpy= 0.628666
Thermal correction to Gibbs Free Energy= 0.484325
Sum of electronic and zero-point Energies= -3392.835947
Sum of electronic and thermal Energies= -3392.788038
Sum of electronic and thermal Enthalpies= -3392.787094
Sum of electronic and thermal Free Energies= -3392.931435

Fe	0.406947000	-0.838349000	-0.075217000
N	-0.622513000	0.651518000	0.954774000
C	-1.993277000	0.620139000	0.908498000
C	-2.538309000	-0.468403000	0.128053000
C	-2.896795000	1.497864000	1.516722000
C	-3.938464000	-0.666926000	-0.035495000
C	-4.276755000	1.317239000	1.360284000
H	-2.518658000	2.317008000	2.109314000
C	-2.034205000	-2.339401000	-1.186761000
C	-4.341689000	-1.776404000	-0.825881000
C	-4.804565000	0.272115000	0.614826000
H	-4.954711000	2.009751000	1.846326000
C	-3.397112000	-2.602631000	-1.396769000
H	-1.252671000	-2.960219000	-1.610817000
H	-5.394021000	-1.978038000	-0.974418000
H	-3.692503000	-3.451674000	-2.001801000
N	-1.629653000	-1.309806000	-0.450709000
C	0.092437000	1.588597000	1.641564000
O	-0.345234000	2.529911000	2.307664000
C	1.617109000	1.431767000	1.558882000
H	2.019500000	2.367138000	1.157627000
N	2.135005000	0.275043000	0.762911000
C	1.929685000	-1.509224000	2.449635000
C	-0.144030000	-2.558551000	2.540555000
C	2.267422000	-1.992675000	3.713047000
C	0.126352000	-3.087794000	3.798305000
H	-1.087422000	-2.746733000	2.038895000
C	1.354140000	-2.796721000	4.393834000
H	3.227548000	-1.740587000	4.149710000
H	-0.612767000	-3.705130000	4.295626000
H	1.595242000	-3.184754000	5.378028000
N	0.740418000	-1.790070000	1.885537000
C	2.880106000	-0.693238000	1.604066000
H	3.417047000	-1.375702000	0.936690000
H	3.624544000	-0.187790000	2.229827000
H	1.983025000	1.360481000	2.587385000
C	-0.005626000	1.049329000	-2.586747000
C	2.031168000	1.274809000	-1.483819000
C	0.314378000	2.065964000	-3.480617000
H	-0.954655000	0.526195000	-2.640620000
C	2.413644000	2.318027000	-2.326624000
C	1.543003000	2.712820000	-3.342017000
H	-0.389932000	2.346129000	-4.255468000
H	3.365140000	2.815799000	-2.171001000
H	1.816997000	3.521939000	-4.011363000
N	0.836715000	0.666411000	-1.614166000
C	2.935245000	0.719494000	-0.408633000
H	3.447092000	-0.160089000	-0.814067000
H	3.696377000	1.448181000	-0.111198000
O	1.116135000	-2.125440000	-0.956676000
Cl	4.524364000	4.354560000	0.449782000
O	5.206090000	5.514968000	1.095786000
O	3.038235000	4.537026000	0.521645000
O	4.902299000	3.089030000	1.161623000
O	4.945345000	4.258581000	-0.985893000
C	4.054139000	-3.416731000	-1.602240000
C	4.678398000	-3.844893000	-0.411954000
C	5.940467000	-3.371027000	-0.056458000
C	6.606834000	-2.452596000	-0.874389000
C	6.000624000	-2.012036000	-2.056093000
C	4.740581000	-2.486132000	-2.412643000
H	4.177834000	-4.558611000	0.234236000
H	6.407191000	-3.720015000	0.860052000

