

Supporting Information for A Systematic Study on the Absorption Features of Interstellar Ices in Presence of Impurities

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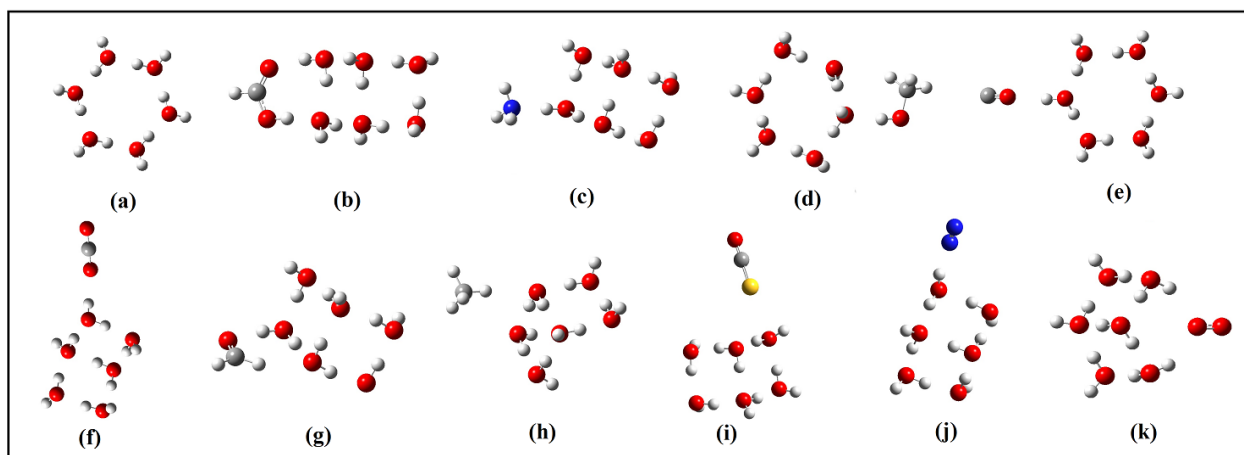
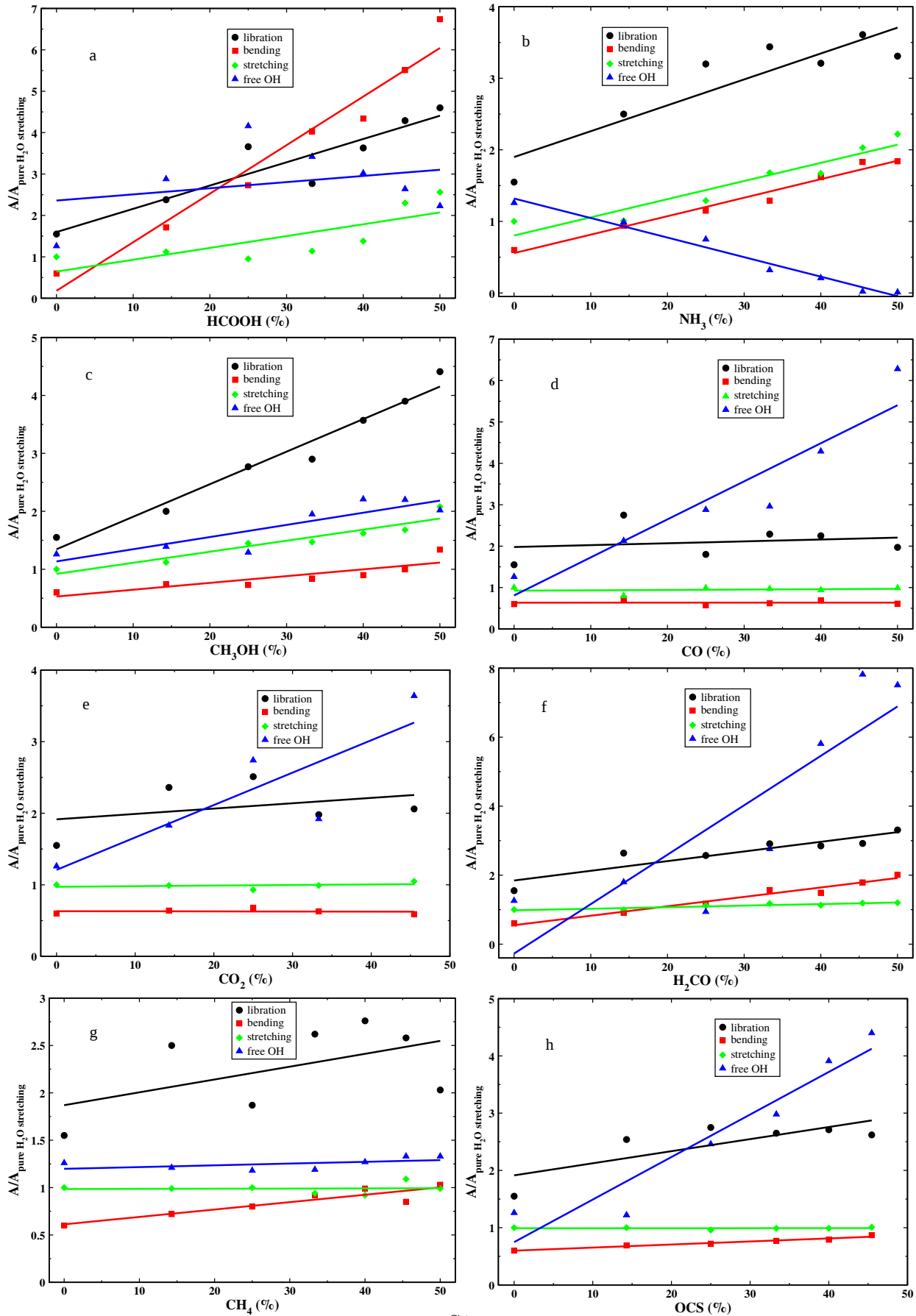


Figure S1: Optimized structures of (a) pure water, (b) $\text{H}_2\text{O} - \text{HCOOH}$, (c) $\text{H}_2\text{O} - \text{NH}_3$, (d) $\text{H}_2\text{O} - \text{CH}_3\text{OH}$, (e) $\text{H}_2\text{O} - \text{CO}$, (f) $\text{H}_2\text{O} - \text{CO}_2$, (g) $\text{H}_2\text{O} - \text{H}_2\text{CO}$, (h) $\text{H}_2\text{O} - \text{CH}_4$, (i) $\text{H}_2\text{O} - \text{OCS}$, (j) $\text{H}_2\text{O} - \text{N}_2$, and (k) $\text{H}_2\text{O} - \text{O}_2$ clusters with a 6 : 1 concentration ratio.



