

Supporting Information for:

The Role of Anharmonicity in Hydrogen Bonded
Systems: The Case of Water Clusters

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Table S1: (H₂O)₂-Cs geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₂ C _s E[MP2/aVDZ]= -152.5302069 a.u.				Harmonic	Anharmonic
6				127	108
dimer				148	123
O	0.003386	0.000000	1.003796	151	124
H	0.765355	0.000000	0.411918	184	152
H	-0.764306	0.000000	0.406268	358	328
O	-2.467024	0.000000	-0.546582	639	514
H	-3.003066	-0.762684	-0.291013	1624	1581
H	-3.003066	0.762684	-0.291013	1643	1593
				3704	3554
				3796	3614
				3904	3720
				3925	3730

Table S2: (H₂O)₃-UUD geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₃ UUD E[MP2/aVDZ]= -228.8088005 a.u.				Harmonic	Anharmonic
9				156	128
3-UUD				172	144
H	-0.606830	-1.095067	0.024601	184	156
O	-1.478308	-0.659353	-0.057842	192	163
H	-2.036784	-1.080040	0.606958	233	177
O	1.310442	-0.949283	-0.050209	217	187
H	1.225115	0.024305	-0.001049	340	269
H	1.982185	-1.177920	0.603515	349	309
O	0.165110	1.606239	0.065606	441	360
H	-0.637413	1.048368	0.022543	568	433
H	0.079627	2.223414	-0.671526	664	586
				858	663
				1631	1592
				1634	1592
				1658	1593
				3575	3419
				3633	3464
				3641	3476
				3890	3700
				3894	3705
				3896	3708

Table S3: (H₂O)₄-S₄ geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₄ S ₄ E[MP2/aVDZ]= -305.0894329 a.u.				Harmonic	Anharmonic
12				49.958	45.75
4-S ₄				78.917	70.52
H	1.214527	2.216388	0.764022	209.193	185.25
O	1.023132	1.651613	0.005269	199.363	182.71
H	1.561716	-0.042153	0.004066	235.054	202.32
H	0.042152	1.561715	-0.004066	235.054	202.32
O	1.651615	-1.023133	-0.005269	252.417	221.88
H	2.216390	-1.214529	-0.764021	252.417	221.89
H	-0.042154	-1.561717	-0.004066	259.03	231.64
O	-1.023134	-1.651612	0.005269	288.225	252.95
H	-1.214531	-2.216387	0.764021	400.093	346.13
H	-1.561714	0.042152	0.004066	431.342	384.29
O	-1.651612	1.023132	-0.005269	447.982	398.04
H	-2.216387	1.214529	-0.764021	447.982	398.05
				748.337	694.58
				819.328	718.26
				819.329	718.27
				989.556	837.26
				1636.002	1595.31
				1651.185	1616.18
				1651.185	1616.18
				1681.262	1658.55
				3395.65	3249.86
				3486.321	3316.26
				3486.321	3316.28
				3523.551	3349.67
				3884.226	3692.17
				3885.528	3694.36
				3884.929	3694.37
				3884.929	3693.04

Table S4: (H₂O)₄-C_i geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₄ C _i E[MP2/aVDZ]= -305.0879996 a.u.				Harmonic	Anharmonic
12				29.112	31.038
4-ci				72.479	61.307
H	1.475188	-2.109404	0.673441	188.505	152.386
O	1.179124	-1.547316	-0.052830	203.743	179.53
H	1.547906	0.190137	0.010773	205.829	179.264
H	0.195931	-1.569030	-0.008950	240.037	209.142
O	1.552007	1.174235	0.054619	244.422	201.629
H	2.175745	1.451261	-0.627398	253.194	221.183
H	-0.195934	1.569029	0.008950	253.596	186.068
O	-1.179128	1.547318	0.052820	269.056	198.351
H	-1.475182	2.109406	-0.673453	385.66	351.967
H	-1.547909	-0.190137	-0.010781	402.176	348.066
O	-1.552011	-1.174236	-0.054610	485.384	443.256
H	-2.175741	-1.451248	0.627419	532.397	472.718
				663.276	634.864
				751.611	690.42
				829.298	700.425
				950.757	796.543
				1647.799	1604.8
				1649.005	1609.547
				1670.445	1627.668
				1680.001	1648.607
				3407.226	3268.108
				3486.798	3325.211
				3502.566	3339.072
				3529.946	3362.762
				3885.796	3695.285
				3886.6	3695.668
				3887.156	3691.255
				3887.539	3695.947

