Electronic Supplementary Information

How flexible is the water molecule structure? Analysis of crystal structures and potential energy surface.

Milan R. Milovanović,[a] Jelena M. Živković,[a] Dragan B. Ninković,[a] Ivana M. Stanković [b] and Snežana D. Zarić [*c,d]

[a]Innovation center of the Faculty of Chemistry, Studentski trg 12-16, Belgrade, 11000, Serbia.
[b]Institute of Chemistry, Technology and Metallurgy, University of Belgrade, Njegoševa 12, 11000 Belgrade, Serbia.
[c]Faculty of Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade, 11000, Serbia.
[d]Texas A&M University at Qatar, Education City, PO Box 23874, Doha, Qatar

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1. Computational results.

Table ESI 1a. Calculated absolute energies of water molecule at CCSD(T)/aug-cc-PV6Z level of theory. The bond angle (H-O-H) and bond lengths (O-H) were systematically varied from 90.0° to 116.5° and from 0.900 Å to 0.955 Å, respectively. The data correspond to Figure 1.

H-O-H (Å) / O-H (°)	0.900	0.905	0.910	0.915	0.920	0.925	0.930	0.935	0.940	0.945	0.950	0.955
93.0	-76.359950547	-76.361410076	-76.362729556	-76.363913608	-76.364966711	-76.365893208	-76.366697308	-76.367383090	-76.367954507	-76.368415395	-76.368769468	-76.369020330
93.5	-76.360333666	-76.361785773	-76.363097898	-76.364274662	-76.365320545	-76.366239889	-76.367036902	-76.367715665	-76.368280132	-76.368734137	-76.369081395	-76.369325510
94.0	-76.360701351	-76.362146120	-76.363450975	-76.364620535	-76.365659280	-76.366571554	-76.367361564	-76.368033391	-76.368590989	-76.369038191	-76.369378716	-76.369616166
94.5	-76.361053711	-76.362491227	-76.363788894	-76.364951332	-76.365983022	-76.366888306	-76.367671394	-76.368336365	-76.368887175	-76.369327657	-76.369661528	-76.369892391
95.0	-76.361390854	-76.362821201	-76.364111762	-76.365267159	-76.366291874	-76.367190250	-76.367966495	-76.368624691	-76.369168792	-76.369602631	-76.369929927	-76.370154283
95.5	-76.361712898	-76.363136151	-76.364419685	-76.365568122	-76.366585941	-76.367477487	-76.368246969	-76.368898467	-76.369435937	-76.369863213	-76.370184011	-76.370401936
96.0	-76.362019945	-76.363436185	-76.364712772	-76.365854326	-76.366865328	-76.367750122	-76.368512918	-76.369157796	-76.369688712	-76.370109500	-76.370423877	-76.370635447
96.5	-76.362312106	-76.363721411	-76.364991129	-76.366125878	-76.367130140	-76.368008259	-76.368764445	-76.369402779	-76.369927217	-76.370341592	-76.370649623	-76.370854913
97.0	-76.362589492	-76.363991940	-76.365254864	-76.366382884	-76.367380482	-76.368252001	-76.369001653	-76.369633518	-76.370151551	-76.370559588	-76.370861347	-76.371060431
97.5	-76.362852213	-76.364247880	-76.365504086	-76.366625452	-76.367616460	-76.368481454	-76.369224645	-76.369850114	-76.370361817	-76.370763589	-76.371059148	-76.371252098
98.0	-76.363100377	-76.364489340	-76.365738903	-76.366853688	-76.367838180	-76.368696722	-76.369433525	-76.370052671	-76.370558116	-76.370953694	-76.371243125	-76.371430012
98.5	-76.363334106	-76.364716432	-76.365959424	-76.367067702	-76.368045749	-76.368897911	-76.369628398	-76.370241292	-76.370740549	-76.371130005	-76.371413378	-76.371594272
99.0	-76.363553501	-76.364929265	-76.366165757	-76.367267599	-76.368239274	-76.369085126	-76.369809368	-76.370416080	-76.370909220	-76.371292622	-76.371570006	-76.371744977
99.5	-76.363758677	-76.365127950	-76.366358014	-76.367453491	-76.368418862	-76.369258475	-76.369976540	-76.370577140	-76.371064231	-76.371441649	-76.371713112	-76.371882227
100.0	-76.363949746	-76.365312599	-76.366536305	-76.367625484	-76.368584622	-76.369418064	-76.370130021	-76.370724576	-76.371205686	-76.371577186	-76.371842796	-76.372006121
100.5	-76.364126823	-76.365483324	-76.366700739	-76.367783691	-76.368736663	-76.369564001	-76.370269917	-76.370858494	-76.371333689	-76.371699338	-76.371959160	-76.372116762
101.0	-76.364290015	-76.365640237	-76.366851430	-76.367928221	-76.368875093	-76.369696394	-76.370396335	-76.370979000	-76.371448345	-76.371808208	-76.372062308	-76.372214250
101.5	-76.364439447	-76.365783452	-76.366988489	-76.368059185	-76.369000023	-76.369815352	-76.370509383	-76.371086200	-76.371549761	-76.371903901	-76.372152342	-76.372298687
102.0	-76.364575229	-76.365913083	-76.367112029	-76.368176694	-76.369111564	-76.369920985	-76.370609170	-76.371180203	-76.371638042	-76.371986523	-76.372229366	-76.372370178
102.5	-76.364697478	-76.366029245	-76.367222164	-76.368280863	-76.369209827	-76.370013403	-76.370695805	-76.371261116	-76.371713295	-76.372056178	-76.372293486	-76.372428825
103.0	-76.364806308	-76.366132052	-76.367319008	-76.368371803	-76.369294923	-76.370092717	-76.370769397	-76.371329048	-76.371775628	-76.372112974	-76.372344807	-76.372474733
