Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Why Is Sulfuric Acid a Much Stronger Acid than Ethanol? Contributions by Inductive/Field Effects and Electron-Delocalization Effects.

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1. B3LYP/6-311++G(p,d) calculations for H_2SO_4 and its n=1–6 alkylogues

a. H_2SO_4 (n=0)
energy = -700.3391294 a.u.
thermally corrected enthalpy = -700.294694 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.000000	0.000002	0.169138
2	8	0	1.110273	-0.594451	-0.859539
3	8	0	0.551330	1.148598	0.838177
4	8	0	-0.551329	-1.148582	0.838200
5	8	0	-1.110273	0.594434	-0.859550
6	1	0	1.671504	0.127976	-1.182263
7	1	0	-1.671505	-0.127999	-1.182260

b. H_2SO_4 (n=1)
energy = -778.9866638 a.u.
thermally corrected enthalpy = -778.882523 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-0.888425	-0.138730	0.014990
2	8	0	-1.828323	1.155163	-0.385420
3	1	0	-2.447319	1.309650	0.344079
4	8	0	-1.193834	-0.476005	1.401302
5	8	0	-1.015001	-1.126298	-1.039146
6	6	0	0.737027	0.636818	-0.101676
7	1	0	0.780168	1.117801	-1.079379
8	1	0	0.782789	1.389867	0.685153
9	6	0	1.851130	-0.392978	0.055493
10	1	0	1.792496	-1.130894	-0.750920
11	1	0	1.751797	-0.910700	1.016336
12	8	0	3.064531	0.351859	-0.006244
13	1	0	3.806938	-0.256830	0.058056

c. H_2SO_4 (n=2)
energy = -857.6388247 a.u.
thermally corrected enthalpy = -857.475087 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.903954	-0.148936	0.002656
2	8	0	-2.904839	1.145730	-0.232673
3	1	0	-3.578668	1.126937	0.463572
4	8	0	-2.164038	-0.647878	1.350034
5	8	0	-2.020397	-1.027114	-1.146734
6	6	0	-0.315239	0.712065	-0.062376
7	1	0	-0.326114	1.269322	-1.000999
8	1	0	-0.325485	1.412524	0.774068
9	6	0	0.853346	-0.270606	0.014024
10	1	0	0.784195	-0.974720	-0.820027
11	1	0	0.773950	-0.853578	0.936909
12	6	0	2.197133	0.467688	-0.026749
13	1	0	2.270231	1.170548	0.809857
14	1	0	2.277769	1.057073	-0.946267
15	6	0	3.381749	-0.485743	0.039697
16	1	0	3.348640	-1.184677	-0.807307
17	1	0	3.338211	-1.075134	0.965947
18	8	0	4.572143	0.301275	-0.001826
19	1	0	5.335647	-0.281849	0.043753

d. H_2SO_4 (n=3)
energy = -936.2880965 a.u.
thermally corrected enthalpy = -936.064933 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-3.008851	-0.168111	0.002340
2	8	0	-4.044154	1.105549	-0.201657
3	1	0	-4.724550	1.044278	0.485634
4	8	0	-3.251192	-0.701258	1.339913
5	8	0	-3.108546	-1.025741	-1.164261
6	6	0	-1.444063	0.735748	-0.050556
7	1	0	-1.474268	1.311142	-0.977875
8	1	0	-1.471743	1.419107	0.799677
9	6	0	-0.247544	-0.214757	0.002688
10	1	0	-0.297120	-0.903960	-0.845047
11	1	0	-0.305148	-0.819104	0.913291
12	6	0	1.079877	0.554731	-0.026231
13	1	0	1.120218	1.247816	0.822858
14	1	0	1.124357	1.172509	-0.931451
15	6	0	2.301590	-0.370219	0.016220
16	1	0	2.257844	-1.061814	-0.834305
17	1	0	2.251234	-0.991167	0.919354
18	6	0	3.629419	0.393950	-0.009460
19	1	0	3.686970	1.077154	0.844987
20	1	0	3.690145	1.012294	-0.911758
21	6	0	4.841100	-0.524900	0.026466
22	1	0	4.824095	-1.202772	-0.838401
23	1	0	4.819139	-1.140474	0.936697
24	8	0	6.014813	0.290752	0.001174
25	1	0	6.790799	-0.276973	0.022782

e. H_2SO_4 (n=4)
energy = -1014.9369871 a.u.
thermally corrected enthalpy = -1014.654417 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-4.163980	-0.189351	0.002704
2	8	0	-5.220224	1.069660	-0.187619
3	1	0	-5.898869	0.989969	0.499513
4	8	0	-4.395364	-0.738232	1.335899
5	8	0	-4.252885	-1.037951	-1.171387
6	6	0	-2.614039	0.739884	-0.045152
7	1	0	-2.655107	1.321978	-0.967871
8	1	0	-2.651709	1.415946	0.810537
9	6	0	-1.401904	-0.191115	-0.001027
10	1	0	-1.440816	-0.874019	-0.854363
11	1	0	-1.448263	-0.803973	0.904484
12	6	0	-0.086976	0.600080	-0.024739
13	1	0	-0.058056	1.286845	0.830247
14	1	0	-0.054678	1.226614	-0.924728
15	6	0	1.150296	-0.304199	0.008562
16	1	0	1.119434	-0.989611	-0.847562
17	1	0	1.113381	-0.934677	0.905764
18	6	0	2.470368	0.474228	-0.011305
19	1	0	2.502615	1.156233	0.847727
20	1	0	2.503893	1.109204	-0.905625
21	6	0	3.709853	-0.427530	0.013496
22	1	0	3.676753	-1.107456	-0.847436
23	1	0	3.673598	-1.064233	0.906791
24	6	0	5.025933	0.357368	-0.003423
25	1	0	5.073449	1.029786	0.860237
26	1	0	5.074826	0.989521	-0.896915
27	6	0	6.252433	-0.541622	0.018147
28	1	0	6.244765	-1.208366	-0.855578
29	1	0	6.242090	-1.169591	0.920163
30	8	0	7.414970	0.291376	0.001737
31	1	0	8.198613	-0.265954	0.014960

