Supplementary Information for the manuscript, "Comparison of CBS-QB3, CBS-APNO, and G3 predictions of gas phase deprotonation data," Emma K. Pokon, Matthew D. Liptak, Steven Feldgus, and George C. Shields, *J. Phys. Chem. A*

The following stationary points and energies, in Hartrees, were used to produce Table 2.

The relevant equations are:

SUPPLEMENTARY MATERIAL

$\Delta H = H(H^+) + H(A^-) - H(AH)$

$\Delta G = G(H^+) + G(A^-) - G(AH)$

$H(H^+) = 1.48$ kcal/mol

$G(H^+) = -6.28$ kcal/mol

1 Hartree = 627.5096 kcal/mol

ammonia CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.939524	-0.270284
2	7	0	0.000000	0.000000	0.115836
3	1	0	-0.813652	-0.469762	-0.270284
4	1	0	0.813652	-0.469762	-0.270284

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.033955	E(Thermal)=	0.036821
E(SCF)=	-56.217749	DE(MP2)=	-0.230461
DE(CBS)=	-0.023289	DE(MP34)=	-0.014272
DE(CCSD)=	-0.003632	DE(Int)=	0.007976
DE(Empirical)=	-0.012716		
CBS-Q (0 K)=	-56.460187	CBS-Q Energy=	-56.457320
CBS-Q Enthalpy=	-56.456376	CBS-Q Free Energy=	-56.478221

ammonia CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.935234	-0.277037
2	7	0	0.000000	0.000000	0.118730
3	1	0	-0.809936	-0.467617	-0.277037
4	1	0	0.809936	-0.467617	-0.277037

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.033849	E(Thermal)=	0.036714
E(SCF)=	-56.223552	DE(SCF)=	-0.000043

DE(MP2)=	-0.243465	DE(CBS)=	-0.017734
DE(QCI)=	-0.020530	DE(Int)=	0.006668
DE(Core)=	-0.057531	DE(Empirical)=	-0.003543
CBS-APNO (0 K)=	-56.525883	CBS-APNO Energy=	-56.523017
CBS-APNO Enthalpy=	-56.522073	CBS-APNO Free Energy=	-56.543875

ammonia G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.939762	-0.271700
2	7	0	0.000000	0.000000	0.116443
3	1	0	-0.813858	-0.469881	-0.271700
4	1	0	0.813858	-0.469881	-0.271700

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.033038	E(Thermal)=	0.035903
E(QCISD(T))=	-56.372097	E(Empiric)=	-0.025544
DE(Plus)=	-0.008799	DE(2DF)=	-0.064223
E(Delta-G3)=	-0.069396	E(G3-Empiric)=	-0.025544
G3(0 K)=	-56.507021	G3 Energy=	-56.504156
G3 Enthalpy=	-56.503212	G3 Free Energy=	-56.525017

NH2- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.787142	-0.537159
2	7	0	0.000000	0.000000	0.153474
3	1	0	0.000000	-0.787142	-0.537159

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.017389	E(Thermal)=	0.020226
E(SCF)=	-55.543233	DE(MP2)=	-0.248356
DE(CBS)=	-0.026299	DE(MP34)=	-0.008348
DE(CCSD)=	-0.005486	DE(Int)=	0.009311
DE(Empirical)=	-0.012165		
CBS-Q (0 K)=	-55.817187	CBS-Q Energy=	-55.814350
CBS-Q Enthalpy=	-55.813406	CBS-Q Free Energy=	-55.834915

NH2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.780345	-0.538692
2	7	0	0.000000	0.000000	0.153912
3	1	0	0.000000	-0.780345	-0.538692

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.017471	E(Thermal)=	0.020308

E(SCF)=	-55.550135	DE(SCF)=	-0.000056
DE(MP2)=	-0.264510	DE(CBS)=	-0.019086
DE(QCI)=	-0.015695	DE(Int)=	0.007606
DE(Core)=	-0.056855	DE(Empirical)=	-0.003283
CBS-APNO (0 K)=	-55.884543	CBS-APNO Energy=	-55.881706
CBS-APNO Enthalpy=	-55.880762	CBS-APNO Free Energy=	-55.902213

NH2- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.789573	-0.529252
2	7	0	0.000000	0.000000	0.151215
3	1	0	0.000000	-0.789573	-0.529252

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.017035	E(Thermal)=	0.019872
E(QCISD(T))=	-55.663099	E(Empiric)=	-0.025544
DE(Plus)=	-0.059995	DE(2DF)=	-0.062549
E(Delta-G3)=	-0.069686	E(G3-Empiric)=	-0.025544
G3(0 K)=	-55.863838	G3 Energy=	-55.861001
G3 Enthalpy=	-55.860057	G3 Free Energy=	-55.881516

methylamine CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.592208	1.065661	0.878498
2	6	0	0.050521	0.705322	0.000000
3	1	0	-0.943308	1.180669	0.000000
4	7	0	0.050521	-0.760792	0.000000
5	1	0	0.592208	1.065661	-0.878498
6	1	0	-0.448939	-1.109189	0.812110
7	1	0	-0.448939	-1.109189	-0.812110

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.063192	E(Thermal)=	0.066612
E(SCF)=	-95.251511	DE(MP2)=	-0.396422
DE(CBS)=	-0.039111	DE(MP34)=	-0.028185
DE(CCSD)=	-0.008521	DE(Int)=	0.013667
DE(Empirical)=	-0.021564		
CBS-Q (0 K)=	-95.668454	CBS-Q Energy=	-95.665033
CBS-Q Enthalpy=	-95.664089	CBS-Q Free Energy=	-95.691371

methylamine CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.593755	1.063609	0.882334
2	6	0	0.052739	0.705399	0.000000

3	1	0	-0.945923	1.171486	0.000000
4	7	0	0.052739	-0.762966	0.000000
5	1	0	0.593755	1.063609	-0.882334
6	1	0	-0.463595	-1.095167	0.808574
7	1	0	-0.463595	-1.095167	-0.808574

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.062974	E(Thermal)=	0.066397
E(SCF)=	-95.260863	DE(SCF)=	-0.000294
DE(MP2)=	-0.417054	DE(CBS)=	-0.030139
DE(QCI)=	-0.040355	DE(Int)=	0.011379
DE(Core)=	-0.111568	DE(Empirical)=	-0.006005
CBS-APNO (0 K)=	-95.791926	CBS-APNO Energy=	-95.788502
CBS-APNO Enthalpy=	-95.787558	CBS-APNO Free Energy=	-95.814826

methylamine G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.592732	1.057132	0.880565
2	6	0	0.051681	0.704303	0.000000
3	1	0	-0.941900	1.176201	0.000000
4	7	0	0.051681	-0.759432	0.000000
5	1	0	0.592732	1.057132	-0.880565
6	1	0	-0.457710	-1.100129	0.812231
7	1	0	-0.457710	-1.100129	-0.812231

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.061530	E(Thermal)=	0.064975
E(QCISD(T))=	-95.541352	E(Empiric)=	-0.044702
DE(Plus)=	-0.009383	DE(2DF)=	-0.101323
E(Delta-G3)=	-0.124889	E(G3-Empiric)=	-0.044702
G3(0 K)=	-95.760119	G3 Energy=	-95.756674
G3 Enthalpy=	-95.755730	G3 Free Energy=	-95.783026

CH3NH- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.084395	0.986973	0.000000
2	6	0	0.591407	-0.011250	0.000000
3	1	0	1.116762	-0.541235	-0.886578
4	7	0	-0.810987	0.140565	0.000000
5	1	0	1.116763	-0.541235	0.886579
6	1	0	-1.189453	-0.820954	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.044633	E(Thermal)=	0.047883
E(SCF)=	-94.576550	DE(MP2)=	-0.414484
DE(CBS)=	-0.042039	DE(MP34)=	-0.022583
DE(CCSD)=	-0.010923	DE(Int)=	0.015032

DE(Empirical)=	-0.020898		
CBS-Q (0 K)=	-95.027811	CBS-Q Energy=	-95.024561
CBS-Q Enthalpy=	-95.023617	CBS-Q Free Energy=	-95.050382

CH3NH- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.087843	0.989366	-0.000024
2	6	0	-0.599630	-0.011826	0.000000
3	1	0	-1.105923	-0.539075	0.884730
4	7	0	0.818617	0.141474	0.000000
5	1	0	-1.105918	-0.539116	-0.884709
6	1	0	1.167146	-0.830538	0.000001

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.045636	E(Thermal)=	0.048906
E(SCF)=	-94.587212	DE(SCF)=	-0.000384
DE(MP2)=	-0.437207	DE(CBS)=	-0.031695
DE(QCI)=	-0.036350	DE(Int)=	0.012372
DE(Core)=	-0.110803	DE(Empirical)=	-0.005723
CBS-APNO (0 K)=	-95.151366	CBS-APNO Energy=	-95.148095
CBS-APNO Enthalpy=	-95.147151	CBS-APNO Free Energy=	-95.173940

CH3NH- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.078877	0.987457	-0.000081
2	6	0	-0.598329	-0.013245	0.000000
3	1	0	-1.106103	-0.536651	0.879690
4	7	0	0.814102	0.141659	0.000002
5	1	0	-1.106082	-0.536783	-0.879621
6	1	0	1.182320	-0.826170	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.044973	E(Thermal)=	0.048244
E(QCISD(T))=	-94.851562	E(Empiric)=	-0.044702
DE(Plus)=	-0.041259	DE(2DF)=	-0.098990
E(Delta-G3)=	-0.126468	E(G3-Empiric)=	-0.044702
G3(0 K)=	-95.118008	G3 Energy=	-95.114737
G3 Enthalpy=	-95.113793	G3 Free Energy=	-95.140576

CBS-QB3 calculation on CH2NH2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.138716	-0.560132	0.841019
2	6	0	0.798890	-0.108736	-0.135651
3	7	0	-0.707955	0.110969	-0.071846

4	1	0	-1.070368	0.288419	0.883411
5	1	0	1.237645	0.918072	-0.077305
6	1	0	-1.143644	-0.770725	-0.330298

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.046041	E(Thermal)=	0.049427
E(SCF)=	-94.554122	DE(MP2)=	-0.413238
DE(CBS)=	-0.041125	DE(MP34)=	-0.023744
DE(CCSD)=	-0.010989	DE(Int)=	0.014869
DE(Empirical)=	-0.020710		
CBS-Q (0 K)=	-95.003017	CBS-Q Energy=	-94.999631
CBS-Q Enthalpy=	-94.998687	CBS-Q Free Energy=	-95.025695