103.5	-76.364901838	-76.366221621	-76.367402675	-76.368449628	-76.369366967	-76.370159039	-76.370830058	-76.371384109	-76.371825150	-76.372157019	-76.372383436	-76.372508008
104.0	-76.364984185	-76.366298069	-76.367473282	-76.368514454	-76.369426071	-76.370212481	-76.370877899	-76.371426409	-76.371861970	-76.372188420	-76.372409479	-76.372528755
104.5	-76.365053476	-76.366361513	-76.367530946	-76.368566396	-76.369472351	-76.370253158	-76.370913033	-76.371456060	-76.371886198	-76.372207286	-76.372423045	-76.372537082
105.0	-76.365109815	-76.366412072	-76.367575783	-76.368605570	-76.369505921	-76.370281183	-76.370935572	-76.371473173	-76.371897946	-76.372213729	-76.372424243	-76.372533096
105.5	-76.365153330	-76.366449866	-76.367607913	-76.368632094	-76.369526897	-76.370296672	-76.370945632	-76.371477863	-76.371897326	-76.372207858	-76.372413183	-76.372516907
106.0	-76.365184142	-76.366475013	-76.367627454	-76.368646086	-76.369535398	-76.370299740	-76.370943326	-76.371470242	-76.371884449	-76.372189786	-76.372389975	-76.372488623
106.5	-76.365202372	-76.366487637	-76.367634526	-76.368647665	-76.369531541	-76.370290504	-76.370928771	-76.371450426	-76.371859431	-76.372159626	-76.372354731	-76.372448355
107.0	-76.365208138	-76.366487858	-76.367629251	-76.368636950	-76.369515444	-76.370269083	-76.370902083	-76.371418531	-76.371822386	-76.372117490	-76.372307563	-76.372396216
107.5	-76.365201583	-76.366475799	-76.367611750	-76.368614064	-76.369487229	-76.370235596	-76.370863381	-76.371374672	-76.371773430	-76.372063493	-76.372248586	-76.372332316
108.0	-76.365182816	-76.366451586	-76.367582147	-76.368579127	-76.369447015	-76.370190162	-76.370812784	-76.371318969	-76.371712678	-76.371997752	-76.372177913	-76.372256771
108.5	-76.365151965	-76.366415342	-76.367540565	-76.368532263	-76.369394925	-76.370132901	-76.370750411	-76.371251540	-76.371640250	-76.371920383	-76.372095661	-76.372169694
109.0	-76.365109159	-76.366367193	-76.367487130	-76.368473596	-76.369331081	-76.370063937	-76.370676382	-76.371172504	-76.371556264	-76.371831503	-76.372001946	-76.372071201
109.5	-76.365054525	-76.366307267	-76.367421967	-76.368403250	-76.369255608	-76.369983392	-76.370590821	-76.371081982	-76.371460839	-76.371731232	-76.371896885	-76.371961408
110.0	-76.364988185	-76.366235692	-76.367345203	-76.368321352	-76.369168630	-76.369891390	-76.370493849	-76.370980097	-76.371354096	-76.371619688	-76.371780597	-76.371840433
110.5	-76.364910292	-76.366152597	-76.367256967	-76.368228029	-76.369070274	-76.369788055	-76.370385592	-76.370866971	-76.371236158	-76.371496994	-76.371653202	-76.371708395
111.0	-76.364820954	-76.366058112	-76.367157388	-76.368123409	-76.368960667	-76.369673515	-76.370266173	-76.370742729	-76.371107147	-76.371363270	-76.371514822	-76.371565414
111.5	-76.364720312	-76.365952369	-76.367046596	-76.368007621	-76.368839937	-76.369547896	-76.370135719	-76.370607495	-76.370967188	-76.371218640	-76.371365577	-76.371411610
112.0	-76.364608498	-76.365835499	-76.366924722	-76.367880796	-76.368708213	-76.369411327	-76.369994359	-76.370461397	-76.370816406	-76.371063229	-76.371205592	-76.371247106
112.5	-76.364485647	-76.365707637	-76.366791900	-76.367743066	-76.368565627	-76.369263938	-76.369842219	-76.370304560	-76.370654927	-76.370897161	-76.371034990	-76.371072025
113.0	-76.364351887	-76.365568917	-76.366648263	-76.367594563	-76.368412310	-76.369105859	-76.369679430	-76.370137115	-76.370482879	-76.370720564	-76.370853897	-76.370886492
113.5	-76.364207372	-76.365419475	-76.366493946	-76.367435421	-76.368248395	-76.368937222	-76.369506124	-76.369959191	-76.370300390	-76.370533565	-76.370662441	-76.370690632
114.0	-76.364052230	-76.365259449	-76.366329085	-76.367265776	-76.368074015	-76.368758160	-76.369322431	-76.369770920	-76.370107592	-76.370336292	-76.370460748	-76.370484572
114.5	-76.363886605	-76.365088977	-76.366153818	-76.367085763	-76.367889308	-76.368568808	-76.369128486	-76.369572433	-76.369904615	-76.370128878	-76.370248948	-76.370268441
115.0	-76.363710631	-76.364908198	-76.365968282	-76.366895521	-76.367694408	-76.368369301	-76.368924422	-76.369363864	-76.369691592	-76.369911452	-76.370027173	-76.370042367
115.5	-76.363524453	-76.364717253	-76.365772619	-76.366695188	-76.367489455	-76.368159777	-76.368710377	-76.369145348	-76.369468657	-76.369684149	-76.369795552	-76.369806482
116.0	-76.363328213	-76.364516284	-76.365566969	-76.366484904	-76.367274586	-76.367940373	-76.368486487	-76.368917021	-76.369235944	-76.369447101	-76.369554221	-76.369560918
116.5	-76.363122056	-76.364305434	-76.365351474	-76.366264811	-76.367049943	-76.367711228	-76.368252890	-76.368679021	-76.368993591	-76.369200445	-76.369303312	-76.369305809

