Acid Catalyzed Coupling of Aromatic Aldehydes and Methyldiazoacetate – A Theoretical Mechanistic Study

Georg Dazinger and Karl A. Kirchner*

Supporting Information

A^Z

total electronic energy E_{tot} = -345.925271823 (Hartree/Particle)
Zero-point correction= 0.123526
Thermal correction to Energy= 0.130003
Thermal correction to Enthalpy= 0.130947
Thermal correction to Gibbs Free Energy= 0.092917
Sum of electronic and zero-point Energies= -345.801746
Sum of electronic and thermal Energies= -345.795269
Sum of electronic and thermal Enthalpies= -345.794325
Sum of electronic and thermal Free Energies= -345.832355

O(1)	-2.578	-0.384	-0.001
C(2)	-1.675	0.550	-0.000
C(3)	-0.309	0.245	-0.000
C(4)	0.163	-1.101	-0.000
C(5)	0.613	1.332	-0.000
C(6)	1.522	-1.337	-0.000
C(7)	1.971	1.075	-0.000
C(8)	2.421	-0.254	-0.000
H(9)	-3.489	-0.043	0.001
H(10)	-2.009	1.588	-0.000
H(11)	-0.548	-1.920	-0.000
H(12)	0.244	2.353	-0.000
H(13)	1.900	-2.353	-0.000
H(14)	2.684	1.891	-0.000
H(15)	3.489	-0.453	-0.000

A^E

total electronic energy E_{tot} = -345.921409717 (Hartree/Particle)
Zero-point correction= 0.123342
Thermal correction to Energy= 0.129882
Thermal correction to Enthalpy= 0.130826
Thermal correction to Gibbs Free Energy= 0.092573
Sum of electronic and zero-point Energies= -345.798068
Sum of electronic and thermal Energies= -345.791528
Sum of electronic and thermal Enthalpies= -345.790584
Sum of electronic and thermal Free Energies= -345.828836

O(1)	3.095	0.248	0.000
C(2)	2.086	-0.558	-0.000
C(3)	0.716	-0.234	-0.000
C(4)	0.226	1.103	-0.000
C(5)	-0.199	-1.325	0.000
C(6)	-1.135	1.329	0.000
C(7)	-1.562	-1.082	0.000
C(8)	-2.026	0.239	0.000
H(9)	2.859	1.194	0.000
H(10)	2.403	-1.600	0.000
H(11)	0.901	1.955	-0.000
H(12)	0.179	-2.343	0.000
H(13)	-1.521	2.343	0.000
H(14)	-2.265	-1.908	0.000
H(15)	-3.095	0.429	0.000

A^Z-A^E interconversion

total electronic energy E_{tot} = -345.899641131 (Hartree/Particle)
Zero-point correction= 0.121017
Thermal correction to Energy= 0.127408
Thermal correction to Enthalpy= 0.128352
Thermal correction to Gibbs Free Energy= 0.090428
Sum of electronic and zero-point Energies= -345.778624
Sum of electronic and thermal Energies= -345.772234
Sum of electronic and thermal Enthalpies= -345.771289
Sum of electronic and thermal Free Energies= -345.809213

O(1)	2.8069	0.3247	-0.0695
C(2)	1.8389	-0.5651	-0.0115
C(3)	0.4847	-0.2451	-0.0121
C(4)	0.0304	1.1121	-0.0218
C(5)	-0.4606	-1.3201	-0.0002
C(6)	-1.3227	1.3715	-0.0073
C(7)	-1.8123	-1.0403	0.0188
C(8)	-2.2382	0.2994	0.0153
H(9)	3.1543	0.7056	0.7527
H(10)	2.1505	-1.6129	-0.0583
H(11)	0.7571	1.9162	-0.0603
H(12)	-0.1052	-2.3464	-0.0012
H(13)	-1.6879	2.3924	-0.0205
H(14)	-2.5417	-1.8423	0.0317
H(15)	-3.3029	0.5153	0.0240

MDA

total electronic energy E_{tot} = -376.630066839 (Hartree/Particle)
Zero-point correction= 0.076766
Thermal correction to Energy= 0.084016
Thermal correction to Enthalpy= 0.084960
Thermal correction to Gibbs Free Energy= 0.044972
Sum of electronic and zero-point Energies= -376.553301
Sum of electronic and thermal Energies= -376.546051
Sum of electronic and thermal Enthalpies= -376.545106
Sum of electronic and thermal Free Energies= -376.585095

C(1)	-0.942	1.042	-0.000
N(2)	-1.834	0.087	-0.001
N(3)	-2.610	-0.745	0.001
C(4)	2.107	-0.970	-0.000
O(5)	1.352	1.590	0.000
C(6)	0.485	0.739	-0.000
O(7)	0.719	-0.598	-0.000
H(8)	-1.302	2.059	-0.001
H(9)	2.116	-2.059	-0.001
H(10)	2.610	-0.582	0.889
H(11)	2.610	-0.582	-0.889

A_1^Z

total electronic energy E_{tot} = -722.579729636 (Hartree/Particle)
Zero-point correction= 0.201407
Thermal correction to Energy= 0.217243
Thermal correction to Enthalpy= 0.218187
Thermal correction to Gibbs Free Energy= 0.153231
Sum of electronic and zero-point Energies= -722.378323
Sum of electronic and thermal Energies= -722.362487
Sum of electronic and thermal Enthalpies= -722.361543
Sum of electronic and thermal Free Energies= -722.426498

O(1)	1.8191	2.6223	0.8275
C(2)	1.4652	1.4344	0.4318
C(3)	2.4336	0.4883	0.0576
C(4)	3.8281	0.7727	0.0716
C(5)	1.9597	-0.7916	-0.3445
C(6)	4.7188	-0.2095	-0.3141
C(7)	2.8697	-1.7637	-0.7269
C(8)	4.2398	-1.4715	-0.7119
H(9)	1.0557	3.1773	1.0615
H(10)	0.3995	1.1790	0.3900
H(11)	4.1751	1.7525	0.3807
H(12)	0.8908	-0.9844	-0.3352
H(13)	5.7852	-0.0125	-0.3120

H(14)	2.5267	-2.7448	-1.0359
H(15)	4.9501	-2.2358	-1.0132
C(16)	-3.1671	0.7949	-0.7814
N(17)	-4.4544	0.5887	-0.9635
N(18)	-5.5616	0.4090	-1.1158
C(19)	-2.5040	-1.8876	1.6117
O(20)	-1.2113	0.0981	0.3389
C(21)	-2.4159	-0.0485	0.1162
O(22)	-3.1634	-1.0068	0.6811
H(23)	-2.7177	1.6010	-1.3407
H(24)	-3.2894	-2.5327	2.0012
H(25)	-2.0415	-1.3158	2.4184
H(26)	-1.7440	-2.4826	1.1001

A_1^E

-722.576185079 (Hartree/Particle)
Zero-point correction= 0.201325
Thermal correction to Energy= 0.217115
Thermal correction to Enthalpy= 0.218059
Thermal correction to Gibbs Free Energy= 0.153382
Sum of electronic and zero-point Energies= -722.374860
Sum of electronic and thermal Energies= -722.359071
Sum of electronic and thermal Enthalpies= -722.358126
Sum of electronic and thermal Free Energies= -722.422803

O(1)	-1.4764	-2.8178	0.0002
C(2)	-1.3559	-1.5280	0.0002
C(3)	-2.4043	-0.5817	0.0000
C(4)	-3.7840	-0.9265	0.0001
C(5)	-2.0095	0.7842	-0.0002
C(6)	-4.7356	0.0735	-0.0000
C(7)	-2.9792	1.7765	-0.0003
C(8)	-4.3322	1.4224	-0.0003
H(9)	-2.3995	-3.1308	0.0002
H(10)	-0.3129	-1.1896	0.0002
H(11)	-4.1116	-1.9635	0.0003
H(12)	-0.9491	1.0214	-0.0002
H(13)	-5.7909	-0.1755	0.0000
H(14)	-2.6910	2.8218	-0.0005
H(15)	-5.0894	2.2006	-0.0004
C(16)	3.2413	-1.0008	-0.0002
N(17)	4.5506	-0.8683	-0.0002
N(18)	5.6766	-0.7510	-0.0004
C(19)	2.3334	2.5392	0.0004
O(20)	1.1621	0.1118	0.0002
C(21)	2.3945	0.1667	0.0001
O(22)	3.0886	1.3139	0.0002
H(23)	2.8522	-2.0074	-0.0002
H(24)	3.0769	3.3343	0.0006
H(25)	1.7093	2.6034	0.8947
H(26)	1.7094	2.6038	-0.8939

A_2^Z

total electronic energy E_{tot} = -722.580393738 (Hartree/Particle)
Zero-point correction= 0.200142
Thermal correction to Energy= 0.215708
Thermal correction to Enthalpy= 0.216652
Thermal correction to Gibbs Free Energy= 0.152906
Sum of electronic and zero-point Energies= -722.380252
Sum of electronic and thermal Energies= -722.364686
Sum of electronic and thermal Enthalpies= -722.363741
Sum of electronic and thermal Free Energies= -722.427488

O(1)	-0.590	-0.427	-0.910
C(2)	0.128	-0.183	0.120
C(3)	1.501	0.139	0.034
C(4)	2.173	0.202	-1.216
C(5)	2.204	0.397	1.239
C(6)	3.519	0.518	-1.245
C(7)	3.552	0.713	1.194
C(8)	4.204	0.773	-0.045
H(9)	-1.579	-0.660	-0.683
H(10)	-0.351	-0.229	1.103
H(11)	1.624	0.001	-2.129
H(12)	1.683	0.346	2.191

