Why Are Esters and Amides Weaker Carbon Acids than Ketones and Acid Fluorides?

Contributions by Resonance and Inductive Effects

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1. Cartesian coordinates, absolute energies, zero-point energy corrections, absolute enthalpies, and number of imaginary frequencies for acetone (1), acetone enolate anion, and their $n = 1-4$ vinylogues

Table S1. Acetone neutral $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.000002	0.182370	-0.000022
2	6	0	-1.293612	-0.613917	-0.001920
3	1	0	-1.294982	-1.354555	-0.811628
4	1	0	-1.389461	-1.171378	0.939487
5	1	0	-2.148278	0.057373	-0.111439
6	6	0	1.293630	-0.613929	0.001921
7	1	0	1.295337	-1.354005	0.812140
8	1	0	1.389087	-1.171995	-0.939151
9	1	0	2.148241	0.057562	0.110643
10	8	0	-0.000005	1.401232	0.000010

E = -193.16626074 a.u.

ZPE correction = 0.083930 a.u.

H = -193.07602 a.u.

0 imaginary frequencies

Table S2. Acetone anion $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.294970	-0.483598	-0.000007
2	1	0	1.840686	-0.121360	0.883571
3	1	0	1.841273	-0.119561	-0.882525
4	1	0	1.313065	-1.583231	-0.001143
5	6	0	-0.133941	0.110530	-0.000007
6	8	0	-0.194570	1.387379	0.000016
7	6	0	-1.192488	-0.789864	0.000013
8	1	0	-2.221041	-0.430806	-0.000193
9	1	0	-1.028668	-1.866485	0.000166

E = -192.56791090 a.u.

ZPE correction = 0.070404 a.u.

H = -192.491898 a.u.

0 imaginary frequencies

Table S3. Acetone neutral n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	1.572429	1.254040	0.000016
2	1	O	2.663248	1.303282	-0.002535
3	1	O	1.190218	1.775372	0.886263
4	1	O	1.185746	1.777792	-0.882792
5	6	O	1.147267	-0.206598	-0.000126
6	8	O	1.986420	-1.101122	0.000029
7	6	O	-0.294132	-0.556899	-0.000072
8	1	O	-0.487859	-1.628830	0.000127
9	6	O	-1.311308	0.321494	-0.000125
10	1	O	-1.093445	1.389983	-0.000353
11	6	O	-2.763979	-0.047840	0.000094
12	1	O	-3.271656	0.369439	0.880536
13	1	O	-3.271883	0.369743	-0.880115
14	1	O	-2.907386	-1.132987	-0.000083

E = -270.56979485 a.u.

ZPE correction = 0.117998 a.u.

H = -270.443554 a.u.

0 imaginary frequencies

Table S4. Acetone anion n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	-1.040067	-0.216523	-0.000185
2	8	O	-1.996858	-1.050509	0.000209
3	6	O	-1.469136	1.263781	-0.000100
4	1	O	-0.648328	1.989812	-0.002986
5	1	O	-2.100096	1.445947	-0.880723
6	1	O	-2.095167	1.447422	0.883740
7	6	O	0.323642	-0.573998	-0.000151
8	1	O	0.511385	-1.650127	-0.000203
9	6	O	1.459212	0.286285	0.000017
10	1	O	1.256743	1.360860	0.000727
11	6	O	2.787962	-0.057959	0.000137
12	1	O	3.111511	-1.098964	-0.000606
13	1	O	3.569142	0.699613	0.000073

E = -269.99092729 a.u.

ZPE correction = 0.103931 a.u.

H = -269.879183 a.u.

0 imaginary frequencies

Table S5. Acetone neutral n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.131635	-0.193887	0.074198
2	8	0	-1.648884	-1.281344	-0.118788
3	6	0	-1.908967	1.101083	-0.058144
4	1	0	-1.473045	1.714237	-0.857723
5	1	0	-2.959432	0.894681	-0.278415
6	1	0	-1.826126	1.689054	0.865273
7	6	0	0.313913	-0.080415	0.485867
8	1	0	0.497279	-0.104933	1.562254
9	6	0	1.331827	0.022438	-0.374494
10	1	0	1.116872	0.040198	-1.445041
11	6	0	2.783220	0.096317	0.007432
12	1	0	2.915705	0.071867	1.094541
13	1	0	3.343719	-0.743647	-0.424624
14	1	0	3.245948	1.016085	-0.375110

E = -270.55881763 a.u.

ZPE correction = 0.117035 a.u.

H = -270.434116 a.u.

1 imaginary frequency

Table S6. Acetone anion n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.041085	-0.204614	0.088993
2	8	0	-1.648789	-1.248253	-0.164984
3	6	0	-1.811222	1.117450	-0.082774
4	1	0	-1.275716	1.754377	-0.798844
5	1	0	-2.844765	0.954424	-0.420698
6	1	0	-1.808228	1.663461	0.870002
7	6	0	0.358060	-0.104148	0.566915
8	1	0	0.491536	-0.115151	1.651497
9	6	0	1.453167	-0.000928	-0.299271
10	1	0	1.185138	-0.003722	-1.365637
11	6	0	2.821258	0.104684	-0.055989
12	1	0	3.230794	0.093785	0.954659
13	1	0	3.530489	0.164184	-0.878348

E = -269.9414498 a.u.

ZPE correction = 0.100783 a.u.

H = -269.832779 a.u.

1 imaginary frequency

Table S7. Acetone neutral n=2 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.569278	1.327824	0.000000
2	1	0	-3.650474	1.480674	0.000004
3	1	0	-2.137627	1.811663	-0.884851
4	1	0	-2.137620	1.811662	0.884848
5	6	0	-2.286513	-0.167851	-0.000002
6	8	0	-3.211270	-0.976460	0.000006
7	6	0	-0.891298	-0.652458	-0.000002
8	1	0	-0.797067	-1.737423	0.000000
9	6	0	0.213065	0.129597	-0.000005
10	1	0	0.104169	1.214483	-0.000007
11	6	0	1.572779	-0.374854	-0.000004
12	1	0	1.697925	-1.458553	-0.000012
13	6	0	2.663017	0.418379	0.000003
14	1	0	2.518503	1.500760	0.000010
15	6	0	4.082191	-0.061063	0.000003
16	1	0	4.141719	-1.154651	-0.000005
17	1	0	4.623429	0.312819	-0.880290
18	1	0	4.623426	0.312806	0.880303

E = -347.97889444 a.u.

ZPE correction = 0.151582 a.u.

H = -347.816918 a.u.

0 imaginary frequencies

Table S8. Acetone anion n=2 parallel

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.190858	-0.165300	-0.000038
2	8	0	3.217221	-0.899829	-0.000025
3	6	0	2.458154	1.349360	-0.000075
4	1	0	1.563223	1.980170	-0.000576
5	1	0	3.062014	1.598438	0.882440
6	1	0	3.062865	1.598173	-0.882071
7	6	0	0.865196	-0.672873	-0.000018
8	1	0	0.801203	-1.762495	-0.000054
9	6	0	-0.340625	0.055703	0.000090
10	1	0	-0.267161	1.146593	0.000172
11	6	0	-1.635156	-0.445554	0.000174
12	1	0	-1.779795	-1.528643	0.000128
13	6	0	-2.800919	0.381061	0.000243
14	1	0	-2.601762	1.458765	0.000127
15	6	0	-4.113529	0.001201	-0.000259
16	1	0	-4.405833	-1.048476	-0.000406
17	1	0	-4.916392	0.734523	-0.000264

E = -347.41329720 a.u.

ZPE correction = 0.137352 a.u.

H = -347.26591 a.u.

0 imaginary frequencies

Table S9. Acetone neutral n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.274246	-0.175762	0.041887
2	8	0	-2.811838	-1.228966	-0.257315
3	6	0	-2.988098	1.155870	-0.085222
4	1	0	-2.454845	1.796647	-0.799573
5	1	0	-4.018706	1.005603	-0.417045
6	1	0	-2.975781	1.685025	0.876622
7	6	0	-0.870365	-0.144810	0.584723
8	1	0	-0.782806	-0.231409	1.669377
9	6	0	0.229268	-0.038378	-0.181843
10	1	0	0.115926	0.043168	-1.264584
11	6	0	1.594327	-0.037400	0.326069
12	1	0	1.714700	-0.127127	1.407282
13	6	0	2.687320	0.063162	-0.452643
14	1	0	2.551341	0.148788	-1.532736
15	6	0	4.103923	0.063633	0.039826
16	1	0	4.624453	0.986558	-0.251789
17	1	0	4.153313	-0.025225	1.130724
18	1	0	4.674329	-0.768181	-0.396533

E = -347.96640051 a.u.

ZPE correction = 0.150381 a.u.

H = -347.806129 a.u.

1 imaginary frequency

Table S10. Acetone anion n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.186611	-0.182657	0.019246
2	8	0	-2.785750	-1.167808	-0.411153
3	6	0	-2.867340	1.186900	-0.094075
4	1	0	-2.939437	1.643508	0.901892
5	1	0	-2.233703	1.856209	-0.690566
6	1	0	-3.864028	1.108493	-0.547075
7	6	0	-0.849517	-0.210098	0.669906
8	1	0	-0.854268	-0.340991	1.754328
9	6	0	0.338543	-0.080578	-0.028779
10	1	0	0.237733	0.041327	-1.115519
11	6	0	1.667982	-0.081065	0.437443
12	1	0	1.843304	-0.209245	1.509248
13	6	0	2.791538	0.074483	-0.412456
14	1	0	2.543757	0.192759	-1.475379
15	6	0	4.134161	0.099034	-0.105701
16	1	0	4.491997	-0.011544	0.918125
17	1	0	4.888110	0.225828	-0.879330

E = -347.372052 a.u.

ZPE correction = 0.134762 a.u.

H = -347.227517 a.u.

1 imaginary frequency

Table S11. Acetone neutral n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	3.672508	1.384371	0.000004
2	1	C	4.745624	1.586347	-0.000001
3	1	C	3.219513	1.848455	0.884800
4	1	O	3.219504	1.848458	-0.884785
5	6	O	3.458316	-0.123012	0.000002
6	8	O	4.420427	-0.888115	-0.000004
7	6	O	2.088746	-0.670041	0.000005
8	1	C	2.043208	-1.758046	0.000016
9	6	O	0.946964	0.062160	-0.000005
10	1	C	1.008795	1.150729	-0.000016
11	6	O	-0.381704	-0.500071	-0.000002
12	1	C	-0.462045	-1.587614	0.000002
13	6	O	-1.515020	0.248939	-0.000004
14	1	C	-1.424078	1.336804	-0.000008
15	6	O	-2.857357	-0.291166	-0.000001
16	1	C	-2.951582	-1.378463	0.000001
17	6	O	-3.974774	0.465445	0.000000
18	1	C	-3.866920	1.551968	-0.000002
19	6	O	-5.376688	-0.062836	0.000003
20	1	C	-5.397953	-1.158012	0.000005
21	1	O	-5.931716	0.290782	0.880270
22	1	O	-5.931719	0.290779	-0.880263

E = -425.38885967 a.u.

ZPE correction = 0.185036 a.u.

H = -425.191216 a.u.

0 imaginary frequencies

Table S12. Acetone anion n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	-3.366796	-0.090503	-0.000030
2	8	O	-4.425906	-0.768326	0.000048
3	6	O	-3.542622	1.435380	0.000025
4	1	O	-2.611160	2.009877	-0.000986
5	1	O	-4.131148	1.719699	-0.881673
6	1	O	-4.129303	1.719913	0.882894
7	6	O	-2.068736	-0.681097	-0.000053
8	1	O	-2.073822	-1.772140	-0.000030
9	6	O	-0.830030	-0.028207	-0.000049
10	1	O	-0.832444	1.064382	-0.000054
11	6	O	0.435541	-0.618225	-0.000012
12	1	O	0.500970	-1.708475	0.000025
13	6	O	1.641907	0.119499	-0.000016
14	1	O	1.532223	1.210020	-0.000064
15	6	O	2.935914	-0.366355	0.000008
16	1	O	3.091370	-1.447743	0.000042
17	6	O	4.098609	0.470184	-0.000015
18	1	O	3.896512	1.546332	-0.000105
19	6	O	5.406032	0.085328	0.000046
20	1	O	5.692722	-0.965610	0.000126
21	1	O	6.212414	0.814330	0.000008

E = -424.83256495 a.u.

ZPE correction = 0.170835 a.u.

H = -424.649495 a.u.

0 imaginary frequencies

Table S13. Acetone neutral n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.138201	1.193289	0.027193
2	1	0	-5.142913	1.122902	-0.397687
3	1	0	-3.547179	1.934196	-0.526522
4	1	0	-4.193975	1.551626	1.063649
5	6	0	-3.448905	-0.156173	-0.019866
6	8	0	-3.985814	-1.140473	-0.500313
7	6	0	-2.070591	-0.238652	0.579530
8	1	0	-2.030705	-0.504904	1.637283
9	6	0	-0.935457	-0.037795	-0.117488
10	1	0	-1.003279	0.220914	-1.175945
11	6	0	0.401245	-0.151621	0.432617
12	1	0	0.479696	-0.424678	1.486113
13	6	0	1.533895	0.056409	-0.281852
14	1	0	1.447676	0.326464	-1.336061
15	6	0	2.876372	-0.056348	0.253257
16	1	0	2.963044	-0.328795	1.306924
17	6	0	3.999680	0.149875	-0.463650
18	1	0	3.902724	0.420571	-1.517033
19	6	0	5.397257	0.037128	0.067491
20	1	0	5.406032	-0.242291	1.126857
21	1	0	5.973357	-0.715724	-0.488789
22	1	0	5.940267	0.986827	-0.039667

E = -425.37585244 a.u.

