High-Valent Nonheme Fe(IV)-Oxo/Ru(IV)-Oxo Complexes Catalyze C-H Activation Reactivity and Hydrogen Tunnelling: A Comparative DFT Investigation

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

Reactions	Spin state	Species	B1+ZPE	B2+ZPE	B2+ G^{corr}
1+BA	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	13.0	12.5	23.6
		^{3}IH	-0.3	-5.7	-5.6
1'+BA	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	8.0	9.6	20.9
		^{3}IH	-6.8	-13.5	-14.4
	S=2	^{5}R+S	5.7	4.4	3.1
		^{5}TS	11.6	9.1	18.9
		^{5}IH	-2.8	-14.9	-17.3
1+EB	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	16.3	16.1	28.5
		^{3}IH	6.5	0.2	-0.6
1'+EB	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	13.6	12.8	24.0
		^{3}IH	-3.4	-8.5	-9.1
	S=2	^{5}R+S	5.7	4.4	3.1
		^{5}TS	15.1	11.3	21.2
		^{5}IH	3.1	-9.5	-12.4

2+EB	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	24.2	24.3	36.5
		^{3}IH	3.4	-1.9	-4.0
2'+EB	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	26.8	26.7	40.1
		^{3}IH	4.7	-0.7	-1.1
	S=2	^{5}R+S	1.3	3.5	4.6
		^{5}TS	19.9	13.7	25.8
		^{5}IH	3.08	-5.0	-5.3
2+DHA	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	21.6	18.8	31.2
		^{3}IH	-0.3	-4.2	5.1
2'+DHA	S=1	^{3}R+S	0.0	0.0	0.0
		^{3}TS	25.0	22.9	36.2
		^{3}IH	-0.4	-5.8	4.5
	S=2	^{5}R+S	1.3	3.5	4.6
		^{5}TS	14.4	9.6	23.2
		^{5}IH	-1.9	-13.3	-4.6

Table S2 Calculated energy of activation and free energy of activation (kcal mol^{-1}) are given as B2+ZPE/B2+G^{corr}_{298K} level of theory.

Complex	Aliphatic hydroxylation $\Delta E/\Delta G^{‡}$	Aromatic hydroxylation $\Delta E/\Delta G^{‡}$
1+EB	16.1/28.5	27.9/39.8
1'+EB	11.3/21.2	15.2/24.5

Table S3 Calculated and experimental bond dissociation energy and enthalpy (kcal mol^{-1}) computed at B3LYP/ and CBS-QB3 method.

	B3LYP		CBS-QB3		Experiment
Substrate	ΔE_{BDE}	ΔH_{BDE}	ΔE_{BDE}	ΔH_{BDE}	
BA	77.2	78.6	76.8	78.1	79.0*
EB	83.1	84.6	82.6	84.2	85.4**

* *J. Org. Chem.* **2005**, *70*, 9521-9528 ** J. Org. Chem. 2019, 84, 13549−13556

Table S4 Calculated % Volume buried and %free space for oxidants computed on the geometry optimized at B1 level of theory

Oxidants	Spin state	% Volume buried	% Free space
1	S=1	89.6	10.4
1'	S=2	89.1	10.9
2	S=1	97.2	2.8
2'	S=2	96.6	3.4

Table S5 Kinetic Isotope Effect (KIE) at 298K computed using different methods**.**

Reactions	Spin state	KIE_{Eyr}	KIE_{Eck}	KIE_{W}
1+BA	S=1	6.5	48.3**(54.5)***	9.9
1'+BA	S=1	5.9	16.4	8.3
	S=2	3.4	3.6	3.6
1+EB	S=1	5.1	27.6	7.7
1'+EB	S=1	5.1	30.4	7.5
	S=2	3.7	4.6	4.2
2+EB	S=1	5.6	127.6	8.6
2'+EB	S=1	5.6	31.1	8.8
	S=2	5.9	73.2	8.6
2+DHA	S=1	6.5	253.8	9.9
2'+DHA	S=1	6.2	658.1	9.7
	S=2	6.3	80.6 **(58)***	9.5

*Experimental value

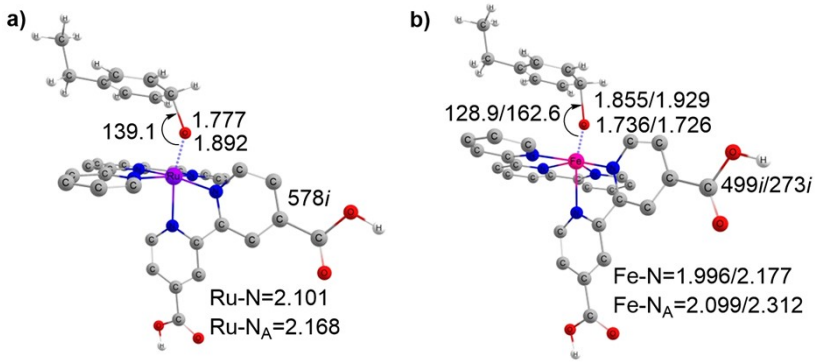

Fig. S1 Optimized geometries of (a) ^3TS_O (b) ^5TS_O with key geometrical parameters computed at B1 level of theory (distances are in Å and angles are in degree).

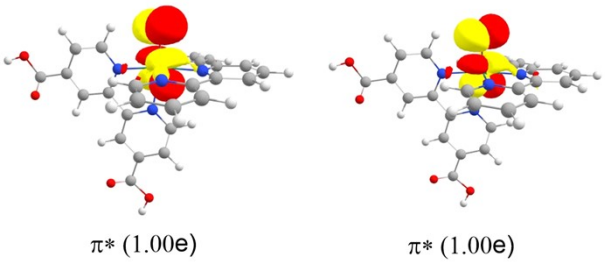

Fig. S2 Spin natural orbitals and their occupations for the oxidant 1.

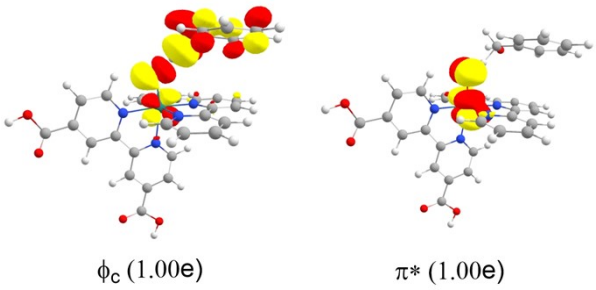

Fig. S3 Spin natural orbitals and their occupations for the transition states of the reaction between complex 1 and BA.

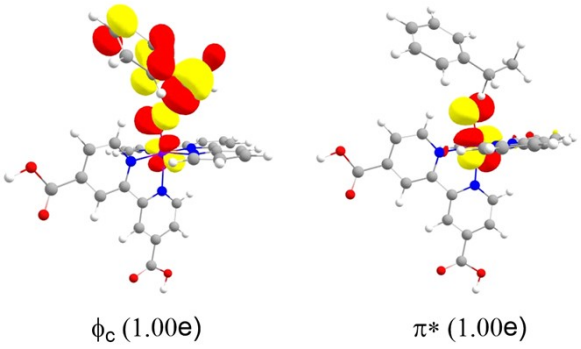

Fig. S4 Spin natural orbitals and their occupations for the transition states of the reaction between complex 1 and EB.

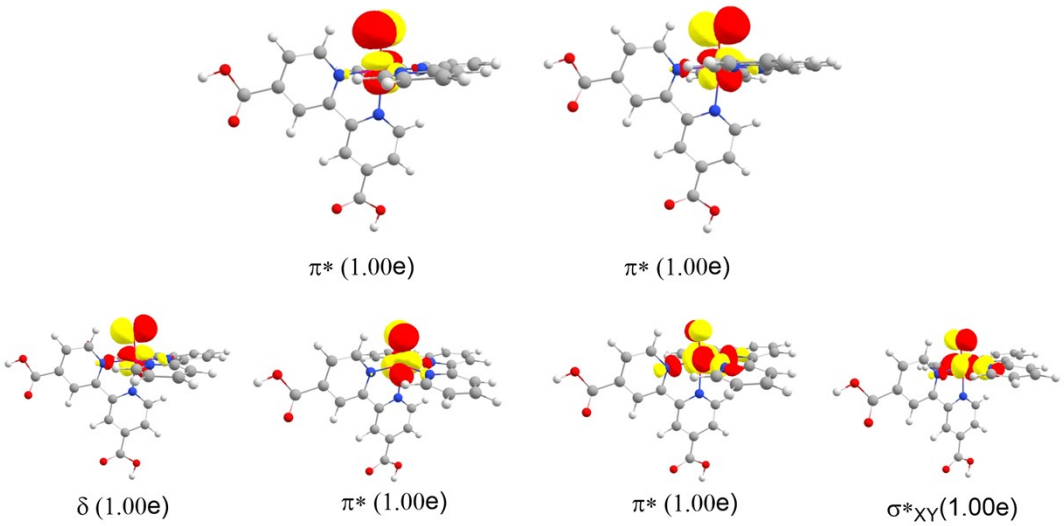

Fig. S5 Spin natural orbitals and their occupations for the oxidants of the complex 1'. Upper panel represents ^{3}R while bottom panel represents ^{5}R.

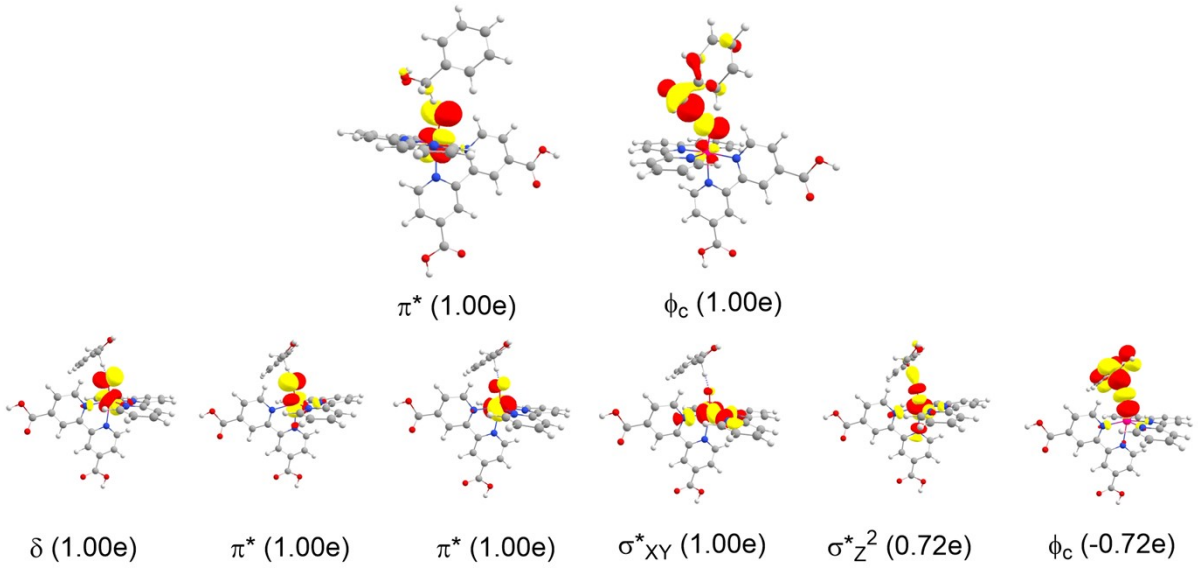

Fig. S6 Spin natural orbitals and their occupations for the transition states of the reaction between complex 1' and BA. Upper panel represents ^{3}R while bottom panel represents ^{5}R.

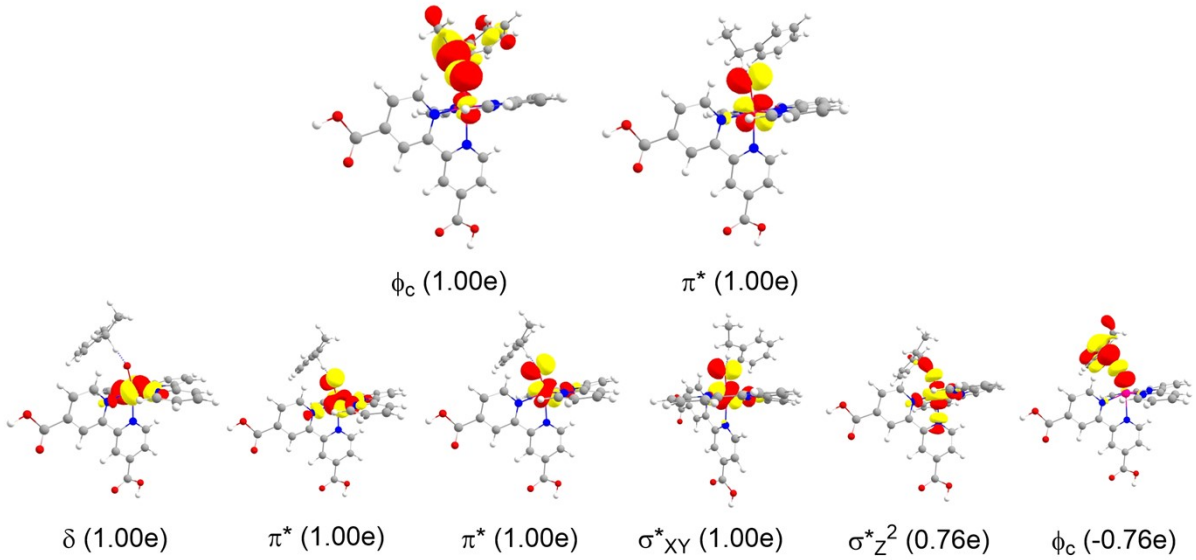

Fig. S7 Spin natural orbitals and their occupations for the transition states of the reaction between the complex 1' and EB. Upper panel represents ^{3}R while bottom panel represents ^{5}R.

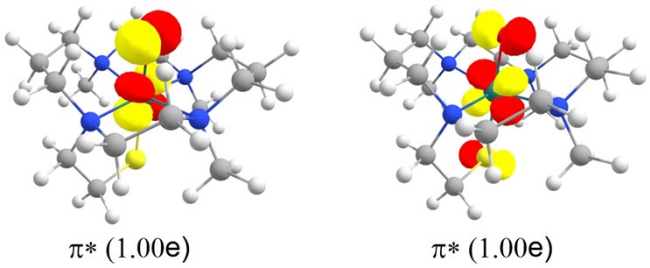

Fig. S8 Spin natural orbitals and their occupations for the oxidant of the complex 2.

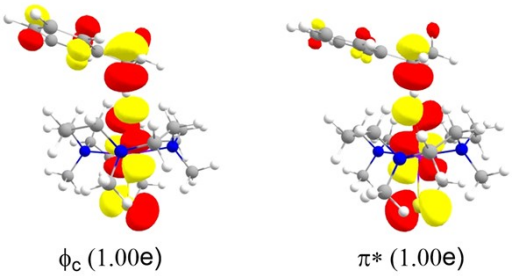

Fig. S9 Spin natural orbitals and their occupations for the transition states of the reaction between complex 2 and EB.

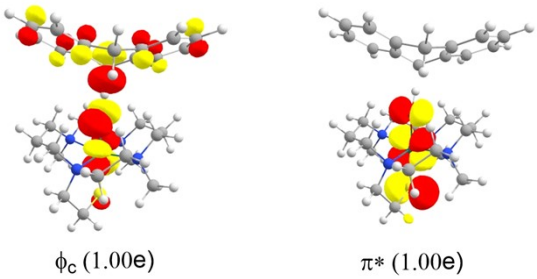

Fig. S10 Spin natural orbitals and their occupations for the transition states of the reaction between complex 2 and DHA.

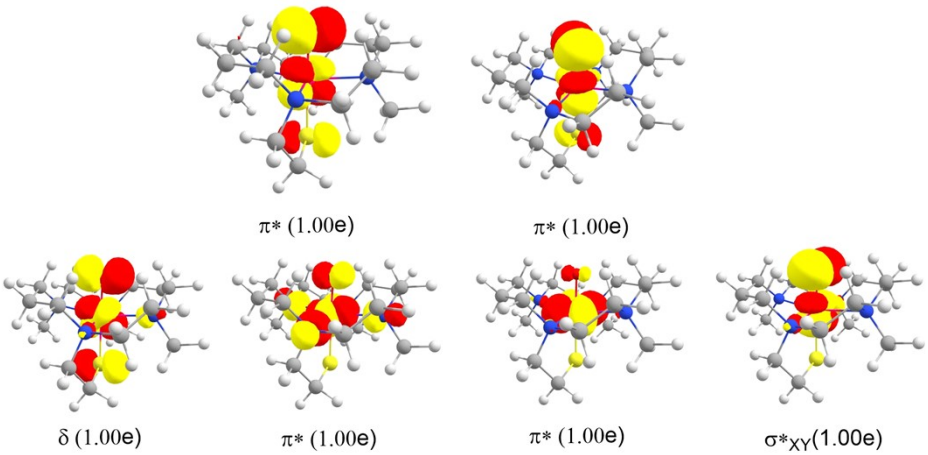

Fig. 11 Spin natural orbitals and their occupations for the oxidants of the complex 2'. Upper panel represents ^{3}R while bottom panel represents ^{5}R.

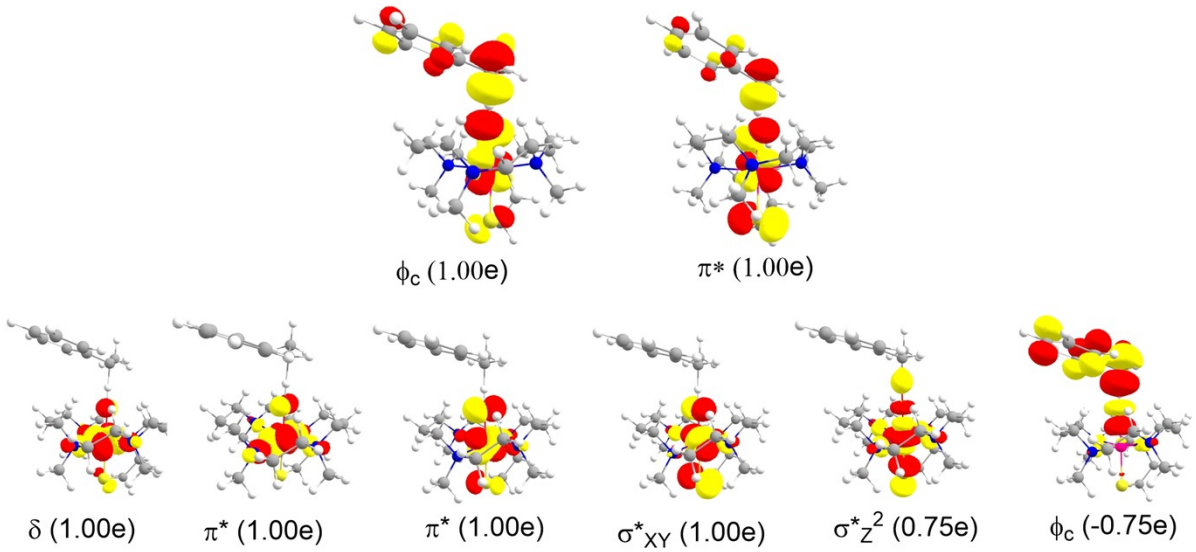

Fig. S12 Spin natural orbitals and their occupations for the transition states of the reaction between the complex 2' and EB. Upper panel represents ^{3}R while bottom panel represents ^{5}R.

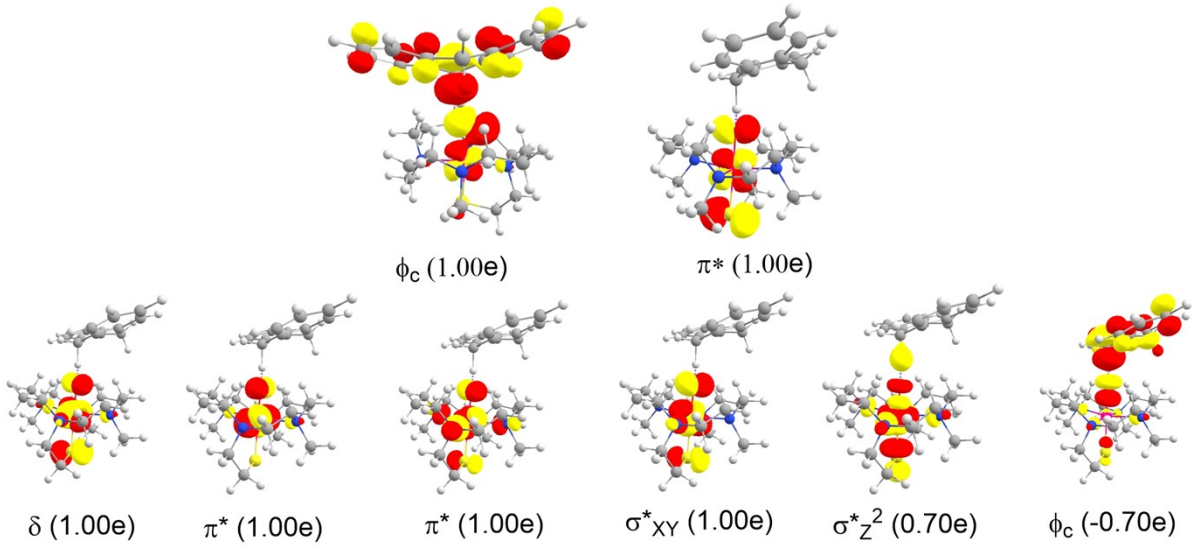

Fig. S13 Spin natural orbitals and their occupations for the transition states of the reaction between the complex 2' and DHA. Upper panel represents ^{3}R while bottom panel represents ^{5}R.

Table S6 Mulliken spin densities and charges for all the investigated oxidants

Species	Spin State	Mulliken Spin Density			Mulliken Charges		
1		**Fe/Ru**	**O**	**Rest**	**Fe/Ru**	**O**	**Rest**
	S=1	0.950	1.015	0.035	1.037	-0.467	-0.57
1'	S=1	1.097	0.948	-0.045	0.591	-0.381	-0.21
	S=2	2.941	0.761	0.298	0.787	-0.368	-0.419
2	S=1	1.012	0.820	0.168	0.404	-0.612	0.208
2'	S=1	1.312	0.741	-0.053	0.171	-0.571	0.4
	S=2	3.122	0.685	0.193	0.272	-0.582	0.31

Table S7 Mulliken spin densities and charges of stationary points along S=1 and S=2.