H(13)	4.047	0.569	-2.191
H(14)	4.099	0.912	2.108
H(15)	5.261	1.020	-0.079
C(16)	-3.678	1.195	-0.536
N(17)	-4.530	2.162	-0.258
N(18)	-5.261	2.986	-0.005
C(19)	-3.249	-2.414	-0.008
O(20)	-4.918	-0.450	0.668
C(21)	-3.974	-0.109	0.002
O(22)	-2.964	-1.026	-0.353
H(23)	-2.890	1.432	-1.237
H(24)	-3.365	-2.514	1.071
H(25)	-2.396	-2.986	-0.372
H(26)	-4.164	-2.728	-0.509

A_2^E

total electronic energy E_{tot} = -722.574445136 (Hartree/Particle)
Zero-point correction= 0.200338
Thermal correction to Energy= 0.215805
Thermal correction to Enthalpy= 0.216749
Thermal correction to Gibbs Free Energy= 0.153553
Sum of electronic and zero-point Energies= -722.374107
Sum of electronic and thermal Energies= -722.358640
Sum of electronic and thermal Enthalpies= -722.357696
Sum of electronic and thermal Free Energies= -722.420892

O(1)	0.412	1.640	-1.378
C(2)	-0.767	1.159	-1.466
C(3)	-1.389	0.131	-0.709
C(4)	-2.738	-0.158	-1.049
C(5)	-0.752	-0.601	0.328
C(6)	-3.431	-1.147	-0.369
C(7)	-1.454	-1.587	0.996
C(8)	-2.789	-1.859	0.651
H(9)	1.073	1.301	-0.668
H(10)	-1.352	1.637	-2.254
H(11)	-3.223	0.401	-1.844
H(12)	0.277	-0.405	0.603
H(13)	-4.461	-1.368	-0.625
H(14)	-0.972	-2.153	1.786
H(15)	-3.329	-2.636	1.183
C(16)	3.423	-0.458	-1.006
N(17)	3.987	-1.639	-1.182
N(18)	4.461	-2.654	-1.327
C(19)	2.098	1.699	1.602
O(20)	2.880	-0.873	1.284
C(21)	2.878	-0.180	0.294
O(22)	2.259	1.089	0.287
H(23)	3.503	0.249	-1.819
H(24)	1.501	1.061	2.254
H(25)	1.608	2.654	1.422
H(26)	3.083	1.856	2.043

A_3^Z

total electronic energy E_{tot} = -722.605040672 (Hartree/Particle)
Zero-point correction= 0.198966
Thermal correction to Energy= 0.214194
Thermal correction to Enthalpy= 0.215138
Thermal correction to Gibbs Free Energy= 0.152388
Sum of electronic and zero-point Energies= -722.406075
Sum of electronic and thermal Energies= -722.390847
Sum of electronic and thermal Enthalpies= -722.389903
Sum of electronic and thermal Free Energies= -722.452653

O(1)	-0.165	-0.053	-0.020
C(2)	0.857	-0.777	-0.015
C(3)	2.204	-0.277	-0.010
C(4)	2.475	1.110	-0.010
C(5)	3.265	-1.206	-0.004
C(6)	3.789	1.550	-0.004
C(7)	4.579	-0.757	0.001
C(8)	4.838	0.618	0.001
H(10)	0.733	-1.871	-0.015
H(11)	1.648	1.812	-0.014
H(12)	3.050	-2.272	-0.004

H(13)	4.009	2.612	-0.005
H(14)	5.400	-1.466	0.005
H(15)	5.865	0.970	0.005
H(9)	-1.344	-0.632	-0.024
C(16)	-3.167	1.129	-0.013
N(17)	-4.240	1.906	-0.007
N(18)	-5.147	2.575	0.003
C(19)	-4.783	-2.173	0.003
O(20)	-2.355	-1.094	-0.016
C(21)	-3.336	-0.280	-0.010
O(22)	-4.565	-0.730	-0.001
H(23)	-2.203	1.617	-0.022
H(24)	-5.865	-2.284	0.010
H(25)	-4.337	-2.610	0.896
H(26)	-4.350	-2.612	-0.896

A_3^E

total electronic energy E_{tot} = -722.602395854 (Hartree/Particle)
Zero-point correction= 0.200059
Thermal correction to Energy= 0.215248
Thermal correction to Enthalpy= 0.216192
Thermal correction to Gibbs Free Energy= 0.153703
Sum of electronic and zero-point Energies= -722.402337
Sum of electronic and thermal Energies= -722.387148
Sum of electronic and thermal Enthalpies= -722.386204
Sum of electronic and thermal Free Energies= -722.448693

O(1)	0.140	-1.599	-0.004
C(2)	-1.074	-1.876	-0.002
C(3)	-2.188	-0.953	-0.003
C(4)	-2.022	0.448	-0.006
C(5)	-3.486	-1.505	-0.001
C(6)	-3.137	1.272	-0.006
C(7)	-4.599	-0.673	-0.001
C(8)	-4.423	0.713	-0.004
H(9)	-1.335	-2.945	-0.000
H(10)	-1.028	0.882	-0.008
H(11)	-3.610	-2.585	0.002
H(12)	-3.017	2.351	-0.009
H(13)	-5.598	-1.097	0.001
H(14)	-5.291	1.365	-0.004
C(15)	3.199	-1.279	-0.005
N(16)	4.498	-1.547	-0.004
N(17)	5.598	-1.790	-0.004
C(18)	3.311	2.399	-0.000
O(19)	1.544	0.415	-0.003
C(20)	2.781	0.073	-0.003
O(21)	3.706	0.993	-0.002
H(22)	2.514	-2.116	-0.006
H(23)	4.251	2.945	0.000
H(24)	2.730	2.615	0.897
H(25)	2.730	2.617	-0.897
H(26)	0.861	-0.402	-0.004

$AB^{H1'}$

total electronic energy E_{tot} = -722.560537615 (Hartree/Particle)
Zero-point correction= 0.201253
Thermal correction to Energy= 0.215763
Thermal correction to Enthalpy= 0.216708
Thermal correction to Gibbs Free Energy= 0.157765
Sum of electronic and zero-point Energies= -722.359284
Sum of electronic and thermal Energies= -722.344774
Sum of electronic and thermal Enthalpies= -722.343830
Sum of electronic and thermal Free Energies= -722.402773
ν = -198cm^{-1}

O(1)	-0.725	-2.519	-1.209
C(2)	-0.297	-1.264	-1.325
C(3)	-1.176	-0.227	-0.826
C(4)	-2.245	-0.531	0.043
C(5)	-0.963	1.104	-1.247
C(6)	-3.087	0.486	0.478
C(7)	-1.813	2.110	-0.808
C(8)	-2.871	1.802	0.056
H(9)	-0.212	-3.131	-1.760
H(10)	0.366	-1.026	-2.157

H(11)	-2.423	-1.558	0.344
H(12)	-0.151	1.331	-1.932
H(13)	-3.916	0.256	1.138
H(14)	-1.664	3.131	-1.144
H(15)	-3.536	2.591	0.393
C(16)	1.428	-1.201	-0.069
N(17)	0.934	-1.212	1.189
N(18)	0.367	-1.160	2.157
C(19)	2.892	2.203	0.117
O(20)	2.551	0.140	-1.642
C(21)	2.156	0.043	-0.503
O(22)	2.227	0.953	0.462
H(23)	1.895	-2.143	-0.340
H(24)	2.870	2.795	1.029
H(25)	2.349	2.701	-0.688
H(26)	3.916	2.000	-0.196

AB^{H1}

total electronic energy E_{tot} = -722.558396044 (Hartree/Particle)
Zero-point correction= 0.201037
Thermal correction to Energy= 0.215613
Thermal correction to Enthalpy= 0.216557
Thermal correction to Gibbs Free Energy= 0.157274
Sum of electronic and zero-point Energies= -722.357359
Sum of electronic and thermal Energies= -722.342783
Sum of electronic and thermal Enthalpies= -722.341839
Sum of electronic and thermal Free Energies= -722.401122
ν = -180cm^{-1}

O(1)	-0.628	-2.669	-1.380
C(2)	-0.347	-1.376	-1.331
C(3)	-1.238	-0.406	-0.720
C(4)	-2.158	-0.765	0.287
C(5)	-1.185	0.927	-1.179
C(6)	-3.021	0.190	0.810
C(7)	-2.057	1.874	-0.654
C(8)	-2.973	1.507	0.337
H(9)	-1.414	-2.895	-0.856
H(10)	0.293	-1.056	-2.150
H(11)	-2.203	-1.780	0.678
H(12)	-0.476	1.201	-1.954
H(13)	-3.731	-0.085	1.582
H(14)	-2.032	2.895	-1.021
H(15)	-3.654	2.248	0.744
C(16)	1.485	-1.332	-0.173
N(17)	1.157	-1.557	1.113
N(18)	0.745	-1.696	2.150
C(19)	2.739	2.118	0.341
O(20)	2.288	0.312	-1.655
C(21)	2.062	0.016	-0.504
O(22)	2.207	0.782	0.572
H(23)	1.935	-2.196	-0.654
H(24)	2.788	2.576	1.326
H(25)	2.073	2.675	-0.319
H(26)	3.731	2.047	-0.107

B^{H1}

total electronic energy E_{tot} = -722.569956349 (Hartree/Particle)
Zero-point correction= 0.202206
Thermal correction to Energy= 0.216989
Thermal correction to Enthalpy= 0.217933
Thermal correction to Gibbs Free Energy= 0.158871
Sum of electronic and zero-point Energies= -722.367750
Sum of electronic and thermal Energies= -722.352967
Sum of electronic and thermal Enthalpies= -722.352023
Sum of electronic and thermal Free Energies= -722.411085