CBS-APNO calculation on CH2NH2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.119535	-0.590998	0.827803
2	6	0	0.802274	-0.105529	-0.143891
3	7	0	-0.711507	0.116977	-0.069751
4	1	0	-1.043568	0.245238	0.896547
5	1	0	1.228555	0.925668	-0.029560
6	1	0	-1.137612	-0.765572	-0.343183

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.046517	E(Thermal)=	0.049887
E(SCF)=	-94.563606	DE(SCF)=	-0.000271
DE(MP2)=	-0.435589	DE(CBS)=	-0.031384
DE(QCI)=	-0.037765	DE(Int)=	0.012397
DE(Core)=	-0.110833	DE(Empirical)=	-0.005665
CBS-APNO (0 K)=	-95.126199	CBS-APNO Energy=	-95.122829
CBS-APNO Enthalpy=	-95.121885	CBS-APNO Free Energy=	-95.148854

G3 calculation on CH2NH2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.117730	-0.554515	0.847575
2	6	0	0.798564	-0.110434	-0.136226
3	7	0	-0.703941	0.111799	-0.074364
4	1	0	-1.060977	0.292624	0.880233
5	1	0	1.218402	0.921338	-0.072648
6	1	0	-1.138950	-0.779437	-0.317257

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.045462	E(Thermal)=	0.048848
E(QCISD(T))=	-94.818186	E(Empiric)=	-0.044702
DE(Plus)=	-0.048508	DE(2DF)=	-0.104490
E(Delta-G3)=	-0.123263	E(G3-Empiric)=	-0.044702
G3(0 K)=	-95.093686	G3 Energy=	-95.090301

G3 Enthalpy= -95.089357 G3 Free Energy= -95.116349

methanamine CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.000432	-0.735676	1.282630
2	1	0	-0.838364	1.153693	0.000000
3	6	0	0.037046	-0.220272	-1.215568
4	6	0	0.037046	-0.220272	1.215568
5	1	0	-0.049053	0.429747	-2.089697
6	1	0	-0.754474	-0.989359	-1.276262
7	1	0	1.000432	-0.735676	-1.282630
8	1	0	-0.754474	-0.989359	1.276262
9	1	0	-0.049053	0.429747	2.089697
10	7	0	0.000000	0.582878	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091073	E(Thermal)=	0.095498
E(SCF)=	-134.289320	DE(MP2)=	-0.565415
DE(CBS)=	-0.055075	DE(MP34)=	-0.041230
DE(CCSD)=	-0.013697	DE(Int)=	0.019364
DE(Empirical)=	-0.030391		
CBS-Q (0 K)=	-134.884690	CBS-Q Energy=	-134.880266
CBS-Q Enthalpy=	-134.879322	CBS-Q Free Energy=	-134.910168

methanamine CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.009469	-0.730514	1.266111
2	1	0	-0.869003	1.121745	0.000000
3	6	0	0.038916	-0.223434	-1.207475
4	6	0	0.038916	-0.223434	1.207475
5	1	0	-0.059470	0.416998	-2.090329
6	1	0	-0.748993	-0.998282	-1.244688
7	1	0	1.009469	-0.730514	-1.266111
8	1	0	-0.748993	-0.998282	1.244688
9	1	0	-0.059470	0.416998	2.090329
10	7	0	0.000000	0.597580	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.090795	E(Thermal)=	0.095235
E(SCF)=	-134.302028	DE(SCF)=	-0.000547
DE(MP2)=	-0.593976	DE(CBS)=	-0.042705
DE(QCI)=	-0.059415	DE(Int)=	0.016099
DE(Core)=	-0.165728	DE(Empirical)=	-0.008460
CBS-APNO (0 K)=	-135.065964	CBS-APNO Energy=	-135.061524
CBS-APNO Enthalpy=	-135.060580	CBS-APNO Free Energy=	-135.091463

methanamine G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.006199	-0.728872	1.259358
2	1	0	-0.860166	1.138327	0.000000
3	6	0	0.037948	-0.223323	-1.204891
4	6	0	0.037948	-0.223323	1.204891
5	1	0	-0.056210	0.418629	-2.083854
6	1	0	-0.747597	-0.996680	-1.249207
7	1	0	1.006199	-0.728872	-1.259358
8	1	0	-0.747597	-0.996680	1.249207
9	1	0	-0.056210	0.418629	2.083854
10	7	0	0.000000	0.593628	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.088798	E(Thermal)=	0.093282
E(QCISD(T))=	-134.716618	E(Empiric)=	-0.063860
DE(Plus)=	-0.010100	DE(2DF)=	-0.138957
E(Delta-G3)=	-0.180387	E(G3-Empiric)=	-0.063860
G3(0 K)=	-135.021124	G3 Energy=	-135.016640
G3 Enthalpy=	-135.015695	G3 Free Energy=	-135.046644

CH3NCH3- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.887926	0.878887	1.241553
2	7	0	0.000002	-0.656704	0.000000
3	6	0	0.000002	0.162305	-1.141456
4	6	0	0.000002	0.162305	1.141456
5	1	0	0.000018	-0.433171	-2.073384
6	1	0	0.887885	0.878919	-1.241537
7	1	0	-0.887926	0.878887	-1.241553
8	1	0	0.887885	0.878919	1.241537
9	1	0	0.000018	-0.433171	2.073384

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.072041	E(Thermal)=	0.076170
E(SCF)=	-133.624931	DE(MP2)=	-0.587034
DE(CBS)=	-0.058104	DE(MP34)=	-0.034501
DE(CCSD)=	-0.016853	DE(Int)=	0.020859
DE(Empirical)=	-0.029560		
CBS-Q (0 K)=	-134.258083	CBS-Q Energy=	-134.253954
CBS-Q Enthalpy=	-134.253009	CBS-Q Free Energy=	-134.283132

CH3NCH3- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	-0.888247	0.881702	1.214183
2	7	0	0.000000	-0.677129	0.000000
3	6	0	0.000000	0.169987	-1.134219
4	6	0	0.000000	0.169987	1.134219
5	1	0	0.000011	-0.413387	-2.075787
6	1	0	0.888238	0.881713	-1.214164
7	1	0	-0.888247	0.881702	-1.214183
8	1	0	0.888238	0.881713	1.214164
9	1	0	0.000011	-0.413387	2.075787

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.072829	E(Thermal)=	0.077002
E(SCF)=	-133.637910	DE(SCF)=	-0.000685
DE(MP2)=	-0.617073	DE(CBS)=	-0.044445
DE(QCI)=	-0.054986	DE(Int)=	0.017150
DE(Core)=	-0.165018	DE(Empirical)=	-0.008135
CBS-APNO (0 K)=	-134.438274	CBS-APNO Energy=	-134.434101
CBS-APNO Enthalpy=	-134.433157	CBS-APNO Free Energy=	-134.463365

CH3NCH3- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.882900	0.879763	1.222103
2	7	0	0.000000	-0.674176	0.000000
3	6	0	0.000000	0.169538	-1.132261
4	6	0	0.000000	0.169538	1.132261
5	1	0	0.000012	-0.417152	-2.069863
6	1	0	0.882890	0.879776	-1.222083
7	1	0	-0.882900	0.879763	-1.222103
8	1	0	0.882890	0.879776	1.222083
9	1	0	0.000012	-0.417152	2.069863

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.071918	E(Thermal)=	0.076134
E(QCISD(T))=	-134.046372	E(Empiric)=	-0.063860
DE(Plus)=	-0.035974	DE(2DF)=	-0.135849
E(Delta-G3)=	-0.182340	E(G3-Empiric)=	-0.063860
G3(0 K)=	-134.392478	G3 Energy=	-134.388262
G3 Enthalpy=	-134.387318	G3 Free Energy=	-134.417603

CBS-QB3 Calculation on CH3NHCH2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.106550	0.250622	-0.457838
2	6	0	-1.249015	-0.348255	-0.080950
3	7	0	-0.062374	0.540021	-0.087209
4	1	0	-1.525356	-0.596756	0.980823
5	1	0	-0.020380	1.222618	0.686971
6	6	0	1.172653	-0.212939	-0.015703

7	1	0	2.051968	0.463937	-0.047212
8	1	0	1.205667	-0.903215	-0.867416
9	1	0	1.289438	-0.850185	0.895046

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.073370	E(Thermal)=	0.077810
E(SCF)=	-133.596021	DE(MP2)=	-0.584268
DE(CBS)=	-0.057073	DE(MP34)=	-0.036059
DE(CCSD)=	-0.016504	DE(Int)=	0.020566
DE(Empirical)=	-0.029437		
CBS-Q (0 K)=	-134.225426	CBS-Q Energy=	-134.220985
CBS-Q Enthalpy=	-134.220041	CBS-Q Free Energy=	-134.250778

CH3NHCH2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.117619	0.298106	-0.346333
2	6	0	-1.246915	-0.358331	-0.101726
3	7	0	-0.057671	0.563588	-0.091114
4	1	0	-1.442493	-0.662663	0.970181
5	1	0	-0.034370	1.176150	0.732888
6	6	0	1.163784	-0.215727	-0.015112
7	1	0	2.056767	0.442366	-0.004584
8	1	0	1.206186	-0.874924	-0.891659
9	1	0	1.234013	-0.879800	0.878335

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.073983	E(Thermal)=	0.078384
E(SCF)=	-133.608663	DE(SCF)=	-0.000544
DE(MP2)=	-0.614130	DE(CBS)=	-0.044043
DE(QCI)=	-0.056646	DE(Int)=	0.017126
DE(Core)=	-0.165031	DE(Empirical)=	-0.008095
CBS-APNO (0 K)=	-134.406042	CBS-APNO Energy=	-134.401642
CBS-APNO Enthalpy=	-134.400697	CBS-APNO Free Energy=	-134.431376

CH3NHCH2- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.107068	0.296466	-0.333568
2	6	0	-1.237798	-0.358296	-0.100550
3	7	0	-0.059180	0.563277	-0.090619
4	1	0	-1.426796	-0.673223	0.963157
5	1	0	-0.026239	1.204786	0.720381
6	6	0	1.155870	-0.216516	-0.014835
7	1	0	2.051961	0.432412	-0.015691
8	1	0	1.178476	-0.878027	-0.885473
9	1	0	1.235492	-0.876476	0.877838

