Supporting information for Origin of the ligand effect in the cobalt catalyzed regioselective hydroboration of 1, 3-diene

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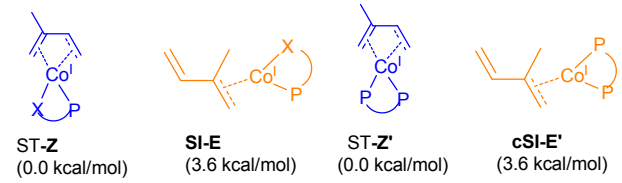
I. Computational Details

The calculations were conducted using Gaussian 09 program [1]. Geometries were optimized using the B3LYP functional [2]. Lanl2dz [3] basis set was used for Ir, a standard 6-31G(d) [4] basis set was used for other atoms. Frequency analyses were carried out to ensure theses stationary points were at either a minimum or transition state. Solvation free energies are calculated with SMD[5] solvation model (solvent =tetrahydrofuran). The energetic results were further improved by single-point energy calculations at ωB97XD [6] level of theory and the basis set SDD [3] for Co and def2-TZVP [7] basis set for other atoms. The solvation model for the single point calculation was the same as described above. The energies presented in this paper are the ωB97XD-calculated single point energies added with B3LYP-optimized thermodynamic corrections.

II. Geometries for the key intermediates



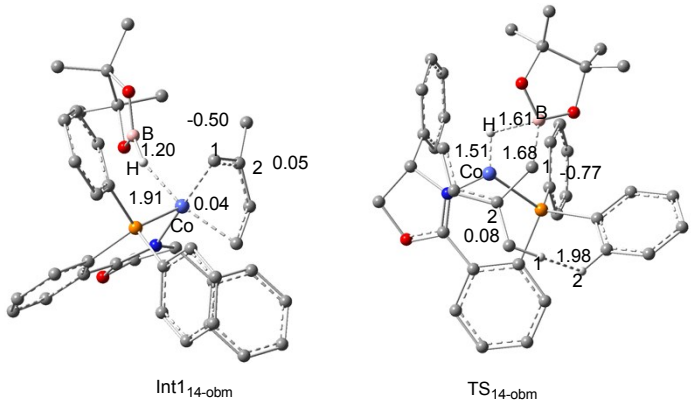


Figure 1. Possible active catalyst for Co(PHOX)$^+$ or Co(dppp)$^+$ catalyzed Hydroboration of 2-methyl 1, 3-diene (irrelevant hydrogen atoms are omitted for clarity). NPA charges are underlined. The bond lengths are given in Å.

III. Free-energy profiles for other possible pathways

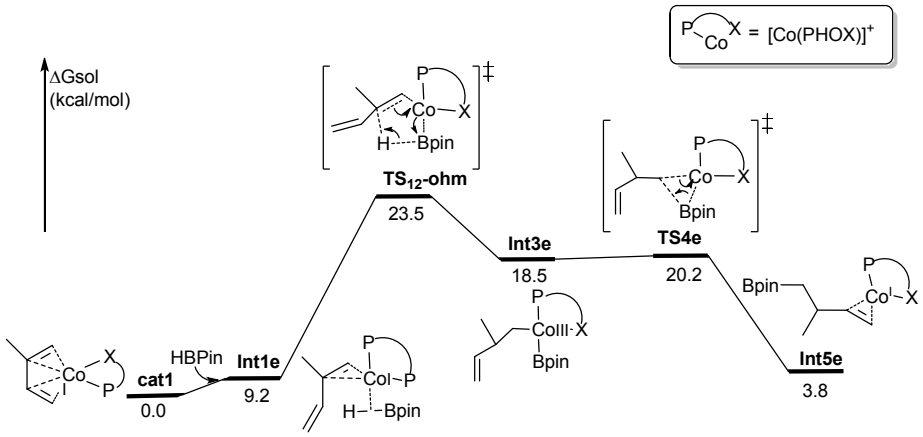


Figure 2. Free energy profiles of pathc and pathd for hydroboration of 2-methyl 1, 3-diene catalyzed by Co(PHOX)Cl_2 in the 1,2- oxidative hydrogen migration pathway

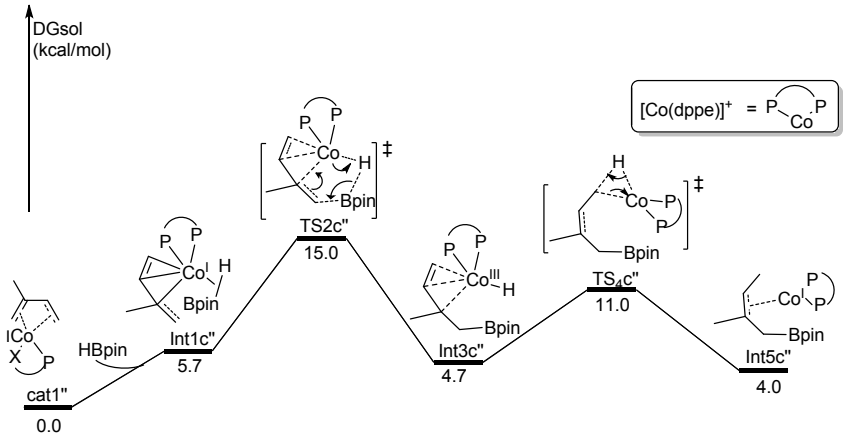


Figure 3 Free energy profiles of 1,4-hydroboration of 2-methyl 1, 3-diene catalyzed by Co(dppe)Cl_2 in the oxidative hydrogen migration pathway

Table 1. Computed barriers for the oxidative hydrogen migration and oxidative boryl migration step in Co(I)/dppe catalyzed hydroboration reactions of 2-methyl-1, 3-diene (ohm=oxidative hydrogen migration; obm=oxdative boryl migration; rhm=reductive hydrogen migration)

TSs	TS"$_{14\text{-ohm}}$= TS"$_{34\text{-ohm}}$=TS2c'		TS"$_{21\text{-ohm}}$=TS"$_{41\text{-ohm}}$	TS"$_{12\text{-ohm}}$	TS"$_{43\text{-ohm}}$
△G (kcal/mol)	15.0		17.4	21.8	27.4
TSs	TS"$_{41\text{-rhm}}$	TS"$_{43\text{-rhm}}$	TS"$_{21\text{-obm}}$	TS"$_{34\text{-obm}}$	
△G (kcal/mol)s	12.7	12.8	38.4	32.3	

IV. Cartesian coordinates and energies from the B3LYP-D3 method and electronic energies from

the ωB97XD method.

ST-Z

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.00001	1.32959	1.40867
C	-0.20135	2.56575	2.77017
C	0.73914	2.63949	3.81293
H	1.59109	1.97282	3.82914
C	0.6062	3.57897	4.8352
H	1.34814	3.61833	5.62761
C	-0.47581	4.46108	4.83977
H	-0.58314	5.19006	5.63768
C	-1.41557	4.40125	3.81077
H	-2.25865	5.08605	3.80096
C	-1.28111	3.46577	2.78312
H	-2.02318	3.44385	1.99434
C	-1.55641	1.54438	0.4351
C	-2.75341	1.03185	0.96389
H	-2.75417	0.49878	1.90917
C	-3.95874	1.2178	0.28476
H	-4.87816	0.82657	0.7114
C	-3.98524	1.89902	-0.93455
H	-4.92412	2.03957	-1.46255
C	-2.79954	2.40856	-1.46648
H	-2.81129	2.95008	-2.40815
C	-1.59263	2.24164	-0.78252
H	-0.68734	2.66966	-1.1994
C	1.3002	2.03951	0.30514
C	1.89361	3.27924	0.56136
H	1.57191	3.85953	1.41897
C	2.89322	3.78765	-0.2742
H	3.34293	4.74997	-0.04781
C	3.29908	3.06955	-1.39692
H	4.06886	3.46237	-2.05381
C	2.70234	1.8425	-1.68389
H	2.99702	1.28675	-2.56694
C	1.71997	1.31128	-0.83503
C	1.12328	0.01336	-1.20537
N	0.59385	-0.87691	-0.4269
C	0.22655	-2.05471	-1.27725
H	0.97485	-2.82858	-1.07964
C	0.41654	-1.50237	-2.70844
H	0.9981	-2.15451	-3.36124
H	-0.53018	-1.24532	-3.19104
O	1.16128	-0.27236	-2.51781
C	-1.14448	-2.64544	-1.02685
C	-1.27152	-4.01618	-0.77177
C	-2.30101	-1.85755	-1.10513
C	-2.53041	-4.59406	-0.59559
H	-0.38265	-4.64068	-0.71898
C	-3.55841	-2.43198	-0.92151
H	-2.22361	-0.79259	-1.30269
C	-3.67708	-3.8015	-0.66806
H	-2.61317	-5.66044	-0.4067
H	-4.4456	-1.8084	-0.98173
H	-4.65831	-4.24899	-0.53712
C	1.4109	-0.88102	3.55702
C	2.49641	-0.82971	2.63688
C	2.53367	-1.88637	1.67396
C	1.55251	-2.88035	1.67488
H	1.08843	-3.25469	2.57917
H	1.48876	-3.55057	0.82485
H	1.1158	-1.83101	3.99352
H	1.25006	-0.0347	4.2169
Co	0.69946	-0.90098	1.6089
H	3.21775	-1.78868	0.83342
C	3.55345	0.24307	2.59839
H	4.39424	-0.06292	3.23533
H	3.94206	0.39765	1.58668
H	3.19787	1.20297	2.9775

Thermal correction to Energy=0.570789

Thermal correction to Enthalpy=0.571733

Thermal correction to Gibbs Free Energy= 0.472544

Sum of electronic and zero-point Energies= -1853.126782

Sum of electronic and thermal Energies= -1853.094250

Sum of electronic and thermal Enthalpies= -1853.093306

Sum of electronic and thermal Free Energies= -1853.192495

SCF Done: E(RwB97XD) = -1854.56437168

HBPin

Number of imaginary frequencies=0

Charge =0 Multiplicity = 1

C	-0.78664	-0.19249	-0.04833
C	0.78667	-0.19227	0.04835
B	-0.00022	1.94252	-0.00036
O	1.08253	1.2039	0.38272
O	-1.08289	1.20352	-0.38331

C	-1.36405	-1.08659	-1.13995
H	-1.09579	-2.13328	-0.95864
H	-2.45673	-1.0118	-1.13954
H	-1.00587	-0.80061	-2.13192
C	-1.47816	-0.47127	1.28922
H	-2.54861	-0.26519	1.18785
H	-1.3553	-1.51594	1.59232
H	-1.0837	0.17208	2.0825
C	1.36443	-1.08564	1.14047
H	1.0964	-2.13257	0.96016
H	2.45709	-1.01062	1.13986
H	1.00628	-0.79893	2.13227
C	1.47822	-0.47163	-1.28907
H	2.54866	-0.26534	-1.18786
H	1.35551	-1.5165	-1.59154

Thermal correction to Energy= 0.201066

Thermal correction to Enthalpy= 0.202010

Thermal correction to Gibbs Free Energy=0.158381

Sum of electronic and zero-point Energies=-411.672325

Sum of electronic and thermal Energies=-411.662795

Sum of electronic and thermal Enthalpies= -411.661851

Sum of electronic and thermal Free Energies= -411.705480

SCF Done: E(RwB97XD) = -411.910605169

Int1a

Number of imaginary frequencies=0

Charge =1 Multiplicity = 1

H	1.72828	-0.93797	-1.60271
C	0.4378	-2.14153	-2.09227
C	-0.86595	-1.87833	-1.57752
B	2.5236	-0.19389	-0.99086
O	3.20735	-0.69897	0.08335
O	3.32076	0.45978	-1.88676
C	4.63935	-0.62406	-0.23503
C	4.68203	0.50616	-1.34109
C	-0.99585	-1.65717	-0.18824
H	-2.54828	-2.40681	1.05221
C	0.24966	-1.51017	0.51033
H	1.04627	-2.23347	0.36946
H	0.2035	-1.12747	1.52548
C	4.89543	1.91145	-0.77819
H	5.91195	2.03193	-0.3907
H	4.74596	2.64419	-1.57586
H	4.18822	2.13925	0.02424
C	5.65664	0.24707	-2.48883
H	5.5865	1.05948	-3.21898
H	6.68827	0.21483	-2.12119
H	5.4437	-0.69149	-3.00522
C	5.40332	-0.30743	1.04799
H	5.27414	-1.12499	1.76402
H	6.47501	-0.2051	0.84498
H	5.05182	0.61482	1.51619
C	5.03464	-2.01327	-0.75176
H	6.10631	-2.0724	-0.96592
H	4.79791	-2.75903	0.01314
H	4.48747	-2.27579	-1.66314
H	-1.71712	-1.77125	-2.24046
H	1.07788	-2.85117	-1.56899
C	-2.33003	-1.49157	0.4896
H	-3.14875	-1.3362	-0.21877
H	-2.31965	-0.66828	1.2135
Co	0.41423	-0.24	-1.08077
H	0.56478	-2.16209	-3.16969
P	0.00147	1.61658	0.08232
C	0.19118	1.56708	1.91032
C	1.40614	1.10167	2.4469
H	2.19947	0.76723	1.78618
C	1.5862	1.03622	3.8275
H	2.53016	0.67919	4.22936
C	0.55397	1.41422	4.69115
H	0.69479	1.35638	5.76658
C	-0.66008	1.85685	4.16696
H	-1.46982	2.14424	4.83139
C	-0.84357	1.93612	2.78373
H	-1.792	2.28896	2.39446
C	-1.64483	2.40447	-0.2109
C	-2.67905	1.67942	-0.81531
H	-2.49976	0.66248	-1.14165
C	-3.93163	2.26442	-1.01909
H	-4.7256	1.68727	-1.48491
C	-4.16077	3.58351	-0.62808
H	-5.13419	4.03867	-0.78623
C	-3.13061	4.32119	-0.03798
H	-3.29918	5.35179	0.26072
C	-1.88065	3.73869	0.16723
H	-1.08944	4.32752	0.62099
C	1.13054	2.9522	-0.48697
C	1.66471	3.88265	0.4121

H	1.46897	3.77309	1.47324
C	2.4431	4.95354	-0.03371
H	2.84554	5.66254	0.68395
C	2.68904	5.11153	-1.396
H	3.28358	5.94575	-1.7555
C	2.17071	4.191	-2.30361
H	2.36725	4.30813	-3.36184
C	1.40096	3.09889	-1.86682
C	0.91507	2.16163	-2.89996
N	0.37965	0.98401	-2.77333
C	0.18682	0.43448	-4.15168
H	0.93226	-0.35707	-4.28225
C	0.5413	1.63582	-5.06136
H	1.29516	1.40772	-5.81678
H	-0.3366	2.07842	-5.53918
O	1.0924	2.61205	-4.15445
C	-1.18711	-0.128	-4.45718
C	-1.30364	-1.33697	-5.15422
C	-2.3506	0.58515	-4.13663
C	-2.55881	-1.83837	-5.50819
H	-0.40838	-1.88919	-5.43312
C	-3.6048	0.08396	-4.48583
H	-2.27657	1.52982	-3.60605
C	-3.71294	-1.13081	-5.16948
H	-2.63218	-2.77692	-6.04982
H	-4.49925	0.64646	-4.23243
H	-4.69003	-1.51739	-5.44403

Thermal correction to Energy=0.774969

Thermal correction to Enthalpy=0.775913

Thermal correction to Gibbs Free Energy=0.653536

Sum of electronic and zero-point Energies= -2264.808610

Sum of electronic and thermal Energies= -2264.765241

Sum of electronic and thermal Enthalpies= -2264.764297

Sum of electronic and thermal Free Energies= -2264.886674

SCF Done: E(RwB97XD) = -2266.49554309

SCF Done: E(RwB97XD) = -2266.47639531

Int3a

Number of imaginary frequencies=0

Charge =1 Multiplicity = 1

H	1.40928	-1.30097	-1.81171
C	0.4818	-2.13053	-2.09227
C	-0.87145	-1.86733	-1.56652
B	2.5016	-0.16639	-0.96886
O	3.20735	-0.69897	0.08335
O	3.31526	0.45428	-1.88676
C	4.63935	-0.62406	-0.23503
C	4.68203	0.50066	-1.34109
C	-1.00135	-1.66267	-0.19374
H	-2.54828	-2.40681	1.05771
C	0.24966	-1.50467	0.50483
H	1.04077	-2.23897	0.36946
H	0.209	-1.12197	1.51998
C	4.89543	1.91145	-0.77819
H	5.91195	2.03193	-0.3907
H	4.74596	2.64419	-1.57586
H	4.18822	2.13925	0.02424
C	5.65664	0.24707	-2.48883
H	5.5865	1.05948	-3.21898
H	6.68827	0.21483	-2.12119
H	5.4437	-0.69149	-3.00522
C	5.40332	-0.30743	1.04799
H	5.27414	-1.12499	1.76402
H	6.47501	-0.2051	0.84498
H	5.05182	0.61482	1.51619
C	5.03464	-2.01327	-0.75176
H	6.10631	-2.0724	-0.96592
H	4.79791	-2.75903	0.01314
H	4.48747	-2.27579	-1.66314
H	-1.71712	-1.82075	-2.24596
H	1.01188	-2.96117	-1.60749
C	-2.33003	-1.49157	0.4896
H	-3.14875	-1.3362	-0.21877
H	-2.31965	-0.66828	1.208
Co	0.41973	-0.2345	-1.08077
H	0.54828	-2.18959	-3.17519
P	0.00147	1.61658	0.08232
C	0.19118	1.56708	1.91032
C	1.40614	1.10167	2.4469
H	2.19947	0.76723	1.78618
C	1.5862	1.03622	3.8275
H	2.53016	0.67919	4.22936
C	0.55397	1.41422	4.69115
H	0.69479	1.35638	5.76658
C	-0.66008	1.85685	4.16696
H	-1.46982	2.14424	4.83139
C	-0.84357	1.93612	2.78373
H	-1.792	2.28896	2.39446

C	-1.64483	2.40447	-0.2109
C	-2.67905	1.67942	-0.81531
H	-2.49976	0.66248	-1.14165
C	-3.93163	2.26442	-1.01909
H	-4.7256	1.68727	-1.48491
C	-4.16077	3.58351	-0.62808
H	-5.13419	4.03867	-0.78623
C	-3.13061	4.32119	-0.03798
H	-3.29918	5.35179	0.26072
C	-1.88065	3.73869	0.16723
H	-1.08944	4.32752	0.62099
C	1.13054	2.9522	-0.48697
C	1.66471	3.88265	0.4121
H	1.46897	3.77309	1.47324
C	2.4431	4.95354	-0.03371
H	2.84554	5.66254	0.68395
C	2.68904	5.11153	-1.396
H	3.28358	5.94575	-1.7555
C	2.17071	4.191	-2.30361
H	2.36725	4.30813	-3.36184
C	1.40096	3.09889	-1.86682
C	0.91507	2.16163	-2.89996
N	0.37965	0.98401	-2.77333
C	0.18682	0.43448	-4.15168
H	0.93226	-0.35707	-4.28225
C	0.5413	1.63582	-5.06136
H	1.29516	1.40772	-5.81678
H	-0.3366	2.07842	-5.53918
O	1.0924	2.61205	-4.15445
C	-1.18711	-0.128	-4.45718
C	-1.30364	-1.33697	-5.15422
C	-2.3506	0.58515	-4.13663
C	-2.55881	-1.83837	-5.50819
H	-0.40838	-1.88919	-5.43312
C	-3.6048	0.08396	-4.48583
H	-2.27657	1.52982	-3.60605
C	-3.71294	-1.13081	-5.16948
H	-2.63218	-2.77692	-6.04982
H	-4.49925	0.64646	-4.23243
H	-4.69003	-1.51739	-5.44403

Thermal correction to Energy=0.776740

Thermal correction to Enthalpy=0.777685

Thermal correction to Gibbs Free Energy=0.656546

Sum of electronic and zero-point Energies= -2264.803931

Sum of electronic and thermal Energies= -2264.760407

Sum of electronic and thermal Enthalpies= -2264.759462

Sum of electronic and thermal Free Energies= -2264.880601

SCF Done: E(RwB97XD) = -2266.49553728

Ts4a

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

H	1.43368	-3.37263	-2.18098
C	0.65669	-3.1332	-2.90529
C	-0.51891	-2.39475	-2.3123
B	1.86568	-1.02616	-0.37145
O	2.49035	-0.63779	0.79104
O	2.73323	-1.61051	-1.26715
C	3.8568	-1.17703	0.77694
C	4.09897	-1.43599	-0.76183
C	-0.88503	-2.3207	-0.96994
H	-2.83786	-3.06933	-0.53038
C	0.1295	-2.25186	0.06
H	0.96325	-2.94984	-0.02809
H	-0.21308	-2.14719	1.08581
C	4.70058	-0.23671	-1.50249
H	5.74748	-0.07923	-1.2239
H	4.6615	-0.42853	-2.57939
H	4.14686	0.68431	-1.29874
C	4.8894	-2.70122	-1.0903
H	4.96942	-2.81256	-2.17612
H	5.90509	-2.64173	-0.68364
H	4.40935	-3.59855	-0.69359
C	4.78268	-0.14563	1.41678
H	4.51686	-0.01537	2.47059
H	5.82467	-0.48129	1.37301
H	4.70868	0.82729	0.92626
C	3.83393	-2.45714	1.62086
H	4.83209	-2.89815	1.7039
H	3.48563	-2.21577	2.62987
H	3.16183	-3.21223	1.20087
H	-1.3287	-2.21197	-3.01665
H	0.29286	-4.07178	-3.34767
C	-2.33453	-2.09529	-0.59978
H	-2.8653	-1.50706	-1.35635
H	-2.4399	-1.60937	0.37452
Co	0.12419	-0.52245	-1.09524

H	1.13494	-2.56892	-3.71428
P	-0.00167	1.22655	0.31273
C	-0.12625	1.18612	2.1513
C	0.39841	0.12051	2.90004
H	0.93668	-0.6736	2.40167
C	0.2644	0.10333	4.28972
H	0.67123	-0.72952	4.85632
C	-0.38572	1.14678	4.94928
H	-0.48966	1.12863	6.03036
C	-0.90343	2.21548	4.214
H	-1.40943	3.03295	4.71941
C	-0.78194	2.23456	2.82514
H	-1.20334	3.06492	2.26831
C	-1.53048	2.16258	-0.14695
C	-2.7746	1.55543	0.09199
H	-2.82281	0.56392	0.5305
C	-3.9615	2.22478	-0.20466
H	-4.91457	1.74327	-0.00541
C	-3.92374	3.51103	-0.74878
H	-4.8475	4.03594	-0.97447
C	-2.69271	4.12453	-0.98782
H	-2.65452	5.12981	-1.39776
C	-1.50193	3.45727	-0.68783
H	-0.55714	3.96103	-0.86265
C	1.36671	2.37657	-0.10957
C	2.04683	3.08974	0.88152
H	1.75629	2.96841	1.91908
C	3.0952	3.95453	0.55703
H	3.61116	4.49403	1.34587
C	3.46909	4.12647	-0.77461
H	4.27784	4.80141	-1.03701
C	2.79857	3.42932	-1.77722
H	3.08332	3.56459	-2.81351
C	1.75594	2.53992	-1.46218
C	1.1076	1.83627	-2.58822
N	0.35767	0.7718	-2.57894
C	0.00378	0.44685	-3.99483
H	0.50257	-0.49523	-4.23714
C	0.6492	1.61198	-4.79083
H	1.37344	1.28586	-5.53974
H	-0.08714	2.27367	-5.25202
O	1.35971	2.37858	-3.78807
C	-1.4789	0.2983	-4.27816
C	-1.89669	-0.65212	-5.21998
C	-2.43209	1.14139	-3.69375
C	-3.24349	-0.76359	-5.56941
H	-1.16487	-1.30933	-5.68531
C	-3.78045	1.02386	-4.03728
H	-2.12756	1.88767	-2.96686
C	-4.18998	0.07353	-4.97508
H	-3.55145	-1.50378	-6.30224
H	-4.50901	1.681	-3.57147
H	-5.23893	-0.01243	-5.24338

Thermal correction to Energy=0.775693

Thermal correction to Enthalpy=0.776637

Thermal correction to Gibbs Free Energy=0.657026

Sum of electronic and zero-point Energies= -2264.800228

Sum of electronic and thermal Energies= -2264.757155

Sum of electronic and thermal Enthalpies= -2264.756211

Sum of electronic and thermal Free Energies= -2264.875822

SCF Done: E(RwB97XD) = -2266.49184607

Int5a

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

H	1.50102	-3.32118	-2.30197
C	0.68907	-3.1153	-2.99738
C	-0.48814	-2.40844	-2.36947
B	1.80397	-1.24612	-0.26126
O	2.43297	-0.82934	0.8983
O	2.71068	-1.72728	-1.1926
C	3.82968	-1.27362	0.84243
C	4.0638	-1.45426	-0.70792
C	-0.80684	-2.28518	-1.02733
H	-2.69013	-3.11464	-0.43353
C	0.26417	-2.23313	-0.00901
H	0.96885	-3.07196	-0.08565
H	-0.08902	-2.14245	1.01787
C	4.56123	-0.18733	-1.41165
H	5.59887	0.03639	-1.14331
H	4.5167	-0.34026	-2.49487
H	3.94777	0.68246	-1.1639
C	4.9484	-2.64208	-1.09408
H	5.02127	-2.70556	-2.18357
H	5.9612	-2.5168	-0.69644
H	4.54508	-3.58959	-0.72458
C	4.70089	-0.2107	1.51133
H	4.44355	-0.13791	2.57304

H	5.76037	-0.48167	1.44262
H	4.56252	0.77428	1.05955
C	3.90417	-2.58459	1.63366
H	4.92759	-2.96985	1.68257
H	3.55788	-2.40709	2.65595
H	3.27054	-3.36384	1.19094
H	-1.32094	-2.24653	-3.04929
H	0.33748	-4.06615	-3.41753
C	-2.24583	-2.12047	-0.59515
H	-2.84209	-1.61573	-1.36029
H	-2.33555	-1.5754	0.34803
Co	0.18849	-0.50618	-1.1294
H	1.11614	-2.54451	-3.83158
P	0.01803	1.24231	0.29303
C	-0.1201	1.22287	2.13525
C	0.36923	0.15232	2.90191
H	0.89529	-0.65895	2.42304
C	0.21992	0.15602	4.2907
H	0.6007	-0.67868	4.87043
C	-0.40753	1.22549	4.93203
H	-0.52099	1.22386	6.01231
C	-0.88778	2.29948	4.17637
H	-1.37688	3.13489	4.66709
C	-0.75173	2.29488	2.78872
H	-1.14847	3.12955	2.21858
C	-1.50946	2.18167	-0.1686
C	-2.75237	1.57454	0.06574
H	-2.80299	0.57969	0.49126
C	-3.9402	2.24965	-0.22422
H	-4.8918	1.76725	-0.0288
C	-3.89938	3.53909	-0.75809
H	-4.8218	4.06829	-0.98176
C	-2.66941	4.1524	-0.99557
H	-2.62852	5.15988	-1.39722
C	-1.4776	3.48219	-0.69814
H	-0.53157	3.9846	-0.8678
C	1.39258	2.38532	-0.12608
C	2.09375	3.07956	0.86194
H	1.81874	2.95235	1.90237
C	3.14776	3.93561	0.52695
H	3.68311	4.46264	1.31306
C	3.49942	4.11914	-0.80854
H	4.31181	4.79067	-1.07629
C	2.80583	3.4399	-1.80794
H	3.07592	3.5829	-2.84716
C	1.76259	2.55738	-1.48211
C	1.0892	1.86566	-2.60162
N	0.33253	0.80612	-2.58648
C	-0.03728	0.48622	-4.00079
H	0.48203	-0.44167	-4.26129
C	0.56588	1.67424	-4.79223
H	1.25251	1.37506	-5.58545
H	-0.19409	2.34752	-5.19444
O	1.32418	2.4131	-3.80429
C	-1.51938	0.30528	-4.26986
C	-1.92591	-0.65472	-5.20579
C	-2.4823	1.12731	-3.67529
C	-3.27399	-0.79774	-5.54079
H	-1.18373	-1.29661	-5.68019
C	-3.83168	0.9804	-4.00384
H	-2.18658	1.87986	-2.95249
C	-4.23016	0.01986	-4.93503
H	-3.57261	-1.54303	-6.26865
H	-4.57053	1.62017	-3.5296
H	-5.28014	-0.08933	-5.19165

Thermal correction to Energy=0.776683

Thermal correction to Enthalpy=0.777627

Thermal correction to Gibbs Free Energy=0.655590

Sum of electronic and zero-point Energies= -2264.800482

Sum of electronic and thermal Energies= -2264.756616

Sum of electronic and thermal Enthalpies= -2264.755672

Sum of electronic and thermal Free Energies= -2264.877708

SCF Done: E(RwB97XD) = -2266.49354288

Int3b

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

H	1.03938	-1.88482	-1.68811
C	0.38769	-0.01366	-2.61196
B	-1.20685	-1.43192	-0.42542
O	-2.18699	-1.62033	-1.36491
O	-1.43172	-2.1381	0.73097
C	-3.04603	-2.71924	-0.89803
C	-2.78728	-2.7001	0.65558
C	-3.70306	-1.73926	1.42196
H	-4.72292	-2.13087	1.49355
H	-3.31325	-1.61081	2.43618
H	-3.74352	-0.75356	0.94824

C	-2.77909	-4.07063	1.32769
H	-2.6154	-3.95661	2.40399
H	-3.74101	-4.57597	1.18749
H	-1.98944	-4.71242	0.93008
C	-4.48027	-2.42328	-1.32737
H	-4.54006	-2.40217	-2.41991
H	-5.15992	-3.20419	-0.96849
H	-4.83115	-1.45981	-0.95056
C	-2.53952	-3.99326	-1.58494
H	-3.16052	-4.85823	-1.33197
H	-2.57529	-3.85654	-2.67016
H	-1.50588	-4.21843	-1.30245
Co	0.44024	-0.44088	-0.72704
C	0.81617	-1.46821	-2.67948
P	-0.29851	1.30795	0.31977
C	-1.65941	2.35744	-0.30619
C	-2.70548	1.76892	-1.03596
H	-2.67955	0.71248	-1.27884
C	-3.76874	2.55452	-1.48473
H	-4.57061	2.09437	-2.05482
C	-3.79572	3.92449	-1.21823
H	-4.62253	4.53216	-1.57457
C	-2.75288	4.51657	-0.50098
H	-2.76583	5.58347	-0.29801
C	-1.6876	3.73975	-0.04568
H	-0.87946	4.2103	0.50592
C	1.16622	2.42253	0.47254
C	1.65993	3.04589	-0.68734
H	1.15198	2.91424	-1.63702
C	2.79317	3.85654	-0.62744
H	3.1559	4.33981	-1.53005
C	3.45516	4.04886	0.5876
H	4.3371	4.68102	0.63405
C	2.97233	3.43411	1.74427
H	3.47371	3.59029	2.69518
C	1.8347	2.62539	1.69032
H	1.4644	2.17143	2.60327
C	-0.74203	0.88714	2.06198
C	-1.7449	1.61067	2.7163
H	-2.27189	2.3952	2.18543
C	-2.08556	1.34295	4.04478
H	-2.87231	1.91825	4.52371
C	-1.41232	0.34687	4.7475
H	-1.66462	0.13457	5.78183
C	-0.40545	-0.38126	4.11723
H	0.12238	-1.15679	4.65896
C	-0.0681	-0.13498	2.77655
C	0.9915	-0.97322	2.18996
N	1.30196	-1.12325	0.9418
C	2.36578	-2.16183	0.85625
H	1.87991	-3.08462	0.51302
C	2.79872	-2.30825	2.33196
H	2.89313	-3.34001	2.67126
H	3.71687	-1.75666	2.55602
O	1.71703	-1.68519	3.07102
C	3.4901	-1.81162	-0.09661
C	4.01541	-2.79426	-0.94493
C	4.04403	-0.52274	-0.11883
C	5.07713	-2.4979	-1.80214
H	3.59526	-3.79782	-0.93409
C	5.09993	-0.22486	-0.98181
H	3.65034	0.25031	0.5362
C	5.61908	-1.21125	-1.82428
H	5.4781	-3.2706	-2.45161
H	5.51888	0.7773	-0.99214
H	6.44337	-0.97891	-2.4922
C	-0.59542	0.54867	-3.57751
H	1.77396	-1.62605	-3.18517
H	0.04728	-2.12905	-3.07551
C	-1.54803	-0.17222	-4.19266
H	-2.22408	0.29148	-4.90543
H	-1.70019	-1.22874	-4.00466
C	-0.44004	2.02181	-3.8902
H	-0.62405	2.64436	-3.00619
H	0.57605	2.24549	-4.24306
H	-1.14133	2.34065	-4.66636
H	1.28112	0.63551	-2.56263

Thermal correction to Energy=0.775459

Thermal correction to Enthalpy=0.776403

Thermal correction to Gibbs Free Energy=0.653779

Sum of electronic and zero-point Energies= -2264.788601

Sum of electronic and thermal Energies= -2264.744788

Sum of electronic and thermal Enthalpies= -2264.743844

Sum of electronic and thermal Free Energies= -2264.866467

SCF Done: E(RwB97XD) = -2266.47734776

ts4b

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

H	1.51773	-1.97056	-1.93207
C	0.43666	-0.40229	-3.04358
B	-1.21707	-1.1604	-1.60292
O	-2.47113	-0.71867	-1.92969
O	-1.17828	-2.52641	-1.37363
C	-3.36111	-1.88243	-2.06053
C	-2.56126	-3.01058	-1.2974
C	-2.89785	-3.11645	0.19606
H	-3.90079	-3.52686	0.35062
H	-2.17993	-3.79008	0.67432
H	-2.83948	-2.14586	0.69762
C	-2.61836	-4.39248	-1.94496
H	-2.03129	-5.10332	-1.3551
H	-3.64954	-4.76083	-1.98231
H	-2.21821	-4.38292	-2.9614
C	-4.71046	-1.51418	-1.44468
H	-5.17793	-0.71717	-2.03144
H	-5.38857	-2.37451	-1.45336
H	-4.60909	-1.16489	-0.41466
C	-3.52896	-2.14361	-3.55949
H	-4.23099	-2.96502	-3.73674
H	-3.931	-1.24424	-4.03594
H	-2.57924	-2.37697	-4.04569
Co	0.45959	-0.39714	-1.11028
C	1.23397	-1.71055	-2.97872
P	-0.33003	1.37968	-0.0975
C	-1.43581	2.70684	-0.73297
C	-2.65948	2.39777	-1.35139
H	-2.94356	1.36561	-1.51235
C	-3.51278	3.42149	-1.76647
H	-4.45649	3.16953	-2.24208
C	-3.15935	4.75911	-1.57981
H	-3.82543	5.55118	-1.90976
C	-1.9472	5.07348	-0.96462
H	-1.6632	6.11044	-0.811
C	-1.09168	4.05712	-0.5377
H	-0.16068	4.3238	-0.05129
C	1.17409	2.30518	0.4327
C	2.08719	2.69773	-0.56077
H	1.90352	2.44639	-1.60251
C	3.22818	3.42643	-0.2246
H	3.92088	3.73151	-1.00352
C	3.47736	3.76027	1.10887
H	4.365	4.32842	1.37179
C	2.5778	3.36929	2.10321
H	2.76272	3.63455	3.14024
C	1.42849	2.64858	1.76917
H	0.72993	2.36828	2.55105
C	-1.11554	0.80063	1.46535
C	-2.27941	1.40968	1.94648
H	-2.72911	2.21977	1.38391
C	-2.87392	0.9912	3.14032
H	-3.78069	1.47769	3.48726
C	-2.29798	-0.03688	3.88368
H	-2.74882	-0.36213	4.81608
C	-1.13212	-0.64886	3.42857
H	-0.67537	-1.44401	4.00551
C	-0.53997	-0.25406	2.21792
C	0.68121	-0.95992	1.80038
N	1.23756	-0.9796	0.6283
C	2.39791	-1.92322	0.69168
H	2.07625	-2.84968	0.19896
C	2.5407	-2.15908	2.2098
H	2.66138	-3.20588	2.48918
H	3.34264	-1.56107	2.65264
O	1.28337	-1.68705	2.7582
C	3.6588	-1.42374	0.01747
C	4.34989	-2.25711	-0.87047
C	4.17756	-0.15231	0.30411
C	5.53967	-1.83121	-1.46487
H	3.96198	-3.24907	-1.09246
C	5.36279	0.27507	-0.29352
H	3.65246	0.50926	0.98764
C	6.04701	-0.56312	-1.17849
H	6.06817	-2.49023	-2.14747
H	5.7535	1.26236	-0.06529
H	6.97269	-0.23016	-1.63887
C	-0.37375	-0.10826	-4.26525
H	2.189	-1.63297	-3.50848
H	0.66684	-2.57427	-3.32449
C	-0.45831	-0.95876	-5.30111
H	-1.01384	-0.68668	-6.19441
H	0.01999	-1.93366	-5.30894
C	-1.04067	1.24547	-4.32241
H	-1.95018	1.26268	-3.71277
H	-0.38708	2.03673	-3.93482
H	-1.31494	1.50673	-5.34864

H	1.14964	0.44603	-2.95373

Thermal correction to Energy=0.774533

Thermal correction to Enthalpy=0.775477

Thermal correction to Gibbs Free Energy=0.653098

Sum of electronic and zero-point Energies= -2264.780067

Sum of electronic and thermal Energies= -2264.736674

Sum of electronic and thermal Enthalpies= -2264.735730

Sum of electronic and thermal Free Energies=-2264.858110

SCF Done: E(RwB97XD) = -2266.46636715

Int5b

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	-0.21399	0.68563	1.59136
C	0.10203	1.64994	3.12332
C	1.0837	1.18517	4.01674
H	1.62997	0.26882	3.80994
C	1.36233	1.89641	5.18375
H	2.12252	1.5296	5.86762
C	0.66018	3.06826	5.4773
H	0.87367	3.61644	6.39037
C	-0.32008	3.53065	4.59779
H	-0.87056	4.43949	4.82309
C	-0.59972	2.82765	3.42391
H	-1.36306	3.19623	2.74667
C	-1.7261	1.42672	0.85274
C	-2.97217	0.96353	1.30821
H	-3.01802	0.17101	2.05056
C	-4.15368	1.51247	0.81114
H	-5.11092	1.15094	1.17531
C	-4.10415	2.5174	-0.15873
H	-5.02434	2.94298	-0.54864
C	-2.8701	2.97474	-0.62556
H	-2.82752	3.7559	-1.37917
C	-1.68397	2.437	-0.12032
H	-0.73115	2.80909	-0.4839
C	1.15645	1.15492	0.45586
C	1.87574	2.33849	0.6526
H	1.61403	2.98903	1.48035
C	2.93053	2.69384	-0.19242
H	3.47586	3.61608	-0.01474
C	3.27669	1.86438	-1.25689
H	4.09457	2.13021	-1.91935
C	2.56666	0.68563	-1.47506
H	2.82863	0.04323	-2.30683
C	1.51001	0.31299	-0.62581
C	0.80343	-0.94322	-0.94728
N	0.0134	-1.6763	-0.21332
C	-0.50726	-2.78356	-1.07175
H	-0.33216	-3.73031	-0.55752
C	0.40752	-2.6912	-2.31616
H	1.20922	-3.43606	-2.31616
H	-0.13218	-2.7219	-3.26242
O	1.02084	-1.3855	-2.19596
C	-1.98637	-2.66173	-1.39895
C	-2.74088	-3.83283	-1.55702
C	-2.59657	-1.42303	-1.62867
C	-4.08198	-3.76833	-1.93746
H	-2.27718	-4.80268	-1.38631
C	-3.93936	-1.35843	-2.005
H	-2.0332	-0.50369	-1.50331
C	-4.68465	-2.52879	-2.16154
H	-4.6539	-4.68409	-2.05578
H	-4.4012	-0.38988	-2.17236
H	-5.72883	-2.47601	-2.4557
C	-0.17263	-2.1996	4.30686
C	-0.10598	-3.6098	2.24368
Co	-0.33669	-1.58206	1.68437
H	-0.3797	-1.31173	3.66059
C	-1.43673	-3.34842	1.9828
H	-1.91953	-3.70434	1.07996
H	-2.12253	-3.01979	2.76172
C	4.16514	-2.02695	3.43168
C	4.28223	-3.48059	2.82077
B	2.10334	-3.0278	3.34122
O	2.88505	-3.8136	2.53902
O	2.79378	-2.01591	3.95635
C	4.7851	-4.52899	3.82102
H	4.65184	-5.52546	3.38937
H	5.8475	-4.39238	4.04579
H	4.22618	-4.49115	4.76153
C	5.07274	-3.57766	1.51797
H	6.11747	-3.28678	1.67361
H	5.06229	-4.61179	1.15986
H	4.64866	-2.94369	0.73556
C	4.24567	-0.91431	2.38033
H	3.99142	0.0432	2.84539
H	5.25569	-0.831	1.96687