Table S5: (H₂O)₅-Cyclic geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₅ Cyclic E[MP2/aVDZ]= -381.3647344 a.u.				Harmonic	Anharmonic
15				23.483	19.545
5-cyclic				42.464	32.803
H	-0.972759	-1.684129	-0.084067	62.567	49.666
H	2.526700	-1.272626	0.968055	65.39	43.205
O	-0.204724	-2.296294	-0.177775	180.843	157.233
O	-2.266352	-0.528691	0.097773	193.115	137.635
H	-1.938217	0.400557	0.073642	200.039	147.745
H	-2.782296	-0.590427	0.910681	228.527	169.05
O	-1.185952	1.982012	-0.081836	235.965	205.269
H	-1.400137	2.719681	0.501615	240.589	206.84
H	-0.200693	1.928468	-0.070905	266.553	214.871
O	1.533013	1.731673	-0.048325	295.769	248.8
H	1.786163	0.783446	0.052976	299.557	260.721
H	2.007636	2.025999	-0.835448	302.504	266.5
O	2.125877	-0.922617	0.163277	410.579	375.47
H	1.306860	-1.457570	0.034316	429.896	375.877
H	-0.355647	-2.755632	-1.012842	453.163	400.484
				466.338	415.693
				512.63	468.686
				721.191	669.636
				787.07	716.823
				865.438	744.253
				881.125	769.378
				984.4	857.331
				1640.467	1598.058
				1652.082	1621.863
				1660.213	1636.922
				1681.013	1627.78
				1688.845	1602.13
				3353.788	3144.346
				3433.326	3275.333
				3442.183	3282.28
				3486.953	3313.942
				3494.005	3324.797
				3882.765	3689.378
				3884.968	3689.106
				3886.789	3694.497
				3886.981	3696.495
				3888.698	3699.29

Table S6: (H₂O)₆-Cyclic chair geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ Cyclic-chair E[MP2/aVDZ]= -457.6397288 a.u.				Harmonic	Anharmonic
18				30.111	14.673
6-cyclic-chair				30.111	14.726
H	-0.831866	2.210850	-0.030212	46.581	23.007
O	0.014001	2.706065	-0.141981	46.581	22.771
H	-0.109130	3.222499	-0.947495	53.624	37.388
H	1.498701	1.825830	0.030840	84.66	59.936
O	-2.336529	1.365123	0.142274	158.866	142.157
H	-2.845374	1.516451	0.947814	182.032	148.22
H	-2.330579	0.385009	0.030202	207.528	158.008
O	-2.350467	-1.340878	-0.142819	207.532	158.432
H	-1.498700	-1.825828	-0.030850	215.862	187.994
H	-2.735917	-1.705653	-0.948478	215.863	187.901
O	-0.014002	-2.706068	0.141981	267.289	201.522
H	0.109123	-3.222494	0.947501	267.292	201.952
H	0.831864	-2.210852	0.030215	295.106	238.832
O	2.336527	-1.365122	-0.142266	299.417	267.349
H	2.330579	-0.385006	-0.030202	299.418	267.318
H	2.845381	-1.516459	-0.947798	331.906	294.916
O	2.350470	1.340882	0.142805	418.876	373.305
H	2.735919	1.705653	0.948466	438.01	381.737
				438.013	381.548
				458.151	408.346
				465.082	423.499
				465.083	423.401
				781.972	710
				803.871	716.86
				803.873	716.873
				900.771	783.664
				900.775	782.382
				978.33	840.525
				1635.857	1579.52
				1648.262	1627.048
				1648.262	1621.4
				1678.842	1624.586
				1678.843	1624.577
				1696.931	1622.203
				3348.465	3145.832
				3420.613	3276.028
				3420.615	3276.04
				3475.999	3304.401
				3476	3304.399
				3494.118	3320.114
				3887.079	3695.808
				3887.151	3695.801
				3887.151	3695.699
				3887.585	3699.897
				3887.585	3699.797
				3887.996	3696.371