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.072487	E(Thermal)=	0.076915
E(QCISD(T))=	-134.001252	E(Empiric)=	-0.063860
DE(Plus)=	-0.046521	DE(2DF)=	-0.142202
E(Delta-G3)=	-0.178926	E(G3-Empiric)=	-0.063860
G3(0 K)=	-134.360275	G3 Energy=	-134.355847
G3 Enthalpy=	-134.354903	G3 Free Energy=	-134.385615

ethylamine CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.054397	1.231248	-0.874539
2	6	0	0.044500	0.572434	-0.000001
3	1	0	0.054399	1.231248	0.874537
4	7	0	1.300936	-0.183812	-0.000001
5	6	0	-1.241631	-0.263616	0.000001
6	1	0	-2.133600	0.371810	0.000001
7	1	0	-1.289044	-0.907655	0.884265
8	1	0	-1.289045	-0.907656	-0.884262
9	1	0	1.339570	-0.792602	0.812875
10	1	0	1.339561	-0.792616	-0.812867

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091484	E(Thermal)=	0.095901
E(SCF)=	-134.300832	DE(MP2)=	-0.567044
DE(CBS)=	-0.055273	DE(MP34)=	-0.040500
DE(CCSD)=	-0.013386	DE(Int)=	0.019443
DE(Empirical)=	-0.030403		
CBS-Q (0 K)=	-134.896511	CBS-Q Energy=	-134.892095
CBS-Q Enthalpy=	-134.891151	CBS-Q Free Energy=	-134.922008

ethylamine CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.055339	1.234831	0.879308
2	6	0	-0.045555	0.578837	0.000000
3	1	0	-0.055338	1.234831	-0.879309
4	7	0	-1.298756	-0.185770	-0.000001
5	6	0	1.235424	-0.264579	0.000000
6	1	0	2.132118	0.367999	0.000001
7	1	0	1.272110	-0.909367	-0.887366
8	1	0	1.272108	-0.909368	0.887367
9	1	0	-1.306787	-0.802047	-0.808834
10	1	0	-1.306793	-0.802038	0.808839

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.091029	E(Thermal)=	0.095441
E(SCF)=	-134.313656	DE(SCF)=	-0.000438
DE(MP2)=	-0.595727	DE(CBS)=	-0.042825
DE(QCI)=	-0.058830	DE(Int)=	0.016202

DE(Core)=	-0.165819	DE(Empirical)=	-0.008466
CBS-APNO (0 K)=	-135.078530	CBS-APNO Energy=	-135.074119
CBS-APNO Enthalpy=	-135.073175	CBS-APNO Free Energy=	-135.104013

ethylamine G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.055940	1.230201	-0.876496
2	6	0	0.042461	0.574461	0.000001
3	1	0	0.055937	1.230199	0.876500
4	7	0	1.295753	-0.183199	0.000002
5	6	0	-1.232752	-0.263765	-0.000001
6	1	0	-2.127668	0.366561	-0.000022
7	1	0	-1.272494	-0.906454	0.885099
8	1	0	-1.272472	-0.906481	-0.885083
9	1	0	1.316109	-0.797916	0.812787
10	1	0	1.316125	-0.797890	-0.812802

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.088898	E(Thermal)=	0.093376
E(QCISD(T))=	-134.726553	E(Empiric)=	-0.063860
DE(Plus)=	-0.010675	DE(2DF)=	-0.140492
E(Delta-G3)=	-0.180819	E(G3-Empiric)=	-0.063860
G3(0 K)=	-135.033501	G3 Energy=	-135.029023
G3 Enthalpy=	-135.028079	G3 Free Energy=	-135.059031

CH3CH2NH- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.079202	1.136290	1.003207
2	6	0	-0.170679	0.516283	0.042360
3	1	0	-0.123696	1.284023	-0.761556
4	7	0	-1.323769	-0.276671	-0.136141
5	6	0	1.208862	-0.231716	-0.023588
6	1	0	2.090286	0.442342	0.033756
7	1	0	1.251733	-0.816481	-0.952063
8	1	0	1.274544	-0.946405	0.810038
9	1	0	-1.376385	-0.870475	0.706975

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.073935	E(Thermal)=	0.078156
E(SCF)=	-133.631784	DE(MP2)=	-0.588600
DE(CBS)=	-0.057986	DE(MP34)=	-0.034239
DE(CCSD)=	-0.016669	DE(Int)=	0.020864
DE(Empirical)=	-0.029567		
CBS-Q (0 K)=	-134.264046	CBS-Q Energy=	-134.259825
CBS-Q Enthalpy=	-134.258881	CBS-Q Free Energy=	-134.289243

CH3CH2NH- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.073680	1.135462	1.006744
2	6	0	-0.164048	0.525124	0.044688
3	1	0	-0.122380	1.292748	-0.760212
4	7	0	-1.324643	-0.276779	-0.132735
5	6	0	1.199699	-0.234382	-0.026419
6	1	0	2.089374	0.429194	0.030008
7	1	0	1.227582	-0.816260	-0.958916
8	1	0	1.254753	-0.952399	0.807623
9	1	0	-1.317050	-0.895740	0.694288

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.074221	E(Thermal)=	0.078438
E(SCF)=	-133.644893	DE(SCF)=	-0.000517
DE(MP2)=	-0.618754	DE(CBS)=	-0.044418
DE(QCI)=	-0.055123	DE(Int)=	0.017259
DE(Core)=	-0.165047	DE(Empirical)=	-0.008140
CBS-APNO (0 K)=	-134.445412	CBS-APNO Energy=	-134.441194
CBS-APNO Enthalpy=	-134.440250	CBS-APNO Free Energy=	-134.470602

CH3CH2NH- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.062700	1.146214	0.997692
2	6	0	-0.163152	0.521930	0.046550
3	1	0	-0.123214	1.286880	-0.757583
4	7	0	-1.323467	-0.271524	-0.129854
5	6	0	1.195735	-0.233435	-0.026795
6	1	0	2.086933	0.417829	0.050388
7	1	0	1.236566	-0.793518	-0.967692
8	1	0	1.244700	-0.965379	0.790882
9	1	0	-1.313519	-0.922332	0.676761

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.072696	E(Thermal)=	0.076969
E(QCISD(T))=	-134.043645	E(Empiric)=	-0.063860
DE(Plus)=	-0.044391	DE(2DF)=	-0.138415
E(Delta-G3)=	-0.182148	E(G3-Empiric)=	-0.063860
G3(0 K)=	-134.399762	G3 Energy=	-134.395489
G3 Enthalpy=	-134.394545	G3 Free Energy=	-134.424989

CH3CHNH2- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.240914	-0.920090	0.872516

2	6	0	-1.208237	-0.197934	-0.013607
3	1	0	-1.354029	-0.848727	-0.892846
4	6	0	0.040370	0.649689	-0.132030
5	1	0	-2.111178	0.427548	0.080935
6	7	0	1.190168	-0.301550	-0.089209
7	1	0	1.281500	-0.777992	0.841436
8	1	0	0.047848	1.292167	0.788584
9	1	0	2.052800	0.227415	-0.192340

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.073304	E(Thermal)=	0.077649
E(SCF)=	-133.602710	DE(MP2)=	-0.587583
DE(CBS)=	-0.057324	DE(MP34)=	-0.035339
DE(CCSD)=	-0.016619	DE(Int)=	0.020684
DE(Empirical)=	-0.029344		
CBS-Q (0 K)=	-134.234930	CBS-Q Energy=	-134.230585
CBS-Q Enthalpy=	-134.229641	CBS-Q Free Energy=	-134.260204

CH3CHNH2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.221534	-0.918533	0.867955
2	6	0	-1.210575	-0.202826	-0.011402
3	1	0	-1.356144	-0.843578	-0.899638
4	6	0	0.042084	0.665146	-0.140619
5	1	0	-2.117324	0.420719	0.092975
6	7	0	1.190116	-0.311670	-0.088510
7	1	0	1.273530	-0.739382	0.854378
8	1	0	0.051837	1.266049	0.812683
9	1	0	2.049765	0.222490	-0.196655

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.074000	E(Thermal)=	0.078399
E(SCF)=	-133.615893	DE(SCF)=	-0.000455
DE(MP2)=	-0.616971	DE(CBS)=	-0.044231
DE(QCI)=	-0.056119	DE(Int)=	0.017243
DE(Core)=	-0.165059	DE(Empirical)=	-0.008080
CBS-APNO (0 K)=	-134.415564	CBS-APNO Energy=	-134.411166
CBS-APNO Enthalpy=	-134.410221	CBS-APNO Free Energy=	-134.440905

CH3CHNH2- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.239855	-0.924523	0.858361
2	6	0	-1.199448	-0.201108	-0.010934
3	1	0	-1.343801	-0.837940	-0.899517
4	6	0	0.039147	0.659849	-0.135669
5	1	0	-2.105457	0.420622	0.087800
6	7	0	1.182201	-0.307417	-0.088652
7	1	0	1.276156	-0.764436	0.844021

8	1	0	0.052297	1.279260	0.800946
9	1	0	2.047063	0.226491	-0.191422

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.072516	E(Thermal)=	0.076932
E(QCISD(T))=	-134.010317	E(Empiric)=	-0.063860
DE(Plus)=	-0.044954	DE(2DF)=	-0.142372
E(Delta-G3)=	-0.180990	E(G3-Empiric)=	-0.063860
G3(0 K)=	-134.369977	G3 Energy=	-134.365561
G3 Enthalpy=	-134.364617	G3 Free Energy=	-134.395315

CH2CH2NH2- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.671175	-0.606362	0.917380
2	6	0	1.259000	-0.356194	-0.078147
3	1	0	2.060276	0.163708	-0.633785
4	6	0	0.045587	0.528273	0.041921
5	7	0	-1.227504	-0.298874	0.099829
6	1	0	-0.972805	-1.100160	-0.484641
7	1	0	0.009785	1.209955	-0.831199
8	1	0	-0.025238	1.191383	0.939892
9	1	0	-1.978186	0.201119	-0.389094