H	3.54742	-1.08727	1.55508
C	5.11845	-1.72866	4.58651
H	6.1607	-1.78084	4.25291
H	4.93683	-0.71686	4.96278
H	4.98399	-2.42648	5.41558
C	0.56178	-3.3498	3.58573
H	0.42645	-1.78947	5.12427
H	-1.14257	-2.51305	4.70752
C	0.72363	-4.41217	1.2241
H	1.39821	-3.75457	0.71676
H	1.28052	-5.16981	1.73476
H	0.06858	-4.86964	0.51239
H	0.52092	-4.23069	4.19174

Thermal correction to Energy= 0.777076

Thermal correction to Enthalpy= 0.778020

Thermal correction to Gibbs Free Energy=0.655649

Sum of electronic and zero-point Energies= -2264.810902

Sum of electronic and thermal Energies= -2264.767556

Sum of electronic and thermal Enthalpies= -2264.766612

Sum of electronic and thermal Free Energies= -2264.888983

SCF Done: E(RwB97XD) = -2266.50056743

Int1c

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.2136	1.68479	1.41398
C	0.5707	3.16056	2.45798
C	1.88617	3.64035	2.58863
H	2.69037	3.19585	2.01171
C	2.17036	4.71482	3.43369
H	3.19185	5.07845	3.51301
C	1.14881	5.31562	4.17211
H	1.37026	6.14845	4.82849
C	-0.15673	4.84294	4.05396
H	-0.96093	5.30941	4.62102
C	-0.44749	3.77193	3.20264
H	-1.4716	3.42272	3.12073
C	-1.59127	1.77189	1.0802
C	-2.46221	1.13155	1.97445
H	-2.05913	0.56426	2.80373
C	-3.84345	1.23172	1.79837
H	-4.51338	0.73741	2.49833
C	-4.36653	1.95374	0.72142
H	-5.44193	2.03112	0.58627
C	-3.5009	2.58178	-0.17588
H	-3.89925	3.14444	-1.01603
C	-2.11889	2.49817	0.00355
H	-1.4621	3.00171	-0.69785
C	0.99813	2.05185	-0.21537
C	1.33403	3.35836	-0.59013
H	1.13053	4.18015	0.09221
C	1.93045	3.63243	-1.82418
H	2.18221	4.65645	-2.08082
C	2.19261	2.59724	-2.71668
H	2.65651	2.80099	-3.67663
C	1.84365	1.29277	-2.37982
H	2.02491	0.48464	-3.07606
C	1.25696	1.00536	-1.13736
C	0.86626	-0.39349	-0.88987
N	0.65041	-1.00709	0.237
C	0.10928	-2.37293	-0.06929
H	0.66112	-3.09389	0.52781
C	0.47602	-2.50449	-1.56566
H	1.4108	-3.05379	-1.72841
H	-0.31792	-2.92604	-2.18097
O	0.69425	-1.13558	-1.99404
C	-1.36979	-2.5228	0.22383
C	-1.79659	-3.52247	1.10392
C	-2.32772	-1.73532	-0.42761
C	-3.16017	-3.73558	1.33458
H	-1.06268	-4.14588	1.61088
C	-3.68927	-1.94235	-0.19692
H	-2.01855	-0.95325	-1.11818
C	-4.10723	-2.94376	0.68207
H	-3.47762	-4.52069	2.01646
H	-4.4201	-1.32553	-0.7091
H	-5.1661	-3.10916	0.85264
C	2.00401	0.38302	4.11828
C	2.83052	0.26894	2.83241
C	3.11132	-0.94892	2.21171
C	2.21631	-2.02539	2.51015
H	1.9233	-2.2395	3.532
H	2.26791	-2.90658	1.87297
H	2.65911	-0.00627	4.91651
H	1.84648	1.44727	4.31047
H	-0.25219	-1.04415	2.327
B	0.64618	-0.3404	4.66322
O	-0.53866	0.31695	4.8435

O	0.73143	-1.52167	5.34906
C	-1.26269	-0.37451	5.92095
C	-0.58199	-1.8039	5.93339
C	-2.75321	-0.37537	5.58634
H	-3.32142	-0.8998	6.36037
H	-3.12222	0.65562	5.54371
H	-2.96098	-0.85557	4.62382
C	-1.01388	0.4417	7.19248
H	-1.35633	1.46959	7.03174
H	-1.5567	0.03178	8.04905
H	0.0532	0.47895	7.44884
C	-1.26697	-2.82734	5.02138
H	-0.63646	-3.72533	4.9648
H	-2.24135	-3.12316	5.41986
H	-1.40266	-2.44501	4.00639
C	-0.36132	-2.39913	7.32179
H	-1.31593	-2.58227	7.82396
H	0.15817	-3.35857	7.22843
H	0.24657	-1.74977	7.95645
Co	1.03229	-0.39848	2.01196
C	4.10377	-1.03452	1.08055
H	4.40345	-0.04734	0.71657
H	5.00663	-1.55537	1.42304
H	3.70047	-1.6121	0.24023
H	3.4135	1.14676	2.57589

Thermal correction to Energy=0.775042

Thermal correction to Enthalpy= 0.775987

Thermal correction to Gibbs Free Energy= 0.653707

Sum of electronic and zero-point Energies= -2264.809828

Sum of electronic and thermal Energies=-2264.766432

Sum of electronic and thermal Enthalpies= -2264.765488

Sum of electronic and thermal Free Energies= -2264.887767

SCF Done: E(RwB97XD) = -2266.4974561

ts2c

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.20337	1.64409	1.44209
C	0.53452	3.1133	2.50465
C	1.83883	3.62557	2.6372
H	2.65182	3.21451	2.04625
C	2.10033	4.68798	3.50194
H	3.11059	5.07901	3.58266
C	1.067	5.24812	4.25739
H	1.27119	6.07508	4.93113
C	-0.22763	4.74272	4.13791
H	-1.03768	5.17589	4.71756
C	-0.49539	3.6829	3.26886
H	-1.50814	3.30445	3.18735
C	-1.59823	1.72233	1.08749
C	-2.47735	1.03152	1.93508
H	-2.07815	0.43019	2.74393
C	-3.85658	1.12654	1.74302
H	-4.5299	0.59313	2.40786
C	-4.36872	1.89461	0.69575
H	-5.44236	1.96464	0.54538
C	-3.49782	2.57358	-0.15977
H	-3.891	3.17113	-0.9773
C	-2.11865	2.49437	0.03622
H	-1.45523	3.0362	-0.63043
C	1.00033	2.0356	-0.17935
C	1.32499	3.34855	-0.54082
H	1.1073	4.16083	0.14343
C	1.92893	3.6369	-1.76814
H	2.17264	4.66558	-2.01719
C	2.20937	2.61017	-2.66728
H	2.67881	2.82546	-3.62201
C	1.8712	1.29928	-2.34054
H	2.0651	0.49708	-3.04283
C	1.2744	0.99824	-1.10487
C	0.8963	-0.40466	-0.86783
N	0.67078	-1.0209	0.25327
C	0.14476	-2.39015	-0.06361
H	0.68936	-3.10986	0.54515
C	0.53615	-2.51986	-1.55152
H	1.47892	-3.05577	-1.70057
H	-0.24246	-2.94881	-2.1808
O	0.74221	-1.1455	-1.97746
C	-1.3404	-2.55026	0.20232
C	-1.77757	-3.53155	1.09956
C	-2.29207	-1.78819	-0.48963
C	-3.14151	-3.75179	1.30344
H	-1.04766	-4.13187	1.63717
C	-3.65414	-2.0061	-0.28628
H	-1.97558	-1.02191	-1.19304
C	-4.08228	-2.98944	0.60974
H	-3.46595	-4.5227	1.99658
H	-4.3807	-1.4092	-0.82952

H	-5.14382	-3.16404	0.76042
C	2.00664	0.3365	4.04514
C	2.84688	0.26218	2.77581
C	3.13702	-0.95394	2.15648
C	2.27531	-2.0428	2.49886
H	2.02851	-2.25368	3.53403
H	2.31585	-2.92887	1.8699
H	2.6108	-0.13643	4.83643
H	1.86803	1.39045	4.29327
H	-0.22798	-1.1023	2.36783
B	0.59457	-0.35907	4.56323
O	-0.53432	0.37331	4.81175
O	0.64323	-1.54253	5.24632
C	-1.22947	-0.26959	5.93726
C	-0.65125	-1.74149	5.89914
C	-2.73425	-0.15986	5.71025
H	-3.2809	-0.64611	6.52561
H	-3.02904	0.89408	5.69074
H	-3.04146	-0.62119	4.769
C	-0.82582	0.51834	7.18904
H	-1.09884	1.56914	7.0529
H	-1.33784	0.14357	8.08062
H	0.25333	0.46919	7.36581
C	-1.45587	-2.7049	5.01945
H	-0.89654	-3.64042	4.91841
H	-2.42597	-2.93761	5.47033
H	-1.62081	-2.30165	4.01633
C	-0.397	-2.37067	7.26771
H	-1.33542	-2.49004	7.82054
H	0.04423	-3.36357	7.13707
H	0.28967	-1.77385	7.87183
Co	1.04827	-0.4283	2.04058
C	4.10027	-1.03194	0.99961
H	4.35631	-0.0428	0.60731
H	5.02849	-1.51624	1.32684
H	3.69532	-1.63915	0.1827
H	3.40164	1.15607	2.51212

Thermal correction to Energy= 0.772740

Thermal correction to Enthalpy= 0.773684

Thermal correction to Gibbs Free Energy= 0.655374

Sum of electronic and zero-point Energies=-2264.781627

Sum of electronic and thermal Energies=-2264.739532

Sum of electronic and thermal Enthalpies= -2264.738588

Sum of electronic and thermal Free Energies=-2264.856898

SCF Done: E(RwB97XD) = -2266.47462398

Int3c

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.2136	1.69109	1.40138
C	0.577	3.16686	2.44538
C	1.89877	3.63405	2.58233
H	2.70297	3.17695	2.01171
C	2.18926	4.70222	3.42739
H	3.21075	5.05955	3.51301
C	1.16771	5.31562	4.15951
H	1.39546	6.14845	4.82219
C	-0.14413	4.85554	4.03506
H	-0.94203	5.32831	4.59582
C	-0.44119	3.79083	3.18374
H	-1.4653	3.44792	3.09553
C	-1.59127	1.78449	1.0739
C	-2.46221	1.15045	1.97445
H	-2.05283	0.58946	2.81003
C	-3.84345	1.25062	1.80467
H	-4.50708	0.76261	2.51093
C	-4.36653	1.96634	0.72772
H	-5.44193	2.03742	0.59257
C	-3.5072	2.58808	-0.18218
H	-3.91185	3.14444	-1.02233
C	-2.12519	2.50447	-0.00905
H	-1.4684	3.00171	-0.71675
C	0.99813	2.05815	-0.23427
C	1.34033	3.36466	-0.60273
H	1.14313	4.18015	0.07961
C	1.93675	3.63873	-1.83678
H	2.19481	4.66275	-2.09342
C	2.19261	2.60354	-2.73558
H	2.65651	2.80729	-3.69553
C	1.83735	1.29907	-2.39872
H	2.01231	0.49094	-3.10126
C	1.24436	1.01166	-1.15626
C	0.85366	-0.38719	-0.91507
N	0.63781	-1.00709	0.2055
C	0.10298	-2.37293	-0.10709
H	0.66112	-3.10019	0.48371
C	0.45712	-2.49819	-1.60346
H	1.3856	-3.04749	-1.77881

H	-0.34312	-2.90714	-2.21877
O	0.67535	-1.12298	-2.02554
C	-1.37609	-2.5291	0.19863
C	-1.79659	-3.52877	1.08502
C	-2.34032	-1.73532	-0.44021
C	-3.15387	-3.73558	1.32828
H	-1.05638	-4.15218	1.57938
C	-3.69557	-1.94235	-0.19692
H	-2.03745	-0.95325	-1.13078
C	-4.10723	-2.94376	0.68837
H	-3.46502	-4.52069	2.01016
H	-4.4327	-1.31923	-0.6965
H	-5.1661	-3.10916	0.87154
C	2.03551	0.41452	4.21278
C	2.81162	0.25004	2.90171
C	3.07352	-0.96782	2.27471
C	2.15331	-2.03169	2.52275
H	1.8099	-2.2395	3.532
H	2.22381	-2.91288	1.89187
H	2.74101	0.10083	5.00471
H	1.85908	1.48507	4.34827
H	-0.27739	-1.01895	2.264
B	0.70918	-0.3152	4.77032
O	-0.51346	0.29805	4.875
O	0.78813	-1.49017	5.46246
C	-1.26899	-0.40601	5.92095
C	-0.54419	-1.8102	5.97749
C	-2.74061	-0.45097	5.51704
H	-3.32772	-0.988	6.27217
H	-3.13482	0.56742	5.44921
H	-2.88538	-0.94377	4.55452
C	-1.09578	0.4291	7.19878
H	-1.45713	1.44439	7.01284
H	-1.6701	0.00658	8.03015
H	-0.04761	0.49155	7.49924
C	-1.14727	-2.85884	5.03398
H	-0.49156	-3.73163	5.0089
H	-2.13425	-3.18616	5.38206
H	-1.24516	-2.47651	4.01269
C	-0.38022	-2.39913	7.37849
H	-1.36003	-2.60117	7.83026
H	0.16447	-3.34597	7.31663
H	0.17727	-1.73087	8.03835
Co	1.01969	-0.39218	1.97416
C	4.08487	-1.05972	1.15615
H	4.40345	-0.07254	0.80477
H	4.97513	-1.59317	1.51124
H	3.69417	-1.6247	0.30323
H	3.4198	1.10896	2.63259

Thermal correction to Energy= 0.773838

Thermal correction to Enthalpy= 0.774782

Thermal correction to Gibbs Free Energy=0.651836

Sum of electronic and zero-point Energies= -2264.799795

Sum of electronic and thermal Energies=-2264.756514

Sum of electronic and thermal Enthalpies= -2264.755570

Sum of electronic and thermal Free Energies= -2264.878516

SCF Done: E(RwB97XD) = -2266.48881283

ts4c

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.00755	1.52708	1.52668
C	0.32907	2.87076	2.74124
C	1.64955	3.09008	3.17492
H	2.46435	2.496	2.76693
C	1.93031	4.07888	4.11559
H	2.95529	4.2444	4.43497
C	0.89429	4.85196	4.64946
H	1.11262	5.61832	5.38737
C	-0.41825	4.63555	4.23158
H	-1.22709	5.23333	4.64164
C	-0.70295	3.65272	3.27872
H	-1.7279	3.50082	2.95724
C	-1.77579	1.67259	1.09933
C	-2.70663	0.90915	1.82316
H	-2.38031	0.21372	2.58917
C	-4.0717	1.03565	1.5598
H	-4.7802	0.44594	2.13403
C	-4.51935	1.90771	0.56548
H	-5.58193	2.0017	0.35986
C	-3.59737	2.66123	-0.16527
H	-3.93957	3.34036	-0.94092
C	-2.23215	2.55012	0.10157
H	-1.52846	3.14827	-0.46874
C	0.89621	2.08195	0.00541
C	1.23124	3.42893	-0.17508
H	0.97236	4.1494	0.593
C	1.90024	3.86574	-1.32184

H	2.15198	4.91663	-1.4301
C	2.23996	2.95317	-2.31733
H	2.76101	3.28033	-3.21163
C	1.90611	1.60954	-2.16423
H	2.16223	0.89837	-2.93984
C	1.24088	1.15685	-1.01151
C	0.91801	-0.28343	-0.95446
N	0.57595	-1.02178	0.06237
C	0.2919	-2.39832	-0.43836
H	0.90145	-3.09909	0.13565
C	0.79519	-2.32923	-1.90303
H	1.75402	-2.83352	-2.05387
H	0.06876	-2.68335	-2.63463
O	1.00278	-0.9146	-2.13509
C	-1.16386	-2.81217	-0.3187
C	-1.46335	-4.15265	-0.04106
C	-2.2119	-1.91846	-0.57304
C	-2.78675	-4.5968	-0.02606
H	-0.65751	-4.85677	0.15576
C	-3.53563	-2.35992	-0.54845
H	-2.00106	-0.87357	-0.77904
C	-3.8267	-3.69967	-0.27965
H	-3.0033	-5.64042	0.18333
H	-4.33852	-1.65443	-0.74118
H	-4.85721	-4.04303	-0.27093
C	-0.39356	-0.3284	4.88741
C	0.91501	-0.27987	4.11848
C	1.689	-1.29702	3.54379
C	1.04226	-2.42047	2.91407
H	0.26879	-2.95378	3.4593
H	1.66754	-3.07504	2.30842
H	-0.10681	-0.25105	5.95281
H	-0.9368	0.60426	4.6894
B	-1.43806	-1.5167	4.85337
O	-2.75661	-1.30524	4.54164
O	-1.18052	-2.79681	5.26752
C	-3.51997	-2.4614	5.01499
C	-2.4092	-3.58242	5.13088
C	-4.63219	-2.74976	4.00882
H	-5.19808	-3.64187	4.29952
H	-5.33064	-1.90676	3.98556
H	-4.24239	-2.89814	2.99901
C	-4.12389	-2.04999	6.36359
H	-4.73615	-1.15437	6.22119
H	-4.76076	-2.83818	6.77724
H	-3.34743	-1.81297	7.09773
C	-2.25684	-4.43336	3.86511
H	-1.36735	-5.06412	3.96543
H	-3.12036	-5.09057	3.7208
H	-2.14325	-3.81846	2.96737
C	-2.52671	-4.48946	6.35485
H	-3.46004	-5.06263	6.32683
H	-1.69484	-5.20053	6.36419
H	-2.4942	-3.92255	7.28755
Co	0.6468	-0.6074	1.96926
H	-0.32823	-1.67322	2.20156
C	3.16701	-1.07635	3.31015
H	3.73915	-1.61542	4.07751
H	3.49354	-1.46203	2.33735
H	3.44041	-0.01814	3.38355
H	1.47853	0.62428	4.34345

Thermal correction to Energy=0.772435

Thermal correction to Enthalpy= 0.773379

Thermal correction to Gibbs Free Energy= 0.651436

Sum of electronic and zero-point Energies= -2264.791265

Sum of electronic and thermal Energies= -2264.748295

Sum of electronic and thermal Enthalpies= -2264.747351

Sum of electronic and thermal Free Energies= -2264.869294

SCF Done: E(RwB97XD) = -2266.47987117

Int5c

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.01062	1.52677	1.52696
C	0.32597	2.87007	2.74259
C	1.64522	3.08756	3.18091
H	2.46056	2.49176	2.77652
C	1.92419	4.07663	4.12183
H	2.94827	4.24068	4.44484
C	0.88752	4.8518	4.65135
H	1.10442	5.61833	5.38951
C	-0.42385	4.63723	4.22888
H	-1.2332	5.23661	4.6356
C	-0.70671	3.65417	3.27572
H	-1.73074	3.50369	2.95068
C	-1.77615	1.67076	1.09805
C	-2.70735	0.90904	1.82325
H	-2.38158	0.21577	2.59146

C	-4.07224	1.03458	1.55851
H	-4.78105	0.44623	2.13375
C	-4.51937	1.90391	0.56155
H	-5.58182	1.9971	0.3549
C	-3.59703	2.65576	-0.17043
H	-3.9388	3.33284	-0.94806
C	-2.23198	2.54566	0.09775
H	-1.52799	3.14264	-0.47341
C	0.89636	2.08329	0.00661
C	1.23192	3.43037	-0.17205
H	0.97258	4.15002	0.59665
C	1.90179	3.86837	-1.31787
H	2.15387	4.91932	-1.4247
C	2.24185	2.95692	-2.31426
H	2.76352	3.28502	-3.20785
C	1.90748	1.6132	-2.163
H	2.16384	0.90289	-2.93933
C	1.24149	1.15931	-1.01122
C	0.91852	-0.28111	-0.95615
N	0.57852	-1.0175	0.06007
C	0.29433	-2.39715	-0.442
H	0.906	-3.0982	0.12565
C	0.79382	-2.32533	-1.90791
H	1.75205	-2.82967	-2.06232
H	0.0653	-2.67773	-2.63828
O	1.00138	-0.91028	-2.13788
C	-1.16066	-2.81273	-0.31929
C	-1.45798	-4.15359	-0.04117
C	-2.21029	-1.92024	-0.57131
C	-2.78082	-4.59929	-0.02337
H	-0.6509	-4.85677	0.15391
C	-3.53346	-2.36325	-0.54391
H	-2.00114	-0.87509	-0.77772
C	-3.82237	-3.70337	-0.27463
H	-2.99569	-5.64319	0.18636
H	-4.33756	-1.65867	-0.73489
H	-4.85244	-4.04795	-0.26377
C	-0.38966	-0.32942	4.88524
C	0.91889	-0.28458	4.1197
C	1.68948	-1.29348	3.53719
C	1.01321	-2.42174	2.90173
H	0.31184	-3.00064	3.51513
H	1.63345	-3.06679	2.27782
H	-0.10612	-0.25156	5.95046
H	-0.93128	0.60402	4.68653
B	-1.436	-1.51613	4.85289
O	-2.75483	-1.30243	4.54347
O	-1.1798	-2.79666	5.26622
C	-3.5192	-2.45747	5.01779
C	-2.40996	-3.58028	5.1317
C	-4.6334	-2.74397	4.0133
H	-5.20033	-3.63515	4.3048
H	-5.33051	-1.89982	3.99106
H	-4.2453	-2.89299	3.00292
C	-4.12039	-2.04543	6.36741
H	-4.73162	-1.14893	6.22612
H	-4.75769	-2.83279	6.78197
H	-3.34239	-1.80962	7.1003
C	-2.26115	-4.43135	3.86561
H	-1.3725	-5.06353	3.96436
H	-3.126	-5.08712	3.72269
H	-2.14804	-3.81654	2.96775
C	-2.52678	-4.48721	6.3558
H	-3.46095	-5.05908	6.32927
H	-1.69588	-5.19943	6.36375
H	-2.49197	-3.9204	7.28849
Co	0.65092	-0.60351	1.96721
H	-0.10943	-1.91979	2.25713
C	3.16828	-1.09153	3.30793
H	3.74205	-1.63278	4.07527
H	3.49429	-1.47407	2.33515
H	3.445	-0.03421	3.38218
H	1.48596	0.61696	4.34642

Thermal correction to Energy= 0.777063

Thermal correction to Enthalpy= 0.778007

Thermal correction to Gibbs Free Energy=0.655526

Sum of electronic and zero-point Energies=-2264.819857

Sum of electronic and thermal Energies=-2264.776515

Sum of electronic and thermal Enthalpies=-2264.775570

Sum of electronic and thermal Free Energies=-2264.898052

SCF Done: E(RwB97XD) =-2266.50844029

Int3d

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	-0.17704	1.52194	1.46389
C	0.11033	2.68226	2.85355
C	1.41769	2.85389	3.34382

H	2.25309	2.35204	2.86175
C	1.65834	3.68463	4.43677
H	2.67322	3.81554	4.8011
C	0.59663	4.34596	5.06139
H	0.78445	4.99052	5.91506
C	-0.70288	4.17779	4.58345
H	-1.53109	4.69268	5.06167
C	-0.9484	3.35223	3.48271
H	-1.96345	3.23639	3.11725
C	-1.91195	1.79338	0.91722
C	-2.93195	0.99531	1.46764
H	-2.68429	0.20865	2.175
C	-4.25846	1.20651	1.10704
H	-5.03655	0.58605	1.54275
C	-4.59006	2.20438	0.18817
H	-5.62707	2.36266	-0.09378
C	-3.58561	2.99866	-0.36947
H	-3.83818	3.77482	-1.08608
C	-2.25304	2.80133	-0.0058
H	-1.48314	3.42865	-0.44389
C	0.87381	2.17906	0.09096
C	1.25115	3.52717	0.06974
H	0.93031	4.18347	0.87144
C	2.04563	4.04323	-0.95779
H	2.32945	5.09138	-0.94366
C	2.46959	3.21188	-1.99158
H	3.08907	3.60108	-2.7935
C	2.09173	1.8708	-1.99847
H	2.41038	1.22406	-2.80692
C	1.30214	1.33908	-0.9654
C	0.93326	-0.08807	-1.07771
N	0.49773	-0.89851	-0.15704
C	0.2711	-2.23157	-0.78491
H	0.97728	-2.93363	-0.32777
C	0.6407	-1.98423	-2.27227
H	1.46418	-2.6047	-2.63137
H	-0.21297	-2.07603	-2.94684
O	1.07895	-0.60314	-2.30011
C	-1.13647	-2.76403	-0.59109
C	-1.33187	-4.12389	-0.32072
C	-2.25375	-1.9358	-0.76283
C	-2.62129	-4.65053	-0.22336
H	-0.4725	-4.77876	-0.19245
C	-3.54258	-2.45997	-0.65943
H	-2.12025	-0.87769	-0.96926
C	-3.72969	-3.81838	-0.39165
H	-2.75811	-5.70878	-0.02009
H	-4.39953	-1.80586	-0.79226
H	-4.7335	-4.22698	-0.31932
C	0.04107	-0.76157	5.00673
C	0.92096	-0.68187	3.75395
C	1.41575	-1.83737	3.05342
C	0.50846	-2.71815	2.48339
H	-0.52257	-2.78409	2.81565
H	0.8634	-3.51031	1.82754
H	0.72422	-0.99636	5.83817
H	-0.33128	0.25211	5.22726
B	-1.20399	-1.7292	5.13814
O	-2.23327	-1.79772	4.22376
O	-1.40947	-2.52888	6.22531
C	-3.33246	-2.53455	4.84767
C	-2.592	-3.35324	5.97798
C	-4.01869	-3.37863	3.77721
H	-4.82044	-3.98185	4.21758
H	-4.46499	-2.72654	3.01941
H	-3.3178	-4.04703	3.2726
C	-4.30141	-1.47835	5.39313
H	-4.62469	-0.83053	4.57189
H	-5.19109	-1.93779	5.83516
H	-3.82432	-0.85073	6.15239
C	-2.08215	-4.7237	5.5136
H	-1.42221	-5.13537	6.28295
H	-2.90608	-5.42703	5.35628
H	-1.50851	-4.64772	4.58402
C	-3.36579	-3.49891	7.28685
H	-4.29321	-4.06117	7.13093
H	-2.75702	-4.04737	8.0122
H	-3.61457	-2.52903	7.723
Co	0.28399	-0.60404	1.81907
H	-1.06474	-0.51918	2.49527
C	2.88507	-1.91105	2.71225
H	3.42935	-2.27741	3.58809
H	3.0989	-2.58341	1.87366
H	3.29273	-0.91653	2.48242
H	1.68588	0.09065	3.88061

Thermal correction to Energy=0.773796

Thermal correction to Enthalpy=0.774740

Thermal correction to Gibbs Free Energy=0.651332

Sum of electronic and zero-point Energies=-2264.800022

Sum of electronic and thermal Energies=-2264.756680

Sum of electronic and thermal Enthalpies=-2264.755736

Sum of electronic and thermal Free Energies=-2264.879144

SCF Done: E(RwB97XD) = -2266.48914187

ts4d

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	-0.18166	1.52824	1.44875
C	0.10821	2.68864	2.84375
C	1.41596	2.85693	3.33406
H	2.25	2.35279	2.85196
C	1.65884	3.68738	4.4268
H	2.67408	3.81572	4.79109
C	0.59893	4.35195	5.05101
H	0.78842	4.9964	5.90439
C	-0.70096	4.18723	4.57287
H	-1.52778	4.70478	5.05066
C	-0.94866	3.36186	3.47245
H	-1.96399	3.24891	3.10683
C	-1.91522	1.8112	0.90633
C	-2.93118	1.00834	1.455
H	-2.68422	0.22061	2.16146
C	-4.26283	1.22184	1.09411
H	-5.04214	0.60205	1.52859
C	-4.59231	2.22157	0.17647
H	-5.62892	2.38181	-0.10587
C	-3.58634	3.01513	-0.3795
H	-3.83743	3.79264	-1.09516
C	-2.25424	2.81532	-0.01544
H	-1.48306	3.44192	-0.45232
C	0.87302	2.18249	0.08348
C	1.24927	3.53086	0.05879
H	0.92453	4.18985	0.85674
C	2.04788	4.04347	-0.96718
H	2.33094	5.09187	-0.95595
C	2.47715	3.20832	-1.9958
H	3.09999	3.59487	-2.79639
C	2.10037	1.86695	-1.99922
H	2.42303	1.21733	-2.80377
C	1.30664	1.33879	-0.96746
C	0.93797	-0.08856	-1.07018
N	0.5061	-0.89674	-0.14826
C	0.27468	-2.23114	-0.77388
H	0.98134	-2.9319	-0.32119
C	0.64444	-1.98659	-2.26149
H	1.46635	-2.60948	-2.61996
H	-0.2097	-2.07749	-2.93565
O	1.08561	-0.6067	-2.29677
C	-1.13265	-2.76402	-0.58515
C	-1.32773	-4.12462	-0.31814
C	-2.25016	-1.93538	-0.7534
C	-2.61701	-4.65151	-0.22059
H	-0.46822	-4.77983	-0.19255
C	-3.53889	-2.45987	-0.64977
H	-2.11699	-0.8768	-0.95757
C	-3.72566	-3.81893	-0.38529
H	-2.75356	-5.71029	-0.01993
H	-4.39599	-1.80542	-0.78002
H	-4.72937	-4.22775	-0.3128
C	0.05535	-0.79867	5.0537
C	0.8655	-0.67735	3.75719
C	1.40336	-1.82144	3.02922
C	0.50317	-2.71166	2.47396
H	-0.52593	-2.78181	2.81137
H	0.85844	-3.50731	1.82712
H	0.76087	-1.07163	5.85165
H	-0.29756	0.21106	5.31373
B	-1.19958	-1.75568	5.15816
O	-2.22199	-1.81017	4.23656
O	-1.40975	-2.55797	6.24228
C	-3.33096	-2.54444	4.85631
C	-2.59564	-3.37064	5.98458
C	-4.01929	-3.38153	3.78173
H	-4.82439	-3.98275	4.21874
H	-4.46155	-2.72464	3.02573
H	-3.32069	-4.05127	3.27571
C	-4.29593	-1.48601	5.4044
H	-4.61506	-0.83357	4.5852
H	-5.18828	-1.94319	5.84338
H	-3.81717	-0.8635	6.16682
C	-2.0909	-4.74136	5.51559
H	-1.43367	-5.15877	6.28415
H	-2.91754	-5.44064	5.35446
H	-1.51579	-4.66403	4.58703
C	-3.37185	-3.51787	7.29182
H	-4.30146	-4.07553	7.13244

H	-2.76648	-4.07169	8.01593
H	-3.6171	-2.54858	7.73126
Co	0.26924	-0.60525	1.80486
H	-0.67712	-0.37076	2.89793
C	2.87825	-1.88748	2.71524
H	3.42464	-2.27141	3.58704
H	3.08763	-2.55176	1.87053
H	3.28789	-0.89534	2.49331
H	1.57968	0.14462	3.83943

Thermal correction to Energy=0.772283

Thermal correction to Enthalpy=0.773227

Thermal correction to Gibbs Free Energy=0.650073

Sum of electronic and zero-point Energies=-2264.795080

Sum of electronic and thermal Energies=-2264.751965

Sum of electronic and thermal Enthalpies=-2264.751020

Sum of electronic and thermal Free Energies=-2264.874174

SCF Done: E(RwB97XD) = -2266.47978647

Int5d

Number of imaginary frequencies=0

Charge =1 Multiplicity = 1

P	-0.17704	1.52194	1.45489
C	0.11033	2.68226	2.85355
C	1.41769	2.85389	3.34382
H	2.25309	2.35204	2.86175
C	1.65834	3.68463	4.43677
H	2.67322	3.81554	4.8011
C	0.59663	4.34596	5.06139
H	0.78445	4.99052	5.91506
C	-0.70288	4.17779	4.58345
H	-1.53109	4.69268	5.06167
C	-0.9484	3.35223	3.48271
H	-1.96345	3.23639	3.11725
C	-1.91195	1.80238	0.91722
C	-2.92295	0.99531	1.46764
H	-2.67529	0.20865	2.175
C	-4.25846	1.20651	1.10704
H	-5.03655	0.58605	1.54275
C	-4.59006	2.20438	0.18817
H	-5.62707	2.36266	-0.09378
C	-3.58561	2.99866	-0.36947
H	-3.83818	3.77482	-1.08608
C	-2.25304	2.80133	-0.0058
H	-1.48314	3.42865	-0.44389
C	0.87381	2.17906	0.09096
C	1.25115	3.52717	0.06974
H	0.93031	4.18347	0.87144
C	2.04563	4.04323	-0.95779
H	2.32945	5.09138	-0.94366
C	2.46959	3.21188	-1.99158
H	3.08907	3.60108	-2.7935
C	2.09173	1.8708	-1.99847
H	2.41038	1.22406	-2.80692
C	1.30214	1.33908	-0.9654
C	0.93326	-0.08807	-1.06871
N	0.50673	-0.89851	-0.14804
C	0.2711	-2.23157	-0.77591
H	0.97728	-2.93363	-0.32777
C	0.6407	-1.98423	-2.26327
H	1.46418	-2.6047	-2.62237
H	-0.21297	-2.07603	-2.93784
O	1.07895	-0.60314	-2.30011
C	-1.13647	-2.76403	-0.59109
C	-1.33187	-4.12389	-0.32072
C	-2.25375	-1.9358	-0.76283
C	-2.62129	-4.65053	-0.22336
H	-0.4725	-4.77876	-0.19245
C	-3.54258	-2.45997	-0.65943
H	-2.12025	-0.87769	-0.96926
C	-3.72969	-3.81838	-0.39165
H	-2.75811	-5.70878	-0.02009
H	-4.39953	-1.80586	-0.79226
H	-4.7335	-4.22698	-0.31932
C	0.05007	-0.77957	5.05173
C	0.84896	-0.67287	3.74495
C	1.40675	-1.82837	3.02642
C	0.50846	-2.71815	2.47439
H	-0.52257	-2.78409	2.80665
H	0.8634	-3.51931	1.83654
H	0.75122	-1.04136	5.85617
H	-0.30428	0.23411	5.29026
B	-1.20399	-1.7382	5.14715
O	-2.22427	-1.79772	4.22376
O	-1.40947	-2.53788	6.23431
C	-3.33246	-2.53455	4.84767
C	-2.592	-3.35324	5.97798
C	-4.01869	-3.37863	3.77721
H	-4.82044	-3.98185	4.21758

H	-4.46499	-2.72654	3.01941
H	-3.3178	-4.04703	3.2726
C	-4.30141	-1.47835	5.39313
H	-4.62469	-0.83053	4.57189
H	-5.19109	-1.93779	5.83516
H	-3.82432	-0.85073	6.15239
C	-2.08215	-4.7237	5.5136
H	-1.42221	-5.13537	6.28295
H	-2.90608	-5.42703	5.35628
H	-1.50851	-4.64772	4.58402
C	-3.36579	-3.49891	7.28685
H	-4.29321	-4.06117	7.13093
H	-2.75702	-4.04737	8.0122
H	-3.61457	-2.52903	7.723
Co	0.28399	-0.61304	1.80107
H	-0.44374	-0.33018	3.08027
C	2.88507	-1.90205	2.73025
H	3.42935	-2.28641	3.60609
H	3.0899	-2.57441	1.89166
H	3.30173	-0.91653	2.50042
H	1.55088	0.16265	3.80861

Thermal correction to Energy=0.776949

Thermal correction to Enthalpy=0.777893

Thermal correction to Gibbs Free Energy=0.654294

Sum of electronic and zero-point Energies=-2264.820594

Sum of electronic and thermal Energies=-2264.777240

Sum of electronic and thermal Enthalpies= -2264.776296

Sum of electronic and thermal Free Energies=-2264.899895

SCF Done: E(RwB97XD) = -2266.50911716

Int1e

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

H	-4.53611	-0.51572	-1.05102
C	-4.35931	-0.06843	1.51141
B	-2.52631	-0.50025	-0.80631
O	-2.03388	-1.48021	0.02962
O	-1.86269	-0.44856	-2.00728
C	-1.11025	-2.31372	-0.75498
C	-0.6986	-1.33869	-1.92351
C	0.51031	-0.4558	-1.59159
H	1.43716	-1.03792	-1.57158
H	0.60959	0.31803	-2.35874
H	0.39451	0.04246	-0.62392
C	-0.50681	-2.00198	-3.28519
H	-0.25211	-1.24333	-4.03204
H	0.31375	-2.72727	-3.25151
H	-1.41076	-2.51644	-3.61898
C	0.02929	-2.75363	0.16014
H	-0.36545	-3.38412	0.96314
H	0.76726	-3.34209	-0.3962
H	0.5393	-1.9019	0.61553
C	-1.90551	-3.53515	-1.22982
H	-1.27269	-4.22749	-1.79394
H	-2.29879	-4.0705	-0.36014
H	-2.74923	-3.24515	-1.8639
H	-4.67174	0.79079	2.09711
Co	-3.97202	0.69522	-0.35039
C	-5.29629	-0.72852	0.70537
C	-6.61142	-0.11136	0.39646
C	-7.18083	0.89275	1.08373
H	-3.54193	-0.64119	1.93602
H	-8.16536	1.26019	0.8084
H	-6.70492	1.36803	1.93444
P	-2.75351	2.41018	0.45198
C	-1.76626	2.27133	1.9919
C	-1.16191	1.04249	2.306
H	-1.31131	0.18009	1.66292
C	-0.37075	0.92105	3.44942
H	0.08863	-0.03466	3.68531
C	-0.17798	2.01757	4.29193
H	0.43313	1.9182	5.18435
C	-0.77641	3.242	3.98718
H	-0.6314	4.09824	4.63956
C	-1.56518	3.37193	2.84315
H	-2.02546	4.32898	2.6189
C	-3.87831	3.84516	0.72149
C	-4.71328	3.84687	1.85506
H	-4.62565	3.06174	2.59847
C	-5.63061	4.87749	2.05719
H	-6.25667	4.8738	2.94493
C	-5.73777	5.91432	1.1267
H	-6.45043	6.71825	1.28597
C	-4.91533	5.91941	-0.00065
H	-4.98122	6.73025	-0.72064
C	-3.99119	4.89139	-0.20373
H	-3.34785	4.92555	-1.07703

C	-1.55741	2.99318	-0.82876
C	-0.36017	3.60658	-0.44107
H	-0.14043	3.73114	0.61324
C	0.56536	4.0571	-1.38444
H	1.48745	4.52502	-1.05249
C	0.29983	3.90536	-2.74335
H	1.01047	4.25277	-3.48691
C	-0.88826	3.30437	-3.1509
H	-1.09895	3.18798	-4.20655
C	-1.82281	2.83465	-2.21086
C	-3.04572	2.21457	-2.75027
N	-3.94773	1.50425	-2.14658
C	-4.95123	1.06153	-3.15978
H	-4.85948	-0.02333	-3.24238
C	-4.45337	1.74902	-4.46094
H	-4.21056	1.04915	-5.26019
H	-5.1403	2.51301	-4.83129
O	-3.23002	2.41225	-4.06441
C	-6.38492	1.41587	-2.82119
C	-7.40648	0.50372	-3.11273
C	-6.7206	2.67123	-2.29732
C	-8.74346	0.83685	-2.88412
H	-7.15662	-0.47139	-3.52604
C	-8.05543	3.00264	-2.06227
H	-5.94	3.38958	-2.06076
C	-9.07022	2.08786	-2.3563
H	-9.52654	0.1219	-3.11997
H	-8.30295	3.97794	-1.65265
H	-10.10944	2.35053	-2.1804
C	-5.23995	-2.23469	0.53368
H	-5.7368	-2.57626	-0.38327
H	-4.21496	-2.60177	0.55139
H	-5.77831	-2.67124	1.38511
H	-7.16055	-0.55824	-0.42609

