1	1	0	2.048134	0.488828	-0.000005
2	6	0	-0.094425	0.350636	0.000007
3	6	0	1.183452	-0.170393	-0.000010
4	8	0	-1.231412	-0.226140	-0.000004
5	1	0	-0.088397	1.483329	0.000011
6	1	0	1.357401	-1.244493	0.000036

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.040412	E(Thermal)=	0.043914
E(QCISD(T))=	-152.758076	E(Empiric)=	-0.057474
DE(Plus)=	-0.042371	DE(2DF)=	-0.125416
E(Delta-G3)=	-0.188164	E(G3-Empiric)=	-0.057474
G3(0 K)=	-153.131090	G3 Energy=	-153.127588
G3 Enthalpy=	-153.126644	G3 Free Energy=	-153.155283

COCH3- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.633625	-0.604091	0.883980
2	6	0	-0.974380	-0.643535	0.000000
3	1	0	-0.399182	-1.593122	0.000000
4	6	0	0.000000	0.668141	0.000000
5	1	0	-1.633625	-0.604091	-0.883980
6	8	0	1.189089	0.331708	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.039086	E(Thermal)=	0.043253
E(SCF)=	-152.316916	DE(MP2)=	-0.572575
DE(CBS)=	-0.056991	DE(MP34)=	-0.024947
DE(CCSD)=	-0.017353	DE(Int)=	0.019461
DE(Empirical)=	-0.027295		
CBS-Q (0 K)=	-152.957530	CBS-Q Energy=	-152.953362
CBS-Q Enthalpy=	-152.952418	CBS-Q Free Energy=	-152.982738

COCH3- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.634208	-0.597033	0.888067
2	6	0	-0.976728	-0.633130	0.000000
3	1	0	-0.392896	-1.576713	0.000000
4	6	0	0.000000	0.674697	0.000000
5	1	0	-1.634208	-0.597033	-0.888067
6	8	0	1.190210	0.315173	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.039358	E(Thermal)=	0.043473
E(SCF)=	-152.331905	DE(SCF)=	-0.000890
DE(MP2)=	-0.603325	DE(CBS)=	-0.045085

DE(QCI)=	-0.046155	DE(Int)=	0.016648
DE(Core)=	-0.166622	DE(Empirical)=	-0.007540
CBS-APNO (0 K)=	-153.145517	CBS-APNO Energy=	-153.141401
CBS-APNO Enthalpy=	-153.140457	CBS-APNO Free Energy=	-153.170778

COCH3- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.643709	-0.588124	0.881093
2	6	0	-0.981958	-0.617176	0.000000
3	1	0	-0.420476	-1.568308	0.000000
4	6	0	0.000000	0.684464	0.000000
5	1	0	-1.643709	-0.588124	-0.881093
6	8	0	1.199955	0.292603	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.038490	E(Thermal)=	0.042657
E(QCISD(T))=	-152.708888	E(Empiric)=	-0.057474
DE(Plus)=	-0.052528	DE(2DF)=	-0.125084
E(Delta-G3)=	-0.183090	E(G3-Empiric)=	-0.057474
G3(0 K)=	-153.088574	G3 Energy=	-153.084408
G3 Enthalpy=	-153.083463	G3 Free Energy=	-153.113839

nitrous acid CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.013696	-0.401591	0.000000
2	7	0	0.000000	0.547417	0.000000
3	8	0	1.084392	0.081668	0.000000
4	1	0	-0.565563	-1.272538	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.020054	E(Thermal)=	0.023208
E(SCF)=	-204.716656	DE(MP2)=	-0.675116
DE(CBS)=	-0.066567	DE(MP34)=	-0.007388
DE(CCSD)=	-0.018598	DE(Int)=	0.019907
DE(Empirical)=	-0.029924		
CBS-Q (0 K)=	-205.474288	CBS-Q Energy=	-205.471134
CBS-Q Enthalpy=	-205.470190	CBS-Q Free Energy=	-205.498264