H	7.589496000	-2.085031000	-0.594605000
H	6.513400000	-1.303426000	-2.699815000
H	4.275915000	-2.145051000	-3.334312000
C	2.696383000	-3.860506000	-1.992557000
H	1.936555000	-3.012123000	-1.504363000
H	2.516554000	-3.712273000	-3.062468000
C	2.170318000	-5.198179000	-1.497350000
H	1.146695000	-5.356894000	-1.847664000
H	2.786067000	-6.024346000	-1.874945000
H	2.161892000	-5.263017000	-0.405292000
S	-6.573010000	0.187687000	0.521077000
O	-7.037901000	-1.207027000	0.455098000
O	-7.159465000	1.119480000	1.494012000
C	-6.974382000	0.924532000	-1.160045000
F	-8.295278000	0.891969000	-1.330505000
F	-6.382024000	0.210874000	-2.122766000
F	-6.544988000	2.184908000	-1.213278000

^{5}IH

Zero-point correction= 0.583532 (Hartree/Particle)
Thermal correction to Energy= 0.631697
Thermal correction to Enthalpy= 0.632641
Thermal correction to Gibbs Free Energy= 0.488204
Sum of electronic and zero-point Energies= -3392.858224
Sum of electronic and thermal Energies= -3392.810059
Sum of electronic and thermal Enthalpies= -3392.809115
Sum of electronic and thermal Free Energies= -3392.953552

Fe	-0.305272000	-0.625708000	0.280285000
N	0.632437000	0.517683000	-0.954306000
C	2.012427000	0.429029000	-0.952698000
C	2.531986000	-0.531651000	-0.016364000
C	2.920818000	1.142230000	-1.733499000
C	3.922102000	-0.777327000	0.142461000
C	4.298702000	0.917151000	-1.586271000
H	2.559634000	1.865819000	-2.448425000
C	1.964210000	-2.115789000	1.613354000
C	4.289691000	-1.758046000	1.103622000
C	4.803594000	-0.008825000	-0.685972000
H	4.989261000	1.479038000	-2.204889000
C	3.319819000	-2.416350000	1.830833000
H	1.156444000	-2.598846000	2.152936000
H	5.333754000	-1.993594000	1.261032000
H	3.590599000	-3.164723000	2.566120000
N	1.597024000	-1.207206000	0.720134000
C	-0.094907000	1.340672000	-1.776459000
O	0.355877000	2.116100000	-2.616119000
C	-1.609718000	1.246300000	-1.589476000
H	-1.974968000	2.248719000	-1.345232000
N	-2.086175000	0.261641000	-0.559024000
C	-2.033610000	-1.788437000	-1.930627000
C	0.023277000	-2.863177000	-2.008577000
C	-2.490026000	-2.502490000	-3.038365000
C	-0.362786000	-3.625289000	-3.106659000
H	1.011259000	-2.963668000	-1.570845000
C	-1.642491000	-3.437823000	-3.630763000
H	-3.488104000	-2.325420000	-3.424092000
H	0.327668000	-4.339789000	-3.539841000
H	-1.973998000	-4.007387000	-4.492668000
N	-0.796729000	-1.967910000	-1.436463000
C	-2.906323000	-0.811447000	-1.175580000
H	-3.423343000	-1.351895000	-0.375748000
H	-3.678442000	-0.391001000	-1.829608000
H	-2.037626000	0.994751000	-2.564107000
C	0.245538000	1.691507000	2.415741000
C	-1.860767000	1.696182000	1.433726000
C	-0.038715000	2.845421000	3.138936000
H	1.208186000	1.196693000	2.495213000
C	-2.214059000	2.867085000	2.104502000
C	-1.288729000	3.443829000	2.973785000
H	0.707483000	3.265631000	3.803491000
H	-3.183956000	3.320423000	1.928643000
H	-1.537195000	4.354527000	3.509151000
N	-0.648746000	1.133726000	1.584907000
C	-2.821528000	0.949052000	0.537519000
H	-3.331333000	0.185375000	1.135247000
H	-3.588044000	1.616406000	0.130561000
O	-0.962414000	-1.779866000	1.509031000
Cl	-4.376521000	4.385463000	-0.924013000
O	-5.015759000	5.412805000	-1.797951000
O	-2.885138000	4.463780000	-1.060424000
O	-4.838101000	3.017880000	-1.334609000
O	-4.758982000	4.628162000	0.504348000
C	-4.557753000	-3.725025000	1.207184000
C	-5.637129000	-2.876477000	0.817708000
C	-5.963908000	-1.745726000	1.556995000
C	-5.238266000	-1.407346000	2.708489000
C	-4.172830000	-2.227720000	3.116342000
C	-3.837231000	-3.360393000	2.385906000
H	-6.216606000	-3.122246000	-0.066385000
H	-6.792728000	-1.119417000	1.238807000
H	-5.502260000	-0.525624000	3.284163000
H	-3.611953000	-1.980571000	4.013429000
H	-3.018143000	-3.995044000	2.714338000
C	-4.194340000	-4.885175000	0.479851000
H	-1.925239000	-1.795749000	1.615288000
H	-3.372913000	-5.479673000	0.872481000
C	-4.879527000	-5.367960000	-0.759394000
H	-4.310083000	-6.169161000	-1.236338000
H	-5.883740000	-5.763943000	-0.544563000
H	-5.014834000	-4.566051000	-1.496416000
S	6.572028000	-0.168556000	-0.626409000
O	6.967145000	-1.554260000	-0.330505000
O	7.164717000	0.548288000	-1.762955000
C	7.058369000	0.827215000	0.891427000
F	8.381148000	0.762515000	1.030203000
F	6.468350000	0.316265000	1.976284000
F	6.682493000	2.095776000	0.735992000