Thermal correction to Energy=0.774684

Thermal correction to Enthalpy=0.775628

Thermal correction to Gibbs Free Energy=0.651844

Sum of electronic and zero-point Energies=-2264.811739

Sum of electronic and thermal Energies=-2264.768276

Sum of electronic and thermal Enthalpies=-2264.767332

Sum of electronic and thermal Free Energies=-2264.891115

SCF Done: E(RwB97XD) = -2266.49347348

$TS_{12\text{-}ohm}$=ts2e

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

H	-4.52604	-0.81076	-1.16544
C	-4.23182	-0.40765	1.65446
B	-2.46508	-0.61699	-0.80725
O	-1.9324	-1.58726	0.01265
O	-1.75011	-0.44953	-1.96562
C	-0.90583	-2.30454	-0.75702
C	-0.52093	-1.24484	-1.85983
C	0.59838	-0.28954	-1.42948
H	1.56447	-0.80275	-1.38808
H	0.67587	0.52422	-2.15656
H	0.40103	0.15313	-0.44831
C	-0.2119	-1.82663	-3.23739
H	0.01519	-1.01629	-3.93741
H	0.66211	-2.48599	-3.19326
H	-1.0548	-2.39412	-3.6379
C	0.22187	-2.69566	0.19417
H	-0.15726	-3.39213	0.94885
H	1.02979	-3.19814	-0.34923
H	0.64083	-1.8289	0.71034
C	-1.58035	-3.56075	-1.32055
H	-0.87044	-4.18297	-1.87448
H	-1.97706	-4.15658	-0.49255
H	-2.4109	-3.30688	-1.98662
H	-4.40042	0.49685	2.22608
Co	-4.10756	0.39759	-0.37003
C	-5.22967	-0.97848	0.88108
C	-6.346	-0.16093	0.38318
C	-6.54549	1.14452	0.67348
H	-3.40789	-1.02654	1.98704
H	-7.32134	1.70815	0.16715
H	-6.00116	1.66695	1.44924
P	-2.99256	2.29148	0.46946
C	-1.954	2.17537	1.9903
C	-1.28683	0.96903	2.2641
H	-1.42209	0.11082	1.61517
C	-0.44595	0.86156	3.3728
H	0.06012	-0.07878	3.57258
C	-0.26118	1.95154	4.22534
H	0.38813	1.86351	5.09157
C	-0.9155	3.15557	3.95965
H	-0.77503	4.01009	4.61535

C	-1.75326	3.27092	2.84876
H	-2.24707	4.2171	2.65559
C	-4.03044	3.79812	0.74942
C	-4.79435	3.90598	1.9261
H	-4.71471	3.1506	2.70377
C	-5.63436	4.99993	2.13302
H	-6.2071	5.07057	3.05329
C	-5.73049	6.00405	1.16634
H	-6.38175	6.8577	1.32932
C	-4.97436	5.90997	-0.00206
H	-5.02855	6.69424	-0.75195
C	-4.12897	4.81678	-0.21005
H	-3.53389	4.77667	-1.11643
C	-1.79389	2.84806	-0.82609
C	-0.60457	3.48343	-0.44923
H	-0.38689	3.6325	0.60196
C	0.316	3.92951	-1.39973
H	1.23101	4.41558	-1.07416
C	0.05554	3.75135	-2.75663
H	0.76282	4.09547	-3.50494
C	-1.12424	3.12827	-3.15378
H	-1.33417	2.98822	-4.20681
C	-2.05245	2.66545	-2.20454
C	-3.27352	2.02887	-2.72833
N	-4.15549	1.29938	-2.11774
C	-5.22244	0.94	-3.10128
H	-5.31566	-0.14789	-3.10047
C	-4.61765	1.43113	-4.43954
H	-4.22956	0.61821	-5.05946
H	-5.29294	2.05717	-5.02299
O	-3.49416	2.24941	-4.03432
C	-6.57637	1.55286	-2.79271
C	-7.72863	0.76402	-2.89364
C	-6.7092	2.91178	-2.47723
C	-8.99261	1.31754	-2.67532
H	-7.63923	-0.28972	-3.14986
C	-7.97022	3.46587	-2.25492
H	-5.82763	3.54041	-2.38773
C	-9.11559	2.67032	-2.35255
H	-9.87757	0.69324	-2.75897
H	-8.0581	4.51939	-2.00506
H	-10.0969	3.10355	-2.18241
C	-5.25473	-2.46513	0.62001
H	-5.75893	-2.71133	-0.31883
H	-4.24238	-2.87345	0.59815
H	-5.80243	-2.95344	1.43712
H	-6.99048	-0.63807	-0.35013

Thermal correction to Energy= 0.771590

Thermal correction to Enthalpy= 0.772535

Thermal correction to Gibbs Free Energy=0.651780

Sum of electronic and zero-point Energies=-2264.772065

Sum of electronic and thermal Energies= -2264.728917

Sum of electronic and thermal Enthalpies=-2264.727973

Sum of electronic and thermal Free Energies=-2264.848728

SCF Done: E(RwB97XD) = -2266.45843248

Int3e

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

H	-4.83251	-0.57292	-0.66622
C	-4.34371	-0.05283	1.48021
B	-2.51071	-0.48985	-0.79591
O	-2.03388	-1.48021	0.02962
O	-1.86269	-0.44856	-2.00728
C	-1.11025	-2.31372	-0.75498
C	-0.6986	-1.33869	-1.92351
C	0.51031	-0.4558	-1.59159
H	1.43716	-1.03792	-1.57158
H	0.60959	0.31803	-2.35874
H	0.39451	0.04246	-0.62392
C	-0.50681	-2.00198	-3.28519
H	-0.25211	-1.24333	-4.03204
H	0.31375	-2.72727	-3.25151
H	-1.41076	-2.51644	-3.61898
C	0.02929	-2.75363	0.16014
H	-0.36545	-3.38412	0.96314
H	0.76726	-3.34209	-0.3962
H	0.5393	-1.9019	0.61553
C	-1.90551	-3.53515	-1.22982
H	-1.27269	-4.22749	-1.79394
H	-2.29879	-4.0705	-0.36014
H	-2.74923	-3.24515	-1.8639
H	-4.71854	0.73879	2.12831
Co	-3.96682	0.70562	-0.33479
C	-5.28069	-0.72852	0.61177
C	-6.63222	-0.11656	0.40166
C	-7.18083	0.88755	1.08893

H	-3.55233	-0.64639	1.92562	C	-6.38492	1.41587	-2.82119
H	-8.17056	1.24979	0.8344	C	-7.40648	0.50372	-3.11273
H	-6.68932	1.37843	1.92404	C	-6.7206	2.67123	-2.29732
P	-2.74831	2.40498	0.44678	C	-8.74346	0.83685	-2.88412
C	-1.76626	2.27133	1.9919	H	-7.15662	-0.47139	-3.52604
C	-1.16191	1.04249	2.306	C	-8.05543	3.00264	-2.06227
H	-1.31651	0.18009	1.66812	H	-5.94	3.38958	-2.06076
C	-0.37075	0.92105	3.44942	C	-9.07022	2.08786	-2.3563
H	0.08863	-0.03466	3.68531	H	-9.52654	0.1219	-3.11997
C	-0.17798	2.01757	4.29193	H	-8.30295	3.97794	-1.65265
H	0.43313	1.9182	5.18435	H	-10.10944	2.35053	-2.1804
C	-0.77641	3.242	3.98718	C	-5.25555	-2.25549	0.54408
H	-0.6314	4.09824	4.63956	H	-5.7576	-2.62826	-0.35207
C	-1.56518	3.37193	2.84315	H	-4.22536	-2.61737	0.55659
H	-2.02546	4.32898	2.6189	H	-5.77831	-2.65564	1.42151
C	-3.88351	3.83996	0.72149	H	-7.20215	-0.55824	-0.41569
C	-4.71328	3.84687	1.85506	Thermal correction to Energy=0.775268			
H	-4.63085	3.05654	2.59847	Thermal correction to Enthalpy=0.776213			
C	-5.63061	4.87749	2.05719	Thermal correction to Gibbs Free Energy=0.654251			
H	-6.25667	4.8738	2.94493	Sum of electronic and zero-point Energies=-2264.779669			
C	-5.73777	5.91432	1.1267	Sum of electronic and thermal Energies=-2264.736129			
H	-6.45043	6.71825	1.28597	Sum of electronic and thermal Enthalpies=-2264.735185			
C	-4.91533	5.91941	-0.00065	Sum of electronic and thermal Free Energies=-2264.857147			
H	-4.98122	6.73025	-0.72064	SCF Done: E(RwB97XD) = -2266.46875373			
C	-3.99119	4.89139	-0.20373				
H	-3.34785	4.92035	-1.07703	ts4e			
C	-1.55741	2.99318	-0.82876	Number of imaginary frequencies=1			
C	-0.36017	3.60658	-0.44107	Charge = 1 Multiplicity = 1			
H	-0.14043	3.73114	0.61324	H	-5.6772	-0.25107	-0.50894
C	0.56536	4.0571	-1.38444	C	-4.60057	-0.39918	1.37612
H	1.48745	4.52502	-1.05249	B	-2.84793	-0.77182	0.22308
C	0.29983	3.90536	-2.74335	O	-1.63403	-0.92745	0.84731
H	1.01047	4.25277	-3.48691	O	-3.13719	-1.80604	-0.65456
C	-0.88826	3.30437	-3.1509	C	-1.1112	-2.25301	0.48643
H	-1.09895	3.18798	-4.20655	C	-1.89401	-2.56316	-0.84838
C	-1.82281	2.83465	-2.21086	C	-1.21379	-1.99471	-2.09977
C	-3.05092	2.20937	-2.75027	H	-0.29992	-2.54441	-2.34625
N	-3.95293	1.49385	-2.15178	H	-1.9006	-2.08189	-2.94778
C	-4.95123	1.06153	-3.16498	H	-0.95751	-0.93811	-1.9713
H	-4.86468	-0.02853	-3.25278	C	-2.25636	-4.02963	-1.06321
C	-4.45337	1.74902	-4.46094	H	-2.83239	-4.13593	-1.98789
H	-4.21056	1.04915	-5.26539	H	-1.3528	-4.64224	-1.1594
H	-5.1403	2.51301	-4.83129	H	-2.85794	-4.42567	-0.24227
O	-3.23002	2.41225	-4.06441	C	0.40393	-2.14269	0.33772

H	0.8536	-1.90073	1.30594
H	0.8305	-3.09359	-0.00035
H	0.68694	-1.36184	-0.37168
C	-1.46441	-3.20174	1.63728
H	-1.04927	-4.20084	1.47165
H	-1.04368	-2.80999	2.5684
H	-2.54698	-3.29821	1.76676
H	-4.68554	0.3079	2.20305
Co	-3.94349	0.71654	-0.12182
C	-5.87916	-0.59744	0.55432
C	-7.08291	0.21375	0.99353
C	-7.33256	0.66735	2.22462
H	-4.22922	-1.33862	1.7986
H	-8.26295	1.1796	2.45317
H	-6.64487	0.52671	3.0548
P	-2.79278	2.33135	0.77406
C	-2.2402	2.3936	2.52243
C	-1.6337	1.27002	3.11077
H	-1.4921	0.36508	2.53105
C	-1.20704	1.32279	4.43827
H	-0.73879	0.4501	4.88477
C	-1.38262	2.48517	5.19187
H	-1.05263	2.51944	6.2262
C	-1.98491	3.60349	4.61282
H	-2.12515	4.51103	5.1928
C	-2.41355	3.56231	3.28564
H	-2.88207	4.43921	2.85257
C	-3.86382	3.81659	0.57248
C	-5.19191	3.7458	1.02601
H	-5.57885	2.82761	1.4597
C	-6.03218	4.85493	0.9185
H	-7.05485	4.78884	1.2785
C	-5.56134	6.04021	0.34922
H	-6.21569	6.9033	0.26672
C	-4.2441	6.1156	-0.10948
H	-3.87079	7.0369	-0.54751
C	-3.39592	5.01191	0.00331
H	-2.37037	5.09096	-0.34351
C	-1.32287	2.67316	-0.27302
C	-0.11428	3.08096	0.29953
H	-0.04183	3.1826	1.37693
C	1.0015	3.35923	-0.49486
H	1.93076	3.67009	-0.0267
C	0.91617	3.24408	-1.88098
H	1.77702	3.46274	-2.50514
C	-0.28177	2.84654	-2.47114
H	-0.35281	2.75859	-3.54867
C	-1.40493	2.54493	-1.68281
C	-2.62365	2.10228	-2.38169
N	-3.67124	1.5126	-1.88721
C	-4.57106	1.14071	-3.02265
H	-4.47178	0.05666	-3.1559
C	-3.92523	1.88988	-4.2118
H	-3.76596	1.26814	-5.09359
H	-4.47555	2.79307	-4.48921
O	-2.62736	2.2994	-3.71043
C	-6.03362	1.47184	-2.80979
C	-7.00882	0.51012	-3.10289
C	-6.4359	2.74353	-2.37704
C	-8.36637	0.81263	-2.97106
H	-6.70699	-0.4781	-3.44319
C	-7.79113	3.04327	-2.23957
H	-5.6919	3.49844	-2.13787
C	-8.75939	2.08069	-2.53884
H	-9.11276	0.06036	-3.20926
H	-8.09046	4.0308	-1.90073
H	-9.81425	2.31923	-2.4384
C	-6.27086	-2.08409	0.38363
H	-7.13311	-2.18995	-0.28361
H	-5.43505	-2.65324	-0.03099
H	-6.54376	-2.50272	1.35804
H	-7.83352	0.36303	0.21725

Thermal correction to Energy=0.774635

Thermal correction to Enthalpy=0.775580

Thermal correction to Gibbs Free Energy=0.654764

Sum of electronic and zero-point Energies=-2264.779102

Sum of electronic and thermal Energies=-2264.736094

Sum of electronic and thermal Enthalpies=-2264.735150

Sum of electronic and thermal Free Energies=-2264.855966

SCF Done: E(RwB97XD) = -2266.47066850

Int5e

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

H	-5.62089	-0.31238	-0.57032
C	-4.56467	-0.51428	1.32386
B	-2.90948	-0.80392	0.25768

O	-1.67663	-0.89138	0.87145	H	-6.99921	4.85055	1.38735
O	-3.12253	-1.8358	-0.64749	C	-5.53739	6.04102	0.33863
C	-1.08329	-2.18152	0.50196	H	-6.18534	6.90825	0.24956
C	-1.84646	-2.52911	-0.83527	C	-4.24259	6.08177	-0.18348
C	-1.18673	-1.93695	-2.08557	H	-3.87943	6.97887	-0.67682
H	-0.2484	-2.44982	-2.32478	C	-3.40255	4.97209	-0.06367
H	-1.86385	-2.05914	-2.93698	H	-2.39379	5.0264	-0.4584
H	-0.97615	-0.87073	-1.9612	C	-1.33161	2.61478	-0.27128
C	-2.13894	-4.0133	-1.04729	C	-0.10839	2.98197	0.29522
H	-2.70238	-4.14906	-1.97545	H	-0.02616	3.0747	1.37252
H	-1.20686	-4.58355	-1.13418	C	1.01032	3.22502	-0.50505
H	-2.72702	-4.4332	-0.22877	H	1.95146	3.5025	-0.04123
C	0.4249	-1.99441	0.35653	C	0.91275	3.1222	-1.89114
H	0.86052	-1.73243	1.32753	H	1.77525	3.31729	-2.52002
H	0.89984	-2.92159	0.01597	C	-0.29964	2.76381	-2.47536
H	0.66986	-1.19804	-0.34911	H	-0.38001	2.68258	-3.55277
C	-1.38484	-3.15371	1.64933	C	-1.42568	2.49223	-1.68108
H	-0.91651	-4.12711	1.48505	C	-2.65947	2.08086	-2.37317
H	-0.98418	-2.74032	2.58295	N	-3.72242	1.5226	-1.86964
H	-2.4607	-3.3111	1.78003	C	-4.63305	1.16488	-3.00298
H	-4.64306	0.1666	2.17291	H	-4.54241	0.081	-3.1446
Co	-3.98788	0.71535	-0.12149	C	-3.98586	1.91642	-4.188
C	-5.84564	-0.66427	0.48934	H	-3.86379	1.30647	-5.08501
C	-7.0338	0.17235	0.92139	H	-4.51201	2.84259	-4.43608
C	-7.29298	0.62437	2.15291	O	-2.66751	2.27135	-3.70233
H	-4.22717	-1.47525	1.72647	C	-6.0899	1.50709	-2.77766
H	-8.21464	1.15742	2.36706	C	-7.07907	0.56799	-3.09652
H	-6.62444	0.46412	2.99264	C	-6.47586	2.77065	-2.30606
P	-2.80619	2.30757	0.7784	C	-8.43196	0.88265	-2.95197
C	-2.25941	2.37406	2.53121	H	-6.78905	-0.41375	-3.46687
C	-1.85895	1.21122	3.20794	C	-7.82646	3.08214	-2.15539
H	-1.84438	0.25952	2.69045	H	-5.72035	3.50725	-2.04664
C	-1.45545	1.28295	4.5415	C	-8.80615	2.14245	-2.48038
H	-1.14827	0.37687	5.05763	H	-9.1868	0.14828	-3.21031
C	-1.44422	2.50478	5.21166	H	-8.11115	4.06302	-1.78599
H	-1.13104	2.554	6.25061	H	-9.85732	2.38957	-2.36644
C	-1.83556	3.66707	4.54376	C	-6.27156	-2.13678	0.28907
H	-1.83014	4.62316	5.059	H	-7.12908	-2.21081	-0.38971
C	-2.24606	3.6054	3.21232	H	-5.44513	-2.72164	-0.12725
H	-2.55989	4.51489	2.71198	H	-6.5641	-2.5638	1.25341
C	-3.85554	3.80907	0.57616	H	-7.77012	0.34672	0.13479
C	-5.16163	3.77352	1.09427				
H	-5.53695	2.87964	1.58243				
C	-5.99395	4.88716	0.98019				

Thermal correction to Energy=0.777020

Thermal correction to Enthalpy=0.777964

Thermal correction to Gibbs Free Energy=0.652149

Sum of electronic and zero-point Energies=-2264.803740

Sum of electronic and thermal Energies=-2264.759865

Sum of electronic and thermal Enthalpies=-2264.758921

Sum of electronic and thermal Free Energies=-2264.884736

SCF Done: E(RwB97XD) = -2266.49262849

$TS_{21\text{-}ohm}$= $TS_{41\text{-}ohm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

H	-4.36695	-0.59637	-1.14842
C	-4.8799	-0.07252	1.28733
B	-2.43144	-0.45722	-0.95699
O	-1.98975	-1.47584	-0.14923
O	-1.72835	-0.351	-2.1294
C	-1.04077	-2.2806	-0.93317
C	-0.57512	-1.25714	-2.04084
C	0.62696	-0.40322	-1.62273
H	1.54689	-0.99586	-1.59409
H	0.76269	0.40292	-2.34998
H	0.47799	0.05183	-0.63869
C	-0.33697	-1.86137	-3.42229
H	-0.05158	-1.07289	-4.12584
H	0.47845	-2.59247	-3.38933
H	-1.23004	-2.35586	-3.81096
C	0.05895	-2.77239	0.00392
H	-0.37309	-3.43157	0.76338
H	0.81147	-3.34518	-0.54927
H	0.55976	-1.94714	0.51517
C	-1.83231	-3.4695	-1.4903
H	-1.18755	-4.15249	-2.05235
H	-2.27429	-4.02763	-0.65905
H	-2.64163	-3.14015	-2.15011
Co	-3.91375	0.68307	-0.45243
C	-5.05539	-1.04306	0.27543
P	-2.69718	2.39305	0.44932
C	-1.64258	2.16908	1.93961
C	-1.08923	0.90141	2.18606
H	-1.34182	0.0603	1.55002
C	-0.22704	0.70909	3.26738
H	0.19111	-0.27681	3.44994
C	0.08694	1.77104	4.1169
H	0.75318	1.61639	4.96076
C	-0.46277	3.03336	3.88211
H	-0.22435	3.8643	4.53979
C	-1.31995	3.23472	2.79951
H	-1.73378	4.22271	2.62678
C	-3.71207	3.90254	0.79535
C	-4.35698	4.04743	2.03652
H	-4.19125	3.32244	2.8275
C	-5.18984	5.13952	2.28301
H	-5.66931	5.23982	3.25252
C	-5.39945	6.10114	1.29263
H	-6.04553	6.95238	1.48599
C	-4.76301	5.96877	0.05769
H	-4.90602	6.72074	-0.71324
C	-3.92499	4.87939	-0.1903
H	-3.42121	4.81167	-1.14875
C	-1.49588	2.98677	-0.84012
C	-0.27963	3.55685	-0.44432
H	-0.03574	3.62154	0.60926
C	0.63885	4.04375	-1.37698
H	1.5745	4.4746	-1.03283
C	0.35102	3.97893	-2.73817
H	1.05601	4.35774	-3.47165
C	-0.85481	3.42472	-3.15699
H	-1.08941	3.37252	-4.2132
C	-1.77824	2.91687	-2.22635
C	-3.01614	2.34141	-2.77404
N	-3.87404	1.56496	-2.19294
C	-4.89497	1.15794	-3.19847
H	-4.68519	0.1125	-3.45183
C	-4.56461	2.08059	-4.39576
H	-4.45843	1.55254	-5.34417
H	-5.27526	2.90386	-4.50757
O	-3.27662	2.65191	-4.05415
C	-6.32236	1.26672	-2.70248
C	-7.20521	0.19417	-2.87914
C	-6.79226	2.44534	-2.10368
C	-8.53659	0.29462	-2.46858
H	-6.85204	-0.72171	-3.34809
C	-8.12098	2.5444	-1.68868
H	-6.11869	3.28538	-1.9513
C	-8.99609	1.46992	-1.8714
H	-9.2122	-0.54268	-2.61754
H	-8.47378	3.46153	-1.22567
H	-10.03114	1.55054	-1.55255
C	-4.1001	-0.34392	2.51288

H	-6.01713	-1.11396	-0.22967
H	-3.85463	0.53509	3.10634
H	-4.48209	-1.96365	0.31505
C	-5.99876	0.95666	1.42704
H	-5.70845	1.80117	2.05386
H	-6.33025	1.35251	0.45803
H	-6.87666	0.48662	1.89306
C	-3.73723	-1.54533	2.98027
H	-3.18	-1.63722	3.90771
H	-3.98326	-2.47228	2.47006

Thermal correction to Energy=0.771275

Thermal correction to Enthalpy=0.772219

Thermal correction to Gibbs Free Energy=0.650825

Sum of electronic and zero-point Energies=-2264.762331

Sum of electronic and thermal Energies=-2264.718726

Sum of electronic and thermal Enthalpies=-2264.717782

Sum of electronic and thermal Free Energies=-2264.839176

SCF Done: E(RwB97XD) = -2266.44923831

$TS_{43\text{-}ohm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

H	-4.60818	-0.49312	-0.91805
C	-4.31428	0.04777	1.47324
B	-2.51831	-0.44693	-0.82747
O	-2.09791	-1.4445	0.02133
O	-1.84928	-0.44015	-2.02515
C	-1.22353	-2.33937	-0.75274
C	-0.73857	-1.39559	-1.91936
C	0.51233	-0.58081	-1.57127
H	1.40531	-1.213	-1.53748
H	0.66429	0.18527	-2.3377
H	0.41026	-0.07577	-0.6055
C	-0.56494	-2.07549	-3.27492
H	-0.26513	-1.33461	-4.02286
H	0.21868	-2.83989	-3.22812
H	-1.48933	-2.54691	-3.6161
C	-0.12333	-2.8533	0.17133
H	-0.56488	-3.45725	0.97027
H	0.57935	-3.48805	-0.37987
H	0.43762	-2.03708	0.6322
C	-2.10188	-3.50194	-1.22955
H	-1.5157	-4.25067	-1.77149
H	-2.55423	-3.98927	-0.36018
H	-2.90659	-3.154	-1.88538
H	-4.78754	0.82249	2.07103
Co	-3.94689	0.77194	-0.3804
C	-5.1184	-0.75087	0.62275
C	-6.57676	-0.5327	0.39253
C	-7.21613	0.5687	0.81442
H	-3.43834	-0.40446	1.92252
H	-8.27434	0.70973	0.61935
H	-6.72021	1.36548	1.35958
P	-2.7533	2.48565	0.42808
C	-1.7775	2.35062	1.97628
C	-1.11439	1.14383	2.25744
H	-1.21652	0.29581	1.58798
C	-0.33039	1.02385	3.40534
H	0.17485	0.0854	3.61516
C	-0.20361	2.09997	4.28637
H	0.40196	2.00157	5.18264
C	-0.86031	3.30164	4.01459
H	-0.76652	4.14165	4.69672
C	-1.6418	3.43049	2.86493
H	-2.1465	4.37043	2.66581
C	-3.88273	3.92267	0.68271
C	-4.79839	3.88349	1.74993
H	-4.7793	3.05933	2.45746
C	-5.71708	4.91638	1.93422
H	-6.40895	4.87757	2.77071
C	-5.74237	5.99885	1.05098
H	-6.45666	6.80403	1.19595
C	-4.83696	6.04739	-0.00998
H	-4.84017	6.89301	-0.69189
C	-3.91092	5.0174	-0.19456
H	-3.20332	5.08168	-1.01485
C	-1.542	3.05982	-0.84002
C	-0.34634	3.66813	-0.43983
H	-0.13982	3.79886	0.6165
C	0.59505	4.10557	-1.37416
H	1.51582	4.5692	-1.0327
C	0.34761	3.9458	-2.73559
H	1.07145	4.28208	-3.47145
C	-0.83983	3.35166	-3.15553
H	-1.03855	3.23002	-4.21314
C	-1.78946	2.89617	-2.22468
C	-3.01794	2.28906	-2.77144

N	-3.92258	1.57679	-2.17294
C	-4.94916	1.18279	-3.17635
H	-4.9064	0.09333	-3.26839
C	-4.43686	1.85697	-4.47802
H	-4.19454	1.14835	-5.27258
H	-5.11302	2.62507	-4.85823
O	-3.20805	2.51153	-4.07939
C	-6.36309	1.59543	-2.81334
C	-7.43074	0.75913	-3.16123
C	-6.63372	2.83426	-2.21727
C	-8.74834	1.15204	-2.91961
H	-7.23318	-0.20314	-3.62881
C	-7.95056	3.22356	-1.96703
H	-5.81756	3.49594	-1.94023
C	-9.01105	2.38536	-2.31943
H	-9.56737	0.49613	-3.20083
H	-8.14585	4.18462	-1.49964
H	-10.03575	2.69293	-2.13159
C	-7.27975	-1.63976	-0.35153
H	-8.33296	-1.4042	-0.52308
H	-6.80724	-1.82056	-1.32677
H	-7.22664	-2.58305	0.20838
H	-4.77826	-1.77256	0.46302

Thermal correction to Energy=0.771219

Thermal correction to Enthalpy=0.772163

Thermal correction to Gibbs Free Energy=0.649182

Sum of electronic and zero-point Energies=-2264.776588

Sum of electronic and thermal Energies=-2264.733122

Sum of electronic and thermal Enthalpies=-2264.732178

Sum of electronic and thermal Free Energies=-2264.855159

SCF Done: E(RwB97XD) = -2266.46371768

$TS_{21\text{-}obm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	-0.32721	1.70833	3.23987
C	0.01667	2.51583	4.86246
C	-0.60411	2.06606	6.03564
H	-1.20856	1.16906	6.01361
C	-0.41957	2.75624	7.23764
H	-0.90932	2.40139	8.14024
C	0.3859	3.89311	7.28083
H	0.52834	4.42631	8.21643
C	1.0032	4.35274	6.11324
H	1.6231	5.24437	6.13761
C	0.81153	3.67783	4.90999
H	1.27075	4.0638	4.00458
C	-0.89386	3.1951	2.28785
C	-2.11655	3.76797	2.67639
H	-2.68898	3.33306	3.49215
C	-2.59743	4.91552	2.04651
H	-3.53887	5.35165	2.3684
C	-1.86676	5.50516	1.0115
H	-2.23813	6.40061	0.52174
C	-0.65011	4.94486	0.61954
H	-0.06897	5.40448	-0.17506
C	-0.16251	3.79863	1.25486
H	0.79626	3.39359	0.94668
C	1.308	1.27025	2.50818
C	2.49335	1.3757	3.24338
H	2.46276	1.75977	4.25647
C	3.72304	0.99878	2.69424
H	4.62554	1.08655	3.29206
C	3.78989	0.52549	1.38629
H	4.74252	0.24319	0.9492
C	2.62142	0.41177	0.63528
H	2.66281	0.04302	-0.38316
C	1.37806	0.75478	1.18882
C	0.18663	0.54594	0.34358
N	-1.03138	0.29896	0.71718
C	-1.82796	-0.00737	-0.51065
H	-1.9583	-1.09501	-0.52888
C	-0.86868	0.43354	-1.64011
H	-0.76126	-0.29661	-2.44299
H	-1.13148	1.40957	-2.05715
O	0.41555	0.56945	-0.97847
C	-3.19204	0.64645	-0.59092
C	-4.29833	-0.11318	-0.99436
C	-3.36177	2.01441	-0.33753
C	-5.55528	0.47863	-1.13501
H	-4.17624	-1.17326	-1.20691
C	-4.61942	2.60428	-0.47112
H	-2.51404	2.62193	-0.0366
C	-5.71881	1.83919	-0.86909
H	-6.40231	-0.12251	-1.45259
H	-4.7366	3.66481	-0.26811
H	-6.69537	2.3022	-0.97721
C	-3.14782	-1.15614	3.43974

B	-1.25721	-1.42302	4.20735
C	-2.87391	-1.66242	2.10265
O	-0.90802	-0.90928	5.42678
O	-0.88407	-2.73413	4.04635
C	-0.29763	-1.98579	6.22926
C	0.02422	-3.08501	5.13463
H	-3.51684	-1.33457	1.28914
C	-3.7029	-1.97616	4.56264
C	-4.2306	-3.19443	4.41198
H	-2.47875	-2.67017	2.00723
H	-4.22174	-3.7128	3.45805
C	-1.33883	-2.41945	7.26548
H	-2.23239	-2.83724	6.79678
H	-0.92524	-3.16963	7.94689
H	-1.63663	-1.55074	7.86158
C	-0.27139	-4.52359	5.55592
H	-0.04894	-5.19943	4.72446
H	0.35427	-4.81817	6.4057
H	-1.31959	-4.65968	5.82965
C	1.44525	-2.98974	4.56212
H	1.52657	-3.66458	3.70469
H	1.67631	-1.97699	4.21714
H	2.19668	-3.28482	5.30132
C	0.92441	-1.4039	6.93768
H	1.62607	-0.95016	6.23455
H	0.60972	-0.63168	7.64637
H	1.44981	-2.18309	7.50044
H	-3.749	-1.4782	5.52916
H	-4.69742	-3.70781	5.2476
C	-3.78939	0.23944	3.40334
H	-3.81603	0.71181	4.3878
H	-3.2923	0.94426	2.69608
H	-4.80809	0.15318	3.00542
H	-0.4445	-1.0696	2.53756
Co	-1.60335	-0.21923	2.56619

Thermal correction to Energy= 0.770885

Thermal correction to Enthalpy=0.771829

Thermal correction to Gibbs Free Energy=0.653174

Sum of electronic and zero-point Energies=-2264.733172

Sum of electronic and thermal Energies=-2264.690399

Sum of electronic and thermal Enthalpies=-2264.689455

Sum of electronic and thermal Free Energies=-2264.808110

SCF Done: E(RwB97XD) = -2266.42258920

$TS_{41\text{-}obm}=TS_{43\text{-}obm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.21559	1.60745	1.48939
C	0.40225	3.07334	2.59688
C	1.62732	3.75116	2.73071
H	2.47309	3.48193	2.10839
C	1.7645	4.80796	3.63183
H	2.71596	5.32631	3.70976
C	0.68243	5.20092	4.42148
H	0.78796	6.02479	5.1212
C	-0.53705	4.53392	4.29883
H	-1.38791	4.83861	4.90154
C	-0.6783	3.47823	3.39704
H	-1.63446	2.97477	3.31602
C	-1.57981	1.60063	1.08201
C	-2.45169	0.8306	1.86534
H	-2.04763	0.19691	2.64613
C	-3.82876	0.88467	1.64395
H	-4.49614	0.28729	2.25823
C	-4.34532	1.69259	0.62956
H	-5.41708	1.73171	0.45639
C	-3.48121	2.45026	-0.16425
H	-3.87756	3.07868	-0.95675
C	-2.10517	2.41111	0.06273
H	-1.44754	3.01549	-0.55397
C	1.0244	2.07081	-0.10707
C	1.32667	3.39711	-0.43646
H	1.0689	4.19206	0.25367
C	1.95557	3.72247	-1.64214
H	2.18148	4.76112	-1.86531
C	2.28297	2.72022	-2.55253
H	2.77419	2.96406	-3.48924
C	1.95767	1.39714	-2.26329
H	2.17869	0.61465	-2.97968
C	1.33432	1.05942	-1.05081
C	0.94173	-0.34795	-0.86738
N	0.67571	-0.99886	0.22512
C	0.12741	-2.34524	-0.1605
H	0.63348	-3.09857	0.43816
C	0.57245	-2.43198	-1.63389
H	1.51596	-2.97171	-1.76299
H	-0.18395	-2.83405	-2.30632
O	0.80634	-1.04687	-2.00674

C	-1.36878	-2.48154	0.05317
C	-1.84811	-3.35995	1.03215
C	-2.28772	-1.79999	-0.75736
C	-3.22011	-3.55945	1.1987
H	-1.14437	-3.90019	1.66036
C	-3.65789	-1.99962	-0.59373
H	-1.93902	-1.11576	-1.52719
C	-4.12745	-2.88122	0.38356
H	-3.57686	-4.25321	1.95468
H	-4.35846	-1.47016	-1.23266
H	-5.19489	-3.04444	0.50211
C	2.18281	0.22143	3.98035
C	3.03804	-0.004	2.73034
C	3.06745	-1.26625	2.14556
C	2.08308	-2.23395	2.4999
H	1.84206	-2.42193	3.54036
H	1.99631	-3.11264	1.86826
H	2.7474	-0.23573	4.81099
H	2.11993	1.2966	4.16275
H	-0.21595	-1.10205	2.40992
B	0.74148	-0.3637	4.55163
O	-0.32778	0.45249	4.80128
O	0.72904	-1.52149	5.28123
C	-1.03331	-0.09871	5.96751
C	-0.55825	-1.60729	5.97158
C	-2.53276	0.10726	5.77485
H	-3.08858	-0.30858	6.62231
H	-2.75473	1.17763	5.72113
H	-2.89768	-0.3647	4.86025
C	-0.54213	0.70624	7.17683
H	-0.74226	1.76778	7.00259
H	-1.05656	0.4049	8.0946
H	0.53493	0.5864	7.3311
C	-1.45045	-2.54503	5.14995
H	-0.95946	-3.52017	5.07121
H	-2.421	-2.69289	5.63414
H	-1.61564	-2.16845	4.13624
C	-0.31269	-2.20098	7.35725
H	-1.24225	-2.2286	7.93641
H	0.05144	-3.22806	7.25679
H	0.43153	-1.6333	7.91978
Co	1.0791	-0.48651	2.04365
H	3.68451	-1.40227	1.2584
C	4.11241	1.009	2.43056
H	4.51542	0.87292	1.42171
H	3.76027	2.03627	2.53252
H	4.94553	0.88981	3.13749

Thermal correction to Energy=0.772460

Thermal correction to Enthalpy=0.773404

Thermal correction to Gibbs Free Energy=0.655512

Sum of electronic and zero-point Energies=-2264.774588

Sum of electronic and thermal Energies=-2264.732565

Sum of electronic and thermal Enthalpies=-2264.731621

Sum of electronic and thermal Free Energies=-2264.849513

SCF Done: E(RwB97XD) = -2266.47030970

TS34-obm

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	-0.15266	0.52573	2.29308
C	-0.08645	1.11781	4.03054
C	0.38649	0.23744	5.01908
H	0.70206	-0.7632	4.74279
C	0.46775	0.65146	6.34937
H	0.83437	-0.03638	7.10614
C	0.07454	1.94237	6.7082
H	0.13294	2.26119	7.74487
C	-0.39487	2.82339	5.73136
H	-0.69952	3.8294	6.00506
C	-0.47563	2.41716	4.39864
H	-0.84332	3.11083	3.64975
C	-1.3045	1.69092	1.45223
C	-2.63935	1.74097	1.8938
H	-2.9557	1.15412	2.75222
C	-3.56633	2.56717	1.25892
H	-4.59079	2.60056	1.61828
C	-3.17703	3.35143	0.17
H	-3.89845	3.99646	-0.32304
C	-1.85393	3.31258	-0.27231
H	-1.53981	3.93138	-1.10811
C	-0.92075	2.4903	0.36522
H	0.10754	2.48986	0.0185
C	1.51123	0.91091	1.58604
C	2.40755	1.73325	2.27639
H	2.116	2.15725	3.23073
C	3.67364	2.02137	1.75893
H	4.35039	2.6586	2.32055

C	4.05947	1.49953	0.52647
H	5.03875	1.7231	0.11488
C	3.17709	0.6898	-0.18596
H	3.46471	0.29024	-1.15149
C	1.91162	0.3767	0.33547
C	1.04179	-0.48645	-0.48893
N	0.06617	-1.25292	-0.10808
C	-0.45571	-1.98277	-1.30186
H	-0.15712	-3.02878	-1.18042
C	0.32735	-1.31881	-2.46211
H	0.8532	-2.02673	-3.10425
H	-0.29438	-0.65839	-3.07114
O	1.32288	-0.49279	-1.79915
C	-1.96034	-1.92564	-1.46537
C	-2.68038	-3.11017	-1.65829
C	-2.64403	-0.70166	-1.47036
C	-4.06316	-3.0765	-1.85438
H	-2.1583	-4.06445	-1.65681
C	-4.02544	-0.66822	-1.65904
H	-2.10318	0.2282	-1.31345
C	-4.73816	-1.85494	-1.85309
H	-4.60927	-4.00279	-2.00768
H	-4.54475	0.28582	-1.65532
H	-5.81326	-1.82621	-2.0049
C	-1.78359	-2.35838	3.26365
B	0.06694	-3.22535	3.02126
C	-2.29867	-1.92922	1.95627
O	1.26916	-2.57239	3.253
O	0.10092	-4.55123	3.31559
C	2.2363	-3.57856	3.74707
C	1.51027	-4.94316	3.40029
H	-2.74631	-0.94237	1.86655
C	-2.39773	-3.55496	3.96562
C	-3.19394	-4.43822	3.35257
H	-2.77836	-2.67117	1.32617
H	-3.42263	-4.40007	2.29281
C	2.38482	-3.31832	5.24886
H	1.43324	-3.43143	5.77696
H	3.11036	-4.00349	5.6983
H	2.74441	-2.29638	5.40461
C	1.63474	-6.02886	4.46672
H	1.07051	-6.91212	4.15319
H	2.68114	-6.32582	4.59775
H	1.2406	-5.70308	5.43161
C	1.88903	-5.51218	2.02657
H	1.22616	-6.35175	1.79786
H	1.77439	-4.76735	1.23295
H	2.92071	-5.8775	2.01562
C	3.5673	-3.3494	3.03779
H	3.46284	-3.38944	1.95137
H	3.96414	-2.36569	3.30748
H	4.30161	-4.10302	3.34303
H	-3.64829	-5.25106	3.91117
H	-0.40876	-3.20924	1.19176
Co	-0.42052	-1.7881	1.69792
C	-2.1242	-3.63698	5.44905
H	-2.44482	-2.72077	5.96284
H	-2.65308	-4.4804	5.90063
H	-1.05416	-3.76648	5.65147
H	-1.6519	-1.5411	3.97393

Thermal correction to Energy= 0.771751

Thermal correction to Enthalpy=0.772695

Thermal correction to Gibbs Free Energy=0.652147

Sum of electronic and zero-point Energies=-2264.749282

Sum of electronic and thermal Energies=-2264.706562

Sum of electronic and thermal Enthalpies= -2264.705618

Sum of electronic and thermal Free Energies=-2264.826165

SCF Done: E(RwB97XD) = -2266.43288505

ST-Z′

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.07648	3.02617	0.86491
C	-1.51862	3.96029	1.1136
C	-2.69804	3.40796	0.29503
C	1.32565	4.08258	1.71465
C	0.97699	5.05518	2.66426
H	-0.06193	5.23352	2.92203
C	1.96413	5.82251	3.29043
H	1.67617	6.57438	4.01961
C	3.30858	5.63002	2.97491
C	3.66575	4.6666	2.02725
H	4.71095	4.51753	1.7709
C	2.6853	3.89637	1.40302
H	2.97391	3.15422	0.66354
C	0.40842	3.39807	-0.91717
C	0.15336	2.44697	-1.91442
H	-0.18608	1.45437	-1.64694