nitrous acid CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.012067	-0.389333	0.000000
2	7	0	0.000000	0.548013	0.000000
3	8	0	1.080976	0.065620	0.000000
4	1	0	-0.551268	-1.246389	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.021443	E(Thermal)=	0.024537
E(SCF)=	-204.741318	DE(SCF)=	-0.001668
DE(MP2)=	-0.709509	DE(CBS)=	-0.054355
DE(QCI)=	-0.032126	DE(Int)=	0.017553
DE(Core)=	-0.175524	DE(Empirical)=	-0.008510
CBS-APNO (0 K)=	-205.684014	CBS-APNO Energy=	-205.680920
CBS-APNO Enthalpy=	-205.679976	CBS-APNO Free Energy=	-205.707871

nitrous acid G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.025730	-0.375233	0.000000
2	7	0	0.000000	0.555823	0.000000
3	8	0	1.096397	0.045475	0.000000
4	1	0	-0.565330	-1.252696	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.020669	E(Thermal)=	0.023782
E(QCISD(T))=	-205.193368	E(Empiric)=	-0.057474
DE(Plus)=	-0.016073	DE(2DF)=	-0.140148
E(Delta-G3)=	-0.215670	E(G3-Empiric)=	-0.057474
G3(0 K)=	-205.602064	G3 Energy=	-205.598951
G3 Enthalpy=	-205.598007	G3 Free Energy=	-205.625942

NO2- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.072837	-0.204398	0.000000
2	7	0	0.000000	0.466556	0.000000
3	8	0	-1.072837	-0.203839	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.007825	E(Thermal)=	0.010758
E(SCF)=	-204.155042	DE(MP2)=	-0.690073
DE(CBS)=	-0.070042	DE(MP34)=	0.000762
DE(CCSD)=	-0.020598	DE(Int)=	0.020974
DE(Empirical)=	-0.029831		
CBS-Q (0 K)=	-204.936025	CBS-Q Energy=	-204.933092
CBS-Q Enthalpy=	-204.932148	CBS-Q Free Energy=	-204.959709

NO2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.069219	-0.203588	0.000000
2	7	0	0.000000	0.465318	0.000000

3	8	0	-1.069219	-0.203565	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.008564	E(Thermal)=	0.011477
E(SCF)=	-204.178848	DE(SCF)=	-0.001788
DE(MP2)=	-0.727066	DE(CBS)=	-0.054979
DE(QCI)=	-0.025309	DE(Int)=	0.018056
DE(Core)=	-0.175308	DE(Empirical)=	-0.008356
CBS-APNO (0 K)=	-205.145034	CBS-APNO Energy=	-205.142121
CBS-APNO Enthalpy=	-205.141177	CBS-APNO Free Energy=	-205.168609

NO2- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.082577	-0.208340	0.000000
2	7	0	0.000000	0.476204	0.000000
3	8	0	-1.082577	-0.208339	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.008298	E(Thermal)=	0.011223
E(QCISD(T))=	-204.618228	E(Empiric)=	-0.057474
DE(Plus)=	-0.052473	DE(2DF)=	-0.132140
E(Delta-G3)=	-0.211360	E(G3-Empiric)=	-0.057474
G3(0 K)=	-205.063377	G3 Energy=	-205.060452
G3 Enthalpy=	-205.059508	G3 Free Energy=	-205.086974

Benzene CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.478169	0.000000
2	6	0	0.000000	1.393785	0.000000
3	6	0	0.000000	-1.393785	0.000000
4	6	0	1.207053	0.696892	0.000000
5	6	0	-1.207053	0.696892	0.000000
6	6	0	-1.207053	-0.696892	0.000000
7	6	0	1.207053	-0.696892	0.000000
8	1	0	2.146157	1.239084	0.000000
9	1	0	-2.146157	1.239084	0.000000
10	1	0	-2.146157	-1.239084	0.000000
11	1	0	2.146157	-1.239084	0.000000
12	1	0	0.000000	-2.478169	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.099177	E(Thermal)=	0.103609
E(SCF)=	-230.773822	DE(MP2)=	-0.939413
DE(CBS)=	-0.090100	DE(MP34)=	-0.035529
DE(CCSD)=	-0.038133	DE(Int)=	0.031320
DE(Empirical)=	-0.043124		