Table ESI 1b. Calculated absolute energies of water molecule at CCSD(T)/aug-cc-PV6Z level of theory. The bond angle (H-O-H) and bond lengths (O-H) were systematically varied from 93.0° to 116.5° and from 0.960 Å to 1.010 Å, respectively. The data correspond to Figure 1.

H-O-H (Å) / O-H (°)	0.960	0.965	0.970	0.975	0.980	0.985	0.990	0.995	1.000	1.005	1.010
93.0	-76.369171476	-76.369226293	-76.369188067	-76.369059984	-76.368845135	-76.368546518	-76.368167040	-76.367709521	-76.367176697	-76.366571222	-76.365895669
93.5	-76.369469978	-76.369518184	-76.369473417	-76.369338861	-76.369117607	-76.368812654	-76.368426909	-76.367963191	-76.367424237	-76.366812700	-76.366131155
94.0	-76.369754035	-76.369795712	-76.369744482	-76.369603533	-76.369375954	-76.369064744	-76.368672810	-76.368202972	-76.367657966	-76.367040445	-76.366352986
94.5	-76.370023742	-76.370058968	-76.370001355	-76.369854091	-76.369620265	-76.369302876	-76.368904830	-76.368428949	-76.367877969	-76.367254542	-76.366561243
95.0	-76.370279193	-76.370308046	-76.370244128	-76.370090625	-76.369850629	-76.369527137	-76.369123057	-76.368641209	-76.368084330	-76.367455072	-76.366756010
95.5	-76.370520482	-76.370543039	-76.370472891	-76.370313227	-76.370067136	-76.369737617	-76.369327578	-76.368839838	-76.368277134	-76.367642119	-76.366937368
96.0	-76.370747705	-76.370764041	-76.370687739	-76.370521988	-76.370269877	-76.369934405	-76.369518480	-76.369024922	-76.368456466	-76.367815768	-76.367105401
96.5	-76.370960958	-76.370971146	-76.370888764	-76.370716999	-76.370458942	-76.370117590	-76.369695852	-76.369196548	-76.368622414	-76.367976103	-76.367260191
97.0	-76.371160335	-76.371164449	-76.371076060	-76.370898353	-76.370634421	-76.370287262	-76.369859782	-76.369354804	-76.368775062	-76.368123210	-76.367401824
97.5	-76.371345934	-76.371344046	-76.371249720	-76.371066144	-76.370796408	-76.370443511	-76.370010361	-76.369499778	-76.368914498	-76.368257175	-76.367530384
98.0	-76.371517851	-76.371510031	-76.371409840	-76.371220463	-76.370944994	-76.370586429	-76.370147677	-76.369631558	-76.369040809	-76.368378083	-76.367645956
98.5	-76.371676183	-76.371662502	-76.371556513	-76.371361406	-76.371080271	-76.370716107	-76.370271821	-76.369750235	-76.369154084	-76.368486023	-76.367748625
99.0	-76.371821030	-76.371801554	-76.371689837	-76.371489067	-76.371202334	-76.370832637	-76.370382885	-76.369855898	-76.369254411	-76.368581080	-76.367838479
99.5	-76.371952488	-76.371927286	-76.371809907	-76.371603540	-76.371311276	-76.370936113	-76.370480960	-76.369948637	-76.369341880	-76.368663345	-76.367915605
100.0	-76.372070658	-76.372039795	-76.371916820	-76.371704922	-76.371407191	-76.371026627	-76.370566138	-76.370028543	-76.369416581	-76.368732905	-76.367980089
100.5	-76.372175638	-76.372139180	-76.372010674	-76.371793309	-76.371490176	-76.371104274	-76.370638512	-76.370095710	-76.369478605	-76.368789850	-76.368032022
101.0	-76.372267530	-76.372225540	-76.372091567	-76.371868798	-76.371560326	-76.371169149	-76.370698176	-76.370150228	-76.369528042	-76.368834271	-76.368071491
101.5	-76.372346435	-76.372298976	-76.372159597	-76.371931487	-76.371617737	-76.371221347	-76.370745225	-76.370192192	-76.369564986	-76.368866259	-76.368098587
102.0	-76.372412455	-76.372359588	-76.372214865	-76.371981474	-76.371662508	-76.371260965	-76.370779754	-76.370221696	-76.369589528	-76.368885905	-76.368113426
102.5	-76.372465692	-76.372407478	-76.372257471	-76.372018860	-76.371694736	-76.371288099	-76.370801858	-76.370238834	-76.369601764	-76.368893302	-76.368116049
103.0	-76.372506250	-76.372442748	-76.372287516	-76.372043743	-76.371714520	-76.371302848	-76.370811634	-76.370243702	-76.369601787	-76.368888543	-76.368106573
103.5	-76.372534233	-76.372465502	-76.372305103	-76.372056225	-76.371721961	-76.371305310	-76.370809181	-76.370236396	-76.369589692	-76.368871723	-76.368085091
104.0	-76.372549746	-76.372475842	-76.372310333	-76.372056407	-76.371717158	-76.371295584	-76.370794596	-76.370217014	-76.369565576	-76.368842937	-76.368051697
104.5	-76.372558088	-76.372473875	-76.372303311	-76.372044393	-76.371700214	-76.371273772	-76.370767978	-76.370185654	-76.369529536	-76.368802279	-76.368006486
105.0	-76.372543786	-76.372459705	-76.372284142	-76.372020285	-76.371671230	-76.371239974	-76.370729428	-76.370142414	-76.369481669	-76.368749848	-76.367949553
105.5	-76.372522528	-76.372433439	-76.372252930	-76.371984189	-76.371630310	-76.371194293	-76.370679047	-76.370087396	-76.369422075	-76.368685741	-76.367880995
106.0	-76.372489229	-76.372395186	-76.372209782	-76.371936208	-76.371577557	-76.371136830	-76.370616936	-76.370020698	-76.369350852	-76.368610055	-76.367800910
106.5	-76.372443998	-76.372345052	-76.372154806	-76.371876450	-76.371513078	-76.371067691	-76.370543199	-76.369942423	-76.369268102	-76.368522918	-76.367709394
107.0	-76.372386946	-76.372283147	-76.372088109	-76.371805021	-76.371436978	-76.370986981	-76.370457938	-76.369852674	-76.369173926	-76.368424377	-76.367606549
107.5	-76.372318184	-76.372209582	-76.372009801	-76.371722030	-76.371349364	-76.370894804	-76.370361260	-76.369751555	-76.369068427	-76.368314558	-76.367492473
108.0	-76.372237825	-76.372124468	-76.371919991	-76.371627585	-76.371250344	-76.370791268	-76.370253269	-76.369639169	-76.368951707	-76.368193566	-76.367367268
108.5	-76.372145982	-76.372027918	-76.371818792	-76.371521797	-76.371140026	-76.370676481	-76.370134072	-76.369515623	-76.368823872	-76.368061503	-76.367231037
109.0	-76.372042769	-76.371920044	-76.371706316	-76.371404777	-76.371018522	-76.370550552	-76.370003778	-76.369381023	-76.368685026	-76.367918473	-76.367083882
109.5	-76.371928302	-76.371800961	-76.371582675	-76.371276637	-76.370885942	-76.370413590	-76.369862494	-76.369235477	-76.368535278	-76.367764582	-76.366925909
110.0	-76.371802697	-76.371670784	-76.371447984	-76.371137491	-76.370742398	-76.370265708	-76.369710332	-76.369079094	-76.368374733	-76.367599936	-76.366757221
110.5	-76.371666073	-76.371529630	-76.371302359	-76.370987452	-76.370588003	-76.370107016	-76.369547401	-76.368911984	-76.368203502	-76.367424644	-76.366577927
111.0	-76.371518547	-76.371377618	-76.371145916	-76.370826636	-76.370422872	-76.369937628	-76.369373815	-76.368734257	-76.368021722	-76.367238813	-76.366388133
111.5	-76.371360241	-76.371214864	-76.370978773	-76.370655160	-76.370247121	-76.369757659	-76.369189686	-76.368546026	-76.367829449	-76.367042554	-76.366187948
112.0	-76.371191274	-76.371041491	-76.370801049	-76.370473142	-76.370060866	-76.369567224	-76.368995129	-76.368347404	-76.367626821	-76.366835979	-76.365977482
112.5	-76.371011769	-76.370857617	-76.370612863	-76.370280700	-76.369864225	-76.369366440	-76.368790259	-76.368138507	-76.367413953	-76.366619198	-76.365756847
113.0	-76.370821850	-76.370663367	-76.370414338	-76.370077956	-76.369657317	-76.369155425	-76.368575194	-76.367919448	-76.367190959	-76.366392326	-76.365526155
113.5	-76.370621641	-76.370458864	-76.370205596	-76.369865029	-76.369440262	-76.368934299	-76.368350052	-76.367690347	-76.366957956	-76.366155478	-76.365285519
114.0	-76.370411268	-76.370244232	-76.369986759	-76.369642044	-76.369213183	-76.368703180	-76.368114951	-76.367451320	-76.366715060	-76.365908769	-76.365035054
114.5	-76.370190858	-76.370019598	-76.369757955	-76.369409123	-76.368976201	-76.368462193	-76.367870013	-76.367202488	-76.366462390	-76.365652317	-76.364774877
115.0	-76.369960540	-76.369785088	-76.369519307	-76.369166392	-76.368729441	-76.368211459	-76.367615360	-76.366944000	-76.366200065	-76.365386240	-76.364505105
115.5	-76.369720443	-76.369540832	-76.369270946	-76.368913978	-76.368473029	-76.367951102	-76.367351114	-76.366675921	-76.365928207	-76.365110658	-76.364225856
116.0	-76.369470699	-76.369286960	-76.369012998	-76.368652009	-76.368207090	-76.367681250	-76.367077401	-76.366398402	-76.365646937	-76.364825693	-76.363937251
116.5	-76.369211439	-76.369023603	-76.368745595	-76.368380613	-76.367931755	-76.367402027	-76.366794346	-76.366111569	-76.365356380	-76.364531467	-76.363639411