f. H_2SO_4 (n=5)
energy = -1093.5857547 a.u.
thermally corrected enthalpy = -1093.243776 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-5.350552	-0.210191	0.003117
2	8	0	-6.420832	1.038279	-0.179236
3	1	0	-7.097626	0.947288	0.508310
4	8	0	-5.574245	-0.768332	1.333790
5	8	0	-5.432067	-1.053657	-1.175209
6	6	0	-3.810834	0.735962	-0.041933
7	1	0	-3.858849	1.321371	-0.962217
8	1	0	-3.855241	1.407986	0.816616
9	6	0	-2.588643	-0.182045	-0.002441
10	1	0	-2.620718	-0.861813	-0.858558
11	1	0	-2.627752	-0.799135	0.900528
12	6	0	-1.282252	0.623256	-0.023682
13	1	0	-1.260365	1.307013	0.833963
14	1	0	-1.257156	1.253594	-0.921270
15	6	0	-0.035282	-0.267775	0.005607
16	1	0	-0.059141	-0.950132	-0.853166
17	1	0	-0.065074	-0.902309	0.900188
18	6	0	1.277032	0.524033	-0.011632
19	1	0	1.302050	1.202447	0.850813
20	1	0	1.302054	1.164224	-0.902827
21	6	0	2.526302	-0.363992	0.007380
22	1	0	2.502349	-1.039955	-0.857031
23	1	0	2.499539	-1.007072	0.896498
24	6	0	3.838977	0.427159	-0.005272
25	1	0	3.864332	1.101277	0.860305
26	1	0	3.865265	1.071765	-0.893033
27	6	0	5.088717	-0.460607	0.010282
28	1	0	5.062168	-1.133670	-0.856395
29	1	0	5.060476	-1.105537	0.898071
30	6	0	6.396728	0.337936	-0.001259
31	1	0	6.437350	1.004652	0.867183
32	1	0	6.438651	0.977084	-0.890133
33	6	0	7.632425	-0.548367	0.013602
34	1	0	7.630950	-1.209457	-0.864476
35	1	0	7.629082	-1.182343	0.911476
36	8	0	8.787328	0.295819	0.001941
37	1	0	9.575991	-0.254447	0.011092

g. H_2SO_4 (n=6)
energy = -1172.2344571 a.u.
thermally corrected enthalpy = -1171.833071 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-6.558627	-0.228793	0.003619
2	8	0	-7.637569	1.012657	-0.176174
3	1	0	-8.312987	0.916183	0.511968
4	8	0	-6.778329	-0.790918	1.333285
5	8	0	-6.634717	-1.070527	-1.176298
6	6	0	-5.025457	0.727968	-0.039773
7	1	0	-5.077878	1.315341	-0.958556
8	1	0	-5.074185	1.397479	0.820507
9	6	0	-3.796870	-0.181617	-0.003095
10	1	0	-3.824105	-0.858755	-0.861453
11	1	0	-3.831682	-0.801990	0.897795
12	6	0	-2.496204	0.632949	-0.021508
13	1	0	-2.478762	1.313226	0.839011
14	1	0	-2.476043	1.267280	-0.916423
15	6	0	-1.242804	-0.249205	0.003287
16	1	0	-1.262238	-0.928141	-0.858295
17	1	0	-1.267484	-0.887693	0.895208
18	6	0	0.063770	0.552113	-0.011354
19	1	0	0.083660	1.228109	0.853172
20	1	0	0.084081	1.195242	-0.900596
21	6	0	1.319698	-0.326541	0.005117
22	1	0	1.300297	-1.001021	-0.860557
23	1	0	1.298318	-0.971682	0.892864
24	6	0	2.627022	0.473745	-0.006790
25	1	0	2.646880	1.146886	0.860036
26	1	0	2.647106	1.120585	-0.893413
27	6	0	3.883771	-0.403804	0.006505
28	1	0	3.864702	-1.075681	-0.861364
29	1	0	3.862930	-1.051915	0.892250
30	6	0	5.190497	0.397228	-0.002995
31	1	0	5.210765	1.067973	0.865366
32	1	0	5.211603	1.045899	-0.887956
33	6	0	6.447379	-0.480539	0.008637
34	1	0	6.425811	-1.150494	-0.860635
35	1	0	6.424575	-1.129175	0.893920
36	6	0	7.749241	0.328103	-0.000294
37	1	0	7.784939	0.991859	0.870633

38	1	0	7.785835	0.970938	-0.886746
39	6	0	8.991738	-0.548639	0.010788
40	1	0	8.994854	-1.206620	-0.869630
41	1	0	8.993726	-1.185805	0.906406
42	8	0	10.140552	0.304112	0.001525
43	1	0	10.933142	-0.240497	0.008723