CBS-Q (0 K)=	-231.789624	CBS-Q Energy=	-231.785192
CBS-Q Enthalpy=	-231.784248	CBS-Q Free Energy=	-231.814754

Benzene CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.486926	0.000000
2	6	0	0.000000	1.399840	0.000000
3	6	0	0.000000	-1.399840	0.000000
4	6	0	1.212297	0.699920	0.000000
5	6	0	-1.212297	0.699920	0.000000
6	6	0	-1.212297	-0.699920	0.000000
7	6	0	1.212297	-0.699920	0.000000
8	1	0	2.153741	1.243463	0.000000
9	1	0	-2.153741	1.243463	0.000000
10	1	0	-2.153741	-1.243463	0.000000
11	1	0	2.153741	-1.243463	0.000000
12	1	0	0.000000	-2.486926	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.098601	E(Thermal)=	0.102995
E(SCF)=	-230.793078	DE(SCF)=	-0.001710
DE(MP2)=	-0.978892	DE(CBS)=	-0.073108
DE(QCI)=	-0.078344	DE(Int)=	0.027232
DE(Core)=	-0.325199	DE(Empirical)=	-0.012051
CBS-APNO (0 K)=	-232.136548	CBS-APNO Energy=	-232.132154
CBS-APNO Enthalpy=	-232.131210	CBS-APNO Free Energy=	-232.161641

Benzene G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.482375	0.000000
2	6	0	0.000000	1.395242	0.000000
3	6	0	0.000000	-1.395242	0.000000
4	6	0	1.208315	0.697621	0.000000
5	6	0	-1.208315	0.697621	0.000000
6	6	0	-1.208315	-0.697621	0.000000
7	6	0	1.208315	-0.697621	0.000000
8	1	0	2.149800	1.241188	0.000000
9	1	0	-2.149800	1.241188	0.000000
10	1	0	-2.149800	-1.241188	0.000000
11	1	0	2.149800	-1.241188	0.000000
12	1	0	0.000000	-2.482375	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.096132	E(Thermal)=	0.100637
E(QCISD(T))=	-231.531280	E(Empiric)=	-0.095790
DE(Plus)=	-0.014041	DE(2DF)=	-0.181857
E(Delta-G3)=	-0.325340	E(G3-Empiric)=	-0.095790

G3(0 K)=	-232.052176	G3 Energy=	-232.047671
G3 Enthalpy=	-232.046727	G3 Free Energy=	-232.077317

C6H5- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.149611	-1.189697
2	6	0	0.000000	1.197991	-0.649921
3	6	0	0.000000	-1.172050	0.751695
4	6	0	0.000000	1.172050	0.751695
5	6	0	0.000000	0.000000	-1.368951
6	6	0	0.000000	-1.197991	-0.649921
7	6	0	0.000000	0.000000	1.555924
8	1	0	0.000000	2.153029	1.247044
9	1	0	0.000000	0.000000	-2.457817
10	1	0	0.000000	-2.149611	-1.189697
11	1	0	0.000000	-2.153029	1.247044

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.083589	E(Thermal)=	0.088106
E(SCF)=	-230.110297	DE(MP2)=	-0.954389
DE(CBS)=	-0.091503	DE(MP34)=	-0.030289
DE(CCSD)=	-0.040965	DE(Int)=	0.032325
DE(Empirical)=	-0.042294		
CBS-Q (0 K)=	-231.153823	CBS-Q Energy=	-231.149306
CBS-Q Enthalpy=	-231.148361	CBS-Q Free Energy=	-231.180671

C6H5- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.154931	-1.191485
2	6	0	0.000000	1.200688	-0.653674
3	6	0	0.000000	-1.173502	0.752867
4	6	0	0.000000	1.173502	0.752867
5	6	0	0.000000	0.000000	-1.377537
6	6	0	0.000000	-1.200688	-0.653674
7	6	0	0.000000	0.000000	1.572525
8	1	0	0.000000	2.156547	1.245759
9	1	0	0.000000	0.000000	-2.468785
10	1	0	0.000000	-2.154931	-1.191485
11	1	0	0.000000	-2.156547	1.245759