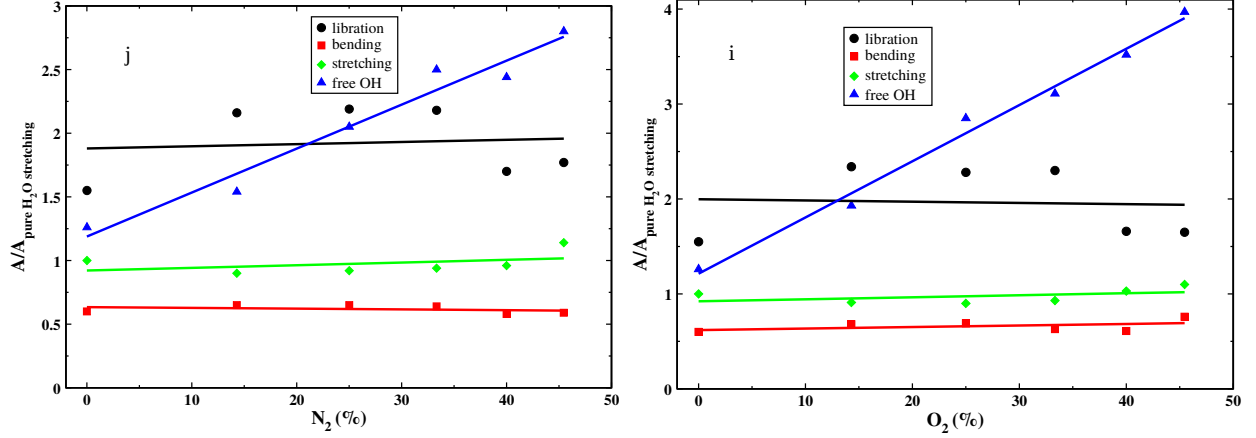


Figure S2: Band strengths of the four fundamental vibration modes of water for (a) $\text{H}_2\text{O} - \text{HCOOH}$, (b) $\text{H}_2\text{O} - \text{NH}_3$, (c) $\text{H}_2\text{O} - \text{CH}_3\text{OH}$, (d) $\text{H}_2\text{O} - \text{CO}$, (e) $\text{H}_2\text{O} - \text{CO}_2$, (f) $\text{H}_2\text{O} - \text{H}_2\text{CO}$, (g) $\text{H}_2\text{O} - \text{CH}_4$, (h) $\text{H}_2\text{O} - \text{OCS}$, (i) $\text{H}_2\text{O} - \text{N}_2$, and (j) $\text{H}_2\text{O} - \text{O}_2$ clusters with various concentrations. The water c-hexamer (chair) configuration has been used for pure water.

S1

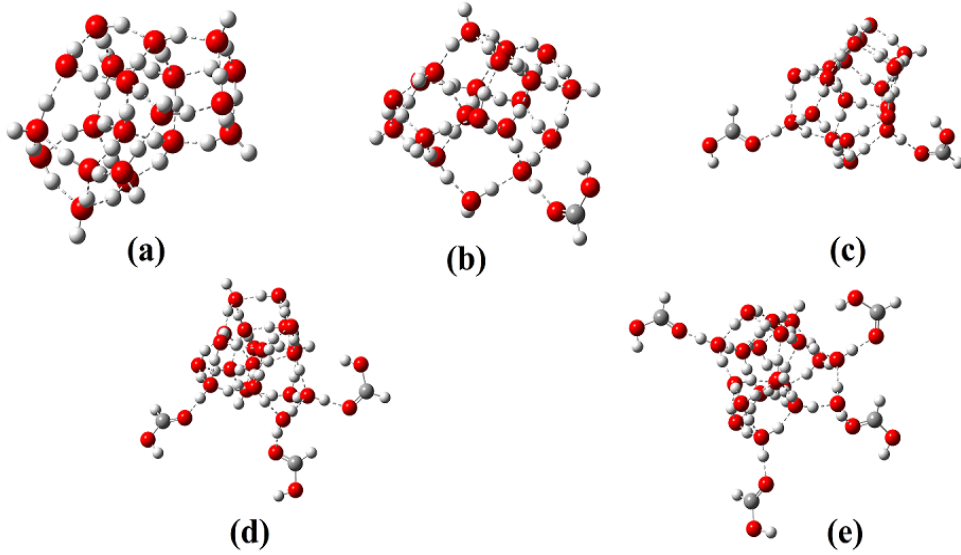


Figure S3: Structure of water clusters containing 20 H_2O molecules with HCOOH as impurity in different concentration ratio: (a) pure water, (b) $\text{H}_2\text{O} : \text{HCOOH} = 20 : 1$, (c) $\text{H}_2\text{O} : \text{HCOOH} = 10 : 1$, (d) $\text{H}_2\text{O} : \text{HCOOH} = 6.67 : 1$, (e) $\text{H}_2\text{O} : \text{HCOOH} = 5 : 1$.

S4

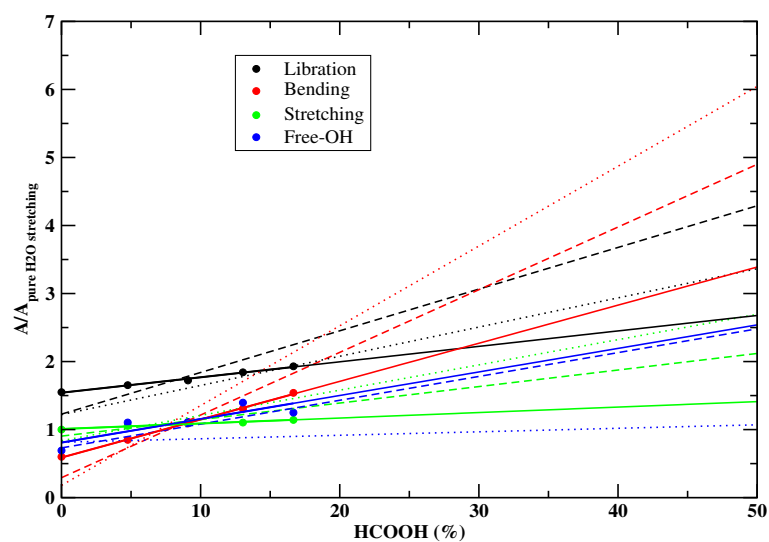


Figure S4: Comparison of the band strength of the four fundamental vibrational modes for water clusters containing 20H₂O, 6H₂O, and 4H₂O molecules with HCOOH as an impurity in different concentrations. Solid lines represent the band strength profiles for 20H₂O cluster, dotted lines for the water c-hexamer (chair) (6H₂O), and dashed lines for water c-tetramer (4H₂O).