Oxidant	Species	Mulliken Spin Density					Mulliken Charges				
1+BA		**Fe/Ru**	**O**	**H**	**C**	**Rest**	**Fe/Ru**	**O**	H	C	**Rest**
	^{3}TS	0.746	0.710	-0.045	0.361	0.228	0.987	-0.642	0.346	-0.144	-0.547
	^{3}I	0.812	0.156	-0.005	0.622	0.415	0.976	-0.762	0.417	-0.012	-0.619
1'+BA	**^{3}TS**	0.858	0.717	-0.043	0.332	0.136	0.574	-0.542	0.323	-0.149	-0.206
	^{3}I	0.983	0.080	-0.004	0.579	0.362	0.564	-0.739	0.421	-0.002	-0.244
	^{5}TS	3.702	0.312	-0.001	-0.170	0.157	0.858	-0.559	0.293	-0.144	-0.448
	^{5}I	2.814	0.170	0.009	0.517	0.49	0.699	-0.786	0.420	0.017	-0.35
1+EB	**^{3}TS**	0.696	0.735	-0.039	0.415	0.193	0.967	-0.610	0.360	-0.400	-0.317

	^{3}**I**	0.699	0.305	0.000	0.732	0.264	0.944	-0.711	0.428	-0.245	-0.416
1'+EB	^{3}**TS**	0.848	0.715	-0.049	0.412	0.074	0.567	-0.538	0.339	-0.396	0.028
	^{3}**I**	0.835	0.220	-0.006	0.738	0.213	0.538	-0.686	0.473	-0.192	-0.133
	^{5}**TS**	3.754	0.288	0.006	-0.255	0.207	0.865	-0.577	0.328	-0.402	-0.214
	^{5}**I**	4.002	0.413	-0.014	-0.659	0.258	0.876	-0.759	0.438	-0.261	-0.294
2-EB	^{3}**TS**	0.784	0.512	-0.066	0.414	0.356	0.297	-0.726	0.345	-0.390	0.474
	^{3}**I**	0.633	0.076	-0.004	0.758	0.537	0.221	-0.791	0.377	-0.180	0.373
2'-EB	^{3}**TS**	1.022	0.524	-0.067	0.411	0.11	0.145	-0.704	0.324	-0.383	0.618
	^{3}**I**	0.906	0.062	-0.004	0.758	0.278	0.079	-0.782	0.372	-0.183	0.514
	^{5}**TS**	3.719	0.107	0.040	-0.386	0.52	0.370	-0.760	0.349	-0.399	0.44
	^{5}**I**	3.902	0.221	0.003	-0.757	0.631	0.300	-0.812	0.385	-0.190	0.317
2-DHA	^{3}**TS**	0.826	0.527	-0.060	0.310	0.397	0.316	-0.722	0.347	-0.539	0.598
	^{3}**I**	0.636	0.076	-0.003	0.626	0.665	0.220	-0.794	0.380	-0.305	0.499
2'+DHA	^{3}**TS**	1.059	0.532	-0.060	0.303	0.166	0.167	-0.700	0.323	-0.534	0.744
	^{3}**I**	0.909	0.065	-0.003	0.621	0.408	0.071	-0.779	0.370	-0.295	0.633
	^{5}**TS**	3.664	0.173	0.037	-0.284	0.41	0.358	-0.755	0.349	-0.546	0.594
	^{5}**I**	3.895	0.228	0.005	-0.619	0.491	0.289	-0.814	0.384	-0.295	0.436

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

Complex 1

Zero-point correction= 0.457518 (Hartree/Particle)
Thermal correction to Energy= 0.500371
Thermal correction to Enthalpy= 0.501315
Thermal correction to Gibbs Free Energy=0.374772
Sum of electronic and zero-point Energies= -3305.138471
Sum of electronic and thermal Energies= 3305.095618
Sum of electronic and thermal Enthalpies= -3305.094674
Sum of electronic and thermal Free Energies= -3305.2212

Ru	-0.362291000	-1.212247000	-0.806819000
N	0.158604000	-2.226876000	0.985851000
N	-2.186548000	-1.717654000	-0.102528000
N	-1.640287000	-0.263869000	-2.237460000
N	1.554551000	-0.468087000	-1.406317000
N	-0.155191000	0.715596000	0.276548000
O	-0.188720000	-2.678141000	-1.814811000
C	2.362587000	-1.135784000	-2.250030000
C	1.966270000	0.705761000	-0.861164000
C	3.617803000	-0.662019000	-2.604144000
H	1.970126000	-2.073966000	-2.626088000
C	3.211664000	1.240817000	-1.191622000
H	4.250529000	-1.235657000	-3.269689000
H	3.567327000	2.164996000	-0.756266000
C	4.047782000	0.551382000	-2.063756000
C	1.026226000	1.356573000	0.072938000
C	-1.073829000	1.249180000	1.097211000
C	1.303715000	2.560192000	0.716868000
C	-0.861902000	2.453789000	1.763643000
H	-2.016415000	0.727200000	1.216087000
H	2.246582000	3.074428000	0.585074000
H	-1.640579000	2.855574000	2.399722000
C	0.349614000	3.115688000	1.570994000
C	0.677953000	4.420193000	2.229661000
O	-0.264963000	4.800735000	3.114885000
O	1.675872000	5.065120000	1.992245000
H	0.027074000	5.655774000	3.483671000
C	5.385407000	1.151016000	-2.366341000
O	6.183450000	0.304995000	-3.050590000
O	5.709253000	2.273639000	-2.050586000
H	7.034691000	0.766534000	-3.171839000
C	-0.934841000	-2.689319000	1.670150000
C	1.388846000	-2.406524000	1.480312000
C	-0.776731000	-3.334550000	2.893023000
C	1.603789000	-3.033382000	2.711554000
H	2.226193000	-2.045195000	0.891807000
H	-1.643843000	-3.691716000	3.436869000
H	2.621825000	-3.110615000	3.078536000
C	-3.268112000	-1.350367000	-0.819401000
C	-2.248449000	-2.439291000	1.035410000
C	-4.531965000	-1.776144000	-0.408489000
C	-3.495439000	-2.869302000	1.493392000
H	-5.421571000	-1.481042000	-0.944864000
H	-3.583830000	-3.447984000	2.405070000
C	-2.963195000	-0.491587000	-1.987033000
C	-1.282823000	0.514231000	-3.267660000
C	-3.949294000	0.096402000	-2.778727000
C	-2.219314000	1.109159000	-4.107661000
H	-0.217311000	0.654641000	-3.410063000
H	-4.992649000	-0.018867000	-2.516166000
H	-1.885797000	1.733105000	-4.929592000
C	-3.572640000	0.901385000	-3.850302000
C	-4.630575000	-2.538083000	0.755369000

C	0.506744000	-3.500452000	3.423671000
H	-4.331900000	1.375573000	-4.463894000
H	-5.607945000	-2.858251000	1.100672000
H	0.635077000	-3.986618000	4.385959000
Cl	-4.753823000	1.618293000	0.582059000
Cl	4.430324000	-0.606818000	1.561279000
O	5.493899000	0.344089000	1.144097000
O	4.126463000	-1.543782000	0.410521000
O	4.841924000	-1.408679000	2.746676000
O	3.165793000	0.150036000	1.881744000
O	-5.357107000	2.774741000	1.279658000
O	-4.159568000	0.658267000	1.586437000
O	-5.792093000	0.890516000	-0.226210000
O	-3.653072000	2.070756000	-0.338012000

Complex ^{3}1'

Zero-point correction= 0.458825 (Hartree/Particle)
Thermal correction to Energy= 0.501191
Thermal correction to Enthalpy= 0.502135
Thermal correction to Gibbs Free Energy= 0.377526
Sum of electronic and zero-point Energies= -3334.683092
Sum of electronic and thermal Energies= -3334.640726
Sum of electronic and thermal Enthalpies= -3334.639782
Sum of electronic and thermal Free Energies= -3334.764

Fe	0.304143000	-1.418130000	0.714022000
N	0.889215000	-2.802636000	-0.663900000
N	2.197589000	-1.304726000	0.949820000
N	0.346549000	0.102152000	1.998936000
N	-1.650607000	-1.406781000	0.267759000
N	0.248821000	0.029424000	-0.817624000
O	0.114629000	-2.549979000	1.871234000
C	-2.545589000	-2.200776000	0.880913000
C	-2.061172000	-0.553292000	-0.704016000
C	-3.892131000	-2.195673000	0.540750000
H	-2.145595000	-2.835111000	1.663331000
C	-3.393027000	-0.521591000	-1.112199000
H	-4.591602000	-2.827600000	1.073378000
H	-3.736184000	0.157841000	-1.880973000
C	-4.320354000	-1.344274000	-0.479565000
C	-1.003215000	0.299212000	-1.269327000
C	1.286090000	0.748517000	-1.271187000
C	-1.236516000	1.319710000	-2.186904000
C	1.127010000	1.783504000	-2.192339000
H	2.278389000	0.511348000	-0.907086000
H	-2.235762000	1.565234000	-2.522721000
H	1.997940000	2.342434000	-2.513555000
C	-0.156442000	2.072035000	-2.654690000
C	-0.440461000	3.160131000	-3.645568000
O	0.657920000	3.880128000	-3.944433000
O	-1.532583000	3.363114000	-4.129398000
H	0.381442000	4.564475000	-4.582895000
C	-5.747205000	-1.258353000	-0.927330000
O	-6.585608000	-1.895899000	-0.086293000
O	-6.100826000	-0.703164000	-1.942668000
H	-7.486912000	-1.751607000	-0.431493000
C	2.232571000	-3.021275000	-0.652997000
C	0.108213000	-3.510951000	-1.487615000
C	2.811073000	-3.967963000	-1.499738000
C	0.621181000	-4.472109000	-2.355254000
H	-0.953290000	-3.297446000	-1.441110000
H	3.883782000	-4.122609000	-1.489715000
H	-0.048049000	-5.021597000	-3.008015000
C	2.667243000	-0.407689000	1.830040000
C	2.983723000	-2.177961000	0.295017000
C	4.034085000	-0.378750000	2.118714000
C	4.352893000	-2.192975000	0.544673000
H	4.445192000	0.361727000	2.791249000
H	5.011091000	-2.874105000	0.018691000
C	1.609793000	0.456448000	2.377660000
C	-0.706691000	0.796723000	2.441027000
C	1.830022000	1.563856000	3.187482000
C	-0.549359000	1.915603000	3.264354000
H	-1.698832000	0.476586000	2.142253000
H	2.842226000	1.863477000	3.430042000
H	-1.437525000	2.459538000	3.567885000
C	0.732424000	2.307037000	3.631745000
C	4.870978000	-1.279431000	1.466687000
C	1.996415000	-4.700370000	-2.360071000
H	0.888552000	3.186327000	4.248945000
H	5.938718000	-1.239816000	1.646900000
H	2.432388000	-5.438393000	-3.026193000
Cl	-4.022757000	1.822576000	1.357629000
O	-4.221949000	2.925467000	2.331496000
O	-5.227806000	1.621466000	0.503088000
O	-3.733747000	0.537294000	2.103969000
O	-2.830866000	2.124114000	0.483508000
Cl	4.765448000	1.801369000	-0.346143000
O	4.368933000	0.560491000	-1.117257000
O	3.606818000	2.178598000	0.543819000
O	5.059450000	2.903042000	-1.292472000
O	5.951920000	1.483520000	0.504752000

Complex ^{5}1'

Zero-point correction= 0.457083 (Hartree/Particle)
Thermal correction to Energy= 0.500238
Thermal correction to Enthalpy= 0.501182
Thermal correction to Gibbs Free Energy= 0.373817
Sum of electronic and zero-point Energies= -3334.674028
Sum of electronic and thermal Energies= -3334.630874
Sum of electronic and thermal Enthalpies= -3334.629929
Sum of electronic and thermal Enthalpies= -3334.757295

Fe	0.215196000	-1.090618000	-1.057645000
N	1.551708000	0.095882000	-2.333589000
N	2.153169000	-1.678241000	-0.501080000
N	-0.086815000	-2.436665000	0.607054000
N	-1.615397000	-0.267547000	-1.484255000
N	0.158466000	0.512712000	0.280389000
O	0.042615000	-2.263182000	-2.168374000
C	-2.458687000	-0.781115000	-2.396477000
C	-1.985945000	0.802329000	-0.735459000
C	-3.716457000	-0.238675000	-2.620003000
H	-2.093964000	-1.649055000	-2.934191000
C	-3.227209000	1.403953000	-0.924555000
H	-4.385239000	-0.685511000	-3.344656000
H	-3.551608000	2.244547000	-0.325688000
C	-4.103415000	0.873152000	-1.868133000
C	-0.987587000	1.245812000	0.250967000
C	1.137600000	0.845566000	1.133155000
C	-1.168750000	2.330829000	1.100006000
C	1.024589000	1.927608000	2.006395000
H	2.051679000	0.266060000	1.121674000
H	-2.083717000	2.909147000	1.098455000
H	1.854923000	2.168360000	2.657904000
C	-0.148611000	2.676830000	1.990605000
C	-0.369830000	3.864675000	2.877124000
O	0.625691000	4.031791000	3.768429000
O	-1.334395000	4.593669000	2.797392000
H	0.406156000	4.826447000	4.290731000
C	-5.443743000	1.528198000	-2.014934000
O	-6.286442000	0.801316000	-2.775251000
O	-5.726351000	2.596931000	-1.523583000
H	-7.135773000	1.282006000	-2.786372000

C	2.870099000	-0.138579000	-2.163555000
C	1.147907000	1.040568000	-3.190613000
C	3.832327000	0.615380000	-2.840004000
C	2.046809000	1.810687000	-3.922712000
H	0.075238000	1.177234000	-3.286089000
H	4.883051000	0.483507000	-2.616539000
H	1.679974000	2.567600000	-4.607566000
C	2.291209000	-2.614606000	0.451640000
C	3.200757000	-1.211446000	-1.198020000
C	3.549539000	-3.154971000	0.727920000
C	4.481076000	-1.726461000	-0.980623000
H	3.673727000	-3.910056000	1.494878000
H	5.333163000	-1.349011000	-1.526606000
C	1.031022000	-2.987379000	1.133861000
C	-1.288492000	-2.704910000	1.128673000
C	0.955699000	-3.826768000	2.244699000
C	-1.433390000	-3.528138000	2.248446000
H	-2.158290000	-2.260861000	0.652464000
H	1.854466000	-4.254073000	2.674476000
H	-2.427278000	-3.686764000	2.653003000
C	-0.293755000	-4.092066000	2.811743000
C	4.644607000	-2.706691000	-0.005657000
C	3.411666000	1.597958000	-3.731039000
H	-0.365942000	-4.731307000	3.686583000
H	5.632375000	-3.109488000	0.192705000
H	4.144251000	2.203376000	-4.255445000
Cl	-4.382996000	-0.859052000	1.427987000
O	-4.844630000	-1.783987000	2.495035000
O	-5.426449000	0.146546000	1.082473000
O	-4.042278000	-1.655958000	0.185543000
O	-3.128277000	-0.152529000	1.875472000
Cl	4.772696000	1.383166000	0.769638000
O	5.416640000	2.360763000	1.674827000
O	3.657239000	2.035657000	-0.002550000
O	4.182478000	0.246972000	1.572155000
O	5.772993000	0.824582000	-0.201679000

Complex 2

Zero-point correction= 0.529867 (Hartree/Particle)
Thermal correction to Energy= 0.560911
Thermal correction to Enthalpy= 0.561855
Thermal correction to Gibbs Free Energy= 0.468299
Sum of electronic and zero-point Energies= -2338.644785
Sum of electronic and thermal Energies= -2338.613741
Sum of electronic and thermal Enthalpies= -2338.612797
Sum of electronic and thermal Free Energies= -2338.7063

Ru	1.671051000	0.045548000	0.129834000
C	-0.777540000	2.070975000	0.237189000
H	-1.156378000	3.012130000	0.658614000
H	-1.562386000	1.322209000	0.318986000
H	-0.547482000	2.198554000	-0.818929000
N	2.800019000	1.721847000	-0.787180000
N	0.439378000	1.648776000	0.993397000
C	2.789788000	1.781846000	-2.274575000
H	3.210513000	0.872370000	-2.698421000
H	3.373128000	2.648746000	-2.617107000
C	2.131634000	2.972884000	-0.280579000
H	1.404081000	3.277064000	-1.035478000
H	2.870577000	3.781597000	-0.196473000
C	4.212494000	1.628750000	-0.303041000
H	4.770397000	2.480464000	-0.722823000
H	4.190260000	1.729486000	0.783904000
C	4.952513000	0.331660000	-0.678251000
H	6.006474000	0.511044000	-0.427753000
H	4.942746000	0.175138000	-1.761771000
C	4.565351000	-0.950311000	0.074280000
H	5.324391000	-1.721582000	-0.126958000
H	4.563028000	-0.734080000	1.142318000
C	3.259508000	-2.167662000	-1.584893000
H	4.020744000	-2.961902000	-1.595473000
H	3.496753000	-1.429223000	-2.349668000
H	2.285822000	-2.582458000	-1.835189000
N	0.486563000	-1.604208000	0.887927000
N	3.220545000	-1.523515000	-0.251298000
S	0.445614000	-0.364074000	-1.934591000
C	-0.780458000	-1.827384000	0.092554000
H	-1.498825000	-1.054969000	0.356188000
H	-1.213732000	-2.787077000	0.413654000
C	-0.575908000	-1.804339000	-1.412958000
H	-1.568736000	-1.710445000	-1.863585000
H	-0.115460000	-2.725020000	-1.794265000
C	2.843489000	-2.522252000	0.801158000
C	1.349945000	-2.831172000	0.774236000
H	1.087237000	-3.332763000	-0.158209000
H	1.108549000	-3.526937000	1.588377000
C	0.130289000	-1.338961000	2.321910000
H	-0.467173000	-2.192005000	2.675662000
H	1.068568000	-1.315343000	2.882668000
C	-0.671189000	-0.052929000	2.581180000
C	0.062801000	1.280606000	2.401798000
H	1.763398000	1.868506000	-2.629946000
C	1.430817000	2.769410000	1.055260000
H	2.158451000	2.517078000	1.827293000
H	0.923593000	3.701640000	1.342504000
H	0.990193000	1.259627000	2.975414000
H	-0.575910000	2.085451000	2.792520000
H	-0.938057000	-0.092269000	3.646481000
H	-1.625628000	-0.056388000	2.048448000
H	3.114109000	-2.084267000	1.762141000
H	3.414875000	-3.452896000	0.664944000
O	2.598636000	0.210208000	1.700029000
O	-3.354108000	0.049732000	0.855208000
O	-3.814625000	1.419855000	-1.175971000
C	-5.790451000	0.014873000	-0.115054000
F	-6.522239000	0.053857000	-1.239552000
F	-6.168142000	1.041315000	0.666164000
F	-6.077891000	-1.127824000	0.532316000
S	-3.976231000	0.115961000	-0.503797000
O	-3.725413000	-1.087067000	-1.331532000

Complex ^{3}2'

Zero-point correction= 0.531445 (Hartree/Particle)
Thermal correction to Energy= 0.562107
Thermal correction to Enthalpy= 0.563051
Thermal correction to Gibbs Free Energy= 0.470492
Sum of electronic and zero-point Energies= -2368.181659
Sum of electronic and thermal Energies= -2368.150997
Sum of electronic and thermal Enthalpies= -2368.150053
Sum of electronic and thermal Free Energies= -2368.2426

Fe	1.795650000	0.032583000	0.174770000
C	-0.668496000	1.969164000	0.210364000
H	-1.038255000	2.924081000	0.607779000
H	-1.462091000	1.235837000	0.325167000
H	-0.445985000	2.061317000	-0.849675000
N	2.928890000	1.635492000	-0.733537000
N	0.549244000	1.562250000	0.975319000
C	3.041227000	1.696897000	-2.217319000
H	3.493984000	0.790528000	-2.611085000
H	3.655249000	2.563342000	-2.503025000
C	2.209303000	2.878395000	-0.302873000

H	1.473753000	3.112621000	-1.074258000
H	2.914990000	3.719790000	-0.255968000
C	4.305835000	1.606956000	-0.151095000
H	4.848176000	2.486997000	-0.530520000
H	4.207740000	1.699401000	0.931191000
C	5.121064000	0.350592000	-0.481435000
H	6.139460000	0.543374000	-0.119477000
H	5.222890000	0.219428000	-1.563524000
C	4.668935000	-0.942564000	0.200469000
H	5.418470000	-1.727531000	0.016023000
H	4.614148000	-0.763943000	1.273714000
C	3.434367000	-2.053376000	-1.576018000
H	4.185384000	-2.857613000	-1.578506000
H	3.724562000	-1.291194000	-2.296979000
H	2.471031000	-2.441043000	-1.897351000
N	0.594230000	-1.532954000	0.804584000
N	3.333477000	-1.465273000	-0.219776000
S	0.715556000	-0.252727000	-1.888774000
C	-0.672695000	-1.698482000	-0.002758000
H	-1.377537000	-0.923115000	0.280963000
H	-1.132258000	-2.655967000	0.285739000
C	-0.431177000	-1.629886000	-1.497889000
H	-1.399659000	-1.444639000	-1.972102000
H	-0.029658000	-2.565743000	-1.907195000
C	2.906488000	-2.509516000	0.757434000
C	1.416879000	-2.776497000	0.638867000
H	1.186990000	-3.200229000	-0.338799000
H	1.111079000	-3.518102000	1.388040000
C	0.230638000	-1.358800000	2.250352000
H	-0.366976000	-2.234507000	2.541984000
H	1.163629000	-1.369113000	2.818272000
C	-0.573764000	-0.097101000	2.576130000
C	0.162427000	1.227685000	2.386189000
H	2.051089000	1.793068000	-2.659481000
C	1.513017000	2.700420000	1.031232000
H	2.238668000	2.484937000	1.815459000
H	0.980768000	3.625494000	1.293706000
H	1.083164000	1.215965000	2.969915000
H	-0.476253000	2.043514000	2.753630000
H	-0.803087000	-0.160096000	3.648728000
H	-1.544361000	-0.093247000	2.073132000
H	3.142190000	-2.136948000	1.754046000
H	3.467899000	-3.441263000	0.591060000
O	2.595234000	0.164256000	1.621633000
O	-3.295983000	0.036187000	0.883188000
O	-3.779536000	1.489236000	-1.084484000
C	-5.722207000	-0.023581000	-0.111517000
F	-6.445106000	0.047848000	-1.240159000
F	-6.137540000	0.951669000	0.714491000
F	-5.979866000	-1.204651000	0.476842000
S	-3.908742000	0.150449000	-0.476408000
O	-3.612770000	-1.001972000	-1.360239000

Complex ^{5}2'

Zero-point correction= 0.528726 (Hartee/Particle)
Thermal correction to Energy= 0.560264
Thermal correction to Enthalpy= 0.561208
Thermal correction to Gibbs Free Energy= 0.466078
Sum of electronic and zero-point Energies= -2368.183683
Sum of electronic and thermal Energies= -2368.152145
Sum of electronic and thermal Enthalpies= -2368.151201
Sum of electronic and thermal Free Energies= -2368.2463