Table S7: (H₂O)₆-Book-1 geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ Book-1 E[MP2/aVDZ]= -457.6418357 a.u.				Harmonic	Anharmonic
18				27.784	16.954
6-book-1				38.786	29.743
H	3.587741	5.431675	4.279365	55.58	46.161
H	4.099179	5.244158	5.738394	69.498	55.939
H	6.184675	5.081186	4.706913	87.655	77.592
H	7.554866	5.712418	4.979451	155.642	125.967
H	7.139008	7.896633	4.985358	182.029	158.487
H	8.512417	7.867699	4.283524	189.464	157.992
H	4.957618	8.810819	5.597089	198.218	172.251
H	4.881584	7.418557	4.933387	227.824	198.432
H	3.803815	4.808027	8.033109	236.666	206.61
H	4.931421	4.005915	7.333809	254.05	208.726
H	6.909855	4.031200	6.465899	255.276	215.672
H	6.905003	2.684257	7.240083	279.262	247.545
O	4.293859	5.700184	4.879957	289.398	247.165
O	7.094090	4.847207	4.962753	297.991	264.35
O	8.032034	7.491761	5.031418	311.099	270.55
O	5.364980	8.271329	4.908550	387.276	347.533
O	6.606979	3.599541	7.305362	403.125	357.057
O	4.017277	4.363336	7.203678	442.628	410.865
				453.943	407.544
				480.956	437.979
				543.016	475.286
				616.587	521.773
				730.608	648.548
				754.782	666.495
				837.913	728.964
				858.437	753.348
				907.688	808.225
				1025.417	900.824
				1631.551	1614.821
				1644.984	1607.997
				1647.123	1614.034
				1666.651	1625.812
				1678.307	1635.642
				1707.409	1670.153
				3285.43	3068.04
				3362.287	3169.735
				3414.879	3265.397
				3515.719	3355.648
				3570.074	3397.803
				3586.175	3415.438
				3734.822	3546.317
				3877.443	3685.701
				3882.208	3691.765
				3884.865	3693.115
				3886.254	3693.712
				3888.919	3697.177

Table S8: (H₂O)₆-Cage geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ Cage E[MP2/aVDZ]= -457.6426191 a.u.				Harmonic	Anharmonic
18				45.07	32.093
6-cage				57.615	45.372
H	0.063746	1.370228	-0.535519	74.365	63.774
O	0.593274	1.729598	0.229481	98.837	86.396
H	0.508196	2.689491	0.179344	123.264	96.798
H	2.159040	0.826090	0.162036	149.371	123.754
H	-1.628481	0.235804	-1.244624	184.474	148.671
O	2.811279	0.098384	0.056408	197.565	133.566
H	1.683728	-1.219015	-0.321381	211.26	171.496
H	3.298495	0.077966	0.889701	224.525	199.508
O	0.851442	-1.722144	-0.484056	233.817	198.349
H	1.128737	-2.606198	-0.753349	243.556	210.998
H	-0.285241	-0.446030	-1.532575	244.769	217.693
H	-0.188665	-1.097262	1.091688	260.953	201.103
O	-0.755781	0.397638	-1.659951	287.883	257.516
O	-0.684248	-0.493866	1.675160	305.397	262.619
H	-2.247829	-0.249640	0.785869	387.678	350.781
H	-0.266370	0.366609	1.492462	403.029	359.416
O	-2.892720	0.022876	0.094390	431.297	394.262
H	-3.651893	-0.562557	0.198037	456.762	398.055
				473.176	422.689
				530.529	473.539
				563.87	457.095
				636.411	525.675
				692.193	582.996
				736.134	656.229
				800.473	697.038
				818.053	701.345
				879.1	752.889
				1011.608	889.284
				1638.827	1613.202
				1647.951	1598.668
				1660.551	1618.276
				1674.142	1621.972
				1681.586	1636.154
				1696.477	1653.73
				3224.341	2980.609
				3442.128	3298.695
				3483.361	3315.976
				3533.046	3348.784
				3590.729	3410.274
				3670.838	3490.487
				3723.936	3520.726
				3761.534	3555.326
				3877.668	3684.213
				3880.204	3691.726
				3883.441	3690.355
				3894.506	3708.601