6+EB

^{3}TS

Zero-point correction= 0.592828 (Hartree/Particle)
Thermal correction to Energy= 0.637228
Thermal correction to Enthalpy= 0.638172
Thermal correction to Gibbs Free Energy= 0.504940
Sum of electronic and zero-point Energies= -3193.352047
Sum of electronic and thermal Energies= -3193.307648
Sum of electronic and thermal Enthalpies= -3193.306703
Sum of electronic and thermal Free Energies= -3193.439935

Fe	-0.675363000	-1.119612000	0.293818000
N	0.988904000	0.053001000	0.071191000
N	-1.071280000	0.219005000	1.732812000
N	-1.426888000	0.217920000	-0.990620000
N	0.489165000	-2.145887000	1.540053000
N	0.141350000	-2.169697000	-1.190842000
O	-2.027821000	-2.187686000	0.451635000
C	-1.773060000	0.057250000	2.863837000
C	-1.905254000	1.090258000	3.788689000
C	-1.281862000	2.310860000	3.531927000
C	-0.531192000	2.471036000	2.363717000
C	-0.447527000	1.394632000	1.489465000
C	0.297455000	1.395958000	0.165139000
C	-0.763296000	1.394993000	-0.921622000
C	-1.069619000	2.465618000	-1.750916000
C	-2.094366000	2.296667000	-2.687311000