Fe	1.763249000	0.038569000	0.184386000
C	-0.699143000	2.109456000	0.343927000
H	-1.062713000	3.051052000	0.781131000
H	-1.491218000	1.368076000	0.427636000
H	-0.491832000	2.248737000	-0.715813000
N	2.894249000	1.722143000	-0.791014000
N	0.522610000	1.664492000	1.065580000
C	2.907253000	1.816818000	-2.272115000
H	3.320744000	0.910940000	-2.711797000
H	3.507941000	2.682167000	-2.590604000
C	2.213730000	2.946133000	-0.257876000
H	1.463166000	3.242004000	-0.993178000
H	2.939099000	3.769661000	-0.186022000
C	4.295872000	1.623708000	-0.283118000
H	4.855450000	2.490661000	-0.670714000
H	4.257134000	1.700185000	0.804921000
C	5.058273000	0.344456000	-0.673766000
H	6.109020000	0.537611000	-0.420224000
H	5.051619000	0.201089000	-1.759174000
C	4.688229000	-0.953198000	0.060505000
H	5.466808000	-1.706332000	-0.142955000
H	4.682944000	-0.751858000	1.131969000
C	3.396805000	-2.158897000	-1.619036000
H	4.151610000	-2.960650000	-1.651906000
H	3.637247000	-1.410598000	-2.374077000
H	2.420649000	-2.565847000	-1.876691000
N	0.579341000	-1.623597000	0.876536000
N	3.360718000	-1.538262000	-0.280971000
S	0.599366000	-0.252028000	-1.809842000
C	-0.680057000	-1.818832000	0.075914000
H	-1.405610000	-1.061930000	0.365642000
H	-1.116290000	-2.794662000	0.340395000
C	-0.442318000	-1.715519000	-1.419645000
H	-1.419785000	-1.577572000	-1.893390000
H	0.024958000	-2.613394000	-1.842407000
C	2.957878000	-2.528985000	0.754947000
C	1.455316000	-2.826904000	0.727767000
H	1.192745000	-3.310257000	-0.214377000
H	1.225956000	-3.545691000	1.526304000
C	0.242820000	-1.375068000	2.316950000
H	-0.353409000	-2.231401000	2.667503000
H	1.186730000	-1.365724000	2.868048000
C	-0.551093000	-0.089338000	2.611389000
C	0.180977000	1.252258000	2.464920000
H	1.889084000	1.928056000	-2.643826000
C	1.540004000	2.747972000	1.099916000
H	2.282266000	2.486777000	1.854881000
H	1.069188000	3.698840000	1.392576000
H	1.117206000	1.215587000	3.023763000
H	-0.452024000	2.039180000	2.902137000
H	-0.817120000	-0.158203000	3.675338000
H	-1.506784000	-0.077197000	2.080461000
H	3.232953000	-2.113923000	1.724538000
H	3.505459000	-3.474550000	0.615272000
O	2.624185000	0.164256000	1.603271000
O	-3.253351000	0.019514000	0.857483000
O	-3.717973000	1.477010000	-1.112879000
C	-5.673383000	-0.026688000	-0.153434000
F	-6.388025000	0.049697000	-1.287004000
F	-6.089374000	0.949763000	0.670784000
F	-5.940891000	-1.207114000	0.431716000
S	-3.856633000	0.139110000	-0.506112000
O	-3.563135000	-1.015244000	-1.388876000

BA

Zero-point correction= 0.133333 (Hartree/Particle)
Thermal correction to Energy= 0.140449
Thermal correction to Enthalpy= 0.141393
Thermal correction to Gibbs Free Energy= 0.101384
Sum of electronic and zero-point Energies= -346.634293

Sum of electronic and thermal Energies= -346.627177
Sum of electronic and thermal Enthalpies= -346.626233
Sum of electronic and thermal Free Energies= -346.66624

C	1.378346000	-1.343919000	0.042510000
C	0.013145000	-1.062864000	0.113119000
C	-0.438988000	0.260863000	0.081725000
C	0.497674000	1.295499000	-0.023967000
C	1.863207000	1.016242000	-0.085419000
C	2.307969000	-0.306760000	-0.053024000
H	1.716499000	-2.376939000	0.061573000
H	-0.713318000	-1.865890000	0.179015000
H	0.156299000	2.328310000	-0.062180000
H	2.578023000	1.830892000	-0.168651000
H	3.370778000	-0.527448000	-0.107680000
C	-1.911451000	0.582269000	0.205932000
H	-2.156632000	0.761025000	1.267262000
H	-2.128252000	1.519178000	-0.332459000
O	-2.684242000	-0.497581000	-0.306854000
H	-3.608871000	-0.336453000	-0.067299000

EB

Zero-point correction= 0.157375 (Hartree/Particle)
Thermal correction to Energy= 0.164699
Thermal correction to Enthalpy= 0.165643
Thermal correction to Gibbs Free Energy= 0.125145
Sum of electronic and zero-point Energies= -310.722853
Sum of electronic and thermal Energies= -310.715528
Sum of electronic and thermal Enthalpies= -310.714584
Sum of electronic and thermal Free Energies= -310.755082

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

DHA

Zero-point correction= 0.217567 (Hartree/Particle)
Thermal correction to Energy= 0.227576
Thermal correction to Enthalpy= 0.228521
Thermal correction to Gibbs Free Energy= 0.181846
Sum of electronic and zero-point Energies= -540.517533
Sum of electronic and thermal Energies= -540.507524
Sum of electronic and thermal Enthalpies= -540.506579
Sum of electronic and thermal Free Energies= -540.55325

C	-3.567119000	0.697799000	-0.496220000
C	-2.414367000	1.390008000	-0.123743000
C	-1.259185000	0.702208000	0.259410000
C	-1.259184000	-0.702208000	0.259409000
C	-2.414366000	-1.390008000	-0.123744000
C	-3.567119000	-0.697799000	-0.496220000
C	-0.000001000	1.432344000	0.684130000
C	0.000001000	-1.432345000	0.684128000
C	1.259185000	-0.702207000	0.259410000
C	1.259183000	0.702208000	0.259407000
C	2.414366000	1.390008000	-0.123744000
H	2.409116000	2.478015000	-0.132903000
C	3.567119000	0.697800000	-0.496220000
C	3.567119000	-0.697799000	-0.496220000
C	2.414368000	-1.390008000	-0.123742000
H	-0.000001000	2.455320000	0.290527000
H	-4.457478000	1.245892000	-0.792846000
H	-2.409117000	2.478014000	-0.132902000
H	-2.409116000	-2.478014000	-0.132903000
H	-4.457477000	-1.245893000	-0.792846000
H	0.000000000	-1.534840000	1.782845000
H	4.457477000	1.245893000	-0.792846000
H	4.457478000	-1.245891000	-0.792846000
H	2.409118000	-2.478014000	-0.132901000
H	0.000000000	1.534833000	1.782847000
H	0.000001000	-2.455319000	0.290520000

1+BA

^{3}TS

Zero-point correction= 0.585577 (Hartree/Particle)
Thermal correction to Energy= 0.636978
Thermal correction to Enthalpy= 0.637922
Thermal correction to Gibbs Free Energy= 0.488560
Sum of electronic and zero-point Energies= -3651.751973
Sum of electronic and thermal Energies= -3651.700571
Sum of electronic and thermal Enthalpies= -3651.699627
Sum of electronic and thermal Free Energies= -3651.8489

Ru	-0.321665000	-0.421596000	-0.676023000
N	-0.134116000	-1.486146000	1.144365000
N	-2.171205000	-0.212454000	0.090917000
N	-1.217573000	0.902569000	-2.087933000
N	1.694881000	-0.490717000	-1.375784000
N	0.605216000	1.286227000	0.292957000
O	-0.701187000	-1.952150000	-1.699170000
C	2.163405000	-1.432559000	-2.212737000
C	2.535326000	0.457597000	-0.887601000
C	3.490951000	-1.471631000	-2.615844000
H	1.430719000	-2.163159000	-2.537596000
C	3.877775000	0.481285000	-1.266937000
H	3.840488000	-2.257076000	-3.274187000
H	4.567757000	1.216990000	-0.875861000
C	4.363101000	-0.493380000	-2.132994000
C	1.935523000	1.434812000	0.041076000
C	-0.024243000	2.154970000	1.100358000
C	2.658468000	2.467618000	0.633423000
C	0.639574000	3.215063000	1.711767000
H	-1.089878000	2.032071000	1.250884000
H	3.720830000	2.586999000	0.466263000
H	0.081936000	3.901604000	2.336184000
C	2.005431000	3.366959000	1.478068000
C	2.814975000	4.474302000	2.078840000
O	2.107929000	5.206971000	2.962714000
O	3.974172000	4.692681000	1.801357000
H	2.707795000	5.903464000	3.290335000
C	5.814974000	-0.446871000	-2.490533000
O	6.214195000	-1.547002000	-3.163780000
O	6.548225000	0.479139000	-2.225395000
H	7.171475000	-1.439787000	-3.319623000
C	-1.290895000	-1.504141000	1.877917000
C	0.967597000	-2.091671000	1.607325000
C	-1.328091000	-2.143789000	3.114388000
C	0.991030000	-2.730371000	2.849331000
H	1.852790000	-2.073047000	0.980209000

H	-2.244991000	-2.157796000	3.692131000
H	1.926318000	-3.165226000	3.186123000
C	-3.064042000	0.552483000	-0.574668000
C	-2.438919000	-0.788684000	1.283352000
C	-4.346888000	0.724223000	-0.053421000
C	-3.708972000	-0.638941000	1.843881000
H	-5.061304000	1.373154000	-0.538624000
H	-3.948297000	-1.088580000	2.799977000
C	-2.522962000	1.182371000	-1.798482000
C	-0.637764000	1.463418000	-3.159348000
C	-3.259569000	2.049280000	-2.607356000
C	-1.323942000	2.324456000	-4.008748000
H	0.401487000	1.203690000	-3.326414000
H	-4.268026000	2.323297000	-2.328544000
H	-0.814841000	2.758983000	-4.862131000
C	-2.654925000	2.623263000	-3.721171000
C	-4.660554000	0.115522000	1.160901000
C	-0.172833000	-2.755038000	3.608903000
H	-3.214067000	3.313877000	-4.344395000
H	-5.645546000	0.259944000	1.591998000
H	-0.191126000	-3.239292000	4.580634000
Cl	-3.186757000	4.057306000	0.552072000
Cl	4.487517000	-1.653210000	1.506235000
O	5.838306000	-1.263973000	1.024355000
O	3.773826000	-2.419954000	0.412565000
O	4.564345000	-2.506386000	2.726126000
O	3.675799000	-0.419415000	1.807798000
O	-3.249101000	5.425137000	1.113415000
O	-3.005792000	3.048601000	1.660841000
O	-4.454528000	3.738156000	-0.191628000
O	-2.023637000	3.928527000	-0.393501000
C	-4.750898000	-4.434496000	1.130577000
C	-4.465120000	-3.703587000	-0.022618000
C	-3.274531000	-3.936895000	-0.731518000
C	-2.375214000	-4.908646000	-0.252296000
C	-2.662651000	-5.631485000	0.901843000
C	-3.853341000	-5.397816000	1.598674000
H	-5.684180000	-4.259430000	1.659797000
H	-5.166343000	-2.964862000	-0.394849000
H	-1.448105000	-5.091658000	-0.790694000
H	-1.961175000	-6.381517000	1.256493000
H	-4.081878000	-5.968532000	2.494574000
C	-2.928406000	-3.177191000	-1.949495000
H	-1.824782000	-2.494951000	-1.699004000
H	-2.534529000	-3.800795000	-2.764768000
O	-3.925336000	-2.294900000	-2.359618000
H	-3.700537000	-1.970181000	-3.244535000

^{3}IH

Zero-point correction= 0.589900 (Hartree/Particle)
Thermal correction to Energy= 0.641843
Thermal correction to Enthalpy= 0.642788
Thermal correction to Gibbs Free Energy= 0.492680
Sum of electronic and zero-point Energies= -3651.780429
Sum of electronic and thermal Energies= -3651.728486
Sum of electronic and thermal Enthalpies= -3651.727541
Sum of electronic and thermal Free Energies= -3651.8776

Ru	-0.030547000	-0.392780000	0.948328000
N	-1.415000000	-0.025121000	-0.617571000
N	-0.491861000	-2.275267000	0.390721000
N	1.305214000	-1.526835000	2.138417000
N	0.467247000	1.609637000	1.448523000
N	1.577851000	0.037778000	-0.373547000
O	-1.380855000	-0.435063000	2.404585000
C	-0.169029000	2.328301000	2.389585000
C	1.470701000	2.173577000	0.726607000
C	0.171487000	3.646080000	2.664855000
H	-0.961232000	1.805432000	2.913829000
C	1.874136000	3.485130000	0.972168000
H	-0.373811000	4.206420000	3.413984000
H	2.660633000	3.957616000	0.398960000
C	1.214669000	4.231611000	1.944156000
C	2.074499000	1.306169000	-0.298733000
C	2.085201000	-0.834027000	-1.262244000
C	3.095783000	1.716889000	-1.150765000
C	3.111380000	-0.481459000	-2.134268000
H	1.684986000	-1.841529000	-1.275641000
H	3.484042000	2.726642000	-1.123825000
H	3.499749000	-1.221390000	-2.822711000
C	3.620431000	0.815513000	-2.078447000
C	4.730639000	1.292584000	-2.964256000
O	5.073444000	0.379074000	-3.893900000
O	5.263394000	2.375021000	-2.854630000
H	5.800760000	0.768608000	-4.415220000
C	1.660834000	5.644542000	2.157013000
O	0.810376000	6.337264000	2.942449000
O	2.679579000	6.106833000	1.695597000
H	1.162072000	7.246036000	2.995162000
C	-1.931953000	-1.177806000	-1.150634000
C	-1.787084000	1.168039000	-1.102502000
C	-2.844781000	-1.117616000	-2.197544000
C	-2.683745000	1.284113000	-2.167056000
H	-1.372630000	2.054232000	-0.634518000
H	-3.260114000	-2.028336000	-2.612559000
H	-2.922870000	2.276391000	-2.534579000
C	0.116790000	-3.301373000	1.021301000
C	-1.438279000	-2.441193000	-0.558076000
C	-0.263624000	-4.612534000	0.726284000
C	-1.840247000	-3.734643000	-0.893222000
H	0.229004000	-5.453383000	1.192546000
H	-2.597700000	-3.900914000	-1.649699000
C	1.167153000	-2.877499000	1.969868000
C	2.256079000	-1.054522000	2.960403000
C	2.009042000	-3.768698000	2.636971000
C	3.112570000	-1.894273000	3.663052000
H	2.315970000	0.024533000	3.046218000
H	1.942933000	-4.828514000	2.430482000
H	3.867356000	-1.468754000	4.315280000
C	2.987966000	-3.272439000	3.491436000
C	-1.249958000	-4.814794000	-0.236936000
C	-3.220300000	0.126364000	-2.715539000
H	3.659462000	-3.956143000	4.000679000
H	-1.546763000	-5.826297000	-0.493366000
H	-3.926024000	0.176437000	-3.538783000
Cl	2.943313000	-4.445040000	-0.902899000
Cl	-0.454289000	4.492630000	-1.415670000
O	0.413254000	5.639783000	-1.032591000
O	-1.219493000	4.025588000	-0.194652000
O	-1.417707000	4.864878000	-2.485050000
O	0.403345000	3.343194000	-1.884040000
O	3.953884000	-4.965894000	-1.848653000
O	1.735245000	-3.941203000	-1.659726000
O	2.502091000	-5.525007000	0.044852000
O	3.504487000	-3.298061000	-0.107425000
C	-7.379975000	-2.166185000	-0.630732000
C	-6.212699000	-1.854014000	0.051526000
C	-5.861555000	-0.495371000	0.305115000
C	-6.750345000	0.516824000	-0.161067000
C	-7.911353000	0.186227000	-0.842136000
C	-8.239930000	-1.156398000	-1.086798000
H	-7.632186000	-3.209189000	-0.808969000
H	-5.556484000	-2.640302000	0.410914000

H	-6.506160000	1.560630000	0.023805000
H	-8.572722000	0.976939000	-1.187620000
H	-9.152216000	-1.410112000	-1.618802000
C	-4.678784000	-0.141977000	0.983501000
H	-1.365062000	-1.285612000	2.879529000
H	-4.422923000	0.895169000	1.186220000
O	-3.817751000	-1.098702000	1.409412000
H	-3.012208000	-0.685140000	1.804994000

1'+BA

^{3}TS

Zero-point correction= 0.587104 (Hartree/Particle)
Thermal correction to Energy= 0.638097
Thermal correction to Enthalpy= 0.639041
Thermal correction to Gibbs Free Energy= 0.491853
Sum of electronic and zero-point Energies= -3681.304656
Sum of electronic and thermal Energies= -3681.253663
Sum of electronic and thermal Enthalpies= -3681.252719
Sum of electronic and thermal Free Energies= -3681.3999

Fe	0.205876000	0.436868000	0.743629000
N	0.849393000	0.441734000	2.690257000
N	1.733118000	1.572311000	0.552960000
N	0.141644000	0.706173000	-1.227836000
N	-1.271894000	-0.910694000	0.971677000
N	1.238641000	-1.341188000	0.394560000
O	-0.882167000	1.726442000	1.110554000
C	-2.536224000	-0.573563000	1.264844000
C	-0.949871000	-2.217568000	0.778473000
C	-3.542810000	-1.525758000	1.409076000
H	-2.721916000	0.488349000	1.363327000
C	-1.910022000	-3.216823000	0.898199000
H	-4.560377000	-1.215264000	1.603555000
H	-1.676436000	-4.260239000	0.725886000
C	-3.222984000	-2.867334000	1.218250000
C	0.462931000	-2.457280000	0.436489000
C	2.540105000	-1.450490000	0.092808000
C	0.998017000	-3.714544000	0.166807000
C	3.140728000	-2.676935000	-0.194577000
H	3.143073000	-0.551276000	0.071137000
H	0.389816000	-4.610624000	0.190298000
H	4.193430000	-2.701071000	-0.450264000
C	2.353388000	-3.826377000	-0.155882000
C	2.889784000	-5.195665000	-0.443699000
O	4.195548000	-5.177438000	-0.769619000
O	2.222730000	-6.206453000	-0.385229000
H	4.456113000	-6.100629000	-0.949314000
C	-4.240290000	-3.963687000	1.294247000
O	-5.444859000	-3.522567000	1.697309000
O	-3.993571000	-5.123532000	1.042534000
H	-6.053468000	-4.283334000	1.646071000
C	1.918592000	1.261433000	2.880514000
C	0.308216000	-0.191839000	3.736305000
C	2.468344000	1.440799000	4.151089000
C	0.805371000	-0.055858000	5.030771000
H	-0.549657000	-0.818686000	3.521571000
H	3.325660000	2.089915000	4.287180000
H	0.335572000	-0.590515000	5.849022000
C	2.041066000	2.026616000	-0.671791000
C	2.423536000	1.915260000	1.655957000
C	3.110938000	2.909754000	-0.835835000
C	3.499370000	2.793270000	1.551666000
H	3.407521000	3.251312000	-1.818056000
H	4.082704000	3.070623000	2.421667000
C	1.150644000	1.486322000	-1.712398000
C	-0.749177000	0.168529000	-2.071227000
C	1.292317000	1.715909000	-3.077397000
C	-0.674399000	0.381157000	-3.449491000
H	-1.540829000	-0.447608000	-1.660039000
H	2.129929000	2.295774000	-3.445102000
H	-1.428492000	-0.073601000	-4.082605000
C	0.362963000	1.156918000	-3.957466000
C	3.839308000	3.284383000	0.288610000
C	1.906194000	0.773572000	5.237317000
H	0.459956000	1.323937000	-5.025792000
H	4.700487000	3.932330000	0.173516000
H	2.324295000	0.901704000	6.231020000
Cl	-4.280411000	-1.207928000	-1.961084000
O	-4.742530000	-0.972390000	-3.350545000
O	-5.266508000	-2.018106000	-1.188493000
O	-4.071447000	0.114142000	-1.259634000
O	-2.954742000	-1.933322000	-1.980074000
Cl	5.348827000	0.447143000	-1.433522000
O	5.063212000	0.302738000	0.045590000
O	4.041943000	0.290896000	-2.172153000
O	6.301257000	-0.605863000	-1.860515000
O	5.895348000	1.812934000	-1.691685000
C	-4.464453000	5.579575000	0.460208000
C	-3.091918000	5.354371000	0.349044000
C	-2.613485000	4.150435000	-0.192273000
C	-3.535827000	3.178246000	-0.619410000
C	-4.904191000	3.405836000	-0.506347000
C	-5.373363000	4.606488000	0.037336000
H	-4.823582000	6.521197000	0.867266000
H	-2.394129000	6.134371000	0.643023000
H	-3.195215000	2.232903000	-1.031736000
H	-5.592134000	2.634722000	-0.839645000
H	-6.441578000	4.784900000	0.126148000
C	-1.157075000	3.857587000	-0.304129000
H	-0.988343000	2.765508000	0.315908000
H	-0.825749000	3.616098000	-1.318466000
O	-0.263619000	4.785744000	0.225241000
H	-0.587929000	5.043407000	1.104286000

^{3}IH

Zero-point correction= 0.591039 (Hartree/Particle)
Thermal correction to Energy= 0.642425
Thermal correction to Enthalpy= 0.643369
Thermal correction to Gibbs Free Energy= 0.496576
Sum of electronic and zero-point Energies= -3681.341565
Sum of electronic and thermal Energies= -3681.290179
Sum of electronic and thermal Enthalpies= -3681.289235
Sum of electronic and thermal Free Energies= -3681.4360

Fe	0.306671000	-0.363106000	-0.693669000
N	1.681579000	-1.084135000	0.629711000
N	-0.016988000	-2.234480000	-0.923452000
N	-1.215345000	-0.260468000	-1.967532000
N	0.643001000	1.571643000	-0.306990000
N	-1.032879000	-0.075995000	0.802458000
O	1.553982000	-0.327940000	-2.044134000
C	1.525163000	2.334882000	-0.971839000
C	-0.094279000	2.111670000	0.695466000
C	1.733196000	3.670735000	-0.650125000
H	2.044086000	1.838079000	-1.782548000
C	0.083794000	3.436653000	1.085643000
H	2.431638000	4.267906000	-1.222818000
H	-0.505794000	3.883420000	1.875244000
C	1.003555000	4.227292000	0.401982000
C	-1.065740000	1.189234000	1.299275000
C	-1.883786000	-1.000916000	1.272997000
C	-1.976547000	1.547930000	2.288028000

C	-2.819245000	-0.708230000	2.263751000
H	-1.832277000	-2.005937000	0.873930000
H	-2.030814000	2.559803000	2.668647000
H	-3.489554000	-1.489985000	2.600706000
C	-2.864751000	0.587670000	2.777013000
C	-3.828188000	1.008255000	3.845860000
O	-4.696039000	0.029954000	4.165692000
O	-3.819672000	2.102014000	4.366894000
H	-5.285527000	0.388589000	4.855898000
C	1.144703000	5.656376000	0.828011000
O	1.870790000	6.381120000	-0.046605000
O	0.680025000	6.101407000	1.852740000
H	1.875941000	7.297252000	0.289689000
C	1.738942000	-2.447842000	0.631786000
C	2.532446000	-0.388787000	1.396610000
C	2.657416000	-3.126182000	1.427898000
C	3.480156000	-1.006570000	2.208353000
H	2.445807000	0.690042000	1.352285000
H	2.685610000	-4.209642000	1.423695000
H	4.157841000	-0.402458000	2.800612000
C	-0.994126000	-2.618621000	-1.764200000
C	0.772815000	-3.106130000	-0.266664000
C	-1.199810000	-3.976541000	-2.013300000
C	0.608509000	-4.473521000	-0.477905000
H	-2.007839000	-4.311092000	-2.649469000
H	1.220212000	-5.196664000	0.047896000
C	-1.737910000	-1.474792000	-2.313748000
C	-1.790475000	0.867058000	-2.406017000
C	-2.886739000	-1.566308000	-3.091385000
C	-2.941848000	0.838640000	-3.196420000
H	-1.339989000	1.814193000	-2.127844000
H	-3.318422000	-2.536145000	-3.305792000
H	-3.381788000	1.782980000	-3.499046000
C	-3.499205000	-0.390561000	-3.532865000
C	-0.389265000	-4.899822000	-1.357246000
C	3.544663000	-2.397479000	2.221387000
H	-4.408960000	-0.443541000	-4.122824000
H	-0.565501000	-5.959278000	-1.502191000
H	4.274564000	-2.911347000	2.838150000
Cl	-2.284873000	4.289261000	-1.303186000
O	-3.383439000	4.616731000	-2.246798000
O	-1.900256000	5.468283000	-0.477040000
O	-1.073078000	3.823674000	-2.084036000
O	-2.709307000	3.157984000	-0.399962000
Cl	-3.458623000	-4.308403000	0.451111000
O	-2.165213000	-4.062293000	1.197445000
O	-3.693350000	-3.126261000	-0.457927000
O	-4.575090000	-4.437601000	1.416247000
O	-3.312229000	-5.541104000	-0.380706000
C	7.629742000	-2.157366000	0.535324000
C	6.427632000	-1.905948000	-0.111944000
C	6.020589000	-0.568545000	-0.389024000
C	6.887246000	0.487091000	0.016213000
C	8.082527000	0.217960000	0.664181000
C	8.466974000	-1.105243000	0.932643000
H	7.927079000	-3.185142000	0.730574000
H	5.788571000	-2.723298000	-0.429124000
H	6.601490000	1.516084000	-0.192496000
H	8.728214000	1.040204000	0.962134000
H	9.406563000	-1.311410000	1.436801000
C	4.795901000	-0.278424000	-1.026248000
H	1.221415000	-0.775961000	-2.839353000
H	4.503878000	0.746906000	-1.246965000
O	3.975154000	-1.264499000	-1.432472000
H	3.101432000	-0.886787000	-1.730112000