O(1)	0.390	1.488	2.477
C(2)	0.177	1.263	1.103
C(3)	1.182	0.350	0.440
C(4)	1.867	-0.618	1.191
C(5)	1.442	0.478	-0.932
C(6)	2.793	-1.456	0.569
C(7)	2.365	-0.366	-1.548
C(8)	3.038	-1.335	-0.800
C(9)	-1.306	0.722	1.081

N(10)	-1.349	-0.497	1.859
N(11)	-1.274	-1.440	2.434
C(12)	-2.953	-1.039	-1.791
O(13)	-1.834	1.397	-1.134
C(14)	-1.878	0.495	-0.343
O(15)	-2.372	-0.721	-0.484
H(16)	1.296	1.803	2.608
H(17)	0.071	2.196	0.530
H(18)	1.702	-0.695	2.262
H(19)	0.933	1.241	-1.514
H(20)	3.328	-2.196	1.156
H(21)	2.570	-0.258	-2.608
H(22)	3.763	-1.984	-1.280
H(23)	-1.940	1.425	1.635
H(24)	-3.321	-2.058	-1.691
H(25)	-2.178	-0.970	-2.555
H(26)	-3.763	-0.343	-2.006

BC^{H1}

total electronic energy E_{tot} = -722.559136033 (Hartree/Particle)
Zero-point correction= 0.198746
Thermal correction to Energy= 0.214083
Thermal correction to Enthalpy= 0.215028
Thermal correction to Gibbs Free Energy= 0.154344
Sum of electronic and zero-point Energies= -722.360390
Sum of electronic and thermal Energies= -722.345053
Sum of electronic and thermal Enthalpies= -722.344108
Sum of electronic and thermal Free Energies= -722.404792
ν = -140cm^{-1}

O(1)	0.311	0.965	-2.455
C(2)	0.064	-0.112	-1.596
C(3)	1.096	-0.342	-0.503
C(4)	1.841	0.739	-0.015
C(5)	1.307	-1.630	0.007
C(6)	2.781	0.531	0.995
C(7)	2.245	-1.829	1.020
C(8)	2.980	-0.750	1.515
C(9)	-1.355	0.015	-1.168
C(10)	-2.823	-1.418	1.970
O(11)	-2.095	-2.037	-0.636
C(12)	-1.946	-0.929	-0.165
O(13)	-2.229	-0.466	1.021
H(14)	1.191	0.862	-2.845
H(15)	-0.057	-1.071	-2.161
H(16)	1.699	1.731	-0.432
H(17)	0.754	-2.478	-0.391
H(18)	3.360	1.368	1.369
H(19)	2.413	-2.828	1.409
H(20)	3.717	-0.909	2.295
H(21)	-2.041	0.384	-1.933
H(22)	-3.062	-0.820	2.845
H(23)	-2.089	-2.189	2.205
H(24)	-3.717	-1.859	1.530
N(25)	-1.323	1.847	-0.262
N(26)	-1.403	2.828	0.237

C^{H}

total electronic energy E_{tot} = -613.127374310 (Hartree/Particle)
Zero-point correction= 0.194549
Thermal correction to Energy= 0.206861
Thermal correction to Enthalpy= 0.207805
Thermal correction to Gibbs Free Energy= 0.153930
Sum of electronic and zero-point Energies= -612.932826
Sum of electronic and thermal Energies= -612.920513
Sum of electronic and thermal Enthalpies= -612.919569
Sum of electronic and thermal Free Energies= -612.973445

O(1)	0.197	2.379	-0.306
C(2)	0.373	1.185	0.190
C(3)	1.596	0.464	0.040
C(4)	1.643	-0.918	0.362
C(5)	2.770	1.105	-0.445
C(6)	2.818	-1.632	0.177
C(7)	3.939	0.386	-0.606
C(8)	3.961	-0.985	-0.301

C(9)	-0.839	0.694	0.906
C(10)	-3.922	-0.612	-0.728
O(11)	-1.276	-1.188	-0.578
C(12)	-1.713	-0.225	0.006
O(13)	-2.969	0.195	0.022
H(14)	0.948	2.692	-0.841
H(15)	0.750	-1.429	0.697
H(16)	2.793	2.173	-0.651
H(17)	2.846	-2.692	0.405
H(18)	4.838	0.880	-0.958
H(19)	4.882	-1.545	-0.431
H(20)	-1.432	1.554	1.221
H(21)	-0.555	0.108	1.784
H(22)	-4.882	-0.123	-0.579
H(23)	-3.933	-1.630	-0.337
H(24)	-3.645	-0.623	-1.784

AB^{Ph2}

total electronic energy E_{tot} = -722.556934401 (Hartree/Particle)
Zero-point correction= 0.201036
Thermal correction to Energy= 0.215656
Thermal correction to Enthalpy= 0.216600
Thermal correction to Gibbs Free Energy= 0.157218
Sum of electronic and zero-point Energies= -722.355898
Sum of electronic and thermal Energies= -722.341278
Sum of electronic and thermal Enthalpies= -722.340334
Sum of electronic and thermal Free Energies= -722.399717
ν = -178cm^{-1}

O(1)	0.3552	-2.6440	0.4605
C(2)	0.0941	-1.3648	0.6587
C(3)	-1.1686	-0.7448	0.3175
C(4)	-1.5499	0.4078	1.0361
C(5)	-2.0302	-1.2751	-0.6665
C(6)	-2.7827	1.0016	0.7901
C(7)	-3.2554	-0.6714	-0.9100
C(8)	-3.6330	0.4640	-0.1801
C(9)	1.5639	-0.3483	-0.6914
N(10)	2.6261	-1.1295	-0.4226
N(11)	3.4376	-1.8440	-0.1171
C(12)	1.0106	3.2686	-0.3448
O(13)	2.0872	1.1931	1.0487
C(14)	1.6302	1.0096	-0.0589
O(15)	1.0528	1.9066	-0.8526
H(16)	-0.3143	-3.0769	-0.0955
H(17)	0.6766	-0.9497	1.4779
H(18)	-0.8873	0.8118	1.7961
H(19)	-1.7466	-2.1428	-1.2590
H(20)	-3.0854	1.8759	1.3562
H(21)	-3.9192	-1.0774	-1.6656
H(22)	-4.5948	0.9288	-0.3717
H(23)	1.2005	-0.4636	-1.7082
H(24)	0.4866	3.8390	-1.1085
H(25)	2.0262	3.6418	-0.2067
H(26)	0.4761	3.2985	0.6058

B^{Ph2}

total electronic energy E_{tot} = -722.568866038
Zero-point correction= 0.201974 (Hartree/Particle)
Thermal correction to Energy= 0.216872
Thermal correction to Enthalpy= 0.217816
Thermal correction to Gibbs Free Energy= 0.157974
Sum of electronic and zero-point Energies= -722.366893
Sum of electronic and thermal Energies= -722.351995
Sum of electronic and thermal Enthalpies= -722.351051
Sum of electronic and thermal Free Energies= -722.410892

O(1)	0.934	-3.025	0.416
C(2)	0.673	-1.746	0.615
C(3)	-0.590	-1.126	0.273
C(4)	-0.971	0.027	0.992
C(5)	-1.452	-1.656	-0.710
C(6)	-2.204	0.621	0.746
C(7)	-2.677	-1.052	-0.954
C(8)	-3.054	0.083	-0.224
H(16)	0.264	-3.458	-0.140

H(17)	1.255	-1.331	1.434
H(18)	-0.309	0.431	1.752
H(19)	-1.168	-2.524	-1.303
H(20)	-2.507	1.495	1.312
H(21)	-3.341	-1.458	-1.710
H(22)	-4.016	0.548	-0.416
C(9)	2.142	-0.729	-0.735
N(10)	3.205	-1.511	-0.467
N(11)	4.016	-2.225	-0.161
C(12)	1.589	2.888	-0.389
O(13)	2.666	0.812	1.005
C(14)	2.209	0.629	-0.103
O(15)	1.631	1.526	-0.897
H(23)	1.779	-0.845	-1.752
H(24)	1.065	3.458	-1.152
H(25)	2.605	3.261	-0.251
H(26)	1.055	2.917	0.562

BC^{Ph2}

total electronic energy E_{tot} = -722.563448537 (Hartree/Particle)
Zero-point correction= 0.200189
Thermal correction to Energy= 0.215321
Thermal correction to Enthalpy= 0.216266
Thermal correction to Gibbs Free Energy= 0.156080
Sum of electronic and zero-point Energies= -722.363259
Sum of electronic and thermal Energies= -722.348127
Sum of electronic and thermal Enthalpies= -722.347183
Sum of electronic and thermal Free Energies= -722.407369
ν = -363cm^{-1}

O(1)	-0.850	-2.728	-0.557
C(2)	-0.783	-1.324	-0.594
C(3)	0.581	-0.715	-0.285
C(4)	0.991	0.461	-0.934
C(5)	1.418	-1.329	0.663
C(6)	2.237	1.009	-0.646
C(7)	2.665	-0.775	0.942
C(8)	3.072	0.394	0.293
C(9)	-1.594	-0.841	0.582
C(10)	-3.027	2.462	-0.358
O(11)	-1.619	1.278	1.676
C(12)	-1.953	0.645	0.710
O(13)	-2.626	1.056	-0.358
H(14)	-0.217	-3.093	-1.193
H(15)	-1.185	-0.902	-1.524
H(16)	0.348	0.928	-1.676
H(17)	1.104	-2.247	1.149
H(18)	2.564	1.908	-1.158
H(19)	3.319	-1.254	1.663
H(20)	4.044	0.824	0.513
H(21)	-1.329	-1.295	1.536
H(22)	-3.592	2.594	-1.277
H(23)	-2.137	3.093	-0.345
H(24)	-3.642	2.666	0.519
N(25)	-3.152	-1.627	0.384
N(26)	-4.044	-2.208	0.089