Table S9: (H₂O)₆-Prism geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ Prism E[MP2/aVDZ]= -457.6430159 a.u.				Harmonic	Anharmonic
18				62.863	45.158
6-prism				70.995	56.732
H	0.280085	-1.115676	-1.505747	75.109	62.578
O	1.233799	-1.200715	-1.323362	88.293	60.929
H	1.541956	-0.278331	-1.281840	99.802	71.03
H	-0.441637	-0.685016	1.573766	146.494	113.207
O	-1.408814	-0.468633	1.450722	169.963	155.623
H	-1.851253	-0.760546	2.256739	175.017	150.095
H	1.288019	-1.285926	0.546403	212.202	183.105
O	1.213913	-0.927730	1.459038	222.945	198.351
H	1.611248	-0.048005	1.336866	237.83	206.345
H	-2.314717	-1.355258	-1.690243	247.886	221.089
O	-1.650089	-0.778247	-1.294237	280.032	245.043
H	-1.753027	-0.882003	-0.324695	288.271	256.298
H	-1.315577	1.367221	-0.914751	295.211	264.947
O	-0.976746	1.863882	-0.152405	359.327	298.119
H	-1.243438	1.290115	0.590232	368.823	317.683
H	0.792641	1.741734	-0.176619	426.906	371.215
O	1.734212	1.447372	-0.158826	429.806	364.518
H	2.256902	2.248508	-0.284693	467.712	403.243
				491.655	416.761
				539.367	480.621
				556.226	467.648
				620.964	525.49
				646.301	540.675
				691.826	566.087
				735.644	640.107
				848.193	788.543
				898.6	779.728
				1040.425	940.258
				1635.773	1606.005
				1648.623	1611.303
				1655.344	1605.427
				1673.696	1623.863
				1690.321	1653.755
				1709.327	1740.965
				3196.981	2949.949
				3437.538	3279.441
				3534.651	3303.495
				3565.241	3366.748
				3667.047	3487.273
				3677.388	3481.929
				3754.628	3546.137
				3771.545	3578.604
				3805.122	3604.428
				3879.817	3687.202
				3883.907	3692.713
				3885.128	3692.285

Table S10: (H₂O)₆-Book-2 geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ Book-2 E[MP2/aVDZ]= -457.6414447 a.u.				Harmonic	Anharmonic
18				23.148	2.588
6-book-2				30.76	19.265
O	2.305230	1.271784	-0.403092	40.5	37.999
H	3.223784	1.463814	-0.178001	68.645	46.964
H	2.286365	0.298477	-0.587624	85.795	68.629
O	2.025571	-1.399657	-0.678701	153.552	123.61
H	1.775147	-1.804813	-1.518038	190.23	165.967
H	1.242649	-1.534250	-0.085401	205.171	178.941
O	-0.089941	-1.445594	1.017708	210.101	182.116
H	-0.072179	-0.521941	1.323776	223.618	199.601
H	-0.930735	-1.500142	0.516594	237.071	207.952
O	-2.367388	-1.241556	-0.605451	251.524	221.758
H	-3.264516	-1.467065	-0.330597	261.723	225.28
H	-2.355823	-0.260300	-0.654295	269.755	230.683
O	-2.008184	1.505372	-0.534949	285.671	251.81
H	-1.750468	1.979067	-1.335618	290.529	261.119
H	-1.242086	1.602725	0.069499	298.742	238.775
O	0.162802	1.465119	1.220103	389.004	352.594
H	0.267342	2.075080	1.960340	408.911	343.277
H	1.014174	1.501505	0.715029	438.343	395.511
				454.005	419.054
				534.342	469.953
				569.3	510.973
				641.683	552.738
				735.916	658.229
				764.676	674.951
				809.39	682.591
				838.307	759.964
				873.898	764.836
				984.818	854.284
				1638.954	1610.144
				1651.162	1596.516
				1656.297	1597.282
				1673.822	1657.14
				1691.713	1591.74
				1702.181	1651.307
				3285.636	3012.266
				3368.044	3124.785
				3408.869	3249.66
				3501.846	3341.809
				3569.866	3398.507
				3583.246	3408.763
				3739.62	3549.213
				3880.092	3687.594
				3881.297	3692.73
				3881.709	3691.074
				3883.806	3691.242
				3886.533	3691.528

