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

Supporting Information

Structure, stability, infrared spectra, and bonding of $OH^m(H_2O)_7$ (m = 0, ±1) clusters. Ab initio study combining the particle swarm optimization algorithm

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Table S1-S3 The Cartesian coordinates for the fifteen structures of anionic $OH^-(H_2O)_7$ clusters, the twelve structures of neutral $OH(H_2O)_7$ clusters, and the twelve structures of cationic $OH^+(H_2O)_7$ clusters, respectively.

Table S4-S6 The total energies of the $OH^-(H_2O)_7$ isomers, the $OH(H_2O)_7$ isomers, and the $OH^+(H_2O)_7$ isomers for CCSD(T), MP2, and DFT methods, respectively.

Figure S1 Relative energies of the fifteen $OH^-(H_2O)_7$ isomers with respect to A6.

Figure S2 Relative energies of the twelve $OH(H_2O)_7$ isomers with respect to N1.

Table S1. The Cartesian coordinates for the fifteen low-energy structures of anionic $OH^-(H_2O)_7$ clusters.

Structure	Atom	*X* (Å)	*Y* (Å)	*Z* (Å)	Structure	Atom	*X* (Å)	*Y* (Å)	*Z* (Å)
A1	H1	-0.2645	-1.4579	1.4817	A2	H1	-0.0378	1.8047	0.1998
	H2	0.9938	-1.3824	-1.3504		H2	0.2560	2.8314	1.3596
	H3	-1.9042	0.9067	-0.6103		H3	0.0479	0.1437	1.8638
	H4	2.0658	1.8967	0.4527		H4	1.3175	-1.8053	-0.5261
	H5	-1.1710	1.7314	1.8027		H5	0.1304	1.8461	-2.0002
	H6	-0.0536	-0.3173	-1.7015		H6	-1.4323	-1.4446	1.0368
	H7	1.8589	-1.2773	0.7005		H7	-2.3555	1.5141	0.3221
	H8	0.2860	-0.0967	1.8956		H8	-0.0043	-0.5241	-1.6550
	H9	-0.5482	2.0639	-1.7196		H9	-1.5954	1.0843	-0.9122
	H10	-1.0074	-1.8702	-0.5214		H10	-0.8186	-1.6977	-1.0928
	H11	-2.1134	-1.1494	0.2278		H11	0.7880	-1.1524	1.4753
	H12	-0.3440	1.6592	0.5056		H12	2.4075	-0.8734	-0.0237
	H13	-3.3645	0.4682	-0.9410		H13	1.7164	1.1047	-0.7521
	H14	1.2557	1.4876	-0.7750		H14	2.4429	1.3024	0.5837
	H15	2.5356	-0.2881	-0.2346		H15	-2.4031	-0.7659	0.0745
	O1	0.4774	-1.0523	1.9823		O1	0.0706	-0.8118	2.0561
	O2	2.4517	-1.2515	-0.0813		O2	1.9970	-1.7359	0.1849
	O3	0.1427	-1.2796	-1.8246		O3	-2.5077	1.0478	-0.5136
	O4	2.1970	1.5839	-0.4538		O4	-0.0640	-1.5113	-1.6880
	O5	-2.7831	0.6262	-0.1870		O5	0.1185	1.2226	-1.2607
	O6	-0.4221	1.3244	-1.1088		O6	-2.1112	-1.6554	0.3617
	O7	-1.5901	-1.9742	0.2671		O7	-0.1856	1.9907	1.1921
	O8	-0.2515	1.7264	1.5046		O8	2.6248	1.0323	-0.3267
A3	H1	0.1088	0.2224	0.6895	A4	H1	0.2066	1.8523	-1.9409
	H2	-1.8136	0.2704	-0.9092		H2	-0.1237	-1.0156	0.6441
	H3	-0.9018	2.0231	-0.0166		H3	-0.0707	0.0782	1.6989
	H4	1.3285	1.3346	-0.8308		H4	0.0172	1.8387	0.4228
	H5	1.9611	-0.8092	1.2433		H5	-1.7836	-1.7497	-0.5658
	H6	0.3317	-0.8895	-1.3408		H6	0.0485	-0.3314	-1.3715
	H7	2.7778	-0.0611	0.2254		H7	2.6663	1.5005	0.4904
	H8	1.4442	-1.7254	-0.7110		H8	1.8524	-1.6151	0.9509
	H9	-0.4810	-0.9058	1.4954		H9	1.7622	1.1542	-0.7166
	H10	-2.9496	0.7120	-0.0039		H10	-1.1715	1.9768	1.3359
	H11	-1.0152	1.9218	1.4905		H11	-2.1621	-1.6046	0.8843
	H12	2.1002	2.2979	0.0970		H12	-2.7190	0.3074	-0.3057
	H13	-2.0836	-1.5961	0.2309		H13	2.6827	-0.7766	0.0016
	H14	-0.7659	-2.3104	-0.0459		H14	0.8287	-1.6538	-1.0693
	H15	-0.2757	1.1623	-2.0737		H15	-1.6082	1.2548	-0.7711
	O1	-0.2120	0.8112	-1.1736		O1	-0.0649	-0.9004	1.6135

	O2	-1.4775	-2.2546	0.6295		O2	2.4768	-1.7154	0.2114
	O3	0.0951	-0.1164	1.6039		O3	2.7002	1.0319	-0.3545
	O4	-2.7319	-0.0009	-0.6221		O4	-0.0691	-1.3290	-1.2663
	O5	-1.2707	2.5091	0.7623		O5	-2.5233	1.2565	-0.4034
	O6	2.2589	1.6110	-0.5638		O6	-2.5738	-1.7200	0.0128
	O7	2.7356	-0.9364	0.6631		O7	0.2030	1.2747	-1.1655
	O8	0.6317	-1.8289	-1.2418		O8	-0.2021	1.9497	1.3911
A5	H1	-0.0001	-1.4403	-0.6289	A6	H1	0.4987	1.3383	-0.8499
	H2	-0.7732	1.3740	1.3490		H2	1.8309	-1.9746	-0.5536
	H3	1.9959	-1.3866	-0.9472		H3	2.1250	0.2966	1.6917
	H4	1.2905	1.5683	-0.6414		H4	-2.1249	-0.2967	1.6916
	H5	-1.9385	-1.4941	0.5485		H5	-1.8310	1.9746	-0.5533
	H6	-1.9961	-1.3865	-0.9473		H6	-0.4987	-1.3382	-0.8500
	H7	2.4279	0.7291	-0.0111		H7	-1.4490	0.7284	-1.3501
	H8	-2.4279	0.7294	-0.0111		H8	-1.5508	-1.8172	0.1775
	H9	0.7734	1.3739	1.3491		H9	-2.8000	0.0982	0.3960
	H10	0.0000	-0.4753	1.7063		H10	2.7999	-0.0983	0.3960
	H11	-1.2903	1.5684	-0.6414		H11	1.5509	1.8171	0.1777
	H12	1.9384	-1.4943	0.5486		H12	1.4490	-0.7282	-1.3501
	H13	0.0000	-0.2656	-1.6619		H13	-0.0640	-0.7612	1.2227
	H14	0.0001	1.7502	-2.4432		H14	0.0640	0.7611	1.2228
	H15	-0.0003	-1.9336	2.2993		H15	0.0000	0.0002	-2.7468
	O1	-2.5859	-1.3824	-0.1691		O1	-2.2477	1.2109	-0.9784
	O2	2.0019	1.5987	0.0798		O2	-0.6408	-2.0011	-0.1178
	O3	-0.0001	-1.4597	1.4591		O3	-2.8961	-0.5308	1.1459
	O4	0.0000	1.3040	-1.5869		O4	2.8962	0.5307	1.1460
	O5	-2.0017	1.5989	0.0798		O5	0.6408	2.0011	-0.1175
	O6	0.0001	1.1101	1.9099		O6	2.2477	-1.2108	-0.9785
	O7	0.0000	-1.2892	-1.5870		O7	0.0000	-0.0001	1.8399
	O8	2.5858	-1.3826	-0.1690		O8	0.0000	0.0001	-1.7800
A7	H1	2.4893	0.6514	0.0591	A8	H1	-0.8393	-0.9964	-0.7584
	H2	-0.7943	0.1639	-2.2952		H2	0.9481	-2.4256	-0.7449
	H3	2.4006	-0.8590	0.0095		H3	-0.6637	1.1897	-0.3982
	H4	0.7183	-1.1822	-1.3612		H4	2.7240	2.0047	-1.0695
	H5	1.0538	2.4864	-0.4675		H5	-3.0066	0.8983	-0.0601
	H6	-3.0122	-0.7558	0.2557		H6	-0.1293	0.5017	-2.3780
	H7	-0.0408	0.7378	1.7989		H7	-0.5381	2.4607	0.4709
	H8	-1.9708	1.7211	0.7362		H8	1.3101	1.3428	-0.9755
	H9	0.8102	-2.4397	-0.5284		H9	-1.0486	-1.4445	0.6812
	H10	-2.4416	0.0633	-0.8535		H10	1.1874	-1.0530	-1.3392
	H11	0.8238	1.2135	-1.2731		H11	2.2400	-0.9671	0.5259
	H12	-0.8741	1.2575	-0.2121		H12	-0.6697	0.3782	1.7139
	H13	1.2785	-0.0448	1.7866		H13	0.6071	-0.4140	1.9798
	H14	-0.6000	-1.3179	1.3448		H14	2.3124	0.5256	0.7919