Table ESI 1c. Calculated energies of water molecule at CCSD(T)/aug-cc-PV6Z level of theory reported with respect to the energy minimum. The bond angle (H-O-H) and bond lengths (O-H) were systematically varied from 93.0° to 116.5° and from 0.900 Å to 1.010 Å, respectively. The data correspond to Figure 1.

H-O-H (Å) / O-H (°)	0.900	0.905	0.910	0.915	0.920	0.925	0.930	0.935	0.940	0.945	0.950	0.955	0.960	0.965	0.970	0.975	0.980	0.985	0.990	0.995	1.000	1.005	1.010
93.0	7.911	6.995	6.168	5.424	4.764	4.182	3.678	3.247	2.889	2.600	2.377	2.220	2.125	2.091	2.115	2.195	2.330	2.517	2.755	3.043	3.377	3.757	4.181
93.5	7.671	6.760	5.936	5.198	4.542	3.965	3.465	3.039	2.684	2.400	2.182	2.028	1.938	1.908	1.936	2.020	2.159	2.350	2.592	2.883	3.222	3.605	4.033
94.0	7.440	6.534	5.715	4.981	4.329	3.757	3.261	2.839	2.489	2.209	1.995	1.846	1.760	1.733	1.766	1.854	1.997	2.192	2.438	2.733	3.075	3.462	3.894
94.5	7.219	6.317	5.503	4.773	4.126	3.558	3.066	2.649	2.304	2.027	1.818	1.673	1.590	1.568	1.604	1.697	1.844	2.043	2.292	2.591	2.937	3.328	3.763
95.0	7.008	6.110	5.300	4.575	3.932	3.368	2.881	2.468	2.127	1.855	1.649	1.508	1.430	1.412	1.452	1.548	1.699	1.902	2.156	2.458	2.807	3.202	3.641
95.5	6.805	5.912	5.107	4.386	3.748	3.188	2.705	2.296	1.959	1.691	1.490	1.353	1.279	1.264	1.308	1.409	1.563	1.770	2.027	2.333	2.686	3.085	3.527
96.0	6.613	5.724	4.923	4.207	3.572	3.017	2.538	2.134	1.801	1.537	1.339	1.206	1.136	1.126	1.174	1.278	1.436	1.646	1.907	2.217	2.574	2.976	3.422
96.5	6.429	5.545	4.748	4.036	3.406	2.855	2.381	1.980	1.651	1.391	1.198	1.069	1.002	0.996	1.048	1.155	1.317	1.531	1.796	2.109	2.470	2.875	3.324
97.0	6.255	5.375	4.583	3.875	3.249	2.702	2.232	1.835	1.510	1.254	1.065	0.940	0.877	0.875	0.930	1.042	1.207	1.425	1.693	2.010	2.374	2.783	3.236
97.5	6.091	5.215	4.426	3.723	3.101	2.558	2.092	1.699	1.378	1.126	0.941	0.820	0.761	0.762	0.821	0.936	1.105	1.327	1.599	1.919	2.286	2.699	3.155
98.0	5.935	5.063	4.279	3.580	2.962	2.423	1.961	1.572	1.255	1.007	0.825	0.708	0.653	0.658	0.721	0.839	1.012	1.237	1.513	1.836	2.207	2.623	3.082
98.5	5.788	4.921	4.141	3.445	2.832	2.297	1.838	1.454	1.141	0.896	0.718	0.605	0.553	0.562	0.628	0.751	0.927	1.156	1.435	1.762	2.136	2.555	3.018
99.0	5.650	4.787	4.011	3.320	2.710	2.179	1.725	1.344	1.035	0.794	0.620	0.510	0.463	0.475	0.545	0.671	0.851	1.083	1.365	1.696	2.073	2.496	2.962
99.5	5.522	4.662	3.891	3.203	2.597	2.071	1.620	1.243	0.937	0.701	0.530	0.424	0.380	0.396	0.469	0.599	0.782	1.018	1.303	1.637	2.018	2.444	2.913
100.0	5.402	4.547	3.779	3.095	2.493	1.970	1.524	1.151	0.849	0.616	0.449	0.346	0.306	0.325	0.402	0.535	0.722	0.961	1.250	1.587	1.971	2.400	2.873
100.5	5.291	4.439	3.676	2.996	2.398	1.879	1.436	1.067	0.768	0.539	0.376	0.277	0.240	0.263	0.344	0.480	0.670	0.912	1.205	1.545	1.932	2.365	2.840
101.0	5.188	4.341	3.581	2.905	2.311	1.796	1.357	0.991	0.696	0.471	0.311	0.216	0.182	0.209	0.293	0.433	0.626	0.872	1.167	1.511	1.901	2.337	2.815
101.5	5.095	4.251	3.495	2.823	2.233	1.721	1.286	0.924	0.633	0.411	0.255	0.163	0.133	0.163	0.250	0.393	0.590	0.839	1.138	1.485	1.878	2.317	2.798
102.0	5.009	4.170	3.417	2.749	2.163	1.655	1.223	0.865	0.577	0.359	0.206	0.118	0.091	0.125	0.215	0.362	0.562	0.814	1.116	1.466	1.863	2.304	2.789
102.5	4.933	4.097	3.348	2.684	2.101	1.597	1.169	0.814	0.530	0.315	0.166	0.081	0.058	0.095	0.189	0.338	0.542	0.797	1.102	1.455	1.855	2.300	2.787
103.0	4.864	4.032	3.288	2.627	2.048	1.547	1.122	0.771	0.491	0.279	0.134	0.052	0.033	0.072	0.170	0.323	0.529	0.788	1.096	1.452	1.855	2.303	2.793
103.5	4.804	3.976	3.235	2.578	2.002	1.505	1.084	0.737	0.460	0.252	0.110	0.031	0.015	0.058	0.159	0.315	0.525	0.786	1.097	1.457	1.863	2.313	2.807