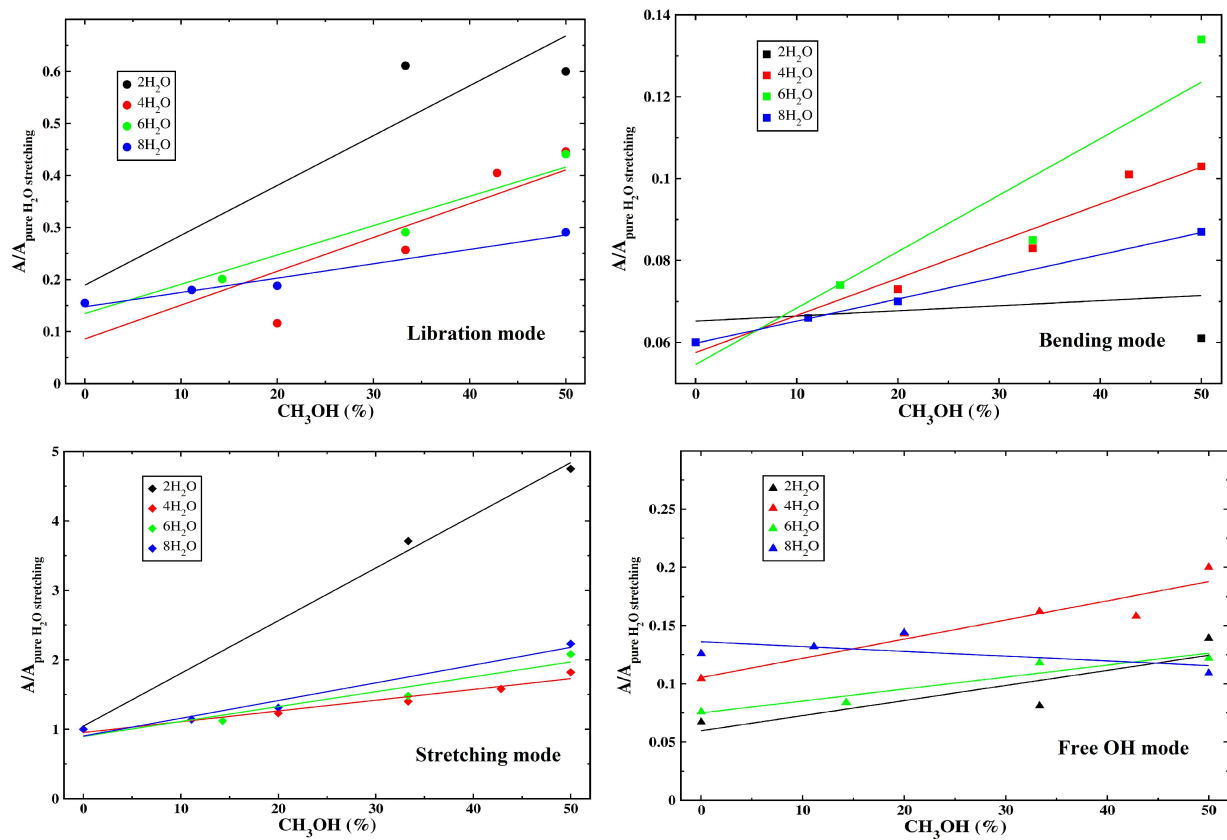


Figure S5: Effect of the cluster size on the band strength profile.

Table S1: Harmonic infrared frequencies and intensities of the complex 4H₂O evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	39.3404	0.0000
2	85.5169	4.1241
3	202.1393	0.0000
4	222.9069	104.7500
5	222.9069	104.7500
6	231.0105	94.8938
7	240.0832	0.6734
8	246.4688	287.8694
9	246.4688	287.8694
10	274.1815	0.0000
11	398.6011	0.0000
12	427.5608	44.2017
13	443.1204	79.6160
14	443.1204	79.6160
15	683.4168	312.1539
16 ^t	778.3957	237.5051
17 ^t	778.3957	237.5051
18 ^t	934.3601	0.0000
19 ^b	1630.3695	176.7723
20 ^b	1647.3535	74.0296
21 ^b	1647.3536	74.0296
22 ^b	1672.6698	0.0000
23 ^s	3411.5900	0.0000
24 ^s	3477.3996	1793.2478
25 ^s	3477.3996	1793.2478
26 ^s	3522.3300	2.0149
27 ^f	3864.6871	144.7620
28 ^f	3865.9912	138.6232
29 ^f	3865.9912	138.6232
30 ^f	3867.1847	0.0000

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH.

Table S2: Harmonic infrared frequencies and intensities of the complex 4H₂O/HCOOH evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	7.4652	2.8797
2	21.6554	0.4836
3	31.8296	0.8007
4	45.1056	0.3993
5	61.0883	3.2003
6	99.9662	7.7802
7	176.7899	26.3202
8	190.2330	26.8829
9	212.6031	80.9785
10	214.8008	65.5508
11	229.1782	167.5034
12	238.5224	82.0767
13	255.2508	249.2937
14	283.6779	26.8213
15	291.4533	55.7068
16	356.4031	83.8068
17	417.6885	49.4695
18	428.1868	57.7373
19	460.8606	57.1370
20	508.1693	55.1486
21	660.2176	284.6155
22	690.3556	83.8851
23 ^t	754.6078	231.9718
24 ^t	824.4685	178.7024
25 ^{t*}	939.4045	72.3782
26 ^{t*}	992.4637	143.3107
27	1085.0300	25.7493
28	1202.3494	398.5316
29	1404.3401	4.1326
30	1450.6121	11.3947
31 ^b	1630.0596	190.6522
32 ^b	1643.5475	74.8871
33 ^b	1650.3969	67.4629
34 ^b	1671.1011	2.8373
35	1727.4428	643.7374
36	3082.2813	261.4632
37 ^{s*}	3180.6017	2093.2108
38 ^{s*}	3305.3198	591.1162
39 ^s	3439.5143	1097.5194
40 ^s	3501.1192	960.3923
41 ^s	3594.2178	538.8467
42 ^f	3844.3939	126.6809
43 ^f	3864.5499	125.4762
44 ^f	3865.8634	156.4890
45 ^f	3866.9802	55.7713

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by HCOOH modes.