2. B3LYP/6-311++G(p,d) calculations for HSO_4^- and its n=1–6 alkylogues

a. HSO_4^- (n=0)
energy = -699.8367546 a.u.
thermally corrected enthalpy = -699.804676 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	0.156350	-0.022050	0.000250
2	8	0	0.825553	1.286369	0.002808
3	8	0	0.299242	-0.817727	1.239568
4	8	0	0.305502	-0.816003	-1.239401
5	8	0	-1.494613	0.440196	-0.003232
6	1	0	-1.987081	-0.389878	-0.001942

b. HSO_4^- (n=1)
energy = -778.4093567 a.u.
thermally corrected enthalpy = -778.321126 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

1	16	0	-0.833574	-0.136871	0.012089
2	8	0	-1.892717	1.151116	-0.361967
3	1	0	-2.127880	1.550889	0.486529
4	8	0	-1.124311	-0.453591	1.417488
5	8	0	-1.106215	-1.130724	-1.020095
6	6	0	0.823319	0.562453	-0.166174
7	1	0	0.873939	0.933842	-1.190349
8	1	0	0.867892	1.392678	0.540468
9	6	0	2.083835	-0.389843	0.102116
10	1	0	1.963223	-1.248532	-0.606995
11	1	0	1.922552	-0.818939	1.124639
12	8	0	3.172560	0.351241	-0.055847

c. HSO_4^- (n=2)
energy = -857.0433579 a.u.
thermally corrected enthalpy = -856.896210 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-1.858006	-0.151391	0.001254
2	8	0	-2.897124	1.152037	-0.201548
3	1	0	-3.275435	1.340573	0.668875
4	8	0	-2.105005	-0.641321	1.359314
5	8	0	-2.080409	-1.016194	-1.145918
6	6	0	-0.234372	0.665992	-0.112051
7	1	0	-0.256541	1.175853	-1.077270
8	1	0	-0.246484	1.408424	0.688468
9	6	0	0.948481	-0.290051	0.012019
10	1	0	0.902282	-1.036122	-0.787617
11	1	0	0.888182	-0.826625	0.964663
12	6	0	2.277559	0.476100	-0.066387
13	1	0	2.332115	1.228360	0.730993
14	1	0	2.355441	1.009751	-1.022170
15	6	0	3.556560	-0.435362	0.066422
16	1	0	3.418387	-1.227563	-0.736579
17	1	0	3.388806	-1.009827	1.032913
18	8	0	4.699034	0.237898	0.002857

d. HSO_4^- (n=3)
energy = -935.6851257 a.u.
thermally corrected enthalpy = -935.478610 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-2.961547	-0.166738	0.004565
2	8	0	-4.009834	1.118940	-0.158414
3	1	0	-4.455787	1.228580	0.693719
4	8	0	-3.185593	-0.700899	1.347259
5	8	0	-3.147515	-1.000939	-1.168748
6	6	0	-1.371431	0.691331	-0.085896
7	1	0	-1.404976	1.244534	-1.026735
8	1	0	-1.382155	1.397677	0.746586
9	6	0	-0.173862	-0.256704	-0.016188
10	1	0	-0.217205	-0.962460	-0.850644
11	1	0	-0.222369	-0.840896	0.907768
12	6	0	1.146559	0.532042	-0.063937
13	1	0	1.167210	1.249506	0.766721
14	1	0	1.177416	1.128422	-0.985078
15	6	0	2.395476	-0.354986	0.006165
16	1	0	2.374057	-1.069776	-0.828066
17	1	0	2.354925	-0.957397	0.924407
18	6	0	3.714185	0.422866	-0.028377
19	1	0	3.757040	1.134281	0.807737
20	1	0	3.782586	1.013726	-0.952018
21	6	0	5.004215	-0.468308	0.051985
22	1	0	4.875634	-1.222984	-0.791496
23	1	0	4.848403	-1.101170	0.986418
24	8	0	6.147831	0.211440	0.023043

e. HSO_4^- (n=4)
energy = -1014.3307749 a.u.
thermally corrected enthalpy = -1014.064863 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-4.115322	-0.181876	0.009604
2	8	0	-5.172447	1.091277	-0.142472
3	1	0	-5.663708	1.154839	0.689507
4	8	0	-4.327673	-0.731850	1.346842
5	8	0	-4.277831	-1.009124	-1.171329
6	6	0	-2.540373	0.702927	-0.072158
7	1	0	-2.582964	1.271640	-1.003224
8	1	0	-2.554977	1.394321	0.772477
9	6	0	-1.335663	-0.237827	-0.024154
10	1	0	-1.379221	-0.928491	-0.871054
11	1	0	-1.379063	-0.840122	0.888378
12	6	0	-0.021344	0.556490	-0.061151
13	1	0	0.002559	1.255890	0.784376
14	1	0	0.004839	1.172103	-0.969399
15	6	0	1.229046	-0.329519	-0.016049
16	1	0	1.212404	-1.023221	-0.866528
17	1	0	1.198706	-0.952989	0.886950
18	6	0	2.538966	0.469708	-0.036870
19	1	0	2.548407	1.164180	0.814141
20	1	0	2.562496	1.097132	-0.938203
21	6	0	3.803867	-0.396601	0.007074
22	1	0	3.791909	-1.089277	-0.846569
23	1	0	3.773327	-1.027088	0.907313
24	6	0	5.114992	0.394955	-0.006614
25	1	0	5.151790	1.082163	0.850069
26	1	0	5.174116	1.015153	-0.911781
27	6	0	6.414073	-0.482615	0.043475
28	1	0	6.291546	-1.213840	-0.821990
29	1	0	6.268303	-1.146229	0.958542
30	8	0	7.553363	0.207040	0.032211