ZPE correction = 0.183905 a.u.

H = -425.179884 a.u.

1 imaginary frequency

Table S14. Acetone anion n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.357269	-0.090198	0.134986
2	8	0	3.942667	-0.655877	1.055199
3	6	0	3.990966	1.154308	-0.490192
4	1	0	4.114816	1.001690	-1.570505
5	1	0	3.306139	2.005023	-0.378797
6	1	0	4.958033	1.386342	-0.028390
7	6	0	2.063167	-0.543498	-0.448931
8	1	0	2.141442	-1.241499	-1.285195
9	6	0	0.835332	-0.128415	0.012514
10	1	0	0.846506	0.569496	0.858527
11	6	0	-0.457178	-0.477206	-0.453131
12	1	0	-0.529854	-1.178067	-1.288521
13	6	0	-1.641195	0.031065	0.098574
14	1	0	-1.510816	0.727840	0.936229
15	6	0	-2.959947	-0.226187	-0.271821
16	1	0	-3.145565	-0.914424	-1.100664
17	6	0	-4.089427	0.361231	0.368841
18	1	0	-3.847016	1.042492	1.192872
19	6	0	-5.420200	0.188295	0.093118
20	1	0	-5.758819	-0.469758	-0.706802
21	1	0	-6.188922	0.701512	0.665894

E = -424.7965073 a.u.

ZPE correction = 0.168488 a.u.

H = -424.616151 a.u.

1 imaginary frequency

Table S15. Acetone neutral n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	4.819937	1.436269	0.000015
2	1	H	5.886880	1.668817	0.000003
3	1	H	4.353992	1.887429	0.884791
4	1	H	4.353965	1.887454	-0.884733
5	6	O	4.648960	-0.076901	-0.000004
6	8	C	5.633318	-0.813854	-0.000032
7	6	O	3.296492	-0.662283	0.000002
8	1	H	3.281297	-1.751133	0.000008
9	6	O	2.133119	0.037778	0.000004
10	1	H	2.165058	1.127641	-0.000001
11	6	O	0.823148	-0.560220	0.000014
12	1	H	0.771788	-1.649475	0.000031
13	6	O	-0.333737	0.158695	0.000003
14	1	H	-0.270259	1.248557	-0.000014
15	6	O	-1.653160	-0.414094	0.000013
16	1	H	-1.722711	-1.502879	0.000036
17	6	O	-2.799133	0.318475	-0.000003
18	1	H	-2.724479	1.407490	-0.000025
19	6	O	-4.131577	-0.243099	0.000008
20	1	H	-4.207097	-1.332069	0.000037
21	6	O	-5.263695	0.492283	-0.000016
22	1	H	-5.176737	1.580656	-0.000045
23	6	O	-6.655118	-0.063474	-0.000006
24	1	H	-6.654402	-1.158952	0.000024
25	1	H	-7.217633	0.278389	0.880266
26	1	H	-7.217628	0.278341	-0.880299

E = -502.79922376 a.u.

ZPE correction = 0.218523 a.u.

H = -502.565908 a.u.

0 imaginary frequencies

Table S16. Acetone anion n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.550993	0.009379	0.000017
2	8	0	-5.653824	-0.584961	-0.000024
3	6	0	-4.569394	1.547524	0.000007
4	1	0	-4.066111	1.959866	0.884553
5	1	0	-4.065321	1.959846	-0.884102
6	1	0	-5.611950	1.877749	-0.000460
7	6	0	-3.295405	-0.679190	-0.000017
8	1	0	-3.365344	-1.767127	-0.000071
9	6	0	-2.037277	-0.081554	0.000011
10	1	0	-1.999624	1.011113	0.000038
11	6	0	-0.790905	-0.724422	-0.000004
12	1	0	-0.773190	-1.816303	0.000007
13	6	0	0.437048	-0.040790	0.000019
14	1	0	0.378974	1.053111	0.000054
15	6	0	1.714056	-0.591521	0.000038
16	1	0	1.809901	-1.679569	0.000084
17	6	0	2.905049	0.176495	-0.000015
18	1	0	2.772532	1.263753	-0.000034
19	6	0	4.203278	-0.288733	-0.000012
20	1	0	4.375319	-1.367433	0.000017
21	6	0	5.356056	0.564900	-0.000022
22	1	0	5.142455	1.638233	-0.000069
23	6	0	6.663653	0.188700	0.000022
24	1	0	6.956248	-0.860427	-0.000051
25	1	0	7.465715	0.922143	-0.000048

E = -502.24994703 a.u.

ZPE correction = 0.204129 a.u.

H = -502.031408 a.u.

0 imaginary frequencies

Table S17. Acetone neutral n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	5.311924	1.071310	-0.596807
2	1	0	6.315098	1.237602	-0.195631
3	1	0	4.706649	1.979851	-0.481313
4	1	0	5.367087	0.869315	-1.674604
5	6	0	4.642313	-0.086439	0.117287
6	8	0	5.182398	-0.679288	1.036387
7	6	0	3.280813	-0.494570	-0.377497
8	1	0	3.270978	-1.252958	-1.162362
9	6	0	2.125268	0.002445	0.107209
10	1	0	2.164113	0.756662	0.895600
11	6	0	0.805972	-0.399473	-0.333255
12	1	0	0.755064	-1.160600	-1.113328
13	6	0	-0.348591	0.112046	0.167293
14	1	0	-0.288014	0.870826	0.949853
15	6	0	-1.669786	-0.276508	-0.258977
16	1	0	-1.734430	-1.035560	-1.040498
17	6	0	-2.818940	0.239859	0.249630
18	1	0	-2.751857	0.998134	1.032035
19	6	0	-4.148968	-0.144963	-0.172382
20	1	0	-4.215040	-0.903811	-0.954689
21	6	0	-5.288007	0.370031	0.335856
22	1	0	-5.212784	1.128039	1.118179
23	6	0	-6.674170	-0.014283	-0.086389
24	1	0	-6.660813	-0.778394	-0.871556
25	1	0	-7.253080	-0.406835	0.761627
26	1	0	-7.229120	0.855300	-0.466219

E = -502.78591592 a.u.

ZPE = 0.217194 a.u.

H = -502.554397 a.u.

1 imaginary frequency

Table S18. Acetone anion n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.542748	-0.095582	-0.171783
2	8	0	5.116255	-0.135452	-1.256000
3	6	0	5.146836	-0.832112	1.022570
4	1	0	5.281454	-0.135260	1.860176
5	1	0	4.440526	-1.596890	1.371490
6	1	0	6.103541	-1.297409	0.759814
7	6	0	3.278235	0.656687	0.078655
8	1	0	3.401358	1.691344	0.405189
9	6	0	2.029514	0.114915	-0.080936
10	1	0	1.984971	-0.928177	-0.414092
11	6	0	0.766284	0.734008	0.129962
12	1	0	0.757730	1.779151	0.447968
13	6	0	-0.451311	0.079976	-0.045252
14	1	0	-0.393436	-0.966105	-0.368268
15	6	0	-1.744011	0.590699	0.139904
16	1	0	-1.846673	1.631249	0.457447
17	6	0	-2.920628	-0.159592	-0.059220
18	1	0	-2.773566	-1.198326	-0.377542
19	6	0	-4.235501	0.251528	0.096679
20	1	0	-4.429206	1.280088	0.411011
21	6	0	-5.364849	-0.594825	-0.131076
22	1	0	-5.122549	-1.615757	-0.445428
23	6	0	-6.689147	-0.286423	-0.005419
24	1	0	-7.018635	0.705015	0.303488
25	1	0	-7.464568	-1.020982	-0.207768

E = -502.2174627 a.u.

ZPE correction = 0.202209 a.u.

H = -502.001278 a.u.

1 imaginary frequency

2. Cartesian coordinates, absolute energies, zero-point energy corrections, absolute enthalpies, and number of imaginary frequencies for acetamide (2), acetamide enolate anion, and their $n = 1-4$ vinylogues

Table S19. Acetamide neutral $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.074027	0.143940	-0.000125
2	8	0	-0.355973	1.336378	0.000005
3	6	0	1.365201	-0.346773	0.000000
4	1	0	1.873459	0.057387	-0.881178
5	1	0	1.871947	0.053472	0.883871
6	1	0	1.460519	-1.437420	-0.002217
7	7	0	-1.038738	-0.827293	0.000045
8	1	0	-0.824333	-1.813086	-0.000305
9	1	0	-2.009687	-0.543334	0.000216

E = -209.2269541 a.u.

ZPE correction = 0.073539 a.u.

H = -209.147193 a.u.

0 imaginary frequencies

Table S20. Acetamide anion $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.070531	0.127945	-0.012914
2	8	0	-0.258283	1.353155	0.008192
3	6	0	1.343305	-0.437264	0.023320
4	1	0	2.217255	0.207609	0.021869
5	1	0	1.495058	-1.510872	-0.078484
6	7	0	-1.056210	-0.805835	-0.108451
7	1	0	-0.867688	-1.675833	0.386113
8	1	0	-1.867902	-0.349383	0.301686

E = -208.6150753 a.u.

ZPE correction = 0.059732 a.u.

H = -208.549872 a.u.

0 imaginary frequencies

Table S21. Acetamide neutral n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.166793	-0.154610	-0.020651
2	8	0	-2.013847	-1.033979	0.117489
3	7	0	-1.506507	1.180927	-0.013601
4	1	0	-0.900625	1.865930	-0.443043
5	1	0	-2.498310	1.382878	-0.031040
6	6	0	0.277091	-0.496993	-0.158536
7	1	0	0.443842	-1.533665	-0.443365
8	6	0	1.311971	0.313826	0.107070
9	1	0	1.121753	1.333312	0.446764
10	6	0	2.755991	-0.081966	0.013324
11	1	0	3.297206	0.573778	-0.682347
12	1	0	3.251618	0.017538	0.988573
13	1	0	2.871285	-1.115972	-0.327488

E = -286.6271423 a.u.

ZPE correction = 0.107515 a.u.

H = -286.511673 a.u.

0 imaginary frequencies

Table S22. Acetamide anion n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.058582	-0.175385	-0.008267
2	8	0	2.064821	-0.935693	-0.016756
3	7	0	1.345355	1.238635	-0.067321
4	1	0	0.705782	1.812946	0.474456
5	1	0	2.303968	1.381377	0.236364
6	6	0	-0.293583	-0.589861	0.023201
7	1	0	-0.438950	-1.667588	0.084828
8	6	0	-1.435587	0.251512	-0.043640
9	1	0	-1.236598	1.320223	-0.180181
10	6	0	-2.767712	-0.084046	0.016350
11	1	0	-3.095125	-1.116866	0.136705
12	1	0	-3.545329	0.671684	-0.072741

E = -286.0412881 a.u.

ZPE correction = 0.093464 a.u.

H = -285.94035 a.u.

0 imaginary frequencies

Table S23. Acetamide neutral n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.148738	-0.143084	0.076719
2	8	0	-1.706246	-1.216956	-0.121535
3	7	0	-1.799953	1.053211	-0.046980
4	1	0	-1.324428	1.934122	0.083153
5	1	0	-2.775871	1.055506	-0.316045
6	6	0	0.295506	-0.045631	0.493211
7	1	0	0.483399	-0.144901	1.563059
8	6	0	1.309517	0.040870	-0.374125
9	1	0	1.084705	0.105396	-1.440458
10	6	0	2.764953	0.034564	-0.002855
11	1	0	3.270503	0.939993	-0.364814
12	1	0	2.904675	-0.027308	1.081880
13	1	0	3.279226	-0.819942	-0.463326

E = -286.6212903 a.u.

ZPE correction = 0.106678 a.u.

H = -286.507148 a.u.

1 imaginary frequency

Table S24. Acetamide anion n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.063300	-0.154142	0.099275
2	8	0	-1.735974	-1.161979	-0.163817
3	7	0	-1.689412	1.089649	-0.035422
4	1	0	-1.090793	1.902898	-0.057173
5	1	0	-2.569205	1.127390	-0.544108
6	6	0	0.339810	-0.093657	0.578738
7	1	0	0.480742	-0.105431	1.660367
8	6	0	1.428119	-0.025115	-0.301564
9	1	0	1.147872	-0.037129	-1.364327
10	6	0	2.799420	0.050545	-0.071701
11	1	0	3.217132	0.049383	0.935739
12	1	0	3.503637	0.065397	-0.900504

E = -286.0052684 a.u.

ZPE correction = 0.090748 a.u.

H = -285.906991 a.u.

1 imaginary frequency

Table S25. Acetamide neutral n=2 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.301293	-0.127592	-0.002420
2	8	0	-3.216147	-0.926976	0.188504
3	7	0	-2.533523	1.232283	-0.050598
4	1	0	-1.890933	1.840837	-0.538456
5	1	0	-3.508213	1.505448	-0.071870
6	6	0	-0.897788	-0.590582	-0.145279
7	1	0	-0.816952	-1.654836	-0.353879
8	6	0	0.211431	0.159238	0.028887
9	1	0	0.116574	1.212980	0.295206
10	6	0	1.567289	-0.349548	-0.081162
11	1	0	1.677823	-1.403997	-0.338109
12	6	0	2.667880	0.402852	0.114244
13	1	0	2.539517	1.455818	0.373690
14	6	0	4.080430	-0.086160	0.007758
15	1	0	4.618258	0.055177	0.955588
16	1	0	4.123218	-1.148735	-0.254405
17	1	0	4.636849	0.477885	-0.753770

E = -364.0356917 a.u.