C^{Ph}

total electronic energy E_{tot} = -613.092784644 (Hartree/Particle)
Zero-point correction= 0.193672
Thermal correction to Energy= 0.206200
Thermal correction to Enthalpy= 0.207145
Thermal correction to Gibbs Free Energy= 0.153323
Sum of electronic and zero-point Energies= -612.899113
Sum of electronic and thermal Energies= -612.886584
Sum of electronic and thermal Enthalpies= -612.885640
Sum of electronic and thermal Free Energies= -612.939461

O(1)	0.344	2.265	0.273
C(2)	0.468	1.005	0.517
C(3)	-0.974	-0.449	-0.301
C(4)	-2.051	0.233	-0.903
C(5)	-1.220	-1.533	0.565
C(6)	-3.352	-0.206	-0.691

C(7)	-2.527	-1.961	0.772
C(8)	-3.590	-1.301	0.147
C(9)	0.453	0.043	-0.577
C(10)	3.848	-1.296	0.108
O(11)	1.454	-2.151	-0.876
C(12)	1.568	-1.019	-0.492
O(13)	2.660	-0.454	0.037
H(14)	0.255	2.814	1.075
H(15)	0.529	0.667	1.551
H(16)	-1.862	1.084	-1.551
H(17)	-0.398	-2.069	1.026
H(18)	-4.180	0.301	-1.176
H(19)	-2.718	-2.814	1.415
H(20)	-4.608	-1.640	0.315
H(21)	0.519	0.549	-1.544
H(22)	4.608	-0.677	0.581
H(23)	4.151	-1.586	-0.899
H(24)	3.637	-2.186	0.703

AB^{OH1}

total electronic energy E_{tot} = -722.567080484 (Hartree/Particle)
Zero-point correction= 0.201666
Thermal correction to Energy= 0.215820
Thermal correction to Enthalpy= 0.216764
Thermal correction to Gibbs Free Energy= 0.159340
Sum of electronic and zero-point Energies= -722.365415
Sum of electronic and thermal Energies= -722.351261
Sum of electronic and thermal Enthalpies= -722.350317
Sum of electronic and thermal Free Energies= -722.407740

O(1)	0.0728	2.2004	0.1676
C(2)	-0.1594	0.9363	0.5345
C(3)	-1.5235	0.4413	0.3348
C(4)	-2.3971	1.0682	-0.5732
C(5)	-1.9570	-0.6770	1.0730
C(6)	-3.6883	0.5791	-0.7313
C(7)	-3.2525	-1.1600	0.9064
C(8)	-4.1150	-0.5342	0.0035
H(9)	1.0079	2.4316	0.3438
H(10)	0.3386	0.5976	1.4465
H(11)	-2.0656	1.9411	-1.1251
H(12)	-1.2948	-1.1430	1.7985
H(13)	-4.3689	1.0665	-1.4214
H(14)	-3.5915	-2.0125	1.4850
H(15)	-5.1260	-0.9079	-0.1233
C(16)	1.0226	-0.0008	-0.7093
N(17)	0.7034	-1.3279	-0.7969
N(18)	0.3041	-2.3720	-0.7340
C(19)	4.5124	-0.5871	0.4721
O(20)	2.7221	1.4424	0.0782
C(21)	2.4191	0.2992	-0.1983
O(22)	3.1626	-0.7821	-0.0593
H(23)	0.7485	0.5154	-1.6283
H(24)	4.9392	-1.5860	0.5178
H(25)	4.4538	-0.1341	1.4622
H(26)	5.0777	0.0540	-0.2044

AB^{OH2}

B^{OH1}

total electronic energy E_{tot} = -722.568667361 (Hartree/Particle)
Zero-point correction= 0.202279
Thermal correction to Energy= 0.216919
Thermal correction to Enthalpy= 0.217863
Thermal correction to Gibbs Free Energy= 0.159104
Sum of electronic and zero-point Energies= -722.366388
Sum of electronic and thermal Energies= -722.351748
Sum of electronic and thermal Enthalpies= -722.350804
Sum of electronic and thermal Free Energies= -722.409564

O(1)	0.117	2.128	0.072
C(2)	-0.059	0.803	0.401
C(3)	-1.468	0.341	0.184
C(4)	-2.247	0.889	-0.844

C(5)	-1.999	-0.662	1.008
C(6)	-3.547	0.431	-1.044
C(7)	-3.302	-1.118	0.801
C(8)	-4.073	-0.574	-0.226
C(9)	0.989	0.010	-0.638
N(10)	0.687	-1.372	-0.717
N(11)	0.311	-2.416	-0.640
C(12)	4.601	-0.743	0.047
O(13)	2.805	1.335	0.155
C(14)	2.460	0.241	-0.219
O(15)	3.186	-0.855	-0.323
H(16)	1.005	2.416	0.346
H(17)	0.306	0.544	1.402
H(18)	-1.847	1.689	-1.459
H(19)	-1.413	-1.063	1.832
H(20)	-4.155	0.864	-1.832
H(21)	-3.715	-1.884	1.448
H(22)	-5.089	-0.923	-0.384
H(23)	0.788	0.429	-1.629
H(24)	5.002	-1.744	-0.090
H(25)	4.680	-0.420	1.085
H(26)	5.089	-0.026	-0.614

B^{Ph1}

total electronic energy E_{tot} = -722.566904057 (Hartree/Particle)
Zero-point correction= 0.202028
Thermal correction to Energy= 0.216832
Thermal correction to Enthalpy= 0.217776
Thermal correction to Gibbs Free Energy= 0.158733
Sum of electronic and zero-point Energies= -722.364876
Sum of electronic and thermal Energies= -722.350072
Sum of electronic and thermal Enthalpies= -722.349128
Sum of electronic and thermal Free Energies= -722.408171

O(1)	0.855	-1.047	1.287
C(2)	0.214	-1.380	0.079
C(3)	-1.112	-0.708	-0.180
C(4)	-1.430	0.518	0.418
C(5)	-2.048	-1.348	-1.006
C(6)	-2.680	1.093	0.195
C(7)	-3.289	-0.762	-1.237
C(8)	-3.606	0.459	-0.636
C(9)	1.296	-0.976	-1.009
N(10)	2.449	-1.834	-0.779
N(11)	3.287	-2.507	-0.508
C(12)	3.543	1.961	-0.382
O(13)	1.003	1.382	-1.272
C(14)	1.758	0.512	-0.941
O(15)	3.003	0.607	-0.504
H(16)	0.232	-1.168	2.018
H(17)	0.089	-2.468	-0.032
H(18)	-0.708	1.017	1.056
H(19)	-1.815	-2.312	-1.454
H(20)	-2.929	2.039	0.666
H(21)	-4.013	-1.262	-1.872
H(22)	-4.576	0.912	-0.810
H(23)	0.948	-1.216	-2.018
H(24)	4.576	1.823	-0.074
H(25)	2.976	2.507	0.372
H(26)	3.479	2.467	-1.346

B^{H2}

total electronic energy E_{tot} = -722.568979133 (Hartree/Particle)
Zero-point correction= 0.201843
Thermal correction to Energy= 0.216786
Thermal correction to Enthalpy= 0.217730
Thermal correction to Gibbs Free Energy= 0.157688
Sum of electronic and zero-point Energies= -722.367136
Sum of electronic and thermal Energies= -722.352193
Sum of electronic and thermal Enthalpies= -722.351249
Sum of electronic and thermal Free Energies= -722.411291

O(1)	-0.348	-0.708	1.793
C(2)	0.041	-1.065	0.504
C(3)	1.473	-0.692	0.210
C(4)	2.089	-1.183	-0.951
C(5)	2.183	0.150	1.074

C(6)	3.403	-0.828	-1.248
C(7)	3.500	0.501	0.772
C(8)	4.108	0.018	-0.387
C(9)	-0.965	-0.341	-0.527
N(10)	-0.744	1.071	-0.419
N(11)	-0.477	2.120	-0.178
C(12)	-4.673	0.142	-0.211
O(13)	-2.732	-1.781	0.175
C(14)	-2.449	-0.679	-0.212
O(15)	-3.240	0.351	-0.446
H(16)	-0.967	-1.366	2.140
H(17)	-0.156	-2.120	0.275
H(18)	1.556	-1.864	-1.613
H(19)	1.719	0.497	1.990
H(20)	3.879	-1.220	-2.140
H(21)	4.053	1.144	1.449
H(22)	5.134	0.289	-0.616
H(23)	-0.722	-0.602	-1.563
H(24)	-5.134	1.100	-0.439
H(25)	-4.831	-0.138	0.831
H(26)	-5.036	-0.641	-0.876

B^{OH2}

total electronic energy E_{tot} = -722.564738425 (Hartree/Particle)
Zero-point correction= 0.202342
Thermal correction to Energy= 0.216967
Thermal correction to Enthalpy= 0.217912
Thermal correction to Gibbs Free Energy= 0.159402
Sum of electronic and zero-point Energies= -722.362397
Sum of electronic and thermal Energies= -722.347771
Sum of electronic and thermal Enthalpies= -722.346827
Sum of electronic and thermal Free Energies= -722.405336