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.074056	E(Thermal)=	0.078675
E(SCF)=	-133.612104	DE(MP2)=	-0.588994
DE(CBS)=	-0.057443	DE(MP34)=	-0.033980
DE(CCSD)=	-0.016835	DE(Int)=	0.020743
DE(Empirical)=	-0.029353		
CBS-Q (0 K)=	-134.243909	CBS-Q Energy=	-134.239291
CBS-Q Enthalpy=	-134.238346	CBS-Q Free Energy=	-134.269608

CH2CH2NH2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.572438	-0.699726	0.910040
2	6	0	1.258042	-0.364528	-0.104607
3	1	0	2.096669	0.264937	-0.478123
4	6	0	0.036129	0.535042	0.044245
5	7	0	-1.211737	-0.303821	0.099261
6	1	0	-0.953753	-1.075485	-0.518481
7	1	0	-0.001500	1.222438	-0.827143
8	1	0	-0.024849	1.193223	0.946809
9	1	0	-1.971869	0.198270	-0.365759

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.074661	E(Thermal)=	0.079052
E(SCF)=	-133.624997	DE(SCF)=	-0.000437

DE(MP2)=	-0.618070	DE(CBS)=	-0.044857
DE(QCI)=	-0.055342	DE(Int)=	0.017436
DE(Core)=	-0.165135	DE(Empirical)=	-0.008082
CBS-APNO (0 K)=	-134.424824	CBS-APNO Energy=	-134.420433
CBS-APNO Enthalpy=	-134.419489	CBS-APNO Free Energy=	-134.450183

CH2CH2NH2-

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.527554	-0.743315	0.893085
2	6	0	1.244263	-0.361136	-0.108316
3	1	0	2.099172	0.263915	-0.435882
4	6	0	0.042557	0.538812	0.045961
5	7	0	-1.203279	-0.303434	0.098023
6	1	0	-0.916818	-1.079469	-0.507671
7	1	0	0.004368	1.229640	-0.821040
8	1	0	-0.043604	1.205181	0.941724
9	1	0	-1.968638	0.182032	-0.382252

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.073082	E(Thermal)=	0.077491
E(QCISD(T))=	-134.015641	E(Empiric)=	-0.063860
DE(Plus)=	-0.049183	DE(2DF)=	-0.143131
E(Delta-G3)=	-0.179623	E(G3-Empiric)=	-0.063860
G3(0 K)=	-134.378356	G3 Energy=	-134.373948
G3 Enthalpy=	-134.373004	G3 Free Energy=	-134.403708

methane CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.629735	0.629735	0.629735
2	6	0	0.000000	0.000000	0.000000
3	1	0	-0.629735	-0.629735	0.629735
4	1	0	0.629735	-0.629735	-0.629735
5	1	0	-0.629735	0.629735	-0.629735

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.044142	E(Thermal)=	0.047012
E(SCF)=	-40.212154	DE(MP2)=	-0.192064
DE(CBS)=	-0.019397	DE(MP34)=	-0.022192
DE(CCSD)=	-0.003628	DE(Int)=	0.007329
DE(Empirical)=	-0.012036		
CBS-Q (0 K)=	-40.410001	CBS-Q Energy=	-40.407130
CBS-Q Enthalpy=	-40.406186	CBS-Q Free Energy=	-40.427319

methane CBS-APNO

Center	Atomic	Atomic	Coordinates (Angstroms)

Number	Number	Type	X	Y	Z
1	1	0	0.630909	0.630909	0.630909
2	6	0	0.000000	0.000000	0.000000
3	1	0	-0.630909	-0.630909	0.630909
4	1	0	0.630909	-0.630909	-0.630909
5	1	0	-0.630909	0.630909	-0.630909

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.043466	E(Thermal)=	0.046335
E(SCF)=	-40.215982	DE(SCF)=	-0.000021
DE(MP2)=	-0.202809	DE(CBS)=	-0.014337
DE(QCI)=	-0.027672	DE(Int)=	0.005874
DE(Core)=	-0.054124	DE(Empirical)=	-0.003307
CBS-APNO (0 K)=	-40.468913	CBS-APNO Energy=	-40.466044
CBS-APNO Enthalpy=	-40.465100	CBS-APNO Free Energy=	-40.486212

methane G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.628989	0.628989	0.628989
2	6	0	0.000000	0.000000	0.000000
3	1	0	-0.628989	-0.628989	0.628989
4	1	0	0.628989	-0.628989	-0.628989
5	1	0	-0.628989	0.628989	-0.628989

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.042658	E(Thermal)=	0.045529
E(QCISD(T))=	-40.355940	E(Empiric)=	-0.025544
DE(Plus)=	-0.001724	DE(2DF)=	-0.056359
E(Delta-G3)=	-0.060717	E(G3-Empiric)=	-0.025544
G3(0 K)=	-40.457626	G3 Energy=	-40.454755
G3 Enthalpy=	-40.453810	G3 Free Energy=	-40.474926

CH3- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.006552	-0.336167
2	6	0	0.000000	0.000000	0.168084
3	1	0	0.871700	-0.503276	-0.336167
4	1	0	-0.871700	-0.503276	-0.336167

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.027417	E(Thermal)=	0.030293
E(SCF)=	-39.518334	DE(MP2)=	-0.205662
DE(CBS)=	-0.021775	DE(MP34)=	-0.017757
DE(CCSD)=	-0.005616	DE(Int)=	0.008598
DE(Empirical)=	-0.011304		
CBS-Q (0 K)=	-39.744432	CBS-Q Energy=	-39.741556

CBS-Q Enthalpy= -39.740612 CBS-Q Free Energy= -39.762572

CH3- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.007174	-0.338587
2	6	0	0.000000	0.000000	0.169293
3	1	0	0.872238	-0.503587	-0.338587
4	1	0	-0.872238	-0.503587	-0.338587

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026923	E(Thermal)=	0.029798
E(SCF)=	-39.522335	DE(SCF)=	-0.000027
DE(MP2)=	-0.218439	DE(CBS)=	-0.015781
DE(QCI)=	-0.024760	DE(Int)=	0.006914
DE(Core)=	-0.053479	DE(Empirical)=	-0.003010
CBS-APNO (0 K)=	-39.803995	CBS-APNO Energy=	-39.801120
CBS-APNO Enthalpy=	-39.800176	CBS-APNO Free Energy=	-39.822114

CH3- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	1.002875	-0.333736
2	6	0	0.000000	0.000000	0.166868
3	1	0	0.868515	-0.501438	-0.333736
4	1	0	-0.868515	-0.501438	-0.333736

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026534	E(Thermal)=	0.029403
E(QCISD(T))=	-39.625220	E(Empiric)=	-0.025544
DE(Plus)=	-0.047528	DE(2DF)=	-0.061434
E(Delta-G3)=	-0.058653	E(G3-Empiric)=	-0.025544
G3(0 K)=	-39.791846	G3 Energy=	-39.788976
G3 Enthalpy=	-39.788032	G3 Free Energy=	-39.809968

methyl alcohol CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.046553	0.662646	0.000000
2	8	0	0.046553	-0.758712	0.000000
3	1	0	-0.868749	-1.051923	0.000000
4	1	0	-0.436739	1.083316	0.892258
5	1	0	-0.436739	1.083316	-0.892258
6	1	0	1.090483	0.979112	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.050597	E(Thermal)=	0.053923

E(SCF)=	-115.086723	DE(MP2)=	-0.421302
DE(CBS)=	-0.043116	DE(MP34)=	-0.022738
DE(CCSD)=	-0.007973	DE(Int)=	0.013955
DE(Empirical)=	-0.022642		
CBS-Q (0 K)=	-115.539941	CBS-Q Energy=	-115.536615
CBS-Q Enthalpy=	-115.535671	CBS-Q Free Energy=	-115.562686

methyl alcohol CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.046873	0.659957	0.000000
2	8	0	0.046873	-0.757590	0.000000
3	1	0	-0.869628	-1.032773	0.000000
4	1	0	-0.439419	1.077519	0.893576
5	1	0	-0.439419	1.077519	-0.893576
6	1	0	1.092238	0.978706	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.050761	E(Thermal)=	0.054084
E(SCF)=	-115.099857	DE(SCF)=	-0.000486
DE(MP2)=	-0.444998	DE(CBS)=	-0.033649
DE(QCI)=	-0.034392	DE(Int)=	0.011779
DE(Core)=	-0.113697	DE(Empirical)=	-0.006344
CBS-APNO (0 K)=	-115.670884	CBS-APNO Energy=	-115.667560
CBS-APNO Enthalpy=	-115.666616	CBS-APNO Free Energy=	-115.693595

methyl alcohol G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.047115	0.664281	0.000000
2	8	0	0.047115	-0.758591	0.000000
3	1	0	-0.878369	-1.048875	0.000000
4	1	0	-0.437097	1.080828	0.891694
5	1	0	-0.437097	1.080828	-0.891694
6	1	0	1.092956	0.970258	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.049415	E(Thermal)=	0.052759
E(QCISD(T))=	-115.374855	E(Empiric)=	-0.044702
DE(Plus)=	-0.012145	DE(2DF)=	-0.109891
E(Delta-G3)=	-0.137026	E(G3-Empiric)=	-0.044702
G3(0 K)=	-115.629204	G3 Energy=	-115.625860
G3 Enthalpy=	-115.624916	G3 Free Energy=	-115.651929

CH3O- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	6	0	0.000056	0.518282	0.000000
2	8	0	0.000056	-0.786372	0.000000
3	1	0	1.029793	1.060877	0.000000
4	1	0	-0.515287	1.060200	0.891878
5	1	0	-0.515287	1.060200	-0.891878

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.033199	E(Thermal)=	0.036104
E(SCF)=	-114.448100	DE(MP2)=	-0.436543
DE(CBS)=	-0.046223	DE(MP34)=	-0.017740
DE(CCSD)=	-0.009572	DE(Int)=	0.015190
DE(Empirical)=	-0.022235		
CBS-Q (0 K)=	-114.932023	CBS-Q Energy=	-114.929119
CBS-Q Enthalpy=	-114.928174	CBS-Q Free Energy=	-114.954251

CH3O- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.524851	0.000000
2	8	0	0.000000	-0.789544	0.000000
3	1	0	1.027137	1.055748	0.000000
4	1	0	-0.513568	1.055749	0.889527
5	1	0	-0.513568	1.055749	-0.889527