	H15	-0.9418	-1.2267	-0.1302		H15	-2.9785	-0.5872	-0.3065
	O1	-1.0890	-1.8077	0.6491		O1	-0.3537	-0.4226	2.1778
	O2	-1.0285	1.8667	0.5651		O2	2.3633	-0.3304	1.2623
	O3	0.4229	0.0134	2.2653		O3	-3.5964	0.1697	-0.3141
	O4	1.5326	1.8798	-1.0510		O4	0.1912	0.3154	-1.4848
	O5	-3.2725	-0.0355	-0.3432		O5	-1.1136	1.6931	0.3528
	O6	-0.5056	0.0903	-1.3739		O6	1.9591	1.9507	-0.4838
	O7	2.7327	-0.1381	0.5856		O7	-1.3155	-1.6830	-0.2311
	O8	1.3451	-1.9275	-1.1557		O8	1.6837	-1.8697	-1.0458
A9	H1	0.9619	-1.1097	-1.1920	A10	H1	2.4372	-0.7851	0.1231
	H2	-2.2804	-1.0389	0.8802		H2	0.9556	1.2251	-1.3029
	H3	-2.3958	-0.4928	-1.2098		H3	-3.0927	0.9753	0.2982
	H4	-1.5568	1.7700	-0.5112		H4	2.1794	1.2972	-0.4112
	H5	-2.5135	0.9752	0.3470		H5	-2.3892	0.1203	-0.7314
	H6	1.5029	1.0839	-1.3731		H6	1.9425	-0.1046	1.3883
	H7	2.6720	0.2066	-0.9727		H7	0.7358	-1.1152	-1.3150
	H8	-1.3466	-1.6004	-1.0658		H8	-0.8198	1.3023	-0.2362
	H9	0.4510	1.2979	0.6010		H9	-0.1742	0.6879	1.7411
	H10	-1.1385	-0.2984	1.5907		H10	-0.0071	2.4499	0.2933
	H11	0.6960	0.1499	2.4558		H11	-2.0877	-1.7879	0.6389
	H12	3.1403	-1.3852	0.6282		H12	0.9736	-2.4691	-0.6551
	H13	2.2405	-0.2374	1.1138		H13	-0.8874	0.0153	-2.2524
	H14	0.6440	2.8241	0.2400		H14	-0.9919	-1.2953	-0.2954
	H15	0.4777	-1.2370	0.2449		H15	-0.2260	-0.8301	1.7178
	O1	0.4528	-1.7141	-0.6169		O1	-0.8332	1.9788	0.4947
	O2	0.3248	1.9979	-0.1422		O2	-1.1567	-1.9586	0.4336
	O3	-2.1174	-0.4356	1.6298		O3	-0.6189	-0.0079	-1.3224
	O4	0.6520	0.0506	1.4948		O4	0.2081	-0.0934	2.1932
	O5	3.1747	-0.4320	0.7861		O5	1.4469	-1.7974	-1.1671
	O6	2.1186	0.4243	-1.7504		O6	2.7201	-0.1273	0.7911
	O7	-2.3176	-1.4606	-1.1181		O7	1.6662	1.8457	-1.0395
	O8	-2.4822	1.4560	-0.5054		O8	-3.2511	0.1993	-0.2588
A11	H1	-1.5999	-0.0358	1.8139	A12	H1	0.0006	2.9403	0.1067
	H2	3.0564	-0.0261	0.0163		H2	-2.9621	-1.1808	0.0378
	H3	2.6527	-0.0018	1.4794		H3	-0.7687	1.2258	1.4236
	H4	0.3935	-0.7526	1.0803		H4	0.7692	1.2255	1.4236
	H5	1.0458	-2.6613	-0.3063		H5	-0.0002	-1.2300	-0.3964
	H6	1.1619	1.1366	-0.9290		H6	1.4027	0.4881	-0.5141
	H7	2.1295	-0.0562	-2.3385		H7	2.5034	1.5305	-0.1795
	H8	-2.2050	-0.4517	-1.2010		H8	-2.5028	1.5314	-0.1794
	H9	0.4094	0.7664	1.0616		H9	0.0004	2.0748	-1.1312
	H10	-2.4134	1.2341	0.0781		H10	-1.4025	0.4886	-0.5140
	H11	1.1197	-1.1838	-0.9041		H11	-0.0004	-1.7648	1.0563
	H12	-2.5856	-0.7206	0.8808		H12	-2.0225	-2.3537	-0.0218

