

Coordinates of the optimized clusters at MP2/6-311++G\*\* (unless stated otherwise). The relative energies are based upon CCSD(T) calculations (aug-cc-pVTZ for n=1-6 and aug-cc-pVDZ n=7-9) and DFT zero point energies.

Frequencies computed using B3LYP+D/6-311++G\*\* (unscaled frequencies shown).

### **n=3**

Cluster 1: +0 kJ/mol

H	0.842113	0.304451	0.004478
O	-2.194382	-0.546489	-0.054221
H	-3.139667	-0.355606	-0.181207
O	2.027798	-0.414536	0.024391
H	2.186452	-1.202335	0.555893
H	2.608016	-0.463053	-0.743735
O	-0.019652	0.917125	-0.039218
H	-0.890674	0.428622	-0.021707
H	-0.002394	1.636335	0.606619

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3018.54	1567.673
3665.92	86.453
3787.58	271.400
3793.92	51.260
3886.08	231.352

Cluster 2: +51.4 kJ/mol

O	0.898572	1.009118	-0.105563
H	1.364343	1.199392	0.729094
H	-0.069312	1.034158	0.085845
O	0.920084	-1.013679	0.115088
H	1.393487	-1.188719	-0.718783
H	-0.045923	-1.058371	-0.081422
O	-1.600176	-0.021130	-0.000269
H	-2.192724	-0.149055	0.751587
H	-2.194593	0.098920	-0.751942

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3275.93	320.122
3430.31	906.158
3701.62	328.813
3714.51	242.918
3763.92	42.047
3843.84	190.034

Cluster 3: +53.3 kJ/mol (DFT optimized structure)

O	0.317485	-1.139756	0.342631
H	-0.510197	-0.540982	0.181231
H	0.474955	-1.204683	1.304227
O	1.620134	0.515152	0.148866
H	1.140881	0.981593	-0.560813
H	2.345969	0.024768	-0.279175
O	-1.542364	0.460030	-0.280840
H	-2.148280	0.215778	-0.993803
H	-2.041273	1.012945	0.335354

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3861.06	193.880
3775.67	44.192
3762.30	256.071
3697.89	122.492
3654.59	344.522

**n=4**

Cluster 1: +0 kJ/mol

H	0.978085	-0.134813	-0.194645
O	-1.078861	2.374987	0.150689
H	-0.921182	3.298123	-0.108165
O	0.022794	0.012434	-0.500741
H	-0.618502	-0.720440	-0.214534
H	-0.313521	0.913236	-0.279406
O	2.442811	-0.279324	0.168877
H	2.801104	-0.576100	1.011200
H	3.127148	-0.443308	-0.488027
O	-1.535997	-1.869304	0.138820
H	-1.962388	-2.417438	-0.527910
H	-2.073590	-1.944681	0.933466

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3903.10	225.499
3901.01	145.500
3808.94	48.822
3806.19	72.588
3679.72	66.804
3283.75	1203.415

Cluster 2: +8.5 kJ/mol

H	0.090302	-0.783858	-0.155589
O	-1.055920	-0.881496	0.576979
H	-1.841346	-0.332277	0.399809
H	-1.355187	-1.735711	0.903609
O	1.022003	-0.736049	-0.673857
H	0.926176	-0.592573	-1.623111
H	1.720838	-0.110492	-0.280484
O	-3.036000	0.923470	-0.145013
H	-3.961826	1.146793	0.042537
H	3.672073	0.398042	0.562710
O	2.836760	0.751714	0.240657
H	2.774665	1.652869	0.571873

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3904.20	194.800
3875.06	182.054
3818.08	170.615
3808.43	91.491
3689.32	53.581
3494.63	839.869

Cluster 3: +9.1 kJ/mol

H	-0.079663	-0.609074	0.310894
O	-0.929292	-0.288430	0.879347
H	-1.748714	0.004683	0.357782
H	-1.157902	-0.896151	1.592664
O	1.063335	-0.995028	-0.305006
H	1.083496	-1.535392	-1.100252
H	1.832024	-0.393948	-0.325215
O	-2.915320	0.548425	-0.435821
H	-3.231725	1.452144	-0.335467
H	-3.640253	0.049908	-0.825646
H	4.034962	0.972006	-0.301569
O	3.085688	0.885978	-0.118328