104.0	4.753	3.928	3.191	2.537	1.965	1.472	1.054	0.710	0.437	0.232	0.093	0.018	0.005	0.052	0.155	0.315	0.528	0.792	1.107	1.469	1.878	2.331	2.828
104.5	4.709	3.888	3.155	2.505	1.936	1.446	1.032	0.692	0.422	0.220	0.085	0.013	0.000	0.053	0.160	0.322	0.538	0.806	1.123	1.489	1.900	2.357	2.856
105.0	4.674	3.857	3.126	2.480	1.915	1.429	1.018	0.681	0.414	0.216	0.084	0.016	0.009	0.062	0.172	0.337	0.557	0.827	1.148	1.516	1.930	2.390	2.892
105.5	4.647	3.833	3.106	2.464	1.902	1.419	1.012	0.678	0.415	0.220	0.091	0.026	0.022	0.078	0.191	0.360	0.582	0.856	1.179	1.550	1.968	2.430	2.935
106.0	4.627	3.817	3.094	2.455	1.897	1.417	1.013	0.683	0.423	0.231	0.105	0.044	0.043	0.102	0.219	0.390	0.615	0.892	1.218	1.592	2.013	2.477	2.985
106.5	4.616	3.809	3.090	2.454	1.899	1.423	1.022	0.695	0.438	0.250	0.128	0.069	0.072	0.134	0.253	0.428	0.656	0.935	1.264	1.641	2.064	2.532	3.043
107.0	4.612	3.809	3.093	2.461	1.909	1.436	1.039	0.715	0.462	0.276	0.157	0.102	0.107	0.173	0.295	0.473	0.704	0.986	1.318	1.698	2.124	2.594	3.107
107.5	4.616	3.817	3.104	2.475	1.927	1.457	1.063	0.743	0.492	0.310	0.194	0.142	0.151	0.219	0.344	0.525	0.758	1.044	1.379	1.761	2.190	2.663	3.179
108.0	4.628	3.832	3.122	2.497	1.952	1.486	1.095	0.778	0.531	0.352	0.239	0.189	0.201	0.272	0.400	0.584	0.821	1.109	1.446	1.832	2.263	2.739	3.257
108.5	4.647	3.855	3.149	2.526	1.985	1.522	1.134	0.820	0.576	0.400	0.290	0.244	0.259	0.333	0.464	0.650	0.890	1.181	1.521	1.909	2.343	2.822	3.343
109.0	4.674	3.885	3.182	2.563	2.025	1.565	1.181	0.869	0.629	0.456	0.349	0.306	0.323	0.400	0.534	0.724	0.966	1.260	1.603	1.994	2.430	2.911	3.435
109.5	4.709	3.922	3.223	2.607	2.072	1.616	1.234	0.926	0.689	0.519	0.415	0.374	0.395	0.475	0.612	0.804	1.049	1.346	1.692	2.085	2.524	3.008	3.534
110.0	4.750	3.967	3.271	2.659	2.127	1.673	1.295	0.990	0.756	0.589	0.488	0.450	0.474	0.557	0.697	0.891	1.139	1.438	1.787	2.183	2.625	3.111	3.640
110.5	4.799	4.020	3.327	2.717	2.189	1.738	1.363	1.061	0.830	0.666	0.568	0.533	0.560	0.645	0.788	0.986	1.236	1.538	1.889	2.288	2.733	3.221	3.753
111.0	4.855	4.079	3.389	2.783	2.257	1.810	1.438	1.139	0.910	0.750	0.655	0.623	0.652	0.741	0.886	1.087	1.340	1.644	1.998	2.399	2.847	3.338	3.872
111.5	4.918	4.145	3.459	2.855	2.333	1.889	1.520	1.224	0.998	0.841	0.748	0.719	0.752	0.843	0.991	1.194	1.450	1.757	2.114	2.518	2.967	3.461	3.997
112.0	4.988	4.218	3.535	2.935	2.416	1.975	1.609	1.316	1.093	0.938	0.849	0.823	0.858	0.952	1.103	1.308	1.567	1.877	2.236	2.642	3.094	3.591	4.129
112.5	5.066	4.299	3.618	3.021	2.505	2.067	1.704	1.414	1.194	1.042	0.956	0.933	0.970	1.067	1.221	1.429	1.690	2.003	2.364	2.773	3.228	3.727	4.268
113.0	5.149	4.386	3.708	3.115	2.602	2.166	1.806	1.519	1.302	1.153	1.069	1.049	1.090	1.189	1.345	1.556	1.820	2.135	2.499	2.911	3.368	3.869	4.413
113.5	5.240	4.480	3.805	3.215	2.704	2.272	1.915	1.631	1.417	1.270	1.190	1.172	1.215	1.317	1.476	1.690	1.956	2.274	2.641	3.055	3.514	4.018	4.564
114.0	5.338	4.580	3.909	3.321	2.814	2.384	2.030	1.749	1.538	1.394	1.316	1.301	1.347	1.452	1.614	1.830	2.099	2.419	2.788	3.205	3.667	4.173	4.721
114.5	5.441	4.687	4.019	3.434	2.930	2.503	2.152	1.874	1.665	1.524	1.449	1.437	1.485	1.593	1.757	1.976	2.248	2.570	2.942	3.361	3.825	4.333	4.884
115.0	5.552	4.800	4.135	3.553	3.052	2.629	2.280	2.004	1.799	1.661	1.588	1.579	1.630	1.740	1.907	2.128	2.403	2.728	3.102	3.523	3.990	4.500	5.053
115.5	5.669	4.920	4.258	3.679	3.181	2.760	2.414	2.142	1.939	1.803	1.734	1.727	1.781	1.893	2.063	2.287	2.563	2.891	3.267	3.691	4.160	4.673	5.229
116.0	5.792	5.046	4.387	3.811	3.315	2.898	2.555	2.285	2.085	1.952	1.885	1.881	1.937	2.053	2.225	2.451	2.730	3.060	3.439	3.865	4.337	4.852	5.410
116.5	5.921	5.179	4.522	3.949	3.456	3.041	2.702	2.434	2.237	2.107	2.042	2.041	2.100	2.218	2.392	2.621	2.903	3.235	3.617	4.045	4.519	5.037	5.597