Table S11: (H₂O)₆-Bag geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ Bag E[MP2/aVDZ]= -457.6406749 a.u.				Harmonic	Anharmonic
18				34.52	19.143
6-bag				43.441	31.32
O	-1.019343	1.600534	-0.468309	52.14	41.607
H	-0.031108	1.700552	-0.379547	63.739	46.097
H	-1.327825	2.455286	-0.793754	80.113	60.845
O	-0.097581	-1.934622	0.494430	155.041	96.86
H	-0.531324	-1.349998	1.145244	174.66	137.822
H	-0.594348	-1.748932	-0.326266	185.945	157.03
O	1.634535	1.716180	-0.186563	194.017	165.697
H	1.952634	2.102384	0.639466	201.3	168.357
H	1.959619	0.779768	-0.155356	205.069	146.157
O	2.346927	-0.868300	0.051856	218.758	183.217
H	2.787546	-1.374963	-0.640749	245.5	215.611
H	1.489115	-1.339457	0.215377	285.615	254.277
O	-1.323517	0.196773	1.963586	288.876	257.572
H	-2.190946	0.206283	2.385829	314.605	285.37
H	-1.403622	0.795711	1.195308	322.694	267.99
O	-1.342826	-0.864363	-1.818698	388.466	347.655
H	-1.339402	0.052150	-1.475837	405.281	362.158
H	-2.236756	-1.008062	-2.151951	443.571	408.86
				484.817	417.319
				496.936	441.206
				557.555	518.588
				636.672	496.85
				663.871	560.178
				711.639	590.752
				776.378	696.028
				863.18	782.337
				948.345	837.053
				997.88	898.908
				1645.187	1597.598
				1648.32	1603.742
				1657.721	1610.457
				1674.334	1641.726
				1696.022	1670.427
				1699.205	1646.646
				3211.049	2992.082
				3311.609	3082.679
				3386.12	3171.372
				3585.022	3419.37
				3614.997	3441.465
				3637.066	3461.929
				3697.503	3496.235
				3872.081	3681.372
				3873.447	3685.329
				3886.013	3695.856
				3891.367	3700.597
				3894.538	3704.123

Table S12: (H₂O)₆-Cyclic boat-1 geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ cyclic-boat-1 E[MP2/aVDZ]= -457.63818 a.u.				Harmonic	Anharmonic
18				20.632	5.326
6-cyclic-boat-1				29.793	17.605
O	-0.964938	-2.122656	-0.415391	36.674	24.765
H	-1.160652	-2.908291	-0.939494	41.638	28.852
H	0.020007	-2.083012	-0.371327	45.019	6.897
O	1.753649	-1.961908	-0.326495	74.246	60.284
H	2.091172	-1.036763	-0.383746	168.773	142.763
H	2.209985	-2.338977	0.435549	197.07	142.454
O	2.667259	0.604895	-0.471102	199.348	138.665
H	2.174156	1.241812	0.097603	207.464	140.864
H	2.698781	1.018903	-1.341761	219.026	180.294
O	-2.289078	0.235629	-0.747605	224.92	191.747
H	-2.267440	0.461980	-1.685016	240.454	130.761
H	-1.814645	-0.626202	-0.681259	267.169	210.066
O	1.284203	2.253456	1.200608	268.854	176.138
H	1.492450	3.190094	1.298353	289.945	255.479
H	0.299201	2.213141	1.158437	299.053	263.03
O	-1.431881	2.122870	1.026545	320.224	283.156
H	-1.748791	1.446036	0.382684	412.288	366.754
H	-1.934270	1.945135	1.831000	416.294	369.825
				441.534	397.626
				457.205	419.658
				501.671	441.132
				504.502	465.801
				740.979	689.511
				757.24	674.255
				824.446	732.625
				874.557	760.472
				904.051	746.86
				960.929	801.559
				1640.725	1607.48
				1644.672	1610.356
				1657.483	1629.177
				1673.981	1622.035
				1684.891	1587.678
				1693.258	1614.259
				3353.965	3116.798
				3417.468	3264.902
				3428.51	3282.241
				3473.869	3307.755
				3485.114	3320.139
				3496.019	3329.18
				3884.526	3692.077
				3884.719	3693.035
				3888.955	3697.741
				3889.176	3698.464
				3890.025	3703.308
				3890.089	3700.526