	H13	1.1690	2.6137	-0.3272		H13	-0.0001	-0.0495	-2.1615
	H14	-1.3126	-1.6563	-0.8705		H14	2.9617	-1.1819	0.0378
	H15	-1.2590	1.7538	-0.7802		H15	2.0216	-2.3545	-0.0218
	O1	-2.2079	1.5197	-0.8330		O1	0.0006	3.0220	-0.8618
	O2	0.5790	1.8618	-0.4567		O2	-0.0004	-2.0798	0.1415
	O3	1.9468	-0.0441	-1.3910		O3	0.0000	0.2170	-1.2322
	O4	-2.2521	-1.3994	-0.9671		O4	2.1713	0.6737	0.1193
	O5	0.5036	-1.8713	-0.4167		O5	2.9748	-2.1540	-0.0152
	O6	0.3213	0.0156	1.6875		O6	-2.1711	0.6745	0.1194
	O7	-2.5577	-0.0694	1.6097		O7	0.0003	1.6257	1.8735
	O8	3.4468	-0.0077	0.9231		O8	-2.9756	-2.1529	-0.0153
A13	H1	-0.8749	-2.4398	-0.5170	A14	H1	-2.0011	-2.8968	0.2663
	H2	4.1075	-0.5812	-0.5737		H2	1.4840	1.4014	0.2917
	H3	1.9758	-1.7988	-0.5961		H3	1.4310	-2.0184	-0.9415
	H4	0.9266	-1.7227	0.5203		H4	1.6270	2.9482	0.1835
	H5	-2.2730	1.0027	0.0545		H5	2.6218	-0.2003	-0.4188
	H6	1.4236	1.8527	0.3174		H6	-0.6925	-2.1538	-0.1121
	H7	-0.5985	2.5130	-0.1366		H7	-1.4441	1.5102	0.8120
	H8	-4.1078	-0.4673	-0.6854		H8	-2.6251	-0.5931	-1.0855
	H9	-2.6577	-0.9623	-0.8067		H9	0.0349	0.0682	1.6920
	H10	2.8121	0.2361	-0.4561		H10	-1.3100	-0.6318	1.4292
	H11	-1.1043	0.7276	1.0426		H11	1.2662	-1.4666	0.4669
	H12	-1.1114	-1.4875	0.6397		H12	-2.5632	0.9251	-1.0452
	H13	-0.0756	-0.6946	2.4168		H13	2.2803	-0.0153	1.8442
	H14	1.1834	0.4972	1.0414		H14	-0.6289	2.2344	-0.2337
	H15	0.1669	2.6699	-1.4581		H15	2.5884	0.5243	-1.7421
	O1	1.3154	-2.3486	-0.1386		O1	-0.9288	0.1079	1.9346
	O2	-3.2750	-0.2460	-1.1199		O2	-1.5538	2.1400	0.0660
	O3	0.1230	3.0456	-0.5694		O3	1.6836	-0.0097	1.0839
	O4	-1.6796	1.4642	0.6759		O4	0.9920	-2.2497	-0.1075
	O5	-1.6185	-2.0540	-0.0249		O5	-3.0355	0.1906	-1.4867
	O6	3.3218	-0.3478	-1.0832		O6	1.3240	2.1864	-0.3255
	O7	1.9106	1.0964	0.6954		O7	2.9324	-0.2940	-1.3560
	O8	-0.0718	-0.5281	1.4644		O8	-1.6725	-2.0260	0.0153
A15	H1	0.3689	1.5060	-0.2511	A15	H13	1.2277	-2.0461	-1.3712
	H2	2.6720	1.4540	-0.1199		H14	-0.6747	0.5816	-1.9242
	H3	-1.7730	1.2186	-0.1402		H15	0.6537	3.0220	-0.1186
	H4	-3.5455	-1.1599	0.2839		O1	-0.5700	0.3525	-0.9897
	H5	-1.3243	-2.2498	0.3455		O2	0.9430	2.1725	0.2362
	H6	0.6951	-0.6567	-0.9165		O3	-1.8491	-1.9501	-0.4082
	H7	3.5275	-0.5875	1.2506		O4	1.4928	-1.2770	-0.8525
	H8	2.4873	-1.5870	0.8730		O5	3.1849	-1.4505	1.5385
	H9	2.9759	0.1232	-0.7682		O6	3.4288	0.8804	-0.3571
	H10	-1.9014	1.9616	1.1915		O7	-2.4242	1.7375	0.4106

	H11	-3.7604	0.2895	0.6408		O8	-4.2337	-0.5633	0.6321
	H12	-1.4095	-1.0868	-0.6540					

Table S2. The Cartesian coordinates for the twelve low-energy structures of neutral $OH(H_2O)_7$ clusters.

Structure	Atom	*X* (Å)	*Y* (Å)	*Z* (Å)	Structure	Atom	*X* (Å)	*Y* (Å)	*Z* (Å)
N1	H1	1.3825	1.7840	0.4064	N2	H1	3.1286	0.5738	1.2911
	H2	-0.2325	1.6240	-1.2245		H2	1.0725	-1.4648	-1.0149
	H3	0.7266	-0.1650	-1.9910		H3	0.5091	0.3472	-2.0414
	H4	3.0576	-0.9985	-1.2721		H4	-2.2497	0.3926	-0.5785
	H5	1.4773	0.7507	1.5160		H5	-1.1697	1.5146	0.9760
	H6	-2.8792	-1.6949	-0.9992		H6	0.5960	0.7363	1.9925
	H7	-0.8048	-0.3431	-1.9590		H7	2.1548	-0.4085	0.5778
	H8	2.2372	-0.0653	-0.3149		H8	2.0519	-2.6022	-0.5577
	H9	-0.4754	3.1316	-0.8753		H9	-0.7198	-0.5756	-1.8855
	H10	-0.5359	-2.1512	0.0533		H10	-3.2125	-0.5888	-1.3211
	H11	0.1511	-1.0306	1.7980		H11	-2.0965	2.6157	0.3679
	H12	-1.5253	1.4389	0.6230		H12	-0.5978	-0.2200	2.0520
	H13	0.9922	-1.9781	0.0023		H13	1.6645	1.6023	-0.4948
	H14	0.0186	-0.4199	3.2242		H14	-1.5638	-1.5727	0.5356
	H15	-2.2495	-0.5604	-0.1452		H15	-0.1503	-2.0722	0.8391
	O1	2.0199	1.1685	0.8133		O1	-0.9859	-1.8309	1.2769
	O2	-0.2840	2.2755	-0.4725		O2	1.3535	1.9783	-1.3528
	O3	-0.1087	0.2778	-2.2434		O3	1.5215	-1.8707	-0.2183
	O4	-2.0369	-1.2728	-0.7899		O4	0.2260	-0.5827	-2.1345
	O5	0.2706	-2.2859	0.5837		O5	-2.3273	-0.5251	-0.9428
	O6	0.1138	-0.1769	2.2955		O6	-1.6071	1.8177	0.1354
	O7	-2.3017	0.9090	0.9321		O7	-0.3484	0.7159	2.2260
	O8	2.1595	-0.8104	-0.9740		O8	2.2405	0.5129	0.9177
N3	H1	1.6568	-1.4819	0.3008	N4	H1	-0.2525	0.5853	-0.8313
	H2	-0.8177	-1.4201	-2.6625		H2	4.1113	-0.7548	-0.3202
	H3	-1.0131	-1.3142	-1.1085		H3	-2.3055	-1.0905	0.7844
	H4	-1.0319	-1.5399	1.0086		H4	-0.4085	0.0740	1.3043
	H5	0.6505	-0.0816	1.7467		H5	-1.6058	-1.0892	-1.2367
	H6	1.7177	1.5574	0.7906		H6	-0.9568	-1.1646	-2.6581
	H7	1.3048	-1.3142	-1.1753		H7	-0.5498	-0.4893	2.7507
	H8	-0.8471	2.3047	-1.7648		H8	-3.1219	-0.0678	0.0019
	H9	2.9163	0.1684	-0.4726		H9	2.6370	-1.0180	0.0871
	H10	-3.3369	1.3362	1.2246		H10	2.8097	1.2720	-0.1319
	H11	-2.4778	1.2873	-0.0561		H11	-1.9005	1.8905	0.0026
	H12	-0.7449	0.7678	-1.5462		H12	2.7254	2.7505	0.3309