ZPE correction = 0.141036 a.u.

H = -363.884536 a.u.

0 imaginary frequencies

Table S26. Acetamide anion n=2 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	2.201915	-0.122801	-0.009996
2	8	0	3.262096	-0.794053	-0.038189
3	7	0	2.347244	1.300336	-0.047878
4	1	0	1.643587	1.819275	0.467396
5	1	0	3.286704	1.552667	0.240970
6	6	0	0.886061	-0.673793	0.021531
7	1	0	0.857067	-1.760980	0.068711
8	6	0	-0.322021	0.039693	-0.020553
9	1	0	-0.253200	1.128216	-0.125192
10	6	0	-1.620418	-0.456451	0.030907
11	1	0	-1.765810	-1.535523	0.124485
12	6	0	-2.783189	0.368641	-0.035361
13	1	0	-2.580711	1.441837	-0.131294
14	6	0	-4.099022	-0.002315	0.005659
15	1	0	-4.397176	-1.046481	0.096744
16	1	0	-4.897903	0.733215	-0.054292

E = -363.4647018 a.u.

ZPE correction = 0.126943 a.u.

H = -363.328161 a.u.

0 imaginary frequencies

Table S27. Acetamide neutral n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.283243	-0.137187	0.042238
2	8	0	-2.837896	-1.182897	-0.278356
3	7	0	-2.896766	1.080077	-0.066734
4	1	0	-2.423839	1.937854	0.177598
5	1	0	-3.844506	1.123220	-0.419973
6	6	0	-0.884697	-0.102000	0.595545
7	1	0	-0.796885	-0.282980	1.667062
8	6	0	0.213100	0.017350	-0.172585
9	1	0	0.093933	0.162188	-1.247705
10	6	0	1.579566	-0.043348	0.326393
11	1	0	1.703619	-0.201165	1.399350
12	6	0	2.670488	0.077163	-0.452709
13	1	0	2.530385	0.230392	-1.524751
14	6	0	4.089356	0.012235	0.028402
15	1	0	4.634750	-0.807447	-0.459842
16	1	0	4.632569	0.936534	-0.213331
17	1	0	4.143084	-0.141226	1.111874

E = -364.0289457 a.u.

ZPE correction = 0.140040 a.u.

H = -363.879225 a.u.

1 imaginary frequency

Table S28. Acetamide anion n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.198540	-0.139816	0.029686
2	8	0	-2.841113	-1.112269	-0.383344
3	7	0	-2.767298	1.126130	-0.084554
4	1	0	-2.162984	1.926469	0.035348
5	1	0	-3.586075	1.227088	-0.676454
6	6	0	-0.864492	-0.160965	0.690305
7	1	0	-0.869558	-0.252121	1.776888
8	6	0	0.321628	-0.071064	-0.019936
9	1	0	0.215056	0.006029	-1.109959
10	6	0	1.651874	-0.066867	0.440468
11	1	0	1.831116	-0.145640	1.516484
12	6	0	2.773342	0.038933	-0.420615
13	1	0	2.521753	0.110456	-1.486851
14	6	0	4.116884	0.065755	-0.120194
15	1	0	4.477631	-0.002596	0.906352
16	1	0	4.868872	0.149691	-0.901457

E = -363.4355351 a.u.

ZPE correction = 0.124726 a.u.

H = -363.30139 a.u.

1 imaginary frequency

Table S29. Acetamide neutral n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.472074	-0.091334	0.013135
2	8	0	-4.417409	-0.847387	0.233071
3	7	0	-3.652493	1.275198	-0.076294
4	1	0	-2.992334	1.841872	-0.590590
5	1	0	-4.616930	1.582105	-0.105208
6	6	0	-2.090536	-0.613393	-0.120730
7	1	0	-2.052344	-1.688413	-0.280063
8	6	0	-0.948427	0.101088	0.005575
9	1	0	-1.000914	1.168812	0.223624
10	6	0	0.378898	-0.460987	-0.096465
11	1	0	0.450203	-1.528952	-0.305475
12	6	0	1.517668	0.262645	0.051759
13	1	0	1.437085	1.330481	0.264070
14	6	0	2.855717	-0.280914	-0.049689
15	1	0	2.938394	-1.348250	-0.262329
16	6	0	3.981379	0.446890	0.102881
17	1	0	3.886567	1.513511	0.316334
18	6	0	5.377195	-0.089503	0.004692
19	1	0	5.931376	0.077504	0.939029
20	1	0	5.384544	-1.163885	-0.208905
21	1	0	5.942166	0.420977	-0.787948

E = -441.4454606 a.u.

ZPE correction = 0.174481 a.u.

H = -441.25865 a.u.

0 imaginary frequencies

Table S30. Acetamide anion n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	3.373552	-0.045603	-0.012402
2	8	O	4.461029	-0.662610	-0.053525
3	7	O	3.433595	1.375800	-0.031615
4	1	O	2.696239	1.856510	0.471941
5	1	O	4.357331	1.693374	0.241097
6	6	O	2.085730	-0.677016	0.015539
7	1	O	2.125008	-1.763826	0.053342
8	6	O	0.845806	-0.039689	-0.016416
9	1	O	0.841632	1.051623	-0.104396
10	6	O	-0.423482	-0.627874	0.030843
11	1	O	-0.487662	-1.715418	0.108934
12	6	O	-1.627515	0.107686	-0.018311
13	1	O	-1.516497	1.195456	-0.098105
14	6	O	-2.924910	-0.372720	0.022724
15	1	O	-3.083472	-1.450926	0.100698
16	6	O	-4.083722	0.465350	-0.031938
17	1	O	-3.876895	1.537899	-0.111428
18	6	O	-5.394595	0.089827	0.002465
19	1	O	-5.687921	-0.956460	0.080023
20	1	O	-6.196343	0.822276	-0.047622

E = -440.8846964 a.u.

ZPE correction = 0.160364 a.u.

H = -440.712556 a.u.

0 imaginary frequencies

Table S31. Acetamide neutral n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.453881	-0.125068	-0.022914
2	8	0	-4.002847	-1.081016	-0.560440
3	7	0	-4.050227	1.101499	0.074907
4	1	0	-3.583043	1.887523	0.502851
5	1	0	-4.982078	1.226804	-0.300425
6	6	0	-2.081970	-0.221256	0.585789
7	1	0	-2.043479	-0.606636	1.604813
8	6	0	-0.947652	0.022647	-0.099611
9	1	0	-1.018863	0.373572	-1.130512
10	6	0	0.388832	-0.156788	0.431972
11	1	0	0.468067	-0.520982	1.457463
12	6	0	1.521130	0.096489	-0.268662
13	1	0	1.433641	0.457136	-1.295283
14	6	0	2.864348	-0.080905	0.246385
15	1	0	2.952586	-0.443960	1.272221
16	6	0	3.986483	0.170570	-0.457896
17	1	0	3.887238	0.532054	-1.483459
18	6	0	5.385306	-0.007665	0.051375
19	1	0	5.945468	-0.720473	-0.570125
20	1	0	5.942953	0.939027	0.019312
21	1	0	5.396288	-0.374574	1.083680

E = -441.4384346 a.u.

ZPE = 0.173563 a.u.

H = -441.253012 a.u.

1 imaginary frequency

Table S32. Acetamide anion n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.363258	0.001115	0.134141
2	8	0	-3.977360	0.043469	1.204318
3	7	0	-3.904936	-0.712088	-0.925971
4	1	0	-3.311603	-0.926902	-1.714525
5	1	0	-4.694021	-1.320882	-0.736544
6	6	0	-2.075491	0.687243	-0.175445
7	1	0	-2.157404	1.692598	-0.589293
8	6	0	-0.848115	0.102436	0.041452
9	1	0	-0.862707	-0.907924	0.467039
10	6	0	0.444041	0.625553	-0.207908
11	1	0	0.518778	1.626345	-0.640412
12	6	0	1.627654	-0.074702	0.066862
13	1	0	1.495601	-1.072470	0.503871
14	6	0	2.946298	0.322965	-0.140097
15	1	0	3.133454	1.308342	-0.574768
16	6	0	4.075621	-0.484395	0.184794
17	1	0	3.832349	-1.461394	0.618317
18	6	0	5.406229	-0.202480	0.026618
19	1	0	5.745491	0.743893	-0.393971
20	1	0	6.175621	-0.911156	0.325038

E = -440.8597631 a.u.

ZPE correction = 0.158434 a.u.

H = -440.689811 a.u.

1 imaginary frequency

Table S33. Acetamide neutral n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.662952	-0.053433	0.025761
2	8	0	-5.625694	-0.781809	0.264282
3	7	0	-4.812316	1.315003	-0.093220
4	1	0	-4.141552	1.854805	-0.622539
5	1	0	-5.769905	1.642037	-0.128444
6	6	0	-3.295355	-0.610758	-0.098848
7	1	0	-3.282956	-1.690901	-0.223743
8	6	0	-2.134604	0.080448	-0.003252
9	1	0	-2.160411	1.155667	0.180057
10	6	0	-0.824091	-0.515265	-0.095435
11	1	0	-0.778449	-1.590905	-0.268955
12	6	0	0.335637	0.186953	0.021766
13	1	0	0.279342	1.262810	0.198675
14	6	0	1.652398	-0.387536	-0.068556
15	1	0	1.713683	-1.462366	-0.245885
16	6	0	2.803913	0.324711	0.054869
17	1	0	2.738847	1.399640	0.233381
18	6	0	4.131796	-0.242114	-0.032877
19	1	0	4.196623	-1.317037	-0.211841
20	6	0	5.271403	0.470358	0.092110
21	1	0	5.196378	1.544757	0.271524
22	6	0	6.656866	-0.094272	0.005214
23	1	0	7.218455	0.090105	0.931956
24	1	0	6.643429	-1.174662	-0.175740
25	1	0	7.228213	0.380961	-0.804675

E = -518.8557122 a.u.

ZPE correction = 0.207868 a.u.

H = -518.633279 a.u.

0 imaginary frequencies

Table S34. Acetamide anion n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	4.559756	0.047226	-0.015955
2	8	O	5.665605	-0.528701	-0.072919
3	7	O	4.557251	1.464129	-0.015151
4	1	O	3.799419	1.913279	0.485993
5	1	O	5.468114	1.828437	0.240418
6	6	O	3.295349	-0.642389	0.010571
7	1	O	3.384188	-1.726258	0.041131
8	6	O	2.034673	-0.061030	-0.014241
9	1	O	1.978059	1.029029	-0.093175
10	6	O	0.790663	-0.713140	0.030199
11	1	O	0.782054	-1.802873	0.098977
12	6	O	-0.439770	-0.039096	-0.010185
13	1	O	-0.387531	1.053116	-0.080077
14	6	O	-1.716580	-0.592779	0.028889
15	1	O	-1.809414	-1.678990	0.097064
16	6	O	-2.908024	0.171319	-0.015273
17	1	O	-2.776393	1.256627	-0.085143
18	6	O	-4.207513	-0.291946	0.019318
19	1	O	-4.380453	-1.368306	0.089100
20	6	O	-5.358692	0.561203	-0.032228
21	1	O	-5.142926	1.631942	-0.102672
22	6	O	-6.668029	0.189972	-0.003938
23	1	O	-6.964000	-0.855985	0.064607
24	1	O	-7.467712	0.924654	-0.049754

E = -518.3026173 a.u.

ZPE correction = 0.193848 a.u.

H = -518.094822 a.u.

0 imaginary frequencies

Table S35. Acetamide neutral n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.644715	-0.043265	0.112958
2	8	0	5.192586	-0.439535	1.136310
3	7	0	5.227767	0.866531	-0.724811
4	1	0	4.753052	1.213552	-1.545549
5	1	0	6.141591	1.234813	-0.491664
6	6	0	3.290194	-0.535335	-0.316712
7	1	0	3.281395	-1.474200	-0.870458
8	6	0	2.135520	0.054255	0.054603
9	1	0	2.178151	0.974364	0.640031
10	6	0	0.816398	-0.450782	-0.261175
11	1	0	0.764536	-1.379916	-0.830740
12	6	0	-0.337865	0.161417	0.111257
13	1	0	-0.275957	1.088379	0.684573
14	6	0	-1.659623	-0.326638	-0.193283
15	1	0	-1.725562	-1.257363	-0.759406
16	6	0	-2.808129	0.296283	0.179535
17	1	0	-2.739659	1.226210	0.747131
18	6	0	-4.138901	-0.186858	-0.121913
19	1	0	-4.206323	-1.114852	-0.693265
20	6	0	-5.277267	0.431947	0.255234
21	1	0	-5.200874	1.359176	0.826639
22	6	0	-6.663975	-0.051528	-0.046738
23	1	0	-7.233956	-0.224682	0.877055
24	1	0	-7.227253	0.694323	-0.625336
25	1	0	-6.650604	-0.986212	-0.618408

E = -518.8485074 a.u.

ZPE correction = 0.206881 a.u.

H = -518.627515 a.u.