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3899.64	192.969
3872.86	170.504
3819.52	182.544
3804.79	78.397
3687.84	54.097
3463.05	883.186

Cluster 4: +53.8 kJ/mol

O	0.424466	-0.426115	0.855331
H	1.317072	-0.313162	0.393991
H	0.009384	-1.203985	0.446354
O	-0.492763	1.028262	-0.224019
H	-0.500102	1.614964	0.551678
H	-1.381312	0.547698	-0.233263
O	2.708819	-0.200459	-0.294900
H	3.539825	-0.419977	0.138086
H	2.936733	0.359078	-1.043426
O	-2.591921	-0.458509	-0.303079
H	-3.055110	-0.605166	-1.135532
H	-3.269249	-0.534014	0.378253

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3896.17	167.130
3861.55	170.630
3801.70	59.529
3779.49	36.266
3754.09	247.751
3504.48	900.166

**n=5**

Cluster 1: +0.0 kJ/mol

O	2.678051	1.249149	-0.721919
H	2.500970	1.901985	-1.405867
H	3.545096	1.472146	-0.369176
O	0.931741	-0.010936	0.684680
H	1.588376	0.504304	0.130159
H	0.857940	-0.964513	0.387854
O	-3.309356	0.066072	-0.812245
H	-4.256284	0.166614	-0.998755
H	0.019345	0.449086	0.736403
O	0.680291	-2.481544	0.016860
H	0.954567	-3.199101	0.596186
H	0.649836	-2.854869	-0.869063
O	-1.267027	1.178299	0.803745
H	-1.563999	1.592123	1.619149
H	-2.060395	0.873476	0.334211

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3908.03	320.436
3907.61	14.394
3877.89	158.115

3813.27	41.669
3810.96	61.635
3692.77	41.175
3584.66	630.289

Cluster 2: +4.3 kJ/mol

O	-2.636367	-1.822255	-0.068511
H	-2.631564	-2.397138	-0.840069
H	-3.111861	-2.303121	0.616267
O	-0.908633	-0.031534	0.504612
H	-1.570903	-0.748845	0.256639
H	-1.204821	0.883972	0.212546
O	1.401092	-0.766252	-0.334451
H	2.313146	-0.422997	-0.140572
H	0.024538	-0.257972	0.194323
O	-1.595070	2.341946	-0.151389
H	-1.849836	2.995707	0.507096
H	-1.958002	2.650933	-0.986945
O	3.872726	0.141534	0.065227
H	4.260885	0.533045	0.852536
H	4.612192	-0.233835	-0.421644

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3911.76	160.858
3906.67	196.059
3904.51	136.178
3812.76	45.542
3810.67	47.537
3808.79	68.342

Cluster 3: +8.5 kJ/mol

O	-0.583870	-1.799128	-0.199256
H	-1.446812	-1.423922	0.036250
H	-0.737937	-2.665201	-0.587180
O	-2.686628	0.000135	0.548205
H	-3.546841	0.000145	0.112380
H	-2.905941	0.000209	1.487547
O	3.276060	0.000302	0.731090
H	4.221210	-0.001130	0.506722
O	-0.583694	1.799105	-0.199475
H	-1.446686	1.424044	0.036070
H	-0.737621	2.665195	-0.587416
O	1.053419	-0.000123	-0.825526
H	0.472268	0.811805	-0.615872
H	1.880160	-0.000121	-0.288456
H	0.472192	-0.811969	-0.615786

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3876.59	84.749
3873.83	284.073
3861.40	148.208
3775.54	30.848
3680.66	59.132
3630.47	649.411
3600.86	332.642

Cluster 4: +46.0 kJ/mol

O	-1.279200	1.867399	-0.021969
H	-1.662762	2.390955	0.692067
H	-1.102971	2.514684	-0.715006
O	2.842331	0.206427	-0.529017
H	3.107917	-0.505584	-1.119387
H	3.663074	0.600513	-0.216782
O	-2.244858	-0.794180	-0.391964
H	-2.319309	0.162949	-0.503071
H	-2.933416	-1.204507	-0.923465
O	0.091435	-1.651567	0.118374
H	-0.860938	-1.362752	-0.100904
H	0.067938	-2.015519	1.019749
O	0.668022	0.125134	0.920017
H	1.504278	0.146377	0.371595
H	0.038043	0.764335	0.514654