C	0.32606	2.76512	-3.26381
H	0.11927	2.01408	-4.02092
C	0.76092	4.03719	-3.63353
C	1.01641	4.99466	-2.64835
H	1.35452	5.98846	-2.92791
C	0.83973	4.68065	-1.30164
H	1.04871	5.43546	-0.54997
C	-3.29126	2.10132	0.84028
H	-3.51935	2.23247	1.90365
P	-2.23402	0.56776	0.74446
H	0.89979	4.28435	-4.68217
H	4.07387	6.22921	3.45945
H	-1.33687	5.00409	0.83534
H	-1.76747	3.94123	2.18186
H	-2.4122	3.30066	-0.75751
H	-3.4962	4.16027	0.31441
C	-2.3417	-0.00528	-1.00451
C	-1.47845	-1.0363	-1.41843
C	-3.25613	0.51892	-1.93094
C	-1.53458	-1.53182	-2.72176
H	-0.76204	-1.45711	-0.7192
C	-3.30017	0.03161	-3.23904
H	-3.94171	1.31065	-1.64916
C	-2.44259	-0.99474	-3.63738
H	-0.86783	-2.33579	-3.0205
H	-4.01048	0.45362	-3.94414
H	-2.48338	-1.37586	-4.65364
C	-3.33428	-0.6202	1.65196
C	-3.6966	-1.86052	1.10432
C	-3.82068	-0.2835	2.92838
C	-4.52131	-2.73721	1.81392
H	-3.34938	-2.14577	0.11732
C	-4.64904	-1.15782	3.63195
H	-3.56362	0.6683	3.38581
C	-5.00019	-2.39008	3.07694
H	-4.79309	-3.69085	1.37053
H	-5.02048	-0.87404	4.61251
H	-5.6444	-3.07167	3.62441
H	-4.24939	1.88223	0.35713
C	-0.12064	-1.18501	2.36156
C	-0.40355	-0.21262	3.33646
C	0.50463	0.86392	3.56895
H	0.55135	1.69396	5.53457
C	1.67826	0.86272	2.77902
H	2.1986	-0.07072	2.58732
H	2.31357	1.74146	2.78975
H	-1.38576	-0.17016	3.79641
H	0.88135	-1.5557	2.17836
C	0.15909	1.95805	4.54325
H	-0.92374	2.09168	4.64361
H	0.61367	2.91064	4.26105
Co	-0.04222	0.76778	1.54448
H	-0.91498	-1.87089	2.08307

Thermal correction to Energy= 0.606884

Thermal correction to Enthalpy=0.607828

Thermal correction to Gibbs Free Energy=0.504983

Sum of electronic and zero-point Energies=-2066.887196

Sum of electronic and thermal Energies=-2066.853115

Sum of electronic and thermal Enthalpies=-2066.852171

Sum of electronic and thermal Free Energies=-2066.955017

SCF Done: E(RwB97XD) = -2068.37674516

TS'12-ohm

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.45094	2.82393	0.90682
C	-1.14624	3.70059	1.32964
C	-2.42951	3.11192	0.70396
C	1.77161	3.85696	1.68245
C	1.64494	5.24778	1.82403
H	0.74389	5.7612	1.5035
C	2.68262	6.00029	2.37648
H	2.5652	7.07413	2.49013
C	3.8672	5.37805	2.77428
C	4.0116	3.99844	2.61605
H	4.93603	3.50989	2.91138
C	2.97009	3.24101	2.07802
H	3.09249	2.16932	1.95137
C	0.71753	3.14987	-0.8903
C	1.78237	2.49596	-1.53326
H	2.37704	1.7718	-0.98728
C	2.07198	2.76728	-2.87056
H	2.90137	2.25815	-3.35376
C	1.30621	3.69171	-3.58479
C	0.25245	4.35082	-2.95147
H	-0.34386	5.07746	-3.49582
C	-0.03876	4.08689	-1.61142
H	-0.85451	4.62785	-1.14426

C	-2.97592	1.82146	1.34016
H	-3.08336	1.95157	2.425
P	-1.92107	0.30447	1.04744
H	1.53335	3.90177	-4.62596
H	4.67493	5.96616	3.20008
H	-1.05966	4.75297	1.04065
H	-1.22214	3.69907	2.42529
H	-2.29526	2.96027	-0.37232
H	-3.21286	3.87347	0.80431
C	-2.0846	0.01401	-0.76021
C	-0.98457	0.16431	-1.61456
C	-3.33038	-0.34531	-1.30498
C	-1.12732	-0.02523	-2.99169
H	-0.01626	0.43199	-1.20922
C	-3.46945	-0.53524	-2.67852
H	-4.18968	-0.49303	-0.6567
C	-2.36819	-0.37329	-3.52472
H	-0.26773	0.10464	-3.64275
H	-4.43593	-0.81409	-3.08836
H	-2.47945	-0.52284	-4.59484
C	-2.89179	-1.07508	1.7821
C	-2.34951	-2.37051	1.70587
C	-4.13058	-0.89223	2.41479
C	-3.04197	-3.45684	2.23815
H	-1.37849	-2.52361	1.2439
C	-4.81807	-1.98453	2.95216
H	-4.57732	0.09344	2.49385
C	-4.27812	-3.26692	2.86231
H	-2.61503	-4.45341	2.16878
H	-5.77717	-1.82809	3.43757
H	-4.81517	-4.11455	3.27792
H	-3.97745	1.62761	0.93948
H	1.32183	1.22355	2.75961
C	-0.42522	-0.26605	3.68661
B	1.23397	-0.36209	1.19241
O	2.32076	-0.03155	0.42041
O	1.08105	-1.71399	1.35819
C	3.11644	-1.25218	0.2102
C	2.06972	-2.39977	0.51333
C	1.32096	-2.90149	-0.72599
H	1.98789	-3.44998	-1.39866
H	0.52491	-3.58445	-0.41299
H	0.85971	-2.08271	-1.28533
C	2.62321	-3.58422	1.30282
H	1.81947	-4.30061	1.4996
H	3.40097	-4.10329	0.73159
H	3.0432	-3.27517	2.26229
C	3.65637	-1.22909	-1.21793
H	4.34163	-0.38395	-1.33936
H	4.21715	-2.1449	-1.43496
H	2.85691	-1.13045	-1.95572
C	4.27515	-1.18932	1.21114
H	4.94711	-2.04625	1.1
H	4.85504	-0.27897	1.02904
H	3.91261	-1.16346	2.24287
Co	0.04348	0.87695	2.05235
C	0.37659	1.78849	4.90883
H	0.18148	1.55717	5.9641
H	1.21969	2.48348	4.86452
H	-0.51275	2.29198	4.51288
C	0.66694	0.48839	4.16997
C	1.97921	-0.13017	4.51283
H	-1.42836	0.02453	3.9945
H	-0.30117	-1.31537	3.44401
C	2.14629	-1.40937	4.86168
H	2.82686	0.55294	4.55032
H	3.1202	-1.78297	5.16475
H	1.32375	-2.11828	4.87659

Thermal correction to Energy=0.807243

Thermal correction to Enthalpy=0.808187

Thermal correction to Gibbs Free Energy= 0.682971

Sum of electronic and zero-point Energies=-2478.517499

Sum of electronic and thermal Energies=-2478.472322

Sum of electronic and thermal Enthalpies=-2478.471378

Sum of electronic and thermal Free Energies=-2478.596594

SCF Done: E(RwB97XD) = -2480.25406865

Int1b’

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.14242	2.95452	0.83282
C	-1.45282	3.92051	0.93881
C	-2.58967	3.33572	0.08875
C	1.3152	4.0335	1.76081
C	0.87875	4.9787	2.70584
H	-0.17826	5.11296	2.90912
C	1.79701	5.76892	3.39932
H	1.43788	6.49964	4.12101

C	3.16472	5.63189	3.16156
C	3.61164	4.69582	2.22346
H	4.67479	4.58778	2.02739
C	2.69691	3.90153	1.52803
H	3.05397	3.18138	0.80229
C	0.59304	3.27598	-0.92861
C	0.44577	2.27694	-1.90237
H	0.13615	1.28042	-1.61148
C	0.69291	2.55724	-3.24825
H	0.56751	1.77462	-3.99138
C	1.10536	3.83355	-3.63703
C	1.25871	4.83333	-2.67304
H	1.57891	5.82924	-2.96577
C	1.00088	4.56088	-1.33057
H	1.12931	5.3477	-0.59326
C	-3.20138	2.06564	0.68515
H	-3.43041	2.24003	1.74273
P	-2.17742	0.50967	0.64379
H	1.30462	4.05047	-4.68262
H	3.87679	6.25071	3.69708
H	-1.23453	4.94466	0.61788
H	-1.76824	3.96361	1.98812
H	-2.25123	3.16448	-0.93944
H	-3.38461	4.08882	0.02508
C	-2.26943	-0.10409	-1.08883
C	-1.4014	-1.13553	-1.48654
C	-3.2175	0.37455	-2.00801
C	-1.48856	-1.67975	-2.76954
H	-0.65204	-1.50475	-0.79353
C	-3.29035	-0.16072	-3.29442
H	-3.90951	1.16402	-1.73792
C	-2.42876	-1.19131	-3.67726
H	-0.81544	-2.48151	-3.05811
H	-4.02382	0.22792	-3.9961
H	-2.49213	-1.61057	-4.67843
C	-3.32003	-0.61372	1.5743
C	-3.75352	-1.83629	1.03854
C	-3.78588	-0.23335	2.84759
C	-4.62882	-2.65508	1.75919
H	-3.42134	-2.15254	0.05573
C	-4.66058	-1.0514	3.55957
H	-3.46979	0.70595	3.29324
C	-5.08449	-2.26658	3.01736
H	-4.95667	-3.59627	1.32491
H	-5.01397	-0.73509	4.53854
H	-5.76534	-2.90387	3.57376
H	-4.16145	1.83149	0.21227
H	0.48708	0.16816	0.1663
C	-0.25448	-1.20121	2.33623
C	-0.4082	-0.22283	3.36533
B	2.0292	0.0858	0.9023
O	2.40882	-1.23878	0.75007
O	2.82242	0.93503	0.15138
C	3.3028	-1.32189	-0.39793
C	3.88865	0.14582	-0.47193
C	0.55667	0.78157	3.46714
H	1.17095	1.54841	5.36554
C	1.77289	0.62006	2.60116
H	2.31952	-0.28215	2.91154
H	2.41329	1.49644	2.65636
C	5.14809	0.34291	0.378
H	6.00398	-0.18507	-0.05027
H	5.39576	1.40775	0.4165
H	5.00689	-0.01179	1.40476
C	4.11871	0.67997	-1.88422
H	4.50861	1.70062	-1.83394
H	4.85718	0.06625	-2.41319
H	3.19764	0.70069	-2.46822
C	4.3337	-2.41716	-0.12622
H	3.82903	-3.38437	-0.06061
H	5.0648	-2.47159	-0.93895
H	4.86739	-2.24966	0.81291
C	2.44663	-1.7028	-1.6145
H	3.0623	-1.84431	-2.50897
H	1.93456	-2.64415	-1.40124
H	1.69152	-0.94157	-1.83082
H	-1.33623	-0.12782	3.92252
H	0.70313	-1.68808	2.17717
C	0.51905	1.84096	4.53306
H	-0.49119	1.96339	4.93627
H	0.87545	2.80715	4.17043
Co	-0.0501	0.66517	1.47003
H	-1.11058	-1.82687	2.10589

Thermal correction to Energy= 0.811737

Thermal correction to Enthalpy=0.812681

Thermal correction to Gibbs Free Energy=0.688415

Sum of electronic and zero-point Energies=-2478.564324

Sum of electronic and thermal Energies= -2478.519579

Sum of electronic and thermal Enthalpies=-2478.518635

Sum of electronic and thermal Free Energies=-2478.642901

SCF Done: E(RwB97XD) = -2480.30373981

TS2b'

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.17602	2.90906	0.78673
C	-1.36115	3.88123	1.20628
C	-2.63123	3.39332	0.49024
C	1.51857	3.95214	1.51062
C	1.2788	4.89897	2.51979
H	0.27877	5.05465	2.91115
C	2.32322	5.67544	3.02987
H	2.11732	6.40647	3.8065
C	3.61847	5.5195	2.53736
C	3.86553	4.58528	1.52807
H	4.87	4.46862	1.13039
C	2.82739	3.80611	1.01794
H	3.02484	3.08751	0.2301
C	0.35125	3.29362	-1.01252
C	0.26092	2.29977	-1.99326
H	0.12361	1.26608	-1.70591
C	0.34793	2.62844	-3.34884
H	0.27137	1.84272	-4.09487
C	0.52965	3.95441	-3.73822
C	0.62624	4.95558	-2.76686
H	0.7746	5.99043	-3.06199
C	0.53917	4.62935	-1.41525
H	0.63704	5.41647	-0.67302
C	-3.20242	2.07661	1.03614
H	-3.29603	2.15675	2.12454
P	-2.20728	0.53684	0.724
H	0.60124	4.20994	-4.79161
H	4.42878	6.12624	2.93079
H	-1.17486	4.92719	0.93995
H	-1.50967	3.84243	2.29219
H	-2.45375	3.32558	-0.58897
H	-3.40209	4.16261	0.62145
C	-2.41455	0.17453	-1.07283
C	-1.60828	-0.81509	-1.66462
C	-3.38539	0.81039	-1.86156
C	-1.77121	-1.15732	-3.00752
H	-0.85029	-1.32273	-1.07473
C	-3.53605	0.4771	-3.20952
H	-4.03442	1.57024	-1.44028
C	-2.73197	-0.50663	-3.78531
H	-1.14686	-1.93125	-3.44504
H	-4.28719	0.98631	-3.80626
H	-2.85515	-0.76818	-4.83221
C	-3.28901	-0.7404	1.5279
C	-3.50019	-1.99063	0.92382
C	-3.90084	-0.48718	2.7687
C	-4.29979	-2.95488	1.54042
H	-3.05728	-2.21546	-0.04001
C	-4.70425	-1.45077	3.38002
H	-3.77029	0.4662	3.27185
C	-4.90485	-2.68932	2.76903
H	-4.45363	-3.91247	1.05141
H	-5.17509	-1.22834	4.33329
H	-5.53046	-3.43847	3.245
H	-4.21705	1.91026	0.65896
H	0.36146	0.06756	0.0243
C	-0.14751	-1.2343	2.412
C	-0.47528	-0.19696	3.31648
B	1.82596	-0.09149	0.44927
O	2.26524	-1.38049	0.57372
O	2.71721	0.73845	-0.17258
C	3.50608	-1.50318	-0.19899
C	3.98131	0.0002	-0.31404
C	0.42665	0.88019	3.4993
H	0.45721	1.79685	5.42398
C	1.65719	0.76834	2.7604
H	2.20764	-0.16669	2.83019
H	2.29614	1.64535	2.71324
C	4.89901	0.44117	0.83294
H	5.88301	-0.03107	0.75412
H	5.03696	1.52545	0.79106
H	4.48076	0.19189	1.81266
C	4.60166	0.38444	-1.65537
H	4.87756	1.44377	-1.64469
H	5.512	-0.19602	-1.84168
H	3.91009	0.22474	-2.48519
C	4.45202	-2.4318	0.55865
H	4.01241	-3.43223	0.61677
H	5.41249	-2.51645	0.03865
H	4.63815	-2.08517	1.57753
C	3.11636	-2.13007	-1.54303

H	3.99456	-2.30339	-2.17274
H	2.63231	-3.09414	-1.35977
H	2.41464	-1.49625	-2.09471
H	-1.47963	-0.11302	3.7211
H	0.84922	-1.65493	2.36055
C	0.10207	2.03142	4.4114
H	-0.97604	2.21489	4.47861
H	0.6073	2.94948	4.10432
Co	0.0358	0.62635	1.45853
H	-0.93997	-1.9147	2.11731

Thermal correction to Energy= 0.809118

Thermal correction to Enthalpy=0.810062

Thermal correction to Gibbs Free Energy=0.691884

Sum of electronic and zero-point Energies=-2478.543716

Sum of electronic and thermal Energies= -2478.500480

Sum of electronic and thermal Enthalpies= -2478.499535

Sum of electronic and thermal Free Energies=-2478.617713

SCF Done: E(RwB97XD) = -2480.29383803

Int3b'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.13722	2.95452	0.82762
C	-1.45282	3.92051	0.93361
C	-2.58967	3.33572	0.08355
C	1.3152	4.0335	1.76081
C	0.87355	4.9735	2.70584
H	-0.18346	5.10776	2.90912
C	1.79181	5.76892	3.39932
H	1.43268	6.49444	4.12101
C	3.15952	5.63189	3.16156
C	3.60644	4.70102	2.22346
H	4.66959	4.59298	2.02739
C	2.69691	3.90673	1.52803
H	3.05397	3.18658	0.79709
C	0.59304	3.27598	-0.93381
C	0.44577	2.28214	-1.90757
H	0.14135	1.28562	-1.61148
C	0.69811	2.56244	-3.25345
H	0.57271	1.77982	-3.99658
C	1.10536	3.83875	-3.63703
C	1.25871	4.83853	-2.67304
H	1.57891	5.83444	-2.96577
C	1.00088	4.56088	-1.33057
H	1.12931	5.3477	-0.59326
C	-3.20658	2.06564	0.68515
H	-3.43041	2.24003	1.74273
P	-2.19303	0.50447	0.63859
H	1.30462	4.05567	-4.68262
H	3.87159	6.25071	3.70228
H	-1.23453	4.94466	0.61268
H	-1.76824	3.96361	1.98292
H	-2.25123	3.16448	-0.94464
H	-3.38461	4.08882	0.01988
C	-2.28503	-0.10929	-1.09403
C	-1.4222	-1.14593	-1.49174
C	-3.2279	0.37455	-2.01321
C	-1.50416	-1.68495	-2.77474
H	-0.68324	-1.52555	-0.79353
C	-3.29555	-0.15552	-3.30482
H	-3.91471	1.16922	-1.74312
C	-2.43916	-1.18611	-3.68766
H	-0.83624	-2.49191	-3.06331
H	-4.02382	0.23832	-4.0065
H	-2.49733	-1.60017	-4.68883
C	-3.33043	-0.61372	1.5743
C	-3.76392	-1.83629	1.03854
C	-3.78588	-0.23335	2.84759
C	-4.63402	-2.65508	1.75919
H	-3.43174	-2.15254	0.05573
C	-4.66058	-1.0514	3.56477
H	-3.46979	0.70595	3.29324
C	-5.08449	-2.26658	3.02256
H	-4.96187	-3.59627	1.33011
H	-5.00877	-0.74029	4.54374
H	-5.76534	-2.90387	3.57896
H	-4.16665	1.83669	0.21227
H	0.20108	0.19936	0.0987
C	-0.27008	-1.19601	2.30503
C	-0.3926	-0.22803	3.34973
B	2.2008	0.0962	1.0479
O	2.46602	-1.22838	0.80207
O	2.88482	0.94023	0.20858
C	3.3132	-1.31669	-0.38753
C	3.90945	0.14062	-0.47713
C	0.56707	0.78157	3.43074
H	1.22295	1.51721	5.33434
C	1.84049	0.59926	2.60636

H	2.38192	-0.25095	3.05714
H	2.44969	1.50164	2.70836
C	5.20009	0.32211	0.3364
H	6.04038	-0.21107	-0.12307
H	5.45296	1.38695	0.3749
H	5.08489	-0.03779	1.36316
C	4.09791	0.68517	-1.88942
H	4.49301	1.70582	-1.84434
H	4.81558	0.07145	-2.44439
H	3.15604	0.71629	-2.44222
C	4.3389	-2.42236	-0.14702
H	3.82903	-3.38957	-0.07101
H	5.0492	-2.48199	-0.98055
H	4.89859	-2.26526	0.77651
C	2.41543	-1.6872	-1.5729
H	3.0051	-1.83391	-2.48297
H	1.89816	-2.62855	-1.34924
H	1.66032	-0.92077	-1.76842
H	-1.30503	-0.13822	3.93292
H	0.68233	-1.67248	2.10437
C	0.55025	1.82016	4.51746
H	-0.45479	1.92699	4.94147
H	0.89105	2.79675	4.16523
Co	-0.1073	0.67557	1.45443
H	-1.12618	-1.83207	2.10589

Thermal correction to Energy=0.810676

Thermal correction to Enthalpy=0.811620

Thermal correction to Gibbs Free Energy=0.688546

Sum of electronic and zero-point Energies=-2478.559604

Sum of electronic and thermal Energies=-2478.515376

Sum of electronic and thermal Enthalpies=-2478.514432

Sum of electronic and thermal Free Energies=-2478.637505

SCF Done: E(RwB97XD) = -2480.30333542

TS4b'

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.28163	2.90866	0.47128
C	-1.20699	3.99206	0.79048
C	-2.48552	3.54406	0.06845
C	1.57255	3.74789	1.49844
C	1.26088	4.27601	2.76275
H	0.24644	4.23621	3.14467
C	2.24584	4.87438	3.55203
H	1.97865	5.28775	4.52054
C	3.56306	4.95012	3.09655
C	3.88569	4.43229	1.84118
H	4.90418	4.49954	1.46887
C	2.90032	3.83955	1.04963
H	3.16516	3.47089	0.06617
C	0.70221	3.40877	-1.25458
C	0.54612	2.4878	-2.29969
H	0.21721	1.47881	-2.07703
C	0.7906	2.86374	-3.62338
H	0.65869	2.13899	-4.4218
C	1.19705	4.16546	-3.91526
C	1.35238	5.09398	-2.88132
H	1.66655	6.10969	-3.10415
C	1.10399	4.72158	-1.56111
H	1.23607	5.45261	-0.76849
C	-3.11275	2.27767	0.66966
H	-3.16518	2.38579	1.75898
P	-2.19003	0.69588	0.33686
H	1.39058	4.45944	-4.9429
H	4.32798	5.41718	3.70984
H	-0.93803	5.01048	0.49045
H	-1.39497	4.01351	1.86959
H	-2.29933	3.41648	-1.00469
H	-3.21964	4.35474	0.15352
C	-2.48258	0.3658	-1.4587
C	-1.59953	-0.47959	-2.15062
C	-3.59378	0.88074	-2.14676
C	-1.82007	-0.80413	-3.49047
H	-0.73498	-0.88315	-1.63254
C	-3.80552	0.56851	-3.49063
H	-4.30849	1.52479	-1.64574
C	-2.92168	-0.27553	-4.16542
H	-1.13039	-1.46703	-4.0057
H	-4.66701	0.98135	-4.00755
H	-3.09251	-0.52121	-5.20953
C	-3.28203	-0.55256	1.16263
C	-3.54977	-1.78822	0.55102
C	-3.8262	-0.30127	2.43434
C	-4.34104	-2.74286	1.19239
H	-3.15501	-2.00529	-0.43637
C	-4.62205	-1.25533	3.07085
H	-3.64498	0.64297	2.93941
C	-4.88015	-2.47979	2.45272

H	-4.54227	-3.68996	0.69991
H	-5.04228	-1.03746	4.04859
H	-5.50021	-3.2212	2.94792
H	-4.14514	2.15477	0.3275
C	-0.10455	-1.13044	1.9874
C	-0.28424	-0.12984	3.05632
B	2.73223	0.02231	2.13817
O	3.86869	-0.71363	2.06055
O	2.14125	0.23965	0.89477
C	4.01565	-1.24531	0.71328
C	3.06291	-0.31523	-0.14709
C	0.65466	0.62888	3.69788
H	0.63792	1.08187	5.79846
C	2.15448	0.57332	3.48833
H	2.60919	0.01133	4.3187
H	2.54802	1.59571	3.60643
C	3.78583	0.8744	-0.77769
H	4.48111	0.53487	-1.55153
H	3.05785	1.53882	-1.25062
H	4.35114	1.44336	-0.03525
C	2.2553	-1.05392	-1.20683
H	1.61618	-0.35191	-1.74733
H	2.9355	-1.51394	-1.93247
H	1.62853	-1.83915	-0.78057
C	5.49511	-1.17247	0.33425
H	6.06877	-1.81457	1.00893
H	5.65701	-1.52876	-0.68883
H	5.89058	-0.15848	0.42017
C	3.57604	-2.71442	0.77557
H	3.71775	-3.21865	-0.18535
H	4.18372	-3.23001	1.52455
H	2.52693	-2.82116	1.06858
H	-1.30994	-0.01312	3.39646
H	0.84277	-1.66676	1.97972
C	0.2248	1.48717	4.86371
H	-0.86361	1.5298	4.971
H	0.61189	2.50831	4.77557
Co	-0.02153	0.64877	0.94233
H	-0.94194	-1.82363	1.92438
H	-0.14953	-0.76242	0.5483

Thermal correction to Energy=0.809295

Thermal correction to Enthalpy=0.810239

Thermal correction to Gibbs Free Energy=0.688213

Sum of electronic and zero-point Energies=-2478.548580

Sum of electronic and thermal Energies=-2478.504623

Sum of electronic and thermal Enthalpies=-2478.503679

Sum of electronic and thermal Free Energies=-2478.625705

SCF Done: E(RwB97XD) = -2480.29304145

Int5b'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.37785	2.8428	0.38951
C	-1.04934	3.95464	0.86672
C	-2.4001	3.57479	0.2452
C	1.76183	3.68729	1.286
C	1.62157	3.95362	2.65835
H	0.71156	3.67162	3.17777
C	2.6358	4.59204	3.37331
H	2.5001	4.80065	4.43092
C	3.81658	4.96831	2.72963
C	3.96957	4.70771	1.36762
H	4.87975	5.00534	0.85448
C	2.95135	4.07473	0.65014
H	3.0842	3.90093	-0.41162
C	0.62921	3.32719	-1.37283
C	0.60425	2.34979	-2.37609
H	0.45145	1.31215	-2.10322
C	0.74882	2.70147	-3.72071
H	0.71912	1.93053	-4.48531
C	0.92085	4.03837	-4.07733
C	0.9464	5.02454	-3.08613
H	1.07998	6.06762	-3.35826
C	0.80038	4.67367	-1.74516
H	0.83521	5.45234	-0.98846
C	-3.01646	2.29583	0.83145
H	-2.98127	2.35403	1.92545
P	-2.17016	0.70638	0.36203
H	1.03303	4.31489	-5.12175
H	4.60645	5.46671	3.2838
H	-0.78009	4.97657	0.58127
H	-1.13079	3.94424	1.95969
H	-2.31306	3.50133	-0.84522
H	-3.09946	4.39786	0.4379
C	-2.50392	0.50875	-1.44313
C	-1.67372	-0.32491	-2.20983
C	-3.61515	1.10372	-2.0633
C	-1.9466	-0.56043	-3.55852

H	-0.81047	-0.78981	-1.74261
C	-3.87761	0.88118	-3.4157
H	-4.29118	1.73917	-1.50104
C	-3.04653	0.04735	-4.16607
H	-1.2989	-1.21682	-4.13318
H	-4.73795	1.35459	-3.87989
H	-3.25767	-0.12988	-5.21665
C	-3.29253	-0.56242	1.11139
C	-3.48583	-1.79847	0.47198
C	-3.93677	-0.3346	2.33925
C	-4.29924	-2.77672	1.04496
H	-3.01481	-1.99735	-0.48563
C	-4.75382	-1.31383	2.90835
H	-3.82036	0.60949	2.86242
C	-4.93526	-2.53821	2.26487
H	-4.44092	-3.72352	0.53166
H	-5.25044	-1.11422	3.8536
H	-5.57143	-3.29887	2.70764
H	-4.07463	2.21701	0.56201
C	-0.16139	-1.19515	1.93712
C	-0.40136	-0.20997	3.02937
B	2.67319	-0.03187	2.31833
O	3.86203	-0.68186	2.2832
O	2.12317	0.15729	1.05208
C	4.09409	-1.19919	0.94184
C	3.12059	-0.32848	0.04466
C	0.49312	0.53365	3.74671
H	0.31242	0.92519	5.85668
C	2.00226	0.45709	3.64882
H	2.38227	-0.16653	4.47486
H	2.41553	1.45599	3.8594
C	3.78495	0.91198	-0.54862
H	4.54464	0.62641	-1.28268
H	3.03602	1.51853	-1.06361
H	4.25802	1.52674	0.22102
C	2.40765	-1.11612	-1.04809
H	1.73981	-0.45888	-1.60942
H	3.1438	-1.52091	-1.74813
H	1.82043	-1.94566	-0.65095
C	5.57897	-1.03236	0.61948
H	6.1665	-1.63815	1.31551
H	5.80071	-1.37615	-0.3966
H	5.90534	0.00483	0.71937
C	3.74082	-2.69176	0.9892
H	3.94426	-3.18602	0.0343
H	4.35186	-3.1713	1.75908
H	2.69007	-2.85808	1.2476
H	-1.44654	-0.09769	3.30645
H	0.78138	-1.74515	2.00364
C	-0.01351	1.36485	4.90282
H	-1.10581	1.43291	4.92398
H	0.39788	2.38083	4.88779
Co	0.01643	0.5719	0.93874
H	-0.99313	-1.89646	1.85766
H	-0.15236	-0.96894	0.65657

Thermal correction to Energy=0.813804

Thermal correction to Enthalpy=0.814748

Thermal correction to Gibbs Free Energy=0.691313

Sum of electronic and zero-point Energies=-2478.579723

Sum of electronic and thermal Energies=-2478.534859

Sum of electronic and thermal Enthalpies=-2478.533914

Sum of electronic and thermal Free Energies=-2478.657349

SCF Done: E(RwB97XD) = -2480.32572116

Int3d'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.52617	2.24276	0.90982
C	-0.78042	3.56042	1.07306
C	-2.12561	3.1871	0.42327
C	1.98245	2.91178	1.82211
C	3.17943	2.17164	1.80616
H	3.24203	1.25086	1.23488
C	4.29666	2.62647	2.50753
H	5.21699	2.04962	2.48176
C	4.23611	3.81555	3.24155
C	3.05256	4.55055	3.26322
H	2.99813	5.47938	3.82386
C	1.93107	4.10731	2.55935
H	1.02758	4.70731	2.58788
C	0.99158	2.43506	-0.8622
C	0.27153	1.74229	-1.84619
H	-0.47547	1.01112	-1.55647
C	0.5154	1.9747	-3.20134
H	-0.05752	1.43091	-3.94946
C	1.49809	2.88597	-3.58989
C	2.23366	3.56726	-2.61712
H	3.00354	4.27483	-2.91481

C	1.97902	3.35139	-1.26209
H	2.55493	3.89427	-0.51986
C	-2.93155	2.11645	1.18178
H	-2.91298	2.35141	2.25167
P	-2.33098	0.36117	1.0383
H	1.69304	3.05996	-4.64372
H	5.10672	4.16251	3.78844
H	-0.39792	4.47894	0.61706
H	-0.93406	3.75924	2.13958
H	-1.97978	2.90005	-0.62447
H	-2.74212	4.09608	0.39995
C	-2.67372	-0.15366	-0.69841
C	-1.97746	-1.23742	-1.26405
C	-3.68465	0.4673	-1.45124
C	-2.28705	-1.68479	-2.55007
H	-1.1905	-1.73046	-0.70129
C	-3.97914	0.02961	-2.74218
H	-4.25342	1.29592	-1.0401
C	-3.28289	-1.04772	-3.29576
H	-1.74924	-2.52892	-2.96826
H	-4.75707	0.52703	-3.31401
H	-3.51716	-1.39259	-4.29866
C	-3.59058	-0.58855	1.99948
C	-3.93436	-1.89335	1.60832
C	-4.19873	-0.04393	3.14574
C	-4.86677	-2.63063	2.33935
H	-3.4872	-2.33485	0.72375
C	-5.13706	-0.78344	3.86894
H	-3.9647	0.96269	3.47786
C	-5.47056	-2.07902	3.47083
H	-5.12524	-3.63536	2.01773
H	-5.60368	-0.34219	4.74639
H	-6.19932	-2.65265	4.03574
H	-3.98383	2.14281	0.87958
C	1.33166	-1.1122	2.66293
C	-0.08522	-1.23841	3.17292
C	-0.69945	-0.12095	3.78783
C	-0.14544	1.16624	3.72002
H	0.9225	1.33265	3.82493
H	-0.76257	2.01459	4.00866
H	1.8996	-0.2741	3.07683
H	1.88917	-2.02285	2.97047
B	1.55347	-1.36769	1.06617
O	1.15404	-2.56869	0.50524
O	2.57929	-0.77154	0.38321
C	2.26835	-3.01144	-0.33382
C	2.94551	-1.6421	-0.74718
C	1.71455	-3.83943	-1.48715
H	2.52478	-4.16235	-2.15659
H	1.22935	-4.73789	-1.0928
H	0.98303	-3.28653	-2.0742
C	3.15683	-3.88235	0.56285
H	2.55939	-4.70342	0.96744
H	3.99492	-4.31252	0.00655
H	3.56423	-3.31222	1.40523
C	2.36443	-1.0366	-2.0241
H	2.7391	-0.01524	-2.14398
H	2.6702	-1.62015	-2.90137
H	1.27522	-0.99416	-1.99667
C	4.46916	-1.6714	-0.81773
H	4.80847	-2.37134	-1.58893
H	4.84304	-0.6763	-1.08428
H	4.91868	-1.95672	0.13689
Co	-0.25827	0.25818	1.76051
H	-1.73418	-0.24783	4.10122
C	-0.68328	-2.61643	3.27192
H	-1.76668	-2.58108	3.39434
H	-0.44203	-3.21529	2.38788
H	-0.26503	-3.13762	4.14748
H	-0.22004	-0.52799	0.51114

Thermal correction to Energy=0.809687

Thermal correction to Enthalpy=0.810632

Thermal correction to Gibbs Free Energy=0.686444

Sum of electronic and zero-point Energies=-2478.564473

Sum of electronic and thermal Energies=-2478.520222

Sum of electronic and thermal Enthalpies=-2478.519278

Sum of electronic and thermal Free Energies=-2478.643465

SCF Done: E(RwB97XD) = -2480.30684622

TS4d'

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	-0.21927	3.34428	0.7243
C	-1.80429	4.31093	0.84498
C	-2.97587	3.75322	0.01468
C	0.97473	4.32063	1.73375
C	0.5623	5.22708	2.7216
H	-0.49101	5.40936	2.90763

C	1.50656	5.91853	3.48585
H	1.17137	6.6195	4.2449
C	2.86939	5.71467	3.27227
C	3.28909	4.81444	2.28878
H	4.34903	4.65687	2.1106
C	2.35028	4.12002	1.52748
H	2.69066	3.42842	0.76177
C	0.35835	3.57238	-1.00945
C	1.15292	2.57842	-1.60591
H	1.40932	1.68069	-1.05003
C	1.63975	2.74933	-2.90351
H	2.25758	1.97597	-3.35189
C	1.33496	3.9053	-3.62307
C	0.54769	4.89903	-3.03723
H	0.31152	5.80423	-3.58909
C	0.06633	4.73743	-1.73811
H	-0.53033	5.53133	-1.30004
C	-3.63867	2.50184	0.61335
H	-3.86388	2.66952	1.67331
P	-2.60293	0.95582	0.50101
H	1.71108	4.03484	-4.63378
H	3.6013	6.25542	3.86498
H	-1.60297	5.35143	0.56876
H	-2.08781	4.32414	1.90434
H	-2.66174	3.56193	-1.01847
H	-3.74069	4.5371	-0.04394
C	-2.78078	0.42788	-1.24654
C	-1.63435	0.09742	-1.9848
C	-4.03905	0.35302	-1.87004
C	-1.74107	-0.29454	-3.32074
H	-0.65766	0.15058	-1.51345
C	-4.14295	-0.03837	-3.20401
H	-4.94314	0.58524	-1.31411
C	-2.99369	-0.36104	-3.93141
H	-0.84601	-0.54461	-3.88297
H	-5.12006	-0.09336	-3.67508
H	-3.07727	-0.66459	-4.97095
C	-3.56896	-0.24852	1.50433
C	-4.0004	-1.48164	0.99248
C	-3.81728	0.04865	2.85669
C	-4.68055	-2.38709	1.81113
H	-3.81894	-1.73588	-0.04679
C	-4.50191	-0.85492	3.66908
H	-3.47968	0.9907	3.28339
C	-4.93544	-2.07631	3.14704
H	-5.01399	-3.33512	1.3988
H	-4.69522	-0.60588	4.70861
H	-5.4673	-2.7808	3.7796
H	-4.59706	2.31083	0.11911
H	1.04388	1.37764	1.07549
C	-0.12507	-0.99676	1.21334
C	-0.10739	-0.41877	2.47375
B	3.07803	-0.42191	1.6061
O	4.02759	-1.3593	1.89297
O	2.91389	-0.21774	0.25191
C	4.4455	-1.98917	0.64408
C	4.00725	-0.92	-0.43239
C	0.8483	0.61205	2.81958
H	0.72603	1.01026	4.93292
C	2.36219	0.38899	2.7615
H	2.63838	-0.09755	3.70986
H	2.8451	1.37729	2.79948
C	5.08183	0.13444	-0.72317
H	5.91877	-0.28958	-1.28663
H	4.64244	0.94058	-1.31955
H	5.47566	0.57152	0.19984
C	3.46927	-1.49877	-1.73849
H	3.16391	-0.68669	-2.40719
H	4.24322	-2.0793	-2.2523
H	2.60575	-2.14761	-1.57327
C	5.94731	-2.25736	0.71826
H	6.15058	-2.97711	1.51701
H	6.31365	-2.68455	-0.22188
H	6.51384	-1.34865	0.93314
C	3.67845	-3.31403	0.54804
H	3.97692	-3.89091	-0.33315
H	3.8944	-3.91249	1.43795
H	2.59619	-3.15271	0.5069
H	-0.97472	-0.56145	3.11781
H	0.75013	-1.01494	0.57248
C	0.44353	1.49608	3.98619
H	-0.63678	1.67721	4.01821
H	0.95858	2.46013	3.95065
Co	-0.38157	1.14993	1.22354
H	-0.95368	-1.64267	0.93939

Thermal correction to Energy=0.808086

Thermal correction to Enthalpy=0.809030

Thermal correction to Gibbs Free Energy=0.682960

Sum of electronic and zero-point Energies=-2478.544505

Sum of electronic and thermal Energies=-2478.500030

Sum of electronic and thermal Enthalpies=-2478.499086

Sum of electronic and thermal Free Energies=-2478.625157

SCF Done: E(RM06) = -2479.35468050

Int5d'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	-0.21023	3.31412	0.67068
C	-1.76421	4.31582	0.83069
C	-2.97574	3.76666	0.0516
C	1.0357	4.24834	1.65919
C	0.67661	5.23578	2.59061
H	-0.36016	5.50499	2.74724
C	1.65928	5.9004	3.33143
H	1.36601	6.66374	4.04505
C	3.00753	5.58817	3.1513
C	3.37427	4.61073	2.22654
H	4.41999	4.36872	2.07225
C	2.39708	3.9406	1.4879
H	2.69939	3.18326	0.77007
C	0.34291	3.5279	-1.07273
C	1.15297	2.5357	-1.65469
H	1.43262	1.65619	-1.07945
C	1.61892	2.68898	-2.96336
H	2.24974	1.91907	-3.39996
C	1.27831	3.81923	-3.70599
C	0.47884	4.81058	-3.13198
H	0.2152	5.69761	-3.70053
C	0.01746	4.66966	-1.82173
H	-0.59373	5.45695	-1.39718
C	-3.62918	2.52645	0.68656
H	-3.79737	2.70235	1.75451
P	-2.63277	0.96191	0.5111
H	1.64001	3.93386	-4.72204
H	3.76696	6.10824	3.72477
H	-1.55671	5.35068	0.52746
H	-2.00775	4.3504	1.89979
H	-2.71011	3.56839	-0.99232
H	-3.73376	4.56127	0.02242
C	-2.91529	0.47244	-1.23445
C	-1.81081	0.25302	-2.06958
C	-4.21256	0.33866	-1.76571
C	-1.99313	-0.09126	-3.4079
H	-0.80781	0.3614	-1.6681
C	-4.39194	-0.00658	-3.10455
H	-5.08182	0.48926	-1.13247
C	-3.28389	-0.22105	-3.92569
H	-1.13082	-0.25418	-4.04672
H	-5.39536	-0.10943	-3.5042
H	-3.42458	-0.48894	-4.96887
C	-3.58298	-0.24143	1.53342
C	-3.95779	-1.50415	1.04318
C	-3.87058	0.07284	2.87478
C	-4.61588	-2.41741	1.86965
H	-3.74996	-1.77155	0.01205
C	-4.53219	-0.83974	3.69545
H	-3.5802	1.0364	3.28912
C	-4.91052	-2.0895	3.1941
H	-4.90464	-3.38407	1.47248
H	-4.75747	-0.57652	4.72568
H	-5.42629	-2.79913	3.83319
H	-4.61499	2.35401	0.23839
H	1.06356	1.35739	1.23946
C	-0.10179	-1.01555	1.04568
C	-0.15271	-0.49599	2.33017
B	3.08394	-0.44018	1.6688
O	3.99717	-1.40538	1.97037
O	3.02428	-0.1449	0.32287
C	4.51137	-1.95618	0.72033
C	4.16789	-0.81349	-0.31724
C	0.77543	0.53703	2.75302
H	0.54305	0.90961	4.85941
C	2.29058	0.30744	2.81733
H	2.48251	-0.24029	3.75179
H	2.77316	1.28835	2.95161
C	5.26873	0.24602	-0.44712
H	6.14918	-0.15041	-0.96304
H	4.88609	1.09158	-1.02329
H	5.58789	0.61444	0.53575
C	3.73736	-1.29787	-1.69917
H	3.50431	-0.4385	-2.33608
H	4.54678	-1.85962	-2.18069
H	2.85272	-1.94051	-1.64885
C	5.99895	-2.24697	0.90043
H	6.12837	-3.02133	1.66321
H	6.44254	-2.6151	-0.03176