Table S3: Harmonic infrared frequencies and intensities of the complex 4H₂O/2HCOOH evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	4.6054	0.4281
2	13.0063	2.9178
3	16.5189	0.8051
4	19.0314	2.3774
5	20.9593	2.6393
6	33.4976	0.4467
7	36.7713	1.8500
8	42.5055	1.8790
9	57.0477	3.6453
10	87.6438	1.4306
11	98.3938	9.9521
12	109.3757	0.0813
13	179.0412	24.1400
14	190.5090	28.2740
15	214.0975	84.9229
16	218.8524	55.4812
17	230.2931	171.1476
18	238.6575	89.3090
19	267.3732	231.1914
20	283.3954	21.6224
21	299.6074	70.4602
22	358.3291	97.5174
23	418.1841	53.6749
24	433.0143	50.5761
25	453.3466	44.2133
26	511.7339	57.2963
27	626.1257	81.2731
28	663.5082	202.0801
29	664.5570	266.9661
30	690.0285	82.0272
31 ^t	746.7845	238.4794
32 ^t	832.5630	181.3816
33 ^{t*}	936.5175	69.8256
34 ^{t*}	992.1307	142.3809
35	1086.4569	25.8243
36	1100.7355	4.5531
37	1117.2066	421.1594
38	1202.1232	398.7897
39	1301.5992	19.3272
40	1403.7379	3.7351
41	1441.6206	5.0048
42	1449.0432	11.3813
43 ^b	1630.1114	189.4041
44 ^b	1643.0592	75.7767
45 ^b	1650.4443	71.8600
46 ^b	1671.6065	3.7550
47	1727.3571	640.6790
48	1740.9364	573.8795
49	3082.1544	256.8737
50 ^{s*}	3108.5982	9.0680
51 ^{s*}	3182.8047	2058.2321
52 ^{s*}	3311.8175	593.5776
53 ^s	3443.5223	1123.8585
54 ^s	3495.5861	975.1779
55 ^s	3593.0205	538.1736
56	3722.9218	111.6916
57 ^f	3843.8168	126.4406
58 ^f	3860.4740	132.4083
59 ^f	3863.8070	104.3051
60 ^f	3865.7512	106.7733

Table S4: Harmonic infrared frequencies and intensities of the complex 4H₂O/3HCOOH evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	4.8748	0.5689
2	8.5054	0.7327
3	10.9091	1.7844
4	14.1204	2.2282
5	16.8372	1.6310
6	19.1432	3.8603
7	22.9673	0.5549
8	28.0702	2.8070
9	34.3674	0.6429
10	40.7401	1.8661
11	45.9916	0.3401
12	54.8514	5.3280
13	66.6228	5.5016
14	89.0988	1.1463
15	99.3575	2.6618
16	110.9935	9.9385
17	174.0921	44.5063
18	177.9118	30.6049
19	188.6541	24.0948
20	209.4056	83.4103
21	212.1508	55.0788
22	234.2838	28.4231
23	245.2791	210.0525
24	261.2989	35.4759
25	284.3732	27.8615
26	314.1459	145.9808
27	352.7412	77.0879
28	410.7784	41.6288
29	418.4381	142.3769
30	451.8321	62.9268
31	486.2526	26.6238
32	515.8604	43.5007
33	626.3452	78.8764
34	658.3748	265.4010
35	664.0178	196.3924
36	686.9044	88.1977
37	687.6686	73.9457
38 ^{t*}	798.2680	156.7957
39 ^t	803.7700	211.1567
40 ^{t*}	926.7114	95.5456
41	949.5463	177.0601
42	1005.8276	134.0566
43	1083.1613	20.4516
44	1083.9241	23.7748
45	1098.4056	4.7221
46	1118.0234	421.3278
47	1198.2543	380.9330
48	1198.3514	418.6655
49	1303.1561	18.8667
50	1400.6093	4.0266
51	1400.7389	2.9534
52	1440.0730	5.2611
53	1445.8193	12.3688
54	1445.9512	8.9357
55 ^b	1630.5379	192.0093
56 ^b	1645.2809	74.7331
57 ^b	1649.3090	90.0689
58 ^b	1670.3929	1.3964
59	1729.0788	813.5933
60	1729.3363	445.0961

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by HCOOH modes.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
61	1741.9079	575.8421
62	3085.0941	261.1337
63	3085.5154	98.0625
64	3110.4187	7.6777
65 ^{s*}	3215.3096	2288.1686
66 ^{s*}	3232.6395	1833.2038
67 ^{s*}	3306.6741	311.8714
68 ^s	3451.6305	978.9670
69 ^s	3473.6093	894.3564
70 ^s	3609.3777	516.6451
71	3723.4615	111.6932
72 ^f	3838.2715	172.2543
73 ^f	3841.3048	97.0635
74 ^f	3857.9521	119.5655
75 ^f	3865.5487	121.3331

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by HCOOH modes.

Table S5: Harmonic infrared frequencies and intensities of the complex 4H₂O/4HCOOH evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	5.2521	0.5902
2	6.6193	1.2706
3	8.8369	0.8598
4	9.6756	1.0009
5	14.2363	3.0419
6	15.7986	1.1225
7	18.3559	3.0357
8	19.2707	2.7650
9	22.1555	0.9922
10	27.4779	3.1848
11	30.7377	0.4104
12	36.6940	0.3940
13	42.5989	1.4605
14	50.4443	2.9039
15	56.1885	2.0333
16	67.8597	3.6648
17	79.8514	11.6336
18	88.6848	0.8582
19	101.4052	1.0586
20	120.4063	2.7295
21	173.0431	53.0876
22	174.6165	79.9014
23	181.6174	16.9912
24	193.2247	8.7228
25	207.4059	98.2327
26	209.4436	56.3457
27	214.9922	15.9518
28	251.9141	48.3664
29	260.0519	27.0848
30	277.2414	21.6313
31	294.7764	138.3103
32	370.6813	53.2423
33	411.5523	157.3717
34	426.8010	160.0370
35	432.4841	46.3694
36	474.7455	4.1043
37	500.7327	25.1590
38	506.2341	58.6370
39	626.8822	79.1196
40	662.8116	197.7640