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.034423	E(Thermal)=	0.037327
E(SCF)=	-114.461599	DE(SCF)=	-0.000636
DE(MP2)=	-0.463038	DE(CBS)=	-0.034849
DE(QCI)=	-0.030245	DE(Int)=	0.012592
DE(Core)=	-0.113014	DE(Empirical)=	-0.006127
CBS-APNO (0 K)=	-115.062493	CBS-APNO Energy=	-115.059589
CBS-APNO Enthalpy=	-115.058645	CBS-APNO Free Energy=	-115.084698

CH3O- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.000000	0.529968	0.000000
2	8	0	0.000000	-0.793233	0.000000
3	1	0	1.021421	1.055352	0.000000
4	1	0	-0.510710	1.055353	0.884577
5	1	0	-0.510710	1.055353	-0.884577

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.034254	E(Thermal)=	0.037160
E(QCISD(T))=	-114.728396	E(Empiric)=	-0.044702
DE(Plus)=	-0.041144	DE(2DF)=	-0.102476
E(Delta-G3)=	-0.137341	E(G3-Empiric)=	-0.044702
G3(0 K)=	-115.019805	G3 Energy=	-115.016899
G3 Enthalpy=	-115.015954	G3 Free Energy=	-115.042009

CH2OH- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.529635	1.078526	0.871318
2	6	0	0.131718	0.785262	0.000000
3	8	0	0.131718	-0.728146	0.000000
4	1	0	-0.784786	-1.043457	0.000000
5	1	0	-0.529635	1.078526	-0.871318

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.033393	E(Thermal)=	0.036665
E(SCF)=	-114.391531	DE(MP2)=	-0.436937
DE(CBS)=	-0.045008	DE(MP34)=	-0.019256
DE(CCSD)=	-0.010128	DE(Int)=	0.015069
DE(Empirical)=	-0.021849		
CBS-Q (0 K)=	-114.876246	CBS-Q Energy=	-114.872974
CBS-Q Enthalpy=	-114.872030	CBS-Q Free Energy=	-114.898746

CH2OH- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.536874	1.063522	0.871613
2	6	0	0.132857	0.784442	0.000000
3	8	0	0.132857	-0.728474	0.000000
4	1	0	-0.786245	-1.005902	0.000000
5	1	0	-0.536874	1.063522	-0.871613

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.034273	E(Thermal)=	0.037517
E(SCF)=	-114.405036	DE(SCF)=	-0.000402
DE(MP2)=	-0.462840	DE(CBS)=	-0.034306
DE(QCI)=	-0.032454	DE(Int)=	0.012637
DE(Core)=	-0.112918	DE(Empirical)=	-0.006019
CBS-APNO (0 K)=	-115.007065	CBS-APNO Energy=	-115.003821
CBS-APNO Enthalpy=	-115.002877	CBS-APNO Free Energy=	-115.029520

CH2OH- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.532055	1.061449	0.869194
2	6	0	0.132842	0.789103	0.000000
3	8	0	0.132842	-0.728682	0.000000
4	1	0	-0.795672	-1.028062	0.000000
5	1	0	-0.532055	1.061449	-0.869194

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.033334	E(Thermal)=	0.036588
E(QCISD(T))=	-114.656917	E(Empiric)=	-0.044702
DE(Plus)=	-0.049208	DE(2DF)=	-0.112001
E(Delta-G3)=	-0.135351	E(G3-Empiric)=	-0.044702
G3(0 K)=	-114.964844	G3 Energy=	-114.961591
G3 Enthalpy=	-114.960647	G3 Free Energy=	-114.987308

water CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.756966	-0.474946
2	8	0	0.000000	0.000000	0.118736
3	1	0	0.000000	-0.756966	-0.474946

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.021100	E(Thermal)=	0.023935
E(SCF)=	-76.056459	DE(MP2)=	-0.258458
DE(CBS)=	-0.027510	DE(MP34)=	-0.007545
DE(CCSD)=	-0.003057	DE(Int)=	0.008266
DE(Empirical)=	-0.013795		
CBS-Q (0 K)=	-76.337459	CBS-Q Energy=	-76.334624
CBS-Q Enthalpy=	-76.333680	CBS-Q Free Energy=	-76.355107

water CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.747663	-0.478434
2	8	0	0.000000	0.000000	0.119608
3	1	0	0.000000	-0.747663	-0.478434

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.021349	E(Thermal)=	0.024185
E(SCF)=	-76.066102	DE(SCF)=	-0.000087
DE(MP2)=	-0.274544	DE(CBS)=	-0.021236
DE(QCI)=	-0.013449	DE(Int)=	0.007056
DE(Core)=	-0.059715	DE(Empirical)=	-0.003884
CBS-APNO (0 K)=	-76.410612	CBS-APNO Energy=	-76.407776
CBS-APNO Enthalpy=	-76.406832	CBS-APNO Free Energy=	-76.428190

water G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.763150	-0.477143
2	8	0	0.000000	0.000000	0.119286
3	1	0	0.000000	-0.763150	-0.477143

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.020515	E(Thermal)=	0.023350
E(QCISD(T))=	-76.207892	E(Empiric)=	-0.025544
DE(Plus)=	-0.012978	DE(2DF)=	-0.074488
E(Delta-G3)=	-0.081653	E(G3-Empiric)=	-0.025544
G3(0 K)=	-76.382040	G3 Energy=	-76.379205
G3 Enthalpy=	-76.378261	G3 Free Energy=	-76.399638

OH- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-0.869388
2	8	0	0.000000	0.000000	0.108674

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.007877	E(Thermal)=	0.010238
E(SCF)=	-75.406983	DE(MP2)=	-0.275367
DE(CBS)=	-0.030524	DE(MP34)=	-0.001647
DE(CCSD)=	-0.003752	DE(Int)=	0.009377
DE(Empirical)=	-0.013588		
CBS-Q (0 K)=	-75.714607	CBS-Q Energy=	-75.712247
CBS-Q Enthalpy=	-75.711303	CBS-Q Free Energy=	-75.730886

OH- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-0.862226
2	8	0	0.000000	0.000000	0.107778

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.008106	E(Thermal)=	0.010467
E(SCF)=	-75.417278	DE(SCF)=	-0.000062
DE(MP2)=	-0.296558	DE(CBS)=	-0.022344
DE(QCI)=	-0.007443	DE(Int)=	0.007915
DE(Core)=	-0.059133	DE(Empirical)=	-0.003697
CBS-APNO (0 K)=	-75.790494	CBS-APNO Energy=	-75.788133
CBS-APNO Enthalpy=	-75.787189	CBS-APNO Free Energy=	-75.806722

OH- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-0.871418
2	8	0	0.000000	0.000000	0.108927

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.007605	E(Thermal)=	0.009966

E(QCISD(T))=	-75.521828	E(Empiric)=	-0.025544
DE(Plus)=	-0.075296	DE(2DF)=	-0.066018
E(Delta-G3)=	-0.079164	E(G3-Empiric)=	-0.025544
G3(0 K)=	-75.760245	G3 Energy=	-75.757884
G3 Enthalpy=	-75.756940	G3 Free Energy=	-75.776493

acetylene CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	1.661692
2	6	0	0.000000	0.000000	0.599026
3	6	0	0.000000	0.000000	-0.599026
4	1	0	0.000000	0.000000	-1.661692

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026713	E(Thermal)=	0.029537
E(SCF)=	-76.848486	DE(MP2)=	-0.305745
DE(CBS)=	-0.028845	DE(MP34)=	-0.015557
DE(CCSD)=	-0.012034	DE(Int)=	0.010936
DE(Empirical)=	-0.014370		
CBS-Q (0 K)=	-77.187388	CBS-Q Energy=	-77.184565
CBS-Q Enthalpy=	-77.183620	CBS-Q Free Energy=	-77.206349

acetylene CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	1.670923
2	6	0	0.000000	0.000000	0.604756
3	6	0	0.000000	0.000000	-0.604756
4	1	0	0.000000	0.000000	-1.670923

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.027041	E(Thermal)=	0.029740
E(SCF)=	-76.853920	DE(SCF)=	-0.000472
DE(MP2)=	-0.319218	DE(CBS)=	-0.023479
DE(QCI)=	-0.029218	DE(Int)=	0.009534
DE(Core)=	-0.107821	DE(Empirical)=	-0.003996
CBS-APNO (0 K)=	-77.301550	CBS-APNO Energy=	-77.298850
CBS-APNO Enthalpy=	-77.297906	CBS-APNO Free Energy=	-77.320439

acetylene G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	1.674293
2	6	0	0.000000	0.000000	0.608148
3	6	0	0.000000	0.000000	-0.608148
4	1	0	0.000000	0.000000	-1.674293

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026290	E(Thermal)=	0.029035
E(QCISD(T))=	-77.094098	E(Empiric)=	-0.031930
DE(Plus)=	-0.006291	DE(2DF)=	-0.061071
E(Delta-G3)=	-0.108849	E(G3-Empiric)=	-0.031930
G3(0 K)=	-77.275949	G3 Energy=	-77.273204
G3 Enthalpy=	-77.272260	G3 Free Energy=	-77.294859

C2H- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-1.561296
2	6	0	0.000000	0.000000	0.750912
3	6	0	0.000000	0.000000	-0.490696

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.014295	E(Thermal)=	0.017047
E(SCF)=	-76.231846	DE(MP2)=	-0.310930
DE(CBS)=	-0.030012	DE(MP34)=	-0.012160
DE(CCSD)=	-0.014028	DE(Int)=	0.011702
DE(Empirical)=	-0.013791		
CBS-Q (0 K)=	-76.586770	CBS-Q Energy=	-76.584018
CBS-Q Enthalpy=	-76.583074	CBS-Q Free Energy=	-76.606178

C2H- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-1.570068
2	6	0	0.000000	0.000000	0.757473
3	6	0	0.000000	0.000000	-0.495795

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.014557	E(Thermal)=	0.017229
E(SCF)=	-76.237128	DE(SCF)=	-0.000401
DE(MP2)=	-0.325474	DE(CBS)=	-0.024275
DE(QCI)=	-0.027754	DE(Int)=	0.010332
DE(Core)=	-0.107116	DE(Empirical)=	-0.003756
CBS-APNO (0 K)=	-76.701016	CBS-APNO Energy=	-76.698344
CBS-APNO Enthalpy=	-76.697400	CBS-APNO Free Energy=	-76.720358

C2H- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-1.574046
2	6	0	0.000000	0.000000	0.761512
3	6	0	0.000000	0.000000	-0.499171