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3898.23	151.363
3884.57	203.634
3862.34	158.163
3803.13	50.054
3776.04	32.566
3754.22	148.970
3717.52	262.598

**n=6**

Cluster 1: +0.0 kJ/mol

O	-4.137126	0.692907	-0.558769
H	-4.533490	1.370518	-1.113687
H	-4.864309	0.111409	-0.320134
O	-0.258484	-2.807134	-0.034286
H	0.019204	-3.512041	0.558529

H	-0.293566	-3.203713	-0.909652
O	1.976500	0.722089	-0.923285
H	2.881303	0.818290	-0.586817
H	0.886041	0.124599	-0.043331
O	-1.841667	1.079976	0.814029
H	-0.664797	0.225826	0.648242
H	-2.051954	1.466840	1.667918
O	0.200259	-0.320721	0.552807
H	1.843045	1.432531	-1.556011
H	0.033596	-1.265783	0.286109
O	4.549431	0.723268	0.292207
H	-2.691728	0.940924	0.347604
H	5.435287	1.109076	0.207250

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3913.24	159.678
3909.60	134.291
3887.80	134.531
3884.12	131.420
3815.52	45.583
3811.98	37.847
3699.88	33.810
3611.53	584.508
3418.58	967.678

Cluster 2: +1.3 kJ/mol

O	4.538937	-0.000601	0.448547
H	5.093159	0.763449	0.629115
H	5.091173	-0.764131	0.637181
O	-0.252456	-1.874898	-0.331277
H	-0.193124	-2.704697	-0.813090
H	0.648130	-1.524756	-0.256042
O	-3.959091	0.028726	0.895412
H	-4.866509	-0.015141	0.580142
H	-2.683614	0.008486	-0.031352
O	-0.247805	1.878832	-0.352955
H	-1.325316	0.819243	-0.570400
H	-0.189264	2.705943	-0.839420
O	-1.918230	0.002920	-0.675632
H	-4.003099	-0.038165	1.853387
H	-1.328018	-0.813645	-0.561485
O	1.890792	0.001124	-0.044194
H	0.652699	1.529315	-0.275115
H	2.860912	0.000744	0.151088

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3913.52	167.161
3912.70	150.100

3879.23	93.39
3876.63	240.503
3815.91	48.103
3813.89	53.783
3647.54	483.501
3617.10	310.371

Cluster 3: +1.6 kJ/mol

O	-2.056255	1.838148	-1.502630
H	-2.399313	1.839059	-2.400852
H	-2.549230	2.529203	-1.051264
O	2.009112	1.880607	1.429530
H	2.295248	1.975909	2.342863
H	2.444345	2.590000	0.948030
O	-1.096763	-0.402913	-0.343581
H	-1.790846	-0.838919	0.173659
H	0.162372	-0.374255	0.132689
O	2.907561	-1.550579	-1.085102
H	1.808022	-0.843698	-0.128785
H	3.426044	-2.311410	-0.806918
O	1.172353	-0.412706	0.500594
H	-1.487663	0.402107	-0.742880
H	1.519505	0.462191	0.816075
O	-3.285146	-1.495718	1.145306
H	2.887611	-1.590014	-2.045571
H	-3.582424	-2.344916	1.507467

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3910.95	236.719
3910.32	76.333
3908.39	120.766
3813.55	25.932
3812.64	57.785
3811.52	40.301
3698.50	18.717
3638.26	690.074

Cluster 4: +42.0 kJ/mol (DFT optimized structure)

O	-2.616617	-1.477627	-0.620481
H	-2.685542	-1.322433	-1.568175
H	-3.370475	-2.015131	-0.355669
O	2.625924	0.152677	-0.743836
H	2.964741	-0.099906	-1.612674
H	3.239050	0.815484	-0.401038
O	1.395313	-1.838663	0.813719
H	2.138776	-1.361516	0.413942
H	1.735657	-2.468803	1.456733

O	-0.109226	0.676397	-0.819177
H	-0.335790	1.521360	-0.326699
H	0.864920	0.540125	-0.739454
O	-0.761611	-0.400743	0.880793
H	0.041836	-1.013081	0.899675
H	-1.467385	-0.833367	0.310806
O	-0.667081	2.822295	0.576383
H	-1.143669	2.679109	1.401845
H	-0.929931	3.687204	0.242404