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.083852	E(Thermal)=	0.088268
E(SCF)=	-230.129413	DE(SCF)=	-0.001593
DE(MP2)=	-0.995147	DE(CBS)=	-0.074339
DE(QCI)=	-0.075425	DE(Int)=	0.028019
DE(Core)=	-0.324340	DE(Empirical)=	-0.011717
CBS-APNO (0 K)=	-231.500105	CBS-APNO Energy=	-231.495689

CBS-APNO Enthalpy= -231.494745 CBS-APNO Free Energy= -231.526866

C6H5- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	2.151545	-1.191971
2	6	0	0.000000	1.197886	-0.653323
3	6	0	0.000000	-1.164479	0.751689
4	6	0	0.000000	1.164479	0.751689
5	6	0	0.000000	0.000000	-1.371239
6	6	0	0.000000	-1.197886	-0.653323
7	6	0	0.000000	0.000000	1.568165
8	1	0	0.000000	2.150291	1.242491
9	1	0	0.000000	0.000000	-2.462995
10	1	0	0.000000	-2.151545	-1.191971
11	1	0	0.000000	-2.150291	1.242491

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.081758	E(Thermal)=	0.086275
E(QCISD(T))=	-230.853314	E(Empiric)=	-0.095790
DE(Plus)=	-0.043886	DE(2DF)=	-0.184164
E(Delta-G3)=	-0.319684	E(G3-Empiric)=	-0.095790
G3(0 K)=	-231.415081	G3 Energy=	-231.410564
G3 Enthalpy=	-231.409620	G3 Free Energy=	-231.441888

Nitric Acid CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.152388	-0.514803	0.000001
2	7	0	-0.152550	0.032296	-0.000006
3	8	0	-0.213641	1.240133	0.000002
4	8	0	-1.020179	-0.787797	0.000002
5	1	0	1.719309	0.273665	0.000002

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026185	E(Thermal)=	0.029730
E(SCF)=	-279.549817	DE(MP2)=	-0.926552
DE(CBS)=	-0.092521	DE(MP34)=	0.003568
DE(CCSD)=	-0.026734	DE(Int)=	0.027030
DE(Empirical)=	-0.040301		
CBS-Q (0 K)=	-280.579142	CBS-Q Energy=	-280.575597
CBS-Q Enthalpy=	-280.574653	CBS-Q Free Energy=	-280.604897

Nitric_acid CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.112603	-0.565986	-0.000002

2	7	0	-0.144308	0.036542	0.000000
3	8	0	-0.146403	1.245457	-0.000001
4	8	0	-1.053561	-0.735741	0.000001
5	1	0	1.709041	0.194364	0.000011

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.027843	E(Thermal)=	0.031259
E(SCF)=	-279.584796	DE(SCF)=	-0.002690
DE(MP2)=	-0.971737	DE(CBS)=	-0.074877
DE(QCI)=	-0.031903	DE(Int)=	0.023610
DE(Core)=	-0.235379	DE(Empirical)=	-0.011487
CBS-APNO (0 K)=	-280.861414	CBS-APNO Energy=	-280.857999
CBS-APNO Enthalpy=	-280.857055	CBS-APNO Free Energy=	-280.887016

Nitric_acid G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	1.100217	-0.618312	-0.000002
2	7	0	-0.143827	0.045403	0.000001
3	8	0	-0.093850	1.269633	-0.000001
4	8	0	-1.097413	-0.707564	0.000001
5	1	0	1.735152	0.132123	0.000015

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026818	E(Thermal)=	0.030274
E(QCISD(T))=	-280.188516	E(Empiric)=	-0.076632
DE(Plus)=	-0.022817	DE(2DF)=	-0.196594
E(Delta-G3)=	-0.290866	E(G3-Empiric)=	-0.076632
G3(0 K)=	-280.748607	G3 Energy=	-280.745151
G3 Enthalpy=	-280.744207	G3 Free Energy=	-280.774234