	H13	-2.3395	-0.8799	0.5186		H13	0.6575	1.6459	-0.1344
	H14	0.7572	-1.2378	2.7962		H14	0.6987	-1.8407	0.8295
	H15	0.2320	1.6719	0.4425		H15	0.6451	-1.8612	-0.6883
	O1	2.0710	-1.3618	-0.5741		O1	-0.7502	-0.9942	-1.7311
	O2	-0.9219	1.6222	-1.0861		O2	-0.6333	-0.7355	1.8210
	O3	0.5615	-1.0642	1.8673		O3	3.3692	-0.3564	0.1497
	O4	0.8305	1.5303	1.2002		O4	-2.8390	-1.0005	-0.0268
	O5	3.2591	1.0921	-0.3147		O5	2.3220	2.1179	-0.2757
	O6	-0.4822	-0.9607	-1.8823		O6	1.2453	-2.0612	0.0538
	O7	-1.7391	-1.6320	0.3393		O7	-0.2262	1.2082	-0.0769
	O8	-3.1571	0.7961	0.4451		O8	-2.8856	1.9665	0.0748
N5	H1	-0.0981	-1.7658	-0.3322	N6	H1	0.2192	0.9478	1.4180
	H2	0.0505	1.7742	0.2038		H2	-2.1262	1.2707	0.6314
	H3	-2.5461	-2.3349	-1.4854		H3	1.6192	-0.7112	1.9426
	H4	3.7815	-1.8673	0.6234		H4	0.2471	1.7763	0.1009
	H5	-2.1786	2.4066	1.6329		H5	-0.4724	-0.2750	-0.2464
	H6	0.5621	-0.3995	-0.0663		H6	1.0955	-0.6424	-1.7927
	H7	-2.2094	-1.2405	1.0568		H7	-3.5776	1.4640	1.1504
	H8	3.4927	0.4462	-0.0346		H8	1.8124	-2.9368	0.9157
	H9	-2.1697	1.3085	-0.8366		H9	-1.3274	-1.4025	-0.8732
	H10	-0.8459	-1.0346	1.6501		H10	2.5399	-0.7886	-1.3511
	H11	-1.0312	1.0403	-1.7856		H11	1.5283	2.9308	-1.6860
	H12	-2.0929	-0.8567	-1.2929		H12	0.8987	-1.9158	0.1869
	H13	1.5305	1.5916	-0.3065		H13	2.1779	0.4989	2.7231
	H14	-1.8203	0.9005	1.4299		H14	-3.3120	-0.5050	-0.3063
	H15	2.3707	-1.5251	0.0758		H15	1.8057	1.4268	-1.4205
	O1	-2.0366	-1.7632	-0.8984		O1	-0.3498	1.2409	0.6713
	O2	0.6026	1.3244	-0.4617		O2	-3.2505	-1.3898	-0.7535
	O3	-1.7443	1.8005	1.0206		O3	1.3517	0.0540	2.4957
	O4	3.3255	-1.3085	-0.0173		O4	1.7648	-2.0105	0.6481
	O5	0.5902	-1.3451	0.2147		O5	1.5764	2.2771	-0.9781
	O6	-1.7775	-0.7916	1.8065		O6	1.9844	-0.2670	-1.9493
	O7	3.4163	1.4375	-0.0602		O7	-0.3997	-1.1295	-0.7342
	O8	-1.9756	0.8406	-1.6708		O8	-3.0684	1.0824	0.4260
N7	H1	0.3925	1.8176	0.0204	N8	H1	0.4717	0.8577	1.4827
	H2	0.5491	0.2646	1.7805		H2	2.9288	0.3704	-0.3391
	H3	1.3513	-1.5170	0.7149		H3	-0.6111	1.7271	-0.2351
	H4	0.4265	-1.5305	-1.0945		H4	-0.7318	-1.2052	-1.2110
	H5	3.6597	0.9884	-1.1184		H5	-2.4480	-0.9871	0.3001
	H6	-0.5684	-0.7897	1.7432		H6	3.8870	1.5027	0.1066
	H7	2.3977	-1.0776	-0.3190		H7	-2.9325	1.1124	-0.1601
	H8	2.6225	1.1394	0.0149		H8	-4.3802	0.5822	-0.0990
	H9	1.0550	2.7384	1.0944		H9	1.4178	1.7200	0.6409
	H10	-2.6314	-2.0881	0.7822		H10	2.6198	-2.0931	-0.8000

	H11	-1.6375	1.5636	-0.9129		H11	0.9046	-1.4739	2.6543
	H12	-3.0676	0.3060	0.3111		H12	1.2528	-1.3101	1.1498
	H13	-1.6398	-1.4444	-0.2331		H13	1.3734	-1.1847	-1.0549
	H14	-0.4852	-1.8400	-2.3440		H14	-0.2344	-0.0154	-2.0599
	H15	-0.6163	0.5757	-1.4975		H15	-1.1233	-1.4918	0.9247
	O1	-0.4582	-1.3185	-1.5322		O1	-0.0321	-0.9427	-1.8609
	O2	1.7184	-1.7654	-0.1627		O2	-1.2797	1.6201	-0.9794
	O3	3.3172	0.5434	-0.3337		O3	-3.5270	0.5272	0.3487
	O4	1.0734	1.8390	0.7444		O4	0.5073	1.7041	1.0012
	O5	-2.1815	-1.2602	0.5714		O5	2.1591	-1.3221	-0.4454
	O6	0.3550	-0.6612	2.0191		O6	2.9967	1.3402	-0.2274
	O7	-0.7170	1.5104	-1.2300		O7	-1.7165	-1.6227	0.1646
	O8	-3.3332	1.2242	0.0559		O8	0.5929	-1.0680	1.8360
N9	H1	-2.6450	1.1725	2.0827	N10	H1	-0.4216	-0.4657	0.7589
	H2	-1.0053	-0.6202	2.0111		H2	1.6047	-1.6467	0.7457
	H3	3.8675	-1.3029	0.1871		H3	-0.9392	1.7717	1.0124
	H4	0.8235	1.8586	-0.0862		H4	-0.6944	-1.6166	-0.2353
	H5	-0.6600	1.6961	0.3670		H5	0.8722	0.1699	-0.9941
	H6	-3.9320	0.0605	-1.2551		H6	-2.8602	0.5111	0.4679
	H7	-0.5362	-0.0423	-2.8919		H7	2.7294	-2.6657	1.0771
	H8	3.1165	2.3901	0.0630		H8	0.2781	3.6207	0.1002
	H9	-0.4429	0.6232	-1.4729		H9	2.2461	0.8391	-1.1225
	H10	-2.4354	-0.3262	-1.3367		H10	-3.7393	0.7558	-0.7727
	H11	0.3997	-1.8853	0.4863		H11	-2.6993	-2.9927	-0.5977
	H12	2.4080	-1.2608	-0.3330		H12	0.4501	2.2337	-0.5955
	H13	-2.6151	0.4256	0.7139		H13	-1.4402	1.2312	2.3930
	H14	0.2754	-1.4916	-0.9941		H14	3.5408	-0.5576	0.1480
	H15	2.8587	0.8706	0.2071		H15	-2.8116	-1.4521	-0.6908
	O1	-0.7587	-0.1896	-1.9642		O1	0.0346	-1.0839	0.1551
	O2	0.8411	-1.9918	-0.3765		O2	3.9428	0.1833	-0.3766
	O3	-2.0444	0.7626	1.4480		O3	-1.3885	1.0048	1.4564
	O4	-0.4044	-1.3841	2.1946		O4	-0.1952	2.8047	-0.1001
	O5	3.2552	-0.7492	-0.3121		O5	-2.2300	-2.2123	-0.9169
	O6	2.4967	1.7573	0.4458		O6	-3.5287	0.0867	-0.1089
	O7	-0.1047	1.8497	-0.4170		O7	1.3069	0.9702	-1.3512
	O8	-3.2154	-0.3260	-0.7370		O8	2.5437	-1.7205	1.0304
N11	H1	0.6645	-1.3944	-0.5422	N12	H1	1.0067	1.7804	-1.0346
	H2	-0.5063	-0.3276	-0.6736		H2	1.6125	-1.5230	0.9159
	H3	2.8495	-1.3122	-0.7527		H3	-2.0768	-3.0773	-0.7826
	H4	4.3568	-0.1533	0.7935		H4	-0.8184	2.4194	0.4537
	H5	1.0080	0.8135	2.3745		H5	2.6043	-1.8043	2.0700
	H6	-1.4724	-1.6850	0.7472		H6	-1.1973	-1.8074	-0.6150
	H7	-2.5338	-2.7440	1.1462		H7	0.5051	-0.2359	-0.4348
	H8	-1.0362	1.7181	-1.0647		H8	-2.0635	1.2320	2.1938