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
41 ^{t*}	680.2702	165.0245
42 ^{t*}	685.5338	74.2193
43 ^{t*}	685.8711	129.0114
44 ^t	703.1086	134.5453
45 ^t	777.4948	157.2018
46 ^{t*}	836.4350	145.9547
47	918.5370	51.5171
48	934.3780	130.8642
49	940.6167	399.9756
50	1005.3540	55.4131
51	1082.2723	15.9752
52	1082.8090	29.1817
53	1083.2383	8.1740
54	1096.9310	4.7996
55	1118.5677	421.7245
56	1194.7613	402.1943
57	1196.6655	678.8383
58	1196.9390	124.3700
59	1303.5269	19.2431
60	1398.1664	2.8858
61	1399.8325	2.3693
62	1400.1243	3.6218
63	1438.1358	3.4116
64	1443.1291	10.6650
65	1444.6815	8.9685
66	1445.0393	12.6099
67 ^b	1633.0557	204.1450
68 ^b	1645.9171	94.0994
69 ^b	1651.0001	68.5795
70 ^b	1672.8271	2.1359
71	1729.8409	773.0317
72	1729.9568	580.0062
73	1730.9646	527.5802
74	1742.3118	572.3800
75	3086.2791	171.0952
76	3087.0204	182.6391
77	3087.9488	105.7546
78	3114.3577	6.5557
79 ^{s*}	3235.8092	2226.0999
80	3251.6769	2145.0628
81 ^{s*}	3269.8018	1271.6200
82 ^{s*}	3338.7804	329.7573
83 ^s	3451.7939	830.3998
84 ^s	3506.2315	849.9293
85 ^s	3580.2425	496.8387
86	3723.2687	112.7727
87 ^f	3837.0764	199.2805
88 ^f	3839.9016	135.3088
89 ^f	3841.2858	85.4332
90 ^f	3859.2614	129.2712

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by HCOOH modes.

Table S7: Harmonic infrared frequencies and intensities of the complex $4\text{H}_2\text{O}/2\text{NH}_3$ evaluated at the B2PLYP/maug-cc-pVTZ level.

Table S6: Harmonic infrared frequencies and intensities of the complex $4\text{H}_2\text{O}/\text{NH}_3$ evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm^{-1}]	IR Int. [Km/mole]
1	17.4723	1.6404
2	24.2573	2.7053
3	42.9718	9.2433
4	56.2828	14.2890
5	77.4675	5.3857
6	176.7386	14.5514
7	205.9991	61.5386
8	210.2974	51.1840
9	220.3754	138.5385
10	234.6966	41.4586
11	240.2432	175.3537
12	253.5984	22.5694
13	262.9908	199.8180
14	269.0541	36.5738
15	288.0112	25.8883
16	411.0477	10.8123
17	438.1929	57.2835
18	462.1627	115.4840
19	649.2280	90.3859
20 ^t	673.7378	245.4033
21 ^t	761.0067	286.3846
22 ^t	785.5912	213.8984
23 ^t	855.6009	110.1452
24	973.8257	54.6453
25	1133.1043	207.9712
26 ^b	1635.5747	161.1828
27 ^b	1648.9602	81.2871
28 ^{b*}	1654.1532	68.4123
29	1659.8070	23.9527
30 ^{b*}	1664.0270	13.9746
31 ^{b*}	1687.1189	4.9894
32 ^s	3278.5997	1998.0299
33 ^s	3358.0759	412.2786
34 ^s	3442.1676	1170.0672
35	3483.9230	0.6553
36 ^s	3499.4250	959.9493
37 ^s	3600.3604	714.2057
38	3600.7264	13.1052
39	3601.5192	18.8438
40 ^f	3865.2764	131.5539
41 ^f	3866.4890	96.2050
42 ^f	3867.7812	62.0566

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by NH_3 modes.

NM	ω [cm^{-1}]	IR Int. [Km/mole]
1	13.2137	3.5154
2	35.8031	4.5193
3	37.7152	15.3999
4	42.6399	0.6394
5	44.0908	1.0833
6	50.2282	25.2398
7	62.5104	1.7351
8	74.8511	7.5826
9	174.7854	0.3931
10	184.1028	49.5918
11	202.3520	59.3483
12	215.2501	3.8987
13	233.8400	170.4567
14	236.8583	13.8898
15	250.5424	28.2234
16	252.5110	43.5646
17	263.8678	24.6139
18	264.6765	198.4026
19	280.7045	30.8723
20	288.8026	34.1641
21	434.2362	2.5448
22	465.8322	178.0575
23	636.4757	5.8561
24	665.1100	92.9446
25 ^t	688.2585	220.0675
26 ^t	740.4480	369.3099
27 ^t	786.8028	188.6747
28 ^t	823.9109	101.1914
29 ^t	894.7322	182.6960
30 ^t	973.9338	41.1551
31	1131.1976	200.1314
32	1131.3535	216.3485
33 ^b	1643.5894	150.8608
34 ^b	1651.7575	100.8326
35 ^{b*}	1656.3567	54.5510
36 ^{b*}	1659.4699	6.3334
37	1660.0271	21.6415
38	1660.6689	23.4365
39 ^{b*}	1680.0902	25.5517
40 ^{b*}	1690.1602	1.1013
41 ^s	3300.1629	879.2415
42 ^s	3307.6453	2808.4413
43 ^s	3377.2024	646.7542
44 ^s	3391.5768	729.5638
45	3483.7965	0.9990
46	3483.9555	1.0499
47 ^s	3578.8775	1603.7262
48 ^s	3582.2181	63.0838
49	3600.8734	18.3990
50	3600.9540	18.6472
51	3601.2568	18.6290
52	3601.5982	18.6555
53 ^f	3866.9165	77.0140
54 ^f	3867.0372	90.8323

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by NH_3 modes.