f. HSO_4^- (n=5)
energy = -1092.9779161 a.u.
thermally corrected enthalpy = -1092.652675 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-5.300035	-0.196095	0.013764
2	8	0	-6.366140	1.067243	-0.130958
3	1	0	-6.886351	1.099431	0.685498
4	8	0	-5.504066	-0.757803	1.346982
5	8	0	-5.446081	-1.018642	-1.172408
6	6	0	-3.736008	0.708344	-0.061235
7	1	0	-3.784954	1.286051	-0.986393
8	1	0	-3.755325	1.390655	0.790551
9	6	0	-2.525179	-0.225089	-0.025293
10	1	0	-2.567730	-0.907982	-0.878526
11	1	0	-2.563620	-0.836778	0.881239
12	6	0	-1.214589	0.574251	-0.057762
13	1	0	-1.189936	1.265378	0.794275
14	1	0	-1.191742	1.198208	-0.960152
15	6	0	0.036353	-0.311441	-0.024198
16	1	0	0.017908	-0.996977	-0.880891
17	1	0	0.008940	-0.943167	0.872786
18	6	0	1.343064	0.490270	-0.041274
19	1	0	1.356368	1.174523	0.817518
20	1	0	1.363457	1.127298	-0.935518
21	6	0	2.607424	-0.376334	-0.012422
22	1	0	2.599879	-1.056230	-0.874828
23	1	0	2.586083	-1.017793	0.878793
24	6	0	3.910125	0.434654	-0.019366
25	1	0	3.913203	1.115194	0.843026
26	1	0	3.927569	1.077995	-0.909698
27	6	0	5.183535	-0.420043	0.009601
28	1	0	5.176144	-1.100015	-0.854441
29	1	0	5.159628	-1.065020	0.899854
30	6	0	6.488943	0.381209	0.006154
31	1	0	6.522656	1.054579	0.873926
32	1	0	6.541073	1.017120	-0.888538
33	6	0	7.794409	-0.486955	0.038314
34	1	0	7.675479	-1.204609	-0.838753
35	1	0	7.656748	-1.166670	0.942541
36	8	0	8.929613	0.210843	0.035433

g. HSO_4^- (n=6)
energy = -1171.6258678 a.u.
thermally corrected enthalpy = -1171.241349 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	16	0	-6.507205	-0.209876	0.018538
2	8	0	-7.588066	1.038584	-0.116308
3	1	0	-8.072858	1.101033	0.721590
4	8	0	-6.693304	-0.786125	1.347927
5	8	0	-6.644231	-1.022880	-1.175467
6	6	0	-4.950572	0.710060	-0.052755
7	1	0	-5.005305	1.293926	-0.973679
8	1	0	-4.973540	1.386299	0.804041
9	6	0	-3.733988	-0.215878	-0.024914
10	1	0	-3.775293	-0.894062	-0.881998
11	1	0	-3.767976	-0.833375	0.877858
12	6	0	-2.426483	0.588296	-0.055356
13	1	0	-2.401418	1.273258	0.801499
14	1	0	-2.407863	1.218628	-0.953280
15	6	0	-1.174244	-0.295656	-0.031650
16	1	0	-1.193975	-0.975068	-0.893022
17	1	0	-1.198200	-0.933669	0.860814
18	6	0	0.131068	0.508092	-0.046572
19	1	0	0.145815	1.187086	0.816058
20	1	0	0.149813	1.149760	-0.937226
21	6	0	1.394334	-0.360060	-0.024724
22	1	0	1.384763	-1.035218	-0.890400
23	1	0	1.374524	-1.005616	0.863132
24	6	0	2.694879	0.451937	-0.030279
25	1	0	2.700871	1.127399	0.835605
26	1	0	2.711717	1.099048	-0.917414
27	6	0	3.966332	-0.404582	-0.008199
28	1	0	3.963695	-1.077848	-0.875970
29	1	0	3.949349	-1.053791	0.877589
30	6	0	5.264244	0.413846	-0.008502
31	1	0	5.263778	1.087529	0.859233
32	1	0	5.278186	1.064449	-0.893564
33	6	0	6.542492	-0.434048	0.013348
34	1	0	6.538104	-1.107644	-0.855678
35	1	0	6.522521	-1.085959	0.898587
36	6	0	7.843495	0.374609	0.014990
37	1	0	7.874018	1.040891	0.888206

38	1	0	7.889693	1.018984	-0.873854
39	6	0	9.151512	-0.485700	0.037233
40	1	0	9.040902	-1.196805	-0.843917
41	1	0	9.025282	-1.173843	0.934446
42	8	0	10.285632	0.217560	0.038727

3. B3LYP/6-311++G(p,d) calculations for CH_3CH_2OH and its n=1–6 alkylogues

a. CH_3CH_2OH (n=0)
energy = -155.09515 a.u.
thermally corrected enthalpy = -155.010309 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.223893	-0.223523	-0.000037
2	1	0	1.292233	-0.859486	-0.885816
3	6	0	-0.081510	0.549683	0.000039
4	1	0	-0.139556	1.194282	-0.887544
5	1	0	-0.139471	1.194160	0.887711
6	8	0	-1.155382	-0.396163	0.000076
7	1	0	-1.991180	0.079601	-0.000570
8	1	0	2.074568	0.463732	0.000181
9	1	0	1.292166	-0.859943	0.885423