O(1)	-0.341	-1.336	2.171
C(2)	0.034	-1.521	0.861
C(3)	1.089	-0.625	0.264
C(4)	2.008	-1.188	-0.634
C(5)	1.186	0.738	0.586
C(6)	3.002	-0.399	-1.214
C(7)	2.184	1.520	0.009
C(8)	3.089	0.956	-0.894
C(9)	-1.402	-1.428	0.017
N(10)	-1.214	-1.867	-1.318
N(11)	-0.892	-2.194	-2.331
C(12)	-2.998	1.721	-1.252
O(13)	-2.054	0.611	1.080
C(14)	-2.000	0.003	0.041
O(15)	-2.404	0.384	-1.155
H(16)	-0.588	-0.410	2.331
H(17)	0.326	-2.570	0.758
H(18)	1.975	-2.252	-0.855
H(19)	0.502	1.196	1.294
H(20)	3.716	-0.847	-1.897
H(21)	2.262	2.570	0.272
H(22)	3.867	1.570	-1.336
H(23)	-2.091	-2.138	0.489
H(24)	-3.282	1.822	-2.296
H(25)	-2.256	2.466	-0.967
H(26)	-3.867	1.777	-0.596

BC^{OH2}

total electronic energy E_{tot} = -722.550872263(Hartree/Particle)
Zero-point correction= 0.200354
Thermal correction to Energy= 0.215291
Thermal correction to Enthalpy= 0.216235
Thermal correction to Gibbs Free Energy= 0.156652
Sum of electronic and zero-point Energies= -722.350518
Sum of electronic and thermal Energies= -722.335582
Sum of electronic and thermal Enthalpies= -722.334638
Sum of electronic and thermal Free Energies= -722.394220

O(1)	0.5615	-0.2183	2.3217
C(2)	-0.1146	0.6056	1.3611
C(3)	-1.2356	0.0038	0.5611
C(4)	-2.4607	0.6840	0.5291
C(5)	-1.1044	-1.2122	-0.1291

C(6)	-3.5354	0.1672	-0.1934
C(7)	-2.1833	-1.7300	-0.8424
C(8)	-3.3971	-1.0395	-0.8796
C(9)	1.1982	0.9471	0.6797
N(10)	0.7908	2.3075	-0.5575
N(11)	0.4325	3.1188	-1.2142
C(12)	3.0353	-2.0690	-0.5096
O(13)	2.2731	0.3897	-1.3983
C(14)	1.9524	0.0232	-0.2976
O(15)	2.2164	-1.1406	0.2795
H(16)	0.6003	-1.1326	1.9944
H(17)	-0.4728	1.4823	1.9046
H(18)	-2.5800	1.6147	1.0776
H(19)	-0.1740	-1.7719	-0.1087
H(20)	-4.4798	0.7009	-0.2104
H(21)	-2.0777	-2.6734	-1.3679
H(22)	-4.2343	-1.4463	-1.4373
H(23)	1.8513	1.5750	1.2861
H(24)	2.5045	-2.3345	-1.4240
H(25)	3.1747	-2.9316	0.1372
H(26)	3.9868	-1.5944	-0.7486

$BB^{H\text{-}Ph1}$

total electronic energy E_{tot} = -722.562462033 (Hartree/Particle)
Zero-point correction= 0.202171
Thermal correction to Energy= 0.216062
Thermal correction to Enthalpy= 0.217006
Thermal correction to Gibbs Free Energy= 0.161024
Sum of electronic and zero-point Energies= -722.360291
Sum of electronic and thermal Energies= -722.346400
Sum of electronic and thermal Enthalpies= -722.345456
Sum of electronic and thermal Free Energies= -722.401438
ν = -38cm^{-1}

O(1)	-1.269	-2.627	-0.467
C(2)	-0.737	-1.877	0.603
C(3)	0.552	-1.169	0.289
C(4)	0.778	-0.635	-0.990
C(5)	1.540	-1.058	1.277
C(6)	1.986	-0.002	-1.273
C(7)	2.745	-0.420	0.989
C(8)	2.968	0.108	-0.284
C(9)	-1.946	-0.862	0.994
N(10)	-3.073	-1.133	0.140
N(11)	-3.910	-1.323	-0.560
C(12)	-1.618	2.590	-0.429
O(13)	-1.004	1.155	1.844
C(14)	-1.582	0.651	0.923
O(15)	-1.968	1.184	-0.225
H(16)	-0.567	-3.187	-0.831
H(17)	-0.616	-2.491	1.504
H(18)	0.020	-0.734	-1.761
H(19)	1.371	-1.475	2.266
H(20)	2.167	0.397	-2.266
H(21)	3.511	-0.342	1.754
H(22)	3.910	0.599	-0.509
H(23)	-2.306	-1.072	2.005
H(24)	-2.092	2.863	-1.369
H(25)	-0.533	2.680	-0.492
H(26)	-2.002	3.187	0.398

$BB^{H\text{-}OH1}$

total electronic energy E_{tot} = -722.562032927 (Hartree/Particle)
Zero-point correction= 0.201718
Thermal correction to Energy= 0.215786
Thermal correction to Enthalpy= 0.216730
Thermal correction to Gibbs Free Energy= 0.159829
Sum of electronic and zero-point Energies= -722.360314
Sum of electronic and thermal Energies= -722.346247
Sum of electronic and thermal Enthalpies= -722.345303
Sum of electronic and thermal Free Energies= -722.402204
ν = -31cm^{-1}

O(1)	-0.244	1.885	-0.727
C(2)	-0.214	0.642	-0.063

C(3)	-1.539	-0.091	-0.034
C(4)	-2.469	0.089	-1.068
C(5)	-1.830	-0.963	1.024
C(6)	-3.680	-0.603	-1.040
C(7)	-3.040	-1.656	1.044
C(8)	-3.964	-1.478	0.011
C(9)	0.927	-0.102	-0.883
N(10)	0.478	-1.383	-1.372
N(11)	0.131	-2.384	-1.692
C(12)	4.252	-1.597	0.014
O(13)	2.595	0.492	0.736
C(14)	2.277	-0.292	-0.112
O(15)	2.933	-1.342	-0.574
H(16)	-0.778	2.506	-0.209
H(17)	0.197	0.732	0.951
H(18)	-2.253	0.788	-1.870
H(19)	-1.124	-1.085	1.843
H(20)	-4.404	-0.453	-1.834
H(21)	-3.268	-2.322	1.870
H(22)	-4.909	-2.010	0.032
H(23)	1.116	0.491	-1.788
H(24)	4.601	-2.506	-0.469
H(25)	4.148	-1.732	1.091
H(26)	4.909	-0.755	-0.202

$BB^{Ph\text{-}H2}$

total electronic energy E_{tot} = -722.565880948 (Hartree/Particle)
Zero-point correction= 0.202155
Thermal correction to Energy= 0.216105
Thermal correction to Enthalpy= 0.217049
Thermal correction to Gibbs Free Energy= 0.160304
Sum of electronic and zero-point Energies= -722.363726
Sum of electronic and thermal Energies= -722.349776
Sum of electronic and thermal Enthalpies= -722.348832
Sum of electronic and thermal Free Energies= -722.405576
ν = -35cm^{-1}

O(1)	0.122	1.682	1.006
C(2)	0.256	0.386	0.465
C(3)	1.630	0.044	-0.050
C(4)	2.050	-1.294	-0.039
C(5)	2.478	1.042	-0.552
C(6)	3.313	-1.629	-0.524
C(7)	3.742	0.701	-1.029
C(8)	4.159	-0.634	-1.018
C(9)	-0.835	0.327	-0.715
N(10)	-1.403	1.634	-0.914
N(11)	-1.802	2.664	-0.991
C(12)	-4.283	-1.163	-0.677
O(13)	-1.682	-1.789	-0.004
C(14)	-1.967	-0.715	-0.457
O(15)	-3.146	-0.251	-0.831
H(16)	0.815	1.813	1.669
H(17)	-0.085	-0.387	1.164
H(18)	1.393	-2.066	0.352
H(19)	2.159	2.080	-0.551
H(20)	3.640	-2.664	-0.508
H(21)	4.404	1.474	-1.406
H(22)	5.145	-0.895	-1.389
H(23)	-0.354	0.084	-1.669
H(24)	-5.145	-0.592	-1.014
H(25)	-4.378	-1.447	0.371
H(26)	-4.123	-2.045	-1.298

$BB^{Ph\text{-}OH2}$

total electronic energy E_{tot} = -722.558588793 (Hartree/Particle)
Zero-point correction= 0.201688
Thermal correction to Energy= 0.215698
Thermal correction to Enthalpy= 0.216642
Thermal correction to Gibbs Free Energy= 0.160087
Sum of electronic and zero-point Energies= -722.356901
Sum of electronic and thermal Energies= -722.342891
Sum of electronic and thermal Enthalpies= -722.341947
Sum of electronic and thermal Free Energies= -722.398502
ν = -39cm^{-1}

O(1)	0.815	-2.818	-1.224
C(2)	0.814	-1.833	-0.224
C(3)	-0.456	-1.029	-0.116
C(4)	-0.900	-0.604	1.144
C(5)	-1.210	-0.729	-1.261
C(6)	-2.090	0.113	1.260
C(7)	-2.401	-0.017	-1.139
C(8)	-2.840	0.406	0.119
C(9)	2.109	-0.950	-0.664
N(10)	3.074	-0.980	0.396
N(11)	3.771	-0.994	1.259
C(12)	1.696	2.748	-0.258
O(13)	1.455	0.781	-2.175
C(14)	1.819	0.526	-1.063
O(15)	2.000	1.334	-0.030
H(16)	-0.054	-3.245	-1.242
H(17)	1.060	-2.255	0.762
H(18)	-0.331	-0.852	2.037
H(19)	-0.866	-1.052	-2.238
H(20)	-2.438	0.428	2.238
H(21)	-2.987	0.207	-2.024
H(22)	-3.771	0.957	0.210
H(23)	2.577	-1.475	-1.503
H(24)	1.962	3.245	0.672
H(25)	0.633	2.853	-0.474
H(26)	2.293	3.118	-1.092