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3918.43	133.544
3891.36	180.938
3871.71	149.730
3817.73	44.235
3809.30	40.410
3783.88	32.932
3714.51	265.566
3434.48	997.402

**n=7**

Cluster 1: +0.0 kJ/mol

O	-2.059100	3.804610	0.841000
H	-1.688087	4.369788	1.523636
H	-2.957799	4.120444	0.714489
O	-0.766847	2.169570	-0.897688
H	-1.209058	2.781496	-0.275894
H	-0.354089	2.716435	-1.570469
O	-1.455336	-1.964101	-0.845738
H	-1.967554	-2.472374	-0.198383
H	-0.531311	-0.793520	-0.422237
O	2.487199	-0.456055	-0.834401
H	1.054517	-0.257837	-0.421315
H	3.214072	-0.466083	-0.180123
O	0.099683	-0.066814	-0.128791
H	-2.001250	-1.933669	-1.636173
H	-0.216892	0.847871	-0.442289
O	-3.172503	-3.462482	0.903244
H	2.764912	-1.023299	-1.557689
H	-3.123641	-4.085487	1.644669
O	4.490481	-0.405411	0.997835
H	4.750860	-1.089134	1.620565
H	5.236104	0.199783	0.963571

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3918.48	136.330
3917.67	128.953

3885.80	162.688
3885.34	69.436
3876.77	129.546
3818.90	34.742
3817.65	34.497
3700.56	29.643
3631.73	540.714
3451.24	1002.109
3444.08	753.301

Cluster 2: +0.2 kJ/mol

O	-1.853049	-0.531436	-1.883200
H	-2.428090	-0.840251	-2.588432
H	-1.403324	-1.304037	-1.507738
O	-0.321856	-2.019769	-0.025077
H	-0.033652	-2.937812	-0.048098
H	-1.445999	-1.362903	1.435123
O	4.425896	-0.145509	-0.019113
H	5.025399	0.500962	-0.401709
H	4.992744	-0.823544	0.358265
O	-2.195373	1.134505	0.003175
H	-2.163046	0.542401	-0.814996
H	-1.346979	1.687554	0.021740
O	0.032818	2.345116	-0.023381
H	0.793695	1.753973	0.075998
H	0.266348	3.186857	0.376985
O	-1.904281	-0.607735	1.836254
H	-2.185134	0.509811	0.795483
H	-2.511332	-0.953526	2.496185
O	1.729644	0.022342	0.066927
H	0.499654	-1.502895	0.005250
H	2.716529	-0.045544	0.043994

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3909.69	150.761
3892.67	173.775
3884.66	154.507
3881.85	187.192
3857.54	136.467
3811.34	52.203
3857.54	136.467
3811.34	52.203
3654.41	348.624
3637.28	565.221
3596.12	350.431
3563.38	463.977

Cluster 3: +2.9 kJ/mol

O	2.774229	-0.692295	0.728248
H	3.714400	-0.838139	0.865751
H	2.096594	0.512176	0.106813
O	1.550568	1.261815	-0.309962
H	1.037674	0.893061	-1.077314
H	0.864439	1.630256	0.358742
O	0.431993	-1.967563	-0.254759
H	2.362771	-1.552213	0.573889
H	-0.410985	-2.117946	0.241456
O	-0.267319	2.023959	1.232549
H	-1.141059	1.804413	0.864015
H	-0.339236	2.876839	1.670483
O	-1.920797	-1.756152	0.953995
H	-2.323828	-0.899219	0.764970
H	-2.393552	-2.129280	1.701598
O	-0.070710	0.097609	-2.041741
H	-0.003316	0.106587	-3.003041
H	0.031899	-0.832190	-1.770677
O	-2.310188	0.871570	-0.259271
H	-3.164778	1.225017	-0.527784
H	-1.846951	0.688426	-1.089791

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3884.79	157.937
3883.86	222.676
3872.95	169.294
3852.72	150.174
3838.23	147.791
3715.46	194.690
3656.59	406.383
3538.18	615.972

Cluster 4: +29.5 kJ/mol (DFT optimized structure)

O	-1.120077	-0.260452	0.836134
H	-2.047518	-0.410563	0.473563
H	-0.953215	0.744480	0.886177
O	-3.479638	-0.757994	-0.161508
H	-3.637504	-0.665755	-1.107318
H	-4.336159	-0.739521	0.278885
O	-0.387978	-0.474269	-1.147461
H	0.153273	-1.219153	-0.785151
H	0.227663	0.318461	-1.172789
O	2.967780	-0.057811	0.361530
H	2.591691	-0.949410	0.432249
H	3.895304	-0.097493	0.613679