H	6.55012	-1.36088	1.22303
C	3.74417	-3.26385	0.47337
H	4.10765	-3.78258	-0.41804
H	3.88391	-3.9234	1.33463
H	2.67009	-3.08594	0.35785
H	-1.0316	-0.69389	2.94745
H	0.79927	-0.98167	0.44528
C	0.28715	1.39622	3.90634
H	-0.80027	1.53994	3.89011
H	0.7694	2.37819	3.90709
Co	-0.40844	1.11316	1.14161
H	-0.90003	-1.67131	0.70498

Thermal correction to Energy=0.812876

Thermal correction to Enthalpy=0.813820

Thermal correction to Gibbs Free Energy=0.687236

Sum of electronic and zero-point Energies=-2478.575750

Sum of electronic and thermal Energies=-2478.531008

Sum of electronic and thermal Enthalpies=-2478.530064

Sum of electronic and thermal Free Energies=-2478.656647

SCF Done: E(RwB97XD) = -2480.31672605

Int1a'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.0098	3.34043	0.80626
C	-1.68227	4.06686	1.06043
C	-2.81262	3.37255	0.28073
C	1.07469	4.45878	1.82796
C	2.22181	5.07262	1.30144
H	2.48868	4.9327	0.25963
C	3.02501	5.88358	2.10729
H	3.90718	6.35364	1.68199
C	2.69328	6.0962	3.4452
C	1.55299	5.48967	3.97771
H	1.28404	5.65541	5.01744
C	0.75228	4.67134	3.18077
H	-0.12209	4.1986	3.61604
C	0.45668	3.82179	-0.92388
C	1.53932	3.1983	-1.5658
H	2.07404	2.39844	-1.06608
C	1.94513	3.58931	-2.84223
H	2.79218	3.09785	-3.31278
C	1.26323	4.60795	-3.51046
C	0.1833	5.23503	-2.88855
H	-0.35271	6.0309	-3.39752
C	-0.21203	4.85172	-1.60551
H	-1.04447	5.37208	-1.14591
C	-3.19765	1.9849	0.81963
H	-3.36684	2.05199	1.89787
P	-1.93532	0.64512	0.53323
H	1.57274	4.91194	-4.50608
H	3.31629	6.7309	4.06861
H	-1.64607	5.13423	0.82078
H	-1.8772	3.99048	2.13348
H	-2.57594	3.31176	-0.78794
H	-3.70388	4.00799	0.35632
C	-1.95818	0.49086	-1.30676
C	-0.80948	0.73408	-2.06644
C	-3.1542	0.15626	-1.969
C	-0.84724	0.65423	-3.46115
H	0.11352	0.99392	-1.56461
C	-3.1917	0.07728	-3.35938
H	-4.0546	-0.05811	-1.40041
C	-2.03742	0.32716	-4.10886
H	0.05252	0.85347	-4.03596
H	-4.12072	-0.18204	-3.85896
H	-2.06959	0.26402	-5.19276
C	-2.83751	-0.88619	1.03779
C	-2.48014	-2.12054	0.46775
C	-3.87861	-0.86077	1.977
C	-3.13055	-3.29549	0.84344
H	-1.70676	-2.16621	-0.29332
C	-4.53359	-2.0375	2.3492
H	-4.2079	0.07677	2.40914
C	-4.1567	-3.25834	1.79025
H	-2.84173	-4.23841	0.3881
H	-5.34574	-1.99432	3.06949
H	-4.66647	-4.17263	2.0793
H	-4.13158	1.65516	0.35167
H	0.23848	1.59284	3.02062
C	1.99008	1.25837	2.47284
C	2.10167	0.67781	1.18067
B	-0.85858	1.26381	3.46154
O	-0.82279	0.24282	4.36815
O	-1.64703	2.31351	3.86193
C	-1.40263	0.71474	5.62293
C	-2.23156	1.99416	5.17627
C	1.38615	-0.51276	0.89402

H	2.18659	-2.10013	-0.27681
C	0.47392	-0.91765	1.91462
H	0.7724	-0.91372	2.95703
H	-0.23995	-1.70095	1.68147
C	-3.7211	1.73314	4.95941
H	-4.23236	1.55517	5.91055
H	-4.17769	2.61096	4.49086
H	-3.89188	0.86768	4.31609
C	-2.0543	3.22177	6.07071
H	-2.62154	4.06189	5.65743
H	-2.43677	3.02374	7.07777
H	-1.00838	3.52514	6.15456
C	-2.23398	-0.42399	6.21236
H	-1.57771	-1.26699	6.44874
H	-2.72561	-0.11031	7.13962
H	-2.99478	-0.77928	5.51392
C	-0.21901	1.02577	6.54805
H	-0.55434	1.34933	7.5384
H	0.38066	0.11915	6.67263
H	0.42924	1.80328	6.13149
H	2.68348	1.16393	0.40474
H	2.02363	0.61309	3.3525
C	1.53437	-1.23182	-0.42064
H	1.98397	-0.60119	-1.19361
H	0.57519	-1.60651	-0.79078
Co	0.05549	1.0772	1.54835
H	2.39576	2.25305	2.62927

Thermal correction to Energy=0.811261

Thermal correction to Enthalpy=0.812205

Thermal correction to Gibbs Free Energy=0.684813

Sum of electronic and zero-point Energies=-2478.566280

Sum of electronic and thermal Energies=-2478.520953

Sum of electronic and thermal Enthalpies=-2478.520009

Sum of electronic and thermal Free Energies=-2478.647401

SCF Done: E(RwB97XD) = -2480.30158458

TS2a’

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.07114	3.33109	0.83365
C	-1.63214	4.06978	1.02402
C	-2.79322	3.35496	0.31621
C	1.08415	4.53423	1.84133
C	1.85812	5.54815	1.24855
H	1.90875	5.64964	0.1724
C	2.57211	6.4531	2.03862
H	3.16342	7.22725	1.55813
C	2.52649	6.3684	3.4296
C	1.75224	5.37513	4.02989
H	1.69834	5.30731	5.11331
C	1.04116	4.4657	3.24631
H	0.42843	3.71794	3.73412
C	0.55821	3.75046	-0.90237
C	1.82407	3.37002	-1.38215
H	2.51581	2.84802	-0.73276
C	2.23366	3.69572	-2.67446
H	3.22163	3.4009	-3.0172
C	1.37904	4.40933	-3.51912
C	0.12589	4.80563	-3.0519
H	-0.54244	5.37273	-3.69323
C	-0.27831	4.48497	-1.7534
H	-1.25292	4.82335	-1.41639
C	-3.16457	1.98345	0.89966
H	-3.29805	2.07448	1.98081
P	-1.91762	0.63724	0.58381
H	1.69426	4.66487	-4.52648
H	3.08222	7.07324	4.04113
H	-1.58355	5.11633	0.7067
H	-1.80819	4.07105	2.10499
H	-2.60229	3.26034	-0.75816
H	-3.67888	3.99663	0.41139
C	-1.95115	0.51712	-1.26071
C	-0.83361	0.85984	-2.03002
C	-3.12793	0.11199	-1.91716
C	-0.88295	0.80491	-3.42577
H	0.07333	1.17749	-1.53574
C	-3.17746	0.05819	-3.30901
H	-4.00237	-0.18004	-1.34293
C	-2.05442	0.40566	-4.06625
H	-0.00762	1.0812	-4.00634
H	-4.09118	-0.25914	-3.80314
H	-2.09566	0.36189	-5.15079
C	-2.82258	-0.89219	1.08248
C	-2.56631	-2.10894	0.42935
C	-3.76911	-0.87394	2.11743
C	-3.22762	-3.2765	0.81073
H	-1.86684	-2.14631	-0.39968
C	-4.43603	-2.04189	2.49415

H	-4.00894	0.05164	2.6287
C	-4.16285	-3.24714	1.84659
H	-3.01738	-4.20699	0.29113
H	-5.17524	-2.00506	3.28922
H	-4.68146	-4.15536	2.13863
H	-4.11722	1.65008	0.47315
H	0.62768	1.45882	2.97447
C	2.03812	1.17772	2.43014
C	2.09511	0.57932	1.10836
B	-0.8193	1.24926	3.43182
O	-0.97476	0.17715	4.26811
O	-1.41723	2.38864	3.92178
C	-1.52264	0.64184	5.54299
C	-2.12275	2.06305	5.17029
C	1.3587	-0.59338	0.87189
H	2.05788	-2.23118	-0.2951
C	0.46377	-0.9534	1.9313
H	0.80715	-0.9614	2.96094
H	-0.28004	-1.71776	1.72986
C	-3.62002	2.04942	4.84739
H	-4.21765	1.87549	5.74729
H	-3.90965	3.02028	4.43273
H	-3.8735	1.27502	4.11884
C	-1.83356	3.17986	6.17465
H	-2.23896	4.12514	5.80041
H	-2.31274	2.96784	7.13644
H	-0.76354	3.31482	6.34736
C	-2.54348	-0.38866	6.02205
H	-2.03732	-1.33818	6.22021
H	-3.02114	-0.06122	6.95175
H	-3.31839	-0.57386	5.27504
C	-0.34021	0.69447	6.51969
H	-0.65838	0.99735	7.52208
H	0.10558	-0.30197	6.59122
H	0.43678	1.38659	6.18
H	2.6713	1.03805	0.31534
H	2.21759	0.51502	3.27842
C	1.4355	-1.33788	-0.43414
H	1.886	-0.73907	-1.23085
H	0.45403	-1.67999	-0.77055
Co	0.08196	1.03683	1.56212
H	2.49532	2.15519	2.54354

Thermal correction to Energy= 0.808847

Thermal correction to Enthalpy=0.809791

Thermal correction to Gibbs Free Energy=0.688183

Sum of electronic and zero-point Energies=-2478.539352

Sum of electronic and thermal Energies=-2478.495454

Sum of electronic and thermal Enthalpies=-2478.494510

Sum of electronic and thermal Free Energies=-2478.616118

SCF Done: E(RwB97XD) = -2480.28632548

Int3a'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.0098	3.34043	0.80626
C	-1.68227	4.06686	1.06043
C	-2.81262	3.37255	0.28073
C	1.07469	4.45878	1.82796
C	2.22181	5.07262	1.30144
H	2.48868	4.9327	0.25963
C	3.02501	5.88358	2.10729
H	3.90718	6.35364	1.68199
C	2.69328	6.0962	3.4452
C	1.55299	5.48967	3.97771
H	1.28404	5.65541	5.01744
C	0.75228	4.67134	3.18077
H	-0.12209	4.1986	3.61604
C	0.45668	3.82179	-0.92388
C	1.53932	3.1983	-1.5658
H	2.07404	2.39844	-1.06608
C	1.94513	3.58931	-2.84223
H	2.79218	3.09785	-3.31278
C	1.26323	4.60795	-3.51046
C	0.1833	5.23503	-2.88855
H	-0.35271	6.0309	-3.39752
C	-0.21203	4.85172	-1.60551
H	-1.04447	5.37208	-1.14591
C	-3.19765	1.9849	0.81963
H	-3.36684	2.05199	1.89787
P	-1.93532	0.64512	0.53323
H	1.57274	4.91194	-4.50608
H	3.31629	6.7309	4.06861
H	-1.64607	5.13423	0.82078
H	-1.8772	3.98358	2.13348
H	-2.57594	3.31176	-0.78794
H	-3.70388	4.00799	0.35632
C	-1.95818	0.49086	-1.30676
C	-0.80948	0.73408	-2.06644

C	-3.1542	0.15626	-1.969
C	-0.84724	0.65423	-3.46115
H	0.11352	0.99392	-1.56461
C	-3.1917	0.07728	-3.35938
H	-4.0546	-0.05811	-1.40041
C	-2.03742	0.32716	-4.10886
H	0.05252	0.85347	-4.03596
H	-4.12072	-0.18204	-3.85896
H	-2.06959	0.26402	-5.19276
C	-2.83751	-0.88619	1.03779
C	-2.48014	-2.12054	0.46775
C	-3.87861	-0.86077	1.977
C	-3.13055	-3.29549	0.84344
H	-1.70676	-2.16621	-0.29332
C	-4.53359	-2.0375	2.3492
H	-4.2079	0.07677	2.40914
C	-4.1567	-3.25834	1.79025
H	-2.84173	-4.23841	0.3881
H	-5.34574	-1.99432	3.06949
H	-4.66647	-4.17263	2.0793
H	-4.13158	1.65516	0.35167
H	0.88018	1.52384	2.91022
C	1.95558	1.27217	2.51424
C	2.08787	0.67091	1.16687
B	-0.88618	1.24311	3.42014
O	-0.81589	0.24972	4.36125
O	-1.64013	2.31351	3.86193
C	-1.40263	0.71474	5.62293
C	-2.22466	1.99416	5.17627
C	1.39995	-0.51276	0.89402
H	2.18659	-2.10703	-0.28371
C	0.47392	-0.91075	1.91462
H	0.7793	-0.91372	2.95703
H	-0.23995	-1.69405	1.68147
C	-3.7211	1.73314	4.95941
H	-4.23236	1.55517	5.91055
H	-4.17769	2.61096	4.49086
H	-3.89188	0.86768	4.31609
C	-2.0543	3.22177	6.07071
H	-2.62154	4.06189	5.65743
H	-2.43677	3.02374	7.07777
H	-1.00838	3.52514	6.15456
C	-2.23398	-0.42399	6.21236
H	-1.57771	-1.26699	6.44874
H	-2.72561	-0.11031	7.13962
H	-2.99478	-0.77928	5.51392
C	-0.21901	1.02577	6.54805
H	-0.55434	1.34933	7.5384
H	0.38066	0.11915	6.67263
H	0.42924	1.80328	6.13149
H	2.73178	1.14323	0.43234
H	2.19613	0.59239	3.3456
C	1.53437	-1.23182	-0.42064
H	1.98397	-0.60119	-1.19361
H	0.57519	-1.59961	-0.79078
Co	0.04859	1.0772	1.54835
H	2.44406	2.23925	2.62927

Thermal correction to Energy= 0.813478

Thermal correction to Enthalpy=0.814422

Thermal correction to Gibbs Free Energy=0.692196

Sum of electronic and zero-point Energies=-2478.554470

Sum of electronic and thermal Energies=-2478.509905

Sum of electronic and thermal Enthalpies=-2478.508960

Sum of electronic and thermal Free Energies=-2478.631187

SCF Done: E(RwB97XD) = -2480.29971940

TS4a'

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.20562	3.10884	0.8801
C	-1.34164	4.08661	1.25244
C	-2.6639	3.63088	0.61107
C	1.43074	4.04415	1.89787
C	2.19082	5.09175	1.35305
H	2.12011	5.33131	0.29755
C	3.04592	5.83755	2.16623
H	3.62937	6.64439	1.73192
C	3.15088	5.55067	3.52812
C	2.3998	4.50905	4.07577
H	2.48427	4.2751	5.13358
C	1.54597	3.75571	3.26755
H	0.98553	2.93283	3.69742
C	0.67957	3.54652	-0.84556
C	1.80345	2.91079	-1.40153
H	2.3509	2.17575	-0.818
C	2.23673	3.22427	-2.68881
H	3.11394	2.73106	-3.09818
C	1.54571	4.17305	-3.44777

C	0.42974	4.81122	-2.90658
H	-0.10889	5.5545	-3.48726
C	0.00137	4.50523	-1.61209
H	-0.86065	5.02798	-1.21236
C	-3.2166	2.2775	1.09303
H	-3.27979	2.25247	2.18602
P	-2.193	0.81749	0.57329
H	1.87983	4.41656	-4.45209
H	3.81707	6.1334	4.15779
H	-1.1416	5.13332	0.99546
H	-1.42753	4.05876	2.34573
H	-2.57922	3.62033	-0.48113
H	-3.4174	4.39255	0.8483
C	-2.22056	0.92037	-1.27074
C	-1.04222	0.87025	-2.02534
C	-3.45386	1.00591	-1.94281
C	-1.08757	0.91398	-3.42137
H	-0.08201	0.80568	-1.52784
C	-3.49818	1.05528	-3.33441
H	-4.38474	1.01355	-1.38271
C	-2.31404	1.00909	-4.0769
H	-0.16318	0.88005	-3.99034
H	-4.45707	1.12127	-3.84043
H	-2.35164	1.04262	-5.16191
C	-3.27052	-0.65344	0.84681
C	-2.94913	-1.84993	0.18563
C	-4.41091	-0.61645	1.66147
C	-3.74381	-2.98544	0.34276
H	-2.08987	-1.89477	-0.47816
C	-5.21138	-1.75047	1.80877
H	-4.68085	0.28929	2.19255
C	-4.87847	-2.93806	1.15518
H	-3.48246	-3.90182	-0.17863
H	-6.09778	-1.7032	2.43522
H	-5.50286	-3.81897	1.27232
H	-4.23185	2.1463	0.703
H	2.11081	0.39368	3.69756
C	2.7919	0.58599	2.86942
C	2.21083	0.26147	1.51636
B	-0.77373	0.4523	3.12571
O	-0.07068	0.9753	4.20596
O	-2.04551	0.06924	3.49303
C	-0.99209	1.10029	5.34145
C	-2.13247	0.08347	4.95352
C	1.25824	-0.70355	1.21001
H	1.70696	-2.31688	-0.11156
C	0.18936	-1.01931	2.15261
H	0.51604	-1.19489	3.18005
H	-0.53358	-1.76535	1.83045
C	-1.86997	-1.35221	5.42738
H	-1.98374	-1.44259	6.51222
H	-2.59209	-2.02129	4.95025
H	-0.86508	-1.69558	5.16191
C	-3.54546	0.50528	5.35011
H	-4.26196	-0.24505	5.00208
H	-3.63758	0.57726	6.43929
H	-3.82358	1.46918	4.91694
C	-0.2227	0.75733	6.61558
H	0.57027	1.49373	6.77959
H	-0.88704	0.78132	7.48661
H	0.23929	-0.23056	6.55979
C	-1.46768	2.55683	5.39536
H	-2.13001	2.72751	6.24967
H	-0.60503	3.22111	5.50209
H	-2.00441	2.84073	4.48429
H	2.8485	0.55747	0.68308
H	3.69434	-0.02742	3.01104
C	1.2264	-1.32997	-0.16609
H	1.78286	-0.73898	-0.90049
H	0.20942	-1.48966	-0.53615
Co	-0.06736	0.85656	1.36586
H	3.10571	1.63142	2.92462

Thermal correction to Energy=0.811893

Thermal correction to Enthalpy=0.812838

Thermal correction to Gibbs Free Energy=0.690835

Sum of electronic and zero-point Energies=-2478.556115

Sum of electronic and thermal Energies=-2478.511629

Sum of electronic and thermal Enthalpies=-2478.510685

Sum of electronic and thermal Free Energies=-2478.632687

SCF Done: E(RwB97XD) = -2480.30337260

Int5a'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.19614	3.12003	0.85569
C	-1.35027	4.09755	1.22139
C	-2.67194	3.6425	0.57951
C	1.41659	4.04496	1.89313

C	2.15131	5.1228	1.36838	C	-5.20811	-1.72773	1.83447
H	2.06881	5.38463	0.31921	H	-4.67763	0.3149	2.19452
C	2.9975	5.86193	2.19312	C	-4.87647	-2.92423	1.19154
H	3.56504	6.68917	1.77518	H	-3.4906	-3.89534	-0.14469
C	3.12265	5.54179	3.54699	H	-6.09032	-1.67886	2.4664
C	2.39291	4.47425	4.07431	H	-5.50031	-3.80396	1.31993
H	2.49286	4.21382	5.1255	H	-4.24682	2.16078	0.67889
C	1.54788	3.72394	3.25403	H	2.14164	0.40566	3.70612
H	1.00508	2.87915	3.66752	C	2.81668	0.5846	2.86787
C	0.69074	3.5637	-0.86127	C	2.22135	0.26009	1.52504
C	1.82869	2.93485	-1.40093	B	-0.7204	0.32245	3.15668
H	2.37499	2.20606	-0.80372	O	-0.03445	0.89578	4.22584
C	2.27259	3.24314	-2.68124	O	-2.01212	-0.00977	3.50749
H	3.1602	2.75845	-3.07815	C	-0.97465	1.07055	5.3419
C	1.58251	4.18324	-3.45678	C	-2.1255	0.05996	4.96543
C	0.45277	4.81052	-2.93183	C	1.2314	-0.66404	1.22735
H	-0.0844	5.54774	-3.52275	H	1.6069	-2.34066	-0.04642
C	0.01308	4.50946	-1.64075	C	0.16775	-0.97311	2.20762
H	-0.86065	5.02254	-1.254	H	0.56331	-1.23328	3.20127
C	-3.22832	2.29571	1.06919	H	-0.55346	-1.72327	1.88208
H	-3.29276	2.27867	2.1625	C	-1.89329	-1.36608	5.48828
P	-2.20032	0.83215	0.55946	H	-2.0234	-1.42292	6.57272
H	1.92503	4.42553	-4.45488	H	-2.62012	-2.03437	5.01855
H	3.78162	6.12154	4.18677	H	-0.88905	-1.7317	5.24328
H	-1.15126	5.1433	0.96332	C	-3.53615	0.51873	5.32605
H	-1.43867	4.07221	2.31444	H	-4.26291	-0.2292	4.99308
H	-2.58504	3.62466	-0.51212	H	-3.64502	0.62815	6.41168
H	-3.42431	4.40834	0.80689	H	-3.79409	1.47544	4.8605
C	-2.23416	0.92037	-1.28518	C	-0.22676	0.74766	6.63467
C	-1.05112	0.89244	-2.03617	H	0.57528	1.47396	6.7905
C	-3.46575	0.97216	-1.96092	H	-0.90176	0.81005	7.49818
C	-1.09398	0.931	-3.43226	H	0.21408	-0.24827	6.61288
H	-0.09294	0.85176	-1.53531	C	-1.42481	2.53754	5.35173
C	-3.50765	1.0127	-3.3525	H	-2.10311	2.73475	6.1887
H	-4.39632	0.96228	-1.40043	H	-0.5566	3.18862	5.4631
C	-2.32266	0.9916	-4.09141	H	-1.93842	2.80889	4.42401
H	-0.16883	0.91574	-4.00095	H	2.86117	0.53134	0.68147
H	-4.46798	1.0559	-3.85854	H	3.71329	-0.03566	3.00882
H	-2.35759	1.0204	-5.17643	C	1.18543	-1.32713	-0.13029
C	-3.2772	-0.6392	0.84669	H	1.79045	-0.78719	-0.86633
C	-2.95715	-1.84097	0.1962	H	0.16822	-1.43367	-0.52048
C	-4.41172	-0.59538	1.66919	Co	-0.06916	0.88964	1.3517
C	-3.74769	-2.97478	0.37144	H	3.14488	1.62884	2.91739
H	-2.10249	-1.89133	-0.47302	Thermal correction to Energy=0.813510			

Thermal correction to Enthalpy=0.814454

Thermal correction to Gibbs Free Energy=0.690832

Sum of electronic and zero-point Energies=-2478.572557

Sum of electronic and thermal Energies=-2478.527572

Sum of electronic and thermal Enthalpies=-2478.526628

Sum of electronic and thermal Free Energies=-2478.650250

SCF Done: E(RwB97XD) = -2480.32034019

Int3b'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.36757	2.76044	0.51328
C	-1.00571	3.4831	1.53099
C	-2.39858	2.9388	1.1733
C	1.89345	3.60944	1.10782
C	1.94542	4.32051	2.31354
H	1.06613	4.4197	2.94034
C	3.13385	4.92896	2.72804
H	3.15454	5.48393	3.66016
C	4.28412	4.82865	1.9458
C	4.24153	4.12291	0.73807
H	5.1289	4.05032	0.11845
C	3.05639	3.51797	0.32334
H	3.03526	2.99553	-0.62987
C	0.14557	3.46903	-1.17378
C	0.54269	2.70599	-2.28124
H	0.90334	1.69234	-2.13325
C	0.47412	3.23477	-3.57136
H	0.78827	2.63283	-4.41918
C	-0.00183	4.53118	-3.76872
C	-0.40233	5.30034	-2.67291
H	-0.76846	6.31198	-2.81956
C	-0.32411	4.77748	-1.3826
H	-0.61813	5.40174	-0.54409
C	-2.6524	1.48118	1.60506
H	-2.40408	1.36184	2.66578
P	-1.67602	0.17254	0.7174
H	-0.0589	4.94381	-4.77178
H	5.20638	5.30053	2.26778
H	-0.99084	4.57425	1.44196
H	-0.7813	3.24726	2.57751
H	-2.58924	3.06112	0.10149
H	-3.14044	3.56186	1.68831
C	-2.15497	0.30448	-1.05785
C	-1.28474	-0.19355	-2.0402
C	-3.4038	0.80808	-1.45762
C	-1.65126	-0.19287	-3.38505
H	-0.31886	-0.60001	-1.75324
C	-3.76365	0.82222	-2.80636
H	-4.11258	1.1805	-0.72196
C	-2.88996	0.31975	-3.77323
H	-0.96824	-0.59356	-4.13135
H	-4.73182	1.21585	-3.09929
H	-3.17418	0.32552	-4.81879
C	-2.4957	-1.39443	1.23612
C	-2.63235	-2.44857	0.31521
C	-2.99763	-1.5592	2.535
C	-3.25074	-3.64118	0.69214
H	-2.27092	-2.33974	-0.70034
C	-3.62381	-2.75001	2.90411
H	-2.8922	-0.77066	3.26958
C	-3.74888	-3.79245	1.9866
H	-3.35106	-4.44505	-0.0314
H	-4.01576	-2.8594	3.91138
H	-4.23649	-4.71832	2.2775
H	-3.71548	1.23696	1.50036
H	2.38625	0.71815	0.4202
C	1.48177	-1.24576	0.95675
B	0.67625	0.01725	2.69827
O	-0.3132	-0.4152	3.54337
O	1.81616	0.41551	3.3528
C	0.21537	-0.41564	4.91579
C	1.52402	0.47434	4.78643
C	1.30073	1.95379	5.1266
H	1.13201	2.09828	6.19865
H	2.19084	2.52198	4.83734
H	0.44614	2.3665	4.58267
C	2.73971	-0.05422	5.54034
H	3.59319	0.60938	5.36969
H	2.54695	-0.08266	6.61975
H	3.01815	-1.05614	5.20751
C	-0.87003	0.16342	5.82317
H	-1.74138	-0.50275	5.82052
H	-0.5183	0.2376	6.85866
H	-1.1961	1.15338	5.49997
C	0.48665	-1.87233	5.30073
H	0.83629	-1.94584	6.33642
H	-0.44347	-2.44404	5.21744

H	1.23249	-2.33041	4.64841
Co	0.52771	0.47102	0.83106
C	2.67754	-0.36019	0.62592
C	1.70151	-2.46775	1.79714
H	3.197	-0.65807	-0.29548
H	3.37471	-0.27446	1.45965
C	2.87843	-2.77048	2.37277
H	3.00021	-3.69972	2.9251
H	3.75553	-2.1366	2.30897
C	0.53425	-3.42112	1.89301
H	-0.32556	-2.95456	2.38444
H	0.19653	-3.73537	0.89298
H	0.80266	-4.32176	2.45246
H	0.95642	-1.56387	0.03572

Thermal correction to Energy=0.811661

Thermal correction to Enthalpy= 0.812605

Thermal correction to Gibbs Free Energy=0.687394

Sum of electronic and zero-point Energies=-2478.539855

Sum of electronic and thermal Energies=-2478.494624

Sum of electronic and thermal Enthalpies=-2478.493680

Sum of electronic and thermal Free Energies=-2478.618891

SCF Done: E(RwB97XD) = -2480.28272042

TS4b'

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.28615	2.86912	1.01611
C	-1.26328	3.10003	2.01594
C	-2.51919	2.47137	1.38472
C	1.50213	4.06746	1.70891
C	2.60406	4.43362	0.91811
H	2.71339	4.03287	-0.08647
C	3.5512	5.33932	1.39567
H	4.39545	5.61539	0.7704
C	3.40469	5.90003	2.66629
C	2.30695	5.5505	3.4543
H	2.1811	5.99128	4.43931
C	1.36372	4.63572	2.98262
H	0.52579	4.36901	3.61668
C	-0.11496	3.67303	-0.59647
C	0.10677	3.00974	-1.80993
H	0.47771	1.99126	-1.81093
C	-0.16148	3.64116	-3.02742
H	0.01225	3.1101	-3.9586
C	-0.65958	4.94298	-3.04229
C	-0.88371	5.61653	-1.83735
H	-1.26464	6.63374	-1.84403
C	-0.60843	4.99015	-0.62357
H	-0.76168	5.53842	0.30179
C	-2.55992	0.9326	1.33897
H	-2.39116	0.52775	2.34494
P	-1.31875	0.04544	0.26297
H	-0.86991	5.43577	-3.98712
H	4.13747	6.61124	3.03618
H	-1.43238	4.17301	2.15766
H	-1.07171	2.66846	3.00371
H	-2.67267	2.89262	0.38551
H	-3.37977	2.79685	1.98297
C	-1.89037	0.28525	-1.47368
C	-1.13272	-0.30148	-2.50269
C	-3.0548	0.98851	-1.81344
C	-1.5265	-0.18363	-3.83441
H	-0.23843	-0.86878	-2.26032
C	-3.4451	1.11249	-3.14973
H	-3.67354	1.44126	-1.04657
C	-2.68323	0.52965	-4.162
H	-0.93475	-0.65251	-4.61563
H	-4.34956	1.66181	-3.39468
H	-2.9909	0.62334	-5.19936
C	-1.76498	-1.71613	0.59141
C	-2.83481	-2.32327	-0.08786
C	-1.07289	-2.44776	1.56829
C	-3.20111	-3.63704	0.20593
H	-3.38032	-1.77835	-0.85178
C	-1.44449	-3.76236	1.85806
H	-0.24882	-1.99248	2.10542
C	-2.50626	-4.36017	1.17765
H	-4.02774	-4.09578	-0.32906
H	-0.89824	-4.32129	2.61311
H	-2.79004	-5.38469	1.40061
H	-3.56021	0.59358	1.04507
H	3.66644	-0.97742	2.33781
C	3.94121	0.03534	2.0402
C	2.91682	0.68564	1.09151
B	1.4028	0.5684	2.59079
O	1.30878	-0.67862	3.18293
O	1.41447	1.58175	3.51895
C	1.04628	-0.50727	4.61663

C	1.42408	1.01455	4.87014
C	2.55307	-0.07698	-0.10937
H	3.92683	0.19447	-1.71768
C	1.77872	-1.21403	0.05559
H	1.72796	-1.72919	1.00861
H	1.417	-1.76585	-0.80606
C	0.41479	1.79446	5.71597
H	0.35694	1.38351	6.72936
H	0.73794	2.8367	5.7989
H	-0.58905	1.78124	5.28484
C	2.82486	1.23728	5.45245
H	3.065	2.30333	5.39776
H	2.86693	0.9306	6.50262
H	3.59642	0.6886	4.90978
C	-0.43728	-0.82077	4.84485
H	-0.64727	-1.8459	4.52789
H	-0.70519	-0.73405	5.90242
H	-1.08667	-0.1527	4.27066
C	1.90369	-1.52227	5.37272
H	1.77093	-1.41404	6.45472
H	1.59849	-2.5367	5.09774
H	2.96542	-1.41575	5.14197
H	3.23626	1.70408	0.86615
H	4.89872	-0.01223	1.50622
C	2.88775	0.46103	-1.4781
H	2.82427	1.55321	-1.52107
H	2.25115	0.03435	-2.25993
Co	0.8581	0.68593	0.72368
H	4.09989	0.64177	2.93339

Thermal correction to Energy=0.811656

Thermal correction to Enthalpy=0.812600

Thermal correction to Gibbs Free Energy=0.689889

Sum of electronic and zero-point Energies=-2478.550328

Sum of electronic and thermal Energies=-2478.505815

Sum of electronic and thermal Enthalpies=-2478.504871

Sum of electronic and thermal Free Energies=-2478.627582

SCF Done: E(RwB97XD) = -2480.27567809

Int5b'

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.35597	2.76044	0.50748
C	-1.01151	3.4831	1.53099
C	-2.41018	2.9504	1.1733
C	1.88765	3.59784	1.10782
C	1.93962	4.31471	2.31354
H	1.06033	4.4139	2.94034
C	3.12805	4.92316	2.72224
H	3.14874	5.48393	3.65436
C	4.27832	4.82285	1.94
C	4.23573	4.11712	0.73807
H	5.1231	4.04452	0.11265
C	3.05059	3.51217	0.32334
H	3.02947	2.98973	-0.62987
C	0.13977	3.46903	-1.17378
C	0.53689	2.70599	-2.28124
H	0.89754	1.69234	-2.13325
C	0.47412	3.23477	-3.57136
H	0.78827	2.63283	-4.41918
C	-0.00183	4.53118	-3.76872
C	-0.40233	5.30034	-2.67291
H	-0.76846	6.31198	-2.82536
C	-0.32411	4.77748	-1.3826
H	-0.61813	5.40174	-0.54409
C	-2.6756	1.49858	1.59926
H	-2.43308	1.37344	2.65998
P	-1.69342	0.20154	0.7058
H	-0.0589	4.94381	-4.77178
H	5.20058	5.30053	2.26198
H	-0.99084	4.57425	1.44196
H	-0.7871	3.24726	2.57751
H	-2.60084	3.07851	0.10149
H	-3.14623	3.57926	1.68831
C	-2.17237	0.31608	-1.06365
C	-1.29634	-0.18775	-2.0402
C	-3.4212	0.81388	-1.46922
C	-1.65706	-0.19287	-3.39085
H	-0.32466	-0.58261	-1.74744
C	-3.77525	0.82222	-2.81796
H	-4.12998	1.1863	-0.73936
C	-2.89576	0.31975	-3.77903
H	-0.97404	-0.59356	-4.13135
H	-4.74342	1.21585	-3.11668
H	-3.17998	0.31972	-4.83039
C	-2.4899	-1.38283	1.23032
C	-2.62655	-2.43697	0.31521
C	-2.99183	-1.5476	2.535
C	-3.24494	-3.62958	0.69214

H	-2.27092	-2.32814	-0.70614
C	-3.61801	-2.73841	2.90411
H	-2.8864	-0.75906	3.26958
C	-3.74308	-3.78665	1.9866
H	-3.34526	-4.43345	-0.0314
H	-4.00996	-2.8478	3.91138
H	-4.23069	-4.71252	2.2775
H	-3.73868	1.26016	1.48876
H	2.40945	0.67175	0.3622
C	1.47017	-1.18196	1.16555
B	0.78065	-0.14515	2.66347
O	-0.2552	-0.4964	3.50277
O	1.86256	0.36911	3.347
C	0.22697	-0.43304	4.89259
C	1.52982	0.46274	4.76903
C	1.30073	1.94219	5.086
H	1.10881	2.09828	6.15225
H	2.19084	2.51038	4.80834
H	0.45194	2.3491	4.52467
C	2.73971	-0.04842	5.55774
H	3.59319	0.61518	5.38709
H	2.52955	-0.05946	6.63135
H	3.02395	-1.05614	5.24811
C	-0.88163	0.15762	5.76517
H	-1.74718	-0.50855	5.76253
H	-0.5415	0.2608	6.80066
H	-1.2077	1.14178	5.41296
C	0.49825	-1.87813	5.32973
H	0.83049	-1.92264	6.37122
H	-0.42607	-2.45564	5.24064
H	1.25569	-2.35361	4.70061
Co	0.49871	0.52322	0.81366
C	2.68334	-0.37179	0.67812
C	1.71891	-2.48515	1.87834
H	3.1506	-0.81467	-0.20848
H	3.41531	-0.22226	1.47125
C	2.91323	-2.81108	2.39597
H	3.06981	-3.78092	2.8613
H	3.77293	-2.1482	2.36697
C	0.55165	-3.44432	1.91621
H	-0.31396	-2.99516	2.41344
H	0.23713	-3.71797	0.90458
H	0.82006	-4.36236	2.44666
H	0.83462	-1.44207	0.29092

Thermal correction to Energy=0.812233
Thermal correction to Enthalpy=0.813178
Thermal correction to Gibbs Free Energy=0.682818
Sum of electronic and zero-point Energies=-2478.552558
Sum of electronic and thermal Energies=-2478.506962
Sum of electronic and thermal Enthalpies=-2478.506018
Sum of electronic and thermal Free Energies=-2478.636377
SCF Done: E(RwB97XD) = -2480.29036635

$TS'_{34\text{-ohm}}$
Number of imaginary frequencies=1
Charge = 1 Multiplicity = 1

P	-0.64894	3.40365	0.49191
C	-2.29085	3.63078	1.35335
C	-3.46537	2.7789	0.83819
C	0.4319	4.6207	1.37655
C	0.2049	4.97954	2.71591
H	-0.65403	4.60093	3.26006
C	1.0724	5.85374	3.37641
H	0.87334	6.12561	4.40909
C	2.18046	6.37952	2.71318
C	2.41625	6.02854	1.38221
H	3.2724	6.43757	0.85345
C	1.55279	5.15631	0.72022
H	1.75009	4.90768	-0.31745
C	-0.85913	4.17682	-1.16745
C	0.09049	3.90982	-2.16931
H	0.90502	3.21883	-1.97725
C	-0.00375	4.53097	-3.41679
H	0.74476	4.32469	-4.17693
C	-1.05215	5.41203	-3.68782
C	-2.00161	5.67926	-2.70028
H	-2.81877	6.36634	-2.90003
C	-1.90305	5.07342	-1.44662
H	-2.64725	5.31361	-0.69531
C	-3.40398	1.28912	1.22039
H	-3.15567	1.18751	2.28378
P	-2.16039	0.30486	0.23364
H	-1.12686	5.89064	-4.65993
H	2.85278	7.06022	3.22689
H	-2.55064	4.69447	1.32888
H	-2.11748	3.38379	2.40619
H	-3.58425	2.88837	-0.24574

H	-4.37976	3.19196	1.28167
C	-2.97597	0.27219	-1.419
C	-2.64876	1.22244	-2.39562
C	-4.00607	-0.64682	-1.68142
C	-3.34448	1.2632	-3.60585
H	-1.84539	1.92807	-2.22206
C	-4.6929	-0.6097	-2.89504
H	-4.27107	-1.39755	-0.94357
C	-4.36606	0.34696	-3.85885
H	-3.0801	2.00904	-4.35014
H	-5.48394	-1.32916	-3.08643
H	-4.90366	0.37529	-4.80234
C	-2.35165	-1.42236	0.84418
C	-1.58606	-2.42842	0.22613
C	-3.21454	-1.77307	1.89299
C	-1.68997	-3.75328	0.64839
H	-0.91724	-2.17	-0.59007
C	-3.30936	-3.10197	2.31749
H	-3.82437	-1.02368	2.38653
C	-2.54999	-4.09355	1.69712
H	-1.10106	-4.52241	0.15631
H	-3.98288	-3.35824	3.13039
H	-2.62833	-5.12585	2.02561
H	-4.3886	0.83437	1.06427
H	0.43666	-0.25377	0.80025
C	1.72468	1.59877	1.5208
B	0.71085	0.64384	-1.01829
O	0.2453	-0.36873	-1.8206
O	1.90458	1.16216	-1.4671
C	1.10703	-0.45657	-3.00852
C	2.41845	0.27055	-2.51725
C	3.42425	-0.66515	-1.83573
H	3.89835	-1.33918	-2.5561
H	4.20873	-0.06574	-1.36364
H	2.9464	-1.27379	-1.06092
C	3.12644	1.12112	-3.56821
H	3.98589	1.62577	-3.11582
H	3.49778	0.49442	-4.38661
H	2.46794	1.88329	-3.99089
C	1.27622	-1.93254	-3.36188
H	0.30879	-2.35359	-3.65308
H	1.96158	-2.05185	-4.2084
H	1.66153	-2.51382	-2.52099
C	0.38753	0.27327	-4.14664
H	0.95135	0.19712	-5.08197
H	-0.5957	-0.17949	-4.30015
H	0.237	1.33244	-3.91809
H	1.62445	2.41196	2.22982
Co	-0.08088	1.17873	0.68609
C	1.35366	0.27761	1.9148
C	0.43298	0.05251	3.06799
C	-0.23474	1.07837	3.63829
H	2.53137	1.71643	0.8067
H	-0.95468	0.89643	4.43153
H	-0.03134	2.11628	3.3998
C	0.24434	-1.37665	3.50612
H	-0.52834	-1.46614	4.27362
H	-0.03071	-2.02106	2.66354
H	1.1834	-1.76544	3.92153
H	2.00911	-0.55847	1.66584