NO3- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.900950	0.880357	0.000000
2	7	0	0.000000	0.000372	0.000000
3	8	0	-0.450475	-0.440342	1.090734
4	8	0	-0.450475	-0.440342	-1.090734

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.014003	E(Thermal)=	0.017165
E(SCF)=	-279.024870	DE(MP2)=	-0.925816
DE(CBS)=	-0.095653	DE(MP34)=	0.006714
DE(CCSD)=	-0.027255	DE(Int)=	0.027858
DE(Empirical)=	-0.040464		
CBS-Q (0 K)=	-280.065484	CBS-Q Energy=	-280.062321
CBS-Q Enthalpy=	-280.061377	CBS-Q Free Energy=	-280.090980

NO3- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	1.253275	0.000000
2	7	0	0.000000	0.000000	0.000000
3	8	0	1.085368	-0.626637	0.000000
4	8	0	-1.085368	-0.626637	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.014955	E(Thermal)=	0.018060
E(SCF)=	-279.057666	DE(SCF)=	-0.002762
DE(MP2)=	-0.975147	DE(CBS)=	-0.075366
DE(QCI)=	-0.028341	DE(Int)=	0.024134
DE(Core)=	-0.235058	DE(Empirical)=	-0.011391
CBS-APNO (0 K)=	-280.346642	CBS-APNO Energy=	-280.343538
CBS-APNO Enthalpy=	-280.342593	CBS-APNO Free Energy=	-280.370340

NO3- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	1.268956	0.000000
2	7	0	0.000000	0.000000	0.000000
3	8	0	1.098948	-0.634478	0.000000
4	8	0	-1.098948	-0.634478	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.014505	E(Thermal)=	0.017648
E(QCISD(T))=	-279.647286	E(Empiric)=	-0.076632
DE(Plus)=	-0.050155	DE(2DF)=	-0.186529
E(Delta-G3)=	-0.287952	E(G3-Empiric)=	-0.076632
G3(0 K)=	-280.234048	G3 Energy=	-280.230906
G3 Enthalpy=	-280.229962	G3 Free Energy=	-280.257771

Furan CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	1.158804
2	6	0	0.000000	1.093837	0.346681
3	6	0	0.000000	0.717370	-0.957759
4	1	0	0.000000	2.048182	0.845010
5	6	0	0.000000	-1.093837	0.346681
6	6	0	0.000000	-0.717370	-0.957759
7	1	0	0.000000	-2.048182	0.845010
8	1	0	0.000000	1.373055	-1.813755
9	1	0	0.000000	-1.373055	-1.813755

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.069069	E(Thermal)=	0.072806

E(SCF)=	-228.701230	DE(MP2)=	-0.860679
DE(CBS)=	-0.082426	DE(MP34)=	-0.026121
DE(CCSD)=	-0.029670	DE(Int)=	0.027312
DE(Empirical)=	-0.039285		
CBS-Q (0 K)=	-229.643028	CBS-Q Energy=	-229.639291
CBS-Q Enthalpy=	-229.638347	CBS-Q Free Energy=	-229.668648

Furan CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	1.163004
2	6	0	0.000000	1.092148	0.347897
3	6	0	0.000000	0.722443	-0.961580
4	1	0	0.000000	2.048891	0.847778
5	6	0	0.000000	-1.092148	0.347897
6	6	0	0.000000	-0.722443	-0.961580
7	1	0	0.000000	-2.048891	0.847778
8	1	0	0.000000	1.382045	-1.817698
9	1	0	0.000000	-1.382045	-1.817698

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.069358	E(Thermal)=	0.073027
E(SCF)=	-228.723303	DE(SCF)=	-0.001877
DE(MP2)=	-0.899039	DE(CBS)=	-0.066904
DE(QCI)=	-0.060660	DE(Int)=	0.023638
DE(Core)=	-0.276408	DE(Empirical)=	-0.011053
CBS-APNO (0 K)=	-229.946249	CBS-APNO Energy=	-229.942580
CBS-APNO Enthalpy=	-229.941636	CBS-APNO Free Energy=	-229.971817