H9	2.4235	-1.9318	-2.1031	H9	-3.2025	-0.9497	-0.4601
H10	2.9072	0.3827	0.7801	H10	2.2547	0.8445	-1.0775
H11	0.7167	0.1452	0.9926	H11	3.4946	-0.4849	0.2262
H12	-3.4371	-0.6452	0.3231	H12	-2.5186	0.6861	0.8091
H13	0.5360	2.3436	0.4949	H13	-0.4516	-0.2786	0.7761
H14	-2.3045	0.8161	-1.1103	H14	-4.0943	0.2549	-0.8538
H15	0.6303	3.5154	-0.5037	H15	4.5047	-0.0892	-0.8730
O1	-0.0034	2.9276	-0.0743	O1	1.3178	0.9177	-1.3593
O2	2.2437	-1.9721	-1.1555	O2	2.5483	-1.7559	1.1079
O3	3.6150	0.0273	0.2032	O3	-2.0453	-2.1369	-0.9950
O4	1.2438	0.8646	1.4391	O4	-1.7402	1.0591	1.3005
O5	-2.3576	-1.7956	1.1621	O5	0.0735	-0.8699	0.2036
O6	-1.3923	0.8911	-1.4473	O6	-3.6796	-0.1676	-0.0913
O7	-3.8969	0.0611	-0.2008	O7	3.8138	0.2762	-0.3068
O8	-0.0526	-0.9467	-0.0392	O8	-0.2332	3.0564	-0.0238

Table S3. The Cartesian coordinates for the twelve low-energy structures of cationic $OH^+(H_2O)_7$ clusters.

Structure	Atom	*X* (Å)	*Y* (Å)	*Z* (Å)	Structure	Atom	*X* (Å)	*Y* (Å)	*Z* (Å)
C1	H1	4.8441	0.8002	-0.5302	C2	H1	-4.0189	-2.1472	1.2736
	H2	-2.3904	-1.5333	-0.2859		H2	1.5543	0.5198	1.3965
	H3	2.9054	-2.3660	-0.2565		H3	1.1771	-1.6804	-0.2945
	H4	0.3986	-0.8657	1.9728		H4	2.8555	-1.5508	1.3373
	H5	-3.1599	4.3676	-0.1880		H5	0.6910	-2.4669	-1.5545
	H6	-3.9326	1.0849	1.4393		H6	-0.9566	-1.2743	-0.7510
	H7	-4.0739	3.7029	-1.2260		H7	-2.5459	-1.2759	-0.2828
	H8	-2.4150	0.0392	0.2498		H8	-1.6753	0.1779	-0.2617
	H9	3.0151	-0.8396	-0.5309		H9	-1.5384	2.2392	-0.0447
	H10	-0.9910	-0.8997	0.3930		H10	-0.5529	1.4260	0.8836
	H11	-3.3013	2.0371	0.3743		H11	5.2102	-0.3946	-1.2762
	H12	1.0557	-1.3537	0.6251		H12	3.2487	-0.6099	0.1702
	H13	-3.2986	-3.6309	0.0249		H13	-4.5176	-2.4187	-0.1575
	H14	4.1870	0.7217	-1.9184		H14	1.1586	1.5469	2.4930
	H15	-3.5126	-3.1635	-1.4249		H15	4.8382	0.9790	-0.7061
	O1	4.0338	0.5225	-0.9858		O1	-3.7282	-2.1902	0.3525
	O2	-3.3382	-2.8398	-0.5302		O2	0.9860	1.2941	1.5772
	O3	-3.4248	3.5063	-0.5376		O3	-1.9668	4.0156	-1.0109
	O4	-3.1532	1.2068	0.8825		O4	-1.4338	1.4000	0.4330
	O5	2.3841	-1.5549	-0.2959		O5	4.4965	0.0836	-0.8330
	O6	0.1955	-1.2834	1.1262		O6	2.4772	-0.9445	0.6850
	O7	6.4866	1.3816	0.6699		O7	-1.8278	-0.7495	-0.7381

	O8	-1.8500	-0.7018	-0.1690		O8	0.3809	-2.0428	-0.7438
C3	H1	-2.3502	2.6502	1.2171	C4	H1	2.9290	-0.2944	-1.8744
	H2	4.4043	-0.3204	0.4521		H2	1.9510	0.0798	0.0353
	H3	2.2312	-0.0342	-0.0518		H3	0.9030	1.3500	0.4362
	H4	0.9981	0.9252	-0.6866		H4	0.3287	3.4179	0.4438
	H5	0.2608	2.7478	-1.4731		H5	-2.7671	1.2452	-0.2784
	H6	-2.3506	1.1548	0.7920		H6	-3.8810	-0.1743	1.3554
	H7	-3.5509	-0.8388	0.3460		H7	6.1813	-0.3813	-0.0046
	H8	-5.3623	-1.8680	-0.9368		H8	-0.5967	-1.7439	2.0260
	H9	-3.0463	-0.9583	1.8070		H9	-0.7059	2.4878	-0.2749
	H10	-5.3719	-0.3505	-1.1548		H10	-3.7321	-1.0440	0.0953
	H11	-1.2426	-1.3908	0.3724		H11	5.8778	-1.8772	-0.1668
	H12	0.7311	-0.6974	-0.3546		H12	-1.5664	-0.9348	1.1150
	H13	-0.5394	2.2444	-0.2196		H13	3.8573	-0.6814	-0.6779
	H14	3.6826	0.3883	1.6265		H14	0.5664	-0.1947	0.9373
	H15	-0.4568	-2.5262	-0.3595		H15	-2.8718	2.4042	-1.3075
	O1	6.1594	-0.8310	-0.4597		O1	-4.5157	-2.4620	-1.1648
	O2	-2.0329	2.0431	0.5365		O2	0.2524	2.6006	-0.0661
	O3	3.5287	-0.1527	0.8410		O3	-2.3338	2.0626	-0.5824
	O4	-2.7742	-0.6618	0.9271		O4	-3.2685	-0.3770	0.6333
	O5	-4.8229	-1.0739	-0.8232		O5	5.4541	-1.0117	-0.0924
	O6	-0.3423	-1.6933	0.1163		O6	-0.6285	-1.1857	1.2381
	O7	1.4268	-0.0189	-0.6589		O7	2.9190	-0.5407	-0.9408
	O8	0.3528	2.2479	-0.6511		O8	1.3119	0.4564	0.7427
C5	H1	1.0620	-3.4509	0.7702	C6	H1	1.7086	-0.9533	2.8113
	H2	1.3299	-1.9248	0.6436		H2	0.5534	-1.5774	0.9911
	H3	2.8805	-0.1406	0.6513		H3	4.2783	-0.1053	0.1702
	H4	-1.8171	-0.8336	-0.8616		H4	-3.7639	0.5580	-1.9370
	H5	-0.5702	-2.4765	-0.6023		H5	3.5577	3.3433	-1.0571
	H6	-4.5320	-0.1932	1.4650		H6	-0.8886	-1.8596	0.1539
	H7	4.6687	-0.6796	-0.8676		H7	2.3509	-0.6899	-1.2034
	H8	0.1858	2.1900	0.0489		H8	3.4429	3.5247	0.4620
	H9	-5.0223	0.8088	0.4040		H9	-2.9592	-2.3751	0.1275
	H10	-1.3828	-2.6034	-1.9401		H10	0.6292	-1.7834	-0.6033
	H11	2.2701	-0.1860	2.0756		H11	2.2243	-0.3492	1.4631
	H12	-1.2732	0.6411	-0.2430		H12	-2.7945	-0.8725	-0.2993
	H13	4.9938	0.6916	-0.2652		H13	1.9893	-1.6464	-2.3855
	H14	0.7019	0.8261	0.6373		H14	3.3893	1.1444	-0.0291
	H15	-2.8823	0.2140	-0.0981		H15	-4.0811	1.0879	-0.5247
	O1	0.5447	4.1126	-0.6513		O1	0.1180	-2.0758	0.2218
	O2	2.0348	-0.2707	1.1410		O2	3.3530	0.1661	0.0907
	O3	-2.0689	0.1557	-0.6778		O3	-3.4727	0.5133	-1.0172
	O4	0.8928	-2.6835	0.2088		O4	1.4265	-0.6774	1.9293
	O5	-1.4249	-2.2405	-1.0454		O5	-5.2274	2.2925	0.7409