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.014228	E(Thermal)=	0.016908
E(QCISD(T))=	-76.450637	E(Empiric)=	-0.031930
DE(Plus)=	-0.041783	DE(2DF)=	-0.061555
E(Delta-G3)=	-0.103075	E(G3-Empiric)=	-0.031930
G3(0 K)=	-76.674753	G3 Energy=	-76.672072
G3 Enthalpy=	-76.671128	G3 Free Energy=	-76.694105

ethylene CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.922619	1.234243
2	6	0	0.000000	0.000000	0.663439
3	6	0	0.000000	0.000000	-0.663439
4	1	0	0.000000	-0.922619	1.234243
5	1	0	0.000000	0.922619	-1.234243
6	1	0	0.000000	-0.922619	-1.234243

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.050306	E(Thermal)=	0.053356
E(SCF)=	-78.062196	DE(MP2)=	-0.328702
DE(CBS)=	-0.031892	DE(MP34)=	-0.027881
DE(CCSD)=	-0.010530	DE(Int)=	0.011832
DE(Empirical)=	-0.017557		
CBS-Q (0 K)=	-78.416620	CBS-Q Energy=	-78.413570
CBS-Q Enthalpy=	-78.412626	CBS-Q Free Energy=	-78.437490

ethylene CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.926240	1.238588
2	6	0	0.000000	0.000000	0.669258
3	6	0	0.000000	0.000000	-0.669258
4	1	0	0.000000	-0.926240	1.238588
5	1	0	0.000000	0.926240	-1.238588
6	1	0	0.000000	-0.926240	-1.238588

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.049977	E(Thermal)=	0.053015
E(SCF)=	-78.068776	DE(SCF)=	-0.000334
DE(MP2)=	-0.344637	DE(CBS)=	-0.024889
DE(QCI)=	-0.040705	DE(Int)=	0.009961
DE(Core)=	-0.107929	DE(Empirical)=	-0.004862
CBS-APNO (0 K)=	-78.532193	CBS-APNO Energy=	-78.529156
CBS-APNO Enthalpy=	-78.528212	CBS-APNO Free Energy=	-78.553038

ethylene G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.922957	1.237550
2	6	0	0.000000	0.000000	0.667432
3	6	0	0.000000	0.000000	-0.667432
4	1	0	0.000000	-0.922957	1.237550
5	1	0	0.000000	0.922957	-1.237550
6	1	0	0.000000	-0.922957	-1.237550

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.048913	E(Thermal)=	0.051972
E(QCISD(T))=	-78.322119	E(Empiric)=	-0.038316
DE(Plus)=	-0.005989	DE(2DF)=	-0.076922
E(Delta-G3)=	-0.112974	E(G3-Empiric)=	-0.038316
G3(0 K)=	-78.507406	G3 Energy=	-78.504347
G3 Enthalpy=	-78.503403	G3 Free Energy=	-78.528256

C2H3- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.013245	-1.108331	0.000000
2	6	0	0.067716	-0.784727	0.000000
3	6	0	0.067716	0.568824	0.000000
4	1	0	1.012026	1.144490	0.000000
5	1	0	-0.811375	1.259255	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.034480	E(Thermal)=	0.037486
E(SCF)=	-77.388065	DE(MP2)=	-0.339604
DE(CBS)=	-0.033760	DE(MP34)=	-0.023766
DE(CCSD)=	-0.012886	DE(Int)=	0.012893
DE(Empirical)=	-0.016825		
CBS-Q (0 K)=	-77.767532	CBS-Q Energy=	-77.764527
CBS-Q Enthalpy=	-77.763582	CBS-Q Free Energy=	-77.789455

C2H3- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.024547	-1.089235	0.000000
2	6	0	0.068578	-0.793029	0.000000
3	6	0	0.068578	0.574318	0.000000
4	1	0	1.014968	1.145780	0.000000
5	1	0	-0.813360	1.255717	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.034646	E(Thermal)=	0.037643
E(SCF)=	-77.394697	DE(SCF)=	-0.000298
DE(MP2)=	-0.356634	DE(CBS)=	-0.025934

DE(QCI)=	-0.038651	DE(Int)=	0.010793
DE(Core)=	-0.107187	DE(Empirical)=	-0.004578
CBS-APNO (0 K)=	-77.882540	CBS-APNO Energy=	-77.879543
CBS-APNO Enthalpy=	-77.878598	CBS-APNO Free Energy=	-77.904441

C2H3- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.018741	-1.098105	0.000000
2	6	0	0.066862	-0.789018	0.000000
3	6	0	0.066862	0.570488	0.000000
4	1	0	1.013946	1.138992	0.000000
5	1	0	-0.797554	1.270292	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.033911	E(Thermal)=	0.036923
E(QCISD(T))=	-77.623257	E(Empiric)=	-0.038316
DE(Plus)=	-0.040659	DE(2DF)=	-0.078773
E(Delta-G3)=	-0.110116	E(G3-Empiric)=	-0.038316
G3(0 K)=	-77.857210	G3 Energy=	-77.854198
G3 Enthalpy=	-77.853254	G3 Free Energy=	-77.879115

formaldehyde CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.938714	-1.118173
2	6	0	0.000000	0.000000	-0.525916
3	8	0	0.000000	0.000000	0.673980
4	1	0	0.000000	-0.938714	-1.118173

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026224	E(Thermal)=	0.029093
E(SCF)=	-113.909684	DE(MP2)=	-0.390330
DE(CBS)=	-0.039099	DE(MP34)=	-0.014896
DE(CCSD)=	-0.009661	DE(Int)=	0.012639
DE(Empirical)=	-0.019325		
CBS-Q (0 K)=	-114.344132	CBS-Q Energy=	-114.341263
CBS-Q Enthalpy=	-114.340319	CBS-Q Free Energy=	-114.365133

formaldehyde CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.937744	-1.119747
2	6	0	0.000000	0.000000	-0.529262
3	8	0	0.000000	0.000000	0.676883
4	1	0	0.000000	-0.937744	-1.119747

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026610	E(Thermal)=	0.029475
E(SCF)=	-113.921615	DE(SCF)=	-0.000781
DE(MP2)=	-0.411178	DE(CBS)=	-0.031385
DE(QCI)=	-0.027600	DE(Int)=	0.010963
DE(Core)=	-0.113099	DE(Empirical)=	-0.005436
CBS-APNO (0 K)=	-114.473522	CBS-APNO Energy=	-114.470657
CBS-APNO Enthalpy=	-114.469713	CBS-APNO Free Energy=	-114.494478

formaldehyde G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.934472	-1.124825
2	6	0	0.000000	0.000000	-0.536364
3	8	0	0.000000	0.000000	0.683479
4	1	0	0.000000	-0.934472	-1.124825

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.026074	E(Thermal)=	0.028944
E(QCISD(T))=	-114.191108	E(Empiric)=	-0.038316
DE(Plus)=	-0.009574	DE(2DF)=	-0.085952
E(Delta-G3)=	-0.132184	E(G3-Empiric)=	-0.038316
G3(0 K)=	-114.431061	G3 Energy=	-114.428190
G3 Enthalpy=	-114.427246	G3 Free Energy=	-114.452021

CHO- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.301134	1.087983	0.000000
2	6	0	0.092938	0.611236	0.000000
3	8	0	0.092938	-0.594425	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.007407	E(Thermal)=	0.010580
E(SCF)=	-113.252841	DE(MP2)=	-0.396455
DE(CBS)=	-0.040792	DE(MP34)=	-0.014475
DE(CCSD)=	-0.011764	DE(Int)=	0.013640
DE(Empirical)=	-0.018572		
CBS-Q (0 K)=	-113.713850	CBS-Q Energy=	-113.710678
CBS-Q Enthalpy=	-113.709734	CBS-Q Free Energy=	-113.735462

CHO- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.184322	1.049898	0.000000
2	6	0	0.084594	0.627702	0.000000
3	8	0	0.084594	-0.602014	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.009051	E(Thermal)=	0.011948
E(SCF)=	-113.267541	DE(SCF)=	-0.000796
DE(MP2)=	-0.420107	DE(CBS)=	-0.031881
DE(QCI)=	-0.028146	DE(Int)=	0.011617
DE(Core)=	-0.112344	DE(Empirical)=	-0.005138
CBS-APNO (0 K)=	-113.845283	CBS-APNO Energy=	-113.842386
CBS-APNO Enthalpy=	-113.841442	CBS-APNO Free Energy=	-113.866607

CHO- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.124326	1.040375	0.000000
2	6	0	0.080309	0.643071	0.000000
3	8	0	0.080309	-0.612350	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.009709	E(Thermal)=	0.012569
E(QCISD(T))=	-113.516172	E(Empiric)=	-0.038316
DE(Plus)=	-0.043662	DE(2DF)=	-0.084568
E(Delta-G3)=	-0.129917	E(G3-Empiric)=	-0.038316
G3(0 K)=	-113.802926	G3 Energy=	-113.800065
G3 Enthalpy=	-113.799121	G3 Free Energy=	-113.824232

hydrogen chloride CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-1.211475
2	17	0	0.000000	0.000000	0.071263

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.006610	E(Thermal)=	0.008971
E(SCF)=	-460.100056	DE(MP2)=	-0.200713
DE(CBS)=	-0.029078	DE(MP34)=	-0.020311
DE(CCSD)=	-0.002724	DE(Int)=	0.010338
DE(Empirical)=	-0.012257		
CBS-Q (0 K)=	-460.348190	CBS-Q Energy=	-460.345829
CBS-Q Enthalpy=	-460.344885	CBS-Q Free Energy=	-460.366073

hydrogen chloride G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	0.000000	0.000000	-1.208869
2	17	0	0.000000	0.000000	0.071110

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.006481	E(Thermal)=	0.008841
E(QCISD(T))=	-460.211570	E(Empiric)=	-0.025544
DE(Plus)=	-0.002202	DE(2DF)=	-0.072002
E(Delta-G3)=	-0.349828	E(G3-Empiric)=	-0.025544
G3(0 K)=	-460.654664	G3 Energy=	-460.652304
G3 Enthalpy=	-460.651360	G3 Free Energy=	-460.672523

Cl- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.000000	0.000000	0.619779