b. CH_3CH_2OH (n=1)
energy = -233.7436282 a.u.
thermally corrected enthalpy = -233.599301 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.033534	-0.339119	0.000069
2	1	0	0.037813	-0.993586	0.878881
3	1	0	0.037946	-0.993708	-0.878655
4	6	0	1.315645	0.478341	0.000090
5	1	0	1.348303	1.125148	0.888239
6	1	0	1.348180	1.125304	-0.887949
7	8	0	2.423713	-0.426793	-0.000098
8	1	0	3.240642	0.080581	0.000042
9	6	0	-1.229799	0.528849	-0.000090
10	1	0	-1.220574	1.187893	0.876645
11	1	0	-1.220543	1.187617	-0.877030
12	6	0	-2.520068	-0.296443	0.000013
13	1	0	-2.576459	-0.940407	0.883041
14	1	0	-3.404508	0.346495	-0.000159
15	1	0	-2.576376	-0.940763	-0.882762

c. CH_3CH_2OH (n=2)
energy = -312.3924133 a.u.
thermally corrected enthalpy = -312.188679 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.253363	-0.344889	0.000095
2	1	0	-1.258713	-1.004715	0.877212
3	1	0	-1.258958	-1.005684	-0.876290
4	6	0	0.036303	0.483759	-0.000548
5	1	0	0.039586	1.143718	0.876642
6	1	0	0.039035	1.143183	-0.878140
7	6	0	1.306551	-0.374117	-0.000723
8	1	0	1.318080	-1.027431	-0.880131
9	1	0	1.317205	-1.029118	0.877442
10	6	0	2.581308	0.455036	0.000673
11	1	0	2.607895	1.101080	0.889531
12	1	0	2.608560	1.103071	-0.886715
13	8	0	3.697546	-0.440242	0.000102
14	1	0	4.509916	0.074422	0.000504
15	6	0	-2.529486	0.504308	-0.000205
16	1	0	-2.523678	1.164411	0.875822
17	1	0	-2.523930	1.163418	-0.876981
18	6	0	-3.812201	-0.332516	0.000448
19	1	0	-3.863174	-0.977047	0.883719
20	1	0	-4.703450	0.301199	0.000206
21	1	0	-3.863413	-0.978059	-0.882070

d. CH_3CH_2OH (n=3)
energy = -391.0411172 a.u.
thermally corrected enthalpy = -390.777979 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.541716	-0.355937	0.000086
2	1	0	-2.545673	-1.016323	0.877127
3	1	0	-2.545911	-1.017029	-0.876422
4	6	0	-1.254704	0.476503	-0.000431
5	1	0	-1.251258	1.137146	0.876318
6	1	0	-1.251665	1.136640	-0.877566
7	6	0	0.023504	-0.369705	-0.000494
8	1	0	0.021224	-1.029432	-0.877490
9	1	0	0.020877	-1.030130	0.875977
10	6	0	1.310515	0.463436	0.000073
11	1	0	1.311215	1.122770	0.877746
12	1	0	1.311452	1.123580	-0.876991
13	6	0	2.583597	-0.390032	-0.000152
14	1	0	2.597117	-1.043799	-0.879219
15	1	0	2.596913	-1.044574	0.878341
16	6	0	3.855445	0.443595	0.000360
17	1	0	3.879995	1.090344	0.888770
18	1	0	3.880165	1.091167	-0.887448
19	8	0	4.974944	-0.447598	0.000045
20	1	0	5.785399	0.070077	0.000688
21	6	0	-3.821559	0.487995	-0.000081
22	1	0	-3.818095	1.148087	0.875953
23	1	0	-3.818338	1.147368	-0.876658
24	6	0	-5.101353	-0.353334	0.000437
25	1	0	-5.150029	-0.998270	0.883598
26	1	0	-5.995037	0.277028	0.000305
27	1	0	-5.150273	-0.998987	-0.882186

e. CH_3CH_2OH (n=4)
energy = -469.6898146 a.u.
thermally corrected enthalpy = -469.367271 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.828733	-0.364968	0.000006
2	1	0	-3.831570	-1.025758	0.876805
3	1	0	-3.831832	-1.025801	-0.876760
4	6	0	-2.543128	0.469619	-0.000205
5	1	0	-2.540922	1.130165	0.876635
6	1	0	-2.541196	1.130139	-0.877067
7	6	0	-1.262798	-0.373520	-0.000395
8	1	0	-1.264896	-1.033854	-0.877282
9	1	0	-1.264900	-1.034253	0.876193
10	6	0	0.023025	0.461097	-0.000212
11	1	0	0.025194	1.121395	0.876815
12	1	0	0.025235	1.121739	-0.876980
13	6	0	1.302453	-0.382955	-0.000341
14	1	0	1.301244	-1.042886	-0.877204
15	1	0	1.301139	-1.043291	0.876217
16	6	0	2.588039	0.452402	-0.000061
17	1	0	2.587585	1.112027	0.877394
18	1	0	2.587781	1.112311	-0.877303
19	6	0	3.862594	-0.398803	-0.000044
20	1	0	3.877262	-1.052833	-0.878901
21	1	0	3.877052	-1.053106	0.878615
22	6	0	5.133036	0.436912	0.000247
23	1	0	5.156461	1.084050	0.888402
24	1	0	5.156768	1.084204	-0.887784
25	8	0	6.254090	-0.452387	0.000375
26	1	0	7.063620	0.066734	0.000076
27	6	0	-5.110109	0.476580	0.000176
28	1	0	-5.107754	1.136404	0.876420
29	1	0	-5.108025	1.136344	-0.876114
30	6	0	-6.388549	-0.366768	0.000403
31	1	0	-6.436213	-1.012134	0.883320
32	1	0	-7.283266	0.262138	0.000511
33	1	0	-6.436477	-1.012205	-0.882448