BC^{Ph1}

total electronic energy E_{tot} = -722.560940757 (Hartree/Particle)
Zero-point correction= 0.199886
Thermal correction to Energy= 0.215027
Thermal correction to Enthalpy= 0.215972
Thermal correction to Gibbs Free Energy= 0.155732
Sum of electronic and zero-point Energies= -722.361054
Sum of electronic and thermal Energies= -722.345913
Sum of electronic and thermal Enthalpies= -722.344969
Sum of electronic and thermal Free Energies= -722.405209
ν = -309cm^{-1}

O(1)	0.172	-0.743	1.881
C(2)	-0.160	-1.043	0.552
C(3)	-1.342	-0.271	-0.039
C(4)	-1.712	0.974	0.488
C(5)	-2.066	-0.835	-1.101
C(6)	-2.820	1.637	-0.034
C(7)	-3.164	-0.159	-1.625
C(8)	-3.541	1.077	-1.092
C(9)	1.032	-0.639	-0.284
C(10)	3.481	1.925	0.923
O(11)	1.154	1.680	-0.514
C(12)	1.700	0.715	-0.044
O(13)	2.813	0.650	0.660
H(14)	-0.610	-0.869	2.438
H(15)	-0.335	-2.118	0.394
H(16)	-1.146	1.411	1.303
H(17)	-1.790	-1.808	-1.499
H(18)	-3.118	2.594	0.382
H(19)	-3.731	-0.599	-2.439
H(20)	-4.401	1.601	-1.498
H(21)	0.982	-0.925	-1.334
H(22)	4.401	1.657	1.437
H(23)	2.841	2.541	1.554
H(24)	3.686	2.432	-0.020
N(25)	2.309	-1.832	0.218
N(26)	2.962	-2.594	0.678

BC^{H2}

total electronic energy E_{tot} = -722.559136033 (Hartree/Particle)
Zero-point correction= 0.198746
Thermal correction to Energy= 0.214083
Thermal correction to Enthalpy= 0.215028
Thermal correction to Gibbs Free Energy= 0.154344
Sum of electronic and zero-point Energies= -722.360390
Sum of electronic and thermal Energies= -722.345053
Sum of electronic and thermal Enthalpies= -722.344108
Sum of electronic and thermal Free Energies= -722.404792

ν = -249cm^{-1}

O(1)	0.084	2.590	-1.236
C(2)	-0.126	1.208	-1.163
C(3)	0.966	0.404	-0.474
C(4)	1.752	1.009	0.513
C(5)	1.189	-0.932	-0.832
C(6)	2.747	0.270	1.154
C(7)	2.182	-1.666	-0.184
C(8)	2.960	-1.066	0.809
C(9)	-1.516	1.025	-0.665
C(10)	-2.815	-2.013	1.105
O(11)	-2.250	-0.965	-1.402
C(12)	-2.058	-0.342	-0.378
O(13)	-2.266	-0.672	0.867
H(14)	0.938	2.757	-1.661
H(15)	-0.293	0.762	-2.176
H(16)	1.599	2.053	0.769
H(17)	0.603	-1.397	-1.621
H(18)	3.359	0.740	1.916
H(19)	2.360	-2.698	-0.467
H(20)	3.739	-1.636	1.304
H(21)	-2.240	1.757	-1.027
H(22)	-2.994	-2.050	2.176
H(23)	-2.078	-2.757	0.801
H(24)	-3.739	-2.132	0.541
N(25)	-1.406	1.974	1.142
N(26)	-1.444	2.473	2.126

BC^{OH1}

total electronic energy E_{tot} = -722.558837069 (Hartree/Particle)
Zero-point correction= 0.200512
Thermal correction to Energy= 0.215412
Thermal correction to Enthalpy= 0.216356
Thermal correction to Gibbs Free Energy= 0.156522
Sum of electronic and zero-point Energies= -722.358325
Sum of electronic and thermal Energies= -722.343425
Sum of electronic and thermal Enthalpies= -722.342481
Sum of electronic and thermal Free Energies= -722.402315

ν = -335cm^{-1}

O(1)	-0.1777	-2.1452	-0.0382
C(2)	0.1231	-0.8561	0.4996
C(3)	1.5432	-0.4378	0.2474
C(4)	2.1743	-0.7478	-0.9658
C(5)	2.2302	0.2854	1.2299
C(6)	3.4842	-0.3293	-1.1904
C(7)	3.5387	0.7086	0.9963
C(8)	4.1642	0.4029	-0.2134
C(9)	-0.9245	-0.1787	-0.3727
C(10)	-4.5886	0.5260	-0.1415
O(11)	-2.7271	-1.3063	0.6975
C(12)	-2.3962	-0.3515	0.0322
O(13)	-3.1558	0.6139	-0.4415
H(14)	-0.9410	-2.5093	0.4471
H(15)	-0.1408	-0.7770	1.5579
H(16)	1.6604	-1.3447	-1.7137
H(17)	1.7538	0.5047	2.1824
H(18)	3.9775	-0.5813	-2.1234
H(19)	4.0715	1.2628	1.7620
H(20)	5.1851	0.7251	-0.3915
H(21)	-0.7085	-0.2386	-1.4393
H(22)	-5.0210	1.4164	-0.5907
H(23)	-4.7331	0.5131	0.9390
H(24)	-4.9925	-0.3817	-0.5902
N(25)	-0.6951	1.6135	-0.2524
N(26)	-0.4075	2.6693	-0.1065

C^{OH}

total electronic energy E_{tot} = -613.091518430 (Hartree/Particle)
Zero-point correction= 0.192966
Thermal correction to Energy= 0.205499
Thermal correction to Enthalpy= 0.206444
Thermal correction to Gibbs Free Energy= 0.152816
Sum of electronic and zero-point Energies= -612.898552
Sum of electronic and thermal Energies= -612.886019

Sum of electronic and thermal Enthalpies= -612.885075
Sum of electronic and thermal Free Energies= -612.938703

O(1)	1.9864	-2.2369	0.5291
C(2)	0.0546	-1.1719	-0.2394
C(3)	-1.1771	-0.5493	-0.0736
C(4)	-1.4456	0.3955	0.9720
C(5)	-2.2213	-0.8733	-1.0036
C(6)	-2.6868	0.9866	1.0614
C(7)	-3.4616	-0.2773	-0.8972
C(8)	-3.6918	0.6492	0.1328
C(9)	1.2955	-1.0305	0.5594
C(10)	2.3765	2.4138	-0.5405
O(11)	3.3491	-0.1262	-0.2997
C(12)	2.2007	0.1162	-0.0242
O(13)	1.5721	1.2755	-0.0976
H(14)	2.9076	-2.0380	0.2744
H(15)	0.1558	-1.8938	-1.0501
H(16)	-0.6715	0.6455	1.6878
H(17)	-2.0201	-1.5934	-1.7910
H(18)	-2.8990	1.7014	1.8487
H(19)	-4.2531	-0.5214	-1.5969
H(20)	-4.6701	1.1129	0.2212
H(21)	1.0743	-0.7174	1.5924
H(22)	1.6838	3.2512	-0.5788
H(23)	2.7984	2.2032	-1.5237
H(24)	3.1751	2.5964	0.1793

CC1

total electronic energy E_{tot} = -613.029853748 (Hartree/Particle)
Zero-point correction= 0.191327
Thermal correction to Energy= 0.203693
Thermal correction to Enthalpy= 0.204637
Thermal correction to Gibbs Free Energy= 0.150513
Sum of electronic and zero-point Energies= -612.838527
Sum of electronic and thermal Energies= -612.826161
Sum of electronic and thermal Enthalpies= -612.825216
Sum of electronic and thermal Free Energies= -612.879340
ν = -200cm^{-1}

O(1)	-0.2994	-1.7305	1.3053
C(2)	-0.0760	-0.4114	0.7581
C(3)	1.3088	-0.0623	0.2964
C(4)	1.9856	-0.8731	-0.6392
C(5)	1.9377	1.0856	0.8088
C(6)	3.2819	-0.5535	-1.0275
C(7)	3.2306	1.4047	0.4091
C(8)	3.9025	0.5872	-0.5075
C(9)	-1.0137	-0.6049	-0.3640
C(10)	-4.0961	1.4838	-0.2324
O(11)	-3.2013	-1.1541	-0.3106
C(12)	-2.4425	-0.2061	-0.3441
O(13)	-2.6855	1.0769	-0.2851
H(14)	0.3972	-2.3342	0.9902
H(15)	-0.4452	0.3050	1.4929
H(16)	1.5171	-1.7614	-1.0585
H(17)	1.4187	1.7125	1.5277
H(18)	3.8062	-1.1847	-1.7368
H(19)	3.7200	2.2839	0.8145
H(20)	4.9109	0.8406	-0.8182
H(21)	-0.7156	-1.2644	-1.1761
H(22)	-4.0752	2.5655	-0.3350
H(23)	-4.5160	1.1826	0.7277
H(24)	-4.6413	1.0155	-1.0523

CC2

total electronic energy E_{tot} = -613.068966855 (Hartree/Particle)
Zero-point correction= 0.191676
Thermal correction to Energy= 0.204144
Thermal correction to Enthalpy= 0.205088
Thermal correction to Gibbs Free Energy= 0.151873
Sum of electronic and zero-point Energies= -612.877291
Sum of electronic and thermal Energies= -612.864823
Sum of electronic and thermal Enthalpies= -612.863879
Sum of electronic and thermal Free Energies= -612.917094
ν = -271cm^{-1}