1 imaginary frequency

Table S36. Acetamide anion n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.544955	-0.133183	-0.125780
2	8	0	5.151921	-0.343362	-1.178406
3	7	0	5.053550	-0.624101	1.065257
4	1	0	4.460249	-0.633117	1.882457
5	1	0	5.822944	-1.282938	1.020078
6	6	0	3.289495	0.662764	0.019302
7	1	0	3.419709	1.728244	0.209837
8	6	0	2.039384	0.107496	-0.077593
9	1	0	1.995049	-0.968850	-0.277216
10	6	0	0.777697	0.750764	0.046561
11	1	0	0.768999	1.826620	0.236093
12	6	0	-0.440160	0.080257	-0.052897
13	1	0	-0.380571	-0.997470	-0.244933
14	6	0	-1.733290	0.608251	0.064143
15	1	0	-1.838433	1.679315	0.253446
16	6	0	-2.908546	-0.163013	-0.045194
17	1	0	-2.758925	-1.232278	-0.235273
18	6	0	-4.224104	0.261201	0.058139
19	1	0	-4.420490	1.319524	0.246748
20	6	0	-5.351496	-0.609137	-0.067512
21	1	0	-5.106668	-1.659916	-0.256394
22	6	0	-6.676267	-0.290286	0.018733
23	1	0	-7.007841	0.730841	0.203780
24	1	0	-7.450254	-1.045056	-0.095583

E = -518.2805436 a.u.

ZPE correction = 0.191960 a.u.

H = -518.074892 a.u.

1 imaginary frequency

3. Cartesian coordinates, absolute energies, zero-point energy corrections, absolute enthalpies, and number of imaginary frequencies for acetic acid (3), acetic acid enolate anion, and their $n = 1-4$ vinylogues

Table S37. Acetic acid neutral $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.088758	0.125663	-0.000005
2	8	0	0.634851	1.208264	0.000000
3	8	0	0.790122	-1.040080	-0.000004
4	1	0	1.737241	-0.804004	0.000029
5	6	0	-1.397392	-0.120158	-0.000006
6	1	0	-1.679872	-0.703810	0.882823
7	1	0	-1.679794	-0.704599	-0.882331
8	1	0	-1.925556	0.833908	-0.000427

E = -229.0961455 a.u.

ZPE correction = 0.061732 a.u.

H = -229.028868 a.u.

0 imaginary frequencies

Table S38. Acetic acid anion $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.052878	0.118600	-0.000565
2	8	0	0.560145	1.224790	0.000139
3	8	0	0.806142	-1.033210	0.000113
4	1	0	1.683963	-0.615621	0.000294
5	1	0	-1.753346	-1.203738	0.000154
6	6	0	-1.403033	-0.176372	0.000049
7	1	0	-2.125450	0.633353	0.000632

E = -228.4956227 a.u.

ZPE correction = 0.047366 a.u.

H = -228.443081 a.u.

0 imaginary frequencies

Table S39. Acetic acid neutral n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	1.152262	-0.144001	0.000038
2	8	O	2.084793	-0.927674	0.000138
3	8	O	1.350354	1.205051	-0.000048
4	1	C	2.315688	1.341379	0.000088
5	6	O	-0.266069	-0.544959	-0.000225
6	1	C	-0.418203	-1.621212	-0.000499
7	6	O	-1.298289	0.313154	-0.000093
8	1	C	-1.086694	1.381526	0.000066
9	6	O	-2.740691	-0.088495	0.000082
10	1	C	-2.864065	-1.176198	-0.002050
11	1	C	-3.256346	0.322547	-0.878508
12	1	C	-3.254840	0.318743	0.881370

E = -306.4990475 a.u.

ZPE correction = 0.095558 a.u.

H = -306.39602 a.u.

0 imaginary frequencies

Table S40. Acetic acid anion n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	-1.011757	-0.305874	0.000000
2	8	O	-2.257121	-0.147022	0.000000
3	8	O	-0.568570	-1.653878	0.000000
4	1	C	-1.409608	-2.141255	0.000000
5	6	O	0.000000	0.663411	0.000000
6	1	C	-0.347162	1.695113	0.000000
7	6	O	1.397536	0.393298	0.000000
8	1	C	1.663399	-0.666354	0.000000
9	1	C	3.473268	0.945509	0.000000
10	6	O	2.439263	1.284424	0.000000
11	1	C	2.275377	2.362629	0.000000

E = -305.9207103 a.u.

ZPE correction = 0.081152 a.u.

H = -305.832384 a.u.

0 imaginary frequencies

Table S41. Acetic acid neutral n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.137753	-0.118243	0.076483
2	8	0	-1.761950	-1.142676	-0.107039
3	8	0	-1.707359	1.108600	-0.048939
4	1	0	-2.643476	0.964904	-0.290747
5	6	0	0.296277	-0.041429	0.490138
6	1	0	0.470291	-0.050910	1.565926
7	6	0	1.310917	0.000127	-0.377608
8	1	0	1.090715	0.007217	-1.446078
9	6	0	2.762757	0.031535	0.001942
10	1	0	3.251288	0.931151	-0.395505
11	1	0	3.295191	-0.831170	-0.420279
12	1	0	2.897279	0.019477	1.088782

E = -306.4874662 a.u.

ZPE correction = 0.094806 a.u.

H = -306.385782 a.u.

1 imaginary frequency

Table S42. Acetic acid anion n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.036641	-0.127491	0.089554
2	8	0	-1.738829	-1.115496	-0.120346
3	8	0	-1.662721	1.111646	-0.093751
4	1	0	-2.577189	0.897084	-0.368941
5	6	0	0.346552	-0.041547	0.561871
6	1	0	0.467462	0.015315	1.643881
7	6	0	1.446228	-0.032231	-0.307373
8	1	0	1.181753	-0.100119	-1.370738
9	6	0	2.810789	0.046191	-0.056484
10	1	0	3.209515	0.122046	0.955616
11	1	0	3.529287	0.026945	-0.872451

E = -305.8751437 a.u.

ZPE correction = 0.078544 a.u.

H = -305.789477 a.u.

1 imaginary frequency

Table S43. Acetic acid neutral n=2 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	2.280750	-0.114600	0.000065
2	8	O	3.280266	-0.813497	0.000156
3	8	O	2.362461	1.248482	0.000033
4	1	O	3.312633	1.465322	0.000135
5	6	O	0.907599	-0.632796	-0.000096
6	1	O	0.843957	-1.717460	-0.000120
7	6	O	-0.201528	0.140055	-0.000175
8	1	O	-0.085426	1.222775	-0.000146
9	6	O	-1.554849	-0.378259	-0.000248
10	1	O	-1.673967	-1.462622	-0.000381
11	6	O	-2.648850	0.409991	-0.000163
12	1	O	-2.507895	1.492576	-0.000169
13	6	O	-4.065515	-0.075360	0.000238
14	1	O	-4.121300	-1.169105	-0.002181
15	1	O	-4.608797	0.299325	-0.878373
16	1	O	-4.606670	0.295128	0.881996

E = -383.9081125 a.u.

ZPE correction = 0.129154 a.u.

H = -383.76934 a.u.

0 imaginary frequencies

Table S44. Acetic acid anion n=2 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	2.181793	-0.120317	-0.000021
2	8	O	3.282387	-0.710841	0.000004
3	8	O	2.225876	1.287702	0.000009
4	1	O	3.180669	1.470985	0.000017
5	6	O	0.888285	-0.685206	-0.000002
6	1	O	0.863438	-1.772759	0.000008
7	6	O	-0.315957	0.043829	-0.000003
8	1	O	-0.214892	1.131688	-0.000012
9	6	O	-1.609867	-0.453889	0.000005
10	1	O	-1.759344	-1.536764	0.000014
11	6	O	-2.773729	0.376425	-0.000003
12	1	O	-2.570976	1.453050	-0.000014
13	1	O	-4.888573	0.732957	-0.000011
14	6	O	-4.086538	-0.001386	0.000002
15	1	O	-4.380345	-1.050775	0.000019

E = -383.3429429 a.u.

ZPE correction = 0.114677 a.u.

H = -383.218972 a.u.

0 imaginary frequencies

Table S45. Acetic acid neutral n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	-2.270987	-0.111851	0.046934
2	8	O	-2.889913	-1.115491	-0.240740
3	8	O	-2.807979	1.129708	-0.076976
4	1	O	-3.718859	1.014653	-0.412514
5	6	O	-0.882688	-0.080843	0.594214
6	1	O	-0.806896	-0.145284	1.678991
7	6	O	0.214536	-0.019423	-0.179166
8	1	O	0.098911	0.042349	-1.261922
9	6	O	1.578077	-0.032118	0.329232
10	1	O	1.698984	-0.099171	1.411779
11	6	O	2.669662	0.034987	-0.455132
12	1	O	2.530632	0.101142	-1.536107
13	6	O	4.087558	0.025910	0.032048
14	1	O	4.617498	0.937199	-0.278329
15	1	O	4.645287	-0.820152	-0.392960
16	1	O	4.140627	-0.044438	1.124006

E = -383.8949586 a.u.

ZPE correction = 0.128208 a.u.

H = -383.757678 a.u.

1 imaginary frequency

Table S46. Acetic acid anion n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.176675	-0.119236	0.038097
2	8	0	-2.842698	-1.093738	-0.294447
3	8	0	-2.741704	1.132887	-0.171564
4	1	0	-3.614741	0.957844	-0.576295
5	6	0	-0.855733	-0.077334	0.683997
6	1	0	-0.869739	-0.070440	1.773536
7	6	0	0.331882	-0.048314	-0.029535
8	1	0	0.230183	-0.056120	-1.121451
9	6	0	1.656322	-0.012590	0.438749
10	1	0	1.827714	0.000289	1.518525
11	6	0	2.785257	0.007879	-0.420678
12	1	0	2.542006	-0.004871	-1.490771
13	6	0	4.125341	0.041408	-0.111550
14	1	0	4.476869	0.054604	0.920214
15	1	0	4.884553	0.054625	-0.890149

E = -383.3045775 a.u.

ZPE correction = 0.112552 a.u.

H = -383.183008 a.u.

1 imaginary frequency

Table S47. Acetic acid neutral n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.447430	-0.073311	0.000064
2	8	0	4.477311	-0.727868	0.000225
3	8	0	3.471197	1.292818	-0.000002
4	1	0	4.411504	1.548796	0.000130
5	6	0	2.099703	-0.649440	-0.000070
6	1	0	2.082216	-1.735768	-0.000101
7	6	0	0.955053	0.075596	-0.000105
8	1	0	1.025985	1.162286	-0.000069
9	6	0	-0.367793	-0.497673	-0.000175
10	1	0	-0.443780	-1.585562	-0.000229
11	6	0	-1.503500	0.247860	-0.000154
12	1	0	-1.414350	1.335635	-0.000104
13	6	0	-2.844182	-0.295702	-0.000162
14	1	0	-2.936713	-1.383101	-0.000277
15	6	0	-3.962347	0.459896	-0.000043
16	1	0	-3.855135	1.546424	-0.000020
17	6	0	-5.363692	-0.069321	0.000253
18	1	0	-5.384485	-1.164483	-0.001413
19	1	0	-5.919439	0.285787	-0.878908
20	1	0	-5.917900	0.282960	0.881558

E = -461.318061 a.u.

ZPE correction = 0.162648 a.u.

H = -461.143604 a.u.

0 imaginary frequencies

Table S.48 Acetic acid anion n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	3.350409	-0.045754	-0.000123
2	8	O	4.475605	-0.578022	0.000076
3	8	O	3.308407	1.356072	0.000065
4	1	H	4.248590	1.605129	0.000142
5	6	O	2.086804	-0.689725	-0.000054
6	1	H	2.129045	-1.776465	0.000005
7	6	O	0.850165	-0.035926	-0.000054
8	1	H	0.880249	1.055649	-0.000108
9	6	O	-0.414911	-0.622740	-0.000003
10	1	H	-0.484625	-1.713124	0.000064
11	6	O	-1.620055	0.117858	-0.000024
12	1	H	-1.507623	1.207739	-0.000094
13	6	O	-2.913930	-0.367185	0.000027
14	1	H	-3.069870	-1.448637	0.000106
15	6	O	-4.076702	0.469257	-0.000010
16	1	H	-3.875183	1.545446	-0.000094
17	1	H	-6.191059	0.811644	-0.000012
18	6	O	-5.383817	0.083545	0.000033
19	1	H	-5.669393	-0.967761	0.000124

E = -460.7621715 a.u.

ZPE correction = 0.148181 a.u.

H = -460.602545 a.u.

0 imaginary frequencies

Table S49. Acetic acid neutral n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	-3.440826	-0.098680	-0.026672
2	8	O	-4.053541	-0.946042	-0.643051
3	8	O	-3.962514	1.129551	0.227939
4	1	O	-4.856507	1.147625	-0.166933
5	6	O	-2.079701	-0.273935	0.558328
6	1	O	-2.053823	-0.683462	1.567164
7	6	O	-0.945725	0.005009	-0.111496
8	1	O	-1.013658	0.411982	-1.120982
9	6	O	0.387675	-0.197094	0.417311
10	1	O	0.464509	-0.607645	1.424959
11	6	O	1.520687	0.094697	-0.266958
12	1	O	1.433797	0.504312	-1.274899
13	6	O	2.863147	-0.098243	0.243294
14	1	O	2.952012	-0.507467	1.251324
15	6	O	3.984445	0.194120	-0.446448
16	1	O	3.883654	0.602643	-1.453893
17	6	O	5.383458	0.005324	0.057228
18	1	O	5.395954	-0.412444	1.069845
19	1	O	5.930709	0.958365	0.074370
20	1	O	5.952825	-0.669166	-0.597586

E = -461.3043873 a.u.

ZPE correction = 0.161647 a.u.

H = -461.131453 a.u.