Table S8: Harmonic infrared frequencies and intensities of the complex 4H₂O/3NH₃ evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	12.5470	2.6010
2	23.2847	18.0759
3	28.7571	23.4249
4	35.7710	0.3934
5	38.9667	0.0081
6	40.5045	3.8999
7	44.8244	0.2126
8	46.5267	10.5312
9	50.6992	8.8616
10	69.7890	5.0744
11	72.6524	9.5767
12	166.7922	5.9217
13	180.8039	37.7349
14	191.1116	39.0754
15	207.3981	10.9113
16	226.1385	96.0046
17	239.4714	55.1417
18	245.0773	9.5193
19	245.6175	62.3353
20	248.1708	26.4263
21	249.2122	68.1865
22	258.4416	35.6050
23	269.5283	80.6776
24	272.4683	30.5828
25	285.7225	20.2189
26	453.0415	74.3332
27	625.3188	29.7964
28	647.1033	149.3482
29	670.2563	144.8666
30	705.1954	132.9061
31 ^t	747.2466	332.8596
32 ^t	768.5970	229.7125
33 ^t	809.9923	25.6758
34 ^t	842.7130	230.7932
35 ^t	871.0453	187.0537
36 ^t	977.2613	31.3718
37	1126.3891	215.3444
38	1128.4031	174.0675
39	1128.4565	237.3456
40 ^b	1645.9709	133.6692
41 ^{b*}	1654.7182	86.0037
42 ^{b*}	1655.6708	67.1056
43 ^{b*}	1658.8667	1.5603
44	1659.6806	25.9239
45	1660.1304	26.0074
46	1660.3043	24.5183
47 ^{b*}	1672.4596	26.6593
48 ^{b*}	1678.8129	23.6462
49 ^b	1693.1435	0.5825
50 ^s	3302.1390	1539.8513
51 ^s	3360.1503	1320.9055
52 ^s	3374.8469	2291.7299
53 ^s	3393.0086	199.4039
54 ^{s*}	3478.9512	630.0948
55	3483.7372	1.4326
56	3483.7543	6.5600
57 ^{s*}	3484.7724	142.9342
58 ^s	3520.0887	1009.6190
59 ^s	3596.2284	723.7876
60	3600.8160	17.3429
61	3600.9676	17.3826
62	3601.0701	18.0350
63	3601.4302	17.6940
64	3601.4607	18.0960
65	3601.5560	18.1230
66 ^f	3867.3234	81.2889

Table S9: Harmonic infrared frequencies and intensities of the complex 4H₂O/4NH₃ evaluated at the B2PLYP/maug-cc-pVTZ level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	4.9193	4.9769
2	9.0775	2.0942
3	17.7847	11.5017
4	19.1211	1.0599
5	22.4392	0.6988
6	25.9838	0.4032
7	27.6254	26.7443
8	35.4482	23.6215
9	39.7909	2.7928
10	42.1429	0.1113
11	46.9852	0.0030
12	62.8166	0.0005
13	72.1392	0.0251
14	74.9466	18.9444
15	158.5797	0.0024
16	174.6287	36.1323
17	178.2147	35.4550
18	201.4197	0.0105
19	233.9639	3.4824
20	235.9429	83.2509
21	237.2040	33.3809
22	239.2784	72.0949
23	239.6302	3.0360
24	242.2423	80.4390
25	243.0833	36.6777
26	246.3526	2.0432
27	261.6961	0.8343
28	266.9875	0.6015
29	269.0885	42.6136
30	273.9278	71.7557
31 ^t	613.8454	0.0116
32	630.4192	212.2155
33	666.2987	0.0041
34	670.4647	0.0071
35	700.3570	199.6747
36	744.5970	379.8388
37 ^t	755.9618	361.3020
38 ^t	799.7584	0.0050
39 ^t	815.2370	0.3721
40 ^t	825.5015	342.7098
41 ^t	846.8651	297.2880
42 ^t	946.2925	0.0017
43	1125.1644	153.1328
44	1125.2155	143.7533
45	1125.4081	503.2784
46	1125.4766	35.6108
47 ^{b*}	1654.5148	120.1771
48 ^{b*}	1654.8637	41.6854
49 ^{b*}	1657.2551	58.5445
50 ^{b*}	1657.8279	12.4900
51	1659.5005	30.4815
52	1659.5303	21.8453
53	1660.0190	25.0784
54	1660.1436	28.1216
55 ^{b*}	1673.3466	67.4843
56 ^{b*}	1674.2718	0.3138
57 ^b	1688.6077	33.8790
58 ^b	1691.9499	0.0133
59 ^s	3369.6234	0.2819
60 ^s	3385.6965	2574.9240

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by NH₃ modes.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
61 ^s	3387.6855	2801.0441
62 ^s	3394.0812	0.7615
63 ^{s*}	3473.3538	0.1108
64	3483.3149	13.0568
65	3483.4935	11.1778
66	3483.6384	2.6130
67 ^{s*}	3484.6015	0.0846
68 ^s	3507.3380	1567.4274
69 ^s	3510.2809	1820.7051
70 ^s	3536.4083	0.1714
71	3600.7487	17.4948
72	3600.7879	17.3727
73	3600.9757	17.5063
74	3601.0932	17.3475
75	3601.1747	17.5682
76	3601.2866	17.5694
77	3601.4175	17.2943
78	3601.5786	17.6734

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH; *vibrations contaminated by NH₃ modes.

Table S10: Harmonic infrared frequencies and intensities of the H₂O^{QM} + 3 H₂O^{MM} complex (Figure 2, left panel).

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	39.0097	3.5702
2	70.0478	0.9941
3	107.4593	248.8304
4	114.6669	81.5288
5	134.1712	121.9418
6	251.1220	19.7407
7	253.1088	18.8069
8	270.4875	7.7664
9	286.0773	10.8931
10	331.3394	156.5948
11	417.2017	11.4416
12	483.9590	107.2607
13 ^t	502.7496	211.3432
14 ^t	539.1224	59.4593
15 ^t	620.5928	2.9662
16 ^t	670.5374	209.1029
17 ^t	734.0061	476.6369
18 ^t	870.1429	201.9038
19 ^b	1407.2265	191.4554
20 ^b	1422.8362	445.8394
21 ^b	1456.6860	64.4541
22 ^b	1764.1323	143.3391
23 ^s	3399.8219	161.5281
24 ^s	3533.5836	119.6470
25 ^s	3561.1437	374.8984
26 ^s	3579.9423	110.7922
27 ^f	3643.1130	84.3280
28 ^f	3647.6874	450.2363
29 ^f	3651.3875	90.6885
30 ^f	3797.0095	37.5965

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH

Table S11: Harmonic infrared frequencies and intensities of the first 4 H₂O^{QM}+16 H₂O^{MM} complex (see Figure 2a in the manuscript, right panel, Configuration 1) evaluated at the B3LYP/6-31g(d) level.