C	-2.765344000	1.077276000	-2.763092000
C	-2.402165000	0.050191000	-1.894544000
C	0.167380000	-3.335197000	2.080724000
C	1.058387000	-4.034273000	2.884749000
C	2.322451000	-3.489585000	3.118186000
C	2.650537000	-2.260030000	2.551779000
C	1.702214000	-1.600878000	1.771467000
C	1.947095000	-0.228386000	1.190133000
C	1.602218000	-0.230389000	-1.266424000
C	1.266100000	-1.633243000	-1.712759000
C	2.028798000	-2.324954000	-2.651497000
C	1.593812000	-3.578320000	-3.079427000
C	0.415372000	-4.110097000	-2.553916000
C	-0.280958000	-3.379022000	-1.598851000
H	-2.225454000	-0.915070000	3.014995000
H	-2.486059000	0.931175000	4.689611000
H	-1.369037000	3.130146000	4.237792000
H	-0.024523000	3.403275000	2.132416000
H	0.986017000	2.241466000	0.075803000
H	-0.521015000	3.398676000	-1.663846000
H	-2.359459000	3.110903000	-3.353542000
H	-3.565914000	0.915594000	-3.474648000
H	-2.892456000	-0.915067000	-1.901826000
H	-0.824520000	-3.700872000	1.842912000
H	0.766294000	-4.988807000	3.306697000
H	3.046119000	-4.018865000	3.729194000
H	3.628850000	-1.816379000	2.692075000
H	2.953995000	-1.891100000	-3.014078000
H	2.171543000	-4.135614000	-3.809465000
H	0.045190000	-5.080754000	-2.862741000
H	-1.189151000	-3.737824000	-1.128684000
H	2.978395000	-0.129315000	0.842678000
H	1.800501000	0.516754000	1.977252000
H	2.681331000	-0.062049000	-1.237124000
H	1.191224000	0.471316000	-1.997610000
Cl	5.547584000	-0.983642000	-0.744724000
O	5.342727000	-1.450920000	-2.152435000
O	4.869618000	0.348190000	-0.565239000
O	7.006327000	-0.837144000	-0.467394000
O	4.944360000	-1.971124000	0.205866000
Cl	1.474520000	5.386403000	0.018208000
O	2.231762000	4.092155000	-0.053431000
O	2.426847000	6.528549000	-0.094505000
O	0.749209000	5.462156000	1.328003000
O	0.484902000	5.441882000	-1.106390000
C	-6.362689000	-0.600799000	-2.049078000
C	-6.504046000	0.768741000	-1.801444000
C	-5.982996000	1.314546000	-0.623516000
C	-5.326686000	0.497983000	0.294152000
C	-5.178737000	-0.886713000	0.064735000
C	-5.708094000	-1.419095000	-1.129660000
H	-6.768073000	-1.032523000	-2.959637000
H	-7.017829000	1.403093000	-2.517531000
H	-6.093494000	2.375632000	-0.419648000
H	-4.929485000	0.926759000	1.210747000
H	-5.612218000	-2.480104000	-1.337259000
C	-4.464110000	-1.720933000	1.055677000
H	-3.231039000	-1.796936000	0.707353000
H	-4.383421000	-1.211980000	2.020533000
C	-4.845037000	-3.184875000	1.208916000
H	-4.730723000	-3.742617000	0.274765000
H	-4.213417000	-3.665271000	1.960968000
H	-5.889373000	-3.284844000	1.530919000

^{3}IH

Zero-point correction= 0.595846 (Hartree/Particle)
Thermal correction to Energy= 0.641729
Thermal correction to Enthalpy= 0.642674
Thermal correction to Gibbs Free Energy= 0.502413
Sum of electronic and zero-point Energies= -3193.379144
Sum of electronic and thermal Energies= -3193.333260
Sum of electronic and thermal Enthalpies= -3193.332316
Sum of electronic and thermal Free Energies= -3193.472577