^{5}TS

Zero-point correction= 0.585828 (Hartree/Particle)
Thermal correction to Energy= 0.637981
Thermal correction to Enthalpy= 0.638926
Thermal correction to Gibbs Free Energy= 0.488184
Sum of electronic and zero-point Energies= -3681.298978
Sum of electronic and thermal Energies= -3681.246825
Sum of electronic and thermal Enthalpies= -3681.245881
Sum of electronic and thermal Free Energies= -3681.3966

Fe	-0.277652000	-0.686822000	0.767286000
N	-1.875925000	-0.486442000	2.252214000
N	-1.918612000	-1.825426000	0.000369000
N	0.321594000	-1.319978000	-1.243429000
N	1.052899000	0.871554000	1.436784000
N	-0.972820000	1.177948000	-0.238184000
O	0.572655000	-1.915603000	1.580890000
C	2.049026000	0.624563000	2.302655000
C	0.974877000	2.079341000	0.830003000
C	3.019389000	1.567817000	2.613227000
H	2.054595000	-0.371606000	2.729079000
C	1.926397000	3.067528000	1.080550000
H	3.819493000	1.329877000	3.302719000
H	1.904571000	4.024026000	0.575198000
C	2.962433000	2.807824000	1.974386000
C	-0.175716000	2.263828000	-0.080245000
C	-2.068757000	1.269352000	-1.001425000
C	-0.461220000	3.468907000	-0.716255000
C	-2.427951000	2.448097000	-1.657997000
H	-2.704415000	0.397224000	-1.089985000
H	0.171324000	4.340811000	-0.607412000
H	-3.338588000	2.474432000	-2.243261000
C	-1.603081000	3.561126000	-1.518216000
C	-1.891587000	4.877460000	-2.171839000
O	-2.965906000	4.824846000	-2.983690000
O	-1.234646000	5.880134000	-1.991502000
H	-3.083093000	5.721157000	-3.351394000
C	3.984882000	3.881899000	2.187122000
O	5.018155000	3.463005000	2.945298000
O	3.883721000	5.004693000	1.746802000
H	5.647294000	4.207581000	2.989548000
C	-3.019420000	-1.159390000	1.995471000
C	-1.797505000	0.301470000	3.331890000
C	-4.139097000	-1.025265000	2.820160000
C	-2.861241000	0.461441000	4.214569000
H	-0.853788000	0.816256000	3.481128000
H	-5.076603000	-1.489880000	2.543347000
H	-2.757385000	1.111139000	5.076979000
C	-1.777989000	-2.461757000	-1.173902000
C	-3.000855000	-1.997902000	0.774263000
C	-2.754552000	-3.361886000	-1.608597000
C	-4.004843000	-2.896009000	0.403972000
H	-2.651456000	-3.881950000	-2.553567000
H	-4.886292000	-3.031482000	1.013582000
C	-0.543317000	-2.114769000	-1.915684000
C	1.471821000	-0.942133000	-1.810385000
C	-0.262123000	-2.536303000	-3.215108000
C	1.813767000	-1.320099000	-3.110923000
H	2.141392000	-0.336328000	-1.209682000
H	-0.963898000	-3.160737000	-3.756279000
H	2.753506000	-0.971222000	-3.524947000
C	0.929279000	-2.126256000	-3.819652000
C	-3.867818000	-3.579854000	-0.801298000
C	-4.054166000	-0.207973000	3.943084000
H	1.155326000	-2.438061000	-4.835084000
H	-4.642015000	-4.270361000	-1.119587000
H	-4.919000000	-0.079442000	4.586472000

Cl	4.199170000	1.424227000	-1.237843000
O	4.903614000	0.684342000	-2.326728000
O	5.071054000	2.470844000	-0.640845000
O	3.806576000	0.435658000	-0.155854000
O	2.938315000	2.036487000	-1.772719000
Cl	-5.599752000	0.199038000	-0.470166000
O	-6.640085000	1.056923000	-1.081720000
O	-4.738151000	1.002821000	0.465282000
O	-4.711591000	-0.380969000	-1.545096000
O	-6.231964000	-0.926661000	0.298716000
C	3.990513000	-5.168960000	-1.271061000
C	3.287402000	-5.052446000	-0.074437000
C	3.304566000	-3.837699000	0.632792000
C	4.013412000	-2.741857000	0.106095000
C	4.699127000	-2.855773000	-1.100081000
C	4.693988000	-4.073942000	-1.788063000
H	3.991471000	-6.115941000	-1.804525000
H	2.739262000	-5.895964000	0.330956000
H	4.016668000	-1.784522000	0.618587000
H	5.214441000	-1.987276000	-1.500138000
H	5.233897000	-4.170184000	-2.726404000
C	2.553962000	-3.661292000	1.900980000
H	3.132925000	-3.101892000	2.655396000
H	1.656176000	-2.907448000	1.680323000
O	2.035157000	-4.857828000	2.396121000
H	1.586244000	-4.674028000	3.235436000

^{5}IH(P+S)

Zero-point correction= 0.465985 (Hartree/Particle)
Thermal correction to Energy= 0.510438
Thermal correction to Enthalpy= 0.511382
Thermal correction to Gibbs Free Energy= 0.380597
Sum of electronic and zero-point Energies= -3335.31085
Sum of electronic and thermal Energies= -3335.266406
Sum of electronic and thermal Enthalpies= -3335.265462
Sum of electronic and thermal Free Energies= -3335.3962

Fe	-0.237738000	1.192864000	-1.030450000
N	-1.602795000	0.161066000	-2.384610000
N	-2.208421000	1.690010000	-0.348727000
N	0.036418000	2.384011000	0.788589000
N	1.626043000	0.209136000	-1.512954000
N	-0.131813000	-0.597902000	0.296298000
O	0.119633000	2.596256000	-2.152983000
C	2.470281000	0.714474000	-2.430826000
C	2.005663000	-0.849553000	-0.760462000
C	3.733791000	0.183759000	-2.649640000
H	2.099578000	1.573774000	-2.977747000
C	3.260052000	-1.434222000	-0.930218000
H	4.397192000	0.626104000	-3.382121000
H	3.593695000	-2.260517000	-0.316922000
C	4.135513000	-0.907372000	-1.875678000
C	1.009974000	-1.324813000	0.223159000
C	-1.106116000	-0.980068000	1.133004000
C	1.199491000	-2.453007000	1.015872000
C	-0.991833000	-2.104810000	1.950182000
H	-2.021049000	-0.401694000	1.150496000
H	2.110683000	-3.035749000	0.976722000
H	-1.818808000	-2.383771000	2.590978000
C	0.185214000	-2.847089000	1.892794000
C	0.414062000	-4.076845000	2.716801000
O	-0.583358000	-4.300768000	3.594982000
O	1.385305000	-4.793373000	2.606191000
H	-0.355774000	-5.119983000	4.073956000
C	5.487776000	-1.540084000	-2.000053000
O	6.314353000	-0.830027000	-2.795053000
O	5.797745000	-2.579857000	-1.464154000
H	7.172120000	-1.295341000	-2.786808000
C	-2.925588000	0.340092000	-2.163959000
C	-1.197266000	-0.674621000	-3.350746000
C	-3.883313000	-0.358236000	-2.901937000
C	-2.094256000	-1.379236000	-4.146872000
H	-0.124362000	-0.775006000	-3.478147000
H	-4.931423000	-0.279852000	-2.643112000
H	-1.725674000	-2.046424000	-4.918447000
C	-2.350254000	2.511076000	0.705991000
C	-3.261028000	1.290051000	-1.080123000
C	-3.611298000	3.000309000	1.054860000
C	-4.545262000	1.760401000	-0.794937000
H	-3.736058000	3.663621000	1.902577000
H	-5.398770000	1.438079000	-1.373059000
C	-1.086275000	2.823700000	1.409904000
C	1.240997000	2.606747000	1.330224000
C	-1.007801000	3.500186000	2.626131000
C	1.389371000	3.267859000	2.552166000
H	2.110356000	2.254130000	0.780307000
H	-1.908352000	3.835736000	3.127850000
H	2.388171000	3.388427000	2.958131000
C	0.246285000	3.716566000	3.205326000
C	-4.709382000	2.621779000	0.286702000
C	-3.459279000	-1.223899000	-3.905689000
H	0.318908000	4.226454000	4.161396000
H	-5.699875000	2.985320000	0.539792000
H	-4.188933000	-1.786357000	-4.479790000
Cl	4.392793000	0.982450000	1.377820000
O	4.727228000	1.974491000	2.437721000
O	5.560403000	0.125931000	1.041225000
O	3.949571000	1.723309000	0.131182000
O	3.241237000	0.127347000	1.835818000
Cl	-4.758565000	-1.482897000	0.635011000
O	-5.354323000	-2.586647000	1.420706000
O	-3.632753000	-1.994759000	-0.222707000
O	-4.200246000	-0.430114000	1.562526000
O	-5.793158000	-0.849913000	-0.252841000
H	0.531423000	3.408071000	-1.815421000

Zero-point correction= 0.119898 (Hartree/Particle)
Thermal correction to Energy= 0.126880
Thermal correction to Enthalpy= 0.127824
Thermal correction to Gibbs Free Energy= 0.088302
Sum of electronic and zero-point Energies= -346.010999
Sum of electronic and thermal Energies= -346.004018
Sum of electronic and thermal Enthalpies= -346.003073
Sum of electronic and thermal Free Energies= -346.0425

C	-1.343803000	1.346481000	-0.000002000
C	0.017826000	1.082791000	0.000046000
C	0.493815000	-0.260207000	0.000051000
C	-0.471350000	-1.308157000	0.000039000
C	-1.827708000	-1.025231000	-0.000016000
C	-2.279847000	0.302750000	-0.000039000
H	-1.686864000	2.378359000	-0.000006000
H	0.736741000	1.895316000	0.000111000
H	-0.130582000	-2.341342000	0.000080000
H	-2.545317000	-1.841999000	-0.000008000
H	-3.344166000	0.519597000	-0.000116000
C	1.866142000	-0.567718000	-0.000039000
H	2.230564000	-1.590915000	-0.000048000
O	2.791288000	0.437989000	-0.000028000
H	3.678867000	0.052807000	-0.000026000

1+EB

^{3}TS

Zero-point correction= 0.609221 (Hartree/Particle)
Thermal correction to Energy= 0.660864

Thermal correction to Enthalpy= 0.661808
Thermal correction to Gibbs Free Energy= 0.514101
Sum of electronic and zero-point Energies= -3615.835390
Sum of electronic and thermal Energies= -3615.783748
Sum of electronic and thermal Enthalpies= -3615.782803
Sum of electronic and thermal Free Energies= -3615.9305

Ru	0.313009000	-0.599524000	0.284785000
N	-0.267508000	-0.925823000	-1.717777000
N	1.747269000	-1.872171000	-0.326567000
N	1.524896000	-0.739840000	2.054401000
N	-1.076592000	0.906123000	0.904227000
N	1.279064000	1.273032000	-0.281012000
O	-0.817008000	-1.937260000	0.964757000
C	-2.262759000	0.626278000	1.468308000
C	-0.721853000	2.200815000	0.683361000
C	-3.152390000	1.620942000	1.861454000
H	-2.487292000	-0.427290000	1.585792000
C	-1.563625000	3.241906000	1.067391000
H	-4.114324000	1.353908000	2.276942000
H	-1.301852000	4.279357000	0.901144000
C	-2.788937000	2.952194000	1.665749000
C	0.586492000	2.404436000	0.031418000
C	2.485029000	1.368786000	-0.862174000
C	1.112276000	3.661530000	-0.258025000
C	3.069355000	2.596827000	-1.167555000
H	3.024612000	0.452337000	-1.070598000
H	0.575311000	4.572258000	-0.023764000
H	4.056133000	2.619657000	-1.612695000
C	2.366887000	3.761202000	-0.864634000
C	2.898669000	5.132470000	-1.143978000
O	4.087392000	5.104616000	-1.777421000
O	2.324736000	6.155142000	-0.835958000
H	4.359645000	6.032996000	-1.905447000
C	-3.667407000	4.101835000	2.045295000
O	-4.824840000	3.703630000	2.607725000
O	-3.366890000	5.264559000	1.877288000
H	-5.342883000	4.511878000	2.782370000
C	0.547986000	-1.813350000	-2.373559000
C	-1.316108000	-0.387450000	-2.358437000
C	0.297642000	-2.159934000	-3.699574000
C	-1.622713000	-0.714485000	-3.681564000
H	-1.931623000	0.320624000	-1.811472000
H	0.952101000	-2.855661000	-4.212485000
H	-2.508868000	-0.272984000	-4.122279000
C	2.700833000	-2.232263000	0.558941000
C	1.674999000	-2.354817000	-1.584915000
C	3.656558000	-3.176031000	0.182952000
C	2.623411000	-3.289375000	-2.008367000
H	4.447693000	-3.467392000	0.857909000
H	2.599470000	-3.690203000	-3.014749000
C	2.605418000	-1.553706000	1.874199000
C	1.361353000	-0.108860000	3.223855000
C	3.561895000	-1.706077000	2.877533000
C	2.264602000	-0.242221000	4.275370000
H	0.479604000	0.516790000	3.306077000
H	4.458458000	-2.281790000	2.687511000
H	2.091829000	0.289220000	5.204931000
C	3.387842000	-1.044758000	4.090690000
C	3.609377000	-3.694723000	-1.111504000
C	-0.802379000	-1.608365000	-4.360481000
H	4.132057000	-1.145370000	4.874283000
H	4.361067000	-4.411027000	-1.425999000
H	-1.009856000	-1.882022000	-5.390495000
Cl	5.674166000	-0.263852000	0.014610000
Cl	-4.594280000	1.275609000	-1.629003000
O	-5.466008000	2.235903000	-2.342111000
O	-5.185349000	0.903112000	-0.303316000
O	-4.404740000	0.027107000	-2.451100000
O	-3.232512000	1.893986000	-1.398882000
O	6.869831000	0.542462000	-0.317944000
O	4.916182000	-0.608226000	-1.246473000
O	6.070567000	-1.536723000	0.706238000
O	4.751228000	0.511306000	0.916023000
C	-3.465306000	-3.517326000	0.321776000
C	-4.358658000	-2.474681000	-0.017567000
C	-5.547877000	-2.293976000	0.681952000
C	-5.879849000	-3.156426000	1.732263000
C	-5.008903000	-4.195529000	2.081392000
C	-3.811898000	-4.370000000	1.393417000
H	-4.124806000	-1.800368000	-0.837755000
H	-6.198969000	-1.471616000	0.402779000
H	-6.810181000	-3.020593000	2.277485000
H	-5.265163000	-4.869315000	2.895044000
H	-3.144918000	-5.177125000	1.681406000
C	-2.190119000	-3.630585000	-0.400003000
H	-2.236529000	-3.182490000	-1.397077000
H	-1.423753000	-2.741628000	0.230853000
C	-1.392002000	-4.920785000	-0.357264000
H	-0.454651000	-4.815721000	-0.914436000
H	-1.135721000	-5.213518000	0.666644000
H	-1.954714000	-5.750863000	-0.807596000

^{3}IH

Zero-point correction= 0.612559 (Hartree/Particle)
Thermal correction to Energy= 0.665345
Thermal correction to Enthalpy= 0.666289
Thermal correction to Gibbs Free Energy= 0.515178
Sum of electronic and zero-point Energies= -3615.851867
Sum of electronic and thermal Energies= -3615.799082
Sum of electronic and thermal Enthalpies= -3615.798137
Sum of electronic and thermal Free Energies= -3615.9492

Ru	0.277817000	-0.481075000	0.337572000
N	-0.302330000	-0.908157000	-1.642934000
N	1.625317000	-1.888397000	-0.172394000
N	1.487101000	-0.559520000	2.111068000
N	-1.042259000	1.088224000	0.902220000
N	1.289130000	1.287855000	-0.361335000
O	-0.982450000	-1.761491000	1.053849000
C	-2.223970000	0.881249000	1.502263000
C	-0.637328000	2.355255000	0.614020000
C	-3.056289000	1.932801000	1.877330000
H	-2.491856000	-0.157771000	1.656813000
C	-1.420148000	3.448375000	0.974031000
H	-4.017853000	1.727215000	2.327137000
H	-1.118506000	4.465563000	0.757191000
C	-2.639290000	3.237032000	1.618650000
C	0.656661000	2.465172000	-0.086015000
C	2.474921000	1.296222000	-0.990682000
C	1.227021000	3.679128000	-0.461430000
C	3.099822000	2.478931000	-1.381639000
H	2.963047000	0.344343000	-1.164831000
H	0.739201000	4.624427000	-0.258595000
H	4.069231000	2.435043000	-1.862015000
C	2.461208000	3.688445000	-1.115961000
C	3.042233000	5.017650000	-1.487504000
O	4.203997000	4.901865000	-2.159609000
O	2.525420000	6.079961000	-1.215176000
H	4.512199000	5.808653000	-2.347290000
C	-3.453297000	4.439795000	1.976370000
O	-4.613767000	4.117667000	2.580183000

O	-3.103858000	5.580443000	1.758239000
H	-5.087450000	4.955689000	2.739853000
C	0.455106000	-1.889791000	-2.231182000
C	-1.317849000	-0.351571000	-2.320874000
C	0.188180000	-2.304435000	-3.534484000
C	-1.641022000	-0.746795000	-3.620988000
H	-1.894023000	0.421679000	-1.819907000
H	0.799017000	-3.071913000	-3.996260000
H	-2.500732000	-0.287440000	-4.094296000
C	2.547068000	-2.251083000	0.745238000
C	1.534076000	-2.452027000	-1.394773000
C	3.436798000	-3.282867000	0.448634000
C	2.417774000	-3.478290000	-1.741216000
H	4.198130000	-3.581983000	1.154041000
H	2.374190000	-3.943477000	-2.718897000
C	2.498411000	-1.469710000	2.004549000
C	1.372692000	0.176742000	3.224277000
C	3.432252000	-1.621220000	3.028933000
C	2.257315000	0.054441000	4.291790000
H	0.545495000	0.877183000	3.247091000
H	4.275536000	-2.286774000	2.898585000
H	2.126877000	0.671681000	5.173937000
C	3.309044000	-0.852770000	4.183481000
C	3.363713000	-3.889460000	-0.806267000
C	-0.873077000	-1.729001000	-4.236661000
H	4.037854000	-0.953300000	4.981487000
H	4.064813000	-4.677636000	-1.059576000
H	-1.094480000	-2.055131000	-5.248346000
Cl	5.534981000	-0.457476000	0.000864000
Cl	-4.549732000	1.305528000	-1.529260000
O	-5.494455000	2.250263000	-2.166008000
O	-5.032977000	0.910171000	-0.166089000
O	-4.388216000	0.070628000	-2.373839000
O	-3.190824000	1.959276000	-1.390535000
O	6.748747000	0.287537000	-0.401834000
O	4.753946000	-0.873536000	-1.224225000
O	5.900565000	-1.684081000	0.784379000
O	4.643054000	0.411590000	0.847671000
C	-3.453085000	-3.839014000	0.121813000
C	-4.213056000	-2.642326000	-0.046856000
C	-5.214990000	-2.294412000	0.847030000
C	-5.506946000	-3.125483000	1.938477000
C	-4.780691000	-4.310914000	2.123015000
C	-3.772045000	-4.666260000	1.238808000
H	-4.011315000	-1.988784000	-0.892093000
H	-5.759280000	-1.368966000	0.685427000
H	-6.294860000	-2.855426000	2.636400000
H	-5.009373000	-4.960640000	2.964358000
H	-3.224831000	-5.591029000	1.396897000
C	-2.420586000	-4.155110000	-0.800463000
H	-2.326264000	-3.506884000	-1.670104000
H	-1.192988000	-2.523645000	0.475488000
C	-1.597413000	-5.408161000	-0.788959000
H	-0.673024000	-5.278434000	-1.363732000
H	-1.318122000	-5.720261000	0.224595000
H	-2.135272000	-6.257171000	-1.242731000

1'+EB

^{3}TS

Zero-point correction= 0.610360 (Hartree/Particle)