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.000000	E(Thermal)=	0.001416
E(SCF)=	-459.565425	DE(MP2)=	-0.203338
DE(CBS)=	-0.031749	DE(MP34)=	-0.015890
DE(CCSD)=	-0.003149	DE(Int)=	0.011456
DE(Empirical)=	-0.012192		
CBS-Q (0 K)=	-459.820287	CBS-Q Energy=	-459.818871
CBS-Q Enthalpy=	-459.817927	CBS-Q Free Energy=	-459.835310

Cl- G3

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.000000	E(Thermal)=	0.001416
E(QCISD(T))=	-459.666548	E(Empiric)=	-0.024876
DE(Plus)=	-0.019581	DE(2DF)=	-0.065206
E(Delta-G3)=	-0.347388	E(G3-Empiric)=	-0.024876
G3(0 K)=	-460.123600	G3 Energy=	-460.122184
G3 Enthalpy=	-460.121239	G3 Free Energy=	-460.138623

propene CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.280465	0.220452	-0.000005
2	6	0	-0.134719	-0.453636	0.000006
3	6	0	1.233553	0.162260	0.000015
4	1	0	-0.166858	-1.542015	0.000023
5	1	0	-1.301617	1.306441	0.000032
6	1	0	-2.238925	-0.286263	0.000028
7	1	0	1.182068	1.253604	-0.000221
8	1	0	1.807479	-0.153276	-0.878426
9	1	0	1.807641	-0.152943	0.878469

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.078519	E(Thermal)=	0.082631
E(SCF)=	-117.113450	DE(MP2)=	-0.499444

DE(CBS)=	-0.048151	DE(MP34)=	-0.039657
DE(CCSD)=	-0.015252	DE(Int)=	0.017619
DE(Empirical)=	-0.026405		
CBS-Q (0 K)=	-117.646220	CBS-Q Energy=	-117.642108
CBS-Q Enthalpy=	-117.641164	CBS-Q Free Energy=	-117.671245

propene CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.283439	-0.223984	-0.000001
2	6	0	0.133597	0.462605	0.000001
3	6	0	-1.237274	-0.164556	0.000000
4	1	0	0.167727	1.552951	-0.000003
5	1	0	1.294207	-1.312475	0.000000
6	1	0	2.246138	0.280164	0.000003
7	1	0	-1.169353	-1.257872	-0.000025
8	1	0	-1.808656	0.146440	-0.883747
9	1	0	-1.808639	0.146401	0.883772

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.078012	E(Thermal)=	0.082117
E(SCF)=	-117.123556	DE(SCF)=	-0.000528
DE(MP2)=	-0.523495	DE(CBS)=	-0.037529
DE(QCI)=	-0.058524	DE(Int)=	0.014735
DE(Core)=	-0.162298	DE(Empirical)=	-0.007323
CBS-APNO (0 K)=	-117.820505	CBS-APNO Energy=	-117.816400
CBS-APNO Enthalpy=	-117.815456	CBS-APNO Free Energy=	-117.845529

propene G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.278865	-0.222075	0.000002
2	6	0	0.130220	0.461369	-0.000003
3	6	0	-1.230459	-0.164127	0.000000
4	1	0	0.164241	1.550113	-0.000005
5	1	0	1.293121	-1.308307	-0.000008
6	1	0	2.240881	0.278889	0.000007
7	1	0	-1.159714	-1.254923	-0.000304
8	1	0	-1.805255	0.141853	-0.880239
9	1	0	-1.805027	0.141375	0.880556

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.076298	E(Thermal)=	0.080465
E(QCISD(T))=	-117.508177	E(Empiric)=	-0.057474
DE(Plus)=	-0.007432	DE(2DF)=	-0.116365
E(Delta-G3)=	-0.169040	E(G3-Empiric)=	-0.057474
G3(0 K)=	-117.782190	G3 Energy=	-117.778023
G3 Enthalpy=	-117.777079	G3 Free Energy=	-117.807259

CH2CHCH2- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.277695	0.177112	0.000186
2	6	0	-0.000007	-0.374578	-0.000001
3	6	0	-1.277713	0.177074	-0.000187
4	1	0	0.000157	-1.475566	-0.000029
5	1	0	1.441600	1.254377	-0.000092
6	1	0	2.161376	-0.455516	-0.000578
7	1	0	-2.161610	-0.455294	0.000633
8	1	0	-1.441374	1.254351	0.000076

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.061690	E(Thermal)=	0.066370
E(SCF)=	-116.463603	DE(MP2)=	-0.517714
DE(CBS)=	-0.050695	DE(MP34)=	-0.030830
DE(CCSD)=	-0.017300	DE(Int)=	0.018640
DE(Empirical)=	-0.025633		
CBS-Q (0 K)=	-117.025446	CBS-Q Energy=	-117.020766
CBS-Q Enthalpy=	-117.019822	CBS-Q Free Energy=	-117.050736

CH2CHCH2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.280547	0.178829	0.052792
2	6	0	0.000013	-0.381037	0.000006
3	6	0	1.280599	0.178838	-0.053084
4	1	0	0.000013	-1.484045	0.000023
5	1	0	-1.417075	1.257470	-0.059454
6	1	0	-2.151821	-0.445350	-0.149143
7	1	0	2.151621	-0.445283	0.150185
8	1	0	1.416875	1.257427	0.060107

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.061524	E(Thermal)=	0.065942
E(SCF)=	-116.472746	DE(SCF)=	-0.000649
DE(MP2)=	-0.543514	DE(CBS)=	-0.039414
DE(QCI)=	-0.051905	DE(Int)=	0.015715
DE(Core)=	-0.162056	DE(Empirical)=	-0.006999
CBS-APNO (0 K)=	-117.200045	CBS-APNO Energy=	-117.195627
CBS-APNO Enthalpy=	-117.194683	CBS-APNO Free Energy=	-117.224943

CH2CHCH2- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.275910	0.176825	-0.056352
2	6	0	0.000002	-0.379537	0.000008

3	6	0	1.275895	0.176827	0.056289
4	1	0	0.000008	-1.481991	-0.000010
5	1	0	-1.412680	1.253844	0.051379
6	1	0	-2.148048	-0.435196	0.167077
7	1	0	2.148089	-0.435202	-0.166866
8	1	0	1.412708	1.253853	-0.051250

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.059961	E(Thermal)=	0.064612
E(QCISD(T))=	-116.832965	E(Empiric)=	-0.057474
DE(Plus)=	-0.041521	DE(2DF)=	-0.119927
E(Delta-G3)=	-0.168390	E(G3-Empiric)=	-0.057474
G3(0 K)=	-117.160316	G3 Energy=	-117.155665
G3 Enthalpy=	-117.154721	G3 Free Energy=	-117.185531

CH3CCH2- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.786152	-0.144744	-0.874034
2	6	0	-1.169951	0.125885	-0.000018
3	1	0	-1.080768	1.248136	-0.000658
4	6	0	0.148587	-0.634919	0.000052
5	6	0	1.225177	0.169483	0.000106
6	1	0	1.174856	1.289720	0.000071
7	1	0	-1.786147	-0.143876	0.874328
8	1	0	2.255337	-0.211929	-0.000546

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.062377	E(Thermal)=	0.066386
E(SCF)=	-116.439736	DE(MP2)=	-0.514281
DE(CBS)=	-0.049998	DE(MP34)=	-0.034530
DE(CCSD)=	-0.018784	DE(Int)=	0.018740
DE(Empirical)=	-0.025507		
CBS-Q (0 K)=	-117.001719	CBS-Q Energy=	-116.997710
CBS-Q Enthalpy=	-116.996765	CBS-Q Free Energy=	-117.026511

CH3CCH2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.785848	-0.130903	0.879140
2	6	0	1.169657	0.130968	0.000000
3	1	0	1.055715	1.246745	-0.000021
4	6	0	-0.150604	-0.656437	0.000000
5	6	0	-1.221888	0.177542	-0.000001
6	1	0	-1.152762	1.294357	0.000003
7	1	0	1.785869	-0.130933	-0.879117
8	1	0	-2.257661	-0.191704	0.000001

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.062488	E(Thermal)=	0.066517
E(SCF)=	-116.449730	DE(SCF)=	-0.000475
DE(MP2)=	-0.539154	DE(CBS)=	-0.038807
DE(QCI)=	-0.056497	DE(Int)=	0.015662
DE(Core)=	-0.161492	DE(Empirical)=	-0.006991
CBS-APNO (0 K)=	-117.174997	CBS-APNO Energy=	-117.170968
CBS-APNO Enthalpy=	-117.170023	CBS-APNO Free Energy=	-117.199831

CH3CCH2- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.781678	-0.126195	-0.874326
2	6	0	-1.158850	0.130296	0.000000
3	1	0	-1.064148	1.245757	-0.000001
4	6	0	0.147900	-0.655960	0.000000
5	6	0	1.212676	0.176392	0.000000
6	1	0	1.166794	1.291915	0.000000
7	1	0	-1.781676	-0.126193	0.874328
8	1	0	2.250351	-0.189652	0.000001

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.061259	E(Thermal)=	0.065335
E(QCISD(T))=	-116.814055	E(Empiric)=	-0.057474
DE(Plus)=	-0.042164	DE(2DF)=	-0.117356
E(Delta-G3)=	-0.166100	E(G3-Empiric)=	-0.057474
G3(0 K)=	-117.135889	G3 Energy=	-117.131814
G3 Enthalpy=	-117.130869	G3 Free Energy=	-117.160748

CH3CHCH- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.094574	-1.259588	-0.000931
2	6	0	-1.161986	-0.163827	-0.000012
3	6	0	0.243231	0.445741	0.000147
4	6	0	1.448997	-0.161816	-0.000085
5	1	0	1.252284	-1.276145	0.000215
6	1	0	0.190879	1.552880	-0.000227
7	1	0	-1.765210	0.131766	-0.880563
8	1	0	-1.764830	0.130497	0.881206

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.062514	E(Thermal)=	0.066572
E(SCF)=	-116.436032	DE(MP2)=	-0.512985
DE(CBS)=	-0.050046	DE(MP34)=	-0.035341
DE(CCSD)=	-0.018130	DE(Int)=	0.018753
DE(Empirical)=	-0.025584		
CBS-Q (0 K)=	-116.996852	CBS-Q Energy=	-116.992794
CBS-Q Enthalpy=	-116.991850	CBS-Q Free Energy=	-117.021781