	O6	-4.2224	0.4252	0.7893		O6	-2.3521	-1.6252	0.1628
	O7	4.2722	0.0599	-0.3872		O7	1.6071	-1.1444	-1.6537
	O8	-0.1050	1.3311	0.3952		O8	3.3429	2.8702	-0.2421
C7	H1	-2.3871	-1.2346	0.1018	C8	H1	0.3096	-1.9762	0.2421
	H2	3.8299	1.1680	-1.6005		H2	-1.0166	-0.9730	0.4336
	H3	2.8471	-0.9699	-0.7456		H3	-0.9290	2.8752	-1.6401
	H4	1.0592	-2.0858	0.4623		H4	2.4056	2.6272	0.2171
	H5	-1.3356	2.1943	-0.1223		H5	3.4906	-0.2985	-1.9501
	H6	1.8725	2.0617	1.7166		H6	1.6440	-3.3570	-0.6948
	H7	2.6906	-2.4433	-1.1901		H7	0.2130	-0.8962	1.5049
	H8	0.6134	-2.4737	1.9149		H8	-1.7619	0.8895	-0.4511
	H9	0.0501	1.5452	0.2606		H9	-1.2257	3.3307	-0.2109
	H10	2.4149	1.3533	0.4556		H10	0.9763	2.2158	-0.2001
	H11	4.6986	0.7228	-0.4228		H11	2.6343	0.4095	-0.8692
	H12	-1.4190	0.1096	0.3634		H12	1.9332	-1.8421	-1.0084
	H13	-3.3936	-2.3638	-1.6513		H13	1.5252	0.1096	3.0383
	H14	-4.3884	-2.1610	-0.4943		H14	-2.9399	-0.1382	-0.3088
	H15	-0.9139	-1.4178	0.8643		H15	1.4671	0.8609	1.6655
	O1	-3.5578	-1.8293	-0.8626		O1	-4.9324	-0.6472	-0.2293
	O2	0.2769	-2.2966	1.0270		O2	0.9780	0.2525	2.2549
	O3	-0.8296	1.3664	-0.1463		O3	-1.9738	-0.0567	-0.3692
	O4	1.6171	1.4605	1.0046		O4	-0.8355	2.6002	-0.7150
	O5	3.7840	0.7231	-0.7414		O5	1.8270	1.8571	0.1225
	O6	2.2395	-1.7300	-0.7204		O6	2.9501	-0.4628	-1.1668
	O7	-2.5750	3.8638	-0.2774		O7	1.2218	-2.4938	-0.7967
	O8	-1.7349	-0.8086	0.7274		O8	-0.3258	-1.5290	0.9285
C9	H1	-4.7589	0.8197	-0.1598	C10	H1	0.9580	0.9565	0.0370
	H2	-0.8974	-1.6029	-0.7277		H2	3.3418	0.5766	0.6117
	H3	4.6388	-0.6592	-0.3832		H3	2.0881	-3.0928	0.3643
	H4	3.1737	1.2355	-0.1384		H4	-0.1759	-0.4921	-0.9705
	H5	-0.4991	1.5277	-0.2001		H5	-0.3923	1.6313	-0.4156
	H6	1.1013	1.5249	-0.6671		H6	-3.0339	-1.0311	0.2099
	H7	-4.5747	0.1992	1.2265		H7	-4.0250	0.6873	1.5494
	H8	0.5602	-1.7724	-0.1602		H8	0.3296	-1.9525	-0.5225
	H9	-3.2005	-1.1931	-0.2936		H9	-1.3127	-1.6859	-0.7582
	H10	0.1424	0.1458	-0.8493		H10	-3.3970	-2.2165	-0.7556
	H11	-2.5442	1.4697	0.7344		H11	-3.0082	1.3445	0.5825
	H12	4.5742	-0.2519	1.0896		H12	-1.8686	3.5729	0.2419
	H13	2.9907	2.6246	-0.8317		H13	2.0572	-1.5671	0.6995
	H14	-1.7830	2.7281	1.2383		H14	-2.2534	3.0668	-1.1465
	H15	-3.0637	-2.5338	-1.0558		H15	2.5926	0.4623	1.9489
	O1	2.0477	-2.4989	1.1097		O1	5.0068	1.1738	-0.4335
	O2	2.5290	1.9586	-0.3056		O2	0.2667	0.9524	-0.6507
	O3	-2.5747	-1.9061	-0.5082		O3	-3.2673	0.4960	0.9817

	O4	0.1618	1.1919	-0.8794		O4	-1.9533	2.7597	-0.2777
	O5	-4.0892	0.4247	0.4185		O5	2.5072	0.2634	1.0051
	O6	0.0373	-1.3023	-0.8295		O6	1.4980	-2.3358	0.4749
	O7	-1.6523	1.8441	0.8710		O7	-0.3585	-1.4883	-1.0996
	O8	4.0580	-0.2448	0.2708		O8	-2.6872	-1.8537	-0.2098
C11	H1	-0.9908	1.6836	-0.6842	C12	H1	0.8495	-1.7145	0.3244
	H2	1.3580	0.7498	-0.3238		H2	-0.3826	-0.3635	-2.9263
	H3	1.5166	-1.2723	-1.0646		H3	0.6336	2.8704	-0.6711
	H4	-0.4126	0.9525	-1.9122		H4	-0.1499	1.3816	2.7977
	H5	-3.2407	2.9449	-0.3829		H5	-0.1210	-2.3116	2.2044
	H6	1.1973	-0.3660	1.5662		H6	-3.1828	-1.5238	-0.6121
	H7	-3.0832	0.4895	-0.0151		H7	-1.9351	-1.5760	0.3099
	H8	-2.6375	2.7264	1.0048		H8	-1.1580	-0.5817	-1.5787
	H9	-0.4899	-1.4588	1.1122		H9	0.2501	1.4385	-1.0994
	H10	2.8892	0.6228	0.0018		H10	0.0990	1.4172	1.2634
	H11	-0.3581	-1.9164	-0.4366		H11	-0.2385	-0.7821	1.8327
	H12	1.2355	-2.6094	-1.8269		H12	3.8879	0.4739	-0.2461
	H13	-3.9549	-0.8022	0.0371		H13	0.8054	-1.1612	-1.1952
	H14	0.7632	-1.0758	2.8954		H14	2.1372	-0.8670	-0.2972
	H15	-1.8106	-1.3090	0.1224		H15	2.4668	1.1427	-0.1924
	O1	-0.3061	1.0483	-0.9556		O1	-2.5544	1.7942	-0.0783
	O2	-1.0084	-1.8904	0.3460		O2	-2.3103	-1.1337	-0.4702
	O3	-3.0792	-0.4693	-0.2008		O3	-0.2949	-0.2784	-1.9660
	O4	-2.6914	2.3282	0.1235		O4	0.7841	1.9396	-0.4529
	O5	0.4216	-0.6802	2.0822		O5	-0.2950	0.8858	1.9814
	O6	2.0434	0.1465	0.0373		O6	-0.2235	-1.7044	1.4578
	O7	0.8095	-1.8191	-1.4681		O7	2.9764	0.3424	0.0480
	O8	4.8129	1.4160	0.0237		O8	1.4224	-1.5756	-0.5090