f. CH_3CH_2OH (n=5)
energy = -548.3385055 a.u.
thermally corrected enthalpy = -547.956559 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.114774	-0.371896	0.000069
2	1	0	-5.116907	-1.032634	0.876923
3	1	0	-5.117155	-1.032816	-0.876647
4	6	0	-3.830054	0.464069	-0.000203
5	1	0	-3.828542	1.124670	0.876585
6	1	0	-3.828846	1.124560	-0.877076
7	6	0	-2.548658	-0.377572	-0.000371
8	1	0	-2.550104	-1.037927	-0.877298
9	1	0	-2.550158	-1.038374	0.876219
10	6	0	-1.263614	0.458257	-0.000131
11	1	0	-1.262044	1.118606	0.876847
12	1	0	-1.261998	1.119035	-0.876786
13	6	0	0.017313	-0.383876	-0.000303
14	1	0	0.015763	-1.044234	-0.877187
15	1	0	0.015741	-1.044610	0.876297
16	6	0	1.302454	0.451808	-0.000110
17	1	0	1.304025	1.112148	0.876889
18	1	0	1.304117	1.112412	-0.876910
19	6	0	2.582651	-0.391094	-0.000166
20	1	0	2.582040	-1.051101	-0.876973
21	1	0	2.581950	-1.051345	0.876458
22	6	0	3.867471	0.445461	0.000020
23	1	0	3.866437	1.105134	0.877440
24	1	0	3.866574	1.105309	-0.877268
25	6	0	5.142843	-0.404534	0.000039
26	1	0	5.158096	-1.058603	-0.878783
27	1	0	5.157968	-1.058753	0.878753
28	6	0	6.412473	0.432432	0.000210
29	1	0	6.435325	1.079623	0.888347
30	1	0	6.435504	1.079716	-0.887853
31	8	0	7.534428	-0.455740	0.000281
32	1	0	8.343415	0.064231	0.000172
33	6	0	-6.397124	0.468192	0.000159
34	1	0	-6.395527	1.128092	0.876348
35	1	0	-6.395781	1.127892	-0.876182
36	6	0	-7.674626	-0.376612	0.000439
37	1	0	-7.721547	-1.021969	0.883416

38	1	0	-8.570101	0.251239	0.000482
39	1	0	-7.721786	-1.022187	-0.882366

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g. CH_3CH_2OH (n=6)
energy = -626.9871897 a.u.
thermally corrected enthalpy = -626.545835 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.400053	-0.377510	-0.000041
2	1	0	-6.401822	-1.038370	0.876735
3	1	0	-6.401887	-1.038341	-0.876838
4	6	0	-5.115916	0.459346	-0.000079
5	1	0	-5.115015	1.119917	0.876751
6	1	0	-5.115090	1.119951	-0.876884
7	6	0	-3.833928	-0.381284	-0.000153
8	1	0	-3.834871	-1.041749	-0.877016
9	1	0	-3.834976	-1.042064	0.876473
10	6	0	-2.549435	0.455411	0.000064
11	1	0	-2.548374	1.115881	0.876953
12	1	0	-2.548267	1.116161	-0.876613
13	6	0	-1.267836	-0.385693	0.000010
14	1	0	-1.269003	-1.046224	-0.876797
15	1	0	-1.269037	-1.046390	0.876690
16	6	0	0.016847	0.450683	0.000109
17	1	0	0.018075	1.111218	0.876948
18	1	0	0.018134	1.111320	-0.876654
19	6	0	1.298216	-0.390743	0.000102
20	1	0	1.297017	-1.051312	-0.876625
21	1	0	1.297031	-1.051306	0.876834
22	6	0	2.582894	0.445639	0.000084
23	1	0	2.584139	1.106157	0.876950
24	1	0	2.584135	1.106114	-0.876814
25	6	0	3.863581	-0.396497	0.000100
26	1	0	3.863289	-1.056707	-0.876556
27	1	0	3.863350	-1.056584	0.876849
28	6	0	5.147903	0.440803	-0.000007
29	1	0	5.146586	1.100648	0.877284
30	1	0	5.146524	1.100511	-0.877402

31	6	0	6.423762	-0.408444	0.000013
32	1	0	6.439280	-1.062689	-0.878671
33	1	0	6.439375	-1.062492	0.878843
34	6	0	7.692934	0.429196	-0.000142
35	1	0	7.715541	1.076602	0.887837
36	1	0	7.715532	1.076293	-0.888344
37	8	0	8.815358	-0.458395	0.000017
38	1	0	9.624077	0.061989	-0.000592
39	6	0	-7.682995	0.461644	0.000017
40	1	0	-7.681954	1.121423	0.876297
41	1	0	-7.681982	1.121496	-0.876208
42	6	0	-8.959930	-0.383985	-0.000001
43	1	0	-9.006557	-1.029518	0.882862
44	1	0	-9.855809	0.243282	0.000027
45	1	0	-9.006570	-1.029457	-0.882909

4. B3LYP/6-311++G(p,d) calculations for $CH_3CH_2O^-$ and its n=1–6 alkylogues

a. $CH_3CH_2O^-$ (n=0)

energy = -154.4829553 a.u.

thermally corrected enthalpy = -154.414423 a.u.