Thermal correction to Energy= 0.661721

Thermal correction to Enthalpy= 0.662665

Thermal correction to Gibbs Free Energy= 0.514708

Sum of electronic and zero-point Energies= -3645.384233

Sum of electronic and thermal Energies= -3645.332872

Sum of electronic and thermal Enthalpies= -3645.331928

Sum of electronic and thermal Free Energies= -3645.4798

Fe	0.008811000	-0.200079000	0.826462000
N	-0.452500000	0.255142000	2.767643000
N	-1.882477000	-0.453820000	0.749699000
N	-0.154745000	-0.645835000	-1.112894000
N	1.956846000	0.307972000	0.882782000
N	-0.087830000	1.821963000	0.294446000
O	0.351793000	-1.806010000	1.358550000
C	2.928478000	-0.554483000	1.216200000
C	2.276489000	1.578302000	0.518822000
C	4.274387000	-0.189756000	1.222388000
H	2.598069000	-1.554189000	1.461126000
C	3.600549000	2.004849000	0.498189000
H	5.033433000	-0.925891000	1.448245000
H	3.874173000	3.009673000	0.200364000
C	4.611566000	1.110475000	0.854340000
C	1.123580000	2.427226000	0.171611000
C	-1.201075000	2.511797000	0.009958000
C	1.228358000	3.749891000	-0.250700000
C	-1.170742000	3.838113000	-0.424624000
H	-2.158480000	2.017960000	0.117305000
H	2.187904000	4.241195000	-0.357601000
H	-2.103838000	4.336458000	-0.659423000
C	0.066639000	4.464809000	-0.556483000
C	0.222320000	5.882992000	-1.014170000
O	-0.958486000	6.465419000	-1.291905000
O	1.292835000	6.443006000	-1.118802000
H	-0.764228000	7.374097000	-1.590280000
C	6.026228000	1.598231000	0.793712000
O	6.908043000	0.673140000	1.211355000
O	6.336972000	2.710036000	0.421916000
H	7.797660000	1.054940000	1.089218000
C	-1.773731000	0.081492000	3.041239000
C	0.381873000	0.617351000	3.747605000
C	-2.275343000	0.291003000	4.326883000
C	-0.050801000	0.840449000	5.053313000
H	1.424505000	0.723552000	3.470336000
H	-3.331894000	0.156875000	4.528345000
H	0.661887000	1.134507000	5.816043000
C	-2.429264000	-0.797959000	-0.426610000
C	-2.594572000	-0.333341000	1.885511000
C	-3.798517000	-1.064655000	-0.500193000
C	-3.963638000	-0.585491000	1.869104000
H	-4.270565000	-1.303447000	-1.442978000
H	-4.564002000	-0.478795000	2.764748000
C	-1.442594000	-0.840224000	-1.518888000
C	0.837436000	-0.687737000	-2.011296000
C	-1.756775000	-1.040338000	-2.859234000
C	0.590552000	-0.917614000	-3.366812000
H	1.853333000	-0.549769000	-1.661279000
H	-2.791821000	-1.130112000	-3.164810000
H	1.435532000	-0.957740000	-4.045266000
C	-0.722289000	-1.081662000	-3.796551000
C	-4.559765000	-0.948632000	0.658544000
C	-1.403954000	0.676200000	5.343501000
H	-0.948069000	-1.235161000	-4.847405000
H	-5.630798000	-1.107216000	0.609317000
H	-1.779269000	0.843961000	6.348309000
Cl	4.293001000	-1.961271000	-1.765821000
O	4.483271000	-2.690000000	-3.042823000
O	5.533074000	-1.985122000	-0.936885000
O	3.162119000	-2.587237000	-0.981367000
O	3.914289000	-0.525038000	-2.047043000
Cl	-4.638024000	2.114631000	-1.319008000
O	-4.254527000	2.231161000	0.139976000
O	-3.444782000	1.572195000	-2.067512000

O	-4.999853000	3.452767000	-1.845508000
O	-5.773734000	1.153405000	-1.448396000
C	-1.034369000	-4.503096000	-0.059238000
C	-1.744803000	-4.477412000	-1.276988000
C	-3.049229000	-4.960396000	-1.362563000
C	-3.683301000	-5.472376000	-0.226999000
C	-2.997523000	-5.500004000	0.991830000
C	-1.691803000	-5.022616000	1.075400000
H	-1.250082000	-4.093908000	-2.165746000
H	-3.568637000	-4.949076000	-2.317446000
H	-4.699218000	-5.852431000	-0.291899000
H	-3.482284000	-5.901568000	1.878041000
H	-1.170337000	-5.052547000	2.027641000
C	0.347478000	-3.979437000	0.005785000
H	0.757036000	-3.723010000	-0.974935000
H	0.275873000	-2.823163000	0.566090000
C	1.372647000	-4.694378000	0.871372000
H	1.487748000	-5.735716000	0.539943000
H	2.343208000	-4.202741000	0.770393000
H	1.089342000	-4.711004000	1.929752000

^{3}IH

Zero-point correction= 0.614417 (Hartree/Particle)
Thermal correction to Energy= 0.666668
Thermal correction to Enthalpy= 0.667613
Thermal correction to Gibbs Free Energy= 0.516614
Sum of electronic and zero-point Energies= -3645.413661
Sum of electronic and thermal Energies= -3645.361410
Sum of electronic and thermal Enthalpies= -3645.360466
Sum of electronic and thermal Free Energies= -3645.5114

Fe	0.459328000	-0.131742000	0.819867000
N	0.481857000	0.465883000	2.754321000
N	-1.379415000	0.347798000	1.007926000
N	-0.146175000	-0.543234000	-1.062878000
N	2.426821000	-0.453411000	0.532831000
N	1.074581000	1.748086000	0.190925000
O	0.155773000	-1.772513000	1.423634000
C	3.030978000	-1.622772000	0.786256000
C	3.144250000	0.577375000	0.006488000
C	4.383348000	-1.835474000	0.517096000
H	2.413267000	-2.412696000	1.192597000
C	4.499780000	0.435818000	-0.273112000
H	4.809488000	-2.813691000	0.698248000
H	5.085025000	1.246775000	-0.689541000
C	5.128375000	-0.787136000	-0.016579000
C	2.372642000	1.813329000	-0.210877000
C	0.288726000	2.823954000	0.056691000
C	2.897449000	2.974169000	-0.769175000
C	0.744940000	4.019068000	-0.506736000
H	-0.740756000	2.756640000	0.386520000
H	3.928205000	3.037593000	-1.096788000
H	0.051953000	4.844528000	-0.621756000
C	2.070766000	4.092068000	-0.925162000
C	2.669950000	5.317454000	-1.544994000
O	1.790400000	6.330799000	-1.633581000
O	3.821226000	5.385932000	-1.920965000
H	2.255615000	7.076853000	-2.057194000
C	6.584781000	-0.902898000	-0.347012000
O	7.086203000	-2.115463000	-0.046818000
O	7.239210000	-0.001920000	-0.826863000
H	8.025950000	-2.106474000	-0.310316000
C	-0.749993000	0.800715000	3.223245000
C	1.529999000	0.484973000	3.584671000
C	-0.934775000	1.184099000	4.552876000
C	1.416476000	0.851669000	4.923694000
H	2.481755000	0.189253000	3.158158000
H	-1.921665000	1.457372000	4.908251000
H	2.294238000	0.850758000	5.560584000
C	-2.183532000	0.188336000	-0.053963000
C	-1.827805000	0.716068000	2.220633000
C	-3.557092000	0.404332000	0.080771000
C	-3.186090000	0.957282000	2.410782000
H	-4.228367000	0.283572000	-0.758268000
H	-3.570038000	1.270353000	3.374505000
C	-1.462961000	-0.250713000	-1.262484000
C	0.580400000	-1.024957000	-2.079323000
C	-2.052429000	-0.374964000	-2.516760000
C	0.044708000	-1.194095000	-3.355763000
H	1.596914000	-1.325837000	-1.863386000
H	-3.087858000	-0.093995000	-2.658081000
H	0.670716000	-1.602684000	-4.140924000
C	-1.283240000	-0.846774000	-3.580180000
C	-4.046581000	0.799118000	1.322452000
C	0.161027000	1.210544000	5.411913000
H	-1.724540000	-0.948274000	-4.566884000
H	-5.106108000	0.997521000	1.436625000
H	0.033764000	1.504927000	6.449108000
Cl	1.779546000	-4.352819000	-0.921698000
O	1.569881000	-5.589375000	-1.700351000
O	2.451507000	-4.637157000	0.384881000
O	0.433806000	-3.699490000	-0.640286000
O	2.615929000	-3.371773000	-1.699027000
Cl	-3.088187000	3.709774000	-0.845046000
O	-2.612787000	3.610833000	0.588890000
O	-2.263758000	2.752975000	-1.672067000
O	-2.884665000	5.097215000	-1.334782000
O	-4.521468000	3.309340000	-0.912119000
C	-4.095223000	-3.315110000	-0.249082000
C	-4.335903000	-3.049179000	-1.633330000
C	-5.507733000	-2.446432000	-2.065452000
C	-6.501552000	-2.077777000	-1.144587000
C	-6.296603000	-2.333868000	0.218947000
C	-5.126611000	-2.935469000	0.663092000
H	-3.576121000	-3.342156000	-2.353911000
H	-5.662149000	-2.267692000	-3.127078000
H	-7.420759000	-1.609923000	-1.484931000
H	-7.065254000	-2.062519000	0.939072000
H	-4.994273000	-3.121688000	1.724384000
C	-2.878610000	-3.919480000	0.146639000
H	-2.145569000	-4.125596000	-0.630343000
H	0.246871000	-2.438941000	0.699113000
C	-2.459593000	-4.261753000	1.539166000
H	-3.293875000	-4.299829000	2.247117000
H	-1.953788000	-5.235142000	1.556137000
H	-1.725630000	-3.532139000	1.915810000

^{5}TS

Zero-point correction= 0.608627 (Hartree/Particle)
Thermal correction to Energy= 0.661137
Thermal correction to Enthalpy= 0.662081
Thermal correction to Gibbs Free Energy= 0.510956
Sum of electronic and zero-point Energies= -3645.381891
Sum of electronic and thermal Energies= -3645.329381
Sum of electronic and thermal Enthalpies= -3645.328437
Sum of electronic and thermal Free Energies= -3645.4795

Fe	-0.279950000	-0.720691000	0.758923000
N	-1.874406000	-0.535183000	2.247960000
N	-1.939672000	-1.814924000	-0.036627000
N	0.307725000	-1.314417000	-1.269105000
N	1.069322000	0.823947000	1.452718000

N	-0.954231000	1.181271000	-0.216389000
O	0.560852000	-1.979735000	1.558944000
C	2.060246000	0.553815000	2.318156000
C	1.007314000	2.039989000	0.862200000
C	3.041679000	1.480893000	2.642447000
H	2.051203000	-0.446296000	2.734907000
C	1.970639000	3.013558000	1.126882000
H	3.835895000	1.225018000	3.332393000
H	1.960668000	3.976918000	0.634449000
C	3.001107000	2.729784000	2.019481000
C	-0.140947000	2.252598000	-0.045452000
C	-2.050133000	1.300270000	-0.975856000
C	-0.408717000	3.470488000	-0.664926000
C	-2.392755000	2.492944000	-1.615815000
H	-2.699469000	0.439498000	-1.074658000
H	0.237528000	4.330910000	-0.546168000
H	-3.304109000	2.541066000	-2.198602000
C	-1.550417000	3.591166000	-1.463159000
C	-1.819904000	4.920280000	-2.098490000
O	-2.895964000	4.894882000	-2.909630000
O	-1.148138000	5.910768000	-1.905718000
H	-2.999856000	5.797936000	-3.264571000
C	4.035739000	3.788483000	2.248833000
O	5.063022000	3.346977000	3.002969000
O	3.950794000	4.917872000	1.822013000
H	5.699244000	4.084615000	3.060723000
C	-3.027188000	-1.186703000	1.977977000
C	-1.781320000	0.220692000	3.349096000
C	-4.141593000	-1.061905000	2.810988000
C	-2.839323000	0.368993000	4.240693000
H	-0.830400000	0.718707000	3.508769000
H	-5.085796000	-1.507775000	2.526252000
H	-2.723464000	0.992313000	5.120838000
C	-1.812997000	-2.417588000	-1.230255000
C	-3.023642000	-1.991351000	0.734178000
C	-2.805205000	-3.288184000	-1.688807000
C	-4.042810000	-2.862106000	0.340412000
H	-2.713350000	-3.780649000	-2.649634000
H	-4.925348000	-3.000563000	0.947693000
C	-0.575358000	-2.067418000	-1.965566000
C	1.462031000	-0.937670000	-1.828489000
C	-0.309112000	-2.444976000	-3.281566000
C	1.789738000	-1.271346000	-3.144864000
H	2.145868000	-0.367529000	-1.208838000
H	-1.025954000	-3.034635000	-3.841758000
H	2.732621000	-0.921064000	-3.550536000
C	0.885930000	-2.033208000	-3.877921000
C	-3.919784000	-3.512152000	-0.884830000
C	-4.041691000	-0.277488000	3.955951000
H	1.099424000	-2.308611000	-4.906562000
H	-4.706267000	-4.179770000	-1.221342000
H	-4.901971000	-0.156697000	4.606895000
Cl	4.187376000	1.395399000	-1.287069000
O	4.803504000	0.610455000	-2.400409000
O	5.132425000	2.408721000	-0.751077000
O	3.808651000	0.436097000	-0.173952000
O	2.928170000	2.052632000	-1.768527000
Cl	-5.596933000	0.268593000	-0.449408000
O	-6.625439000	1.160525000	-1.031743000
O	-4.717454000	1.031264000	0.503437000
O	-4.723954000	-0.296463000	-1.544606000
O	-6.244807000	-0.867151000	0.291280000
C	3.285929000	-3.782979000	0.608130000
C	3.164428000	-4.996308000	-0.102939000
C	3.799286000	-5.163860000	-1.329892000
C	4.545250000	-4.117752000	-1.888554000
C	4.659404000	-2.899899000	-1.208585000
C	4.042769000	-2.740086000	0.027637000
H	2.587299000	-5.814708000	0.316398000
H	3.714126000	-6.111247000	-1.855711000
H	5.031268000	-4.252022000	-2.851304000
H	5.205870000	-2.066091000	-1.639865000
H	4.128313000	-1.782821000	0.532491000
C	2.618371000	-3.544947000	1.906080000
H	3.198955000	-2.850649000	2.526522000
H	1.648815000	-2.844502000	1.667283000
C	2.086047000	-4.720197000	2.711874000
H	1.592730000	-4.364541000	3.621595000
H	1.354267000	-5.307238000	2.147189000
H	2.900513000	-5.394065000	3.009215000

^{5}IH(P+S)

Zero-point correction= 0.465985 (Hartree/Particle)
Thermal correction to Energy= 0.510437
Thermal correction to Enthalpy=0.511382
Thermal correction to Gibbs Free Energy= 0.380601
Sum of electronic and zero-point Energies= -3335.31085
Sum of electronic and thermal Energies= -3335.266406
Sum of electronic and thermal Enthalpies= -3335.265462
Sum of electronic and thermal Free Energies= -3335.3962

Fe	-0.238249000	-1.193352000	1.030046000
N	-1.604095000	-0.162767000	2.384272000
N	-2.208488000	-1.690248000	0.346890000
N	0.037021000	-2.383091000	-0.789765000
N	1.625967000	-0.210676000	1.513068000
N	-0.131968000	0.598662000	-0.295103000
O	0.118530000	-2.597575000	2.151690000
C	2.470110000	-0.716994000	2.430488000
C	2.005752000	0.848663000	0.761563000
C	3.733701000	-0.186679000	2.649813000
H	2.099246000	-1.576718000	2.976637000
C	3.260203000	1.433023000	0.931939000
H	4.397022000	-0.629793000	3.381903000
H	3.593986000	2.259878000	0.319478000
C	4.135565000	0.905157000	1.876921000
C	1.010110000	1.325067000	-0.221544000
C	-1.106267000	0.981931000	-1.131342000
C	1.200000000	2.453817000	-1.013383000
C	-0.991621000	2.107294000	-1.947609000
H	-2.021504000	0.404032000	-1.149185000
H	2.111437000	3.036150000	-0.973928000
H	-1.818550000	2.387124000	-2.588088000
C	0.185758000	2.849019000	-1.889827000
C	0.414939000	4.079388000	-2.712825000
O	-0.582091000	4.303934000	-3.591290000
O	1.386149000	4.795820000	-2.601301000
H	-0.354335000	5.123542000	-4.069512000
C	5.487877000	1.537634000	2.001997000
O	6.314420000	0.826633000	2.796168000
O	5.797907000	2.577981000	1.467239000
H	7.172216000	1.291906000	2.788444000
C	-2.926740000	-0.342097000	2.163015000
C	-1.199180000	0.672386000	3.351126000
C	-3.884974000	0.355403000	2.901125000
C	-2.096696000	1.376124000	4.147430000
H	-0.126348000	0.773064000	3.478951000
H	-4.932955000	0.276895000	2.641802000
H	-1.728638000	2.042896000	4.919614000
C	-2.349671000	-2.510454000	-0.708587000
C	-3.261457000	-1.291372000	1.078349000
C	-3.610402000	-2.999936000	-1.058210000
C	-4.545398000	-1.762105000	0.792469000
H	-3.734636000	-3.662589000	-1.906524000

H	-5.399183000	-1.440737000	1.370721000
C	-1.085311000	-2.822040000	-1.412285000
C	1.241916000	-2.605120000	-1.330924000
C	-1.006082000	-3.496946000	-2.629317000
C	1.391076000	-3.264619000	-2.553658000
H	2.110855000	-2.253212000	-0.779953000
H	-1.906329000	-3.831876000	-3.132000000
H	2.390121000	-3.384562000	-2.959209000
C	0.248384000	-3.712487000	-3.208063000
C	-4.708845000	-2.622616000	-0.289960000
C	-3.461582000	1.220489000	3.905643000
H	0.321581000	-4.221085000	-4.164776000
H	-5.699096000	-2.986442000	-0.543592000
H	-4.191623000	1.782305000	4.479880000
Cl	4.393575000	-0.980887000	-1.378828000
O	4.728453000	-1.971543000	-2.439899000
O	5.560398000	-0.123302000	-1.042289000
O	3.951993000	-1.723277000	-0.132633000
O	3.240722000	-0.126574000	-1.835443000
Cl	-4.759349000	1.482679000	-0.634754000
O	-5.355445000	2.586318000	-1.420340000
O	-3.634468000	1.994967000	0.223927000
O	-4.199620000	0.430743000	-1.562417000
O	-5.794033000	0.848437000	0.252078000
H	0.529970000	-3.409319000	1.813512000

Zero-point correction= 0.143166 (Hartree/Particle)
Thermal correction to Energy= 0.150630
Thermal correction to Enthalpy= 0.151574
Thermal correction to Gibbs Free Energy= 0.110407
Sum of electronic and zero-point Energies= -310.090182
Sum of electronic and thermal Energies= -310.082719
Sum of electronic and thermal Enthalpies= -310.081774
Sum of electronic and thermal Free Energies= -310.1229

C	0.461515000	0.295909000	0.000006000
C	0.015516000	-1.057677000	-0.000004000
C	-1.337755000	-1.365909000	0.000002000
C	-2.302059000	-0.349666000	0.000004000
C	-1.889683000	0.990733000	-0.000005000
C	-0.541076000	1.309527000	-0.000005000
H	0.747957000	-1.859584000	-0.000016000
H	-1.650435000	-2.407247000	0.000002000
H	-3.359689000	-0.597738000	0.000017000
H	-2.631208000	1.785737000	-0.000017000
H	-0.228482000	2.351359000	-0.000017000
C	1.833015000	0.646866000	0.000012000
H	2.076269000	1.706841000	0.000030000
C	2.965458000	-0.332506000	-0.000005000
H	3.931004000	0.181288000	0.000220000
H	2.942376000	-0.992318000	0.880584000
H	2.942615000	-0.991998000	-0.880841000

2+EB
^{3}TS

Zero-point correction= 0.681700 (Hartree/Particle)
Thermal correction to Energy= 0.721437
Thermal correction to Enthalpy= 0.722381
Thermal correction to Gibbs Free Energy= 0.607393
Sum of electronic and zero-point Energies= -2649.329054
Sum of electronic and thermal Energies= -2649.289316
Sum of electronic and thermal Enthalpies= -2649.288372
Sum of electronic and thermal Free Energies= -2649.4033

Ru	-0.563277000	-0.491868000	0.127104000
C	1.701573000	1.042379000	1.747399000
H	1.944818000	1.927763000	2.350997000
H	2.482396000	0.911843000	1.001997000
H	1.690378000	0.155370000	2.377653000
N	-1.512506000	-0.789002000	2.112846000
N	0.373234000	1.243608000	1.094511000
C	-1.136534000	-2.031089000	2.842224000
H	-1.392169000	-2.911375000	2.255859000
H	-1.662752000	-2.071681000	3.807292000
C	-1.059313000	0.375688000	2.951862000
H	-0.205612000	0.037492000	3.542165000
H	-1.850145000	0.656679000	3.661344000
C	-2.993107000	-0.775295000	1.916649000
H	-3.468982000	-0.901925000	2.902662000
H	-3.267853000	0.207975000	1.538813000
C	-3.547118000	-1.856948000	0.972353000
H	-4.637332000	-1.812558000	1.088957000
H	-3.260681000	-2.857226000	1.313868000
C	-3.297193000	-1.687945000	-0.533280000
H	-3.937471000	-2.400713000	-1.075279000
H	-3.589368000	-0.681569000	-0.824076000
C	-1.560892000	-3.329336000	-0.980567000
H	-2.274764000	-3.881217000	-1.609938000
H	-1.607382000	-3.711637000	0.038509000
H	-0.549653000	-3.497424000	-1.344301000
N	0.485038000	-0.306560000	-1.778072000
N	-1.886969000	-1.883259000	-0.998655000
S	1.090562000	-2.101207000	0.603506000
C	1.897284000	-0.839969000	-1.718309000
H	2.531092000	-0.113946000	-1.213678000
H	2.272420000	-0.929635000	-2.749330000
C	2.014988000	-2.164115000	-0.984318000
H	3.074704000	-2.318457000	-0.756613000
H	1.660049000	-3.018924000	-1.574194000
C	-1.749304000	-1.336956000	-2.388447000
C	-0.287460000	-1.130998000	-2.772166000
H	0.216123000	-2.095054000	-2.863040000
H	-0.238819000	-0.656699000	-3.761205000
C	0.524201000	1.133294000	-2.192606000
H	1.065009000	1.189742000	-3.149428000
H	-0.510956000	1.442088000	-2.350544000
C	1.207433000	2.087282000	-1.197507000
C	0.471175000	2.380947000	0.115213000
H	-0.060932000	-2.047689000	3.014830000
C	-0.657228000	1.588015000	2.121627000
H	-1.523639000	1.985961000	1.595533000
H	-0.272542000	2.370103000	2.793223000
H	-0.548885000	2.685505000	-0.112065000
H	0.984450000	3.209069000	0.625018000
H	1.260533000	3.054437000	-1.716984000
H	2.247663000	1.807785000	-1.012120000
H	-2.266754000	-0.379163000	-2.395260000
H	-2.228322000	-2.015086000	-3.111147000
O	-1.845433000	0.830786000	-0.586648000
O	4.198692000	1.110083000	-0.467239000
O	4.923409000	0.077317000	1.683839000
C	6.767965000	0.729167000	-0.097050000
F	7.686907000	-0.081929000	0.450128000
F	6.921259000	1.954130000	0.434592000
F	7.016008000	0.814092000	-1.415474000
S	5.051983000	0.087434000	0.213167000
O	5.044604000	-1.235497000	-0.454653000
C	-5.087529000	1.668078000	-0.135016000
C	-5.808518000	1.289671000	1.019692000
C	-7.001839000	0.576162000	0.932207000
C	-7.515977000	0.215149000	-0.317117000
C	-6.823408000	0.585610000	-1.473770000
C	-5.630247000	1.300205000	-1.386349000
H	-5.430277000	1.584869000	1.996392000

H	-7.540258000	0.312993000	1.839244000
H	-8.448821000	-0.336970000	-0.388591000
H	-7.219484000	0.320956000	-2.450951000
H	-5.112708000	1.583243000	-2.298248000
C	-3.807402000	2.386550000	-0.014829000
H	-3.650740000	2.777234000	0.996356000
H	-2.769366000	1.465384000	-0.178494000
C	-3.426729000	3.388521000	-1.092209000
H	-2.481869000	3.882576000	-0.844701000
H	-3.293122000	2.907614000	-2.067415000
H	-4.192738000	4.168760000	-1.206592000

^{3}IH(P+S)