Furan G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	1.163494
2	6	0	0.000000	1.094601	0.347967
3	6	0	0.000000	0.713166	-0.962125
4	1	0	0.000000	2.049686	0.850978
5	6	0	0.000000	-1.094601	0.347967
6	6	0	0.000000	-0.713166	-0.962125
7	1	0	0.000000	-2.049686	0.850978
8	1	0	0.000000	1.370847	-1.820008
9	1	0	0.000000	-1.370847	-1.820008

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.067615	E(Thermal)=	0.071366
E(QCISD(T))=	-229.364770	E(Empiric)=	-0.083018
DE(Plus)=	-0.015133	DE(2DF)=	-0.172299
E(Delta-G3)=	-0.292334	E(G3-Empiric)=	-0.083018
G3(0 K)=	-229.859940	G3 Energy=	-229.856189
G3 Enthalpy=	-229.855245	G3 Free Energy=	-229.885538

C4OH3- (3) CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.107411	0.319620	0.000000
2	6	0	-0.556543	-1.005435	0.000000
3	6	0	0.802347	-1.082798	0.000000
4	1	0	-1.352131	-1.743353	0.000000
5	6	0	0.000000	1.110745	0.000000
6	6	0	1.132409	0.350096	0.000000
7	1	0	-0.193877	2.177536	0.000000
8	1	0	2.136024	0.773211	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.054319	E(Thermal)=	0.058116
E(SCF)=	-228.044895	DE(MP2)=	-0.877279
DE(CBS)=	-0.084400	DE(MP34)=	-0.020857
DE(CCSD)=	-0.032763	DE(Int)=	0.028408
DE(Empirical)=	-0.038504		
CBS-Q (0 K)=	-229.015971	CBS-Q Energy=	-229.012174
CBS-Q Enthalpy=	-229.011230	CBS-Q Free Energy=	-229.042223

C4OH3- (3) CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.108251	0.321019	0.000000
2	6	0	-0.561198	-0.997162	0.000000
3	6	0	0.805024	-1.095399	0.000000
4	1	0	-1.359071	-1.736315	0.000000
5	6	0	0.000000	1.109715	0.000000
6	6	0	1.135488	0.351056	0.000000
7	1	0	-0.189593	2.179368	0.000000
8	1	0	2.138791	0.779539	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.055180	E(Thermal)=	0.058871
E(SCF)=	-228.066825	DE(SCF)=	-0.001682
DE(MP2)=	-0.917301	DE(CBS)=	-0.067548
DE(QCI)=	-0.057959	DE(Int)=	0.024540
DE(Core)=	-0.275483	DE(Empirical)=	-0.010724
CBS-APNO (0 K)=	-229.317803	CBS-APNO Energy=	-229.314111
CBS-APNO Enthalpy=	-229.313167	CBS-APNO Free Energy=	-229.343985

C4OH3- (3) G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.111419	0.318666	0.000000

2	6	0	-0.555190	-0.993543	0.000000
3	6	0	0.809952	-1.086836	0.000000
4	1	0	-1.356349	-1.731278	0.000000
5	6	0	0.000000	1.114702	0.000000
6	6	0	1.130455	0.337683	0.000000
7	1	0	-0.198471	2.182368	0.000000
8	1	0	2.134872	0.767546	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.053718	E(Thermal)=	0.057493
E(QCISD(T))=	-228.695427	E(Empiric)=	-0.083018
DE(Plus)=	-0.047140	DE(2DF)=	-0.173875
E(Delta-G3)=	-0.286030	E(G3-Empiric)=	-0.083018
G3(0 K)=	-229.231772	G3 Energy=	-229.227998
G3 Enthalpy=	-229.227053	G3 Free Energy=	-229.257987