Table ESI 1d. Calculated absolute energies of water molecule at CCSD(T)/aug-cc-PV6Z level of theory. The bond angle (H-O-H) and bond lengths (O-H) were systematically varied per 0.1° and 0.001 Å, respectively, in order to find energies of 0.5, 1.0 and 2.0 kcal/mol in respect to the energy minimum. The data are related to Figure 1b,c.

H-O-H (Å) / O-H (°)	0.952	0.953	0.954	0.955	0.957	0.958	0.959	0.961	0.962	0.963	0.964	0.965	0.966
93.1	-	-	-	-	-	-	-	-	-	-	-76.369282678	-76.369285830	-76.369285261
93.2	-	-	-	-	-	-	-	-	-	-	-76.369341897	-76.369344784	-76.369343952
93.3	-	-	-	-	-	-	-	-	-	-	-76.369400537	-76.369403162	-76.369402067
96.3	-	-	-	-	-	-	-	-	-76.370893708	-76.370896209	-76.370894955	-	-
96.4	-	-	-	-	-	-	-	-	-76.370935309	-76.370937565	-76.370936066	-	-
96.5	-	-	-	-	-	-	-	-	-76.370976355	-76.370978366	-76.370976623	-	-
98.6	-	-	-	-	-	-	-	-76.371710800	-76.371711579	-76.371708583	-	-	-
98.7	-	-	-	-	-	-	-	-76.371740075	-76.371740619	-76.371737391	-	-	-
98.8	-	-	-	-	-	-	-	-76.371768811	-76.371769122	-76.371765663	-	-	-
104.3	-	-	-	-	-76.372555002	-76.372558143	-76.372557431	-	-	-	-	-	-
104.4	-	-	-	-	-76.372554750	-76.372558088	-76.372557582	-	-	-	-	-	-
104.5	-	-	-	-	-76.372553984	-76.372557537	-76.372557238	-	-	-	-	-	-
110.2	-	-76.371777655	-76.371785264	-76.371788945	-	-	-	-	-	-	-	-	-
110.3	-	-76.371751616	-76.371759040	-76.371762536	-	-	-	-	-	-	-	-	-
110.4	-	-76.371725137	-76.371732377	-76.371735688	-	-	-	-	-	-	-	-	-
112.7	-	-76.370999065	-76.370994333	-76.370985739	-	-	-	-	-	-	-	-	-
112.8	-	-76.370961957	-76.370957049	-76.370948279	-	-	-	-	-	-	-	-	-
112.9	-	-76.370924434	-76.370919350	-76.370910404	-	-	-	-	-	-	-	-	-
116.3	-76.369418339	-76.369419146	-76.369416022	-	-	-	-	-	-	-	-	-	-
116.4	-76.369367440	-76.369368079	-76.369364787	-	-	-	-	-	-	-	-	-	-
116.5	-76.369316159	-76.369316633	-76.369313175	-	-	-	-	-	-	-	-	-	-

Table ESI 1e. Calculated energies of water molecule at CCSD(T)/aug-cc-PV6Z level of theory reported to the energy minimum. The bond angle (H-O-H) and bond lengths (O-H) were systematically varied per 0.1° and 0.001 Å, respectively, in order to find energies of 0.5, 1.0 and 2.0 kcal/mol in respect to the energy minimum. The data are related to Figure 1b,c.

H-O-H (Å) / O-H (°)	0.952	0.953	0.954	0.955	0.957	0.958	0.959	0.961	0.962	0.963	0.964	0.965	0.966
93.1	-	-	-	-				-	-	-	2.055	2.053	2.054
93.2	-	-	-	-	-	-	-	-	-	-	2.018	2.016	2.017
93.3	-	-	-	-	-	-	-	-	-	-	1.981	1.980	1.980
96.3	-	-	-	-	-	-	-	-	1.044	1.043	1.044	-	-
96.4	-	-	-	-	-	-	-	-	1.018	1.017	1.018	-	-
96.5	-	-	-	-	-	-	-	-	0.993	0.991	0.992	-	-
98.6	-	-	-	-	-	-	-	0.532	0.531	0.533	-	-	-
98.7	-	-	-	-	-	-	-	0.513	0.513	0.515	-	-	-
98.8	-	-	-	-	-	-	-	0.495	0.495	0.497	-	-	-
104.3	-	-	-	-	0.002	0.000	0.000	-	-	-	-	-	-
104.4	-	-	-	-	0.002	**0.000**	0.000	-	-	-	-	-	-
104.5	-	-	-	-	0.003	0.000	0.001	-	-	-	-	-	-
110.2	-	0.490	0.485	0.483	-	-	-	-	-	-	-	-	-
110.3	-	0.506	0.501	0.499	-	-	-	-	-	-	-	-	-
110.4	-	0.523	0.518	0.516	-	-	-	-	-	-	-	-	-
112.7	-	0.980	0.978	0.978	-	-	-	-	-	-	-	-	-
112.8	-	1.003	1.001	1.002	-	-	-	-	-	-	-	-	-
112.9	-	1.026	1.024	1.025	-	-	-	-	-	-	-	-	-
116.3	1.970	1.970	1.972	-	-	-	-	-	-	-	-	-	-
116.4	2.002	2.002	2.004	-	-	-	-	-	-	-	-	-	-
116.5	2.034	2.034	2.036	-	-	-	-	-	-	-	-	-	-

Table ESI 1f. Calculated absolute energies of water molecule at CCSD(T)/aug-cc-PV6Z level of theory. The bond angle (H-O-H) and bond lengths (O-H) were systematically varied per 0.1° and 0.001 Å, respectively, in order to find energies of 0.5, 1.0 and 2.0 kcal/mol in respect to the energy minimum. The data are related to Figure 1d,e.