Zero-point correction= 0.536478 (Hartree/Particle)
Thermal correction to Energy= 0.569498
Thermal correction to Enthalpy= 0.570442
Thermal correction to Gibbs Free Energy= 0.472085
Sum of electronic and zero-point Energies=-2339.207053
Sum of electronic and thermal Energies= -2339.174034
Sum of electronic and thermal Enthalpies= -2339.173090
Sum of electronic and thermal Free Energies= -2339.2714

Ru	1.532599000	0.055387000	0.061773000
C	-0.900779000	2.318436000	0.405743000
H	-1.283214000	3.243523000	0.866154000
H	-1.665190000	1.546540000	0.483073000
H	-0.727064000	2.490050000	-0.657294000
N	2.651803000	1.764319000	-0.940068000
N	0.347903000	1.891791000	1.078654000
C	2.519745000	1.795165000	-2.421738000
H	2.908424000	0.875344000	-2.856714000
H	3.068827000	2.653770000	-2.836355000
C	2.031034000	3.028919000	-0.399718000
H	1.259091000	3.324853000	-1.112021000
H	2.786058000	3.828353000	-0.394856000
C	4.101837000	1.669059000	-0.579418000
H	4.623359000	2.499171000	-1.083013000
H	4.194117000	1.844944000	0.494586000
C	4.832812000	0.357338000	-0.946995000
H	5.901011000	0.601725000	-0.873117000
H	4.673846000	0.117305000	-2.003570000
C	4.629540000	-0.893682000	-0.063619000
H	5.480467000	-1.573879000	-0.242686000
H	4.653713000	-0.589660000	0.982961000
C	3.386925000	-2.406329000	-1.516031000
H	4.154388000	-3.198400000	-1.476896000
H	3.599485000	-1.755554000	-2.366828000
H	2.413614000	-2.863263000	-1.700270000
N	0.545996000	-1.645036000	0.989658000
N	3.359678000	-1.626161000	-0.272638000
S	0.255700000	-0.467190000	-1.809277000
C	-0.734874000	-2.004519000	0.276755000
H	-1.500352000	-1.276451000	0.544601000
H	-1.072285000	-2.987549000	0.639660000
C	-0.594971000	-2.003358000	-1.235685000
H	-1.602865000	-1.994154000	-1.662992000
H	-0.048298000	-2.870864000	-1.624350000
C	2.989508000	-2.461231000	0.897063000
C	1.492376000	-2.812686000	0.945217000
H	1.223507000	-3.405880000	0.068988000
H	1.314057000	-3.448745000	1.823280000
C	0.245749000	-1.231862000	2.411878000
H	-0.311899000	-2.064913000	2.865192000
H	1.206410000	-1.132311000	2.918399000
C	-0.592102000	0.055522000	2.616401000
C	0.080307000	1.440097000	2.476116000
H	1.466863000	1.871484000	-2.693241000
C	1.392035000	2.933203000	0.997301000
H	2.150536000	2.724336000	1.754159000
H	0.977782000	3.928888000	1.229641000
H	1.033810000	1.426060000	3.004128000
H	-0.577251000	2.178964000	2.961270000
H	-0.903343000	0.003435000	3.669177000
H	-1.525575000	0.021181000	2.048250000
H	3.254894000	-1.895961000	1.789297000
H	3.553809000	-3.409819000	0.896160000
O	2.646552000	0.225766000	1.803278000
O	-3.278262000	-0.028487000	0.837944000
O	-3.706444000	1.341189000	-1.203084000
C	-5.706107000	-0.037441000	-0.157190000
F	-6.425201000	0.007745000	-1.289683000
F	-6.079936000	0.995562000	0.617425000
F	-6.013999000	-1.174975000	0.489530000
S	-3.886748000	0.041910000	-0.526786000
O	-3.644873000	-1.166298000	-1.350035000
H	3.142241000	1.048387000	1.918243000

Zero-point correction= 0.143166 (Hartree/Particle)
Thermal correction to Energy= 0.150630
Thermal correction to Enthalpy= 0.151574
Thermal correction to Gibbs Free Energy= 0.110406
Sum of electronic and zero-point Energies= -310.090182
Sum of electronic and thermal Energies= -310.082718
Sum of electronic and thermal Enthalpies= -310.081774
Sum of electronic and thermal Free Energies= -310.12294

C	0.461522000	-0.295893000	-0.000008000
C	-0.541055000	-1.309519000	-0.000006000
C	-1.889670000	-0.990747000	0.000007000
C	-2.302067000	0.349641000	0.000009000
C	-1.337776000	1.365902000	-0.000001000
C	0.015495000	1.057694000	-0.000012000
H	-0.228451000	-2.351348000	-0.000009000
H	-2.631175000	-1.785769000	0.000012000
H	-3.359699000	0.597703000	0.000019000
H	-1.650480000	2.407233000	-0.000003000
H	0.747917000	1.859616000	-0.000023000
C	1.833016000	-0.646841000	-0.000021000
H	2.076261000	-1.706817000	0.000026000
C	2.965464000	0.332499000	0.000013000
H	3.931004000	-0.181315000	-0.000302000
H	2.942362000	0.992381000	-0.880519000
H	2.942684000	0.991904000	0.880915000

2'+EB

^{3}TS

Zero-point correction= 0.682950 (Hartree/Particle)
Thermal correction to Energy= 0.722439
Thermal correction to Enthalpy= 0.723383
Thermal correction to Gibbs Free Energy= 0.609381
Sum of electronic and zero-point Energies=-2678.863820
Sum of electronic and thermal Energies= -2678.824331
Sum of electronic and thermal Enthalpies=-2678.823386
Sum of electronic and thermal Free Energies= -2678.9373

Fe	0.639497000	0.563293000	0.066327000
C	-1.584517000	-0.924521000	1.701832000
H	-1.791530000	-1.804471000	2.326533000
H	-2.388865000	-0.834151000	0.976929000
H	-1.581103000	-0.024492000	2.310787000
N	1.629732000	0.898145000	1.957765000
N	-0.268124000	-1.113381000	1.018398000
C	1.350567000	2.158228000	2.703475000

H	1.605776000	3.028698000	2.104283000
H	1.940436000	2.171656000	3.631816000
C	1.166415000	-0.227540000	2.833066000
H	0.306381000	0.131474000	3.400620000
H	1.950102000	-0.485312000	3.559649000
C	3.103078000	0.811209000	1.734665000
H	3.600061000	0.900878000	2.713834000
H	3.325997000	-0.177712000	1.341455000
C	3.685367000	1.876171000	0.797229000
H	4.775210000	1.759278000	0.850351000
H	3.482326000	2.884095000	1.173688000
C	3.325039000	1.748194000	-0.684504000
H	3.926151000	2.470212000	-1.258755000
H	3.587965000	0.747774000	-1.018584000
C	1.575644000	3.407001000	-0.944071000
H	2.252992000	3.972552000	-1.601651000
H	1.693938000	3.757524000	0.079599000
H	0.544447000	3.597341000	-1.230524000
N	-0.494793000	0.419599000	-1.702118000
N	1.886891000	1.959701000	-1.032153000
S	-0.911396000	2.129476000	0.689939000
C	-1.910750000	0.917181000	-1.547731000
H	-2.498174000	0.171906000	-1.019275000
H	-2.352571000	1.011125000	-2.551624000
C	-1.988480000	2.225868000	-0.786791000
H	-3.025669000	2.355488000	-0.462192000
H	-1.710749000	3.095511000	-1.396472000
C	1.666981000	1.481268000	-2.430110000
C	0.186489000	1.293310000	-2.712627000
H	-0.319542000	2.259424000	-2.714646000
H	0.055600000	0.867802000	-3.716297000
C	-0.534914000	-0.994811000	-2.193445000
H	-1.121301000	-1.004168000	-3.124457000
H	0.492665000	-1.280785000	-2.421703000
C	-1.160280000	-2.003125000	-1.222361000
C	-0.386263000	-2.270818000	0.068875000
H	0.291715000	2.221643000	2.947551000
C	0.770114000	-1.452625000	2.031528000
H	1.633178000	-1.857861000	1.506721000
H	0.390845000	-2.227277000	2.714231000
H	0.626000000	-2.583736000	-0.177970000
H	-0.882537000	-3.089083000	0.610683000
H	-1.179008000	-2.961756000	-1.759548000
H	-2.208143000	-1.771566000	-1.014554000
H	2.184372000	0.528873000	-2.524220000
H	2.096222000	2.196603000	-3.148373000
O	1.792163000	-0.631468000	-0.656259000
O	-4.167362000	-1.153244000	-0.396647000
O	-4.903399000	-0.198139000	1.786259000
C	-6.738394000	-0.790202000	-0.025822000
F	-7.662227000	-0.000016000	0.543749000
F	-6.893248000	-2.033197000	0.461745000
F	-6.979509000	-0.829699000	-1.347970000
S	-5.025152000	-0.156954000	0.315576000
O	-5.016819000	1.189166000	-0.304667000
C	4.982747000	-1.757197000	-0.177918000
C	5.588265000	-1.700045000	1.096474000
C	6.833061000	-1.103777000	1.283828000
C	7.514014000	-0.543270000	0.198759000
C	6.936437000	-0.595105000	-1.073476000
C	5.691421000	-1.192762000	-1.260523000
H	5.074819000	-2.149255000	1.944167000
H	7.279107000	-1.086146000	2.274828000
H	8.487111000	-0.081771000	0.340847000
H	7.462912000	-0.173435000	-1.925802000
H	5.265441000	-1.229865000	-2.258842000
C	3.647515000	-2.364720000	-0.339634000
H	3.364006000	-2.958434000	0.535892000
H	2.698860000	-1.380916000	-0.349597000
C	3.319271000	-3.070218000	-1.645173000
H	2.311713000	-3.495483000	-1.612584000
H	3.355480000	-2.387426000	-2.500852000
H	4.024495000	-3.889669000	-1.842383000

^{3}IH(P+S)

Zero-point correction= 0.539032 (Hartree/Particle)
Thermal correction to Energy= 0.571203
Thermal correction to Enthalpy= 0.572147
Thermal correction to Gibbs Free Energy= 0.476278
Sum of electronic and zero-point Energies=-2368.808947
Sum of electronic and thermal Energies= -2368.776776
Sum of electronic and thermal Enthalpies= -2368.775832
Sum of electronic and thermal Free Energies=-2368.8717

Fe	1.707693000	0.033506000	0.138467000
C	-0.732043000	2.135926000	0.368512000
H	-1.107174000	3.068209000	0.817144000
H	-1.511347000	1.380877000	0.449435000
H	-0.538195000	2.290488000	-0.692036000
N	2.841311000	1.716393000	-0.831993000
N	0.503124000	1.699561000	1.073106000
C	2.784371000	1.787917000	-2.316235000
H	3.184398000	0.878234000	-2.760426000
H	3.362024000	2.652950000	-2.675802000
C	2.181140000	2.954186000	-0.297479000
H	1.424250000	3.251019000	-1.025337000
H	2.914167000	3.772546000	-0.245413000
C	4.273425000	1.645594000	-0.417818000
H	4.801089000	2.499728000	-0.873079000
H	4.328667000	1.790533000	0.664190000
C	5.024833000	0.357702000	-0.802787000
H	6.084636000	0.564189000	-0.602266000
H	4.969195000	0.193431000	-1.883630000
C	4.693487000	-0.930050000	-0.031124000
H	5.481451000	-1.671458000	-0.245283000
H	4.716231000	-0.714178000	1.036725000
C	3.377857000	-2.192385000	-1.640147000
H	4.142257000	-2.985702000	-1.676133000
H	3.586052000	-1.463235000	-2.424068000
H	2.401710000	-2.622993000	-1.858889000
N	0.608290000	-1.614820000	0.910556000
N	3.366951000	-1.535594000	-0.320385000
S	0.527980000	-0.283638000	-1.763153000
C	-0.666130000	-1.862123000	0.146581000
H	-1.405498000	-1.117799000	0.435701000
H	-1.067983000	-2.844736000	0.438587000
C	-0.463498000	-1.775934000	-1.354321000
H	-1.450518000	-1.661232000	-1.815155000
H	0.023075000	-2.662624000	-1.777958000
C	2.999229000	-2.501611000	0.750546000
C	1.498398000	-2.811150000	0.774660000
H	1.214039000	-3.328231000	-0.143310000
H	1.299543000	-3.506879000	1.601453000
C	0.292039000	-1.337236000	2.351797000
H	-0.281213000	-2.198289000	2.728621000
H	1.243550000	-1.291246000	2.883220000
C	-0.527191000	-0.062024000	2.632383000
C	0.175699000	1.295572000	2.477753000
H	1.749617000	1.886088000	-2.641870000
C	1.507394000	2.789393000	1.068129000
H	2.248692000	2.583783000	1.842829000

H	1.036319000	3.750907000	1.327202000
H	1.111874000	1.274325000	3.034899000
H	-0.473372000	2.070551000	2.913983000
H	-0.794251000	-0.127509000	3.696457000
H	-1.482373000	-0.070280000	2.100618000
H	3.292141000	-2.055096000	1.698809000
H	3.546327000	-3.449489000	0.619398000
O	2.672277000	0.092402000	1.770438000
O	-3.247504000	-0.005026000	0.851165000
O	-3.701249000	1.458900000	-1.117494000
C	-5.666369000	-0.034502000	-0.163946000
F	-6.378754000	0.048976000	-1.298633000
F	-6.077894000	0.943040000	0.661479000
F	-5.942882000	-1.214282000	0.418228000
S	-3.847863000	0.120627000	-0.512746000
O	-3.561615000	-1.033151000	-1.398739000
H	3.215673000	0.881087000	1.894983000

Zero-point correction= 0.143165 (Hartree/Particle)
Thermal correction to Energy= 0.150630
Thermal correction to Enthalpy= 0.151574
Thermal correction to Gibbs Free Energy= 0.110398
Sum of electronic and zero-point Energies= -310.090184
Sum of electronic and thermal Energies= -310.082719
Sum of electronic and thermal Enthalpies= -310.081775
Sum of electronic and thermal Free Energies= -310.12295

C	0.461527000	-0.295839000	0.000005000
C	-0.541035000	-1.309506000	0.000005000
C	-1.889655000	-0.990785000	0.000002000
C	-2.302107000	0.349593000	0.000000000
C	-1.337852000	1.365883000	-0.000004000
C	0.015436000	1.057730000	-0.000003000
H	-0.228382000	-2.351319000	0.000008000
H	-2.631138000	-1.785828000	0.000002000
H	-3.359749000	0.597610000	0.000003000
H	-1.650589000	2.407204000	-0.000012000
H	0.747817000	1.859686000	-0.000027000
C	1.833023000	-0.646781000	0.000011000
H	2.076271000	-1.706758000	-0.000139000
C	2.965555000	0.332477000	0.000013000
H	3.931040000	-0.181445000	0.000889000
H	2.943209000	0.991516000	-0.881173000
H	2.942176000	0.992693000	0.880274000

^{5}TS

Zero-point correction= 0.679262 (Hartree/Particle)
Thermal correction to Energy= 0.719892
Thermal correction to Enthalpy= 0.720836
Thermal correction to Gibbs Free Energy= 0.603719
Sum of electronic and zero-point Energies=-2678.874864
Sum of electronic and thermal Energies= -2678.834234
Sum of electronic and thermal Enthalpies=-2678.833290
Sum of electronic and thermal Free Energies= -2678.9504

Fe	0.603207000	0.812139000	0.040734000
C	-1.128130000	0.081553000	2.649434000
H	-1.190401000	-0.521145000	3.568559000
H	-2.085648000	0.019719000	2.130603000
H	-0.955172000	1.126621000	2.905338000
N	2.075591000	1.735523000	1.510651000
N	-0.024496000	-0.427957000	1.794228000
C	1.939895000	3.175019000	1.839513000
H	2.028559000	3.783619000	0.941029000
H	2.716749000	3.477313000	2.558784000
C	1.843701000	0.948590000	2.764387000
H	1.160345000	1.531566000	3.385053000
H	2.785785000	0.856358000	3.325031000
C	3.432110000	1.476361000	0.941971000
H	4.177314000	1.854607000	1.661262000
H	3.558766000	0.396981000	0.862694000
C	3.722845000	2.125841000	-0.426404000
H	4.806339000	2.022550000	-0.570080000
H	3.542704000	3.205395000	-0.390873000
C	3.086605000	1.503662000	-1.682454000
H	3.581831000	1.934882000	-2.568288000
H	3.285292000	0.433751000	-1.672426000
C	1.306466000	3.071361000	-2.212186000
H	1.789879000	3.319754000	-3.170754000
H	1.656879000	3.761820000	-1.445115000
H	0.231114000	3.214440000	-2.299708000
N	-0.945221000	0.145301000	-1.340143000
N	1.614924000	1.680374000	-1.825843000
S	-0.819887000	2.683069000	0.369895000
C	-2.271168000	0.783926000	-1.049122000
H	-2.681901000	0.326129000	-0.154079000
H	-2.970525000	0.562127000	-1.866084000
C	-2.176545000	2.280231000	-0.805040000
H	-3.131653000	2.592550000	-0.374955000
H	-2.026398000	2.857237000	-1.726390000
C	1.056630000	0.722503000	-2.821635000
C	-0.464941000	0.550794000	-2.697030000
H	-0.961927000	1.487560000	-2.954429000
H	-0.791608000	-0.190193000	-3.439912000
C	-1.059237000	-1.344836000	-1.218932000
H	-1.854161000	-1.673625000	-1.903983000
H	-0.110453000	-1.764416000	-1.560425000
C	-1.407743000	-1.888672000	0.180603000
C	-0.351698000	-1.801472000	1.294009000
H	0.956054000	3.365043000	2.268110000
C	1.258340000	-0.450703000	2.547361000
H	1.962585000	-1.062260000	1.985003000
H	1.109740000	-0.913443000	3.535942000
H	0.581760000	-2.241523000	0.944324000
H	-0.711592000	-2.396158000	2.147823000
H	-1.575387000	-2.964407000	0.030217000
H	-2.371368000	-1.504338000	0.525287000
H	1.547081000	-0.235112000	-2.655668000
H	1.285048000	1.057747000	-3.846388000
O	1.671396000	-0.567590000	-0.320385000
O	-4.078057000	-0.520701000	1.424386000
O	-6.547687000	-0.135531000	1.585459000
C	-5.589395000	-1.460164000	-0.482335000
F	-6.656148000	-1.241013000	-1.262880000
F	-5.749141000	-2.646630000	0.124675000
F	-4.505562000	-1.573725000	-1.301603000
S	-5.341235000	-0.085611000	0.750286000
O	-5.173565000	1.104464000	-0.116706000
C	4.524869000	-2.214119000	-0.205385000
C	4.851627000	-2.365412000	1.160704000
C	6.088669000	-1.966433000	1.658943000
C	7.040751000	-1.400400000	0.804776000
C	6.740061000	-1.245542000	-0.551654000
C	5.501248000	-1.644519000	-1.050578000
H	4.122509000	-2.819139000	1.828761000
H	6.316834000	-2.105975000	2.712333000
H	8.008730000	-1.092747000	1.190008000
H	7.478467000	-0.819337000	-1.225845000
H	5.293749000	-1.525356000	-2.109881000
C	3.184581000	-2.597680000	-0.682755000
H	2.690565000	-3.296254000	0.000833000
H	2.408029000	-1.519549000	-0.491136000
C	2.977882000	-2.973806000	-2.138655000

H	1.922909000	-3.193826000	-2.332883000
H	3.281116000	-2.176202000	-2.826398000
H	3.556843000	-3.869721000	-2.404538000

^{5}IH(P+S)

Zero-point correction= 0.538033 (Hartree/Particle)
Thermal correction to Energy= 0.570474
Thermal correction to Enthalpy= 0.571418
Thermal correction to Gibbs Free Energy= 0.475456
Sum of electronic and zero-point Energies=-2368.810330
Sum of electronic and thermal Energies= -2368.777890
Sum of electronic and thermal Enthalpies= -2368.776946
Sum of electronic and thermal Free Energies= -2368.8729

Fe	-1.680604000	0.031184000	-0.100760000
C	0.190705000	2.620109000	0.221918000
H	0.432201000	3.638143000	-0.120319000
H	1.122246000	2.065038000	0.344143000
H	-0.300307000	2.666997000	1.193503000
N	-3.348818000	1.422236000	0.599408000
N	-0.696523000	1.954934000	-0.770717000
C	-3.647297000	1.477333000	2.049990000
H	-3.917509000	0.489789000	2.421602000
H	-4.474658000	2.175873000	2.248755000
C	-2.884507000	2.777798000	0.162010000
H	-2.401661000	3.244982000	1.022747000
H	-3.751733000	3.404535000	-0.094426000
C	-4.566176000	0.994857000	-0.156943000
H	-5.383587000	1.687282000	0.103926000
H	-4.340382000	1.100720000	-1.218359000
C	-5.054181000	-0.445449000	0.105252000
H	-6.071378000	-0.487054000	-0.306389000
H	-5.178140000	-0.627089000	1.178280000
C	-4.293501000	-1.602232000	-0.569157000
H	-4.908766000	-2.513353000	-0.489022000
H	-4.164025000	-1.361959000	-1.622867000
C	-3.058611000	-2.580111000	1.281927000
H	-3.605046000	-3.529848000	1.166446000
H	-3.589283000	-1.949146000	1.995623000
H	-2.074258000	-2.780253000	1.702089000
N	-0.020043000	-1.313673000	-0.610557000
N	-2.938401000	-1.890486000	-0.017472000
S	-0.847100000	-0.125500000	2.105651000
C	1.060564000	-1.271821000	0.423302000
H	1.614956000	-0.345551000	0.303698000
H	1.771838000	-2.090767000	0.251239000
C	0.535948000	-1.311278000	1.851074000
H	1.368268000	-1.033870000	2.503144000
H	0.191031000	-2.306469000	2.158365000
C	-2.136497000	-2.706216000	-0.975966000
C	-0.630960000	-2.679060000	-0.670699000
H	-0.439572000	-3.163201000	0.288646000
H	-0.113190000	-3.281237000	-1.430681000
C	0.521849000	-0.896238000	-1.943494000
H	1.362622000	-1.562286000	-2.186842000
H	-0.269279000	-1.072236000	-2.677359000
C	1.051953000	0.549418000	-2.048938000
C	0.064515000	1.729862000	-2.039641000
H	-2.761983000	1.802744000	2.597048000
C	-1.911805000	2.778083000	-1.022764000
H	-2.411738000	2.379956000	-1.905713000
H	-1.629570000	3.822553000	-1.230445000
H	-0.659458000	1.623699000	-2.853806000
H	0.637271000	2.642182000	-2.264240000
H	1.545183000	0.599484000	-3.029603000
H	1.853845000	0.726036000	-1.326993000
H	-2.317905000	-2.293211000	-1.966634000
H	-2.473326000	-3.755545000	-0.960739000
O	-2.426158000	-0.031542000	-1.889342000
O	3.150868000	1.324791000	0.276824000
O	5.369635000	1.286755000	1.438350000
C	4.905475000	-0.439686000	-0.501397000
F	5.849545000	-1.308943000	-0.118064000
F	5.433398000	0.374688000	-1.428111000
F	3.919269000	-1.155045000	-1.112577000
S	4.222077000	0.517697000	0.942679000
O	3.696695000	-0.550401000	1.825540000
H	-1.973212000	0.380727000	-2.634010000