1 imaginary frequency

Table S50. Acetic acid anion n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	3.343893	-0.043331	-0.111596
2	8	O	3.982641	-0.362152	-1.105880
3	8	O	3.880024	-0.349676	1.126457
4	1	O	4.728418	-0.798505	0.939755
5	6	O	2.066458	0.690168	-0.038919
6	1	O	2.154638	1.774144	0.026701
7	6	O	0.839200	0.065500	-0.051848
8	1	O	0.852188	-1.027874	-0.118305
9	6	O	-0.447979	0.647283	0.005630
10	1	O	-0.518947	1.735397	0.076443
11	6	O	-1.635264	-0.100285	-0.024074
12	1	O	-1.507171	-1.187645	-0.093802
13	6	O	-2.951130	0.350892	0.023576
14	1	O	-3.133699	1.426504	0.091448
15	6	O	-4.084674	-0.513991	-0.011870
16	1	O	-3.846200	-1.581707	-0.079956
17	6	O	-5.413389	-0.186833	0.027033
18	1	O	-5.746727	0.848500	0.094019
19	1	O	-6.186501	-0.950609	-0.008506

E = -460.7282824 a.u.

ZPE correction = 0.146281 a.u.

H = -460.570906 a.u.

1 imaginary frequency

Table S51. Acetic acid neutral n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	4.634828	-0.028965	0.000075
2	8	O	5.682905	-0.654688	0.000272
3	8	O	4.621499	1.337727	-0.000056
4	1	H	5.554662	1.618420	0.000093
5	6	O	3.304283	-0.641379	-0.000067
6	1	H	3.316142	-1.727762	-0.000108
7	6	O	2.138810	0.052383	-0.000072
8	1	H	2.180488	1.140616	-0.000025
9	6	O	0.834547	-0.555724	-0.000128
10	1	H	0.787097	-1.645197	-0.000189
11	6	O	-0.324395	0.160002	-0.000098
12	1	H	-0.262480	1.249722	-0.000041
13	6	O	-1.642209	-0.415963	-0.000132
14	1	H	-1.710081	-1.504814	-0.000202
15	6	O	-2.788908	0.315566	-0.000070
16	1	H	-2.714900	1.404560	-0.000003
17	6	O	-4.120872	-0.246843	-0.000071
18	1	H	-4.196210	-1.335784	-0.000172
19	6	O	-5.252868	0.488784	0.000034
20	1	H	-5.165472	1.577101	0.000081
21	6	O	-6.644388	-0.066392	0.000194
22	1	H	-6.644274	-1.161858	-0.000794
23	1	H	-7.207038	0.276760	-0.879450
24	1	H	-7.206128	0.275107	0.881085

E = -538.7284183 a.u.

ZPE correction = 0.196132 a.u.

H = -538.518288 a.u.

0 imaginary frequencies

Table S52. Acetic acid anion n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	4.535341	0.042918	-0.000354
2	8	O	5.675923	-0.447841	0.000314
3	8	O	4.431730	1.436822	0.000202
4	1	H	5.358232	1.733072	0.000535
5	6	O	3.295664	-0.656507	-0.000181
6	1	H	3.385326	-1.740136	0.000026
7	6	O	2.038409	-0.056440	-0.000205
8	1	H	2.018469	1.034959	-0.000395
9	6	O	0.797467	-0.704110	-0.000051
10	1	H	0.781273	-1.796308	0.000142
11	6	O	-0.433583	-0.023614	-0.000128
12	1	H	-0.378013	1.070063	-0.000327
13	6	O	-1.707058	-0.579765	0.000029
14	1	H	-1.798565	-1.668277	0.000235
15	6	O	-2.902090	0.183087	-0.000056
16	1	H	-2.774651	1.270860	-0.000267
17	6	O	-4.197340	-0.288792	0.000091
18	1	H	-4.363848	-1.368419	0.000295
19	6	O	-5.355029	0.558513	-0.000014
20	1	H	-5.147957	1.633079	-0.000219
21	1	H	-7.467170	0.901675	0.000024
22	6	O	-6.659951	0.173858	0.000119
23	1	H	-6.945310	-0.877305	0.000323

E = -538.1795342 a.u.

ZPE correction = 0.181674 a.u.

H = -537.984252 a.u.

0 imaginary frequencies

Table S53. Acetic acid neutral n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.631426	-0.000620	0.097946
2	8	0	-5.236916	-0.006529	1.149964
3	8	0	-5.140478	-0.555083	-1.032797
4	1	0	-6.022883	-0.909047	-0.805919
5	6	0	-3.286973	0.608795	-0.117847
6	1	0	-3.287299	1.669039	-0.366934
7	6	0	-2.134311	-0.068097	0.050572
8	1	0	-2.175362	-1.126075	0.312218
9	6	0	-0.817453	0.513321	-0.092274
10	1	0	-0.767513	1.573869	-0.342268
11	6	0	0.336970	-0.185173	0.065918
12	1	0	0.275862	-1.245560	0.317518
13	6	0	1.657995	0.374035	-0.072995
14	1	0	1.723327	1.435565	-0.317086
15	6	0	2.806391	-0.335715	0.080624
16	1	0	2.738112	-1.397273	0.325229
17	6	0	4.136812	0.216916	-0.057707
18	1	0	4.204017	1.277720	-0.306750
19	6	0	5.274926	-0.490708	0.100439
20	1	0	5.198399	-1.551171	0.348640
21	6	0	6.661618	0.061786	-0.036487
22	1	0	7.225818	-0.046001	0.900729
23	1	0	6.649203	1.123654	-0.305746
24	1	0	7.230174	-0.479070	-0.806103

E = -538.7144904 a.u.

ZPE correction = 0.195084 a.u.

H = -538.505909 a.u.

1 imaginary frequency

Table S54. Acetic acid anion n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	O	4.527044	-0.140576	-0.107574
2	8	O	5.145078	-0.486414	-1.104010
3	8	O	5.036836	-0.472604	1.130141
4	1	O	5.861807	-0.965946	0.951933
5	6	O	3.280981	0.650616	-0.039047
6	1	O	3.416032	1.729827	0.022745
7	6	O	2.032154	0.083402	-0.051176
8	1	O	1.988440	-1.008815	-0.109332
9	6	O	0.774440	0.738523	-0.000807
10	1	O	0.767104	1.829126	0.059892
11	6	O	-0.445386	0.062354	-0.025683
12	1	O	-0.387443	-1.030630	-0.085427
13	6	O	-1.735915	0.604122	0.016310
14	1	O	-1.838549	1.690397	0.074519
15	6	O	-2.914038	-0.171422	-0.012472
16	1	O	-2.767645	-1.256121	-0.072269
17	6	O	-4.227387	0.267674	0.024778
18	1	O	-4.419910	1.341647	0.084786
19	6	O	-5.358543	-0.606936	-0.011646
20	1	O	-5.117683	-1.673617	-0.072420
21	1	O	-7.459042	-1.032642	-0.014969
22	6	O	-6.681613	-0.273580	0.019433
23	1	O	-7.008842	0.763850	0.078794

E = -538.1487257 a.u.

ZPE correction = 0.179968 a.u.

H = -537.955547 a.u.

1 imaginary frequency

4. Cartesian coordinates, absolute energies, zero-point energy corrections, absolute enthalpies, and number of imaginary frequencies for acetyl fluoride, the acetyl fluoride enolate anion, and their $n = 1-4$ vinylogues

Table S55. Acetyl fluoride neutral $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.075386	-0.854936	0.000000
2	1	0	-0.967392	-1.494607	0.882521
3	1	0	-0.967392	-1.494607	-0.882521
4	1	0	-2.055981	-0.377497	0.000000
5	6	0	0.000000	0.188397	0.000000
6	8	0	-0.091491	1.375031	0.000000
7	9	0	1.241668	-0.403812	0.000000

E = -253.10986 a.u.

ZPE correction = 0.049019 a.u.

H = -253.05577 a.u.

0 imaginary frequencies

Table S56. Acetyl fluoride anion $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	0.180651	0.000000
2	8	0	-0.828534	1.093392	0.000000
3	9	0	-0.605382	-1.171416	0.000000
4	6	0	1.373158	0.094518	0.000000
5	1	0	1.958810	1.008689	0.000000
6	1	0	1.878951	-0.864092	0.000000

E = -252.5278779 a.u.

ZPE correction = 0.034864 a.u.

H = -252.488071 a.u.

0 imaginary frequencies

Table S57. Acetyl fluoride neutral n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.136793	-0.314879	0.000000
2	8	0	2.300882	-0.039948	0.000000
3	9	0	0.752591	-1.638544	0.000000
4	6	0	0.000000	0.609371	0.000000
5	1	0	0.284505	1.658357	0.000000
6	6	0	-1.287602	0.224770	0.000000
7	1	0	-1.513715	-0.840248	0.000000
8	6	0	-2.454416	1.159945	0.000000
9	1	0	-3.087816	0.981881	0.879541
10	1	0	-2.144185	2.209373	0.000000
11	1	0	-3.087816	0.981881	-0.879541

E = -330.5138806 a.u.

ZPE correction = 0.082792 a.u.

H = -330.423797 a.u.

0 imaginary frequencies

Table S58. Acetyl fluoride anion n=1 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.062354	-0.247066	0.000000
2	8	0	-2.280984	-0.105128	0.000000
3	9	0	-0.617560	-1.630628	0.000000
4	6	0	0.000000	0.655798	0.000000
5	1	0	-0.295618	1.703840	0.000000
6	6	0	1.387792	0.325178	0.000000
7	1	0	1.611905	-0.742801	0.000000
8	6	0	2.455373	1.180200	0.000000
9	1	0	2.326818	2.263017	0.000000
10	1	0	3.477948	0.807959	0.000000

E = -329.9500493 a.u.

ZPE correction = 0.068623 a.u.

H = -329.874476 a.u.

0 imaginary frequencies

Table S59. Acetyl fluoride neutral n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.147336	-0.134552	0.068788
2	8	0	-1.825950	-1.099858	-0.092412
3	9	0	-1.697420	1.115899	-0.091739
4	6	0	0.275591	-0.047490	0.488602
5	1	0	0.435701	0.019451	1.564249
6	6	0	1.294560	-0.049901	-0.376181
7	1	0	1.081287	-0.113294	-1.443910
8	6	0	2.742225	0.020634	0.010021
9	1	0	3.220018	0.901156	-0.439137
10	1	0	2.871138	0.074918	1.095924
11	1	0	3.285998	-0.858607	-0.359559

E = -330.5010431 a.u.

ZPE correction = 0.081926 a.u.

H = -330.412356 a.u.

1 imaginary frequency

Table S60. Acetyl fluoride anion n=1 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.034330	-0.176846	0.102534
2	8	0	-1.784887	-1.078289	-0.163077
3	9	0	-1.665514	1.135694	-0.103177
4	6	0	0.326818	-0.091894	0.571020
5	1	0	0.455043	-0.071891	1.652578
6	6	0	1.423628	-0.037985	-0.310266
7	1	0	1.155059	-0.069684	-1.373048
8	6	0	2.780750	0.041689	-0.053502
9	1	0	3.175290	0.085261	0.961841
10	1	0	3.502130	0.051598	-0.866864

E = -329.9027055 a.u.

ZPE correction = 0.06571 a.u.

H = -329.829942 a.u.

1 imaginary frequency

Table S61. Acetyl fluoride neutral n=2 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.194059	-1.959363	0.000000
2	8	0	1.264175	-3.155219	0.000000
3	9	0	2.356938	-1.214101	0.000000
4	6	0	-0.007317	-1.133077	0.000000
5	1	0	-0.935504	-1.697950	0.000000
6	6	0	0.000000	0.220703	0.000000
7	1	0	0.957536	0.738510	0.000000
8	6	0	-1.191847	1.041072	0.000000
9	1	0	-2.154726	0.528957	0.000000
10	6	0	-1.153865	2.389770	0.000000
11	1	0	-0.178597	2.880392	0.000000
12	6	0	-2.348593	3.290221	0.000000
13	1	0	-2.341206	3.948508	0.879885
14	1	0	-2.341206	3.948508	-0.879885
15	1	0	-3.286763	2.725782	0.000000

E = -407.9233939 a.u.

ZPE correction = 0.116299 a.u.

H = -407.797620 a.u.

0 imaginary frequencies

Table S62. Acetyl fluoride anion n=2 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.204456	-0.140135	-0.000188
2	8	0	-3.310915	-0.660054	0.000040
3	9	0	-2.204263	1.299128	0.000112
4	6	0	-0.909613	-0.681277	-0.000115
5	1	0	-0.876304	-1.769005	-0.000228
6	6	0	0.297022	0.051491	0.000071
7	1	0	0.198589	1.138612	0.000143
8	6	0	1.583383	-0.454605	0.000110
9	1	0	1.725992	-1.538220	0.000328
10	6	0	2.755842	0.367939	-0.000127
11	1	0	2.564165	1.446125	-0.000339
12	6	0	4.061107	-0.027358	-0.000038
13	1	0	4.339637	-1.080847	0.000618
14	1	0	4.873898	0.695273	-0.000124

E = -407.3705568 a.u.

ZPE correction = 0.102163 a.u.

H = -407.259326 a.u.

0 imaginary frequencies

Table S63. Acetyl fluoride neutral n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.274062	-0.126393	0.044377
2	8	0	-2.945348	-1.085572	-0.175949
3	9	0	-2.792364	1.128383	-0.182874
4	6	0	-0.898868	-0.051175	0.596061
5	1	0	-0.836761	0.020804	1.680958
6	6	0	0.202418	-0.069450	-0.175577
7	1	0	0.091850	-0.135706	-1.258377
8	6	0	1.562059	-0.010074	0.336532
9	1	0	1.680439	0.051434	1.419358
10	6	0	2.653572	-0.025367	-0.451101
11	1	0	2.514323	-0.087138	-1.532211
12	6	0	4.070406	0.036334	0.032464
13	1	0	4.590904	0.908694	-0.386347
14	1	0	4.125191	0.096779	1.124712
15	1	0	4.634969	-0.848998	-0.291171

E = -407.9086485 a.u.