O	1.365370	1.521971	-1.013282
H	2.117636	1.060558	-0.562020
H	1.707062	1.963638	-1.798828
O	1.090956	-2.215332	0.336761
H	1.254936	-3.154756	0.186839
H	0.544952	-2.149494	1.132501
O	-0.559663	2.241403	0.782424
H	-0.513901	2.873988	1.506186
H	0.235102	2.336162	0.224889

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3913.80	141.920
3890.04	176.030
3882.19	145.601
3870.28	145.090
3858.46	133.692
3814.29	45.887
3774.62	20.033
3696.88	332.629
3618.39	353.347

**n=8**

Cluster 1: +0.0 kJ/mol

O	-2.697763	0.279511	-1.540445
H	-3.476092	0.423741	-2.085189
H	-2.145612	1.248124	-0.475224
O	0.633122	-1.957084	-0.481247
H	-1.182971	-2.083467	-0.211884
H	1.249305	-1.210277	-0.638053
O	-1.722847	1.710918	0.318045
H	-0.749044	1.921404	0.122071
H	-1.802544	1.065855	1.091507
O	-2.133240	-1.988865	-0.019082
H	-2.735879	-0.634609	-1.211608
H	-2.482298	-2.885237	-0.046296
O	-1.927714	-0.135144	2.054843
H	-2.147286	-0.953150	1.577358
H	-2.420664	-0.142619	2.879698
O	2.437422	0.202804	-0.876052
H	3.226434	0.021180	-0.323196
H	2.784953	0.274044	-1.771335
O	0.685064	2.232440	-0.227990
H	1.374834	1.568455	-0.419781
H	1.127512	3.050068	0.011905
O	4.576743	-0.379930	0.700278
H	5.280156	0.202682	0.999116
H	4.917528	-1.269194	0.830602

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3916.18	140.528
3889.44	140.677
3880.41	137.713
3875.95	161.713
3854.89	117.014
3842.48	97.046
3818.34	43.170
3579.12	572.098
3528.04	517.562
3491.52	476.631
3457.35	781.537

Cluster 2: +3.7 kJ/mol

O	-0.441394	1.343010	-1.386338
H	-0.696743	-0.518919	-1.865930
H	-1.299314	1.584133	-0.949958
O	0.049355	-0.196107	2.330439
H	-0.735313	-0.625145	1.941712
H	0.034154	-0.372851	3.274823
O	1.896933	-1.836653	-0.844495
H	2.113896	-0.784231	0.249658
H	2.360275	-2.672594	-0.939947
O	-0.752152	-1.469360	-1.664879
H	-1.152035	-1.865127	-2.446661
H	1.008495	-1.940296	-1.225204
O	2.158140	-0.042442	0.933304
H	2.170102	0.853551	0.463888
H	1.344580	-0.105124	1.534865
O	-2.064743	-1.207745	0.845350
H	-2.662871	-1.908298	1.124438
H	-1.730099	-1.494578	-0.022697
O	-2.715641	1.469730	-0.032010
H	-3.221253	2.141056	0.432524
H	-2.784579	0.659069	0.489681
O	2.018379	2.194117	-0.258366
H	2.717684	2.774953	-0.569518
H	1.283393	2.256295	-0.884141

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3887.09	175.873
3881.37	161.534
3862.03	130.499
3852.65	145.418
3848.01	124.649
3776.27	167.675
3766.50	167.403

3561.21	306.488
3546.46	891.193
3488.25	1040.013
3458.09	710.167
3424.85	740.963

Cluster 3: +18.2 kJ/mol

O	0.686008	1.711850	1.220965
H	0.902905	0.964467	1.836938
H	-1.099192	1.851049	0.820127
O	1.849918	-1.586529	-0.308670
H	2.558857	-2.200193	-0.527160
H	2.124706	-0.738837	-0.699430
O	-1.828423	1.599487	0.213677
H	-2.229977	0.725818	0.548231
H	-1.364571	1.354691	-0.694661
O	2.085551	1.107900	-1.222476
H	2.033549	1.667673	-0.434500
H	2.783876	1.497189	-1.760045
O	-0.688263	0.834724	-1.849211
H	0.266240	1.009464	-1.883913
H	-0.773027	-0.133818	-1.869181
O	1.085853	-0.666129	2.285926
H	1.488953	-1.216510	1.599366
H	1.356855	-1.037427	3.129359
O	-0.852765	-1.876303	-1.075779
H	-1.050867	-2.656011	-1.604718
H	0.073170	-1.989813	-0.794075
O	-2.556300	-0.725108	0.865822
H	-2.107573	-1.359682	0.282163
H	-3.427512	-1.078787	1.064897