C4OH3- (2) CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.122598	0.342553	0.000000
2	6	0	0.000000	1.119413	0.000000
3	6	0	1.111102	0.334565	0.000000
4	1	0	-0.139627	2.193864	0.000000
5	6	0	-0.773865	-1.054372	0.000000
6	6	0	0.619262	-1.018323	0.000000
7	1	0	1.243219	-1.907124	0.000000
8	1	0	2.138197	0.685142	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.054018	E(Thermal)=	0.057850
E(SCF)=	-228.053613	DE(MP2)=	-0.874295
DE(CBS)=	-0.083854	DE(MP34)=	-0.022175
DE(CCSD)=	-0.032726	DE(Int)=	0.028216
DE(Empirical)=	-0.038505		
CBS-Q (0 K)=	-229.022933	CBS-Q Energy=	-229.019101
CBS-Q Enthalpy=	-229.018157	CBS-Q Free Energy=	-229.049202

C4OH3- (2) CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.122887	0.347100	0.000000
2	6	0	0.000000	1.115794	0.000000
3	6	0	1.117597	0.335896	0.000000
4	1	0	-0.137623	2.192973	0.000000
5	6	0	-0.779579	-1.051513	0.000000
6	6	0	0.617934	-1.024022	0.000000
7	1	0	1.239552	-1.916870	0.000000
8	1	0	2.145456	0.690166	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.054688	E(Thermal)=	0.058421
E(SCF)=	-228.075978	DE(SCF)=	-0.001707
DE(MP2)=	-0.914345	DE(CBS)=	-0.067309
DE(QCI)=	-0.059109	DE(Int)=	0.024389
DE(Core)=	-0.275505	DE(Empirical)=	-0.010724
CBS-APNO (0 K)=	-229.325601	CBS-APNO Energy=	-229.321867
CBS-APNO Enthalpy=	-229.320923	CBS-APNO Free Energy=	-229.351801

C4OH3- (2) G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	-1.121476	0.348654	0.000000
2	6	0	0.000000	1.118786	0.000000
3	6	0	1.116401	0.328578	0.000000
4	1	0	-0.140003	2.196244	0.000000
5	6	0	-0.779572	-1.062103	0.000000
6	6	0	0.616523	-1.012400	0.000000
7	1	0	1.245736	-1.901041	0.000000
8	1	0	2.145968	0.678402	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.053232	E(Thermal)=	0.057053
E(QCISD(T))=	-228.704556	E(Empiric)=	-0.083018
DE(Plus)=	-0.045809	DE(2DF)=	-0.172604
E(Delta-G3)=	-0.286430	E(G3-Empiric)=	-0.083018
G3(0 K)=	-229.239185	G3 Energy=	-229.235363
G3 Enthalpy=	-229.234419	G3 Free Energy=	-229.265421

Supplementary Information Table Experimental values for deprotonation reactions in the NIST database. Numbers in boldface are the values (with the smallest error bars) used to determine the difference between calculated and experimental values. All values in kcal/mol. Values are ordered from best agreement (exp. 1) with calculated values to worst agreement.