Fe	-0.863590000	-0.762306000	0.297980000
N	1.025801000	-0.073104000	0.063832000
N	-0.922343000	0.654609000	1.705956000
N	-1.273823000	0.714304000	-0.986445000
N	-0.025263000	-2.053161000	1.550471000
N	-0.369269000	-2.014382000	-1.161409000
O	-2.522287000	-1.422207000	0.501216000
C	-1.679208000	0.708279000	2.811074000
C	-1.551467000	1.755105000	3.720974000
C	-0.611347000	2.754986000	3.473560000
C	0.182713000	2.691616000	2.324172000
C	-0.004779000	1.618637000	1.462783000
C	0.715315000	1.407247000	0.140619000
C	-0.320388000	1.674135000	-0.939931000
C	-0.352491000	2.786533000	-1.769919000
C	-1.411527000	2.897009000	-2.676622000
C	-2.388156000	1.903396000	-2.722129000
C	-2.286857000	0.814667000	-1.858633000
C	-0.650171000	-3.110931000	2.096462000
C	0.028253000	-4.018490000	2.900482000
C	1.392734000	-3.827693000	3.125887000
C	2.033855000	-2.730641000	2.553831000
C	1.289429000	-1.846632000	1.775357000
C	1.880302000	-0.586691000	1.187588000
C	1.541645000	-0.524536000	-1.272020000
C	0.852476000	-1.799499000	-1.695728000
C	1.398868000	-2.682167000	-2.624407000
C	0.644918000	-3.783988000	-3.026953000
C	-0.627622000	-3.978996000	-2.487814000
C	-1.100353000	-3.075036000	-1.543564000
H	-2.390349000	-0.098249000	2.947029000
H	-2.181126000	1.778153000	4.602544000
H	-0.492368000	3.578443000	4.169797000
H	0.922139000	3.453550000	2.096597000
H	1.602716000	2.039079000	0.040075000
H	0.425804000	3.540881000	-1.702840000
H	-1.468496000	3.752399000	-3.341606000
H	-3.224561000	1.962537000	-3.408094000
H	-3.018719000	0.014956000	-1.847844000
H	-1.704984000	-3.198289000	1.864355000
H	-0.503480000	-4.860284000	3.328392000
H	1.952839000	-4.528602000	3.735971000
H	3.095641000	-2.562203000	2.688090000
H	2.401711000	-2.512281000	-2.999269000
H	1.049342000	-4.485600000	-3.749061000
H	-1.241757000	-4.823423000	-2.778155000
H	-2.067499000	-3.170260000	-1.063859000
H	2.902247000	-0.755964000	0.840033000
H	1.928710000	0.176842000	1.969183000
H	2.627837000	-0.638694000	-1.242718000
H	1.321593000	0.250286000	-2.011752000
Cl	5.208028000	-2.197954000	-0.681791000
O	4.793575000	-2.692943000	-2.032543000
O	4.837614000	-0.744256000	-0.555297000
O	6.683636000	-2.347072000	-0.518690000
O	4.496332000	-2.978121000	0.379863000
Cl	2.906908000	4.924498000	-0.040318000
O	3.297877000	3.475441000	-0.073842000
O	4.125996000	5.772964000	-0.172064000
O	2.223332000	5.221174000	1.260473000
O	1.969646000	5.209629000	-1.174939000

C	-5.987025000	-0.553558000	-2.191400000
C	-6.098126000	0.817150000	-2.468904000
C	-6.083454000	1.738535000	-1.409469000
C	-5.963568000	1.300674000	-0.098991000
C	-5.856128000	-0.088797000	0.212863000
C	-5.868375000	-1.004784000	-0.882419000
H	-6.000185000	-1.272053000	-3.006438000
H	-6.199074000	1.161800000	-3.493531000
H	-6.169777000	2.801656000	-1.615921000
H	-5.957837000	2.020016000	0.716045000
H	-5.789409000	-2.069587000	-0.687950000
C	-5.751516000	-0.513251000	1.561908000
H	-3.194506000	-0.728132000	0.587137000
H	-5.749797000	0.259942000	2.326381000
C	-5.661880000	-1.941282000	2.003008000
H	-4.732021000	-2.414164000	1.656117000
H	-5.685399000	-2.016859000	3.092647000
H	-6.487724000	-2.547899000	1.606777000

^{5}TS

Zero-point correction= 0.590693 (Hartree/Particle)
Thermal correction to Energy= 0.636642
Thermal correction to Enthalpy= 0.637586
Thermal correction to Gibbs Free Energy= 0.496633
Sum of electronic and zero-point Energies= -3193.346198
Sum of electronic and thermal Energies= -3193.300250
Sum of electronic and thermal Enthalpies= -3193.299305
Sum of electronic and thermal Free Energies= -3193.440259