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
1	28.5053	1.6212
2	32.4112	0.3452
3	40.5682	1.9422
4	42.6937	0.9658
5	45.5125	2.8291
6	47.0457	2.4796
7	51.1545	1.5206
8	53.0040	0.4852
9	57.4113	4.9283
10	58.9090	1.5004
11	62.8440	3.3091
12	64.6577	0.5053
13	67.1132	0.4600
14	71.0670	1.0092
15	72.1009	5.5430
16	78.5377	1.2279
17	79.5809	2.8592
18	84.0856	0.3164
19	88.1866	0.5336
20	91.6244	1.1620
21	95.9146	1.9115
22	131.1634	139.0258
23	147.4509	6.2284
24	155.1556	1.5936
25	157.0881	12.4196
26	163.8254	4.8492
27	169.5773	3.8618
28	173.1802	11.6779
29	177.8697	22.1882
30	179.4412	3.0508
31	189.5523	12.2882
32	193.8849	18.7990
33	199.5633	30.2086
34	203.7815	44.7590
35	205.2272	29.8834
36	210.7469	42.9633
37	212.8473	18.5861
38	215.6034	104.3096
39	219.2947	9.1183
40	221.2358	136.0590
41	223.7398	14.6743
42	226.9991	92.7095
43	229.4667	11.8754
44	231.1955	180.5173
45	235.9253	6.3462
46	239.8566	146.4113
47	249.2394	2.9212
48	254.8166	52.0837
49	260.4354	12.2059
50	270.0093	13.8498
51	280.9175	13.8528
52	284.5581	1.3055
53	286.3104	31.7468
54	307.5132	4.0551
55	308.3710	4.8097
56	314.4016	25.2868
57	319.3857	8.4817
58	330.7679	1.3826
59	334.6995	4.4240
60	347.3954	4.9640

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
61	387.1876	8.8358
62	426.8869	78.1914
63	432.7664	47.4011
64	449.0251	78.8810
65	455.8202	9.0749
66	458.4089	52.9014
67	461.3395	7.1542
68	468.0311	44.1926
69	476.0688	5.2943
70	483.8486	73.9300
71	500.1090	30.3953
72	500.9839	36.5412
73	508.1366	20.0694
74	512.3840	13.9454
75	532.3995	46.0624
76	535.4481	4.4789
77	543.6866	60.5730
78	545.4049	57.7011
79	557.0745	41.0189
80	560.6706	18.2338
81	581.7986	25.4989
82	585.3805	214.1458
83	588.1325	72.1128
84 ^t	593.3498	6.1937
85 ^t	598.2759	204.0196
86 ^t	620.7530	378.5822
87 ^t	623.3143	58.9759
88 ^t	629.3486	219.1103
89 ^t	639.6399	56.7824
90 ^t	642.7590	240.6043
91 ^t	648.3193	65.9335
92 ^t	658.9772	36.8759
93 ^t	676.8776	176.4931
94 ^t	679.7026	594.2500
95 ^t	685.0436	47.0063
96 ^t	690.6345	554.1850
97 ^t	695.3495	353.6124
98 ^t	699.7148	156.7689
99 ^t	704.2320	32.3584
100 ^t	721.7785	334.5258
101 ^t	725.6449	111.7286
102 ^t	728.6757	454.3782
103 ^t	747.1205	168.5362
104 ^t	753.5614	192.6962
105 ^t	765.5413	275.9737
106 ^t	766.1653	425.8765
107 ^t	772.0067	356.3800
108 ^t	803.0436	327.2798
109 ^t	818.6290	277.6746
110 ^t	839.8062	313.0187
111 ^t	850.6360	671.1597
112 ^t	929.4103	415.2180
113 ^t	955.5738	180.7041
114 ^t	966.2260	55.4464
115 ^b	1401.1608	328.9992
116 ^b	1404.9892	279.6521
117 ^b	1406.8655	454.2350
118 ^b	1412.4834	218.9410

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
119 ^b	1415.0050	217.1485
120 ^b	1416.7673	553.3807
121 ^b	1423.8136	320.7421
122 ^b	1427.0557	239.2493
123 ^b	1431.3527	280.4839
124 ^b	1433.6066	107.3301
125 ^b	1436.1459	143.6834
126 ^b	1442.3811	59.3969
127 ^b	1456.0330	69.7821
128 ^b	1465.8850	261.4679
129 ^b	1481.4184	129.4706
130 ^b	1490.6689	54.4350
131 ^b	1759.3916	113.0751
132 ^b	1781.9431	109.2325
133 ^b	1805.1440	185.2649
134 ^b	1821.5031	81.3961
135 ^s	3277.1620	1061.3522
136 ^s	3379.4017	1450.1515
137 ^s	3415.3773	260.6407
138 ^s	3441.1055	54.0971
139 ^s	3501.0930	137.3189
140 ^s	3510.2084	280.1448
141 ^s	3515.4119	164.7163
142 ^s	3527.1563	98.4213
143 ^s	3532.0223	374.1860
144 ^s	3535.9755	331.7897
145 ^s	3539.5696	667.4359
146 ^s	3541.9090	42.2047
147 ^s	3546.9082	185.0747
148 ^s	3549.9374	209.7596
149 ^s	3555.5498	189.4891
150 ^s	3558.8959	76.1871
151 ^s	3563.2840	189.8014
152 ^s	3568.4433	217.3753
153 ^s	3575.4761	97.1563
154 ^s	3576.5391	86.9267
155 ^s	3579.7822	19.6952
156 ^s	3589.8658	38.6004
157 ^s	3590.2134	57.5165
158 ^s	3603.0421	149.2000
159 ^s	3618.1897	266.3486
160 ^s	3620.8200	224.9253
161 ^s	3622.0658	233.3283
162 ^s	3623.0520	397.9328
163 ^s	3624.0959	35.3011
164 ^s	3626.6346	276.1415
165 ^s	3630.3037	955.2942
166 ^s	3631.8424	16.4537
167 ^s	3633.8572	248.7481
168 ^f	3646.1348	108.4691
169 ^f	3650.9996	175.2420
170 ^f	3652.3329	128.0414
171 ^f	3652.8838	205.0487
172 ^f	3653.3844	33.2033
173 ^f	3653.8800	205.2072
174 ^f	3654.0193	86.2440

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^ffree OH.

Table S12: Harmonic infrared frequencies and intensities of the first 4 $\text{H}_2\text{O}^{QM}+16$ H_2O^{MM} complex (Figure 2b, right panel, Configuration 2) evaluated at the B3LYP/6-31g(d) level.