Zero-point correction= 0.143166 (Hartree/Particle)
Thermal correction to Energy= 0.150630
Thermal correction to Enthalpy= 0.151574
Thermal correction to Gibbs Free Energy= 0.110406
Sum of electronic and zero-point Energies= -310.090182
Sum of electronic and thermal Energies= -310.082719
Sum of electronic and thermal Enthalpies= -310.081774
Sum of electronic and thermal Free Energies= -310.12294

C	0.461518000	-0.295901000	-0.000002000
C	-0.541069000	-1.309525000	-0.000004000
C	-1.889676000	-0.990740000	0.000001000
C	-2.302063000	0.349655000	0.000005000
C	-1.337768000	1.365906000	0.000000000
C	0.015505000	1.057685000	-0.000005000
H	-0.228462000	-2.351353000	-0.000008000
H	-2.631197000	-1.785749000	0.000000000
H	-3.359696000	0.597716000	0.000012000
H	-1.650457000	2.407240000	-0.000001000
H	0.747938000	1.859597000	-0.000012000
C	1.833016000	-0.646851000	0.000000000
H	2.076273000	-1.706824000	0.000013000
C	2.965465000	0.332502000	0.000003000
H	3.931005000	-0.181307000	-0.000046000
H	2.942491000	0.992182000	-0.880687000
H	2.942542000	0.992116000	0.880744000

2+DHA

^{3}TS

Zero-point correction= 0.742161 (Hartree/Particle)
Thermal correction to Energy= 0.784790
Thermal correction to Enthalpy= 0.785734
Thermal correction to Gibbs Free Energy= 0.664650
Sum of electronic and zero-point Energies= -2879.127866
Sum of electronic and thermal Energies= -2879.085237
Sum of electronic and thermal Enthalpies= -2879.084293
Sum of electronic and thermal Free Energies= -2879.2053

Ru	0.115516000	-1.050616000	-0.052709000
C	-2.078710000	0.163639000	-2.002976000
H	-2.263428000	0.817384000	-2.866561000
H	-2.796925000	0.413757000	-1.225914000
H	-2.238403000	-0.875683000	-2.283362000
N	0.83310000	-2.140836000	-1.848067000
N	-0.680703000	0.373393000	-1.520376000
C	0.240360000	-3.486090000	-2.082716000
H	0.436194000	-4.143820000	-1.238320000
H	0.667007000	-3.928277000	-2.994969000
C	0.454889000	-1.275410000	-3.020355000
H	-0.484659000	-1.663146000	-3.418478000
H	1.206596000	-1.372702000	-3.816038000
C	2.316602000	-2.280967000	-1.729784000

H	2.682345000	-2.798522000	-2.631477000
H	2.741995000	-1.278541000	-1.722663000
C	2.814055000	-3.053311000	-0.494781000
H	3.886052000	-3.214229000	-0.664887000
H	2.374095000	-4.055292000	-0.457456000
C	2.726185000	-2.352145000	0.868300000
H	3.319115000	-2.927267000	1.595777000
H	3.167219000	-1.361833000	0.777822000
C	0.844071000	-3.469990000	1.926420000
H	1.536263000	-3.878714000	2.677497000
H	0.749555000	-4.174863000	1.101170000
H	-0.143658000	-3.352925000	2.366712000
N	-0.722141000	-0.079583000	1.712528000
N	1.350456000	-2.167829000	1.430793000
S	-1.771424000	-2.464309000	0.137062000
C	-2.190744000	-0.379518000	1.900344000
H	-2.768615000	0.218021000	1.198695000
H	-2.478835000	-0.052979000	2.911370000
C	-2.544340000	-1.840272000	1.684007000
H	-3.631691000	-1.899421000	1.570503000
H	-2.248738000	-2.486017000	2.520804000
C	1.407195000	-1.173151000	2.551029000
C	0.024815000	-0.629542000	2.897473000
H	-0.588520000	-1.418292000	3.336421000
H	0.127493000	0.151468000	3.662268000
C	-0.536538000	1.404778000	1.602233000
H	-0.974075000	1.861250000	2.502863000
H	0.539480000	1.588665000	1.597203000
C	-1.182603000	2.059464000	0.369130000
C	-0.542699000	1.777280000	-0.995396000
H	-0.840098000	-3.399006000	-2.192741000
C	0.283702000	0.191864000	-2.648158000
H	1.237065000	0.613907000	-2.335028000
H	-0.063734000	0.746318000	-3.532726000
H	0.522425000	1.993599000	-0.938477000
H	-0.998711000	2.448478000	-1.737419000
H	-1.057767000	3.140508000	0.521390000
H	-2.263202000	1.898070000	0.340069000
H	2.043260000	-0.359178000	2.207980000
H	1.856870000	-1.633303000	3.444115000
O	1.603256000	0.204470000	0.098426000
O	-4.334490000	1.346550000	0.149746000
O	-5.379574000	-0.228689000	-1.476813000
C	-6.954649000	1.253307000	0.046723000
F	-8.014946000	0.452903000	-0.145506000
F	-7.001167000	2.236486000	-0.868655000
F	-7.067356000	1.812780000	1.263826000
S	-5.369094000	0.295109000	-0.096575000
O	-5.467177000	-0.710958000	0.987200000
C	6.622981000	-1.146296000	-0.709574000
C	5.526034000	-0.484838000	-1.258754000
C	4.841630000	0.510335000	-0.536951000
C	5.293936000	0.844310000	0.759705000
C	6.400082000	0.181382000	1.295842000
C	7.062307000	-0.815591000	0.575445000
C	3.667708000	1.215626000	-1.091673000
C	4.552081000	1.909694000	1.541758000
C	3.928181000	2.970372000	0.657435000
C	3.487873000	2.609492000	-0.634746000
C	2.879754000	3.585393000	-1.444013000
H	2.556220000	3.315954000	-2.447342000
C	2.707640000	4.890139000	-0.987398000
C	3.149616000	5.243293000	0.290583000
C	3.760864000	4.283533000	1.100712000
H	3.552128000	1.091004000	-2.172847000
H	7.145744000	-1.903383000	-1.288326000
H	5.205098000	-0.719042000	-2.271880000
H	6.752345000	0.453012000	2.288868000
H	7.923234000	-1.318220000	1.007345000
H	3.749505000	1.426078000	2.123710000
H	2.241010000	5.632461000	-1.629222000
H	3.026888000	6.260686000	0.651262000
H	4.114407000	4.560265000	2.091842000
H	2.560566000	0.599582000	-0.557658000
H	5.217922000	2.371311000	2.280668000

^{3}IH

Zero-point correction= 0.745863 (Hartree/Particle)
Thermal correction to Energy= 0.789734
Thermal correction to Enthalpy= 0.790679
Thermal correction to Gibbs Free Energy= 0.663384
Sum of electronic and zero-point Energies= -2879.162856
Sum of electronic and thermal Energies= -2879.118984
Sum of electronic and thermal Enthalpies= -2879.118040
Sum of electronic and thermal Free Energies= -2879.2453

Ru	0.076897000	-0.553995000	0.496898000
C	2.227184000	1.754695000	0.858505000
H	2.422470000	2.835773000	0.830428000
H	3.004204000	1.253194000	0.286907000
H	2.280600000	1.395115000	1.884426000
N	-0.881295000	0.287896000	2.333243000
N	0.878573000	1.482264000	0.276254000
C	-0.427644000	-0.310922000	3.618445000
H	-0.638062000	-1.378592000	3.638643000
H	-0.938576000	0.175401000	4.463024000
C	-0.489072000	1.740408000	2.360035000
H	0.385360000	1.826200000	3.007969000
H	-1.289199000	2.339378000	2.817128000
C	-2.361708000	0.122360000	2.235428000
H	-2.814671000	0.530938000	3.153267000
H	-2.725127000	0.734835000	1.408466000
C	-2.851364000	-1.326614000	2.059797000
H	-3.942649000	-1.283419000	2.170598000
H	-2.503838000	-1.953330000	2.887782000
C	-2.610780000	-2.007654000	0.705126000
H	-3.218137000	-2.924450000	0.662634000
H	-2.943942000	-1.339767000	-0.086234000
C	-0.793827000	-3.548475000	1.195571000
H	-1.481594000	-4.386514000	1.007695000
H	-0.813884000	-3.295588000	2.255161000
H	0.222743000	-3.851667000	0.953736000
N	1.073951000	-1.408538000	-1.229383000
N	-1.193203000	-2.373773000	0.384392000
S	1.810801000	-1.498504000	1.724529000
C	2.518032000	-1.745523000	-0.941862000
H	3.107879000	-0.831732000	-0.966932000
H	2.890300000	-2.388598000	-1.754052000
C	2.725591000	-2.408574000	0.409344000
H	3.794414000	-2.355950000	0.640193000
H	2.420220000	-3.462795000	0.425132000
C	-1.096882000	-2.690156000	-1.077775000
C	0.349259000	-2.683634000	-1.558300000
H	0.902475000	-3.506607000	-1.102142000
H	0.371025000	-2.853519000	-2.643127000
C	1.004487000	-0.451102000	-2.379679000
H	1.525543000	-0.914291000	-3.231580000
H	-0.051877000	-0.336849000	-2.631341000
C	1.629073000	0.931885000	-2.127516000
C	0.878598000	1.871479000	-1.177085000
H	0.649030000	-0.183309000	3.724982000
C	-0.152421000	2.302435000	0.984323000
H	-1.043067000	2.344547000	0.357521000

H	0.208924000	3.334690000	1.104299000
H	-0.164723000	1.921369000	-1.485013000
H	1.324721000	2.874214000	-1.249026000
H	1.611044000	1.437666000	-3.103280000
H	2.687557000	0.861059000	-1.864206000
H	-1.660220000	-1.916003000	-1.596547000
H	-1.553055000	-3.670452000	-1.284673000
O	-1.407303000	0.142878000	-0.793437000
O	4.697094000	0.681659000	-1.133639000
O	5.528363000	1.103839000	1.179392000
C	7.291783000	0.695894000	-0.749860000
F	8.273475000	0.386466000	0.112005000
F	7.373807000	2.009631000	-1.022773000
F	7.509084000	0.020193000	-1.891659000
S	5.628358000	0.273620000	-0.037305000
O	5.698032000	-1.191669000	0.173041000
C	-6.976736000	-2.318319000	-0.751766000
C	-6.870055000	-1.174925000	0.025086000
C	-6.049883000	-0.089197000	-0.376931000
C	-5.332871000	-0.190116000	-1.603411000
C	-5.455195000	-1.350715000	-2.368262000
C	-6.266106000	-2.411847000	-1.956981000
C	-5.930956000	1.082870000	0.425442000
C	-4.451915000	0.945960000	-2.081685000
C	-4.344656000	2.133763000	-1.146701000
C	-5.089589000	2.176132000	0.066965000
C	-4.966733000	3.316836000	0.902457000
H	-5.542140000	3.352059000	1.824725000
C	-4.138846000	4.374030000	0.556068000
C	-3.405181000	4.324567000	-0.638506000
C	-3.515364000	3.208618000	-1.473587000
H	-6.501060000	1.143758000	1.349469000
H	-7.613099000	-3.137662000	-0.428582000
H	-7.422906000	-1.093557000	0.958235000
H	-4.910165000	-1.424666000	-3.307408000
H	-6.348106000	-3.302992000	-2.572799000
H	-3.439553000	0.560231000	-2.273169000
H	-4.064332000	5.241587000	1.206153000
H	-2.760315000	5.152084000	-0.920161000
H	-2.951534000	3.176580000	-2.403713000
H	-2.022896000	0.779590000	-0.403105000
H	-4.820080000	1.295813000	-3.059206000

2'+DHA

^{3}TS

Zero-point correction= 0.743538 (Hartree/Particle)

Thermal correction to Energy= 0.785946

Thermal correction to Enthalpy= 0.786890

Thermal correction to Gibbs Free Energy= 0.666315

Sum of electronic and zero-point Energies= -2908.661321

Sum of electronic and thermal Energies= -2908.618914

Sum of electronic and thermal Enthalpies= -2908.617970

Sum of electronic and thermal Free Energies= -2908.7385

Fe	0.211263000	-1.366117000	0.165203000
C	-1.505725000	0.308111000	-1.839260000
H	-1.463878000	1.088491000	-2.611577000
H	-2.325902000	0.548050000	-1.168411000
H	-1.715829000	-0.656803000	-2.292891000
N	1.134962000	-2.267906000	-1.565306000
N	-0.203930000	0.283022000	-1.104331000
C	0.558863000	-3.528496000	-2.113301000
H	0.559979000	-4.315255000	-1.362720000
H	1.150395000	-3.853754000	-2.981699000
C	1.007633000	-1.232763000	-2.644535000
H	0.103392000	-1.461784000	-3.210808000
H	1.856308000	-1.307501000	-3.338327000
C	2.573253000	-2.513876000	-1.252791000
H	3.056369000	-2.899185000	-2.164698000
H	3.030742000	-1.554292000	-1.020659000
C	2.831436000	-3.506658000	-0.112089000
H	3.913220000	-3.696173000	-0.110679000
H	2.374052000	-4.477729000	-0.326954000
C	2.484279000	-3.028297000	1.299701000
H	2.870793000	-3.758463000	2.027897000
H	2.978830000	-2.075629000	1.476922000
C	0.366637000	-4.132575000	1.712625000
H	0.863077000	-4.720274000	2.499716000
H	0.411603000	-4.679859000	0.772752000
H	-0.684738000	-4.007311000	1.958614000
N	-0.895810000	-0.634618000	1.799626000
N	1.032731000	-2.815036000	1.575524000
S	-1.672164000	-2.598180000	-0.288918000
C	-2.387567000	-0.780381000	1.626999000
H	-2.745678000	-0.018149000	0.940932000
H	-2.865562000	-0.577682000	2.597768000
C	-2.784282000	-2.142028000	1.092226000
H	-3.808126000	-2.060807000	0.713864000
H	-2.766013000	-2.927526000	1.858891000
C	0.901132000	-2.047914000	2.850447000
C	-0.491851000	-1.457947000	2.985611000
H	-1.226286000	-2.255212000	3.105670000
H	-0.542546000	-0.843777000	3.894247000
C	-0.582224000	0.809007000	2.051561000
H	-1.170948000	1.125544000	2.925530000
H	0.477800000	0.869457000	2.301959000
C	-0.902410000	1.753218000	0.887851000
C	-0.045823000	1.580964000	-0.365804000
H	-0.472549000	-3.364651000	-2.419998000
C	0.915821000	0.172565000	-2.082281000
H	1.841357000	0.439511000	-1.575736000
H	0.764467000	0.883868000	-2.907297000
H	1.002209000	1.663059000	-0.088051000
H	-0.289324000	2.388618000	-1.071887000
H	-0.681926000	2.764151000	1.257299000
H	-1.968282000	1.759540000	0.645867000
H	1.637802000	-1.247602000	2.818845000
H	1.115025000	-2.700793000	3.710731000
O	1.601822000	-0.402939000	0.738546000
O	-4.009399000	1.539268000	-0.009014000
O	-4.877741000	0.431778000	-2.067959000
C	-6.568780000	1.768834000	-0.534424000
F	-7.641657000	1.147308000	-1.049285000
F	-6.374683000	2.906936000	-1.222993000
F	-6.846866000	2.096727000	0.739528000
S	-5.066156000	0.679423000	-0.624674000
O	-5.433613000	-0.496844000	0.198692000
C	5.588417000	1.444641000	-3.400661000
C	4.854333000	2.416743000	-2.719869000
C	4.311495000	2.161560000	-1.457200000
C	4.512650000	0.898822000	-0.856348000
C	5.273414000	-0.065491000	-1.545600000
C	5.802891000	0.197746000	-2.805544000
C	3.508737000	3.220863000	-0.731500000
C	3.948312000	0.618863000	0.481026000
C	3.711206000	1.791120000	1.349921000
C	3.499518000	3.062759000	0.775507000
C	3.259898000	4.160432000	1.607345000
H	3.110501000	5.141831000	1.162243000
C	3.212447000	4.016065000	2.994386000
C	3.417020000	2.756718000	3.567593000
C	3.665447000	1.658538000	2.750104000
H	3.877306000	4.218103000	-1.001612000

H	6.004124000	1.663986000	-4.380073000
H	4.706366000	3.394971000	-3.172407000
H	5.467772000	-1.023674000	-1.067957000
H	6.393709000	-0.558150000	-3.315879000
H	2.718102000	0.067799000	0.421522000
H	3.025525000	4.881144000	3.624341000
H	3.392969000	2.637058000	4.647346000
H	3.842833000	0.680839000	3.192815000
H	2.468134000	3.190971000	-1.096793000
H	4.460684000	-0.199734000	0.997401000

^{3}IH

Zero-point correction= 0.747014 (Hartree/Particle)
Thermal correction to Energy= 0.790679
Thermal correction to Enthalpy= 0.791623
Thermal correction to Gibbs Free Energy= 0.664970
Sum of electronic and zero-point Energies= -2908.701867
Sum of electronic and thermal Energies= -2908.658202
Sum of electronic and thermal Enthalpies= -2908.657258
Sum of electronic and thermal Free Energies= -2908.7839

Fe	0.036672000	0.923129000	-0.122981000
C	1.943311000	-1.375254000	-1.051085000
H	2.035040000	-2.457439000	-1.217966000
H	2.812906000	-1.050483000	-0.487026000
H	1.946434000	-0.848380000	-2.001784000
N	-1.149565000	0.499688000	-1.910406000
N	0.682273000	-1.104130000	-0.294133000
C	-0.840979000	1.282188000	-3.141115000
H	-0.970794000	2.347659000	-2.967265000
H	-1.507216000	0.964777000	-3.957316000
C	-0.856724000	-0.934537000	-2.234021000
H	-0.036696000	-0.944887000	-2.953878000
H	-1.725107000	-1.397371000	-2.724125000
C	-2.599382000	0.685722000	-1.609635000
H	-3.171771000	0.423059000	-2.513675000
H	-2.892822000	-0.026300000	-0.836861000
C	-2.993586000	2.103848000	-1.179677000
H	-4.089153000	2.110115000	-1.120109000
H	-2.740235000	2.829189000	-1.959652000
C	-2.497131000	2.562166000	0.193094000
H	-2.988569000	3.514467000	0.445558000
H	-2.787423000	1.819622000	0.933029000
C	-0.618179000	3.987523000	-0.381202000
H	-1.193744000	4.844454000	0.000494000
H	-0.799378000	3.879816000	-1.449197000
H	0.444996000	4.176113000	-0.254606000
N	1.290279000	1.413156000	1.475804000
N	-1.019253000	2.753098000	0.335459000
S	1.617808000	1.868453000	-1.448525000
C	2.719065000	1.643081000	1.051738000
H	3.200942000	0.685359000	0.875357000
H	3.256012000	2.115199000	1.888867000
C	2.822876000	2.479423000	-0.209674000
H	3.833590000	2.348693000	-0.608702000
H	2.663201000	3.550419000	-0.029178000
C	-0.712045000	2.888403000	1.791233000
C	0.772115000	2.697732000	2.047137000
H	1.339310000	3.516733000	1.602830000
H	0.967546000	2.729034000	3.127243000
C	1.258318000	0.344965000	2.525514000
H	1.920284000	0.666773000	3.343550000
H	0.234545000	0.295762000	2.898757000
C	1.710738000	-1.042960000	2.057832000
C	0.791699000	-1.746683000	1.060220000
H	0.193723000	1.118663000	-3.436334000
C	-0.459764000	-1.740288000	-1.011146000
H	-1.297588000	-1.841892000	-0.321338000
H	-0.185412000	-2.757692000	-1.324713000
H	-0.213962000	-1.792953000	1.473815000
H	1.156971000	-2.772656000	0.906674000
H	1.709341000	-1.674531000	2.957313000
H	2.747641000	-1.039850000	1.711656000
H	-1.278412000	2.114512000	2.305634000
H	-1.033926000	3.875338000	2.157429000
O	-1.213582000	0.239128000	1.117180000
O	4.700563000	-0.947731000	0.791397000
O	5.265124000	-1.138201000	-1.630481000
C	7.235377000	-1.088923000	0.133235000
F	8.149394000	-0.743690000	-0.787824000
F	7.239768000	-2.428809000	0.243914000
F	7.618015000	-0.573943000	1.314930000
S	5.548736000	-0.471730000	-0.343787000
O	5.713144000	1.000323000	-0.391306000
C	-7.138258000	1.633920000	-0.313537000
C	-6.842202000	0.411050000	-0.924241000
C	-6.054462000	-0.546058000	-0.285120000
C	-5.526948000	-0.264599000	1.007827000
C	-5.846489000	0.975685000	1.617766000
C	-6.640536000	1.909636000	0.968255000
C	-5.812278000	-1.897711000	-0.925005000
C	-4.668222000	-1.206215000	1.647958000
C	-4.223164000	-2.396905000	1.001218000
C	-4.716502000	-2.731383000	-0.293029000
C	-4.227056000	-3.867272000	-0.937353000
H	-4.604127000	-4.120216000	-1.926457000
C	-3.277262000	-4.694604000	-0.329890000
C	-2.803614000	-4.385206000	0.953181000
C	-3.266818000	-3.252720000	1.607374000
H	-6.752350000	-2.473924000	-0.873435000
H	-7.759073000	2.361643000	-0.828212000
H	-7.242751000	0.194542000	-1.912735000
H	-5.454377000	1.185436000	2.610172000
H	-6.877203000	2.852636000	1.453487000
H	-1.885784000	-0.351536000	0.752527000
H	-2.915561000	-5.577819000	-0.848380000
H	-2.074079000	-5.030178000	1.434979000
H	-2.899101000	-3.004447000	2.600079000
H	-5.620001000	-1.775792000	-1.999978000
H	-4.288138000	-0.977581000	2.640321000

^{5}TS

Zero-point correction= 0.739867 (Hartree/Particle)
Thermal correction to Energy= 0.782502
Thermal correction to Enthalpy= 0.783446
Thermal correction to Gibbs Free Energy= 0.663228
Sum of electronic and zero-point Energies= -2908.673525
Sum of electronic and thermal Energies= -2908.630891
Sum of electronic and thermal Enthalpies= -2908.629946
Sum of electronic and thermal Free Energies= -2908.7501

Fe	-0.051412000	-0.130522000	0.940305000
C	2.116132000	2.090483000	0.116202000
H	2.284397000	3.075362000	-0.344515000
H	2.859975000	1.399860000	-0.276280000
H	2.264965000	2.155285000	1.192829000
N	-0.822776000	1.451295000	2.382093000
N	0.739788000	1.621450000	-0.195357000
C	-0.285015000	1.477017000	3.764089000
H	-0.469881000	0.528789000	4.266360000
H	-0.753913000	2.289409000	4.340493000
C	-0.445621000	2.738873000	1.713489000