H-O-H (Å) / O-H (°)	0.918	0.919	0.920	0.929	0.930	0.931	0.937	0.938	0.939	0.957	0.958	0.959	0.979	0.980	0.981	0.988	0.989	0.990	1.001	1.002	1.003
106.2	-76.369195718	-76.369368043	-76.369535333	-	-	-	-	-	-	-	-	-	-	-	-	-	-		-	-	-
106.1	-76.369195564	-76.369368106	-76.369535613	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
106.0	-76.369194909	-76.369367675	-76.369535403	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.7	-	-	-	-76.370826293	-76.370945727	-76.371060744	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.6	-	-	-	-76.370826047	-76.370946189	-76.371061419	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.5	-	-	-	-76.370825308	-76.370945634	-76.371061293	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.4	-	-	-	-	-	-	-76.371659443	-76.371743516	-76.371823171	-	-	-	-	-	-	-	-	-	-	-	-
105.3	-	-	-	-	-	-	-76.371659425	-76.371743711	-76.371823577	-	-	-	-	-	-	-	-	-	-	-	-
105.2	-	-	-	-	-	-	-76.371658915	-76.371743412	-76.371823491	-	-	-	-	-	-	-	-	-	-	-	-
104.5	-	-	-	-	-	-	-	-	-	-76.372555002	-76.372558143	-76.372557431	-	-	-	-	-	-	-	-	-
104.4	-	-	-	-	-	-	-	-	-	-76.372554750	-76.372558088	-76.372557582	-	-	-	-	-	-	-	-	-
104.3	-	-	-	-	-	-	-	-	-	-76.372553984	-76.372557537	-76.372557238	-	-	-	-	-	-	-	-	-
103.7	-	-	-	-	-	-	-	-	-	-	-	-	-76.371795446	-76.371721509	-76.371644272	-	-	-	-	-	-
103.6	-	-	-	-	-	-	-	-	-	-	-	-	-76.371795720	-76.371721983	-76.371644944	-	-	-	-	-	-
103.5	-	-	-	-	-	-	-	-	-	-	-	-	-76.371795499	-76.371721967	-76.371645133	-	-	-	-	-	-
103.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-76.371018656	-76.370916688	-76.370811624	-	-	-
103.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-76.371018755	-76.370916983	-76.370812115	-	-	-
103.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-76.371018367	-76.370916791	-76.370812119	-	-	-
102.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-76.369466606	-76.369327125	-76.369184837
102.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-76.369466794	-76.369327506	-76.369185409
102.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-76.369466484	-76.369327400	-76.369185495

Table ESI 1g. Calculated energies of water molecule at CCSD(T)/aug-cc-PV6Z level of theory reported to the energy minimum. The bond angle (H-O-H) and bond lengths (O-H) were systematically varied per 0.1° and 0.001 Å, respectively, in order to find energies of 0.5, 1.0 and 2.0 kcal/mol in respect to the energy minimum. The data are related to Figure 1d,e.

H-O-H (Å) / O-H (°)	0.918	0.919	0.920	0.929	0.930	0.931	0.937	0.938	0.939	0.957	0.958	0.959	0.979	0.980	0.981	0.988	0.989	0.990	1.001	1.002	1.003
106.2	2.110	2.002	1.897	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
106.1	2.110	2.002	1.897	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
106.0	2.110	2.002	1.897	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.7	-	-	-	1.087	1.012	0.940	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.6	-	-	-	1.087	1.011	0.939	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.5	-	-	-	1.087	1.012	0.939	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-
105.4	-	-	-	-	-	-	0.564	0.511	0.461	-	-	-	-	-	-	-	-	-	-	-	-
105.3	-	-	-	-	-	-	0.564	0.511	0.461	-	-	-	-	-	-	-	-	-	-	-	-
105.2	-	-	-	-	-	-	0.564	0.511	0.461	-	-	-	-	-	-	-	-	-	-	-	-
104.5	-	-	-	-	-	-	-	-	-	0.002	0.000	0.000	-	-	-	-	-	-	-	-	-
104.4	-	-	-	-	-	-	-	-	-	0.002	**0.000**	0.000	-	-	-	-	-	-	-	-	-
104.3	-	-	-	-	-	-	-	-	-	0.003	0.000	0.001	-	-	-	-	-	-	-	-	-
103.7	-	-	-	-	-	-	-	-	-	-	-	-	0.479	0.525	0.573	-	-	-	-	-	-
103.6	-	-	-	-	-	-	-	-	-	-	-	-	0.478	0.525	0.573	-	-	-	-	-	-
103.5	-	-	-	-	-	-	-	-	-	-	-	-	0.479	0.525	0.573	-	-	-	-	-	-
103.3	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.966	1.030	1.096	-	-	-
103.2	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.966	1.030	1.096	-	-	-
103.1	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	0.966	1.030	1.096	-	-	-
102.8	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.940	2.027	2.117
102.7	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.940	2.027	2.116
102.6	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	-	1.940	2.027	2.116

Table ESI 2. Calculated energies of change in the bond angle of water molecule in model systems based on crystal structures (Figure 4) at wB97xD/def2-TZVPP and CCSD(T)/aug-cc-PV6Z level of theory.