number of imaginary frequencies = 0

Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.183385	-0.204704	0.000010
2	1	0	1.279462	-0.845225	-0.886015
3	6	0	-0.218648	0.484213	0.000007
4	1	0	-0.185663	1.192616	-0.890560
5	1	0	-0.185752	1.192975	0.890307
6	8	0	-1.247828	-0.363171	0.000009
7	1	0	2.006471	0.532578	-0.000332
8	1	0	1.279686	-0.844630	0.886428

b. $CH_3CH_2O^-$ (n=1)
energy = -233.1322338 a.u.
thermally corrected enthalpy = -233.004400 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.093696	-0.371213	-0.000231
2	1	0	0.093413	-1.028114	0.881056
3	1	0	0.093432	-1.027665	-0.881848
4	6	0	1.454018	0.411019	-0.000042
5	1	0	1.369803	1.116501	0.891015
6	1	0	1.370136	1.116748	-0.890938
7	8	0	2.544032	-0.355797	0.000156
8	6	0	-1.157157	0.511535	0.000005
9	1	0	-1.129202	1.173667	0.876357
10	1	0	-1.129429	1.173820	-0.876228
11	6	0	-2.481857	-0.262585	0.000099
12	1	0	-2.559524	-0.908882	0.881867
13	1	0	-3.353400	0.406568	0.000205
14	1	0	-2.559690	-0.908801	-0.881716

c. $CH_3CH_2O^-$ (n=2)
energy = -311.7814683 a.u.
thermally corrected enthalpy = -311.594323 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-1.199912	-0.356879	0.000077
2	1	0	-1.219497	-1.016932	0.878382
3	1	0	-1.221560	-1.021637	-0.874651
4	6	0	0.110907	0.440340	-0.003578
5	1	0	0.125466	1.105334	0.872225
6	1	0	0.122716	1.101478	-0.882259
7	6	0	1.383051	-0.414692	-0.003402
8	1	0	1.400243	-1.067254	-0.887352
9	1	0	1.395164	-1.074456	0.875301
10	6	0	2.723070	0.399274	0.003639
11	1	0	2.621808	1.097862	0.898540
12	1	0	2.624818	1.108983	-0.882790
13	8	0	3.830499	-0.342527	0.000836
14	6	0	-2.464902	0.511496	-0.000758
15	1	0	-2.445921	1.174499	0.873661
16	1	0	-2.447672	1.170295	-0.878391
17	6	0	-3.767271	-0.296789	0.002475
18	1	0	-3.828488	-0.941085	0.886265
19	1	0	-4.650352	0.351674	0.001958
20	1	0	-3.830375	-0.945048	-0.878282

d. $CH_3CH_2O^-$ (n=3)
energy = -390.4303577 a.u.
thermally corrected enthalpy = -390.183842 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.486728	-0.352670	0.000353
2	1	0	-2.498363	-1.012663	0.878334
3	1	0	-2.500056	-1.016096	-0.875026
4	6	0	-1.186736	0.460282	-0.002528
5	1	0	-1.174096	1.123304	0.873199
6	1	0	-1.176422	1.120445	-0.880448
7	6	0	0.086078	-0.397362	-0.002879
8	1	0	0.073821	-1.057295	-0.881016
9	1	0	0.071595	-1.061509	0.872044
10	6	0	1.388729	0.413283	0.000569
11	1	0	1.394047	1.073927	0.879568
12	1	0	1.395704	1.078755	-0.874785
13	6	0	2.668501	-0.428629	-0.000616
14	1	0	2.691032	-1.082782	-0.883363
15	1	0	2.690308	-1.086397	0.879453
16	6	0	4.000518	0.398794	0.001626
17	1	0	3.892928	1.100372	0.893635
18	1	0	3.893928	1.103403	-0.888108
19	8	0	5.115078	-0.331858	0.000998
20	6	0	-3.758601	0.503687	-0.000128
21	1	0	-3.747195	1.165578	0.874853
22	1	0	-3.748594	1.162587	-0.877384
23	6	0	-5.050112	-0.320935	0.002309
24	1	0	-5.104389	-0.965569	0.885916
25	1	0	-5.938809	0.318431	0.002097
26	1	0	-5.105955	-0.968331	-0.879178

e. $CH_3CH_2O^-$ (n=4)
energy = -469.0791275 a.u.
thermally corrected enthalpy = -468.773226 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.771131	-0.355955	0.000026
2	1	0	-3.779339	-1.017199	0.876812
3	1	0	-3.779379	-1.017448	-0.876572
4	6	0	-2.477504	0.466654	-0.000116
5	1	0	-2.470326	1.127972	0.876540
6	1	0	-2.470414	1.127793	-0.876907
7	6	0	-1.201949	-0.384158	-0.000094
8	1	0	-1.209784	-1.045608	-0.876781
9	1	0	-1.209920	-1.045784	0.876460
10	6	0	0.093768	0.436015	0.000081
11	1	0	0.101702	1.097567	0.876945
12	1	0	0.101776	1.097811	-0.876597
13	6	0	1.370781	-0.414894	0.000014
14	1	0	1.361111	-1.077034	-0.876578
15	1	0	1.361093	-1.077208	0.876474
16	6	0	2.669449	0.402261	0.000102
17	1	0	2.672322	1.065296	0.877368
18	1	0	2.672325	1.065475	-0.877030
19	6	0	3.953232	-0.433418	0.000014
20	1	0	3.978663	-1.089238	-0.881436
21	1	0	3.978733	-1.089320	0.881400
22	6	0	5.281413	0.400415	0.000005
23	1	0	5.170976	1.102891	0.890874
24	1	0	5.170909	1.102951	-0.890808
25	8	0	6.399388	-0.324996	-0.000068
26	6	0	-5.046973	0.494047	-0.000063
27	1	0	-5.039879	1.154377	0.875993
28	1	0	-5.039920	1.154126	-0.876308
29	6	0	-6.333019	-0.338495	0.000085
30	1	0	-6.384859	-0.984230	0.882857
31	1	0	-7.224395	0.296424	0.000016
32	1	0	-6.384899	-0.984478	-0.882504