Fe	1.152158000	0.122961000	0.709462000
O	2.768393000	0.309279000	1.175243000
N	-0.968758000	-0.141677000	0.125344000
C	-1.036913000	-0.828858000	-1.196863000
C	-1.676190000	-0.915455000	1.186942000
C	-1.369906000	1.306000000	0.069560000
N	0.104873000	1.560418000	1.959632000
N	0.849243000	1.663061000	-0.803845000
N	1.326401000	-1.342056000	-0.844177000
N	0.558282000	-1.451319000	2.020277000
C	0.176610000	-1.695017000	-1.454380000
C	-0.737782000	-1.818952000	1.956322000
C	-1.200821000	-2.951968000	2.625355000
C	-0.306105000	-3.692422000	3.395488000
C	1.029528000	-3.291394000	3.472098000
C	1.426665000	-2.168085000	2.758606000
C	0.127816000	-2.773727000	-2.337406000
C	1.302012000	-3.472034000	-2.612736000
C	2.492793000	-3.082788000	-1.995738000
C	2.461352000	-2.016488000	-1.106178000
C	1.770600000	2.244719000	-1.584938000
C	1.422488000	3.209200000	-2.527851000
C	0.081186000	3.568760000	-2.655106000
C	-0.878990000	2.959761000	-1.841823000
C	-0.450611000	2.006265000	-0.924560000
C	-1.084885000	1.921681000	1.434023000
C	-1.928449000	2.824534000	2.072310000
C	-1.513959000	3.362373000	3.294283000
C	-0.284120000	2.985597000	3.833140000
H	1.467969000	1.744809000	3.500869000
H	0.065559000	3.385358000	4.777884000
H	-2.149342000	4.068053000	3.819398000
H	-2.879275000	3.098205000	1.624357000
H	-2.420414000	1.437740000	-0.209865000
H	-2.121114000	-0.212916000	1.897757000
H	-2.498485000	-1.501719000	0.766886000
H	-1.949049000	-1.425659000	-1.286219000
H	-1.078618000	-0.071154000	-1.984972000
H	-2.239029000	-3.245854000	2.520595000
H	-0.820494000	-3.059080000	-2.778568000
H	-0.645194000	-4.577035000	3.924668000
H	1.287358000	-4.314287000	-3.296887000
H	1.753913000	-3.842802000	4.060113000
H	2.452313000	-1.816532000	2.754949000
H	3.347419000	-1.678336000	-0.580162000
H	3.425706000	-3.600158000	-2.186986000
H	2.797967000	1.925673000	-1.441862000
H	2.189874000	3.663177000	-3.143982000
H	-0.219705000	4.315744000	-3.382384000
Cl	-4.980175000	3.260961000	-0.873778000
O	-4.136404000	4.049493000	-1.829471000
O	-4.538403000	1.826805000	-0.891723000
O	-4.815849000	3.811308000	0.511046000
O	-6.412722000	3.347013000	-1.280215000
Cl	-3.521946000	-4.222843000	-0.752762000
O	-2.290565000	-5.026016000	-0.488597000
O	-3.865201000	-3.410975000	0.464554000
O	-4.660656000	-5.130130000	-1.080869000
O	-3.278144000	-3.290948000	-1.906385000
H	-1.930894000	3.219764000	-1.913887000
C	0.502706000	2.074783000	3.132312000
C	6.314605000	-0.634480000	-0.443785000
C	6.787040000	-0.830063000	-1.738833000
C	6.817430000	0.238338000	-2.641912000
C	6.372850000	1.501642000	-2.236454000
C	5.899420000	1.698048000	-0.940722000
C	5.866776000	0.633989000	-0.014791000
H	6.299292000	-1.464960000	0.257444000
H	7.136420000	-1.811701000	-2.044655000
H	7.185732000	0.088515000	-3.652286000
H	6.398286000	2.334960000	-2.932347000
H	5.562684000	2.685357000	-0.641563000
C	5.332313000	0.792440000	1.360160000
H	4.162658000	0.542749000	1.271008000
H	5.683709000	-0.011675000	2.015906000
C	5.410785000	2.154263000	2.037340000
H	4.893974000	2.932071000	1.467871000
H	4.954564000	2.109920000	3.029982000
H	6.454834000	2.467199000	2.159638000

^{5}IH

Zero-point correction= 0.591966 (Hartree/Particle)
Thermal correction to Energy= 0.639370
Thermal correction to Enthalpy= 0.640314
Thermal correction to Gibbs Free Energy= 0.495841
Sum of electronic and zero-point Energies= -3193.371198
Sum of electronic and thermal Energies= -3193.323794
Sum of electronic and thermal Enthalpies= -3193.322850
Sum of electronic and thermal Free Energies= -3193.467324