Table S13: (H₂O)₆-Cyclic boat-2 geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₆ cyclic-boat-2 E[MP2/aVDZ]= -457.6379985 a.u.				Harmonic	Anharmonic
18				21.082	6.192
6-cyclic-boat-2				29.924	16.303
O	-1.038094	-2.228715	-0.562432	36.939	17.379
H	-1.339570	-2.751800	0.190588	41.381	15.693
H	-0.064309	-2.145562	-0.434192	44.09	3.551
O	1.640603	-1.893245	-0.179736	70.979	63.192
H	1.995123	-0.983505	-0.316871	169.645	143.261
H	2.316444	-2.482609	-0.534248	179.452	68.191
O	2.600126	0.644203	-0.487223	181.913	70.343
H	2.163344	1.300520	0.106904	194.051	117.251
H	2.622735	1.073810	-1.350603	218.406	189.601
O	-2.224278	0.218622	-0.776667	220.646	147.006
H	-2.194849	0.426655	-1.718131	230.091	195.415
H	-1.806698	-0.672992	-0.704780	259.364	203.019
O	1.360426	2.435788	1.154653	274.12	217.891
H	1.613419	2.364733	2.083356	286.24	246.945
H	0.383016	2.308201	1.152187	299.802	261.726
O	-1.327847	1.982967	1.104123	320.45	278.326
H	-1.658354	1.367475	0.408385	406.742	374.669
H	-1.995195	2.676393	1.164084	408.123	374.478
				434.615	398.621
				452.49	419.202
				518.71	460.948
				526.839	473.21
				744.265	660.36
				770.941	669.609
				794.93	692.04
				825.69	719.28
				918.2	775.608
				937.767	802.682
				1643.142	1601.187
				1651.868	1621.343
				1660.255	1625.841
				1675.376	1624.769
				1684.61	1569.055
				1695.072	1611.977
				3356.313	3098.671
				3413.577	3266.739
				3436.039	3285.357
				3476.064	3313.884
				3489.321	3321.488
				3500.481	3330.342
				3882.689	3691.082
				3882.759	3691.831
				3887.762	3696.95
				3888.161	3697.692
				3892.784	3704.907
				3892.794	3704.059

Table S14: (H₂O)₈-S4 geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₈ S4 E[MP2/aVDZ]=-610.2105722 a.u.				Harmonic	Anharmonic
24				69.203	54.706
8-S4				73.283	56.288
H	-1.348963	-0.813717	1.532407	74.274	63.439
O	-0.061639	-1.900221	1.365265	74.274	63.403
H	0.752336	-1.381895	1.517644	78.806	65.95
H	0.274391	-2.704981	-2.102680	108.537	93.55
O	2.002094	0.064076	1.476004	164.848	141.267
O	-2.002081	-0.064082	1.476021	165.971	139.435
H	-2.704981	-0.274413	2.102678	165.971	139.45
H	-2.141419	0.008498	-0.419807	174.654	149.77
H	-0.752321	1.381885	1.517657	189.989	166.653
O	0.061652	1.900213	1.365274	207.401	182.177
H	0.008499	2.141413	0.419821	207.892	183.401
H	1.348975	0.813710	1.532397	207.893	183.402
O	1.900213	-0.061646	-1.365275	276.159	252.326
O	-1.900224	0.061649	-1.365262	281.796	254.301
H	-1.381897	-0.752324	-1.517646	289.12	260.482
H	-0.274421	2.704997	-2.102653	292.352	268.364
O	0.064067	-2.002082	-1.476019	292.352	268.279
H	-0.008494	-2.141417	0.419811	305.42	278.815
H	0.813704	-1.348967	-1.532409	305.421	279.027
H	2.141414	-0.008498	-0.419823	317.162	292.318
H	2.705002	0.274410	2.102651	448.977	401.933
O	-0.064082	2.002090	-1.476006	454.833	404.75
H	-0.813716	1.348971	-1.532393	484.399	427.556
H	1.381891	0.752331	-1.517657	484.4	427.465
				505.023	459.581
				558.832	493.129
				558.832	493.222
				567.851	497.561
				624.251	533.533
				668.652	581.487
				690.335	594.01
				690.336	594.062
				727.534	616.114
				727.534	616.07
				741.89	626.016
				827.643	799.891
				975.564	879.393
				975.565	879.361
				1044.677	943.338
				1070.102	965.122
				1635.952	1596.657
				1642.906	1609.015
				1642.906	1609.105
				1657.515	1623.761
				1680.517	1704.929
				1690.188	1643.809
				1690.188	1643.747
				1714.779	1680.84
				3221.746	2963.902
				3246.884	2984.411
				3275.206	3028.786
				3275.208	3028.754
				3602.329	3422.353
				3608.037	3425.331
				3608.037	3425.318
				3618.664	3431.774
				3666.032	3463.437
				3693.072	3484.688
				3693.072	3484.659
				3711.541	3497.777
				3878.265	3685.044
				3878.288	3685.47
				3878.288	3685.333
				3878.364	3685.839