CH3CHCH- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.085952	-1.262029	-0.000050
2	6	0	1.163705	-0.164581	0.000000
3	6	0	-0.240866	0.451823	0.000000
4	6	0	-1.455942	-0.166773	0.000000
5	1	0	-1.220761	-1.277143	0.000002
6	1	0	-0.190782	1.558692	0.000002
7	1	0	1.762085	0.128794	0.884778
8	1	0	1.762117	0.128873	-0.884730

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.062541	E(Thermal)=	0.066587
E(SCF)=	-116.446077	DE(SCF)=	-0.000486
DE(MP2)=	-0.538277	DE(CBS)=	-0.039047
DE(QCI)=	-0.056609	DE(Int)=	0.015725
DE(Core)=	-0.161438	DE(Empirical)=	-0.007011
CBS-APNO (0 K)=	-117.170678	CBS-APNO Energy=	-117.166632
CBS-APNO Enthalpy=	-117.165687	CBS-APNO Free Energy=	-117.195611

CH3CHCH- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-1.078294	-1.257659	-0.000088
2	6	0	-1.159032	-0.163162	0.000000
3	6	0	0.236665	0.445235	-0.000002
4	6	0	1.452572	-0.160406	0.000001
5	1	0	1.237490	-1.271445	0.000000
6	1	0	0.183965	1.551141	0.000005
7	1	0	-1.762225	0.124051	-0.880070
8	1	0	-1.762169	0.123914	0.880154

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.061271	E(Thermal)=	0.065359
E(QCISD(T))=	-116.810674	E(Empiric)=	-0.057474
DE(Plus)=	-0.040143	DE(2DF)=	-0.118862
E(Delta-G3)=	-0.165682	E(G3-Empiric)=	-0.057474
G3(0 K)=	-117.131564	G3 Energy=	-117.127476
G3 Enthalpy=	-117.126532	G3 Free Energy=	-117.156521

isocyanic acid CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.327301	-1.412304	0.000000
2	7	0	0.369463	-1.104618	0.000000
3	6	0	0.000000	0.048858	0.000000

4	8	0	-0.489193	1.106436	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.021129	E(Thermal)=	0.024385
E(SCF)=	-167.826376	DE(MP2)=	-0.574064
DE(CBS)=	-0.056249	DE(MP34)=	-0.004799
DE(CCSD)=	-0.017060	DE(Int)=	0.018127
DE(Empirical)=	-0.025745		
CBS-Q (0 K)=	-168.465038	CBS-Q Energy=	-168.461782
CBS-Q Enthalpy=	-168.460837	CBS-Q Free Energy=	-168.487929

isocyanic acid CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.343006	-1.356222	0.000000
2	7	0	0.365199	-1.115884	0.000000
3	6	0	0.000000	0.049616	0.000000
4	8	0	-0.487425	1.108714	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.021068	E(Thermal)=	0.024309
E(SCF)=	-167.842946	DE(SCF)=	-0.001489
DE(MP2)=	-0.600935	DE(CBS)=	-0.046002
DE(QCI)=	-0.027199	DE(Int)=	0.015838
DE(Core)=	-0.170903	DE(Empirical)=	-0.007288
CBS-APNO (0 K)=	-168.659857	CBS-APNO Energy=	-168.656616
CBS-APNO Enthalpy=	-168.655672	CBS-APNO Free Energy=	-168.682721

isocyanic acid G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.583555	-1.152916	0.000000
2	7	0	0.583435	-1.023614	0.000000
3	6	0	0.000000	0.052232	0.000000
4	8	0	-0.708450	1.000603	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.020351	E(Thermal)=	0.023635
E(QCISD(T))=	-168.243681	E(Empiric)=	-0.051088
DE(Plus)=	-0.011070	DE(2DF)=	-0.115371
E(Delta-G3)=	-0.194453	E(G3-Empiric)=	-0.051088
G3(0 K)=	-168.595313	G3 Energy=	-168.592028
G3 Enthalpy=	-168.591084	G3 Free Energy=	-168.618189

NCO- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	8	0	0.000000	0.000000	1.156005
2	7	0	0.000000	0.000000	-1.259709
3	6	0	0.000000	0.000000	-0.071679

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.010785	E(Thermal)=	0.013441
E(SCF)=	-167.268790	DE(MP2)=	-0.582239
DE(CBS)=	-0.058402	DE(MP34)=	-0.000284
DE(CCSD)=	-0.017816	DE(Int)=	0.018828
DE(Empirical)=	-0.025650		
CBS-Q (0 K)=	-167.923569	CBS-Q Energy=	-167.920913
CBS-Q Enthalpy=	-167.919969	CBS-Q Free Energy=	-167.944878

NCO- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	1.159463
2	7	0	0.000000	0.000000	-1.263548
3	6	0	0.000000	0.000000	-0.071811

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.011061	E(Thermal)=	0.013678
E(SCF)=	-167.284415	DE(SCF)=	-0.001366
DE(MP2)=	-0.611519	DE(CBS)=	-0.046873
DE(QCI)=	-0.022738	DE(Int)=	0.016533
DE(Core)=	-0.170427	DE(Empirical)=	-0.007170
CBS-APNO (0 K)=	-168.116913	CBS-APNO Energy=	-168.114296
CBS-APNO Enthalpy=	-168.113352	CBS-APNO Free Energy=	-168.138168

NCO- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	8	0	0.000000	0.000000	1.171566
2	7	0	0.000000	0.000000	-1.279306
3	6	0	0.000000	0.000000	-0.069564

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.010602	E(Thermal)=	0.013268
E(QCISD(T))=	-167.677955	E(Empiric)=	-0.051088
DE(Plus)=	-0.034926	DE(2DF)=	-0.107876
E(Delta-G3)=	-0.190986	E(G3-Empiric)=	-0.051088
G3(0 K)=	-168.052229	G3 Energy=	-168.049562
G3 Enthalpy=	-168.048618	G3 Free Energy=	-168.073515

acetaldehyde CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z

1	1	0	1.582503	-0.680934	0.878930
2	6	0	0.000000	0.462155	0.000000
3	6	0	0.929940	-0.723112	0.000000
4	8	0	-1.201564	0.390808	0.000000
5	1	0	0.506578	1.453995	0.000000
6	1	0	1.582503	-0.680934	-0.878930
7	1	0	0.361292	-1.652850	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.054656	E(Thermal)=	0.058565
E(SCF)=	-152.971421	DE(MP2)=	-0.559162
DE(CBS)=	-0.055458	DE(MP34)=	-0.027131
DE(CCSD)=	-0.014147	DE(Int)=	0.018438
DE(Empirical)=	-0.028223		
CBS-Q (0 K)=	-153.582448	CBS-Q Energy=	-153.578539
CBS-Q Enthalpy=	-153.577595	CBS-Q Free Energy=	-153.607397

acetaldehyde CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.583123	-0.679361	0.884492
2	6	0	0.000000	0.466028	0.000000
3	6	0	0.935579	-0.723239	0.000000
4	8	0	-1.205354	0.387001	0.000000
5	1	0	0.502432	1.458292	0.000000
6	1	0	1.583123	-0.679361	-0.884492
7	1	0	0.360682	-1.652307	0.000000

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.054725	E(Thermal)=	0.058629
E(SCF)=	-152.986763	DE(SCF)=	-0.000964
DE(MP2)=	-0.588019	DE(CBS)=	-0.044112
DE(QCI)=	-0.045901	DE(Int)=	0.015765
DE(Core)=	-0.167586	DE(Empirical)=	-0.007911
CBS-APNO (0 K)=	-153.770767	CBS-APNO Energy=	-153.766863
CBS-APNO Enthalpy=	-153.765919	CBS-APNO Free Energy=	-153.795710

acetaldehyde G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	1.596158	-0.652426	0.881200
2	6	0	0.000000	0.464061	0.000000
3	6	0	0.947952	-0.700428	0.000000
4	8	0	-1.217967	0.361565	0.000000
5	1	0	0.477994	1.465163	0.000000
6	1	0	1.596158	-0.652426	-0.881200
7	1	0	0.385709	-1.634626	0.000000

Temperature=	298.150000	Pressure=	1.000000

E(ZPE)=	0.053512	E(Thermal)=	0.057473
E(QCISD(T))=	-153.386019	E(Empiric)=	-0.057474
DE(Plus)=	-0.011637	DE(2DF)=	-0.125314
E(Delta-G3)=	-0.187863	E(G3-Empiric)=	-0.057474
G3(0 K)=	-153.714796	G3 Energy=	-153.710835
G3 Enthalpy=	-153.709890	G3 Free Energy=	-153.739821

CHOCH2- CBS-QB3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.042439	0.498454	0.000089
2	6	0	0.100588	0.345307	-0.000032
3	6	0	-1.182579	-0.168043	-0.000001
4	8	0	1.224718	-0.225365	0.000016
5	1	0	0.093195	1.484504	0.000009
6	1	0	-1.356557	-1.243619	-0.000029

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.040952	E(Thermal)=	0.044469
E(SCF)=	-152.360525	DE(MP2)=	-0.576964
DE(CBS)=	-0.058398	DE(MP34)=	-0.019418
DE(CCSD)=	-0.016451	DE(Int)=	0.019491
DE(Empirical)=	-0.027756		
CBS-Q (0 K)=	-152.999069	CBS-Q Energy=	-152.995552
CBS-Q Enthalpy=	-152.994608	CBS-Q Free Energy=	-153.023302

CHOCH2- CBS-APNO

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.045129	0.500486	0.000051
2	6	0	0.101356	0.347231	0.000004
3	6	0	-1.185293	-0.169054	-0.000019
4	8	0	1.226646	-0.225801	0.000001
5	1	0	0.091471	1.483461	-0.000003
6	1	0	-1.355890	-1.246602	0.000036

Temperature=	298.150000	Pressure=	1.000000
E(ZPE)=	0.041205	E(Thermal)=	0.044671
E(SCF)=	-152.375777	DE(SCF)=	-0.001024
DE(MP2)=	-0.607615	DE(CBS)=	-0.045322
DE(QCI)=	-0.040195	DE(Int)=	0.016461
DE(Core)=	-0.167354	DE(Empirical)=	-0.007682
CBS-APNO (0 K)=	-153.187303	CBS-APNO Energy=	-153.183837
CBS-APNO Enthalpy=	-153.182893	CBS-APNO Free Energy=	-153.211477

CHOCH2- G3

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z