ZPE correction = 0.115335 a.u.

H = -407.784358 a.u.

1 imaginary frequency

Table S64. Acetyl fluoride anion n=2 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.174600	-0.157118	0.040983
2	8	0	-2.881691	-1.047331	-0.344903
3	9	0	-2.730789	1.153855	-0.177468
4	6	0	-0.871990	-0.124198	0.683896
5	1	0	-0.884760	-0.150811	1.772727
6	6	0	0.317400	-0.062767	-0.035224
7	1	0	0.213675	-0.039688	-1.126023
8	6	0	1.634712	-0.031362	0.436273
9	1	0	1.805289	-0.044487	1.515890
10	6	0	2.768207	0.013733	-0.421677
11	1	0	2.529753	0.026506	-1.492286
12	6	0	4.102004	0.043354	-0.100486
13	1	0	4.443719	0.032576	0.934472
14	1	0	4.868548	0.080005	-0.870926

E = -407.3293465 a.u.

ZPE correction = 0.099682 a.u.

H = -407.220718 a.u.

1 imaginary frequency

Table S65. Acetyl fluoride neutral n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.906124	-1.866255	0.000000
2	8	0	-4.098925	-1.983571	0.000000
3	9	0	-2.117140	-3.002438	0.000000
4	6	0	-2.126370	-0.637229	0.000000
5	1	0	-2.724684	0.269599	0.000000
6	6	0	-0.769761	-0.592016	0.000000
7	1	0	-0.216972	-1.529774	0.000000
8	6	0	0.000000	0.623809	0.000000
9	1	0	-0.545290	1.567829	0.000000
10	6	0	1.359647	0.638052	0.000000
11	1	0	1.891245	-0.315047	0.000000
12	6	0	2.169961	1.834898	0.000000
13	1	0	1.643821	2.790712	0.000000
14	6	0	3.519946	1.824062	0.000000
15	1	0	4.031438	0.859546	0.000000
16	6	0	4.394736	3.039017	0.000000
17	1	0	5.052900	3.048935	0.880051
18	1	0	5.052900	3.048935	-0.880051
19	1	0	3.808083	3.963746	0.000000

E = -485.3336168 a.u.

ZPE correction = 0.149778 a.u.

H = -485.172167 a.u.

0 imaginary frequencies

Table S.66 Acetyl fluoride anion n=3 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.368754	-0.067086	-0.000117
2	8	0	4.496449	-0.531218	-0.000467
3	9	0	3.286899	1.361531	0.000291
4	6	0	2.102637	-0.685601	-0.000102
5	1	0	2.133456	-1.773027	-0.000267
6	6	0	0.864873	-0.023974	0.000145
7	1	0	0.897237	1.066610	0.000314
8	6	0	-0.394682	-0.612535	0.000208
9	1	0	-0.463321	-1.702827	0.000180
10	6	0	-1.604705	0.126274	0.000317
11	1	0	-1.496703	1.216237	0.000332
12	6	0	-2.892053	-0.367842	0.000383
13	1	0	-3.040232	-1.450233	0.001062
14	6	0	-4.063604	0.460100	-0.000385
15	1	0	-3.872719	1.537832	-0.001042
16	6	0	-5.363782	0.057862	-0.000353
17	1	0	-5.635584	-0.996978	0.000663
18	1	0	-6.180442	0.775166	-0.000700

E = -484.7884597 a.u.

ZPE correction = 0.135624 a.u.

H = -484.641600 a.u.

0 imaginary frequencies

Table S67. Acetyl fluoride neutral n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.440010	-0.117243	0.018956
2	8	0	-4.106204	-1.100588	-0.074481
3	9	0	-3.943623	1.084219	-0.427167
4	6	0	-2.092620	0.049403	0.615413
5	1	0	-2.080977	0.296953	1.675787
6	6	0	-0.953963	-0.092117	-0.091129
7	1	0	-1.016242	-0.334319	-1.152564
8	6	0	0.374918	0.052690	0.463764
9	1	0	0.447921	0.290866	1.525567
10	6	0	1.509031	-0.089024	-0.265487
11	1	0	1.423263	-0.327101	-1.327273
12	6	0	2.850226	0.053055	0.262742
13	1	0	2.939476	0.290845	1.324199
14	6	0	3.970140	-0.090262	-0.474954
15	1	0	3.867319	-0.327867	-1.535654
16	6	0	5.369511	0.050333	0.041593
17	1	0	5.910117	0.843841	-0.493278
18	1	0	5.385706	0.287431	1.110951
19	1	0	5.942260	-0.874922	-0.112760

E = -485.3181249 a.u.

ZPE correction = 0.148741 a.u.

H = -485.158207 a.u.

1 imaginary frequency

Table S68. Acetyl fluoride anion n=3 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	3.340814	-0.030173	-0.144457
2	8	0	4.015844	-0.355808	-1.080753
3	9	0	3.857915	-0.423762	1.123868
4	6	0	2.080174	0.697437	-0.041519
5	1	0	2.168532	1.778643	0.053109
6	6	0	0.850882	0.065249	-0.061811
7	1	0	0.867304	-1.025292	-0.157940
8	6	0	-0.430741	0.643243	0.017186
9	1	0	-0.503467	1.728543	0.118889
10	6	0	-1.620742	-0.105361	-0.033216
11	1	0	-1.493456	-1.189785	-0.136056
12	6	0	-2.931251	0.348173	0.030725
13	1	0	-3.110572	1.421385	0.133176
14	6	0	-4.070257	-0.511971	-0.029692
15	1	0	-3.838321	-1.577844	-0.133156
16	6	0	-5.393464	-0.174485	0.023211
17	1	0	-5.716489	0.861105	0.125318
18	1	0	-6.174004	-0.929113	-0.034686

E = -484.7512811 a.u.

ZPE correction = 0.133343 a.u.

H = -484.654388 a.u.

1 imaginary frequency

Table S69. Acetyl fluoride neutral n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-1.834608	-4.257541	0.000000
2	8	0	-1.775583	-5.455087	0.000000
3	9	0	-3.075785	-3.644797	0.000000
4	6	0	-0.735946	-3.304790	0.000000
5	1	0	0.250061	-3.760848	0.000000
6	6	0	-0.893169	-1.954906	0.000000
7	1	0	-1.903352	-1.549314	0.000000
8	6	0	0.191036	-1.013269	0.000000
9	1	0	1.206963	-1.408670	0.000000
10	6	0	0.000000	0.336893	0.000000
11	1	0	-1.023566	0.715692	0.000000
12	6	0	1.053511	1.313467	0.000000
13	1	0	2.079496	0.943315	0.000000
14	6	0	0.835357	2.656831	0.000000
15	1	0	-0.194250	3.018991	0.000000
16	6	0	1.877662	3.657493	0.000000
17	1	0	2.908286	3.298579	0.000000
18	6	0	1.644844	4.987648	0.000000
19	1	0	0.609380	5.333729	0.000000
20	6	0	2.700622	6.049711	0.000000
21	1	0	2.604592	6.700978	0.880128
22	1	0	3.708672	5.621222	0.000000
23	1	0	2.604592	6.700978	-0.880128

E = -562.7441216 a.u.

ZPE correction = 0.183320 a.u.

H = -562.54697 a.u.

0 imaginary frequencies

Table S70. Acetyl fluoride anion n=4 parallel.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.549400	0.022223	0.000026
2	8	0	5.692534	-0.395933	-0.000076
3	9	0	4.402618	1.439833	0.000080
4	6	0	3.309337	-0.656287	0.000081
5	1	0	3.389973	-1.740892	0.000226
6	6	0	2.049878	-0.049514	-0.000026
7	1	0	2.032910	1.041020	-0.000176
8	6	0	0.813931	-0.696440	0.000023
9	1	0	0.796136	-1.788445	0.000165
10	6	0	-0.420079	-0.014041	-0.000102
11	1	0	-0.364699	1.079329	-0.000238
12	6	0	-1.688725	-0.572766	-0.000056
13	1	0	-1.778128	-1.661305	-0.000014
14	6	0	-2.888089	0.188080	-0.000055
15	1	0	-2.764636	1.275974	-0.000097
16	6	0	-4.177920	-0.291532	-0.000010
17	1	0	-4.338052	-1.371968	-0.000002
18	6	0	-5.342591	0.549183	0.000026
19	1	0	-5.143902	1.624996	0.000017
20	6	0	-6.641912	0.151411	0.000067
21	1	0	-6.916378	-0.902518	0.000063
22	1	0	-7.456450	0.870883	0.000102

E = -562.2048049 a.u.

ZPE correction = 0.169118 a.u.

H = -562.022285 a.u.

0 imaginary frequencies

Table S71. Acetyl fluoride neutral n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.627195	-0.053539	-0.107567
2	8	0	5.289690	-0.387188	-1.040036
3	9	0	5.117380	-0.233416	1.166840
4	6	0	3.299109	0.605219	-0.088340
5	1	0	3.319650	1.693924	-0.087119
6	6	0	2.138626	-0.081614	-0.073283
7	1	0	2.169897	-1.171711	-0.068484
8	6	0	0.828481	0.528157	-0.064991
9	1	0	0.784713	1.617806	-0.074235
10	6	0	-0.328738	-0.184210	-0.043085
11	1	0	-0.270049	-1.274175	-0.033683
12	6	0	-1.647911	0.394034	-0.030991
13	1	0	-1.713737	1.483067	-0.040008
14	6	0	-2.794945	-0.334531	-0.008904
15	1	0	-2.723464	-1.423705	0.000039
16	6	0	-4.126675	0.230570	0.004667
17	1	0	-4.199532	1.319733	-0.003827
18	6	0	-5.260084	-0.501778	0.027487
19	1	0	-5.175697	-1.590324	0.035846
20	6	0	-6.650326	0.057216	0.043025
21	1	0	-7.200209	-0.274601	0.935032
22	1	0	-6.647071	1.152693	0.032412
23	1	0	-7.226833	-0.291614	-0.825351

E = -562.7283015 a.u.

ZPE correction = 0.182274 a.u.

H = -562.532672 a.u.

1 imaginary frequency

Table S72. Acetyl fluoride anion n=4 perpendicular.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	4.520867	-0.157261	-0.126262
2	8	0	5.184065	-0.579812	-1.030439
3	9	0	5.046853	-0.390525	1.168477
4	6	0	3.288152	0.629440	-0.096229
5	1	0	3.429296	1.709186	-0.086094
6	6	0	2.034510	0.060767	-0.081567
7	1	0	1.990510	-1.032506	-0.093092
8	6	0	0.783842	0.718845	-0.054017
9	1	0	0.777453	1.810800	-0.036172
10	6	0	-0.440493	0.043065	-0.045852
11	1	0	-0.385227	-1.051312	-0.061854
12	6	0	-1.724581	0.591248	-0.019342
13	1	0	-1.822898	1.679213	-0.003515
14	6	0	-2.908774	-0.180253	-0.011355
15	1	0	-2.769041	-1.267027	-0.028094
16	6	0	-4.215567	0.270697	0.015133
17	1	0	-4.399308	1.347587	0.032704
18	6	0	-5.355836	-0.595650	0.021112
19	1	0	-5.126208	-1.666048	0.003096
20	6	0	-6.672599	-0.244486	0.046213
21	1	0	-6.985877	0.798671	0.064975
22	1	0	-7.460028	-0.993822	0.048258

E = -562.1705906 a.u.

ZPE correction = 0.167074 a.u.

H = -561.990388 a.u.

1 imaginary frequency

5. Cartesian coordinates, absolute energies, zero-point energy corrections, absolute enthalpies, and number of imaginary frequencies for methylpropane, the methylpropyl anion, and their $n = 1-4$ vinyllogues

Table S73. Methylpropane neutral $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.000000	1.463124	-0.095884
2	1	0	0.000000	1.522101	-1.193093
3	1	0	0.886629	1.998970	0.265969
4	1	0	-0.886629	1.998970	0.265969
5	6	0	0.000000	0.000000	0.372609
6	1	0	0.000000	0.000000	1.473725
7	6	0	-1.267103	-0.731562	-0.095884
8	1	0	-1.318178	-0.761051	-1.193093
9	1	0	-2.174473	-0.231642	0.265969
10	1	0	-1.287844	-1.767328	0.265969
11	6	0	1.267103	-0.731562	-0.095884
12	1	0	1.318178	-0.761051	-1.193093
13	1	0	1.287844	-1.767328	0.265969
14	1	0	2.174473	-0.231642	0.265969

E = -158.4641151 a.u.

ZPE correction = 0.131915 a.u.

H = -158.325565 a.u.

0 imaginary frequencies

Table S74. Methylpropane anion $n=0$.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	0.028982	0.089335	-0.364941
2	1	0	0.042878	0.033185	-1.471564
3	6	0	0.887839	-1.128776	0.115713
4	1	0	0.889806	-1.179348	1.215631
5	1	0	1.930029	-1.005773	-0.204089
6	1	0	0.521166	-2.104381	-0.274884
7	6	0	-1.430344	-0.154803	0.074910
8	1	0	-1.508681	-0.074838	1.170854
9	1	0	-1.800165	-1.154124	-0.211781
10	1	0	-2.088577	0.608846	-0.355393
11	6	0	0.513213	1.462986	0.055126
12	1	0	1.535485	1.671657	-0.307411
13	1	0	0.479924	1.592321	1.153793

E = -157.7889596 a.u.