Fe	-1.240867000	0.441063000	0.597322000
O	-2.970470000	0.682121000	1.027142000
N	0.952502000	0.190986000	0.085334000
C	1.228955000	0.813887000	-1.240277000
C	1.770092000	0.811981000	1.164643000
C	1.011914000	-1.306885000	0.074239000
N	-0.548339000	-1.168643000	1.910222000
N	-1.193258000	-1.178257000	-0.894374000
N	-0.985224000	1.837454000	-1.015216000
N	-0.296939000	1.903829000	1.859952000
C	0.228355000	1.893705000	-1.596527000
C	1.049437000	1.968189000	1.821975000
C	1.739510000	3.021024000	2.421935000
C	1.015492000	4.000460000	3.100448000
C	-0.376775000	3.910465000	3.157490000
C	-0.999219000	2.849775000	2.511557000
C	0.529849000	2.876137000	-2.540606000
C	-0.455984000	3.791952000	-2.900939000

C	-1.717290000	3.712931000	-2.305663000
C	-1.940313000	2.724296000	-1.356857000
C	-2.183719000	-1.553723000	-1.718074000
C	-2.018416000	-2.589921000	-2.634028000
C	-0.788660000	-3.244829000	-2.690525000
C	0.244015000	-2.850315000	-1.835361000
C	-0.000565000	-1.806295000	-0.949192000
C	0.542313000	-1.805595000	1.435915000
C	1.136063000	-2.860188000	2.121555000
C	0.573589000	-3.255190000	3.338560000
C	-0.551436000	-2.591221000	3.827078000
H	-1.961252000	-0.993159000	3.408261000
H	-1.010075000	-2.872720000	4.767785000
H	1.014328000	-4.072930000	3.899349000
H	2.010106000	-3.358055000	1.712358000
H	2.013107000	-1.688124000	-0.152602000
H	1.962056000	0.061138000	1.936708000
H	2.745315000	1.126091000	0.782012000
H	2.244498000	1.218386000	-1.271252000
H	1.175767000	0.041903000	-2.014081000
H	2.819075000	3.075815000	2.332782000
H	1.526455000	2.923278000	-2.963597000
H	1.531920000	4.829282000	3.573723000
H	-0.241647000	4.563316000	-3.633479000
H	-0.972212000	4.652697000	3.676232000
H	-2.077704000	2.735631000	2.493620000
H	-2.889290000	2.618260000	-0.842610000
H	-2.508952000	4.407994000	-2.559983000
H	-3.120826000	-1.014154000	-1.630683000
H	-2.839100000	-2.870700000	-3.283784000
H	-0.630165000	-4.054468000	-3.395386000
Cl	4.081276000	-4.153208000	-0.626009000
O	3.158079000	-4.644762000	-1.700092000
O	4.027506000	-2.654496000	-0.575834000
O	3.649153000	-4.707792000	0.697992000
O	5.475268000	-4.593277000	-0.922971000
Cl	4.694056000	3.130868000	-0.650121000
O	4.693407000	3.676485000	0.744911000
O	4.588937000	1.631975000	-0.594567000
O	5.961169000	3.512842000	-1.340188000
O	3.520956000	3.679169000	-1.402897000
H	1.213004000	-3.340472000	-1.852383000
C	-1.087359000	-1.545449000	3.079694000
C	-6.522226000	0.774247000	0.200793000
C	-6.998291000	1.375753000	-0.954442000
C	-6.991220000	0.678063000	-2.172036000
C	-6.503108000	-0.635929000	-2.213024000
C	-6.022562000	-1.249180000	-1.063147000
C	-6.012677000	-0.559532000	0.186061000
H	-6.533718000	1.318447000	1.141582000
H	-7.381640000	2.391255000	-0.914100000
H	-7.365001000	1.150423000	-3.075140000
H	-6.504618000	-1.183399000	-3.151269000
H	-5.661663000	-2.271145000	-1.114234000
C	-5.517245000	-1.139643000	1.384550000
H	-3.733360000	0.075531000	1.067553000
H	-5.640944000	-0.559659000	2.297496000
C	-5.012178000	-2.540600000	1.529310000
H	-4.443856000	-2.877944000	0.656622000
H	-4.370666000	-2.634579000	2.409913000
H	-5.842320000	-3.251734000	1.662406000