Thermal correction to Energy=0.808198

Thermal correction to Enthalpy=0.809142

Thermal correction to Gibbs Free Energy=0.684356

Sum of electronic and zero-point Energies=-2478.523945

Sum of electronic and thermal Energies=-2478.479226

Sum of electronic and thermal Enthalpies=-2478.478282

Sum of electronic and thermal Free Energies=-2478.603068

SCF Done: E(RwB97XD) = -2480.26488368

$TS'_{21\text{-}ohm}=TS'_{41\text{-}ohm}$

Number of imaginary frequencies=1

Charge =1 Multiplicity = 1

P	0.34161	2.9313	0.78379
C	-1.23091	3.85028	1.20207
C	-2.47419	3.39618	0.42073
C	1.63751	3.96275	1.59797
C	1.37259	4.74951	2.72933
H	0.37176	4.80512	3.14601
C	2.39182	5.49209	3.33157
H	2.16804	6.10351	4.20105
C	3.68731	5.45331	2.81614
C	3.96153	4.67197	1.69046
H	4.96604	4.64372	1.27806
C	2.94593	3.93263	1.08564
H	3.1686	3.34338	0.20076
C	0.57747	3.38482	-0.9884
C	0.76346	2.41902	-1.98348
H	0.81063	1.37324	-1.71575

C	0.91558	2.80445	-3.31942
H	1.05136	2.0431	-4.08228
C	0.88761	4.15248	-3.67118
C	0.71558	5.12502	-2.68088
H	0.70426	6.17848	-2.94554
C	0.56435	4.74646	-1.3493
H	0.45515	5.51732	-0.59194
C	-3.05053	2.03608	0.84959
H	-3.20965	2.03651	1.93401
P	-1.97456	0.56733	0.48253
H	1.00479	4.44975	-4.70947
H	4.47816	6.03162	3.28463
H	-1.05646	4.91536	1.01735
H	-1.40928	3.73264	2.27694
H	-2.26601	3.40492	-0.65477
H	-3.25746	4.14672	0.58359
C	-2.03734	0.3881	-1.35668
C	-1.12544	-0.4735	-1.98613
C	-3.03717	0.99604	-2.13311
C	-1.21597	-0.72619	-3.35553
H	-0.32076	-0.92429	-1.41702
C	-3.11609	0.7528	-3.50519
H	-3.76813	1.65971	-1.68403
C	-2.20974	-0.11243	-4.11959
H	-0.50433	-1.39974	-3.82512
H	-3.89307	1.23586	-4.09069
H	-2.27837	-0.30641	-5.18612
C	-3.02985	-0.87072	0.98819
C	-2.5735	-2.16987	0.7037
C	-4.27564	-0.72203	1.61761
C	-3.33857	-3.2857	1.03976
H	-1.62168	-2.31519	0.20041
C	-5.04002	-1.8426	1.95697
H	-4.673	0.26174	1.84279
C	-4.57475	-3.12526	1.67124
H	-2.97081	-4.28041	0.80472
H	-6.00335	-1.70576	2.43985
H	-5.1712	-3.99414	1.93299
H	-4.03382	1.89183	0.39019
H	0.07486	2.41595	4.02872
C	-0.68604	0.43553	3.61433
B	1.61636	-0.27486	0.68627
O	1.81043	-0.27097	-0.67446
O	2.60519	-0.97808	1.33797
C	3.15573	-0.80263	-0.94782
C	3.43023	-1.66167	0.34116
C	2.90466	-3.09948	0.24627
H	3.50725	-3.703	-0.4397
H	2.95091	-3.56282	1.23653
H	1.86418	-3.12607	-0.09384
C	4.87672	-1.66136	0.82975
H	4.95438	-2.25051	1.74877
H	5.53841	-2.11467	0.08322
H	5.23368	-0.65188	1.0444
C	3.10342	-1.58413	-2.2577
H	2.86676	-0.90608	-3.08395
H	4.07447	-2.04433	-2.47111
H	2.34635	-2.3715	-2.23468
C	4.08749	0.40674	-1.08986
H	5.1022	0.09803	-1.36019
H	3.70806	1.06336	-1.87877
H	4.13976	0.98304	-0.16067
Co	0.10915	0.79074	1.64683
C	0.31539	1.41907	3.66621
C	1.57453	1.11464	3.06387
H	2.28606	1.92029	2.92816
H	2.03829	0.15349	3.25477
C	-0.28458	-0.82274	2.98408
H	0.34951	-0.75188	1.59043
H	0.6252	-1.29715	3.35338
H	-1.08491	-1.53244	2.79016
C	-2.04695	0.62291	4.2292
H	-2.31017	1.68222	4.32022
H	-2.82785	0.10328	3.66879
H	-2.04929	0.19897	5.24224

Thermal correction to Energy= 0.808772

Thermal correction to Enthalpy=0.809716

Thermal correction to Gibbs Free Energy=0.688855

Sum of electronic and zero-point Energies=-2478.528983

Sum of electronic and thermal Energies=-2478.485082

Sum of electronic and thermal Enthalpies=-2478.484138

Sum of electronic and thermal Free Energies=-2478.604999

SCF Done: E(RwB97XD) = -2480.27727617

$TS'_{21\text{-}obm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

C	-0.11917	-0.86633	-1.94118

B	-0.29084	0.24824	-0.55326	C	2.97078	4.99963	-0.56061
C	0.18931	-2.22898	-1.41379	H	2.48871	4.63061	-2.63193
O	-0.11144	1.59153	-0.70731	H	3.47852	5.04367	1.53459
O	-1.17151	-0.0829	0.45117	H	2.90354	6.0799	-0.65138
C	-1.10474	2.27169	0.14174	C	4.70577	0.05382	-1.47501
C	-1.48686	1.14467	1.18378	C	4.71435	-1.14397	-2.20752
H	0.59061	-2.9335	-2.14703	C	5.75759	0.96784	-1.65848
C	-1.52984	-0.60345	-2.45341	C	5.74747	-1.42457	-3.10497
C	-2.53465	-1.48145	-2.48241	H	3.9192	-1.87254	-2.07325
H	-0.54807	-2.68177	-0.75566	C	6.78923	0.6858	-2.55285
H	-2.4481	-2.4876	-2.08448	H	5.76543	1.9055	-1.11097
P	2.36393	-2.86842	0.53081	C	6.78526	-0.5088	-3.27894
C	1.10674	-3.805	1.49405	H	5.73773	-2.35633	-3.66291
C	1.39152	-5.10715	1.93982	H	7.59582	1.40097	-2.68643
C	-0.10044	-3.19754	1.8734	H	7.58844	-0.72207	-3.97836
C	0.48006	-5.7896	2.74557	C	-2.2608	2.67452	-0.78069
H	2.31825	-5.59573	1.65298	H	-2.74808	1.80379	-1.22799
C	-1.00637	-3.88532	2.68323	H	-3.0165	3.25109	-0.23813
H	-0.34354	-2.19877	1.52546	H	-1.86986	3.30162	-1.58792
C	-0.72004	-5.18023	3.11875	C	-2.96372	1.09753	1.57144
H	0.70778	-6.7979	3.07915	H	-3.13443	0.27459	2.27264
H	-1.94126	-3.40932	2.96529	H	-3.26459	2.0278	2.06564
H	-1.4301	-5.71478	3.74316	H	-3.60663	0.93932	0.70314
C	3.5468	-2.38733	1.89283	C	-0.61499	1.15261	2.44621
C	3.22962	-4.15837	-0.46003	H	-0.81244	0.24398	3.02368
C	4.61749	-4.36074	-0.39008	H	0.45149	1.1769	2.20158
C	2.47528	-4.95884	-1.3388	H	-0.84217	2.01464	3.08091
C	5.23402	-5.33515	-1.17855	C	-0.46098	3.51766	0.74181
H	5.23161	-3.77195	0.28074	H	0.44906	3.28467	1.29677
C	3.09376	-5.93144	-2.12333	H	-0.19457	4.21462	-0.05783
H	1.39735	-4.84535	-1.3897	H	-1.16284	4.0246	1.41339
C	4.4762	-6.1195	-2.0484	H	2.90492	-1.99731	2.69178
H	6.30778	-5.48203	-1.1053	H	3.97929	-3.31882	2.27691
H	2.49406	-6.5468	-2.78784	C	4.65906	-1.36932	1.58618
H	4.95729	-6.87808	-2.6588	H	5.26621	-1.68584	0.73119
P	3.34789	0.37339	-0.26589	H	5.04006	0.75447	1.44076
C	4.18176	0.07662	1.37291	H	3.4778	0.35687	2.16626
C	3.17014	2.20434	-0.33162	H	5.33767	-1.36539	2.44825
C	2.83246	2.80045	-1.55847	H	-1.67004	0.39005	-2.87747
C	3.39479	3.02923	0.7813	H	-3.49053	-1.20952	-2.92073
C	2.739	4.18576	-1.67305	C	0.86971	-0.45969	-3.06189
H	2.65574	2.18246	-2.43387	H	0.78015	0.60144	-3.31011
C	3.29415	4.41876	0.66535	H	1.93034	-0.64276	-2.81202
H	3.65906	2.60576	1.74442	H	0.66373	-1.05795	-3.95793

H	1.00427	-0.74183	0.59264
Co	1.6094	-1.15488	-0.6371

Thermal correction to Energy= 0.807124

Thermal correction to Enthalpy=0.808068

Thermal correction to Gibbs Free Energy=0.685927

Sum of electronic and zero-point Energies=-2478.498039

Sum of electronic and thermal Energies=-2478.453788

Sum of electronic and thermal Enthalpies=-2478.452844

Sum of electronic and thermal Free Energies=-2478.574985

SCF Done: E(RwB97XD) = -2480.24155590

$TS'_{34\text{-}obm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

C	0.21738	-0.89099	-1.95629
B	-0.04694	0.27155	-0.27895
C	0.16278	-2.2073	-1.33142
O	0.07273	1.62673	-0.29718
O	-1.14886	-0.18416	0.40289
C	-1.12622	2.19796	0.34398
C	-1.721	0.955	1.12691
H	0.636	-3.04136	-1.84665
C	-0.85738	-0.21452	-2.75879
C	-2.09648	-0.72244	-2.83651
H	-0.73386	-2.46847	-0.77777
H	-2.39209	-1.61427	-2.29427
P	2.43627	-2.82392	0.64451
C	1.26085	-3.69743	1.75564
C	1.65283	-4.8948	2.38102
C	-0.00187	-3.15698	2.03737
C	0.79515	-5.53573	3.27342
H	2.62117	-5.33653	2.16265
C	-0.85701	-3.80435	2.93305
H	-0.32031	-2.24029	1.55315
C	-0.46145	-4.99056	3.55148
H	1.10597	-6.46162	3.74874
H	-1.83594	-3.38173	3.14149
H	-1.12978	-5.49306	4.24482
C	3.81541	-2.41166	1.83653
C	3.09826	-4.15996	-0.43717
C	4.46184	-4.24767	-0.76262
C	2.20955	-5.09943	-0.99273
C	4.92469	-5.24881	-1.61888
H	5.17709	-3.54748	-0.34561
C	2.67561	-6.09623	-1.84973
H	1.15662	-5.07409	-0.72965
C	4.03362	-6.17197	-2.16765
H	5.98447	-5.3084	-1.84982
H	1.97751	-6.81983	-2.26063
H	4.39565	-6.95138	-2.83171
P	3.32202	0.4072	-0.23705
C	4.31601	0.08596	1.30386
C	3.14991	2.23684	-0.26395
C	2.87645	2.87621	-1.48448
C	3.2678	3.01463	0.89706
C	2.73665	4.26106	-1.54351
H	2.78654	2.29337	-2.39677
C	3.12369	4.40332	0.83595
H	3.47924	2.55511	1.85723
C	2.85973	5.02933	-0.38221
H	2.53707	4.74173	-2.49704
H	3.22664	4.99314	1.74235
H	2.75649	6.10958	-0.42926
C	4.52343	0.07807	-1.59555
C	4.34867	-1.03475	-2.43348
C	5.63566	0.91338	-1.80119
C	5.25996	-1.30737	-3.45684
H	3.50725	-1.70831	-2.28852
C	6.54698	0.6376	-2.81938
H	5.78229	1.78925	-1.17588
C	6.35939	-0.47101	-3.65041
H	5.10918	-2.17199	-4.09661
H	7.40161	1.29126	-2.96813
H	7.0683	-0.67936	-4.44647
C	-2.03157	2.71254	-0.77846
H	-2.34357	1.90823	-1.44933
H	-2.92774	3.19104	-0.37107
H	-1.48675	3.45897	-1.36436
C	-3.24216	0.82691	1.08057
H	-3.55056	-0.07717	1.61493
H	-3.71928	1.68412	1.56799
H	-3.61201	0.75723	0.05569
C	-1.22923	0.84607	2.57586
H	-1.54152	-0.11774	2.98939
H	-0.13792	0.90403	2.63862
H	-1.65267	1.63758	3.2019
C	-0.67779	3.36266	1.22303
H	0.06535	3.05793	1.9625

H	-0.22805	4.13929	0.59772
H	-1.53438	3.80072	1.74722
H	3.30446	-2.08331	2.74998
H	4.32291	-3.35031	2.08732
C	4.85255	-1.34997	1.4306
H	5.37151	-1.62962	0.50732
H	5.15504	0.79064	1.31064
H	3.68304	0.32481	2.16714
H	5.62221	-1.34314	2.21243
H	-2.85143	-0.25543	-3.46262
H	1.14071	-0.67001	0.8509
Co	1.56471	-1.07034	-0.46715
C	-0.41957	0.99332	-3.55293
H	0.34212	0.71235	-4.29343
H	-1.25998	1.43771	-4.09313
H	0.02015	1.75884	-2.90455
H	1.1733	-0.73381	-2.50356

Thermal correction to Energy= 0.806456

Thermal correction to Enthalpy= 0.807400

Thermal correction to Gibbs Free Energy=0.683093

Sum of electronic and zero-point Energies=-2478.501616

Sum of electronic and thermal Energies=-2478.456849

Sum of electronic and thermal Enthalpies=-2478.455905

Sum of electronic and thermal Free Energies=-2478.580212

SCF Done: E(RwB97XD) = -2480.24419235

$TS'_{41\text{-}obm}=TS'_{43\text{-}obm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.153	2.94126	0.78626
C	-1.39374	3.9029	1.1748
C	-2.65683	3.35737	0.49412
C	1.45911	3.96555	1.59744
C	1.20618	4.70623	2.76387
H	0.21617	4.72101	3.20971
C	2.21934	5.45878	3.36253
H	2.00209	6.03441	4.25774
C	3.49967	5.47792	2.80849
C	3.76302	4.74121	1.6513
H	4.75658	4.75504	1.21212
C	2.75395	3.98953	1.04879
H	2.97121	3.41467	0.15539
C	0.41221	3.30501	-0.99758
C	0.57117	2.2694	-1.92512
H	0.57246	1.24429	-1.58074
C	0.73703	2.5539	-3.2828
H	0.84969	1.73971	-3.99292
C	0.7547	3.87643	-3.72379
C	0.61264	4.91964	-2.80332
H	0.63687	5.95185	-3.14069
C	0.44449	4.63767	-1.44945
H	0.35768	5.45922	-0.74361
C	-3.16933	2.02426	1.06663
H	-3.21298	2.09171	2.16099
P	-2.16049	0.50968	0.68913
H	0.88504	4.09824	-4.77923
H	4.28615	6.06596	3.27238
H	-1.23689	4.94607	0.88104
H	-1.53153	3.89427	2.26229
H	-2.50012	3.2823	-0.58755
H	-3.45527	4.0963	0.63337
C	-2.30734	0.26292	-1.13424
C	-1.43551	-0.61732	-1.79246
C	-3.35169	0.84993	-1.8683
C	-1.6004	-0.90477	-3.14789
H	-0.62182	-1.08023	-1.24409
C	-3.50459	0.57469	-3.22804
H	-4.05962	1.5216	-1.39459
C	-2.63186	-0.30391	-3.87129
H	-0.92063	-1.59679	-3.63698
H	-4.31284	1.04375	-3.78154
H	-2.75776	-0.52112	-4.92795
C	-3.2259	-0.8642	1.32299
C	-2.89626	-2.18821	0.97938
C	-4.36863	-0.63759	2.1049
C	-3.69072	-3.2517	1.40061
H	-2.01673	-2.39294	0.37691
C	-5.16452	-1.70762	2.52583
H	-4.66139	0.36583	2.39133
C	-4.8293	-3.01405	2.17586
H	-3.42269	-4.26675	1.12245
H	-6.049	-1.51185	3.12509
H	-5.44936	-3.84359	2.50252
H	-4.1956	1.84802	0.72787
H	0.30752	-0.00035	0.30889
C	-0.30627	-0.88618	2.8475
C	-0.4075	0.31266	3.62614
B	2.10467	0.03781	1.09851

O	2.43262	-1.29776	1.12644
O	2.79047	0.73435	0.12833
C	3.26949	-1.58435	-0.03459
C	3.83384	-0.15399	-0.39648
C	0.61644	1.2339	3.3817
C	1.84583	0.80061	2.6292
H	2.32156	-0.02344	3.17641
H	2.52829	1.64624	2.54493
C	5.12285	0.19927	0.35644
H	5.97309	-0.38419	-0.01049
H	5.34749	1.25955	0.20586
H	5.02517	0.02265	1.43239
C	4.00713	0.12117	-1.88776
H	4.36806	1.14369	-2.03641
H	4.74508	-0.56161	-2.3231
H	3.06888	0.01436	-2.43603
C	4.32101	-2.61176	0.38108
H	3.82968	-3.55463	0.64116
H	5.01706	-2.81106	-0.4413
H	4.89419	-2.28071	1.24981
C	2.36377	-2.17901	-1.11967
H	2.94252	-2.49693	-1.99269
H	1.84931	-3.05517	-0.71312
H	1.60934	-1.45974	-1.45039
H	0.6425	-1.40971	2.77446
Co	-0.0756	0.71571	1.54347
H	-1.16781	-1.54329	2.80998
C	-1.59515	0.66864	4.47914
H	-1.4174	0.32971	5.50894
H	-1.76644	1.7505	4.51838
H	-2.50593	0.17094	4.13413
H	0.61141	2.22361	3.82618

Thermal correction to Energy=0.808927

Thermal correction to Enthalpy=0.809872

Thermal correction to Gibbs Free Energy=0.690630

Sum of electronic and zero-point Energies=-2478.544934

Sum of electronic and thermal Energies=-2478.501555

Sum of electronic and thermal Enthalpies=-2478.500610

Sum of electronic and thermal Free Energies=-2478.619852

SCF Done: E(RwB97XD) = -2480.29678535

ST-Z''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	-0.20734	1.18278	0.19125
P	-0.04398	0.50318	-2.90835
C	0.23302	2.56102	-0.99111
C	-0.2929	2.29768	-2.4096
H	1.32787	2.57311	-0.99968
H	-0.1134	3.53124	-0.61858
H	0.20596	2.95894	-3.12413
H	-1.3643	2.50186	-2.48608
C	-1.52528	0.12748	-3.9432
C	-1.42178	-0.37665	-5.24778
C	-2.80371	0.28208	-3.376
C	-2.5711	-0.70382	-5.97314
H	-0.44838	-0.50895	-5.70772
C	-3.94796	-0.03593	-4.10586
H	-2.912	0.64324	-2.35625
C	-3.83413	-0.53128	-5.4081
H	-2.47382	-1.09032	-6.98359
H	-4.92818	0.09836	-3.65699
H	-4.72544	-0.7828	-5.97535
C	1.3408	0.52853	-4.1235
C	1.41133	1.52164	-5.11662
C	2.31411	-0.48102	-4.11142
C	2.43635	1.50988	-6.06228
H	0.65521	2.29954	-5.17236
C	3.33342	-0.49978	-5.06691
H	2.27529	-1.25943	-3.35747
C	3.39972	0.49807	-6.04019
H	2.4765	2.2854	-6.82166
H	4.07098	-1.29734	-5.05205
H	4.192	0.48453	-6.78302
C	-1.86425	1.60917	0.88124
C	-2.20548	1.15771	2.16863
C	-2.81338	2.34613	0.1556
C	-3.46283	1.4292	2.70847
H	-1.47987	0.61169	2.76466
C	-4.07047	2.6199	0.69973
H	-2.57958	2.7338	-0.83001
C	-4.40072	2.15864	1.97428
H	-3.70463	1.0789	3.70785
H	-4.78695	3.20226	0.12734
H	-5.37748	2.37424	2.39704
C	0.88573	1.49018	1.644
C	0.94864	2.77444	2.21395

C	1.63739	0.45604	2.22034
C	1.75447	3.01726	3.32503
H	0.3576	3.58692	1.80091
C	2.43562	0.69872	3.34259
H	1.60148	-0.54127	1.79739
C	2.49758	1.97856	3.89413
H	1.79546	4.01485	3.75281
H	3.00426	-0.11528	3.7834
H	3.11653	2.16752	4.76649
C	0.27274	-2.61118	-2.06119
C	-1.04295	-2.39957	-1.62974
C	-1.33375	-2.15116	-0.25097
H	-3.2311	-2.82155	0.44451
C	-0.23794	-2.08448	0.63297
H	0.62237	-2.73945	0.52684
H	-0.42559	-1.74666	1.64814
H	-1.83939	-2.25565	-2.3548
H	1.00485	-3.13298	-1.45181
C	-2.74926	-1.87152	0.17651
H	-3.33749	-1.41754	-0.62672
H	-2.79217	-1.22333	1.05427
Co	0.07909	-0.77625	-1.00116
H	0.45816	-2.6459	-3.13013

Thermal correction to Energy=0.575998

Thermal correction to Enthalpy=0.576943

Thermal correction to Gibbs Free Energy=0.474927

Sum of electronic and zero-point Energies=-2027.604867

Sum of electronic and thermal Energies=-2027.571617

Sum of electronic and thermal Enthalpies=-2027.570673

Sum of electronic and thermal Free Energies=-2027.672688

SCF Done: E(RwB97XD) = -1987.71472961

Int1a''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.02777	2.24512	-0.42603
P	0.65891	-0.29923	-2.13023
C	1.2324	2.44627	-1.83358
C	0.90344	1.39355	-2.90194
H	2.24232	2.29805	-1.43718
H	1.177	3.45555	-2.25596
H	1.68142	1.34748	-3.67032
H	-0.03915	1.64736	-3.39738
C	-0.51276	-1.16202	-3.24414
C	-0.32893	-1.08946	-4.63956
C	-1.576	-1.91475	-2.72967
C	-1.20324	-1.7517	-5.49627
H	0.5007	-0.52868	-5.05783
C	-2.44702	-2.58328	-3.59564
H	-1.71933	-1.97266	-1.65613
C	-2.26353	-2.49976	-4.97632
H	-1.05685	-1.68786	-6.57036
H	-3.26684	-3.1654	-3.18584
H	-2.94355	-3.01856	-5.64517
C	2.25966	-1.16795	-2.40428
C	3.47788	-0.48886	-2.23168
C	2.28448	-2.52944	-2.74652
C	4.69104	-1.15517	-2.40304
H	3.49415	0.56416	-1.96611
C	3.50128	-3.19437	-2.91445
H	1.35622	-3.06973	-2.90395
C	4.70534	-2.51057	-2.74185
H	5.62459	-0.61472	-2.27795
H	3.5046	-4.24614	-3.18519
H	5.65065	-3.02825	-2.8774
C	-1.51707	2.92828	-1.16751
C	-2.44647	2.07798	-1.78582
C	-1.73235	4.31384	-1.20356
C	-3.56305	2.60657	-2.43692
H	-2.30129	1.00377	-1.75301
C	-2.85647	4.83806	-1.84673
H	-1.03222	4.99158	-0.72515
C	-3.77047	3.98657	-2.46755
H	-4.27168	1.93542	-2.9179
H	-3.01267	5.91289	-1.86265
H	-4.64469	4.39456	-2.96909
C	0.50357	3.49005	0.83092
C	-0.35941	3.68796	1.92697
C	1.69604	4.2236	0.75854
C	-0.02558	4.60361	2.92461
H	-1.2908	3.13252	1.98975
C	2.0245	5.13843	1.76494
H	2.37873	4.09875	-0.07546
C	1.16701	5.32764	2.8463
H	-0.69951	4.75434	3.76319
H	2.94924	5.70371	1.69356
H	1.42182	6.04031	3.62434
C	-0.03571	0.04913	2.14768

C	1.36802	-0.12163	1.65088
C	1.60655	-1.24647	0.85303
C	0.49182	-2.03163	0.42864
H	-0.28186	-2.3285	1.1295
H	0.66427	-2.7507	-0.36816
H	-0.31205	-0.79342	2.79689
H	-0.15422	0.99846	2.66855
H	-1.37271	-0.23197	-0.30913
B	-1.66128	-0.10457	1.35142
O	-2.45997	1.01622	1.50182
O	-2.34251	-1.26861	1.6634
C	-3.75217	0.59109	2.04816
C	-3.76626	-0.95097	1.70637
C	-4.8498	1.41403	1.37456
H	-5.84195	1.07627	1.7014
H	-4.74737	2.46698	1.65649
H	-4.79953	1.35068	0.28699
C	-3.72241	0.88451	3.55183
H	-3.53324	1.95128	3.70758
H	-4.67944	0.63726	4.02644
H	-2.93267	0.3207	4.06029
C	-4.34344	-1.26671	0.31919
H	-4.14755	-2.31869	0.08801
H	-5.42544	-1.10733	0.28721
H	-3.88176	-0.65615	-0.45937
C	-4.42616	-1.84012	2.75864
H	-5.48921	-1.59222	2.86341
H	-4.35623	-2.88991	2.44951
H	-3.94725	-1.74478	3.73531
Co	0.07688	-0.04843	0.02438
C	2.46843	0.77285	2.151
H	3.36714	0.67832	1.53475
H	2.16471	1.82254	2.1782
H	2.73816	0.485	3.17711
H	2.58662	-1.36923	0.3987

Thermal correction to Energy=0.781293

Thermal correction to Enthalpy=0.782237

Thermal correction to Gibbs Free Energy=0.659445

Sum of electronic and zero-point Energies=-2439.286308

Sum of electronic and thermal Energies=-2439.242611

Sum of electronic and thermal Enthalpies=-2439.241667

Sum of electronic and thermal Free Energies=-2439.364459

SCF Done: E(RwB97XD) = -2440.99056744

TS2a''

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.02891	2.24541	-0.4293
P	0.65913	-0.30058	-2.13541
C	1.23006	2.4477	-1.83989
C	0.89802	1.39403	-2.90652
H	2.24091	2.29957	-1.44589
H	1.17386	3.45661	-2.26302
H	1.67431	1.34673	-3.67655
H	-0.04553	1.64802	-3.40007
C	-0.51527	-1.16404	-3.24548
C	-0.33564	-1.0932	-4.63891
C	-1.57709	-1.91835	-2.72665
C	-1.21531	-1.75387	-5.49461
H	0.49277	-0.53045	-5.06042
C	-2.45094	-2.58521	-3.58903
H	-1.71696	-1.97715	-1.65256
C	-2.27416	-2.501	-4.97038
H	-1.07222	-1.68896	-6.56924
H	-3.26971	-3.16912	-3.17857
H	-2.95632	-3.01798	-5.63906
C	2.25931	-1.16746	-2.40749
C	3.47786	-0.48948	-2.23021
C	2.28351	-2.52823	-2.75265
C	4.69072	-1.15613	-2.40246
H	3.49208	0.56294	-1.96233
C	3.50001	-3.19349	-2.91893
H	1.35502	-3.06771	-2.91147
C	4.70438	-2.51077	-2.74428
H	5.62452	-0.61652	-2.27311
H	3.50283	-4.24468	-3.1919
H	5.64945	-3.02872	-2.87788
C	-1.51762	2.93005	-1.16568
C	-2.44685	2.08166	-1.78589
C	-1.73411	4.31802	-1.20132
C	-3.5644	2.6094	-2.43604
H	-2.30094	1.00755	-1.75323
C	-2.85667	4.84138	-1.84341
H	-1.03153	4.99372	-0.7235
C	-3.77303	3.98923	-2.46367
H	-4.27285	1.94029	-2.9165
H	-3.01381	5.91607	-1.85897
H	-4.64541	4.39914	-2.96442

C	0.50642	3.49074	0.82887
C	-0.35333	3.69208	1.92532
C	1.70225	4.2229	0.75583
C	-0.01809	4.60747	2.92271
H	-1.28531	3.13759	1.98862
C	2.03209	5.13746	1.75943
H	2.38178	4.09713	-0.0811
C	1.17524	5.33026	2.84373
H	-0.69145	4.759	3.76161
H	2.95738	5.7018	1.68764
H	1.43374	6.04275	3.62157
C	-0.06188	0.04578	2.17235
C	1.34684	-0.11305	1.64504
C	1.60181	-1.2421	0.86117
C	0.49523	-2.02529	0.41214
H	-0.29695	-2.31318	1.09609
H	0.68262	-2.7513	-0.37395
H	-0.27229	-0.7854	2.85887
H	-0.14763	0.99773	2.69624
H	-1.30513	-0.25423	-0.44047
B	-1.64125	-0.09436	1.47033
O	-2.44919	1.01969	1.54467
O	-2.33151	-1.26508	1.69597
C	-3.75812	0.58939	2.04788
C	-3.75794	-0.95221	1.70419
C	-4.84133	1.41139	1.35524
H	-5.83679	1.07177	1.66218
H	-4.74426	2.4642	1.63868
H	-4.76845	1.34937	0.2679
C	-3.75925	0.87833	3.55467
H	-3.57473	1.94515	3.71512
H	-4.72327	0.62934	4.00896
H	-2.97903	0.31495	4.0766
C	-4.30577	-1.26951	0.30659
H	-4.10471	-2.32087	0.07728
H	-5.38784	-1.11181	0.25761
H	-3.83178	-0.65444	-0.46405
C	-4.43425	-1.84622	2.742
H	-5.49791	-1.5995	2.83255
H	-4.35687	-2.89291	2.43167
H	-3.96969	-1.75189	3.72584
Co	0.09219	-0.04735	-0.00165
H	2.58998	-1.36663	0.42602
C	2.44251	0.77047	2.1738
H	3.35487	0.6672	1.57693
H	2.14989	1.82305	2.19238
H	2.68893	0.48296	3.20513

Thermal correction to Energy=0.778268

Thermal correction to Enthalpy=0.779213

Thermal correction to Gibbs Free Energy=0.661397

Sum of electronic and zero-point Energies=-2439.269504

Sum of electronic and thermal Energies=-2439.227115

Sum of electronic and thermal Enthalpies=-2439.226171

Sum of electronic and thermal Free Energies=-2439.343987

SCF Done: E(RwB97XD) = -2440.98368481

Int3a''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.02257	2.23992	-0.43123
P	0.66411	-0.30443	-2.14063
C	1.2272	2.44627	-1.83878
C	0.89824	1.39355	-2.90714
H	2.23712	2.29805	-1.44238
H	1.1718	3.45555	-2.26116
H	1.67622	1.34748	-3.67552
H	-0.04435	1.64736	-3.40258
C	-0.50756	-1.16722	-3.25454
C	-0.32373	-1.09466	-4.64476
C	-1.5708	-1.92515	-2.74007
C	-1.20324	-1.7517	-5.50667
H	0.5059	-0.52868	-5.06303
C	-2.44182	-2.58848	-3.60604
H	-1.71413	-1.98826	-1.66653
C	-2.26353	-2.49976	-4.98672
H	-1.05685	-1.68266	-6.58076
H	-3.26164	-3.1758	-3.20144
H	-2.94355	-3.01336	-5.66077
C	2.26486	-1.16795	-2.40948
C	3.48308	-0.48886	-2.23168
C	2.28967	-2.52944	-2.75172
C	4.69624	-1.15517	-2.40304
H	3.49415	0.56416	-1.96611
C	3.50648	-3.19437	-2.91445
H	1.36142	-3.06973	-2.90915
C	4.71054	-2.51057	-2.74185
H	5.62979	-0.61472	-2.27275
H	3.5098	-4.24614	-3.18519

H	5.65585	-3.02825	-2.8722
C	-1.52227	2.92828	-1.16751
C	-2.45167	2.08318	-1.79102
C	-1.73755	4.31904	-1.20356
C	-3.56825	2.61177	-2.44212
H	-2.30649	1.00897	-1.75821
C	-2.85647	4.84326	-1.84673
H	-1.03222	4.99158	-0.72515
C	-3.77567	3.99177	-2.46755
H	-4.27688	1.94582	-2.9231
H	-3.01267	5.91809	-1.86265
H	-4.64469	4.40496	-2.96909
C	0.49837	3.48485	0.83092
C	-0.35941	3.68796	1.92697
C	1.69604	4.2184	0.75854
C	-0.02558	4.60361	2.92461
H	-1.2908	3.13252	1.98975
C	2.0245	5.13323	1.75974
H	2.37353	4.09355	-0.08066
C	1.16701	5.32764	2.8463
H	-0.69951	4.75434	3.76319
H	2.94924	5.69851	1.68836
H	1.42702	6.04031	3.62434
C	-0.07211	0.03873	2.19968
C	1.33162	-0.11123	1.63008
C	1.59095	-1.24647	0.85823
C	0.48662	-2.02643	0.39744
H	-0.31826	-2.3025	1.0723
H	0.67987	-2.7611	-0.37856
H	-0.22885	-0.78302	2.91649
H	-0.12822	0.99326	2.72575
H	-1.24271	-0.28917	-0.60033
B	-1.63528	-0.08377	1.58022
O	-2.44437	1.02662	1.58502
O	-2.33211	-1.25821	1.731
C	-3.76777	0.59629	2.05856
C	-3.76106	-0.94577	1.71677
C	-4.8394	1.41923	1.35376
H	-5.83675	1.08147	1.6494
H	-4.74217	2.47218	1.63569
H	-4.75273	1.35588	0.26619
C	-3.78481	0.88451	3.56743
H	-3.60084	1.95128	3.72838
H	-4.75224	0.63726	4.01084
H	-3.01067	0.3207	4.09669
C	-4.29144	-1.26671	0.31399
H	-4.09035	-2.31869	0.08801
H	-5.37344	-1.10733	0.25601
H	-3.80896	-0.65095	-0.45417
C	-4.44696	-1.84012	2.74824
H	-5.51001	-1.59222	2.83221
H	-4.36663	-2.88471	2.43911
H	-3.98885	-1.74478	3.73531
Co	0.09768	-0.05363	-0.02762
C	2.43203	0.76245	2.1666
H	3.34634	0.65232	1.57115
H	2.14911	1.81734	2.1834
H	2.67576	0.4746	3.1979
H	2.58142	-1.37443	0.4299

Thermal correction to Energy=0.780108

Thermal correction to Enthalpy=0.781053

Thermal correction to Gibbs Free Energy=0.660487

Sum of electronic and zero-point Energies=-2439.285339

Sum of electronic and thermal Energies=-2439.242242

Sum of electronic and thermal Enthalpies=-2439.241298

Sum of electronic and thermal Free Energies=-2439.361863

SCF Done: E(RwB97XD) = -2440.99238319

TS4a''

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	-0.25757	2.2787	-0.5042
P	0.41581	-0.14954	-2.33446
C	1.06139	2.53088	-1.80047
C	0.79198	1.57543	-2.96737
H	2.02548	2.30438	-1.33221
H	1.08499	3.57252	-2.13888
H	1.62848	1.55518	-3.67352
H	-0.09385	1.89975	-3.52306
C	-0.66118	-0.8369	-3.66213
C	-0.19182	-0.87429	-4.98802
C	-1.96089	-1.28287	-3.38874
C	-1.01116	-1.34287	-6.01344
H	0.81868	-0.54969	-5.22059
C	-2.77881	-1.75741	-4.41783
H	-2.32731	-1.25961	-2.36732
C	-2.3065	-1.78583	-5.72987
H	-0.63744	-1.3673	-7.03303

H	-3.783	-2.10517	-4.19199	O	-1.76265	0.04007	1.41221
H	-2.94189	-2.15422	-6.5301	O	-2.15886	-0.73798	3.52924
C	1.98605	-1.09097	-2.55589	C	-3.25185	-0.05273	1.52959
C	3.23657	-0.47167	-2.3949	C	-3.41475	-0.9546	2.81768
C	1.94399	-2.47248	-2.80869	C	-3.84053	-0.6559	0.26145
C	4.4151	-1.21294	-2.49781	H	-4.91728	-0.80844	0.3969
H	3.30416	0.59431	-2.19635	H	-3.70368	0.02627	-0.58131
C	3.12364	-3.2124	-2.90513	H	-3.38501	-1.6152	0.01089
H	0.98961	-2.96997	-2.95624	C	-3.76338	1.37618	1.7195
C	4.36132	-2.58512	-2.75061	H	-3.4621	1.99079	0.8669
H	5.37454	-0.71628	-2.38416	H	-4.8561	1.39067	1.77508
H	3.07394	-4.2779	-3.11037	H	-3.37438	1.8286	2.63658
H	5.27872	-3.16066	-2.83109	C	-3.49436	-2.45808	2.52256
C	-1.70278	3.18521	-1.20436	H	-3.40886	-3.00557	3.46543
C	-2.63629	2.47738	-1.97909	H	-4.44768	-2.72642	2.05707
C	-1.86305	4.57149	-1.04268	H	-2.68468	-2.79207	1.866
C	-3.70353	3.14179	-2.58698	C	-4.56338	-0.54823	3.73986
H	-2.52483	1.40403	-2.10507	H	-5.52653	-0.63679	3.22558
C	-2.93466	5.23114	-1.64534	H	-4.58257	-1.21412	4.60756
H	-1.15585	5.1366	-0.44331	H	-4.45368	0.47485	4.10507
C	-3.85528	4.51917	-2.41854	Co	-0.37646	-0.00606	-0.24137
H	-4.4161	2.58282	-3.18699	H	2.12422	-1.1132	0.1626
H	-3.05017	6.30286	-1.51085	C	2.58574	0.5669	2.10901
H	-4.68824	5.03671	-2.88555	H	3.31538	0.42407	1.30599
C	0.27986	3.33114	0.90856	H	2.38744	1.63997	2.21524
C	-0.55014	3.42214	2.03977	H	3.04945	0.24011	3.05046
C	1.49183	4.04012	0.90745	H	-1.05236	-1.41439	-0.62257
C	-0.17894	4.19806	3.13738				
H	-1.49878	2.89763	2.0561				
C	1.86384	4.81476	2.01012				
H	2.15406	4.00711	0.04906				
C	1.03226	4.89469	3.1271				
H	-0.83733	4.26256	3.99919				
H	2.80335	5.3595	1.98893				
H	1.32195	5.49933	3.98143				
C	0.29646	-0.11458	2.99003				
C	1.3116	-0.2045	1.86686				
C	1.24698	-1.06995	0.80262				
C	0.13167	-1.92386	0.39614				
H	-0.54227	-2.28295	1.17173				
H	0.42073	-2.7225	-0.28368				
H	0.57292	-0.83185	3.77834				
H	0.39925	0.87032	3.47061				
B	-1.22567	-0.28745	2.65418				

Thermal correction to Energy= 0.778658

Thermal correction to Enthalpy=0.779602

Thermal correction to Gibbs Free Energy=0.659364

Sum of electronic and zero-point Energies=-2439.270934

Sum of electronic and thermal Energies=-2439.227952

Sum of electronic and thermal Enthalpies=-2439.227007

Sum of electronic and thermal Free Energies=-2439.347246

SCF Done: E(RwB97XD) = -2440.97802394

Int5a''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	-0.436	2.35336	-0.65577
P	0.56551	-0.12528	-2.24073
C	0.83597	2.65777	-2.01591
C	0.73143	1.55206	-3.07034
H	1.82931	2.662	-1.55372