ZPE correction = 0.114788 a.u.

H = -157.667495 a.u.

0 imaginary frequencies

Table S75. Methylpropane neutral n=1.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	1.015326	0.451437	-0.041082
2	1	0	1.132119	1.103667	-0.923056
3	6	0	1.765884	1.136213	1.120578
4	1	0	1.709225	0.527000	2.031547
5	1	0	1.337271	2.119853	1.348991
6	1	0	2.824775	1.280375	0.871889
7	6	0	1.650643	-0.902912	-0.380861
8	1	0	1.587126	-1.596423	0.467515
9	1	0	2.711755	-0.775251	-0.625875
10	1	0	1.163095	-1.375287	-1.241721
11	6	0	-0.466111	0.388741	0.262350
12	1	0	-0.922621	1.357517	0.484437
13	6	0	-1.249387	-0.696424	0.296665
14	1	0	-0.820762	-1.675380	0.080050
15	6	0	-2.719773	-0.684975	0.615660
16	1	0	-3.311162	-1.092289	-0.216274
17	1	0	-2.941887	-1.308045	1.493240
18	1	0	-3.079882	0.329589	0.821590

E = -235.8620705 a.u.

ZPE correction = 0.165263 a.u.

H = -235.687936 a.u.

0 imaginary frequencies

Table S76. Methylpropane anion n=1.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-0.962618	-0.019822	-0.359798
2	1	0	-1.069045	0.055216	-1.473555
3	6	0	-2.060095	-1.003763	0.088423
4	1	0	-2.072187	-1.080395	1.185559
5	1	0	-1.871407	-2.009895	-0.311682
6	1	0	-3.057769	-0.683617	-0.252294
7	6	0	-1.312308	1.386719	0.174739
8	1	0	-1.333479	1.377422	1.273914
9	1	0	-2.296194	1.721684	-0.199334
10	1	0	-0.569050	2.131508	-0.133778
11	6	0	0.397637	-0.512595	0.064645
12	1	0	0.481126	-1.594275	0.212234
13	6	0	1.584339	0.217320	-0.072695
14	1	0	1.451315	1.277107	-0.331724
15	6	0	2.921069	-0.164549	0.058005
16	1	0	3.204966	-1.180172	0.338008
17	1	0	3.723579	0.565552	-0.027256

E = -235.227548 a.u.

ZPE correction = 0.148006 a.u.

H = -235.070399 a.u.

0 imaginary frequencies

Table S77. Methylpropane neutral n=2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.232731	-0.064193	-0.381216
2	1	0	-2.625412	-0.178392	-1.406092
3	6	0	-3.065331	-1.002537	0.519177
4	1	0	-2.741134	-0.924607	1.564523
5	1	0	-2.958263	-2.050243	0.212505
6	1	0	-4.130771	-0.744970	0.471569
7	6	0	-2.425656	1.401741	0.027733
8	1	0	-2.074024	1.578638	1.052294
9	1	0	-3.487942	1.670563	-0.009289
10	1	0	-1.884662	2.083318	-0.639075
11	6	0	-0.792313	-0.518398	-0.413656
12	1	0	-0.649308	-1.554807	-0.730487
13	6	0	0.301825	0.197545	-0.091973
14	1	0	0.196940	1.233963	0.229122
15	6	0	1.662493	-0.322501	-0.144267
16	1	0	1.775332	-1.359968	-0.466677
17	6	0	2.763350	0.383900	0.173507
18	1	0	2.643047	1.420582	0.495398
19	6	0	4.170165	-0.137074	0.124573
20	1	0	4.650161	-0.083897	1.112155
21	1	0	4.793105	0.458662	-0.557686
22	1	0	4.202119	-1.179742	-0.211524

E = -313.2702 a.u.

ZPE correction = 0.19871 a.u.

H = -313.060423 a.u.

0 imaginary frequencies

Table S78. Methylpropane anion n=2.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-2.151002	-0.030162	-0.378498
2	1	0	-2.523311	-0.070556	-1.427815
3	6	0	-3.173686	-0.844662	0.446029
4	1	0	-2.935345	-0.785340	1.517157
5	1	0	-3.147865	-1.904974	0.161287
6	1	0	-4.203130	-0.477703	0.292915
7	6	0	-2.224908	1.448503	0.037571
8	1	0	-1.891513	1.576178	1.076778
9	1	0	-3.256439	1.822221	-0.041481
10	1	0	-1.589550	2.079993	-0.595110
11	6	0	-0.771442	-0.635457	-0.281828
12	1	0	-0.736566	-1.718989	-0.433429
13	6	0	0.425012	0.035132	-0.123591
14	1	0	0.367116	1.122530	0.002231
15	6	0	1.744737	-0.477011	-0.093726
16	1	0	1.884787	-1.555878	-0.210042
17	6	0	2.890857	0.329017	0.093178
18	1	0	2.677213	1.400212	0.209417
19	6	0	4.226791	-0.019486	0.150663
20	1	0	4.556456	-1.053770	0.048394
21	1	0	4.999990	0.730836	0.300905

E = -312.6606584 a.u.

ZPE correction = 0.182347 a.u.

H = -312.467315 a.u.

0 imaginary frequencies

Table S79. Methylpropane neutral n=3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.401161	-0.063917	-0.337344
2	1	0	-3.836431	-0.225743	-1.338401
3	6	0	-4.221231	-0.927537	0.646185
4	1	0	-3.854942	-0.799220	1.672403
5	1	0	-4.151971	-1.993346	0.396435
6	1	0	-5.280961	-0.644448	0.623254
7	6	0	-3.541499	1.427638	-0.007218
8	1	0	-3.149889	1.652850	0.993033
9	1	0	-4.597106	1.723223	-0.024175
10	1	0	-3.006964	2.054635	-0.730394
11	6	0	-1.975816	-0.558561	-0.398291
12	1	0	-1.870863	-1.612964	-0.666648
13	6	0	-0.850449	0.143437	-0.152896
14	1	0	-0.918101	1.196969	0.118557
15	6	0	0.487815	-0.412419	-0.227538
16	1	0	0.567467	-1.465913	-0.502931
17	6	0	1.623314	0.285466	0.018992
18	1	0	1.543847	1.338768	0.295236
19	6	0	2.961284	-0.268858	-0.056537
20	1	0	3.037724	-1.322325	-0.334506
21	6	0	4.092419	0.422656	0.189718
22	1	0	4.009619	1.475551	0.467307
23	6	0	5.481960	-0.137915	0.114803
24	1	0	6.000820	-0.048393	1.079926
25	1	0	6.092958	0.406768	-0.619136
26	1	0	5.474976	-1.196352	-0.169207

E = -390.6798596 a.u.

ZPE correction = 0.232257 a.u.

H = -390.434375 a.u.

0 imaginary frequencies

Table S80. Methylpropane anion n=3.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-3.326020	0.009190	-0.335305
2	1	0	-3.781120	-0.100528	-1.342147
3	6	0	-4.297219	-0.697191	0.638094
4	1	0	-3.957881	-0.573417	1.675520
5	1	0	-4.341950	-1.774655	0.432239
6	1	0	-5.319577	-0.293575	0.553803
7	6	0	-3.298484	1.516166	-0.035871
8	1	0	-2.879500	1.709508	0.960888
9	1	0	-4.314357	1.934891	-0.064420
10	1	0	-2.687813	2.061939	-0.765117
11	6	0	-1.967840	-0.653718	-0.324134
12	1	0	-1.989109	-1.737624	-0.472644
13	6	0	-0.746085	-0.046004	-0.184253
14	1	0	-0.738135	1.040210	-0.048005
15	6	0	0.546770	-0.645843	-0.192244
16	1	0	0.606222	-1.730138	-0.319624
17	6	0	1.735667	0.072322	-0.040196
18	1	0	1.619769	1.156681	0.086515
19	6	0	3.054076	-0.395478	-0.026533
20	1	0	3.227588	-1.468204	-0.148320
21	6	0	4.188271	0.446450	0.137408
22	1	0	3.953896	1.511547	0.254724
23	6	0	5.520182	0.112907	0.168417
24	1	0	5.855909	-0.918474	0.061233
25	1	0	6.290148	0.869036	0.303061

E = -390.0874644 a.u.

ZPE correction = 0.216171 a.u.

H = -389.858191 a.u.

0 imaginary frequencies

Table S81. Methylpropane neutral n=4.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.588086	-0.055408	-0.299622
2	1	0	-5.048614	-0.258148	-1.281706
3	6	0	-5.399442	-0.856512	0.742692
4	1	0	-5.009584	-0.683013	1.753412
5	1	0	-5.351122	-1.934322	0.545238
6	1	0	-6.455051	-0.558135	0.727249
7	6	0	-4.696937	1.452561	-0.039550
8	1	0	-4.281304	1.719095	0.940610
9	1	0	-5.747675	1.765090	-0.049677
10	1	0	-4.167367	2.034474	-0.802899
11	6	0	-3.173134	-0.576854	-0.368225
12	1	0	-3.090553	-1.642604	-0.596232
13	6	0	-2.031048	0.115311	-0.171694
14	1	0	-2.076895	1.179580	0.059065
15	6	0	-0.706011	-0.465119	-0.249975
16	1	0	-0.647497	-1.529338	-0.486195
17	6	0	0.447781	0.224246	-0.051576
18	1	0	0.387810	1.288230	0.185783
19	6	0	1.767966	-0.350450	-0.131495
20	1	0	1.828346	-1.413752	-0.371660
21	6	0	2.921576	0.338629	0.069267
22	1	0	2.862808	1.401796	0.310015
23	6	0	4.246447	-0.239471	-0.013331
24	1	0	4.301034	-1.303064	-0.255375
25	6	0	5.394085	0.441868	0.185673
26	1	0	5.333559	1.505001	0.427325
27	6	0	6.772024	-0.144382	0.102509
28	1	0	7.313248	-0.027190	1.052257
29	1	0	7.375462	0.362207	-0.664262
30	1	0	6.742073	-1.212422	-0.140981

E = -468.0900741 a.u.

ZPE correction = 0.265669 a.u.

H = -467.808954 a.u.

0 imaginary frequencies

Table S82. Methylpropane anion n=4.

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms)		
			X	Y	Z
1	6	0	-4.506544	0.080291	-0.296766
2	1	0	-4.989225	-0.067800	-1.283773
3	6	0	-5.467060	-0.545131	0.739639
4	1	0	-5.089943	-0.385340	1.758691
5	1	0	-5.557317	-1.628464	0.587030
6	1	0	-6.475721	-0.108573	0.669332
7	6	0	-4.415496	1.597719	-0.077099
8	1	0	-3.965161	1.826727	0.897971
9	1	0	-5.415197	2.052822	-0.103375
10	1	0	-3.804523	2.081577	-0.848448
11	6	0	-3.172298	-0.631270	-0.294341
12	1	0	-3.236283	-1.718629	-0.395972
13	6	0	-1.931040	-0.067781	-0.198813
14	1	0	-1.871414	1.020589	-0.106206
15	6	0	-0.664947	-0.733439	-0.206000
16	1	0	-0.664570	-1.823166	-0.290014
17	6	0	0.553412	-0.074523	-0.107557
18	1	0	0.504229	1.017991	-0.024485
19	6	0	1.848482	-0.626613	-0.099565
20	1	0	1.944692	-1.712420	-0.179880
21	6	0	3.024956	0.135891	0.006168
22	1	0	2.881787	1.220397	0.084946
23	6	0	4.343141	-0.306275	0.023267
24	1	0	4.535849	-1.379480	-0.052967
25	6	0	5.469233	0.562945	0.136066
26	1	0	5.223617	1.628336	0.209950
27	1	0	7.566999	0.999848	0.253799
28	6	0	6.797687	0.236939	0.162993
29	1	0	7.135021	-0.796936	0.095454

E = -467.510259 a.u.

ZPE correction = 0.250043 a.u.

H = -467.24504 a.u.

0 imaginary frequencies

6. Cartesian coordinates and absolute energies of the delocalized and localized structures of acetone (1), acetone enolate anion, acetamide (2), acetamide enolate anion, acetic acid (3), acetic acid enolate anion, acetyl fluoride (4), acetyl fluoride enolate anion, methylpropane (5), and the methylpropyl anion, derived from the BLW method

Table S83. Delocalized CH₃COCH₃

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.0000011224	-1.3247205896	0.0000000000
C	6.0	0.0000010971	-0.1051731871	0.0000000000
C	6.0	1.2976730979	0.6857899301	0.0000000000
H	1.0	2.1467455884	-0.0012465670	0.0000000000
H	1.0	1.3505398085	1.3380565581	-0.8820392583
H	1.0	1.3505398085	1.3380565581	0.8820392583
C	6.0	-1.2976730539	0.6857900393	0.0000000000
H	1.0	-2.1467455358	-0.0012464226	0.0000000000
H	1.0	-1.3505398442	1.3380559714	0.8820397314
H	1.0	-1.3505398442	1.3380559714	-0.8820397314

E = -193.0482662344 a.u.

ZPE correction = 0.0827827 a.u.

H = -192.9605801 a.u.