f. $CH_3CH_2O^-$ (n=5)
energy = -547.7278488 a.u.
thermally corrected enthalpy = -547.362551 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-5.054516	-0.360980	0.000039
2	1	0	-5.060131	-1.021956	0.876908
3	1	0	-5.060227	-1.022359	-0.876526
4	6	0	-3.764702	0.467340	-0.000219
5	1	0	-3.759979	1.128477	0.876404
6	1	0	-3.760151	1.128175	-0.877070
7	6	0	-2.486749	-0.379453	-0.000202
8	1	0	-2.491617	-1.040447	-0.876974
9	1	0	-2.491831	-1.040758	0.876335
10	6	0	-1.195737	0.447645	0.000085
11	1	0	-1.190685	1.108689	0.876929
12	1	0	-1.190547	1.109069	-0.876472
13	6	0	0.082244	-0.399533	0.000000
14	1	0	0.076162	-1.060965	-0.876721
15	1	0	0.076107	-1.061233	0.876518
16	6	0	1.375704	0.424139	0.000160
17	1	0	1.381916	1.085693	0.877034
18	1	0	1.381954	1.085952	-0.876518
19	6	0	2.654947	-0.423442	0.000058
20	1	0	2.646948	-1.085613	-0.876530
21	1	0	2.646979	-1.085781	0.876518
22	6	0	3.951518	0.397019	0.000107
23	1	0	3.952757	1.060057	0.877375
24	1	0	3.952718	1.060221	-0.877039
25	6	0	5.237381	-0.435467	-0.000006
26	1	0	5.264442	-1.091209	-0.881464
27	1	0	5.264536	-1.091304	0.881378
28	6	0	6.563482	0.401669	-0.000035
29	1	0	6.451324	1.103871	0.890832
30	1	0	6.451258	1.103920	-0.890855
31	8	0	7.683224	-0.321022	-0.000091
32	6	0	-6.333137	0.484755	-0.000083
33	1	0	-6.328401	1.145020	0.875950
34	1	0	-6.328489	1.144625	-0.876415
35	6	0	-7.615645	-0.352939	0.000169
36	1	0	-7.665306	-0.998521	0.883066
37	1	0	-8.508883	0.278954	0.000069

38	1	0	-7.665390	-0.998917	-0.882434

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g. $CH_3CH_2O^-$ (n=6)
energy = -626.3765372 a.u.
thermally corrected enthalpy = -625.951842 a.u.
number of imaginary frequencies = 0
Cartesian Coordinates

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-6.337627	-0.366436	-0.000057
2	1	0	-6.341623	-1.027237	0.876883
3	1	0	-6.341719	-1.027767	-0.876597
4	6	0	-5.050138	0.465407	-0.000387
5	1	0	-5.046991	1.126457	0.876218
6	1	0	-5.047213	1.126063	-0.877290
7	6	0	-3.770539	-0.378719	-0.000370
8	1	0	-3.773537	-1.039338	-0.877313
9	1	0	-3.774004	-1.040045	0.876039
10	6	0	-2.482227	0.452350	0.000275
11	1	0	-2.478899	1.112961	0.877272
12	1	0	-2.478530	1.113713	-0.876156
13	6	0	-1.202938	-0.392476	0.000177
14	1	0	-1.206892	-1.053403	-0.876651
15	1	0	-1.207045	-1.053850	0.876666
16	6	0	0.086779	0.436580	0.000480
17	1	0	0.090816	1.097635	0.877320
18	1	0	0.090961	1.098003	-0.876081
19	6	0	1.366114	-0.408576	0.000401
20	1	0	1.361037	-1.070100	-0.876256
21	1	0	1.361097	-1.070189	0.876992
22	6	0	2.658223	0.417225	0.000383
23	1	0	2.663404	1.078891	0.877183
24	1	0	2.663317	1.078955	-0.876368
25	6	0	3.938870	-0.428219	0.000281
26	1	0	3.931873	-1.090550	-0.876195
27	1	0	3.932099	-1.090429	0.876850
28	6	0	5.234115	0.394355	0.000045
29	1	0	5.234411	1.057534	0.877213
30	1	0	5.234174	1.057392	-0.877229
31	6	0	6.521206	-0.436225	-0.000069
32	1	0	6.549084	-1.092102	-0.881404

33	1	0	6.549389	-1.091873	0.881426
34	6	0	7.846215	0.402670	-0.000415
35	1	0	7.733267	1.104900	0.890321
36	1	0	7.732991	1.104615	-0.891341
37	8	0	8.966799	-0.318692	-0.000467
38	6	0	-7.618038	0.476546	-0.000247
39	1	0	-7.614842	1.136761	0.875784
40	1	0	-7.614874	1.136309	-0.876618
41	6	0	-8.898344	-0.364351	-0.000011
42	1	0	-8.946686	-1.009857	0.882949
43	1	0	-9.792770	0.265616	-0.000164
44	1	0	-8.946706	-1.010311	-0.882638

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[42] *Gaussian 09 Revision C.01*, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A. Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. J. Montgomery, J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, T. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, O. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, D. J. Fox., Gaussian, Inc.: Wallingford, CT, **2010**.