Table S4. The total energies (Hartree) of the fifteen $OH^-(H_2O)_7$ isomers with (E_0) and without (E_e) ZPVE correction for CCSD(T), MP2, and DFT methods combining different basis sets.

	E_e	E_0							
	CCSD(T)[a]	CCSD(T)[a]	MP2[b]	B3LYPD3[b]	wB97XD[b]	M062X[b]	B3LYP[b]	BLYP[b]	MP2[c]
A1	-610.62428	-610.43513	-610.02517	-611.12546	-610.90131	-610.83442	-611.10015	-610.97629	-609.58823
A2	-610.62330	-610.43443	-610.02416	-611.12464	-610.90048	-610.83433	-611.10334	-610.97515	-609.58665
A3	-610.62325	-610.43490	-610.02382	-611.12490	-610.90058	-610.83601	-611.10108	-610.97515	-609.58630
A4	-610.62171	-610.43317	-610.02260	-611.12324	-610.89905	-610.83485	-611.10105	-610.97256	-609.58559
A5	-610.61451	-610.42647	-610.01665	-611.11834	-610.89286	-610.82841	-611.09633	-610.96885	-609.58023
A6	-610.62487	-610.43544	-610.02483	-611.12536	-610.90154	-610.83710	-611.10263	-610.97399	-609.58683
A7	-610.62270	-610.43321	-610.02236	-611.12442	-610.90043	-610.83472	-611.10263	-610.97424	-609.58546
A8	-610.62244	-610.43412	-610.02391	-611.12394	-610.89985	-610.83416	-611.10224	-610.97412	-609.58783
A9	-610.62236	-610.43376	-610.02320	-611.12371	-610.89959	-610.83413	-611.10255	-610.97412	-609.58597
A10	-610.62129	-610.43221	-610.02158	-611.12153	-610.89752	-610.83271	-611.09905	-610.97355	-609.58517
A11	-610.61952	-610.43271	-610.02275	-611.12331	-610.89867	-610.83345	-611.10477	-610.97718	-609.58732
A12	-610.61780	-610.43141	-610.02081	-611.12035	-610.89670	-610.83281	-611.10050	-610.97201	-609.58498
A13	-610.61668	-610.42906	-610.01935	-611.11935	-610.89485	-610.82829	-611.10178	-610.97420	-609.58348
A14	-610.61565	-610.42851	-610.01856	-611.11817	-610.89360	-610.82697	-611.10015	-610.97217	-609.58361
A15	-610.61246	-610.42749	-610.01710	-611.11654	-610.89277	-610.82590	-611.09982	-610.97171	-609.58240

[a] The CCSD(T) method with extrapolated complete basis set (CBS) scheme was used.

[b] These total energies were obtained using the aug-cc-pVDZ basis set for ZPVE, and aug-cc-pVTZ for single point energy.

[c] The MP2 energies denotes MP2/6-311++G** energies.

Table S5. The total energies (Hartree) of the twelve $OH(H_2O)_7$ isomers with (E_0) and without (E_e) ZPVE correction for CCSD(T), MP2, and DFT methods combining with different basis sets.

	E_e	E_0							
	CCSD(T)[a]	CCSD(T)[a]	MP2[b]	B3LYPD3[b]	wB97XD[b]	M062X[b]	B3LYP[b]	BLYP[b]	MP2[c]
N1	-610.45729	-610.26901	-609.85227	-610.96357	-610.74034	-610.67123	-610.94337	-610.81952	-609.43127
N2	-610.45489	-610.26708	-609.85057	-610.96095	-610.73819	-610.66921	-610.94176	-610.81212	-609.42925
N3	-610.45531	-610.26746	-609.85087	-610.96016	-610.73876	-610.67125	-610.94083	-610.81226	-609.42929
N4	-610.45449	-610.26711	-609.85050	-610.95937	-610.73840	-610.66884	-610.94129	-610.81119	-609.42864
N5	-610.45463	-610.26701	-609.85006	-610.95918	-610.73790	-610.66933	-610.94143	-610.81339	-609.42787
N6	-610.45375	-610.26680	-609.85025	-610.95755	-610.73648	-610.66885	-610.94162	-610.81257	-609.42883
N7	-610.45446	-610.26680	-609.85032	-610.95947	-610.73806	-610.66751	-610.94140	-610.81270	-609.42767
N8	-610.45180	-610.26516	-609.84824	-610.95818	-610.73599	-610.66716	-610.94037	-610.81321	-609.42784
N9	-610.45163	-610.26499	-609.84870	-610.95735	-610.73579	-610.66406	-610.94171	-610.81337	-609.42633
N10	-610.45126	-610.26489	-609.84847	-610.95706	-610.73631	-610.66663	-610.94194	-610.81296	-609.42624
N11	-610.45063	-610.26411	-609.84769	-610.95609	-610.73521	-610.66363	-610.94090	-610.81181	-609.42617
N12	-610.45023	-610.26376	-609.84727	-610.95567	-610.73468	-610.66310	-610.94058	-610.81275	-609.42916

[a] The CCSD(T) method with extrapolated complete basis set (CBS) scheme was used.

[b] These total energies were obtained using the aug-cc-pVDZ basis set for ZPVE, and aug-cc-pVTZ for single point energy.

[c] The MP2 energies denotes MP2/6-311++G** energies.

Table S6. The total energies (Hartree) of the twelve $OH^+(H_2O)_7$ isomers with (E_0) and without (E_e) ZPVE correction for CCSD(T), MP2, and DFT methods combining with different basis sets.

	E_e	E_0			
	CCSD(T)[a]	CCSD(T)[a]	MP2[b]	B3LYPD3[b]	wB97XD[b]
C1	-610.13583	-609.95336	-609.53842	-610.64194	-610.42793
C2	-610.14230	-609.95798	-609.54298	-610.64678	-610.43211
C3	-610.14266	-609.95781	-609.54284	-610.64677	-610.43212
C4	-610.14210	-609.95763	-609.54257	-610.64624	-610.43162
C5	-610.14215	-609.95755	-609.54256	-610.64630	-610.43170
C6	-610.14107	-609.95640	-609.54150	-610.64522	-610.43083
C7	-610.14039	-609.95593	-609.54093	-610.64437	-610.43004
C8	-610.14276	-609.95620	-609.54124	-610.64500	-610.42971
C9	-610.14060	-609.95578	-609.54051	-610.64499	-610.42872
C10	-610.14176	-609.95547	-609.54046	-610.64423	-610.42928
C11	-610.14280	-609.95572	-609.54082	-610.64420	-610.42621
C12	-610.14031	-609.95315	-609.53839	-610.64448	-610.42671

[a] The CCSD(T) method with extrapolated complete basis set (CBS) scheme was used.