0 imaginary frequencies

Table S84. Localized CH₃COCH₃

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.0000008419	-1.3301934182	0.0000000000
C	6.0	0.0000009552	-0.1207464045	0.0000000000
C	6.0	1.3246986943	0.6984549050	0.0000000000
H	1.0	2.1656149075	0.0008006543	0.0000000000
H	1.0	1.3817551194	1.3359620340	-0.8881073435
H	1.0	1.3817551194	1.3359620340	0.8881073435
C	6.0	-1.3246985812	0.6984546356	0.0000000000
H	1.0	-2.1656152692	0.0008011465	0.0000000000
H	1.0	-1.3817550518	1.3359613377	0.8881076565
H	1.0	-1.3817550518	1.3359613377	-0.8881076565

E = -193.0307431604 a.u.

ZPE correction = 0.0848296 a.u.

H = -192.9411973 a.u.

0 imaginary frequencies

Table S85. Delocalized CH₃COCH₂⁻

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.1735868961	1.3290267932	0.0000000000
C	6.0	-0.1047468437	0.0525114275	0.0000000000
C	6.0	1.3280462943	-0.5324324341	0.0000000000
H	1.0	1.3545265225	-1.6324078703	0.0000000000
H	1.0	1.8725363248	-0.1657415266	-0.8831780222
H	1.0	1.8725363248	-0.1657415266	0.8831780222
C	6.0	-1.1579573180	-0.8559098830	0.0000000000
H	1.0	-2.1893501199	-0.5041773903	0.0000000000
H	1.0	-0.9807999231	-1.9298796785	0.0000000000

E = -192.4506291738 a.u.

ZPE correction = 0.07028777 a.u.

H = -192.3753367 a.u.

0 imaginary frequencies

Table S86. Localized CH₃COCH₂⁻

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.1605308542	1.3099805667	0.0000000000
C	6.0	-0.0760243431	0.0926281467	0.0000000000
C	6.0	1.3760989940	-0.5168621122	0.0000000000
H	1.0	1.3665317097	-1.6121980551	0.0000000000
H	1.0	1.9065534100	-0.1599461457	-0.8897361873
H	1.0	1.9065534100	-0.1599461457	0.8897361873
C	6.0	-1.2301070117	-0.8963490043	0.0000000000
H	1.0	-2.2395337108	-0.5011923606	0.0000000000
H	1.0	-1.0283372381	-1.9608669786	0.0000000000

E = -192.3680199341 a.u.

ZPE correction = 0.0748781 a.u.

H = -192.2885617 a.u.

0 imaginary frequencies

Table S87. Delocalized NH₂COCH₃

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.2024599512	1.3072186708	0.0000000000
C	6.0	-0.0202130691	0.0953589828	0.0000000000
C	6.0	1.3741063747	-0.5101491495	0.0000000000
H	1.0	1.3853903207	-1.6054278635	0.0000000000
H	1.0	1.9128892226	-0.1492151160	-0.8824959671
H	1.0	1.9128892226	-0.1492151160	0.8824959671
N	7.0	-1.0629643933	-0.7928432655	0.0000000000
H	1.0	-2.0058356153	-0.4262727180	0.0000000000
H	1.0	-0.9296414533	-1.7928999780	0.0000000000

E = -209.1089281413 a.u.

ZPE correction = 0.0739212 a.u.

H = -209.0296596 a.u.

0 imaginary frequencies

Table S88. Localized NH₂COCH₃

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.1984284921	1.3134499007	0.0000000000
C	6.0	-0.0034950813	0.1307579819	0.0000000000
C	6.0	1.4130780499	-0.4966619319	0.0000000000
H	1.0	1.3889520490	-1.5900082468	0.0000000000
H	1.0	1.9479920625	-0.1536380866	-0.8887284611
H	1.0	1.9479920625	-0.1536380866	0.8887284611
N	7.0	-1.1136168060	-0.8176232614	0.0000000000
H	1.0	-2.0488317451	-0.4437212802	0.0000000000
H	1.0	-0.9694814411	-1.8123625421	0.0000000000

E = -209.0588795619 a.u.

ZPE correction = 0.079381 a.u.

H = -208.9749926 a.u.

0 imaginary frequencies

Table S89. Delocalized $\text{NH}_2\text{COCH}_2^-$

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.1252421666	1.3261363714	0.0000000000
C	6.0	0.0989263382	0.0750340688	0.0000000000
C	6.0	1.3288830390	-0.5895920370	0.0000000000
H	1.0	2.2495808732	-0.0137778769	0.0000000000
H	1.0	1.3986455847	-1.6769274715	0.0000000000
N	7.0	-1.0764580811	-0.7450727239	0.0000000000
H	1.0	-1.9724292135	-0.2838493499	0.0000000000
H	1.0	-1.0353434149	-1.7536209996	0.0000000000

E = -208.4919017363 a.u.

ZPE correction = 0.0581998 a.u.

H = -208.4282587 a.u.

0 imaginary frequencies

Table S90. Localized $\text{NH}_2\text{COCH}_2^-$

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.1204481132	1.3289919415	0.0000000000
C	6.0	0.0712370538	0.1337227785	0.0000000000
C	6.0	1.3906624438	-0.6117498192	0.0000000000
H	1.0	2.2974836365	-0.0210003473	0.0000000000
H	1.0	1.4096973881	-1.6949383954	0.0000000000
N	7.0	-1.1258998592	-0.7408433582	0.0000000000
H	1.0	-2.0381125410	-0.3154924816	0.0000000000
H	1.0	-1.0180570496	-1.7403603369	0.0000000000

E = -208.4001697985 a.u.

ZPE correction = 0.0681611 a.u.

H = -208.3274893 a.u.

0 imaginary frequencies

Table S91. Delocalized CH_3COOH

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.2552745401	1.3150770461	0.0000000000
C	6.0	0.0159775747	0.1330442565	0.0000000000
C	6.0	1.3990174644	-0.4638993984	0.0000000000
H	1.0	2.1463919862	0.3312207724	0.0000000000
H	1.0	1.5313474846	-1.0999725098	-0.8825382396
H	1.0	1.5313474846	-1.0999725098	0.8825382396
O	8.0	-0.9447125233	-0.8308595388	0.0000000000
H	1.0	-1.8064120186	-0.3721677582	0.0000000000

E = -228.9774346276 a.u.

ZPE correction = 0.0617808 a.u.

H = -228.9109629 a.u.

0 imaginary frequencies

Table S92. Localized CH₃COOH

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.2481426995	1.3343312710	0.0000000000
C	6.0	0.0268607627	0.1752071034	0.0000000000
C	6.0	1.4226293904	-0.4697052294	0.0000000000
H	1.0	2.1795637743	0.3174890906	0.0000000000
H	1.0	1.5363090359	-1.0949052780	-0.8881005303
H	1.0	1.5363090359	-1.0949052780	0.8881005303
O	8.0	-0.9890423164	-0.8567347360	0.0000000000
H	1.0	-1.8468040708	-0.3983065837	0.0000000000

E = -228.9368684139 a.u.

ZPE correction = 0.06502528 a.u.

H = -228.8673545 a.u.

0 imaginary frequencies

Table S93. Delocalized ⁻CH₂COOH

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.1742526183	1.3232442217	0.0000000000
C	6.0	0.0861358220	0.0858495819	0.0000000000
C	6.0	1.2890713025	-0.5943981871	0.0000000000
H	1.0	2.2191897598	-0.0338801337	0.0000000000
H	1.0	1.3253064489	-1.6797019597	0.0000000000
O	8.0	-1.0765914373	-0.7613876522	0.0000000000
H	1.0	-1.7900738537	-0.1011503053	0.0000000000

E = -228.3771789232 a.u.

ZPE correction = 0.0475105 a.u.

H = -228.3245128 a.u.

0 imaginary frequencies

Table S94. Localized ⁻CH₂COOH

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.1672816718	1.3198349910	0.0000000000
C	6.0	0.0608844053	0.1390365284	0.0000000000
C	6.0	1.3613473284	-0.6179165238	0.0000000000
H	1.0	2.2706733267	-0.0321183778	0.0000000000
H	1.0	1.3454073827	-1.6975232427	0.0000000000
O	8.0	-1.1272187235	-0.7523807037	0.0000000000
H	1.0	-1.8650266239	-0.1203571059	0.0000000000

E = -228.2818329505 a.u.

ZPE correction = 0.0538732 a.u.

H = -228.2234313 a.u.

0 imaginary frequencies

Table S95. Delocalized CH₃COF

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.0932064900	1.3738432516	0.0001233650
C	6.0	0.0001269161	0.1872410742	0.0000076618
C	6.0	-1.0756776915	-0.8559676739	-0.0000100733
H	1.0	-2.0532944858	-0.3722245499	-0.0000920380
H	1.0	-0.9700357180	-1.4956843086	0.8832601487
H	1.0	-0.9699355065	-1.4958205770	-0.8831645864
F	9.0	1.2445929756	-0.4013612163	-0.0001244778

E = -252.9905148632 a.u.

ZPE correction = 0.04863376 a.u.

H = -252.9372814 a.u.

0 imaginary frequencies

Table S96. Localized CH₃COF

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	0.0840608994	1.3536887290	0.0001847457
C	6.0	0.1156857807	0.1784996829	0.0000420780
C	6.0	1.2905217972	-0.8069391304	0.0000973967
H	1.0	2.2259757457	-0.2430090867	-0.0002831174
H	1.0	1.2364039771	-1.4375560777	-0.8892604789
H	1.0	1.2365383399	-1.4372409711	0.8896022405
F	9.0	-1.1252534911	-0.5631304572	-0.0003828646

E = -252.9603672697 a.u.

ZPE correction = 0.05013458 a.u.

H = -252.9057266 a.u.

0 imaginary frequencies

Table S97. Delocalized ⁻CH₂COF

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.8310486129	1.0929075841	0.0000000000
C	6.0	-0.0008721058	0.1815599815	0.0000000000
C	6.0	1.3732260049	0.0958996424	0.0000000000
H	1.0	1.9611252791	1.0089470193	0.0000000000
H	1.0	1.8766797202	-0.8640916184	0.0000000000
F	9.0	-0.6024132855	-1.1722716090	0.0000000000

FINAL R-B3LYP ENERGY IS -252.4088499539

ZPE Correction: 21.845188 KCAL/MOL

Enthalpy: add 24.953 kcal/mol to the above electronic energy

E = -252.4088499539 a.u.

ZPE correction = 0.0348130 a.u.

H = -252.3691338 a.u.

0 imaginary frequencies

Table S98. Localized $\bar{\text{C}}\text{H}_2\text{COF}$

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
O	8.0	-0.8464677955	1.0703100630	0.0000000000
C	6.0	-0.0547320398	0.1925941851	0.0000000000
C	6.0	1.4436295563	0.1021959881	0.0000000000
H	1.0	1.9937556735	1.0331841023	0.0000000000
H	1.0	1.9012107979	-0.8738152402	0.0000000000
F	9.0	-0.6606991924	-1.1815180984	0.0000000000
FINAL R-B3LYP ENERGY IS -252.3179971121				
ZPE Correction: 24.570474 KCAL/MOL				
Enthalpy: add 27.418 kcal/mol to the above electronic energy				
E = -252.3179971121 a.u.				
ZPE correction = 0.03915613 a.u.				
H = -252.2743031 a.u.				
0 imaginary frequencies				

Table S99. Delocalized $\text{H}_3\text{CCH}(\text{CH}_3)_2$

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
C	6.0	-0.0000005015	1.4605407530	-0.0930658400
H	1.0	-0.0000056793	1.5076191211	-1.1918334818
H	1.0	0.8868745102	2.0024542806	0.2603932996
H	1.0	-0.8868691456	2.0024579352	0.2604032593
C	6.0	-0.0000000992	0.0000004547	0.3827315966
H	1.0	0.0000000364	0.0000035212	1.4847949946
C	6.0	-1.2648632038	-0.7302729549	-0.0930673474
H	1.0	-1.3056344125	-0.7538104301	-1.1918360211
H	1.0	-2.1776101279	-0.2331727209	0.2603977102
H	1.0	-1.2907394229	-1.7692842675	0.2603990079
C	6.0	1.2648637492	-0.7302731351	-0.0930668965
H	1.0	1.3056374076	-0.7538063050	-1.1918351577
H	1.0	1.2907380437	-1.7692843116	0.2603991862
H	1.0	2.1776088452	-0.2331729407	0.2604026902
E = -158.3406036466 a.u.				
ZPE correction = 0.13256790 a.u.				
H = -158.2015438 a.u.				
0 imaginary frequencies				

Table S100. Delocalized $\text{H}_2\text{CCH}(\text{CH}_3)_2$

Atomic Symbol	Atomic Number	Coordinates (Angstroms)		
		X	Y	Z
C	6.0	0.0277209921	0.0879315817	-0.3697774001
H	1.0	0.0412799804	0.0293056939	-1.4770296173
C	6.0	0.8897386195	-1.1251830186	0.1189038528
H	1.0	0.9036275421	-1.1573365797	1.2203013008
H	1.0	1.9284269541	-1.0073308274	-0.2131886915
H	1.0	0.5150184107	-2.1055963884	-0.2507875236
C	6.0	-1.4312115149	-0.1565284941	0.0720140926
H	1.0	-1.4985037951	-0.1075444321	1.1709851495
H	1.0	-1.8109332776	-1.1443044436	-0.2397653054
H	1.0	-2.0824656260	0.6272165813	-0.3320942442
C	6.0	0.5112916119	1.4650216080	0.0476758485
H	1.0	1.5425325999	1.6596145001	-0.2980390958
H	1.0	0.4650325029	1.5910212187	1.1467656337

E = -157.6663124694 a.u.

ZPE correction = 0.11584208 a.u.

H = -157.5441308 a.u.

0 imaginary frequencies