Reaction	ΔGgas (exp. 1)	ΔGgas (exp. 2)	ΔGgas (exp. 3)	ΔGgas (exp. 4)	ΔHgas (exp. 1)	ΔHgas (exp. 2)	ΔHgas (exp. 3)	ΔHgas (exp. 4)	ΔHgas (exp. 5)
$NH_3 \rightarrow NH_2^- + H^+$	**396.9±0.4**[a]	396.1±0.7[b]			**404.30±0.3**[a]	403.60±0.8[b]			
$CH_3NH_2 \rightarrow CH_3NH^- + H^+$	**395.7±0.7**[b]				**403.20±0.8**[b]				
$CH_3NHCH_3 \rightarrow CH_3NCH_3^- + H^+$	**389.2±0.6**[b]				**396.40±0.9**[b]				
$CH_3CH_2NH_2 \rightarrow CH_3CH_2NH^- + H^+$	**391.7±0.7**[b]				**399.3±1.1**[b]				
$CH_4 \rightarrow CH_3^- + H^+$	409.9±3.6[c]	**408.6±0.9**[d]			418.0±3.5[c]	**416.70±0.8**[d]			
$CH_3OH \rightarrow CH_3O^- + H^+$	375.2±1.1[e]	**375.1±0.6**[f]	374.6±2.1[g]	374±2[h]	381.8±1.0[e]	**381.50±0.4**[f]	381.2±2.0[g]	380.6±2.1[h]	
$H_2O \rightarrow OH^- + H^+$	**384.1±0.2**[i]				**390.70±0.1**[i]				
$C_2H_2 \rightarrow C_2H^- + H^+$	**369.8±0.6**[j]	368.5±2[h]	368±5[k]	376.8±0.6[l]	378.0±0.7[j]	**379.80±0.5**[f]	376.7±2.1[h]	375.8±9.2[m]	385.0±0.7[l]
$C_2H_4 \rightarrow C_2H_3^- + H^+$	**401±0.5**[j]	399.1±2.1[n]			**409.40±0.6**[j]	407.5±2.0[n]	407.0±3.0[e]	406.0±2.0[o]	
$CH_2O \rightarrow CHO^- + H^+$	**385.6±0.8**[p]	394±4.5[q]			**393.50±0.7**[p]				
$HCl \rightarrow Cl^- + H^+$	328.3±2[r]	328.1±0.2[s]	**328.1±0.1**[t]		**333.40±0.1**[s]	333.6±2.1[r]			
$CH_3CHCH_2 \rightarrow CH_2CHCH_2^- + H^+$	**383.60±0.5**[u]	384.1±2.0[h]	382.5±1.6[v]		390.7±2.1[h]	**390.20±0.7**[u]	389.1±1.5[v]		
$CH_3CHCH_2 \rightarrow CH_3CCH_2^- + H^+$	398.1±2.1[w]				405.8±2[w]				
$CHNO \rightarrow CNO^- + H^+$	**333.6±0.5**[x]	338.3±2[y]			**340.0±0.4**[x]	344.7±2.1[y]			
$CHOCH_3 \rightarrow CHOCH_2^- + H^+$	359.7±2[z]	359±2[h]			366.5±2.9[z]	365.8±3.7[aa]	365.8±2.2[h]		
$CHOCH_3 \rightarrow COCH_3^- + H^+$	383.3±2[bb]	382.1±1.1[cc]			391.0±2.1[bb]	389.80±0.9[cc]	387.0±8.0[e]		
$HNO_2 \rightarrow NO_2^- + H^+$	**333.7±0.3**[dd]				**340.20±0.2**[dd]				
$C_6H_6 \rightarrow C_6H_5^- + H^+$	**392.9±0.4**[ee]	390.9±2[f]	390.1±6.5[ff]	389.2±5.5[gg]	400.7±2.5[f]	**401.70±0.5**[ee]	401.0±10[e]	401.80±0.5[hh]	398.0±5.6[gg]
$HNO_3 \rightarrow NO_3^- + H^+$	**317.8±0.2**[ii]				**324.50±0.2**[ii]	324.50±0.5[jj]	327.7±5.8[kk]	329.9±4.8[ll]	
$C_4H_4O \rightarrow C_4H_3O^- + \alpha\text{-}H^+$ [mm]	**382.9±0.2**[nn]	380±3[oo]			**391.10±0.4**[nn]	388.2±3.1[oo]			

[a] Ref. [26] [b] Ref. [27] [c] Ref. [28] [d] Ref. [29] [e] Ref. [30] [f] Ref. [31] [g] Ref. [32] [h] Ref. [33] [i] Ref. [34] [j] Ref. [35] [k] Ref. [36] [l] Ref. [37] [m] Ref. [62] [n] Ref. [38] [o] Ref. [63] [p] Ref. [39] [q] Ref. [40] [r] Ref. [41] [s] Ref. [42] [t] Ref. [43] [u] Ref. [44] [v] Ref. [45] [w] Ref. [38] [x] Ref. [46] [y] Ref. [47] [z] Ref. [48] [aa] Ref. [64] [bb] Ref. [49] [cc] Ref. [50] [dd] Ref. [51] [ee] Ref. [52] [ff] Ref. [53] [gg] Ref. [54] [hh] Ref. [60] [ii] Ref. [55] [jj] Ref. [61] [kk] Ref. [65] [ll] Ref. [66] [mm] α- indicates original position relative to oxygen atom [nn] Ref. [56] [oo] Ref. [57]