[b] These total energies were obtained using the aug-cc-pVDZ basis set for ZPVE, and aug-cc-pVTZ for single point energy.

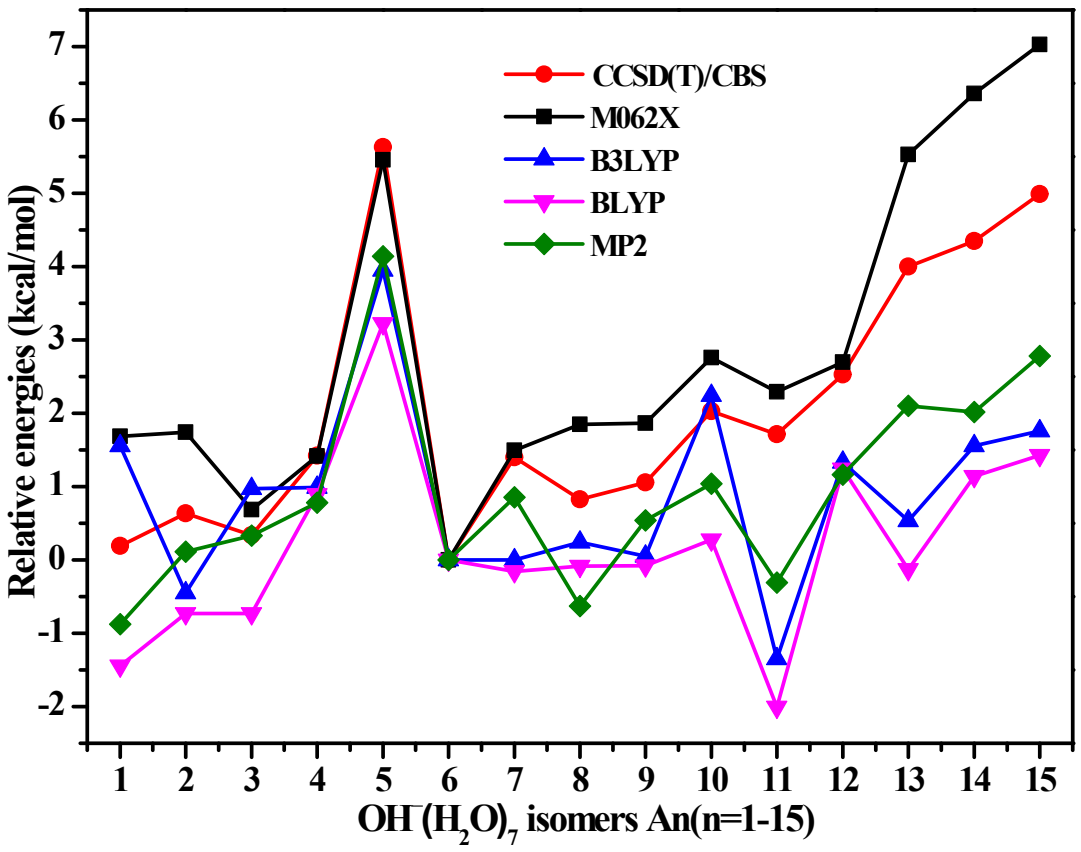

Figure S1. Relative energies (kcal/mol) of the fifteen $OH^-(H_2O)_7$ isomers with ZPVE correction with respect to A6 at CCSD(T), MP2, and DFT (BLYP, B3LYP and M06-2X) levels, respectively. The MP2 energies denotes MP2/6-311++G** energies. The DFT energies were obtained using the aug-cc-pVDZ basis set for ZPVE and aug-cc-pVTZ for single point energy.

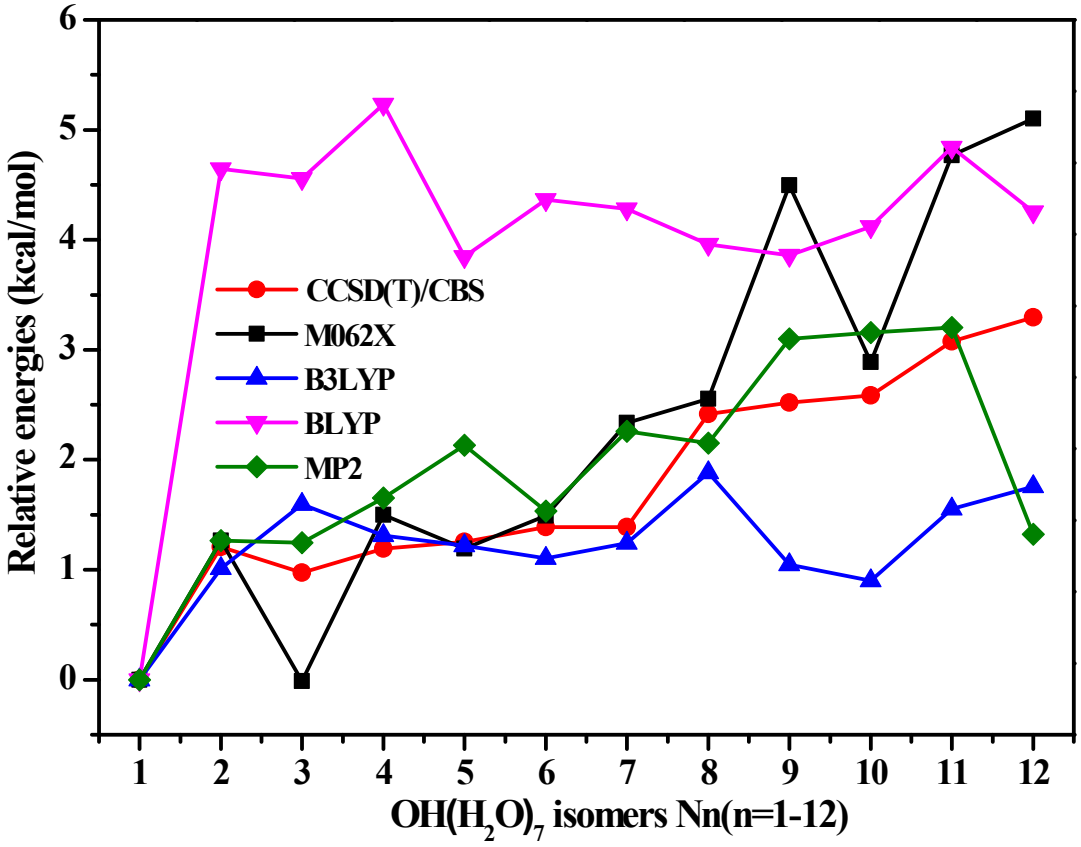

Figure S2. Relative energies (kcal/mol) of the twelve $OH(H_2O)_7$ isomers with ZPVE correction with respect to N1 at CCSD(T), MP2, and DFT (BLYP, B3LYP and M06-2X) levels, respectively. The MP2 energies denotes MP2/6-311++G** energies. The DFT energies were obtained using aug-cc-pVDZ basis set for ZPVE and aug-cc-pVTZ for single point energy.