Table S15: (H₂O)₈-D2d geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₈ D2d E[MP2/aVDZ]= -610.2106012 a.u.				Harmonic	Anharmonic
24				70.989	57.224
8-D2d				74.529	64.419
H	2.146397	0.283150	0.351411	75.666	63.657
O	1.917663	0.261579	-1.330631	77.456	67.24
H	1.251793	0.950763	-1.520737	77.456	67.243
H	1.454428	-0.575482	-1.528721	109.549	96.907
O	-0.281248	2.066115	-1.343578	164.163	140.505
O	0.265747	-2.053960	-1.365122	170.915	148.549
O	2.067823	0.267528	1.343824	176.373	150.787
H	-1.471804	0.589098	-1.506726	176.373	150.743
H	-0.286745	2.145950	-0.351158	189.557	167.766
H	-0.401758	2.960443	-1.685082	207.596	184.984
H	0.382283	-2.945195	-1.715962	208.214	181.961
H	-1.269167	-0.937147	-1.514703	208.216	181.962
H	0.282627	-2.142658	-0.373583	271.075	248.922
H	2.962588	0.384533	1.685402	276.47	249.65
H	0.952647	-1.267224	1.506750	278.297	258.535
H	0.591052	1.456387	1.520988	283.471	257.351
O	0.263199	-1.931104	1.310733	283.471	257.351
H	-2.142197	-0.286335	0.373476	301.101	273.351
H	-0.935188	1.253715	1.528843	316.444	289.919
O	-0.248001	1.919354	1.330865	316.445	290.071
H	-0.573594	-1.469898	1.514602	440.545	403.433
O	-2.052239	-0.279577	1.365022	466.768	411.037
O	-1.932776	-0.249724	-1.310820	466.769	410.994
H	-2.943032	-0.399675	1.715786	512.882	461.802
				520.547	460.535
				534.87	482.809
				552.603	481.072
				552.605	481.002
				609.065	524.89
				690.977	593.83
				690.979	593.768
				699.833	609.797
				711.917	601.083
				711.918	601.072
				738.687	632.85
				849.116	798.26
				930.472	832.983
				1031.334	920.736
				1031.335	920.754
				1093.989	975.719
				1641.328	1621.979
				1641.328	1621.971
				1644.984	1609.169
				1652.018	1619.624
				1669.335	1632.65
				1669.335	1632.641
				1697.029	1638.164
				1712.623	1720.299
				3225.633	2966.365
				3250.208	3002.634
				3250.208	3002.636
				3309.627	3067.848
				3601.816	3421.523
				3601.817	3421.434
				3618.37	3432.094
				3620.303	3434.183
				3667.33	3466.507
				3668.089	3466.87
				3713.691	3502.059
				3713.693	3501.982
				3878.584	3686.861
				3878.584	3686.799
				3878.637	3686.276
				3878.71	3686.677

Table S16: (H₂O)₉-D2dDD geometry, harmonic and VPT2 fundamental frequencies

(H ₂ O) ₉ D2dDD E[MP2/aVDZ]= -686.4871616 a.u.				Harmonic	Anharmonic
27				44.991	23.742
9-D2dDD				57.695	34.869
H	-2.588062	0.410981	-0.043732	60.12	41.613
O	-2.424043	-1.268084	0.082306	68.373	54.912
H	-1.854987	-1.407021	0.864333	73.223	59.117
H	-1.858003	-1.534886	-0.668225	73.473	60.109
O	-0.450380	-1.161191	2.129009	79.054	63.239
O	-0.439747	-1.510473	-1.939160	107.829	92.669
O	-2.473271	1.398039	-0.114465	159.86	135.841
H	0.812753	-1.817580	0.903948	167.994	143.666
H	-0.373915	-0.168952	2.098685	168.999	146.174
H	-0.476926	-1.396937	3.064268	172.884	149.138
H	-0.433751	-1.877386	-2.831560	185.134	160.879
H	0.827071	-1.966347	-0.628332	200.837	177.561
H	-0.348657	-0.525289	-2.047874	206.683	179.993
H	-3.362827	1.769117	-0.155826	211.888	186.205
H	-1.109402	1.412133	-1.436340	249.636	170.827
H	-1.136384	1.643393	1.209676	268.719	246.593
O	-0.317621	1.164674	-1.951814	272.696	245.739
H	2.391698	1.263676	-0.069070	278.087	253.79
H	0.400983	1.747816	1.210113	286.02	256.551
O	-0.354217	1.490301	1.774595	293.435	260.906
H	0.428465	1.497786	-1.415258	302.211	272.627
O	1.709086	1.983298	-0.118801	304.255	271.782
O	1.407187	-2.021795	0.156152	316.995	289.427
H	2.204770	2.801206	-0.247852	326.187	296.79
O	3.317878	-0.152237	-0.069170	447.827	413.336
H	2.662905	-0.892808	0.033374	449.83	414.215
H	4.015288	-0.339163	0.570457	458.655	415.191
				495.474	451.479
				516.23	469.147
				519.243	474.496
				543.495	484.433
				561.477	482.799
				599.195	522.908
				623.189	543.691
				671.119	579.765
				697.78	596.475
				705.903	613.675
				711.077	612.463
				717.395	602.852
				751.114	647.068
				833.118	729.579
				887.73	778.241
				926.571	846.065
				975.922	879.909
				1031.154	932.249
				1076.008	952.841
				1640.825	1627.719
				1644.915	1610.515
				1650.971	1607.318
				1658.496	1608.126
				1666.133	1638.174
				1672.141	1640.358
				1689.513	1650.263