H	0.67502	3.64506	-2.46166
H	1.59476	1.55377	-3.74348
H	-0.16052	1.69493	-3.68679
C	-0.4682	-1.06011	-3.44817
C	-0.00077	-1.3371	-4.74587
C	-1.78046	-1.4226	-3.11004
C	-0.82781	-1.96697	-5.67495
H	1.0119	-1.06722	-5.02995
C	-2.60665	-2.057	-4.04159
H	-2.16063	-1.20342	-2.11646
C	-2.13108	-2.33066	-5.32396
H	-0.45509	-2.17469	-6.67385
H	-3.61869	-2.33773	-3.76366
H	-2.77144	-2.82426	-6.04926
C	2.25016	-0.86396	-2.41677
C	3.38502	-0.06426	-2.2001
C	2.43119	-2.23604	-2.65855
C	4.66677	-0.61442	-2.25135
H	3.27973	0.99685	-1.99276
C	3.71453	-2.78515	-2.70603
H	1.57243	-2.87861	-2.82498
C	4.83482	-1.9769	-2.50628
H	5.53232	0.02296	-2.09439
H	3.83672	-3.84618	-2.90435
H	5.83175	-2.40567	-2.54726
C	-1.96195	3.21552	-1.26462
C	-2.68301	2.62752	-2.32119
C	-2.42554	4.42732	-0.72952
C	-3.8183	3.2473	-2.84199
H	-2.3692	1.67171	-2.73342
C	-3.57405	5.03794	-1.24256
H	-1.89002	4.90746	0.08315
C	-4.26928	4.45471	-2.30126
H	-4.35454	2.7845	-3.66585
H	-3.91825	5.9746	-0.81307
H	-5.15804	4.93325	-2.70213
C	0.21439	3.45459	0.67141
C	0.11413	3.06046	2.01581
C	0.8488	4.67208	0.37256
C	0.63504	3.86052	3.03377
H	-0.37732	2.12743	2.26372
C	1.37531	5.46873	1.3911
H	0.92888	5.01189	-0.65581
C	1.27022	5.06474	2.72316
H	0.54724	3.54363	4.06946
H	1.86516	6.40537	1.14095
H	1.67999	5.68476	3.51515
C	0.21323	-0.79847	2.90618
C	1.12116	-0.93504	1.69694
C	0.84095	-1.71649	0.62381
C	-0.34911	-2.61001	0.36243
H	-0.80996	-2.98192	1.28575
H	-0.05018	-3.47719	-0.23368
H	0.36394	-1.65402	3.58095
H	0.53736	0.07615	3.49101
B	-1.30829	-0.6054	2.59906
O	-1.72567	0.08073	1.44408
O	-2.3419	-1.00665	3.36801
C	-3.19936	0.33062	1.59778
C	-3.59871	-0.76746	2.65641
C	-3.88265	0.18242	0.24704
H	-4.96221	0.32811	0.36564
H	-3.513	0.94136	-0.44551
H	-3.72022	-0.80493	-0.19044
C	-3.35091	1.75768	2.12701
H	-2.92689	2.4681	1.4146
H	-4.40805	2.00801	2.25521
H	-2.85172	1.89014	3.0916
C	-4.01721	-2.10972	2.04335
H	-4.07207	-2.85557	2.84128
H	-5.00208	-2.04335	1.57046
H	-3.29895	-2.46542	1.2987
C	-4.64313	-0.3185	3.67668
H	-5.58672	-0.06633	3.18063
H	-4.83929	-1.13496	4.37763
H	-4.30861	0.54608	4.25322
Co	-0.3711	0.168	-0.19215
H	1.64726	-1.83571	-0.09373
C	2.47269	-0.27187	1.81752
H	3.08819	-0.42688	0.92695
H	2.37221	0.80677	1.98881
H	3.01317	-0.67951	2.6833
H	-1.1587	-2.0765	-0.19195

Thermal correction to Energy=0.783388

Thermal correction to Enthalpy=0.784332

Thermal correction to Gibbs Free Energy=0.662413

Sum of electronic and zero-point Energies=-2439.300784

Sum of electronic and thermal Energies=-2439.256863

Sum of electronic and thermal Enthalpies=-2439.255919

Sum of electronic and thermal Free Energies=-2439.377838

SCF Done: E(RwB97XD) = -2441.00812428

Int1b''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.02777	2.24512	-0.42603
P	0.65891	-0.29923	-2.13023
C	1.2324	2.44627	-1.83358
C	0.90344	1.39355	-2.90194
H	2.24232	2.29805	-1.43718
H	1.177	3.45555	-2.25596
H	1.68142	1.34748	-3.67032
H	-0.03915	1.64736	-3.39738
C	-0.51276	-1.16202	-3.24414
C	-0.32893	-1.08946	-4.63956
C	-1.576	-1.91475	-2.72967
C	-1.20324	-1.7517	-5.49627
H	0.5007	-0.52868	-5.05783
C	-2.44702	-2.58328	-3.59564
H	-1.71933	-1.97266	-1.65613
C	-2.26353	-2.49976	-4.97632
H	-1.05685	-1.68786	-6.57036
H	-3.26684	-3.1654	-3.18584
H	-2.94355	-3.01856	-5.64517
C	2.25966	-1.16795	-2.40428
C	3.47788	-0.48886	-2.23168
C	2.28448	-2.52944	-2.74652
C	4.69104	-1.15517	-2.40304
H	3.49415	0.56416	-1.96611
C	3.50128	-3.19437	-2.91445
H	1.35622	-3.06973	-2.90395
C	4.70534	-2.51057	-2.74185
H	5.62459	-0.61472	-2.27795
H	3.5046	-4.24614	-3.18519
H	5.65065	-3.02825	-2.8774
C	-1.51707	2.92828	-1.16751
C	-2.44647	2.07798	-1.78582
C	-1.73235	4.31384	-1.20356
C	-3.56305	2.60657	-2.43692
H	-2.30129	1.00377	-1.75301
C	-2.85647	4.83806	-1.84673
H	-1.03222	4.99158	-0.72515
C	-3.77047	3.98657	-2.46755
H	-4.27168	1.93542	-2.9179
H	-3.01267	5.91289	-1.86265
H	-4.64469	4.39456	-2.96909
C	0.50357	3.49005	0.83092
C	-0.35941	3.68796	1.92697
C	1.69604	4.2236	0.75854
C	-0.02558	4.60361	2.92461
H	-1.2908	3.13252	1.98975
C	2.0245	5.13843	1.76494
H	2.37873	4.09875	-0.07546
C	1.16701	5.32764	2.8463
H	-0.69951	4.75434	3.76319
H	2.94924	5.70371	1.69356
H	1.42182	6.04031	3.62434
C	-0.03571	0.04913	2.14768
C	1.36802	-0.12163	1.65088
C	1.60655	-1.24647	0.85303
C	0.49182	-2.03163	0.42864
H	-0.28186	-2.3285	1.1295
H	0.66427	-2.7507	-0.36816
H	-0.31205	-0.79342	2.79689
H	-0.15422	0.99846	2.66855
H	-1.37271	-0.23197	-0.30913
B	-1.66128	-0.10457	1.35142
O	-2.45997	1.01622	1.50182
O	-2.34251	-1.26861	1.6634
C	-3.75217	0.59109	2.04816
C	-3.76626	-0.95097	1.70637
C	-4.8498	1.41403	1.37456
H	-5.84195	1.07627	1.7014
H	-4.74737	2.46698	1.65649
H	-4.79953	1.35068	0.28699
C	-3.72241	0.88451	3.55183
H	-3.53324	1.95128	3.70758
H	-4.67944	0.63726	4.02644
H	-2.93267	0.3207	4.06029
C	-4.34344	-1.26671	0.31919
H	-4.14755	-2.31869	0.08801
H	-5.42544	-1.10733	0.28721
H	-3.88176	-0.65615	-0.45937
C	-4.42616	-1.84012	2.75864
H	-5.48921	-1.59222	2.86341
H	-4.35623	-2.88991	2.44951

H	-3.94725	-1.74478	3.73531
Co	0.07688	-0.04843	0.02438
C	2.46843	0.77285	2.151
H	3.36714	0.67832	1.53475
H	2.16471	1.82254	2.1782
H	2.73816	0.485	3.17711
H	2.58662	-1.36923	0.3987

Thermal correction to Energy=0.781293

Thermal correction to Enthalpy=0.782237

Thermal correction to Gibbs Free Energy=0.659445

Sum of electronic and zero-point Energies=-2439.286308

Sum of electronic and thermal Energies=-2439.242611

Sum of electronic and thermal Enthalpies=-2439.241667

Sum of electronic and thermal Free Energies=-2439.364459

SCF Done: E(RwB97XD) = -2440.99056744

TS2b''

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.02891	2.24541	-0.4293
P	0.65913	-0.30058	-2.13541
C	1.23006	2.4477	-1.83989
C	0.89802	1.39403	-2.90652
H	2.24091	2.29957	-1.44589
H	1.17386	3.45661	-2.26302
H	1.67431	1.34673	-3.67655
H	-0.04553	1.64802	-3.40007
C	-0.51527	-1.16404	-3.24548
C	-0.33564	-1.0932	-4.63891
C	-1.57709	-1.91835	-2.72665
C	-1.21531	-1.75387	-5.49461
H	0.49277	-0.53045	-5.06042
C	-2.45094	-2.58521	-3.58903
H	-1.71696	-1.97715	-1.65256
C	-2.27416	-2.501	-4.97038
H	-1.07222	-1.68896	-6.56924
H	-3.26971	-3.16912	-3.17857
H	-2.95632	-3.01798	-5.63906
C	2.25931	-1.16746	-2.40749
C	3.47786	-0.48948	-2.23021
C	2.28351	-2.52823	-2.75265
C	4.69072	-1.15613	-2.40246
H	3.49208	0.56294	-1.96233
C	3.50001	-3.19349	-2.91893
H	1.35502	-3.06771	-2.91147
C	4.70438	-2.51077	-2.74428
H	5.62452	-0.61652	-2.27311
H	3.50283	-4.24468	-3.1919
H	5.64945	-3.02872	-2.87788
C	-1.51762	2.93005	-1.16568
C	-2.44685	2.08166	-1.78589
C	-1.73411	4.31802	-1.20132
C	-3.5644	2.6094	-2.43604
H	-2.30094	1.00755	-1.75323
C	-2.85667	4.84138	-1.84341
H	-1.03153	4.99372	-0.7235
C	-3.77303	3.98923	-2.46367
H	-4.27285	1.94029	-2.9165
H	-3.01381	5.91607	-1.85897
H	-4.64541	4.39914	-2.96442
C	0.50642	3.49074	0.82887
C	-0.35333	3.69208	1.92532
C	1.70225	4.2229	0.75583
C	-0.01809	4.60747	2.92271
H	-1.28531	3.13759	1.98862
C	2.03209	5.13746	1.75943
H	2.38178	4.09713	-0.0811
C	1.17524	5.33026	2.84373
H	-0.69145	4.759	3.76161
H	2.95738	5.7018	1.68764
H	1.43374	6.04275	3.62157
C	-0.06188	0.04578	2.17235
C	1.34684	-0.11305	1.64504
C	1.60181	-1.2421	0.86117
C	0.49523	-2.02529	0.41214
H	-0.29695	-2.31318	1.09609
H	0.68262	-2.7513	-0.37395
H	-0.27229	-0.7854	2.85887
H	-0.14763	0.99773	2.69624
H	-1.30513	-0.25423	-0.44047
B	-1.64125	-0.09436	1.47033
O	-2.44919	1.01969	1.54467
O	-2.33151	-1.26508	1.69597
C	-3.75812	0.58939	2.04788
C	-3.75794	-0.95221	1.70419
C	-4.84133	1.41139	1.35524
H	-5.83679	1.07177	1.66218
H	-4.74426	2.4642	1.63868

H	-4.76845	1.34937	0.2679
C	-3.75925	0.87833	3.55467
H	-3.57473	1.94515	3.71512
H	-4.72327	0.62934	4.00896
H	-2.97903	0.31495	4.0766
C	-4.30577	-1.26951	0.30659
H	-4.10471	-2.32087	0.07728
H	-5.38784	-1.11181	0.25761
H	-3.83178	-0.65444	-0.46405
C	-4.43425	-1.84622	2.742
H	-5.49791	-1.5995	2.83255
H	-4.35687	-2.89291	2.43167
H	-3.96969	-1.75189	3.72584
Co	0.09219	-0.04735	-0.00165
H	2.58998	-1.36663	0.42602
C	2.44251	0.77047	2.1738
H	3.35487	0.6672	1.57693
H	2.14989	1.82305	2.19238
H	2.68893	0.48296	3.20513

Thermal correction to Energy=0.778268

Thermal correction to Enthalpy=0.779213

Thermal correction to Gibbs Free Energy=0.661397

Sum of electronic and zero-point Energies=-2439.269504

Sum of electronic and thermal Energies=-2439.227115

Sum of electronic and thermal Enthalpies=-2439.226171

Sum of electronic and thermal Free Energies=-2439.343987

SCF Done: E(RwB97XD) = -2440.98368481

Int3b''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.02254	2.23994	-0.43122
P	0.66407	-0.30436	-2.1407
C	1.2271	2.44635	-1.83881
C	0.89814	1.39364	-2.90717
H	2.23704	2.29814	-1.44244
H	1.17167	3.45564	-2.26116
H	1.6761	1.34761	-3.67558
H	-0.04448	1.64744	-3.40258
C	-0.50759	-1.16716	-3.25459
C	-0.32377	-1.09459	-4.64482
C	-1.57082	-1.92511	-2.74012
C	-1.20329	-1.75163	-5.50672
H	0.50584	-0.5286	-5.06309
C	-2.44185	-2.58843	-3.60609
H	-1.71414	-1.98823	-1.66658
C	-2.26357	-2.4997	-4.98677
H	-1.05692	-1.68258	-6.58082
H	-3.26165	-3.17577	-3.20148
H	-2.94359	-3.0133	-5.66082
C	2.26484	-1.16783	-2.4096
C	3.48305	-0.48871	-2.2318
C	2.28969	-2.52931	-2.75187
C	4.69623	-1.15499	-2.4032
H	3.4941	0.5643	-1.9662
C	3.50651	-3.19421	-2.91464
H	1.36144	-3.06962	-2.9093
C	4.71055	-2.51038	-2.74205
H	5.62976	-0.61452	-2.27291
H	3.50985	-4.24596	-3.1854
H	5.65587	-3.02803	-2.87242
C	-1.52235	2.92829	-1.16741
C	-2.45174	2.08319	-1.79094
C	-1.73767	4.31905	-1.20338
C	-3.56836	2.61179	-2.44198
H	-2.30653	1.00899	-1.7582
C	-2.85663	4.84326	-1.84649
H	-1.03235	4.99158	-0.72496
C	-3.77582	3.99178	-2.46733
H	-4.27697	1.94584	-2.92298
H	-3.01287	5.91809	-1.86235
H	-4.64487	4.40497	-2.96882
C	0.49836	3.48484	0.83095
C	-0.35939	3.68791	1.92704
C	1.69602	4.2184	0.75856
C	-0.02554	4.60353	2.92469
H	-1.29077	3.13245	1.98983
C	2.02451	5.1332	1.75978
H	2.37348	4.09359	-0.08067
C	1.16704	5.32758	2.84637
H	-0.69944	4.75423	3.7633
H	2.94924	5.6985	1.68838
H	1.42708	6.04023	3.62441
C	-0.07204	0.03867	2.19963
C	1.33168	-0.11125	1.63
C	1.59101	-1.24647	0.85811
C	0.48667	-2.02643	0.39732
H	-0.31819	-2.30253	1.0722

H	0.67991	-2.76107	-0.3787
H	-0.22875	-0.7831	2.91643
H	-0.12815	0.99318	2.72574
H	-1.24271	-0.28917	-0.60036
B	-1.63523	-0.08384	1.58021
O	-2.44433	1.02655	1.58509
O	-2.33203	-1.25829	1.73096
C	-3.7677	0.59617	2.05865
C	-3.76098	-0.94587	1.7168
C	-4.83938	1.41913	1.35393
H	-5.83671	1.08133	1.64958
H	-4.74216	2.47206	1.63592
H	-4.75274	1.35584	0.26636
C	-3.7847	0.88432	3.56753
H	-3.60073	1.95109	3.72853
H	-4.75211	0.63705	4.01097
H	-3.01054	0.3205	4.09674
C	-4.29141	-1.26676	0.31401
H	-4.09031	-2.31873	0.08798
H	-5.3734	-1.10739	0.25608
H	-3.80896	-0.65096	-0.45413
C	-4.44684	-1.84028	2.74825
H	-5.5099	-1.5924	2.83226
H	-4.36651	-2.88486	2.43907
H	-3.98871	-1.74497	3.73531
Co	0.09769	-0.05363	-0.02767
H	2.58146	-1.3744	0.42975
C	2.43208	0.76242	2.16651
H	3.34638	0.65234	1.57104
H	2.14915	1.81732	2.18336
H	2.67586	0.47455	3.1978

Thermal correction to Energy=0.780098

Thermal correction to Enthalpy=0.781042

Thermal correction to Gibbs Free Energy=0.660478

Sum of electronic and zero-point Energies=-2439.285342

Sum of electronic and thermal Energies=-2439.242241

Sum of electronic and thermal Enthalpies=-2439.241297

Sum of electronic and thermal Free Energies=-2439.361861

SCF Done: E(RwB97XD) = -2440.99238319

TS4b''

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	-0.32021	2.21405	-0.40341
P	0.88764	-0.2893	-1.81939
C	1.15565	2.49197	-1.51844
C	1.14855	1.39992	-2.59707
H	2.05204	2.42744	-0.89146
H	1.13529	3.4916	-1.96526
H	2.05936	1.41394	-3.20386
H	0.3047	1.55286	-3.2789
C	-0.11424	-1.21157	-3.05099
C	0.41387	-1.57893	-4.30018
C	-1.45372	-1.51116	-2.75916
C	-0.38796	-2.23214	-5.23559
H	1.45217	-1.3667	-4.53845
C	-2.25329	-2.16838	-3.69598
H	-1.87318	-1.23098	-1.7956
C	-1.72045	-2.52836	-4.93476
H	0.02832	-2.51314	-6.19861
H	-3.28758	-2.4002	-3.45838
H	-2.34054	-3.04046	-5.66471
C	2.53241	-1.10667	-1.86002
C	3.72042	-0.36089	-1.83235
C	2.60971	-2.50878	-1.89818
C	4.95973	-1.0031	-1.86848
H	3.69312	0.72385	-1.7907
C	3.84944	-3.148	-1.92811
H	1.70237	-3.10454	-1.93113
C	5.02716	-2.39692	-1.91964
H	5.87121	-0.41204	-1.86739
H	3.89398	-4.23241	-1.97128
H	5.99161	-2.8949	-1.95796
C	-1.71042	2.98325	-1.31846
C	-2.86696	2.23075	-1.57151
C	-1.63478	4.30168	-1.80353
C	-3.92926	2.78181	-2.2911
H	-2.93247	1.21082	-1.2046
C	-2.69679	4.85039	-2.52092
H	-0.75343	4.90802	-1.61209
C	-3.84493	4.09107	-2.76568
H	-4.81954	2.18892	-2.47986
H	-2.62942	5.87031	-2.8882
H	-4.67047	4.52113	-3.32526
C	-0.00848	3.24292	1.08266
C	-0.89355	4.24423	1.50882
C	1.13624	2.96549	1.85285
C	-0.62754	4.96928	2.67295

H	-1.78828	4.46458	0.93603
C	1.39993	3.69921	3.00867
H	1.81507	2.16719	1.56157
C	0.51946	4.70309	3.42115
H	-1.31914	5.74394	2.9913
H	2.29178	3.48548	3.59118
H	0.72531	5.27091	4.32378
C	0.6425	-0.95631	2.94687
C	0.0381	-1.53031	1.66763
C	-1.29731	-1.18589	1.30361
C	-1.8527	0.1002	1.4612
H	-1.51878	0.78163	2.23794
H	-2.86325	0.27417	1.10413
H	0.25149	0.0504	3.13802
H	0.25567	-1.57493	3.77153
B	2.21458	-0.88851	3.10899
O	3.09782	-0.55121	2.11417
O	2.80994	-1.1112	4.31726
C	4.45108	-0.75502	2.65046
C	4.20606	-0.69507	4.20927
C	5.35991	0.33604	2.09112
H	6.36815	0.25398	2.51184
H	5.43746	0.22624	1.00492
H	4.97728	1.33653	2.30654
C	4.91238	-2.13243	2.16051
H	4.87347	-2.15765	1.06775
H	5.9403	-2.34228	2.47293
H	4.26827	-2.93008	2.54452
C	4.28281	0.72218	4.79118
H	3.9049	0.7057	5.81764
H	5.31114	1.09679	4.80985
H	3.6684	1.42387	4.21684
C	5.05915	-1.65029	5.04096
H	6.12309	-1.40593	4.94683
H	4.78496	-1.56022	6.09653
H	4.91233	-2.69081	4.74374
Co	-0.29679	0.03188	0.04529
H	-1.83524	-1.90004	0.67746
C	0.55113	-2.90035	1.27789
H	0.02494	-3.30427	0.40776
H	1.62157	-2.87278	1.05525
H	0.40677	-3.59655	2.11573
H	0.98725	-0.39156	0.67968

Thermal correction to Energy=0.777242

Thermal correction to Enthalpy=0.778186

Thermal correction to Gibbs Free Energy=0.654304

Sum of electronic and zero-point Energies=-2439.265471

Sum of electronic and thermal Energies=-2439.221869

Sum of electronic and thermal Enthalpies=-2439.220925

Sum of electronic and thermal Free Energies=-2439.344807

SCF Done: E(RwB97XD) = -2440.96896623

Int5b''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.52641	2.68601	-0.66478
P	0.67224	0.08103	-2.35277
C	1.4206	2.78811	-2.30694
C	0.85307	1.71673	-3.24945
H	2.48518	2.61527	-2.11557
H	1.32325	3.78703	-2.73848
H	1.46554	1.60306	-4.15083
H	-0.1549	1.99458	-3.57177
C	-0.64001	-0.80972	-3.27053
C	-0.42663	-1.25505	-4.59174
C	-1.89526	-0.99673	-2.67715
C	-1.45708	-1.87494	-5.29671
H	0.54444	-1.12818	-5.05673
C	-2.92343	-1.61822	-3.38939
H	-2.06624	-0.66044	-1.65807
C	-2.70619	-2.05643	-4.69636
H	-1.28524	-2.21724	-6.31306
H	-3.89248	-1.76305	-2.92128
H	-3.5069	-2.54141	-5.24727
C	2.22173	-0.84216	-2.70416
C	3.43511	-0.18134	-2.95427
C	2.21709	-2.24754	-2.65007
C	4.61314	-0.90682	-3.14517
H	3.47503	0.90153	-3.01659
C	3.39458	-2.96883	-2.84407
H	1.28667	-2.78337	-2.48609
C	4.5969	-2.30066	-3.0879
H	5.54132	-0.37936	-3.34555
H	3.37045	-4.05426	-2.81152
H	5.51314	-2.86363	-3.23886
C	-1.07583	3.51375	-1.0173
C	-2.28587	2.84175	-0.79401
C	-1.0954	4.81555	-1.55179

C	-3.49613	3.46562	-1.11335
H	-2.28514	1.84599	-0.372
C	-2.30513	5.43279	-1.86343
H	-0.16713	5.35784	-1.71047
C	-3.51104	4.75439	-1.6463
H	-4.43153	2.94128	-0.93935
H	-2.30755	6.43902	-2.2722
H	-4.45333	5.23673	-1.88962
C	1.44533	3.84308	0.43397
C	0.76314	4.73227	1.2797
C	2.8484	3.78679	0.49319
C	1.47265	5.55726	2.15444
H	-0.32026	4.79156	1.24962
C	3.55333	4.61756	1.36389
H	3.40293	3.09448	-0.1346
C	2.86697	5.50432	2.19658
H	0.93324	6.2454	2.79887
H	4.63809	4.57079	1.39206
H	3.41663	6.15025	2.87481
C	-0.85824	0.23432	2.86511
C	0.42288	0.30876	2.02633
C	0.93963	-0.8254	1.28386
C	0.18447	-1.55144	0.3786
H	-0.90031	-1.56421	0.40776
H	0.66787	-2.31817	-0.21901
H	-0.57336	-0.18987	3.83865
H	-1.1658	1.26864	3.08458
H	-0.33445	1.29153	1.05191
B	-2.16936	-0.52035	2.41222
O	-2.8456	-0.38308	1.21082
O	-2.81928	-1.32732	3.29614
C	-4.19135	-0.93818	1.41441
C	-3.9661	-1.92707	2.622
C	-4.65434	-1.59469	0.11726
H	-5.63154	-2.07058	0.25418
H	-4.76131	-0.83485	-0.66452
H	-3.94869	-2.35205	-0.23226
C	-5.10049	0.24725	1.75999
H	-5.05474	0.98338	0.9509
H	-6.14227	-0.067	1.87656
H	-4.784	0.73965	2.68466
C	-3.53579	-3.33625	2.19487
H	-3.20355	-3.88768	3.07931
H	-4.36269	-3.88896	1.73768
H	-2.70278	-3.30815	1.48447
C	-5.12147	-2.01053	3.61788
H	-6.02527	-2.39856	3.1349
H	-4.85465	-2.6928	4.43065
H	-5.35078	-1.03777	4.05837
H	2.02262	-0.97723	1.29286
C	1.48397	1.16441	2.69649
H	2.4229	1.19445	2.13105
H	1.13679	2.19206	2.84323
H	1.70002	0.75041	3.6957
Co	0.39411	0.53357	-0.10903

Thermal correction to Energy=0.782451

Thermal correction to Enthalpy=0.783395

Thermal correction to Gibbs Free Energy=0.658776

Sum of electronic and zero-point Energies=-2439.291806

Sum of electronic and thermal Energies=-2439.248172

Sum of electronic and thermal Enthalpies=-2439.247228

Sum of electronic and thermal Free Energies=-2439.371848

SCF Done: E(RwB97XD) = -2440.99524003

Int1c''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.04634	1.26434	0.13805
P	0.05019	0.65877	-2.9895
C	0.29664	2.69434	-1.03363
C	-0.27727	2.42063	-2.431
H	1.38295	2.81211	-1.09503
H	-0.12201	3.61764	-0.62003
H	0.15186	3.12267	-3.15129
H	-1.36013	2.56612	-2.45634
C	-1.48352	0.20166	-3.91645
C	-1.44986	-0.25917	-5.24086
C	-2.72053	0.24719	-3.2479
C	-2.62783	-0.64845	-5.88555
H	-0.50973	-0.30905	-5.77918
C	-3.89467	-0.13049	-3.89744
H	-2.77148	0.56557	-2.21008
C	-3.8512	-0.58041	-5.22031
H	-2.58397	-1.00023	-6.91231
H	-4.84297	-0.07857	-3.36976
H	-4.76527	-0.87876	-5.7252
C	1.31085	0.81914	-4.3265

C	1.19623	1.83736	-5.29012
C	2.36391	-0.09826	-4.44358
C	2.1197	1.94138	-6.32975
H	0.37261	2.54444	-5.24953
C	3.28262	-0.00099	-5.49113
H	2.48024	-0.88875	-3.71231
C	3.16589	1.02143	-6.4328
H	2.01676	2.73608	-7.06292
H	4.09	-0.72378	-5.56806
H	3.88237	1.09992	-7.24524
C	-1.64202	1.48052	0.86635
C	-1.89614	0.98972	2.15945
C	-2.68645	2.11565	0.17577
C	-3.16094	1.11628	2.73476
H	-1.09915	0.52737	2.73367
C	-3.95046	2.24684	0.75571
H	-2.52519	2.53642	-0.81015
C	-4.19374	1.74159	2.03304
H	-3.33442	0.73541	3.73714
H	-4.74068	2.75346	0.20891
H	-5.17624	1.84529	2.48385
C	1.08584	1.69086	1.59998
C	1.11759	3.01844	2.06374
C	1.77609	0.70526	2.32024
C	1.83894	3.35243	3.20884
H	0.57146	3.79875	1.54254
C	2.4839	1.04081	3.47855
H	1.78406	-0.31956	1.97135
C	2.521	2.36286	3.92213
H	1.86034	4.38368	3.54911
H	3.00698	0.26467	4.03007
H	3.07402	2.62256	4.82014
H	1.82008	-1.15322	-1.52695
C	0.75429	-2.47306	-2.03939
C	-0.62124	-2.28021	-1.70086
B	2.50707	-0.28734	-0.82093
O	3.34346	-1.01677	-0.02283
O	3.10367	0.80866	-1.38159
C	4.71166	-0.53302	-0.234
C	4.48792	0.89618	-0.8878
C	-0.97859	-2.06412	-0.35156
H	-2.76072	-2.91132	0.44103
C	0.12774	-1.87442	0.54094
H	0.98673	-2.54097	0.51095
H	-0.11147	-1.52962	1.54347
C	4.544	2.0583	0.10845
H	5.56461	2.21046	0.47417
H	4.22964	2.97715	-0.39717
H	3.88846	1.8999	0.96669
C	5.38567	1.20767	-2.08516
H	5.12771	2.19184	-2.48805
H	6.43867	1.23316	-1.78392
H	5.26933	0.47679	-2.88755
C	5.43027	-0.52532	1.11143
H	5.48801	-1.54692	1.49992
H	6.45353	-0.1495	1.00273
H	4.91035	0.0906	1.84778
C	5.37677	-1.5484	-1.17399
H	6.423	-1.29199	-1.36739
H	5.34887	-2.53737	-0.70669
H	4.85534	-1.61429	-2.13433
H	-1.3755	-2.21155	-2.48116
H	1.37024	-3.12348	-1.41972
C	-2.41865	-1.94119	0.0614
H	-3.06237	-1.66664	-0.77967
H	-2.55032	-1.21176	0.86301
Co	0.44019	-0.59669	-1.05259
H	1.0077	-2.50301	-3.09637

Thermal correction to Energy=0.780658

Thermal correction to Enthalpy=0.781603

Thermal correction to Gibbs Free Energy=0.658106

Sum of electronic and zero-point Energies=-2439.282120

Sum of electronic and thermal Energies=-2439.238046

Sum of electronic and thermal Enthalpies=-2439.237102

Sum of electronic and thermal Free Energies=-2439.360599

SCF Done: E(RwB97XD) = -2440.98383316

TS2c''

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.02585	1.22429	0.15624
P	0.07171	0.65222	-2.98601
C	0.2474	2.66464	-1.01372
C	-0.3131	2.3928	-2.41496
H	1.32958	2.81237	-1.06806
H	-0.20328	3.56831	-0.5916
H	0.08869	3.12397	-3.12141

H	-1.40025	2.50142	-2.44121
C	-1.38742	0.19001	-4.02388
C	-1.2623	-0.18567	-5.36998
C	-2.66538	0.17123	-3.43564
C	-2.389	-0.55468	-6.11066
H	-0.29064	-0.18473	-5.85105
C	-3.78867	-0.18509	-4.17982
H	-2.78615	0.4228	-2.38566
C	-3.65283	-0.55021	-5.52233
H	-2.27296	-0.84068	-7.15208
H	-4.76877	-0.18389	-3.71112
H	-4.52682	-0.83257	-6.10181
C	1.41497	0.81863	-4.23929
C	1.45225	1.91992	-5.11178
C	2.36398	-0.20019	-4.40882
C	2.42392	2.00771	-6.10912
H	0.71277	2.71143	-5.03964
C	3.32732	-0.11963	-5.41622
H	2.36205	-1.06315	-3.75231
C	3.36463	0.98805	-6.26422
H	2.43838	2.86996	-6.76942
H	4.0499	-0.92218	-5.53453
H	4.11749	1.05406	-7.04419
C	-1.66063	1.44089	0.89636
C	-1.85891	1.20327	2.26767
C	-2.7655	1.8333	0.12291
C	-3.123	1.34657	2.84223
H	-1.02326	0.9183	2.89814
C	-4.0276	1.98399	0.70011
H	-2.65404	2.0467	-0.93324
C	-4.21195	1.73563	2.06117
H	-3.25154	1.16084	3.9047
H	-4.86406	2.30322	0.08483
H	-5.19385	1.85254	2.51006
C	1.07469	1.68342	1.6031
C	1.06987	3.01553	2.05614
C	1.80607	0.72825	2.32344
C	1.79258	3.38275	3.18997
H	0.4924	3.77382	1.53677
C	2.51559	1.09659	3.47078
H	1.8534	-0.29621	1.97952
C	2.51401	2.4223	3.90415
H	1.7843	4.41731	3.52056
H	3.07206	0.3426	4.02025
H	3.06836	2.70744	4.79354
H	1.47633	-1.50391	-1.89699
C	0.25615	-2.51046	-2.21022
C	-0.96536	-2.18475	-1.50522
B	2.36668	-0.2121	-0.78812
O	3.25292	-0.99258	-0.08558
O	2.96935	0.89795	-1.33325
C	4.61316	-0.51055	-0.33387
C	4.37797	0.94523	-0.91854
C	-0.92202	-2.07393	-0.10595
H	-2.52662	-2.90291	1.00015
C	0.38759	-2.02449	0.47744
H	1.15616	-2.73094	0.17992
H	0.44009	-1.7557	1.52839
C	4.51201	2.07114	0.11232
H	5.55234	2.18813	0.43271
H	4.19611	3.01392	-0.3464
H	3.89438	1.89982	0.99551
C	5.21716	1.2894	-2.14945
H	4.9459	2.28745	-2.50761
H	6.28383	1.30147	-1.89937
H	5.0577	0.58625	-2.96846
C	5.38663	-0.56074	0.98327
H	5.44531	-1.59644	1.33255
H	6.41	-0.19365	0.84831
H	4.9054	0.03433	1.76226
C	5.23685	-1.49234	-1.33471
H	6.27712	-1.23534	-1.55814
H	5.21908	-2.4982	-0.90408
H	4.67859	-1.51877	-2.2758
H	-1.88642	-2.02079	-2.05369
H	0.85968	-3.33532	-1.8307
C	-2.18119	-1.90539	0.69701
H	-2.98518	-1.43452	0.12349
H	-2.01595	-1.32922	1.60844
Co	0.44977	-0.63642	-1.06677
H	0.21936	-2.46329	-3.29566

Thermal correction to Energy=0.777955

Thermal correction to Enthalpy=0.778899

Thermal correction to Gibbs Free Energy=0.659985

Sum of electronic and zero-point Energies=-2439.258646

Sum of electronic and thermal Energies=-2439.215792

Sum of electronic and thermal Enthalpies=-2439.214848

Sum of electronic and thermal Free Energies=-2439.333762

SCF Done: E(RwB97XD) = -2440.97095221

Int3c''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.04634	1.26434	0.13805
P	0.05019	0.65877	-2.9895
C	0.29664	2.69434	-1.03363
C	-0.27727	2.42063	-2.431
H	1.38295	2.81211	-1.09503
H	-0.12201	3.61764	-0.62003
H	0.15186	3.12267	-3.15129
H	-1.36013	2.56612	-2.45634
C	-1.48352	0.20166	-3.91645
C	-1.44986	-0.25917	-5.24086
C	-2.72053	0.24719	-3.2479
C	-2.62783	-0.64845	-5.88555
H	-0.50973	-0.30905	-5.77918
C	-3.89467	-0.13049	-3.89744
H	-2.77148	0.56557	-2.21008
C	-3.8512	-0.58041	-5.22031
H	-2.58397	-1.00023	-6.91231
H	-4.84297	-0.07857	-3.36976
H	-4.76527	-0.87876	-5.7252
C	1.31085	0.81914	-4.3265
C	1.19623	1.83736	-5.29012
C	2.36391	-0.09826	-4.44358
C	2.1197	1.94138	-6.32975
H	0.37261	2.54444	-5.24953
C	3.28262	-0.00099	-5.49113
H	2.48024	-0.88875	-3.71231
C	3.16589	1.02143	-6.4328
H	2.01676	2.73608	-7.06292
H	4.09	-0.72378	-5.56806
H	3.88237	1.09992	-7.24524
C	-1.64202	1.48052	0.86635
C	-1.89614	0.98972	2.15945
C	-2.68645	2.11565	0.17577
C	-3.16094	1.11628	2.73476
H	-1.09915	0.52737	2.73367
C	-3.95046	2.24684	0.75571
H	-2.52519	2.53642	-0.81015
C	-4.19374	1.74159	2.03304
H	-3.33442	0.73541	3.73714
H	-4.74068	2.75346	0.20891
H	-5.17624	1.84529	2.48385
C	1.08584	1.69086	1.59998
C	1.11759	3.01844	2.06374
C	1.77609	0.70526	2.32024
C	1.83894	3.35243	3.20884
H	0.57146	3.79875	1.54254
C	2.4839	1.04081	3.47855
H	1.78406	-0.31956	1.97135
C	2.521	2.36286	3.92213
H	1.86034	4.38368	3.54911
H	3.00698	0.26467	4.03007
H	3.07402	2.62256	4.82014
H	1.59958	-1.53052	-1.69845
C	0.79349	-2.45836	-2.03449
C	-0.62614	-2.27041	-1.69596
B	2.48747	-0.26774	-0.80133
O	3.33856	-1.01677	-0.02773
O	3.10367	0.80866	-1.38159
C	4.71166	-0.53302	-0.2389
C	4.48792	0.89618	-0.8878
C	-0.97859	-2.06901	-0.35646
H	-2.76562	-2.91132	0.44593
C	0.12774	-1.87442	0.54094
H	0.98183	-2.54587	0.51095
H	-0.11147	-1.52962	1.54347
C	4.544	2.0583	0.10845
H	5.56461	2.21046	0.47417
H	4.22964	2.97715	-0.39717
H	3.88846	1.8999	0.96669
C	5.38567	1.20767	-2.08516
H	5.12771	2.19184	-2.48805
H	6.43867	1.23316	-1.78392
H	5.26933	0.47679	-2.88755
C	5.43027	-0.52532	1.11143
H	5.48801	-1.54692	1.49992
H	6.45353	-0.1495	1.00273
H	4.91035	0.0906	1.84778
C	5.37677	-1.5484	-1.17399
H	6.423	-1.29199	-1.36739
H	5.34887	-2.53737	-0.70669
H	4.85534	-1.61429	-2.13433
H	-1.3706	-2.24585	-2.48116
H	1.32614	-3.22638	-1.45892

C	-2.41865	-1.94119	0.0614
H	-3.06237	-1.66664	-0.77967
H	-2.55032	-1.21176	0.86301
Co	0.44509	-0.59179	-1.04769
H	0.993	-2.53731	-3.10127

Thermal correction to Energy= 0.782786

Thermal correction to Enthalpy=0.783730

Thermal correction to Gibbs Free Energy=0.660959

Sum of electronic and zero-point Energies=-2439.280905

Sum of electronic and thermal Energies=-2439.236791

Sum of electronic and thermal Enthalpies=-2439.235847

Sum of electronic and thermal Free Energies=-2439.358617

SCF Done: E(RwB97XD) = -2440.98838681

TS4c''

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.20385	1.31659	0.33214
P	-0.12519	0.58012	-2.68252
C	0.50337	2.68034	-0.90246
C	-0.23662	2.39509	-2.21597
H	1.58626	2.69978	-1.06762
H	0.22169	3.65686	-0.4948
H	0.13526	3.0277	-3.02816
H	-1.3034	2.60846	-2.10624
C	-1.7571	0.27276	-3.47282
C	-2.05041	0.7191	-4.77305
C	-2.7667	-0.3473	-2.72157
C	-3.32475	0.53429	-5.30906
H	-1.28444	1.20225	-5.37183
C	-4.04256	-0.5272	-3.25945
H	-2.56023	-0.67918	-1.70897
C	-4.32162	-0.09085	-4.55531
H	-3.53916	0.879	-6.31658
H	-4.81478	-1.01002	-2.6673
H	-5.31179	-0.23589	-4.97745
C	1.08485	0.50554	-4.06443
C	2.13675	1.42916	-4.15942
C	0.99191	-0.51511	-5.02573
C	3.0669	1.34149	-5.19655
H	2.23938	2.22628	-3.42988
C	1.92465	-0.6024	-6.05985
H	0.17709	-1.23169	-4.98324
C	2.96453	0.32533	-6.14804
H	3.86763	2.07267	-5.2633
H	1.83237	-1.39136	-6.8007
H	3.68656	0.26054	-6.95667
C	-1.59215	1.43267	0.75215
C	-2.20095	0.3587	1.42192
C	-2.3563	2.58155	0.49087
C	-3.53883	0.42464	1.81215
H	-1.62243	-0.52891	1.65677
C	-3.69685	2.64397	0.87453
H	-1.91493	3.44304	0.00022
C	-4.29215	1.56623	1.53255
H	-3.98985	-0.41314	2.33632
H	-4.2731	3.54035	0.6644
H	-5.33462	1.61912	1.83221
C	1.01441	1.89509	1.87933
C	1.76908	3.07659	1.92391
C	0.84611	1.15142	3.05739
C	2.34044	3.50497	3.12435
H	1.91972	3.67691	1.03295
C	1.4151	1.58237	4.25417
H	0.26896	0.23222	3.04871
C	2.16452	2.7606	4.29088
H	2.91769	4.42497	3.14496
H	1.27235	0.99724	5.15807
H	2.60534	3.0979	5.22437
H	2.59003	-2.90079	-1.73867
C	1.80772	-2.93824	-2.49522
C	0.43414	-2.65913	-1.94523
B	2.38551	-0.44266	-0.23405
O	2.99334	-0.16217	0.96118
O	3.2751	-0.51993	-1.28061
C	4.44242	-0.27591	0.76893
C	4.5869	-0.0703	-0.78778
C	0.04998	-2.61052	-0.61119
H	-1.41799	-3.94401	0.15868
C	0.98103	-2.08028	0.37163
H	1.98328	-2.51472	0.36144
H	0.62476	-2.00926	1.39992
C	4.73936	1.39788	-1.19957
H	5.72072	1.79144	-0.91635
H	4.63787	1.47624	-2.28595
H	3.97305	2.02624	-0.73407
C	5.66322	-0.91677	-1.46202
H	5.65159	-0.7362	-2.5415