NM	ω [cm^{-1}]	IR Int. [Km/mole]
1	29.4016	1.2924
2	34.4375	0.6290
3	40.5656	1.6279
4	44.5388	1.2326
5	47.5478	0.5182
6	49.2499	4.4372
7	52.7161	1.1206
8	53.7670	0.7604
9	58.1400	3.8023
10	62.8023	2.1220
11	65.0382	1.4900
12	65.4195	1.0334
13	68.9622	1.6328
14	71.1636	2.8146
15	75.3263	4.0105
16	77.6513	1.4318
17	79.5630	1.9564
18	86.9075	2.3428
19	88.7674	0.0132
20	92.6829	0.4316
21	97.2538	2.3252
22	132.9698	136.0213
23	144.3282	7.0450
24	150.9225	8.8323
25	160.4446	11.5643
26	163.9774	15.3603
27	166.9931	18.7482
28	174.8622	3.9430
29	178.6797	9.5964
30	186.2172	5.2561
31	189.8802	22.8351
32	196.0450	18.6789
33	200.1828	70.0050
34	201.5062	8.6800
35	202.0414	8.0519
36	208.0234	21.2606
37	211.9547	44.9818
38	216.4440	154.2248
39	217.8326	186.4806
40	218.1099	26.3216
41	221.6619	28.3099
42	224.3879	13.6861
43	227.4102	2.3297
44	229.1919	70.6417
45	230.9956	94.8355
46	243.1731	117.8833
47	249.4187	0.5086
48	253.8914	22.9344
49	257.2356	35.1484
50	267.5344	24.9850
51	280.0676	6.8173
52	285.7365	23.7669
53	296.6659	17.1441
54	304.8541	3.0164
55	308.4159	0.7582
56	314.4300	7.5522
57	317.0437	9.2531
58	327.0967	1.0243
59	338.1423	9.0936
60	366.0320	9.0877

NM	ω [cm^{-1}]	IR Int. [Km/mole]
61	381.8881	2.8750
62	425.0003	72.9104
63	433.1753	46.5032
64	449.7627	54.6515
65	453.1267	32.8363
66	454.2652	31.3116
67	457.6722	30.6715
68	461.6648	46.8946
69	472.4824	9.8892
70	485.9271	79.1355
71	489.0285	21.2511
72	504.9767	27.4262
73	512.8253	6.2202
74	520.2208	42.0235
75	531.5264	37.2553
76	534.9918	6.2757
77	548.5225	54.6906
78	551.0483	47.1921
79	557.6667	22.4631
80	567.0486	44.8651
81	577.5475	247.0326
82	582.7791	105.7169
83	589.4278	39.6372
84 ^t	593.7719	63.8280
85 ^t	602.0192	207.8189
86 ^t	607.5690	235.3652
87 ^t	620.9062	128.9013
88 ^t	630.0995	226.7652
89 ^t	642.3136	46.5019
90 ^t	646.4580	155.7202
91 ^t	656.2139	245.2327
92 ^t	659.7475	92.3092
93 ^t	668.0591	88.0836
94 ^t	678.1031	752.6557
95 ^t	687.1452	86.4196
96 ^t	702.2325	266.3036
97 ^t	704.8812	97.3595
98 ^t	711.5869	144.5530
99 ^t	715.1892	66.1333
100 ^t	725.8863	598.8691
101 ^t	726.0798	18.1883
102 ^t	730.7761	246.5783
103 ^t	736.1656	277.1486
104 ^t	744.0336	554.7832
105 ^t	761.4750	271.4461
106 ^t	775.7715	563.7792
107 ^t	786.5512	479.5887
108 ^t	805.5061	212.9173
109 ^t	826.6848	229.7506
110 ^t	845.7629	191.2681
111 ^t	887.6214	524.4212
112 ^t	923.2407	210.8728
113 ^t	950.0147	288.1648
114 ^t	1014.9949	128.1520
115 ^b	1401.2013	312.9877
116 ^b	1403.0314	627.4395
117 ^b	1404.8169	265.9060
118 ^b	1411.9292	63.9287
119 ^b	1414.1855	237.2331
120 ^b	1414.6760	480.1803
121 ^b	1424.0139	304.7906
122 ^b	1426.0145	322.1644
123 ^b	1430.3473	297.6835
124 ^b	1434.2284	77.0402
125 ^b	1442.9373	116.7008

NM	ω [cm ⁻¹]	IR Int. [Km/mole]
126 ^b	1444.1623	105.5626
127 ^b	1459.2322	55.3003
128 ^b	1465.8496	252.0918
129 ^b	1482.2478	140.3077
130 ^b	1505.1507	42.7361
131 ^b	1775.8533	82.3784
132 ^b	1780.7273	68.7098
133 ^b	1801.6979	332.8605
134 ^b	1807.9136	66.8586
135 ^s	3312.7170	920.6313
136 ^s	3377.7305	741.7304
137 ^s	3421.1305	761.8361
138 ^s	3445.3287	168.4186
139 ^s	3485.4299	175.0443
140 ^s	3509.6340	116.0370
141 ^s	3525.2414	27.1764
142 ^s	3527.9472	11.8392
143 ^s	3529.5426	406.7703
144 ^s	3536.2221	608.4735
145 ^s	3539.1759	168.8773
146 ^s	3542.1608	517.6770
147 ^s	3544.0015	105.2415
148 ^s	3551.6796	422.3966
149 ^s	3556.2138	104.4402
150 ^s	3559.4252	140.9715
151 ^s	3562.5905	344.5012
152 ^s	3566.5079	71.2504
153 ^s	3568.8607	31.6257
154 ^s	3577.3367	111.0585
155 ^s	3577.8583	220.6935
156 ^s	3583.4466	183.5092
157 ^s	3590.2972	17.7387
158 ^s	3591.3690	14.5938
159 ^s	3611.7321	8.8719
160 ^s	3618.8579	235.6198
^c 161 ^s	3623.1189	386.5676
162 ^s	3624.3597	98.4237
163 ^s	3627.3709	210.1150
164 ^s	3628.9811	88.7231
165 ^s	3630.5375	639.2414
166 ^s	3631.3807	548.9593
167 ^s	3632.6677	305.9009
168 ^f	3646.2015	105.3221
169 ^f	3651.1285	183.1653
170 ^f	3652.3160	143.6466
171 ^f	3652.6720	169.0597
172 ^f	3653.3819	24.7682
173 ^f	3653.5148	97.5307
174 ^f	3654.0199	236.1947

Notes. ^tOH torsion; ^bOH scissoring; ^sOH stretching; ^f free OH.