O(1)	-2.3714	-2.2124	-0.2230
C(2)	-0.4128	-1.0910	0.3937
C(3)	0.9240	-0.5792	0.1752
C(4)	1.4928	-0.4326	-1.1089
C(5)	1.6925	-0.2534	1.3137
C(6)	2.7915	0.0374	-1.2426
C(7)	2.9930	0.2151	1.1718
C(8)	3.5414	0.3635	-0.1050
C(9)	-1.3861	-1.3986	-0.5696
C(10)	-1.8269	2.6820	-0.3618
O(11)	-2.6957	0.3840	1.0490
C(12)	-1.8107	0.4087	0.2626
O(13)	-1.2757	1.3167	-0.4939
H(14)	-3.0633	-2.2662	-0.9007
H(15)	-0.6639	-1.4314	1.3975
H(16)	0.9344	-0.7078	-1.9979
H(17)	1.2638	-0.3752	2.3045
H(18)	3.2308	0.1379	-2.2292
H(19)	3.5805	0.4584	2.0505
H(20)	4.5595	0.7225	-0.2169
H(21)	-1.2745	-1.1182	-1.6159
H(22)	-1.6331	3.0413	0.6488
H(23)	-2.8968	2.6557	-0.5686
H(24)	-1.2878	3.2654	-1.1034

$AB^{H2\cdot}$

total electronic energy E_{tot} = -722.563918281 (Hartree/Particle)
Zero-point correction= 0.201573
Thermal correction to Energy= 0.215842
Thermal correction to Enthalpy= 0.216786
Thermal correction to Gibbs Free Energy= 0.158702
Sum of electronic and zero-point Energies= -722.362346
Sum of electronic and thermal Energies= -722.348077
Sum of electronic and thermal Enthalpies= -722.347132
Sum of electronic and thermal Free Energies= -722.405217
ν = -221cm^{-1}

O(1)	-0.3988	-1.6104	1.0253
C(2)	0.1921	-1.2407	-0.1111
C(3)	1.5134	-0.6271	0.0085
C(4)	2.3467	-0.5781	-1.1258
C(5)	1.9613	-0.0989	1.2350
C(6)	3.6159	-0.0203	-1.0299
C(7)	3.2354	0.4549	1.3211
C(8)	4.0597	0.4959	0.1931
C(9)	-1.0325	0.1492	-0.9200
C(10)	-4.4026	0.5679	0.6142
O(11)	-2.7743	-1.3672	-0.4292
C(12)	-2.4140	-0.2091	-0.4103
O(13)	-3.0780	0.8334	0.0559
N(14)	-0.5773	1.3805	-0.5459
N(15)	-0.0647	2.2797	-0.1180
H(16)	-1.2103	-2.1127	0.8275
H(17)	0.0287	-1.8942	-0.9694
H(18)	2.0082	-0.9975	-2.0703
H(19)	1.3253	-0.1570	2.1118
H(20)	4.2645	0.0037	-1.8990
H(21)	3.5891	0.8484	2.2681
H(22)	5.0537	0.9254	0.2668
H(23)	-0.8834	-0.0059	-1.9875
H(24)	-4.7666	1.5388	0.9413
H(25)	-4.3148	-0.1248	1.4519
H(26)	-5.0443	0.1452	-0.1591

AB^{H2}

total electronic energy E_{tot} = -722.560435321 (Hartree/Particle)
Zero-point correction= 0.201248
Thermal correction to Energy= 0.215733
Thermal correction to Enthalpy= 0.216677
Thermal correction to Gibbs Free Energy= 0.157930
Sum of electronic and zero-point Energies= -722.359187
Sum of electronic and thermal Energies= -722.344703
Sum of electronic and thermal Enthalpies= -722.343759
Sum of electronic and thermal Free Energies= -722.402506
ν = -246cm^{-1}

O(1)	0.3277	-0.8747	1.5014
C(2)	-0.1236	0.2156	0.8784
C(3)	-1.5239	0.2027	0.4863
C(4)	-2.1357	1.4166	0.1125
C(5)	-2.2679	-0.9945	0.4861
C(6)	-3.4746	1.4312	-0.2556
C(7)	-3.6078	-0.9678	0.1161
C(8)	-4.2090	0.2392	-0.2568
C(9)	0.9699	0.2417	-0.8780
C(10)	4.3278	-0.0019	0.6756
O(11)	2.7260	1.8131	-0.5823
C(12)	2.3420	0.6829	-0.4330
O(13)	2.9684	-0.3053	0.2295
N(14)	0.8596	-1.0580	-1.2494
N(15)	0.6904	-2.1575	-1.3929
H(16)	1.2464	-0.7623	1.7974
H(17)	0.3055	1.1754	1.1704
H(18)	-1.5641	2.3413	0.1234
H(19)	-1.8024	-1.9218	0.8012
H(20)	-3.9506	2.3651	-0.5341
H(21)	-4.1887	-1.8839	0.1256
H(22)	-5.2562	0.2536	-0.5416
H(23)	0.4652	0.9124	-1.5674
H(24)	4.6804	-0.9156	1.1487
H(25)	4.3095	0.8301	1.3806
H(26)	4.9439	0.2554	-0.1863

$AB^{Ph1'}$

total electronic energy E_{tot} = -722.559724832 (Hartree/Particle)
Zero-point correction= 0.201161
Thermal correction to Energy= 0.215623
Thermal correction to Enthalpy= 0.216567
Thermal correction to Gibbs Free Energy= 0.157960
Sum of electronic and zero-point Energies= -722.358564
Sum of electronic and thermal Energies= -722.344102
Sum of electronic and thermal Enthalpies= -722.343158
Sum of electronic and thermal Free Energies= -722.401765
ν = -209cm^{-1}

O(1)	-0.3516	-0.4190	1.8507
C(2)	0.2972	0.4378	1.0725
C(3)	1.5801	0.1069	0.4478
C(4)	1.8909	-1.1992	0.0209
C(5)	2.5288	1.1368	0.3062
C(6)	3.1445	-1.4670	-0.5158
C(7)	3.7837	0.8573	-0.2259
C(8)	4.0915	-0.4428	-0.6353
C(9)	-0.9742	0.6536	-0.5635
N(10)	-1.5805	1.8721	-0.4907
N(11)	-2.0330	2.8815	-0.3082
C(12)	-4.1256	-1.2524	-0.0714
O(13)	-1.4475	-1.6557	-0.4389
C(14)	-1.9003	-0.5326	-0.4369
O(15)	-3.1646	-0.1735	-0.2725
H(16)	-0.1469	-1.3417	1.6201
H(17)	0.1774	1.4556	1.4384
H(18)	1.1514	-1.9938	0.0677
H(19)	2.2931	2.1441	0.6391
H(20)	3.3858	-2.4716	-0.8461
H(21)	4.5211	1.6477	-0.3164
H(22)	5.0698	-0.6600	-1.0518
H(23)	-0.2734	0.6170	-1.3929
H(24)	-5.0882	-0.7559	0.0253
H(25)	-3.8740	-1.8027	0.8360
H(26)	-4.1114	-1.9205	-0.9329

AB^{Ph1}

total electronic energy E_{tot} = -722.557211384 (Hartree/Particle)
Zero-point correction= 0.200994
Thermal correction to Energy= 0.215522
Thermal correction to Enthalpy= 0.216466
Thermal correction to Gibbs Free Energy= 0.157575
Sum of electronic and zero-point Energies= -722.356218
Sum of electronic and thermal Energies= -722.341689
Sum of electronic and thermal Enthalpies= -722.340745

Sum of electronic and thermal Free Energies= -722.399637

ν = -231cm^{-1}

O(1)	-0.4310	-0.0293	1.8706
C(2)	0.1983	0.7811	1.0129
C(3)	1.4663	0.3027	0.4831
C(4)	1.8025	-1.0650	0.5126
C(5)	2.3692	1.2430	-0.0545
C(6)	3.0347	-1.4764	0.0191
C(7)	3.5981	0.8208	-0.5434
C(8)	3.9292	-0.5391	-0.5085
C(9)	-1.0090	0.8034	-0.6536
N(10)	-1.9074	1.8154	-0.5009
N(11)	-2.6017	2.6628	-0.2547
C(12)	-3.4535	-1.8858	0.0639
O(13)	-1.0153	-1.5236	-1.1148
C(14)	-1.6121	-0.5849	-0.6552
O(15)	-2.7904	-0.5905	-0.0293
H(16)	-1.1457	0.4196	2.3466
H(17)	0.1177	1.8527	1.2030
H(18)	1.1057	-1.7858	0.9229
H(19)	2.1135	2.2998	-0.0689
H(20)	3.3013	-2.5275	0.0441
H(21)	4.3008	1.5434	-0.9440
H(22)	4.8898	-0.8682	-0.8919
H(23)	-0.3181	1.0135	-1.4656
H(24)	-4.4042	-1.6827	0.5517
H(25)	-2.8436	-2.5681	0.6573
H(26)	-3.6049	-2.2944	-0.9357

BF_4^--associated Pathway

$A^Z \cdot MDA \cdot BF_4^-$

total electronic energy E_{tot} = -1147.26030597 (Hartree/Particle)