H	6.65692	-0.64979	-1.08545
H	5.50655	-1.98484	-1.2957
C	5.12648	0.77989	1.63372
H	4.94154	0.56454	2.69054
H	6.21006	0.77093	1.4714
H	4.74901	1.78324	1.42616
C	4.84592	-1.67856	1.2396
H	5.93008	-1.82043	1.18473
H	4.53622	-1.80987	2.28079
H	4.37101	-2.46286	0.64154
H	-0.37579	-2.80694	-2.66052
H	1.79569	-3.94863	-2.92939
C	-1.38148	-2.918	-0.23278
H	-2.05412	-2.87473	-1.09485
H	-1.76934	-2.26525	0.55236
Co	0.50116	-0.61051	-0.78354
H	2.08454	-2.24658	-3.2951

Thermal correction to Energy=0.781221

Thermal correction to Enthalpy=0.782165

Thermal correction to Gibbs Free Energy=0.660961

Sum of electronic and zero-point Energies=-2439.270778

Sum of electronic and thermal Energies=-2439.227213

Sum of electronic and thermal Enthalpies=-2439.226269

Sum of electronic and thermal Free Energies=-2439.347473

SCF Done: E(RwB97XD) = -2440.97827691

Int5c''

Number of imaginary frequencies=0

Charge = 1 Multiplicity = 1

P	0.16251	1.27172	0.38995
P	-0.14465	0.55966	-2.61218
C	0.48561	2.66075	-0.80747
C	-0.28886	2.36645	-2.10403
H	1.56307	2.69967	-0.98978
H	0.17605	3.62468	-0.38671
H	0.03328	3.02435	-2.91623
H	-1.35712	2.54666	-1.94561
C	-1.73593	0.24887	-3.48917
C	-2.16067	1.12397	-4.50521
C	-2.53603	-0.85283	-3.16416
C	-3.3634	0.8994	-5.16875
H	-1.54409	1.97301	-4.7872
C	-3.73867	-1.08098	-3.83421
H	-2.2186	-1.54069	-2.38734
C	-4.15806	-0.20229	-4.83454
H	-3.68064	1.58236	-5.95189
H	-4.34901	-1.94226	-3.5775
H	-5.09196	-0.37579	-5.3596
C	1.07055	0.53367	-3.9968
C	2.071	1.5064	-4.12422
C	0.98773	-0.48709	-4.95919
C	2.96528	1.46544	-5.19646
H	2.15834	2.30941	-3.39873
C	1.89073	-0.53413	-6.02005
H	0.20129	-1.23349	-4.89245
C	2.88143	0.44288	-6.14214
H	3.72704	2.23388	-5.2893
H	1.80836	-1.32685	-6.75839
H	3.5758	0.41376	-6.97666
C	-1.64132	1.4619	0.75148
C	-2.58415	0.58427	0.2032
C	-2.08895	2.52575	1.55669
C	-3.94833	0.76187	0.4452
H	-2.25911	-0.24	-0.41859
C	-3.45119	2.70307	1.7949
H	-1.37508	3.21107	2.00724
C	-4.38518	1.82134	1.24289
H	-4.66798	0.07219	0.0097
H	-3.78342	3.52886	2.41847
H	-5.44197	1.96004	1.43111
C	0.92073	1.74914	1.98813
C	1.73671	2.87607	2.1323
C	0.64428	0.95516	3.11464
C	2.26931	3.20743	3.38007
H	1.96753	3.50685	1.27722
C	1.18109	1.28528	4.35772
H	-0.0063	0.08967	3.02675
C	1.99624	2.41234	4.49416
H	2.89534	4.08959	3.47955
H	0.95878	0.66713	5.22273
H	2.41119	2.66913	5.46356
H	2.46027	-2.88728	-1.89605
C	1.52498	-3.16415	-2.38071
C	0.29821	-2.80371	-1.57684
B	2.4342	-0.47719	-0.2621
O	3.06127	0.21978	0.74455
O	3.31284	-0.8633	-1.2587
C	4.50705	0.0752	0.57061

C	4.6278	-0.28399	-0.96477
C	0.20903	-2.57379	-0.2096
H	-1.07845	-3.69183	1.07569
C	1.34039	-2.00337	0.51631
H	2.30398	-2.48854	0.32892
H	1.19361	-1.81884	1.57843
C	4.80876	0.94059	-1.86911
H	5.79691	1.38848	-1.73798
H	4.69975	0.63584	-2.91175
H	4.05288	1.70804	-1.66031
C	5.68816	-1.33328	-1.30501
H	5.66342	-1.54393	-2.38095
H	6.69172	-0.97063	-1.055
H	5.51567	-2.27382	-0.77204
C	5.17432	1.38586	0.98664
H	4.98968	1.56818	2.04808
H	6.25896	1.33491	0.83309
H	4.78569	2.23984	0.42573
C	4.95329	-1.05348	1.50977
H	6.03934	-1.19043	1.48319
H	4.66663	-0.79588	2.53407
H	4.48458	-2.00784	1.2571
H	-0.63943	-3.05964	-2.06782
H	1.51896	-4.25341	-2.54591
C	-1.10499	-2.74751	0.51555
H	-1.95308	-2.80451	-0.17151
H	-1.29149	-1.94876	1.24273
Co	0.53704	-0.61676	-0.75446
H	1.51334	-2.69182	-3.36608

Thermal correction to Energy=0.782859

Thermal correction to Enthalpy=0.783803

Thermal correction to Gibbs Free Energy=0.660035

Sum of electronic and zero-point Energies=-2439.279951

Sum of electronic and thermal Energies=-2439.235798

Sum of electronic and thermal Enthalpies=-2439.234853

Sum of electronic and thermal Free Energies=-2439.358622

SCF Done: E(RwB97XD) = -2440.98850427

$TS''_{21\text{-ohm}=}TS''_{41\text{-ohm}}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.37111	2.93034	0.85059
C	-1.1923	3.86887	1.26126
C	-2.44068	3.42971	0.48104
C	1.67583	3.9563	1.65574
C	1.42118	4.71628	2.80894
H	0.42816	4.7457	3.24598
C	2.44068	5.46024	3.40716
H	2.22582	6.04999	4.29369
C	3.72718	5.44975	2.86646
C	3.991	4.69409	1.72177
H	4.98807	4.68608	1.29084
C	2.97405	3.95256	1.12076
H	3.18762	3.38243	0.22102
C	0.60719	3.3562	-0.92585
C	0.77242	2.3663	-1.90012
H	0.79842	1.32488	-1.61057
C	0.92148	2.71841	-3.24538
H	1.03665	1.93777	-3.99193
C	0.91411	4.05889	-3.62646
C	0.76386	5.05574	-2.65674
H	0.76736	6.10324	-2.94435
C	0.61352	4.7094	-1.31625
H	0.51895	5.49827	-0.57526
C	-3.02144	2.06023	0.87959
H	-3.16328	2.02594	1.96527
P	-1.96443	0.59149	0.45214
H	1.02941	4.33119	-4.67173
H	4.51849	6.03037	3.33123
H	-1.00222	4.93009	1.06954
H	-1.37556	3.7632	2.33663
H	-2.23759	3.46488	-0.59478
H	-3.22073	4.17843	0.66677
C	-2.05619	0.47515	-1.39225
C	-1.20421	-0.41882	-2.05999
C	-3.02816	1.16287	-2.13634
C	-1.3256	-0.62199	-3.43523
H	-0.41969	-0.93368	-1.51733
C	-3.13687	0.9686	-3.51442
H	-3.716	1.85115	-1.65804
C	-2.29005	0.07246	-4.1674
H	-0.66158	-1.32276	-3.93411
H	-3.89186	1.51341	-4.07394
H	-2.38252	-0.0843	-5.23824
C	-3.02547	-0.85582	0.91372
C	-2.53913	-2.14861	0.64962
C	-4.30267	-0.72353	1.4799
C	-3.30749	-3.27463	0.94193

H	-1.55967	-2.28039	0.19824
C	-5.06984	-1.85427	1.77657
H	-4.72113	0.25517	1.68922
C	-4.57601	-3.13042	1.50995
H	-2.91644	-4.26438	0.72404
H	-6.05771	-1.73073	2.21112
H	-5.17522	-4.0068	1.73828
H	-4.01269	1.9423	0.42995
H	-0.05213	2.35984	4.1007
C	-0.74152	0.37102	3.60766
B	1.62497	-0.29146	0.68508
O	1.68575	-0.52174	-0.66778
O	2.74846	-0.74436	1.33468
C	3.05126	-0.97058	-0.995
C	3.54955	-1.52526	0.39049
C	3.19444	-2.99841	0.63112
H	3.79599	-3.66381	0.00397
H	3.39315	-3.2462	1.67817
H	2.13667	-3.19741	0.42935
C	5.02589	-1.28554	0.69847
H	5.26154	-1.67845	1.69225
H	5.66374	-1.80262	-0.02695
H	5.27648	-0.22272	0.68785
C	2.9553	-2.00158	-2.11634
H	2.5628	-1.52773	-3.02175
H	3.94505	-2.40667	-2.3542
H	2.29681	-2.83241	-1.85328
C	3.82702	0.26153	-1.47379
H	4.84126	-0.00773	-1.78483
H	3.31513	0.70769	-2.33099
H	3.89752	1.02186	-0.68961
Co	0.10951	0.791	1.677
C	0.23049	1.38066	3.72011
C	1.51496	1.12918	3.15631
H	2.21082	1.95442	3.06549
H	1.99846	0.17198	3.31475
C	-0.28444	-0.85536	2.95995
H	0.43047	-0.73407	1.58392
H	0.62499	-1.31462	3.34957
H	-1.05477	-1.58206	2.71424
C	-2.12725	0.51015	4.17781
H	-2.42068	1.56006	4.28477
H	-2.8755	-0.01548	3.58012
H	-2.15094	0.06258	5.18045

Thermal correction to Energy=0.808772

Thermal correction to Enthalpy=0.809716

Thermal correction to Gibbs Free Energy=0.688855

Sum of electronic and zero-point Energies=-2478.528983

Sum of electronic and thermal Energies=-2478.485082

Sum of electronic and thermal Enthalpies=-2478.484138

Sum of electronic and thermal Free Energies=-2478.604999

SCF Done: E(RwB97XD) = -2480.27727617

$TS''_{12\text{-ohm}}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.2423	1.07171	0.3643
P	-0.12033	1.53373	-2.72161
C	0.29144	2.82245	-0.24501
C	-0.51459	2.94477	-1.54726
H	1.35163	3.02538	-0.42296
H	-0.06981	3.53642	0.50222
H	-0.30692	3.90176	-2.03444
H	-1.58852	2.91334	-1.34394
C	-1.71518	1.21809	-3.59452
C	-1.76553	1.05645	-4.98827
C	-2.89241	1.03004	-2.84824
C	-2.9683	0.73121	-5.62086
H	-0.87247	1.19938	-5.58803
C	-4.09244	0.71451	-3.48446
H	-2.8831	1.1272	-1.76545
C	-4.13376	0.56361	-4.87321
H	-2.99092	0.61671	-6.70078
H	-4.9956	0.586	-2.89459
H	-5.06906	0.31724	-5.36709
C	0.94359	2.29353	-4.01204
C	0.5779	3.51602	-4.60448
C	2.10773	1.64891	-4.45004
C	1.37015	4.08341	-5.60109
H	-0.3357	4.02162	-4.30436
C	2.89567	2.21491	-5.45593
H	2.39975	0.70619	-4.00288
C	2.53117	3.43337	-6.02878
H	1.07761	5.02887	-6.04848
H	3.79256	1.70189	-5.79109
H	3.14481	3.87424	-6.80897
C	-1.46151	0.8028	1.02498

C	-1.8288	-0.49813	1.41108
C	-2.38418	1.84549	1.20508
C	-3.08674	-0.75	1.95683
H	-1.12318	-1.31665	1.29825
C	-3.64746	1.58938	1.74452
H	-2.12829	2.86646	0.94064
C	-4.00191	0.29314	2.1194
H	-3.35134	-1.75952	2.25823
H	-4.34944	2.40753	1.87754
H	-4.98262	0.09699	2.5426
C	1.28596	0.99055	1.87158
C	1.54567	2.14026	2.63393
C	1.75729	-0.24983	2.32676
C	2.26867	2.04839	3.82443
H	1.19027	3.11359	2.31119
C	2.47022	-0.33947	3.52291
H	1.57687	-1.14743	1.74279
C	2.72951	0.80936	4.27285
H	2.46683	2.94647	4.40232
H	2.82685	-1.30685	3.86501
H	3.28733	0.7395	5.20208
H	1.31928	-1.10319	-0.40925
C	0.88	-1.45301	-3.24641
B	2.55553	0.09166	-1.32931
O	3.07492	1.27267	-0.85949
O	3.51997	-0.77972	-1.76097
C	4.53852	1.16467	-0.79945
C	4.83553	-0.15215	-1.64548
C	5.33967	0.1083	-3.06984
H	6.35588	0.51521	-3.06342
H	5.35888	-0.83861	-3.61864
H	4.69698	0.80528	-3.61186
C	5.764	-1.16018	-0.96419
H	5.85633	-2.04946	-1.59527
H	6.76592	-0.73982	-0.82539
H	5.38114	-1.47656	0.00831
C	5.11854	2.45478	-1.38062
H	4.82621	3.30108	-0.75077
H	6.21294	2.41717	-1.40118
H	4.75644	2.64815	-2.39281
C	4.91441	1.05458	0.68181
H	6.00007	0.99926	0.81116
H	4.55339	1.94097	1.21142
H	4.46241	0.17923	1.15431
H	1.91429	-1.57466	-3.54659
Co	0.63808	-0.25002	-1.42
C	-1.07444	-2.03685	-1.826
H	-1.73265	-2.01361	-2.69989
H	-1.41894	-2.7971	-1.12135
H	-1.24153	-1.05385	-1.31694
C	0.37525	-2.22988	-2.21705
C	1.11435	-3.34384	-1.59303
C	2.05279	-4.06972	-2.21161
H	0.80973	-3.60943	-0.58202
H	0.21012	-0.98525	-3.95997
H	2.54367	-4.89739	-1.70906
H	2.35384	-3.87232	-3.23637

Thermal correction to Energy=0.777024

Thermal correction to Enthalpy=0.777968

Thermal correction to Gibbs Free Energy=0.654014

Sum of electronic and zero-point Energies=-2439.242288

Sum of electronic and thermal Energies=-2439.198286

Sum of electronic and thermal Enthalpies=-2439.197342

Sum of electronic and thermal Free Energies=-2439.321296

SCF Done: E(RwB97XD) = -2440.94470844

$TS"_{43\text{-ohm}}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.26659	1.09655	0.43285
P	-0.01793	1.66321	-2.64354
C	0.3842	2.86821	-0.10999
C	-0.35983	3.06837	-1.44012
H	1.45509	3.0479	-0.23973
H	0.01482	3.56641	0.64817
H	-0.08268	4.02746	-1.88616
H	-1.44192	3.08645	-1.27859
C	-1.64222	1.39469	-3.47357
C	-1.78734	1.44129	-4.86799
C	-2.75406	1.04913	-2.68389
C	-3.02352	1.16554	-5.45758
H	-0.94301	1.70017	-5.49788
C	-3.98696	0.77956	-3.27727
H	-2.66589	0.9927	-1.60215
C	-4.12463	0.83701	-4.66637
H	-3.12294	1.21217	-6.53822
H	-4.83891	0.52384	-2.65373
H	-5.08463	0.62582	-5.1282

C	1.06544	2.34864	-3.95646
C	0.88849	3.65776	-4.43546
C	2.04351	1.53759	-4.54922
C	1.68481	4.14536	-5.472
H	0.11925	4.30121	-4.01869
C	2.8328	2.02307	-5.59341
H	2.19013	0.52407	-4.19381
C	2.65882	3.32976	-6.05244
H	1.53857	5.16028	-5.82995
H	3.58287	1.38069	-6.04606
H	3.27485	3.71001	-6.86201
C	-1.48093	0.8158	0.93922
C	-1.94462	-0.51045	1.00496
C	-2.36059	1.86023	1.26879
C	-3.25648	-0.78505	1.39292
H	-1.27081	-1.32808	0.76384
C	-3.67312	1.58226	1.65366
H	-2.03052	2.89406	1.23562
C	-4.12333	0.26123	1.71533
H	-3.59958	-1.81427	1.44559
H	-4.34238	2.39865	1.90937
H	-5.14461	0.04882	2.01749
C	1.25374	0.95633	1.96881
C	1.26406	1.99192	2.91832
C	1.96834	-0.22166	2.23258
C	1.98419	1.85149	4.10408
H	0.70916	2.90911	2.7447
C	2.68166	-0.3615	3.42486
H	1.97334	-1.02316	1.50147
C	2.69267	0.67476	4.35986
H	1.98845	2.65942	4.82989
H	3.22966	-1.27885	3.62012
H	3.24968	0.5667	5.28595
H	0.83679	-1.33212	-0.45694
C	0.36113	-1.44293	-2.96963
B	2.43922	0.20775	-1.24752
O	3.00108	1.46071	-1.27021
O	3.36025	-0.79768	-1.1716
C	4.45546	1.32098	-1.07458
C	4.69459	-0.21926	-1.36729
C	5.09925	-0.52624	-2.81353
H	6.11579	-0.18001	-3.02537
H	5.06509	-1.60851	-2.96963
H	4.42116	-0.0581	-3.53273
C	5.65352	-0.91792	-0.40483
H	5.72098	-1.97944	-0.66242
H	6.6591	-0.48965	-0.47903
H	5.31908	-0.84064	0.63196
C	5.15401	2.27844	-2.03827
H	4.8999	3.31078	-1.77809
H	6.24213	2.17337	-1.96504
H	4.85546	2.11015	-3.07471
C	4.75003	1.73402	0.37092
H	5.82442	1.7032	0.57909
H	4.40766	2.76211	0.52624
H	4.23849	1.09428	1.09422
H	1.19121	-1.36464	-3.6655
Co	0.54421	-0.15656	-1.36881
C	0.46888	-2.31526	-1.87199
C	1.56215	-3.31052	-1.67639
C	2.16543	-3.85203	-2.74336
H	-0.62304	-1.22176	-3.37527
H	2.91303	-4.63188	-2.62813
H	1.91966	-3.56058	-3.75957
C	1.86339	-3.75825	-0.26985
H	0.94409	-3.98643	0.28601
H	2.49192	-4.6529	-0.26326
H	2.39253	-2.9665	0.27375
H	-0.4701	-2.59184	-1.38489

Thermal correction to Energy=0.777121

Thermal correction to Enthalpy=0.778065

Thermal correction to Gibbs Free Energy=0.653704

Sum of electronic and zero-point Energies=-2439.244636

Sum of electronic and thermal Energies=-2439.200643

Sum of electronic and thermal Enthalpies=-2439.199698

Sum of electronic and thermal Free Energies=-2439.324059

SCF Done: E(RwB97XD) = -2440.94621588

$TS"_{41\text{-rhm}}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

C	-1.37786	-1.61007	3.02728
C	-0.07422	-0.97833	3.45994
C	1.18977	-1.59181	3.44046
C	1.48494	-2.5276	2.40546
H	0.70753	-3.1512	1.9724
H	2.47455	-2.97385	2.37338
H	-2.074	-0.83092	2.68642

H	-1.2665	-2.30332	2.18564	H	0.8931	-5.41344	-2.42561
B	-2.09967	-2.39091	4.2126	H	-2.99212	-4.15394	-1.07125
O	-3.17628	-3.20279	3.99625	H	-1.51491	-5.90282	-2.04323
O	-1.72222	-2.29715	5.52143	C	2.05077	-0.45321	-1.72292
C	-3.73158	-3.54175	5.30954	C	1.88769	-0.55316	-3.11706
C	-2.50209	-3.2873	6.2702	C	3.28346	-0.02855	-1.20756
C	-4.23322	-4.9826	5.26374	C	2.94257	-0.24051	-3.97222
H	-4.60244	-5.29541	6.24675	H	0.94373	-0.89141	-3.53627
H	-5.06139	-5.06139	4.55247	C	4.33721	0.28834	-2.06809
H	-3.45067	-5.6764	4.94887	H	3.41512	0.05387	-0.13328
C	-4.90278	-2.57991	5.54466	C	4.16859	0.18142	-3.44862
H	-5.6197	-2.68495	4.72456	H	2.8095	-0.32804	-5.04657
H	-5.42205	-2.79901	6.48302	H	5.28791	0.61595	-1.6577
H	-4.56785	-1.5378	5.57061	H	4.98911	0.42436	-4.11749
C	-1.595	-4.51161	6.44271	C	-1.30363	2.02486	2.35133
H	-0.67511	-4.2054	6.95045	C	-1.18444	2.49887	3.66885
H	-2.07661	-5.28681	7.04702	C	-2.58361	1.92528	1.78223
H	-1.32112	-4.94788	5.47664	C	-2.31701	2.87401	4.39223
C	-2.85274	-2.6931	7.63189	H	-0.20374	2.59748	4.12538
H	-3.48538	-3.38093	8.20381	C	-3.71527	2.30254	2.50831
H	-1.93657	-2.52266	8.20612	H	-2.71166	1.56276	0.76627
H	-3.37471	-1.73852	7.53639	C	-3.58468	2.77728	3.8143
H	2.23292	-1.37205	1.06346	H	-2.20641	3.24886	5.40567
C	2.30691	-1.08918	4.32693	H	-4.69702	2.22941	2.04925
H	2.41709	-1.75909	5.18913	H	-4.46494	3.07412	4.37683
H	3.26753	-1.07207	3.80083	C	1.49284	2.66223	1.90146
H	2.10044	-0.08662	4.71329	C	1.25163	4.04611	1.84637
H	-0.19173	-0.15586	4.1621	C	2.76569	2.20091	2.26857
P	0.19249	1.45352	1.44208	C	2.27106	4.94744	2.14917
P	0.63786	-0.79735	-0.60594	H	0.26759	4.42041	1.57804
C	-0.18592	1.81726	-0.36292	C	3.78283	3.10721	2.57671
C	-0.59483	0.52338	-1.08256	H	2.95624	1.13213	2.31143
H	0.73701	2.21469	-0.79861	C	3.53668	4.47929	2.51542
H	-0.95149	2.59398	-0.45501	H	2.07751	6.01522	2.10309
H	-0.61793	0.65517	-2.16962	H	4.76419	2.74128	2.86496
H	-1.59056	0.19553	-0.76599	H	4.32722	5.18475	2.75445
C	-0.06341	-2.40504	-1.13692	Co	0.85634	-0.69458	1.56643
C	0.766	-3.40169	-1.6773	Thermal correction to Energy=0.777729			
C	-1.4205	-2.69464	-0.91175	Thermal correction to Enthalpy=0.778673			
C	0.24271	-4.65399	-2.00147	Thermal correction to Gibbs Free Energy=0.652949			
H	1.81732	-3.19901	-1.85648	Sum of electronic and zero-point Energies=-2439.276257			
C	-1.9396	-3.94688	-1.24118	Sum of electronic and thermal Energies=-2439.232587			
H	-2.08289	-1.95008	-0.47946	Sum of electronic and thermal Enthalpies=-2439.231642			
C	-1.10949	-4.92847	-1.787	Sum of electronic and thermal Free Energies=-2439.357367			

SCF Done: E(RwB97XD) = -2440.97560969

TS"$_{43\text{-}rhm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	-0.71002	0.92457	0.54466
P	-0.18878	1.07856	-2.52621
C	-1.03504	2.552	-0.32529
C	-1.39951	2.30369	-1.7969
H	-0.10092	3.1208	-0.26146
H	-1.80615	3.13378	0.19059
H	-1.39497	3.23559	-2.37224
H	-2.40111	1.87056	-1.88908
C	-0.89913	0.60164	-4.14893
C	-0.12338	0.59663	-5.31827
C	-2.22813	0.14534	-4.20918
C	-0.67248	0.15917	-6.52556
H	0.90525	0.94173	-5.29285
C	-2.77361	-0.28497	-5.41804
H	-2.84625	0.12315	-3.31503
C	-1.99631	-0.2788	-6.57916
H	-0.06326	0.16546	-7.42474
H	-3.80469	-0.6248	-5.45321
H	-2.42168	-0.61492	-7.52015
C	1.2963	2.09353	-2.87851
C	1.19267	3.25822	-3.66169
C	2.54447	1.73721	-2.34494
C	2.31477	4.04898	-3.90152
H	0.2396	3.54312	-4.09941
C	3.66625	2.53338	-2.58877
H	2.64167	0.83701	-1.74496
C	3.55357	3.68802	-3.36327
H	2.22363	4.94425	-4.50958
H	4.62822	2.24873	-2.17212
H	4.42716	4.30563	-3.55072
C	-2.30241	0.47713	1.35248
C	-2.28775	-0.37887	2.46806
C	-3.53949	0.90389	0.84503
C	-3.48085	-0.79401	3.0589
H	-1.34189	-0.70105	2.89426
C	-4.73271	0.48489	1.43821
H	-3.58913	1.57372	-0.00792
C	-4.70695	-0.36631	2.54331
H	-3.4517	-1.44584	3.92734
H	-5.68127	0.83135	1.03803
H	-5.63534	-0.68936	3.00483
C	0.42429	1.33242	1.92075
C	0.00623	2.14428	2.98947
C	1.74794	0.8687	1.88076
C	0.90308	2.48911	3.9992
H	-1.01994	2.49755	3.03962
C	2.64092	1.21651	2.89686
H	2.07671	0.23558	1.06086
C	2.221	2.02555	3.95352
H	0.57361	3.11671	4.82214
H	3.66326	0.85166	2.86444
H	2.91729	2.29316	4.7431
C	1.70084	-2.91053	-2.44982
C	0.34699	-2.2664	-2.12876
C	-0.41988	-2.55393	-0.93244
C	0.14791	-2.25168	0.30013
H	1.22339	-2.17863	0.43291
H	-0.45347	-2.31462	1.20118
H	1.50185	-3.95262	-2.73817
H	2.08513	-2.43138	-3.364
B	2.90754	-2.91876	-1.4289
O	3.35827	-1.83109	-0.70727
O	3.68542	-4.02839	-1.26461
C	4.70073	-2.17101	-0.21601
C	4.66978	-3.74813	-0.22432
C	4.89777	-1.53506	1.15687
H	5.86162	-1.83232	1.58419
H	4.89828	-0.44376	1.06256
H	4.10796	-1.82052	1.85578
C	5.6943	-1.57555	-1.22133
H	5.52408	-0.49669	-1.2983
H	6.72949	-1.73513	-0.90398
H	5.56909	-2.0107	-2.21778
C	4.12367	-4.36049	1.07174
H	3.94275	-5.42717	0.91019
H	4.83362	-4.25504	1.8983
H	3.1753	-3.89972	1.36773
C	5.98548	-4.42096	-0.61022
H	6.77262	-4.18249	0.11379
H	5.85246	-5.50706	-0.61751
H	6.32159	-4.11775	-1.60412
Co	0.01551	-0.56994	-1.06447
H	1.21369	-0.69943	-1.85342

C	-1.89265	-2.87039	-1.04492
H	-2.02304	-3.95285	-1.17964
H	-2.44476	-2.57417	-0.14792
H	-2.34232	-2.3842	-1.91738
H	-0.27225	-2.20956	-3.02561

Thermal correction to Energy=0.777787

Thermal correction to Enthalpy=0.778731

Thermal correction to Gibbs Free Energy=0.654291

Sum of electronic and zero-point Energies=-2439.268329

Sum of electronic and thermal Energies=-2439.224675

Sum of electronic and thermal Enthalpies=-2439.223730

Sum of electronic and thermal Free Energies=-2439.348170

SCF Done: E(RwB97XD) = -2440.96877730

$TS''_{21\text{-obm}}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

C	-0.11917	-0.86633	-1.94118
B	-0.29084	0.24824	-0.55326
C	0.18931	-2.22898	-1.41379
O	-0.11144	1.59153	-0.70731
O	-1.17151	-0.0829	0.45117
C	-1.10474	2.27169	0.14174
C	-1.48686	1.14467	1.18378
H	0.59061	-2.9335	-2.14703
C	-1.52984	-0.60345	-2.45341
C	-2.53465	-1.48145	-2.48241
H	-0.54807	-2.68177	-0.75566
H	-2.4481	-2.4876	-2.08448
P	2.36393	-2.86842	0.53081
C	1.10674	-3.805	1.49405
C	1.39152	-5.10715	1.93982
C	-0.10044	-3.19754	1.8734
C	0.48006	-5.7896	2.74557
H	2.31825	-5.59573	1.65298
C	-1.00637	-3.88532	2.68323
H	-0.34354	-2.19877	1.52546
C	-0.72004	-5.18023	3.11875
H	0.70778	-6.7979	3.07915
H	-1.94126	-3.40932	2.96529
H	-1.4301	-5.71478	3.74316
C	3.5468	-2.38733	1.89283
C	3.22962	-4.15837	-0.46003
C	4.61749	-4.36074	-0.39008
C	2.47528	-4.95884	-1.3388
C	5.23402	-5.33515	-1.17855
H	5.23161	-3.77195	0.28074
C	3.09376	-5.93144	-2.12333
H	1.39735	-4.84535	-1.3897
C	4.4762	-6.1195	-2.0484
H	6.30778	-5.48203	-1.1053
H	2.49406	-6.5468	-2.78784
H	4.95729	-6.87808	-2.6588
P	3.34789	0.37339	-0.26589
C	4.18176	0.07662	1.37291
C	3.17014	2.20434	-0.33162
C	2.83246	2.80045	-1.55847
C	3.39479	3.02923	0.7813
C	2.739	4.18576	-1.67305
H	2.65574	2.18246	-2.43387
C	3.29415	4.41876	0.66535
H	3.65906	2.60576	1.74442
C	2.97078	4.99963	-0.56061
H	2.48871	4.63061	-2.63193
H	3.47852	5.04367	1.53459
H	2.90354	6.0799	-0.65138
C	4.70577	0.05382	-1.47501
C	4.71435	-1.14397	-2.20752
C	5.75759	0.96784	-1.65848
C	5.74747	-1.42457	-3.10497
H	3.9192	-1.87254	-2.07325
C	6.78923	0.6858	-2.55285
H	5.76543	1.9055	-1.11097
C	6.78526	-0.5088	-3.27894
H	5.73773	-2.35633	-3.66291
H	7.59582	1.40097	-2.68643
H	7.58844	-0.72207	-3.97836
C	-2.2608	2.67452	-0.78069
H	-2.74808	1.80379	-1.22799
H	-3.0165	3.25109	-0.23813
H	-1.86986	3.30162	-1.58792
C	-2.96372	1.09753	1.57144
H	-3.13443	0.27459	2.27264
H	-3.26459	2.0278	2.06564
H	-3.60663	0.93932	0.70314
C	-0.61499	1.15261	2.44621
H	-0.81244	0.24398	3.02368
H	0.45149	1.1769	2.20158

H	-0.84217	2.01464	3.08091
C	-0.46098	3.51766	0.74181
H	0.44906	3.28467	1.29677
H	-0.19457	4.21462	-0.05783
H	-1.16284	4.0246	1.41339
H	2.90492	-1.99731	2.69178
H	3.97929	-3.31882	2.27691
C	4.65906	-1.36932	1.58618
H	5.26621	-1.68584	0.73119
H	5.04006	0.75447	1.44076
H	3.4778	0.35687	2.16626
H	5.33767	-1.36539	2.44825
H	-1.67004	0.39005	-2.87747
H	-3.49053	-1.20952	-2.92073
C	0.86971	-0.45969	-3.06189
H	0.78015	0.60144	-3.31011
H	1.93034	-0.64276	-2.81202
H	0.66373	-1.05795	-3.95793
H	1.00427	-0.74183	0.59264
Co	1.6094	-1.15488	-0.6371

Thermal correction to Energy=0.807124

Thermal correction to Enthalpy=0.808068

Thermal correction to Gibbs Free Energy=0.685927

Sum of electronic and zero-point Energies=-2478.498039

Sum of electronic and thermal Energies=-2478.453788

Sum of electronic and thermal Enthalpies=-2478.452844

Sum of electronic and thermal Free Energies=-2478.574985

SCF Done: E(RwB97XD) = -2480.24155590

$TS''_{34\text{-}obm}$

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

C	0.21738	-0.89099	-1.95629
B	-0.04694	0.27155	-0.27895
C	0.16278	-2.2073	-1.33142
O	0.07273	1.62673	-0.29718
O	-1.14886	-0.18416	0.40289
C	-1.12622	2.19796	0.34398
C	-1.721	0.955	1.12691
H	0.636	-3.04136	-1.84665
C	-0.85738	-0.21452	-2.75879
C	-2.09648	-0.72244	-2.83651
H	-0.73386	-2.46847	-0.77777
H	-2.39209	-1.61427	-2.29427
P	2.43627	-2.82392	0.64451
C	1.26085	-3.69743	1.75564
C	1.65283	-4.8948	2.38102
C	-0.00187	-3.15698	2.03737
C	0.79515	-5.53573	3.27342
H	2.62117	-5.33653	2.16265
C	-0.85701	-3.80435	2.93305
H	-0.32031	-2.24029	1.55315
C	-0.46145	-4.99056	3.55148
H	1.10597	-6.46162	3.74874
H	-1.83594	-3.38173	3.14149
H	-1.12978	-5.49306	4.24482
C	3.81541	-2.41166	1.83653
C	3.09826	-4.15996	-0.43717
C	4.46184	-4.24767	-0.76262
C	2.20955	-5.09943	-0.99273
C	4.92469	-5.24881	-1.61888
H	5.17709	-3.54748	-0.34561
C	2.67561	-6.09623	-1.84973
H	1.15662	-5.07409	-0.72965
C	4.03362	-6.17197	-2.16765
H	5.98447	-5.3084	-1.84982
H	1.97751	-6.81983	-2.26063
H	4.39565	-6.95138	-2.83171
P	3.32202	0.4072	-0.23705
C	4.31601	0.08596	1.30386
C	3.14991	2.23684	-0.26395
C	2.87645	2.87621	-1.48448
C	3.2678	3.01463	0.89706
C	2.73665	4.26106	-1.54351
H	2.78654	2.29337	-2.39677
C	3.12369	4.40332	0.83595
H	3.47924	2.55511	1.85723
C	2.85973	5.02933	-0.38221
H	2.53707	4.74173	-2.49704
H	3.22664	4.99314	1.74235
H	2.75649	6.10958	-0.42926
C	4.52343	0.07807	-1.59555
C	4.34867	-1.03475	-2.43348
C	5.63566	0.91338	-1.80119
C	5.25996	-1.30737	-3.45684
H	3.50725	-1.70831	-2.28852
C	6.54698	0.6376	-2.81938

H	5.78229	1.78925	-1.17588
C	6.35939	-0.47101	-3.65041
H	5.10918	-2.17199	-4.09661
H	7.40161	1.29126	-2.96813
H	7.0683	-0.67936	-4.44647
C	-2.03157	2.71254	-0.77846
H	-2.34357	1.90823	-1.44933
H	-2.92774	3.19104	-0.37107
H	-1.48675	3.45897	-1.36436
C	-3.24216	0.82691	1.08057
H	-3.55056	-0.07717	1.61493
H	-3.71928	1.68412	1.56799
H	-3.61201	0.75723	0.05569
C	-1.22923	0.84607	2.57586
H	-1.54152	-0.11774	2.98939
H	-0.13792	0.90403	2.63862
H	-1.65267	1.63758	3.2019
C	-0.67779	3.36266	1.22303
H	0.06535	3.05793	1.9625
H	-0.22805	4.13929	0.59772
H	-1.53438	3.80072	1.74722
H	3.30446	-2.08331	2.74998
H	4.32291	-3.35031	2.08732
C	4.85255	-1.34997	1.4306
H	5.37151	-1.62962	0.50732
H	5.15504	0.79064	1.31064
H	3.68304	0.32481	2.16714
H	5.62221	-1.34314	2.21243
H	-2.85143	-0.25543	-3.46262
H	1.14071	-0.67001	0.8509
Co	1.56471	-1.07034	-0.46715
C	-0.41957	0.99332	-3.55293
H	0.34212	0.71235	-4.29343
H	-1.25998	1.43771	-4.09313
H	0.02015	1.75884	-2.90455
H	1.1733	-0.73381	-2.50356

Thermal correction to Energy=0.806456

Thermal correction to Enthalpy=0.807400

Thermal correction to Gibbs Free Energy=0.683093

Sum of electronic and zero-point Energies=-2478.501616

Sum of electronic and thermal Energies=-2478.456849

Sum of electronic and thermal Enthalpies=-2478.455905

Sum of electronic and thermal Free Energies=-2478.580212

SCF Done: E(RwB97XD) = -2480.24419235

TS14-obm

Number of imaginary frequencies=1

Charge = 1 Multiplicity = 1

P	0.24849	1.61534	1.51042
C	0.41849	3.09977	2.59727
C	1.61267	3.83839	2.68089
H	2.44797	3.60792	2.02988
C	1.73098	4.90742	3.57077
H	2.65779	5.47275	3.60893
C	0.66176	5.25284	4.39857
H	0.75251	6.08636	5.08886
C	-0.5269	4.52527	4.32629
H	-1.36855	4.79222	4.95905
C	-0.6498	3.45737	3.43661
H	-1.58259	2.90774	3.39562
C	-1.54737	1.58055	1.1005
C	-2.41944	0.83622	1.9089
H	-2.01968	0.24509	2.72406
C	-3.79519	0.87174	1.67619
H	-4.46222	0.29529	2.31058

C	-4.31151	1.63443	0.62738
H	-5.38247	1.65948	0.44689
C	-3.44738	2.36496	-0.19092
H	-3.8424	2.95884	-1.01028
C	-2.07239	2.34402	0.04534
H	-1.41616	2.9274	-0.59247
C	1.04937	2.05504	-0.09837
C	1.33163	3.37822	-0.4575
H	1.06138	4.18489	0.21363
C	1.95372	3.68708	-1.67121
H	2.16399	4.72405	-1.91634
C	2.29328	2.67106	-2.56138
H	2.77973	2.90208	-3.50381
C	1.98258	1.35044	-2.24552
H	2.20779	0.55646	-2.94789
C	1.36576	1.02969	-1.02541
C	0.97529	-0.37487	-0.8178
N	0.70109	-0.99791	0.2871
C	0.14526	-2.34764	-0.07227
H	0.6358	-3.09072	0.55209
C	0.60377	-2.47333	-1.53869
H	1.54696	-3.0185	-1.64604
H	-0.14768	-2.88969	-2.20796
O	0.84479	-1.09775	-1.94317
C	-1.35469	-2.46483	0.12738
C	-1.85265	-3.31094	1.12516
C	-2.25865	-1.80192	-0.71533
C	-3.22824	-3.49794	1.2782
H	-1.16084	-3.8372	1.77812
C	-3.63188	-1.98946	-0.56529
H	-1.89531	-1.14313	-1.50036
C	-4.12012	-2.83967	0.43055
H	-3.59937	-4.16766	2.0488
H	-4.32043	-1.47541	-1.22934
H	-5.18998	-2.99412	0.53838
C	2.10556	0.16071	3.92583
C	3.06515	0.0741	2.75928
C	3.16586	-1.15954	2.11638
C	2.24969	-2.19036	2.46853
H	2.05145	-2.427	3.50845
H	2.18112	-3.04741	1.80536
H	2.51108	-0.43612	4.75382
H	1.99037	1.19906	4.23754
H	-0.13313	-1.07847	2.55419

B	0.54309	-0.49976	4.28552
O	-0.43716	0.38754	4.67395
O	0.53034	-1.66062	5.03026
C	-1.03057	-0.12646	5.91361
C	-0.68738	-1.66492	5.83466
C	-2.5199	0.20668	5.91958
H	-3.00219	-0.20699	6.81208
H	-2.65719	1.29244	5.93881
H	-3.0324	-0.1864	5.03866
C	-0.32431	0.60208	7.06389
H	-0.44648	1.68122	6.93001
H	-0.74817	0.32569	8.03431
H	0.74787	0.38198	7.08365
C	-1.73346	-2.4939	5.07873
H	-1.33649	-3.50143	4.91958
H	-2.66269	-2.58206	5.65083
H	-1.9647	-2.06522	4.09905
C	-0.3685	-2.32444	7.17512
H	-1.23801	-2.29176	7.84109
H	-0.10806	-3.37522	7.01447
H	0.47299	-1.84208	7.6772
Co	1.13854	-0.46778	2.10947
H	3.78236	-1.23259	1.22178
C	4.0553	1.17999	2.51506
H	4.40017	1.19023	1.47556
H	3.64839	2.15962	2.76641
H	4.93759	1.03051	3.15248

Thermal correction to Energy=0.772460

Thermal correction to Enthalpy=0.773404

Thermal correction to Gibbs Free Energy=0.655512

Sum of electronic and zero-point Energies= -2264.774588

Sum of electronic and thermal Energies= -2264.732565

Sum of electronic and thermal Enthalpies= -2264.731621

Sum of electronic and thermal Free Energies= -2264.849513

SCF Done: E(RwB97XD) = -2266.47030970

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