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3891.34	170.656
3859.05	94.704
3852.82	60.416
3852.09	234.137
3848.51	110.277
3770.36	159.562
3710.38	391.869
3673.38	319.518
3601.38	422.459
3492.82	653.616
3455.81	917.188
3396.03	549.854

Cluster 4: +35.5 kJ/mol (DFT optimized structure)

O	-1.792107	-1.414350	-0.686234
H	-1.247939	-1.003332	-1.423093
H	-2.389280	-2.071836	-1.061405
O	-0.333403	2.284329	-0.736177
H	-1.096812	1.975432	-0.207650
H	-0.542319	3.166235	-1.065451
O	0.123612	-0.219293	2.088817
H	-0.743487	0.120270	1.737418
H	0.820200	0.335447	1.646238
O	1.797258	1.382001	0.676606
H	2.394197	1.995025	1.121868
H	1.150309	1.910159	0.153105
O	-2.063801	0.760053	0.834133
H	-2.277765	-0.016163	0.265343
H	-2.862918	1.013507	1.311534
O	-0.118223	-0.161572	-2.221243
H	-0.142720	0.783995	-2.000880
H	0.780229	-0.463813	-2.015074
O	2.161644	-0.967901	-0.657924
H	2.987333	-1.421337	-0.865489
H	2.376937	-0.101017	-0.259593
O	0.261940	-1.993180	0.928834
H	1.026181	-1.688732	0.359791
H	-0.564842	-1.869212	0.377483

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3853.38	60.657
3851.11	195.362
3850.69	177.737
3845.42	131.411
3843.58	134.440
3749.54	491.741
3680.28	190.631
3576.12	423.450
3565.72	503.530
3445.84	770.280
3419.96	3419.96

**n=9**

Cluster 1: +0.0 kJ/mol

O	0.912155	1.864102	1.369670
H	1.266465	2.496327	2.004086
H	1.655178	1.664159	0.761982
O	0.379823	0.541629	-2.005254

H	-0.354428	1.132620	-1.796974
H	-0.000128	-0.328010	-2.169259
O	-0.040825	-0.556979	2.381527
H	0.363840	0.292633	2.089355
H	-1.050085	-1.266692	1.322311
O	-0.040366	-2.347116	-1.225840
H	0.820991	-2.259455	-0.761157
H	-0.036943	-3.198631	-1.674660
O	-1.647587	-1.640895	0.611848
H	-1.068851	-2.001180	-0.139711
H	-2.239529	-0.886389	0.258820
O	2.578595	0.887459	-0.549533
H	3.351277	1.249764	-0.993444
H	1.879497	0.807060	-1.236028
O	-1.243904	2.363724	-0.407884
H	-1.449681	3.289603	-0.569623
H	-0.548880	2.368527	0.274544
O	1.925246	-1.622904	0.419229
H	2.544039	-2.146414	0.936338
H	2.418922	-0.834382	0.134187
O	-2.979870	0.271956	-0.311538
H	-2.526514	1.137368	-0.304711
H	-3.916491	0.428235	-0.163223

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3882.50	154.738
3861.08	96.349
3859.03	129.256
3854.62	151.217
3851.14	168.351
3849.91	106.927
3755.28	559.685
3660.38	217.824
3532.94	719.969
3520.00	283.135
3468.35	730.366

Cluster 2: +0.3 kJ/mol

O	0.227224	1.726233	0.084280
H	0.152575	0.441674	1.531135
H	-0.574272	1.788288	-0.494567
O	-2.024555	1.473618	-1.369091
H	-2.457566	2.073720	-1.982928
H	-2.691933	1.242032	-0.689480
O	-0.774064	-1.104757	-1.559899
H	-1.248501	-0.293669	-1.790776
H	-1.273818	-1.493424	-0.826702
O	0.427234	-0.394179	1.949975