Zero-point correction= 0.215585

Thermal correction to Energy= 0.236959

Thermal correction to Enthalpy= 0.237903

Thermal correction to Gibbs Free Energy= 0.160099

Sum of electronic and zero-point Energies= -1147.044721

Sum of electronic and thermal Energies= -1147.023347

Sum of electronic and thermal Enthalpies= -1147.022403

Sum of electronic and thermal Free Energies= -1147.100207

O(1)	1.5694	-2.1601	-0.5260
C(2)	1.5480	-0.9299	-0.2386
C(3)	2.7692	-0.1852	-0.0913
C(4)	4.0306	-0.8083	-0.2136
C(5)	2.6767	1.1945	0.1858
C(6)	5.1829	-0.0545	-0.0570
C(7)	3.8419	1.9396	0.3388
C(8)	5.0869	1.3174	0.2192
H(9)	0.5858	-2.6181	-0.6028
H(10)	0.5872	-0.4267	-0.0934
H(11)	4.0787	-1.8710	-0.4251
H(12)	1.6957	1.6535	0.2638
H(13)	6.1576	-0.5229	-0.1462
H(14)	3.7837	3.0021	0.5510
H(15)	5.9938	1.9024	0.3414
C(16)	-2.7467	0.8660	-0.0956
C(17)	-1.1511	4.1474	-0.0032
O(18)	-0.4917	1.5704	-0.1079
C(19)	-1.6865	1.8456	-0.0739
O(20)	-2.1495	3.1195	-0.0187
N(21)	-3.9951	1.2639	-0.0927
N(22)	-5.0803	1.5989	-0.0901
H(23)	-2.5686	-0.2027	-0.1168
H(24)	-1.7012	5.0881	0.0055
H(25)	-0.5158	4.0867	-0.8906
H(26)	-0.5259	4.0678	0.8902
F(27)	-2.6650	-2.2379	-0.5283
B(28)	-1.5967	-2.6952	0.2200
F(29)	-0.9626	-1.6278	0.8767
F(30)	-1.8996	-3.7239	1.0574
F(31)	-0.5613	-3.1835	-0.7612

AB^H

total electronic energy E_{tot} = -1147.24174298 (Hartree/Particle)

Zero-point correction= 0.217614
Thermal correction to Energy= 0.237453
Thermal correction to Enthalpy= 0.238397
Thermal correction to Gibbs Free Energy= 0.166942
Sum of electronic and zero-point Energies= -1147.024129
Sum of electronic and thermal Energies= -1147.004290
Sum of electronic and thermal Enthalpies= -1147.003346
Sum of electronic and thermal Free Energies= -1147.074801
ν = -194cm^{-1}

O(1)	0.7677	-1.5725	0.7658
C(2)	0.0922	-0.9575	-0.1986
C(3)	-1.3760	-1.1707	-0.1693
C(4)	-2.0114	-1.5963	1.0075
C(5)	-2.1302	-0.9763	-1.3365
C(6)	-3.3863	-1.8140	1.0155
C(7)	-3.5063	-1.1980	-1.3228
C(8)	-4.1358	-1.6132	-0.1473
H(9)	1.7453	-1.6504	0.5132
H(10)	0.5639	-0.9509	-1.1830
H(11)	-1.4178	-1.7747	1.8973
H(12)	-1.6399	-0.6516	-2.2488
H(13)	-3.8739	-2.1495	1.9256
H(14)	-4.0838	-1.0555	-2.2308
H(15)	-5.2071	-1.7903	-0.1393
C(16)	0.3934	0.9419	0.0315
C(17)	-2.7069	2.9420	0.1633
O(18)	-0.9533	1.9639	-1.6314
C(19)	-0.7549	1.7741	-0.4555
O(20)	-1.5278	2.2032	0.5548
N(21)	0.6396	1.0367	1.3727
N(22)	0.8273	0.8937	2.4639
H(23)	1.3317	1.0358	-0.5292
H(24)	-3.1782	3.2474	1.0959
H(25)	-3.3721	2.2983	-0.4153
H(26)	-2.4273	3.8112	-0.4345
F(27)	3.1544	0.4962	0.7626
B(28)	3.5207	-0.2827	-0.3531
F(29)	2.7057	0.1247	-1.4468
F(30)	4.8458	-0.2169	-0.6423
F(31)	3.1306	-1.6504	-0.0493

B^H

total electronic energy E_{tot} = -1147.24320338 (Hartree/Particle)
Zero-point correction= 0.218545
Thermal correction to Energy= 0.238748
Thermal correction to Enthalpy= 0.239692
Thermal correction to Gibbs Free Energy= 0.167014
Sum of electronic and zero-point Energies= -1147.024659
Sum of electronic and thermal Energies= -1147.004456
Sum of electronic and thermal Enthalpies= -1147.003511
Sum of electronic and thermal Free Energies= -1147.076190

O(1)	0.6417	-1.8198	0.1241
C(2)	-0.0686	-0.8519	-0.5314
C(3)	-1.5545	-1.0640	-0.3673
C(4)	-2.0463	-1.7556	0.7480
C(5)	-2.4520	-0.5822	-1.3300
C(6)	-3.4186	-1.9443	0.9058
C(7)	-3.8243	-0.7741	-1.1688
C(8)	-4.3103	-1.4505	-0.0487
H(9)	1.5882	-1.8225	-0.1821
H(10)	0.2096	-0.7204	-1.5850
H(11)	-1.3473	-2.1706	1.4656
H(12)	-2.0769	-0.0613	-2.2056
H(13)	-3.7911	-2.4878	1.7689
H(14)	-4.5112	-0.4063	-1.9250
H(15)	-5.3783	-1.6045	0.0731
C(16)	0.3853	0.6479	0.0524
C(17)	-2.0959	3.3920	0.4146
O(18)	-0.6859	2.0989	-1.4940
C(19)	-0.5464	1.7841	-0.3394
O(20)	-1.1596	2.3281	0.7167
N(21)	0.4993	0.5100	1.4477
N(22)	0.5682	0.2422	2.5215
H(23)	1.4166	0.8271	-0.3330

H(24)	-2.4583	3.7375	1.3808
H(25)	-2.9143	2.9999	-0.1915
H(26)	-1.5895	4.1947	-0.1237
F(27)	2.9895	-0.1245	1.0402
B(28)	3.5339	-0.3134	-0.2516
F(29)	2.9359	0.6788	-1.0946
F(30)	4.8905	-0.2413	-0.2693
F(31)	3.0652	-1.5852	-0.7267

BC^H

total electronic energy E_{tot} = -1147.22467143 (Hartree/Particle)
Zero-point correction= 0.214400
Thermal correction to Energy= 0.235412
Thermal correction to Enthalpy= 0.236356
Thermal correction to Gibbs Free Energy= 0.161000
Sum of electronic and zero-point Energies= -1147.010271
Sum of electronic and thermal Energies= -1146.989260
Sum of electronic and thermal Enthalpies= -1146.988315
Sum of electronic and thermal Free Energies= -1147.063671
ν = -150cm^{-1}

O(1)	0.4573	-1.8305	-0.6375
C(2)	-0.3044	-0.7116	-0.8768
C(3)	-1.7584	-0.9471	-0.4923
C(4)	-2.0521	-1.8660	0.5210
C(5)	-2.7981	-0.2631	-1.1336
C(6)	-3.3761	-2.0773	0.9054
C(7)	-4.1208	-0.4783	-0.7442
C(8)	-4.4116	-1.3822	0.2782
C(9)	0.2974	0.5677	-0.4066
C(10)	-1.5495	3.5916	0.7249
O(11)	-0.7151	2.2995	-1.5180
C(12)	-0.4901	1.8364	-0.4190
O(13)	-0.8263	2.3308	0.7565
N(14)	0.6216	0.0965	1.6217
N(15)	0.9306	-0.0935	2.6632
H(16)	1.4113	-1.6469	-0.8500
H(17)	-0.2852	-0.3965	-1.9622
H(18)	-1.2441	-2.4211	0.9830
H(19)	-2.5811	0.4277	-1.9429
H(20)	-3.5982	-2.7926	1.6914
H(21)	-4.9227	0.0491	-1.2518
H(22)	-5.4416	-1.5542	0.5758
H(23)	1.3938	0.7006	-0.4935
H(24)	-1.6720	3.8719	1.7686
H(25)	-2.5175	3.4470	0.2427
H(26)	-0.9694	4.3391	0.1822
F(27)	3.1202	-1.1207	0.9604
B(28)	3.5141	-0.4040	-0.1642
F(29)	3.0408	0.9446	-0.0307
F(30)	4.8507	-0.4427	-0.4152
F(31)	2.7711	-0.9417	-1.2997

C^H

total electronic energy E_{tot} = -1037.80643559 (Hartree/Particle)
Zero-point correction= 0.207456
Thermal correction to Energy= 0.225894
Thermal correction to Enthalpy= 0.226838
Thermal correction to Gibbs Free Energy= 0.155413
Sum of electronic and zero-point Energies= -1037.598980
Sum of electronic and thermal Energies= -1037.580542
Sum of electronic and thermal Enthalpies= -1037.579598
Sum of electronic and thermal Free Energies= -1037.651023

O(1)	0.2443	-0.8640	-0.8930
C(2)	-0.4797	-0.3040	-0.0418
C(3)	-1.9100	-0.6340	-0.0063
C(4)	-2.8191	0.1136	0.7672
C(5)	-2.3765	-1.7179	-0.7766
C(6)	-4.1701	-0.2205	0.7636
C(7)	-3.7238	-2.0532	-0.7622
C(8)	-4.6212	-1.3047	0.0073
C(9)	0.1052	0.7047	0.9238
C(10)	0.5058	3.6617	-1.2749
O(11)	-0.8041	2.9583	0.9566

C(12)	-0.1012	2.1342	0.4168
O(13)	0.5996	2.3380	-0.7072
H(14)	1.4701	-0.6188	-0.9139
H(15)	1.1764	0.5156	1.0361
H(16)	-2.4823	0.9699	1.3414
H(17)	-1.6661	-2.2850	-1.3673
H(18)	-4.8706	0.3631	1.3519
H(19)	-4.0788	-2.8953	-1.3474
H(20)	-5.6747	-1.5681	0.0164
H(21)	-0.3757	0.6291	1.8979
H(22)	1.1163	3.6335	-2.1758
H(23)	0.8913	4.4012	-0.5702
H(24)	-0.5327	3.8996	-1.5145
F(25)	4.5988	-1.1979	-0.1190
B(26)	3.3130	-1.1739	0.2856
F(27)	3.0501	-0.3606	1.3645
F(28)	2.5437	-0.3964	-0.9221
F(29)	2.6615	-2.3689	0.3284