H	0.491135000	3.070523000	2.165429000
H	-1.200343000	3.507417000	1.936326000
C	-2.303981000	1.268444000	2.421279000
H	-2.725399000	2.063236000	3.059015000
H	-2.680839000	1.411715000	1.408029000
C	-2.796260000	-0.088286000	2.965230000
H	-3.870831000	0.043224000	3.151067000
H	-2.365375000	-0.289794000	3.951432000
C	-2.685644000	-1.325416000	2.056024000
H	-3.292279000	-2.133030000	2.498183000
H	-3.108847000	-1.085541000	1.082596000
C	-0.814135000	-2.533407000	3.026304000
H	-1.476931000	-3.375931000	3.281388000
H	-0.771121000	-1.842953000	3.868490000
H	0.197283000	-2.902605000	2.868007000
N	0.885599000	-1.704833000	-0.258013000
N	-1.307934000	-1.838550000	1.821283000
S	1.775373000	-0.492376000	2.393318000
C	2.344163000	-1.878599000	0.050024000
H	2.903487000	-1.071676000	-0.418573000
H	2.694402000	-2.815757000	-0.410707000
C	2.645890000	-1.868610000	1.540925000
H	3.724208000	-1.716038000	1.649288000
H	2.382595000	-2.812589000	2.034848000
C	-1.275336000	-2.744948000	0.639105000
C	0.143598000	-2.956209000	0.091683000
H	0.743594000	-3.495032000	0.826874000
H	0.078305000	-3.603948000	-0.793871000
C	0.699686000	-1.337048000	-1.697430000
H	1.174483000	-2.122637000	-2.306069000
H	-0.374625000	-1.357942000	-1.893557000
C	1.295486000	0.016430000	-2.134445000
C	0.618984000	1.311519000	-1.654279000
H	0.793887000	1.628928000	3.737681000
C	-0.267253000	2.643838000	0.195699000
H	-1.213931000	2.382885000	-0.275299000
H	0.039627000	3.635734000	-0.171664000
H	-0.445466000	1.272676000	-1.884258000
H	1.060271000	2.149219000	-2.216048000
H	1.193199000	0.030086000	-3.228852000
H	2.373034000	0.052387000	-1.953541000
H	-1.906972000	-2.302933000	-0.129432000
H	-1.693761000	-3.730223000	0.900945000
O	-1.443211000	0.025592000	-0.131692000
O	4.415472000	0.195646000	-1.437261000
O	5.498606000	1.524952000	0.374045000
C	7.035771000	0.236931000	-1.351394000
F	8.105354000	0.274646000	-0.540996000
F	7.094788000	1.300340000	-2.171560000
F	7.121009000	-0.873609000	-2.104857000
S	5.459256000	0.249770000	-0.367523000
O	5.543216000	-0.986179000	0.445995000
C	-5.548490000	-3.398458000	-1.837651000
C	-5.985740000	-2.312865000	-1.077623000
C	-5.278504000	-1.107088000	-1.067720000
C	-4.110871000	-0.981578000	-1.851323000
C	-3.683023000	-2.081501000	-2.619092000
C	-4.389854000	-3.280228000	-2.612393000
C	-5.738645000	0.054729000	-0.210991000
C	-3.351095000	0.285261000	-1.844771000
C	-4.102976000	1.506067000	-1.488425000
C	-5.269395000	1.410046000	-0.698945000
C	-5.969897000	2.572447000	-0.363916000
H	-6.877737000	2.492897000	0.230602000
C	-5.527941000	3.827055000	-0.786005000
C	-4.372030000	3.927574000	-1.567071000
C	-3.671748000	2.776535000	-1.915298000
H	-6.832302000	0.045835000	-0.124318000
H	-6.113286000	-4.326484000	-1.834700000
H	-6.894380000	-2.400751000	-0.485548000
H	-2.794518000	-1.978441000	-3.238433000
H	-4.049421000	-4.115307000	-3.218499000
H	-2.402587000	0.146584000	-0.935014000
H	-6.087631000	4.718807000	-0.518104000
H	-4.028263000	4.898318000	-1.913529000
H	-2.785392000	2.849731000	-2.541718000
H	-5.369381000	-0.097454000	0.818587000
H	-2.714110000	0.411393000	-2.726305000

^{5}IH

Zero-point correction= 0.742314 (Hartree/Particle)
Thermal correction to Energy= 0.787517
Thermal correction to Enthalpy= 0.788461
Thermal correction to Gibbs Free Energy= 0.657827
Sum of electronic and zero-point Energies= -2908.704213
Sum of electronic and thermal Energies= -2908.659010
Sum of electronic and thermal Enthalpies= -2908.658066
Sum of electronic and thermal Free Energies= -2908.7887

Fe	-0.086546000	-0.658525000	0.349338000
C	-2.452778000	-1.554048000	-1.605799000
H	-2.742833000	-1.866850000	-2.620201000
H	-3.167666000	-0.809169000	-1.261214000
H	-2.515649000	-2.405512000	-0.928972000
N	0.693556000	-2.782102000	0.061009000
N	-1.074608000	-0.997607000	-1.624258000
C	0.274416000	-3.826979000	1.024078000
H	0.580024000	-3.562100000	2.035667000
H	0.718495000	-4.798776000	0.757724000
C	0.167606000	-3.155376000	-1.293251000
H	-0.754144000	-3.718222000	-1.132065000
H	0.874777000	-3.836388000	-1.790618000
C	2.182516000	-2.659977000	0.050919000
H	2.601699000	-3.655658000	-0.170291000
H	2.446586000	-1.984812000	-0.763220000
C	2.832312000	-2.155512000	1.356557000
H	3.901649000	-2.381825000	1.255029000
H	2.495045000	-2.747921000	2.213589000
C	2.771075000	-0.650991000	1.681106000
H	3.464556000	-0.455354000	2.515944000
H	3.150765000	-0.096888000	0.824153000
C	1.087256000	-0.518746000	3.413396000
H	1.838178000	-0.137963000	4.124946000
H	1.045080000	-1.605590000	3.484847000
H	0.104376000	-0.143266000	3.691541000
N	-0.946032000	1.325303000	0.798586000
N	1.429089000	-0.112344000	2.035270000
S	-1.730328000	-1.445744000	1.850903000
C	-2.348698000	1.226592000	1.312533000
H	-3.018654000	1.025903000	0.478323000
H	-2.648494000	2.200099000	1.731882000
C	-2.539297000	0.126368000	2.350101000
H	-3.615724000	-0.054638000	2.434926000
H	-2.161462000	0.404017000	3.342505000
C	1.372866000	1.370794000	1.906895000
C	-0.063021000	1.918508000	1.849336000
H	-0.548620000	1.753027000	2.812700000
H	-0.005541000	3.008023000	1.713055000
C	-0.906550000	2.116888000	-0.472906000
H	-1.349591000	3.103861000	-0.264814000
H	0.145814000	2.261161000	-0.726583000
C	-1.657246000	1.510497000	-1.677645000
C	-1.047876000	0.289527000	-2.389329000

H	-0.812432000	-3.915035000	1.021974000
C	-0.118661000	-1.970251000	-2.221807000
H	0.803029000	-1.430912000	-2.434878000
H	-0.523775000	-2.369373000	-3.165412000
H	-0.004385000	0.493467000	-2.625197000
H	-1.600487000	0.137531000	-3.329444000
H	-1.661146000	2.307624000	-2.434563000
H	-2.711746000	1.340793000	-1.444355000
H	1.914780000	1.659698000	1.007334000
H	1.885333000	1.850998000	2.756752000
O	1.271780000	0.044741000	-0.818033000
O	-4.723460000	0.839126000	-0.912631000
O	-5.714553000	-1.419137000	-0.534772000
C	-7.319600000	0.683301000	-0.572834000
F	-8.303265000	0.035976000	0.072087000
F	-7.535178000	0.561401000	-1.894057000
F	-7.401133000	1.988018000	-0.257604000
S	-5.657838000	-0.007284000	-0.109042000
O	-5.575055000	0.233998000	1.351334000
C	3.118008000	4.192723000	-0.842240000
C	3.344647000	3.030887000	-1.566703000
C	4.324990000	2.090767000	-1.153976000
C	5.088714000	2.368826000	0.016449000
C	4.837017000	3.537613000	0.734020000
C	3.861160000	4.449256000	0.318994000
C	4.525977000	0.869168000	-1.862887000
C	6.204538000	1.432088000	0.431200000
C	6.177089000	0.062332000	-0.215143000
C	5.390687000	-0.157940000	-1.382120000
C	5.457809000	-1.423277000	-2.019543000
H	4.867825000	-1.586849000	-2.918329000
C	6.254084000	-2.439189000	-1.511326000
C	7.006375000	-2.222258000	-0.348024000
C	6.961986000	-0.976059000	0.284973000
H	2.056987000	0.568664000	-0.620484000
H	2.367223000	4.903120000	-1.177226000
H	2.768141000	2.823743000	-2.464852000
H	5.420545000	3.746919000	1.628461000
H	3.687070000	5.356137000	0.890912000
H	7.165626000	1.911613000	0.176060000
H	6.294397000	-3.401238000	-2.014813000
H	7.629039000	-3.014843000	0.056905000
H	7.559079000	-0.807028000	1.178970000
H	3.940782000	0.683720000	-2.759656000
H	6.224333000	1.331855000	1.525015000

1+EB$_O$

^{3}TS$_O$

Zero-point correction= 0.614203 (Hartree/Particle)

Thermal correction to Energy= 0.665733

Thermal correction to Enthalpy= 0.666677

Thermal correction to Gibbs Free Energy= 0.518269

Sum of electronic and zero-point Energies= -3615.818854

Sum of electronic and thermal Energies= -3615.767324

Sum of electronic and thermal Enthalpies= -3615.766380

Sum of electronic and thermal Free Energies= -3615.9147

Ru	-0.239223000	-0.785417000	-0.090339000
N	0.339649000	-1.090397000	1.929070000
N	-1.931109000	-0.301146000	0.878245000
N	-1.455181000	-0.101313000	-1.692545000
N	1.656717000	-1.045711000	-1.067604000
N	0.654753000	1.187883000	0.002160000
O	-0.562989000	-2.616041000	-0.442128000
C	2.087439000	-2.209835000	-1.582539000
C	2.466136000	0.043873000	-1.100491000
C	3.339915000	-2.347566000	-2.164795000
H	1.386405000	-3.032370000	-1.496951000
C	3.731969000	-0.025479000	-1.683503000
H	3.662043000	-3.306620000	-2.550835000
H	4.398353000	0.826454000	-1.702685000
C	4.177406000	-1.231300000	-2.215292000
C	1.916546000	1.275286000	-0.502924000
C	0.066102000	2.278869000	0.518735000
C	2.615716000	2.479605000	-0.459702000
C	0.705118000	3.513945000	0.576358000
H	-0.952003000	2.191247000	0.875992000
H	3.628269000	2.562391000	-0.832136000
H	0.174256000	4.366150000	0.981263000
C	2.006538000	3.610461000	0.086335000
C	2.785846000	4.889134000	0.093748000
O	2.142366000	5.879216000	0.744211000
O	3.871263000	5.023204000	-0.428222000
H	2.713966000	6.668062000	0.687206000
C	5.551511000	-1.267840000	-2.805232000
O	5.949598000	-2.522997000	-3.104177000
O	6.226636000	-0.284330000	-3.011217000
H	6.860049000	-2.446512000	-3.446788000
C	-0.664904000	-0.822597000	2.820685000
C	1.542983000	-1.482397000	2.368426000
C	-0.442881000	-0.952360000	4.189892000
C	1.826310000	-1.609389000	3.730794000
H	2.303345000	-1.699156000	1.625330000
H	-1.239118000	-0.738226000	4.893876000
H	2.833688000	-1.886900000	4.023037000
C	-2.964240000	0.196921000	0.161854000
C	-1.940930000	-0.368613000	2.229640000
C	-4.127969000	0.600326000	0.818993000
C	-3.086213000	0.021041000	2.926532000
H	-4.937616000	1.066275000	0.275662000
H	-3.115130000	-0.016227000	4.009278000
C	-2.694396000	0.304643000	-1.287115000
C	-1.116932000	-0.014633000	-2.987679000
C	-3.607714000	0.826300000	-2.204912000
C	-1.991424000	0.475532000	-3.951085000
H	-0.117222000	-0.349817000	-3.239675000
H	-4.552399000	1.225834000	-1.860981000
H	-1.675395000	0.531042000	-4.987147000
C	-3.253228000	0.909875000	-3.547387000
C	-4.182212000	0.496219000	2.208293000
C	0.818343000	-1.341984000	4.649610000
H	-3.949506000	1.331255000	-4.265414000
H	-5.069036000	0.832196000	2.735211000
H	1.002983000	-1.425900000	5.716352000
Cl	-3.255447000	3.919794000	-0.136458000
Cl	4.932072000	-0.990150000	1.525984000
O	6.152409000	-0.734285000	0.717811000
O	4.155674000	-2.131250000	0.902962000
O	5.270639000	-1.345357000	2.933810000
O	4.046003000	0.229295000	1.516760000
O	-3.347296000	5.396670000	-0.136952000
O	-2.804973000	3.427462000	1.217693000
O	-4.597720000	3.314010000	-0.450481000
O	-2.259927000	3.451934000	-1.161422000
C	-4.600063000	-3.037284000	-0.417400000
C	-3.961995000	-3.124823000	0.839232000
C	-2.646409000	-3.527478000	0.956754000
C	-1.846874000	-3.822562000	-0.209684000
C	-2.547637000	-3.815678000	-1.477785000
C	-3.855964000	-3.397167000	-1.567564000
H	-4.532487000	-2.888582000	1.734979000
H	-2.188836000	-3.628906000	1.936832000

H	-1.085157000	-4.588443000	-0.081276000
H	-2.003929000	-4.118966000	-2.367695000
H	-4.344957000	-3.369054000	-2.539286000
C	-6.055883000	-2.651700000	-0.526840000
H	-6.316262000	-1.960975000	0.284967000
H	-6.224057000	-2.110353000	-1.466750000
C	-7.000722000	-3.869695000	-0.474187000
H	-8.045934000	-3.551842000	-0.557933000
H	-6.789693000	-4.566709000	-1.292601000
H	-6.884439000	-4.416308000	0.468088000

1'+EB$_O$

^{3}TS$_O$

Zero-point correction= 0.615344 (Hartree/Particle)
Thermal correction to Energy= 0.666639
Thermal correction to Enthalpy= 0.667583
Thermal correction to Gibbs Free Energy= 0.519842
Sum of electronic and zero-point Energies= -3645.37445
Sum of electronic and thermal Energies= -3645.323162
Sum of electronic and thermal Enthalpies= -3645.322217
Sum of electronic and thermal Free Energies= -3645.4699

Fe	-0.141204000	-0.617737000	0.462517000
N	-0.583872000	-1.111739000	2.404785000
N	-1.645423000	-1.757220000	0.150493000
N	-0.279937000	-0.406597000	-1.518893000
N	1.296783000	0.746612000	0.853213000
N	-1.281989000	1.135453000	0.640445000
O	1.044111000	-1.886596000	0.467090000
C	2.599147000	0.438024000	0.942605000
C	0.903267000	2.042445000	0.974353000
C	3.576914000	1.402559000	1.176414000
H	2.836316000	-0.608620000	0.804128000
C	1.830244000	3.055535000	1.199004000
H	4.621619000	1.124110000	1.196303000
H	1.536328000	4.095148000	1.274778000
C	3.184110000	2.732531000	1.300350000
C	-0.548647000	2.261200000	0.846187000
C	-2.613182000	1.229140000	0.514182000
C	-1.157083000	3.512008000	0.924765000
C	-3.288574000	2.448681000	0.576119000
H	-3.183094000	0.322517000	0.354257000
H	-0.583533000	4.417148000	1.083211000
H	-4.364446000	2.462695000	0.448592000
C	-2.544310000	3.608352000	0.785409000
C	-3.160081000	4.971383000	0.872188000
O	-4.494890000	4.944000000	0.700040000
O	-2.527562000	5.985160000	1.078500000
H	-4.807388000	5.866524000	0.760839000
C	4.158504000	3.852345000	1.496212000
O	5.416934000	3.415213000	1.679834000
O	3.840485000	5.022254000	1.509246000
H	5.984773000	4.207248000	1.724970000
C	-1.599254000	-2.012258000	2.493268000
C	0.044821000	-0.715337000	3.515990000
C	-2.004788000	-2.520222000	3.728529000
C	-0.307271000	-1.182625000	4.780894000
H	0.854556000	-0.008056000	3.377450000
H	-2.820487000	-3.231849000	3.785016000
H	0.229216000	-0.831337000	5.655520000
C	-2.083092000	-1.906584000	-1.111048000
C	-2.212375000	-2.381208000	1.200254000
C	-3.150635000	-2.767653000	-1.377810000
C	-3.279632000	-3.252138000	0.992097000
H	-3.552712000	-2.866547000	-2.376774000
H	-3.764566000	-3.752330000	1.822010000
C	-1.329959000	-1.081438000	-2.071658000
C	0.490152000	0.369238000	-2.292662000
C	-1.637333000	-0.960392000	-3.423183000
C	0.247692000	0.514277000	-3.660760000
H	1.320396000	0.892694000	-1.832714000
H	-2.507957000	-1.461330000	-3.828226000
H	0.911266000	1.150542000	-4.236095000
C	-0.833175000	-0.151563000	-4.229412000
C	-3.745757000	-3.436489000	-0.312005000
C	-1.351987000	-2.098955000	4.885275000
H	-1.060598000	-0.042098000	-5.285315000
H	-4.606708000	-4.068778000	-0.495347000
H	-1.657110000	-2.483295000	5.853705000
Cl	4.027646000	1.689766000	-2.253432000
O	4.393630000	1.769465000	-3.688591000
O	5.086708000	2.288191000	-1.388456000
O	3.823234000	0.246906000	-1.855278000
O	2.727391000	2.423049000	-2.016630000
Cl	-5.533536000	-0.395610000	-1.153901000
O	-5.106228000	-0.565913000	0.287192000
O	-4.317283000	0.007181000	-1.951493000
O	-6.571705000	0.658543000	-1.244245000
O	-6.041781000	-1.703804000	-1.667884000
C	3.908071000	-4.308391000	-0.137593000
C	3.851751000	-3.179320000	-0.985936000
C	2.646781000	-2.634106000	-1.378380000
C	1.410203000	-3.143760000	-0.846834000
C	1.474361000	-4.361831000	-0.084594000
C	2.691697000	-4.891748000	0.288200000
H	4.774208000	-2.736998000	-1.353958000
H	2.640064000	-1.766544000	-2.028998000
H	0.505308000	-2.959490000	-1.414759000
H	0.548511000	-4.834365000	0.232013000
H	2.725262000	-5.791588000	0.899025000
C	5.234943000	-4.867516000	0.314282000
H	5.132697000	-5.940372000	0.521087000
H	5.968930000	-4.768307000	-0.495261000
C	5.779902000	-4.160342000	1.571931000
H	6.743267000	-4.589354000	1.869677000
H	5.926517000	-3.090679000	1.386408000
H	5.084933000	-4.263982000	2.412997000

^{5}TS$_O$

Zero-point correction= 0.613210 (Hartree/Particle)
Thermal correction to Energy= 0.665767
Thermal correction to Enthalpy= 0.666712
Thermal correction to Gibbs Free Energy= 0.514535
Sum of electronic and zero-point Energies= -3645.38023
Sum of electronic and thermal Energies= -3645.327679
Sum of electronic and thermal Enthalpies= -3645.326735
Sum of electronic and thermal Free Energies= -3645.4789

Fe	0.090936000	-0.293320000	0.597257000
N	-1.496053000	-0.412140000	2.114051000
N	-1.187619000	-1.894978000	-0.029422000
N	0.869821000	-0.943456000	-1.354951000
N	0.971744000	1.674226000	0.827208000
N	-1.326553000	1.206119000	-0.446644000
O	1.270091000	-1.081523000	1.580707000
C	2.173995000	1.814340000	1.404798000
C	0.351622000	2.758671000	0.292557000
C	2.824130000	3.043434000	1.501199000
H	2.633556000	0.906915000	1.769534000
C	0.938146000	4.019566000	0.366363000
H	3.816195000	3.091493000	1.929685000
H	0.465597000	4.897281000	-0.056491000

C	2.184906000	4.164889000	0.981429000
C	-0.951661000	2.506140000	-0.365397000
C	-2.496318000	0.900886000	-1.019943000
C	-1.755505000	3.525926000	-0.870902000
C	-3.358147000	1.864370000	-1.549411000
H	-2.792873000	-0.139393000	-1.054414000
H	-1.473580000	4.569615000	-0.806411000
H	-4.301518000	1.553370000	-1.979234000
C	-2.974213000	3.200090000	-1.474478000
C	-3.815619000	4.323980000	-1.995149000
O	-4.937188000	3.890371000	-2.600061000
O	-3.519283000	5.495424000	-1.886965000
H	-5.426693000	4.683186000	-2.889983000
C	2.787602000	5.535963000	1.016200000
O	3.975357000	5.560307000	1.649207000
O	2.260870000	6.515857000	0.533780000
H	4.304114000	6.477667000	1.597006000
C	-2.442259000	-1.358678000	1.922568000
C	-1.587362000	0.416827000	3.160389000
C	-3.543103000	-1.463693000	2.776781000
C	-2.637627000	0.351777000	4.071973000
H	-0.793348000	1.150929000	3.260418000
H	-4.345947000	-2.154701000	2.553698000
H	-2.675621000	1.043123000	4.907074000
C	-0.892341000	-2.560055000	-1.158345000
C	-2.234453000	-2.234173000	0.741962000
C	-1.667371000	-3.654569000	-1.554367000
C	-3.043896000	-3.322177000	0.403069000
H	-1.448220000	-4.193644000	-2.468370000
H	-3.920657000	-3.569925000	0.983666000
C	0.276695000	-2.031359000	-1.903338000
C	1.956496000	-0.413535000	-1.929385000
C	0.764310000	-2.595437000	-3.082468000
C	2.507543000	-0.937686000	-3.101163000
H	2.421145000	0.442245000	-1.448221000
H	0.279568000	-3.459045000	-3.523226000
H	3.409366000	-0.488665000	-3.499816000
C	1.893651000	-2.038569000	-3.687885000
C	-2.747703000	-4.029225000	-0.759601000
C	-3.635886000	-0.598703000	3.863848000
H	2.287884000	-2.472534000	-4.602201000
H	-3.378302000	-4.860757000	-1.057154000
H	-4.492154000	-0.656624000	4.528440000
Cl	5.198533000	1.043418000	-0.635144000
O	5.134326000	-0.314365000	-1.272487000
O	6.458016000	1.732758000	-0.991176000
O	5.098068000	0.886783000	0.862356000
O	4.014628000	1.849857000	-1.112693000
Cl	-5.693376000	-0.964281000	-0.228125000
O	-7.005932000	-0.525056000	-0.754087000
O	-5.063147000	0.126391000	0.592806000
O	-4.762885000	-1.293224000	-1.369631000
O	-5.860198000	-2.187611000	0.633093000
C	3.114705000	-4.204932000	0.167962000
C	2.166113000	-4.457946000	1.188950000
C	1.946351000	-3.543931000	2.197858000
C	2.639845000	-2.290525000	2.199905000
C	3.648066000	-2.071508000	1.206591000
C	3.844564000	-2.997953000	0.200599000
H	1.618466000	-5.397805000	1.179981000
H	1.225726000	-3.749419000	2.983926000
H	2.697209000	-1.735254000	3.129144000
H	4.227983000	-1.152997000	1.217000000
H	4.579279000	-2.780903000	-0.569450000
C	3.385033000	-5.234934000	-0.901568000
H	2.487843000	-5.845353000	-1.064589000
H	3.605559000	-4.727587000	-1.848743000
C	4.566602000	-6.158823000	-0.539520000
H	4.739185000	-6.891134000	-1.335878000
H	5.486686000	-5.581468000	-0.401107000
H	4.368903000	-6.704475000	0.389640000