H	0.499733	-0.194902	2.890314
H	1.877863	-0.710286	1.097138
O	-1.864836	-1.877617	0.959682
H	-2.105372	-2.754616	1.273918
H	-1.102906	-1.608047	1.494421
O	-3.352250	0.513966	0.755387
H	-4.245776	0.601866	1.096507
H	-3.096289	-0.408267	0.910049
O	2.630604	-0.709103	0.454766
H	2.306989	-1.086399	-0.480884
H	2.914391	0.249683	0.346421
O	3.090104	1.801819	0.264533
H	2.301761	2.274870	-0.029459
H	3.851968	2.299787	-0.044742
O	1.806532	-1.464486	-1.717358
H	2.079140	-2.265317	-2.172999
H	0.820876	-1.392295	-1.770111

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3890.88	203.780
3885.98	127.120
3872.14	122.044
3865.28	169.447
3861.52	100.807
3839.13	124.696
3838.61	162.517
3703.64	245.830
3648.28	472.374
3595.70	158.955
3562.50	791.245
3443.98	1293.410

Cluster 3: 28.6 kJ/mol

O	-0.757858	-0.393683	2.008763
H	-0.000030	-1.017577	1.867547
H	-0.954590	-0.410327	2.951955
O	-2.502217	1.522733	-0.460582
H	-2.732781	0.581305	-0.494022
H	-3.248894	2.010040	-0.818856
O	-0.078306	-2.221774	-1.348982
H	-0.971014	-2.009864	-1.016032
H	-0.190476	-2.996034	-1.909541
O	0.004754	2.140844	-0.759902
H	-0.973478	1.958616	-0.654759
H	0.393575	1.356306	-1.218634
O	1.274313	0.071037	-1.966194
H	1.474015	0.179310	-2.902152
H	0.816384	-0.792785	-1.895833

O	-2.376927	-1.259554	-0.054119
H	-1.993209	-1.045770	0.818089
H	-3.130965	-1.828581	0.132649
O	1.271083	-1.830423	1.196046
H	1.060646	-2.235076	0.343946
H	2.065389	-1.304778	1.042031
O	2.743380	0.599041	0.370959
H	3.642011	0.925633	0.486304
H	2.628442	0.455155	-0.581528
O	0.483352	1.847330	1.193053
H	1.377648	1.492652	0.956616
H	-0.060689	1.054985	1.455065

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3890.05	165.250
3856.41	114.640
3854.55	170.403
3849.50	117.540
3848.87	124.115
3844.55	101.773
3742.61	546.839
3675.52	158.135
3607.38	479.367
3589.21	368.212
3464.61	706.544

Cluster 4: +28.6 kJ/mol (DFT optimized structure)

O	0.895737	-1.997836	0.574742
H	0.049133	-1.910978	1.051776
H	0.650278	-2.025696	-0.364705
O	-0.102926	-0.937022	-1.828745
H	-1.076756	-0.950024	-1.687913
H	0.057860	-1.033149	-2.773981
O	4.290315	0.448446	-0.576778
H	5.175401	0.155861	-0.332077
H	4.391799	1.284305	-1.045580
O	-2.682252	-0.833316	-0.938310
H	-2.876213	0.140674	-0.911354
H	-3.438039	-1.276577	-1.339012
O	-2.732593	1.779223	-0.628406
H	-3.352670	2.500915	-0.769078
H	-2.213411	1.968823	0.172721
O	2.187810	0.165085	0.988918
H	1.752504	-0.750673	0.822968
H	3.002775	0.265196	0.413338
O	1.021672	1.143452	-0.484641
H	0.361701	1.343405	0.229886

H	0.647842	0.379185	-1.000864
O	-1.621740	-1.187805	1.552957
H	-2.123044	-1.625288	2.250386
H	-2.166478	-1.212186	0.734257
O	-0.887632	1.453693	1.418418
H	-1.143220	0.543708	1.688821
H	-0.647732	1.938881	2.216107

Frequency (cm <sup>-1</sup> )	Intensity (km/mol)
3906.94	131.552
3888.08	161.743
3863.62	81.966
3860.01	119.614
3857.19	188.142
3854.55	87.353
3809.85	40.985
3718.12	403.929
3651.00	375.628
3625.26	358.068
3501.08	691.980
3467.95	802.562
3420.65	749.214