	1707.558	1658.948
	1720.898	1683.39
	3221.51	2967.587
	3242.06	2988.781
	3249.258	3010.057
	3304.902	3067.772
	3348.444	3102.794
	3593.662	3414.685
	3597.115	3417.931
	3614.736	3429.498
	3616.959	3430.474
	3658.228	3460.979
	3659.077	3461.287
	3708.475	3497.445
	3708.862	3497.182
	3876.665	3686.273
	3878.173	3686.049
	3878.299	3685.921
	3880.157	3687.105
	3885.346	3695.886

Table S17: H₂SO₄(H₂O) geometry, harmonic and VPT2 fundamental frequencies

H ₂ SO ₄ (H ₂ O) E[MP2/aVDZ]= -775.3458802 a.u.				Harmonic	Anharmonic
10				3887.781	3694.528
H2SO4-H2O				3733.235	3545.039
S	0.594190	-0.065769	0.143077	3722.734	3541.646
O	-0.214132	0.380971	1.295342	3172.862	2945.480
O	1.862273	-0.793093	0.274174	1620.165	1577.788
O	-0.334112	-0.921767	-0.868343	1453.450	1396.675
O	0.864057	1.318115	-0.711711	1330.499	1300.628
H	-1.277205	-0.613504	-0.717426	1172.736	1141.371
H	1.583553	1.115936	-1.338730	1138.873	1126.240
O	-2.688060	0.087604	-0.122458	855.957	831.166
H	-2.287680	0.396082	0.709225	819.075	736.895
H	-3.430800	-0.470822	0.143212	771.369	751.470
				526.735	477.687
				511.707	502.904
				497.648	487.206
				466.156	448.141
				396.599	372.399
				360.305	330.203
				328.152	296.560
				259.267	235.336
				224.939	204.486
				208.898	179.443
				137.960	118.165
				45.977	40.137

Table S18: H₂SO₄(H₂O)₂ geometry, harmonic and VPT2 fundamental frequencies

H ₂ SO ₄ (H ₂ O) ₂ E[MP2/aVDZ]= -851.6269964 a.u.				Harmonic	Anharmonic
13				3884.527	3691.217
H2SO4(H2O)2				3883.685	3690.883
S	0.000001	0.504634	-0.000002	3714.655	3525.088
O	-1.140821	1.219550	-0.606426	3713.239	3520.517
O	1.140821	1.219554	0.606419	3215.067	2983.631
O	-0.541711	-0.506215	1.148028	3197.540	2970.746
O	0.541713	-0.506221	-1.148027	1624.996	1581.114
H	-1.448275	-0.806066	0.844591	1623.617	1580.673
H	1.448277	-0.806070	-0.844588	1447.579	1394.481
O	-2.970177	-0.884504	0.091208	1382.478	1321.975
H	-3.164585	-1.590702	-0.539602	1276.065	1251.246
H	-2.819416	-0.092411	-0.454865	1132.028	1118.696
O	2.970179	-0.884504	-0.091204	875.745	828.584
H	3.164586	-1.590699	0.539610	851.220	768.089
H	2.819417	-0.092409	0.454865	841.460	770.290
				799.446	782.300
				555.162	483.167
				532.784	450.468
				514.718	506.623
				509.025	503.222
				490.017	480.415
				396.624	378.554
				358.798	340.215
				326.295	284.612
				313.603	284.533
				239.285	206.594
				236.115	187.627
				229.115	190.677
				218.636	200.765
				146.685	123.850