Refcode[a]	H-O-H[b] (^{0})	O-H[b] (Å)	Optimal H-O-H[c] (^{0})	$\Delta E_{H\text{-}O\text{-}H}$[d] (kcal/mol) wB97xD/ def2-TZVPP	$\Delta E_{H\text{-}O\text{-}H}$[d] (kcal/mol) CCSD(T)/ aug-cc-PV6Z
ARGIND11[1]	113.92	0.909-0.915	106.5	0.70	0.82
CYSTAC01[2]	110.46	0.929-0.980	104.5	0.41	0.52
IBISEU02[3]	111.78	0.980-0.981	103.5	0.87	0.99
FIJBOP01[4]	110.14	0.903-0.938	106.0	0.19	0.25
Ih[5]	109.46	1.000	103.0	0.57	0.66

[a]Crystal structures were solved by neutron diffraction analysis having R factor ≤ 0.05. [b]Original bond angles and bond lengths of a water molecule from the crystal structure. [c]The values are estimated based on the results of calculations (Table ESI 1) by taking the bond angle value that corresponds to energy minimum at bond length closest to the average of the original bond lengths. [d]The difference in absolute energies of a water molecule having the original bond angle and the optimal bond angle. In both geometries of water molecule bond lengths are the original ones.

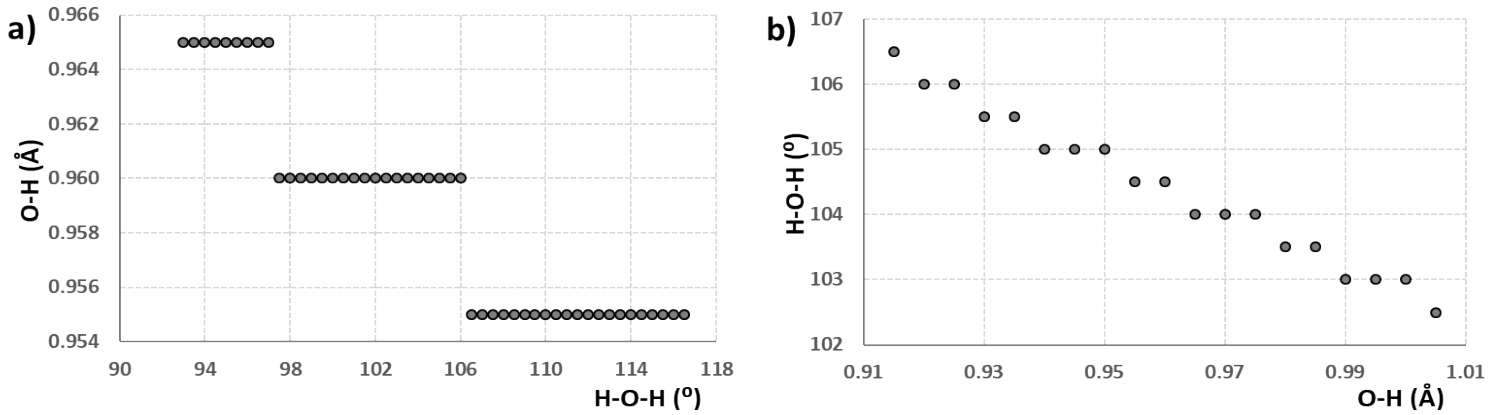

Figure ESI 1. (a) Optimal bond lengths (O-H) at particular bond angles (H-O-H). (b) Optimal bond angles (H-O-H) at particular bond lengths (O-H). The reported data arise from the calculated energies of water molecule depending of the bond angle and the bond length (see Table ESI 1c) calculated at CCSD(T)/aug-cc-PV6Z level of theory. The bond angle and bond lengths were systematically varied per 0.5^o and 0.005 Å, from 93.0^o to 116.5^o and from 0.915 Å to 1.005 Å, respectively. The data are related to Figure 1c,e.

2. CSD analysis results.

Distributions of the considered geometric parameters, i.e. the bond angles and bond lengths, of water molecules found in CSD are given bellow.

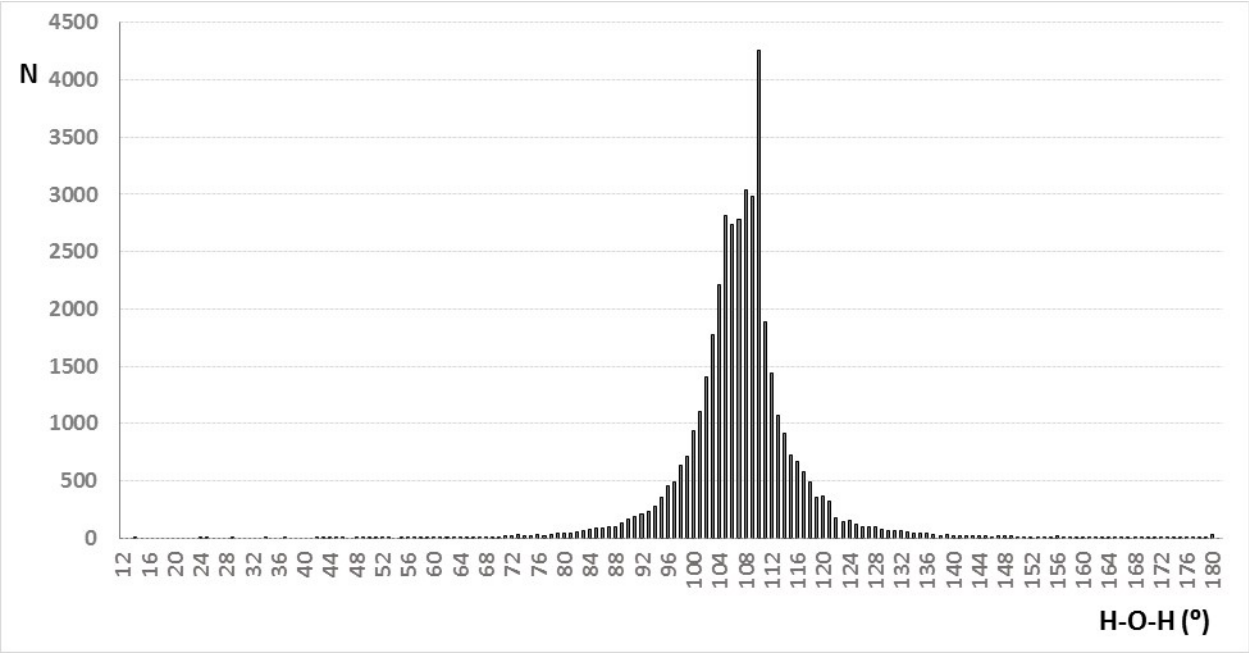

Figure ESI 2. Full distribution of the bond angle of crystal structures that contain non-coordinated water molecule(s). The structures are solved by X-ray diffraction analysis having R factor ≤ 0.05.

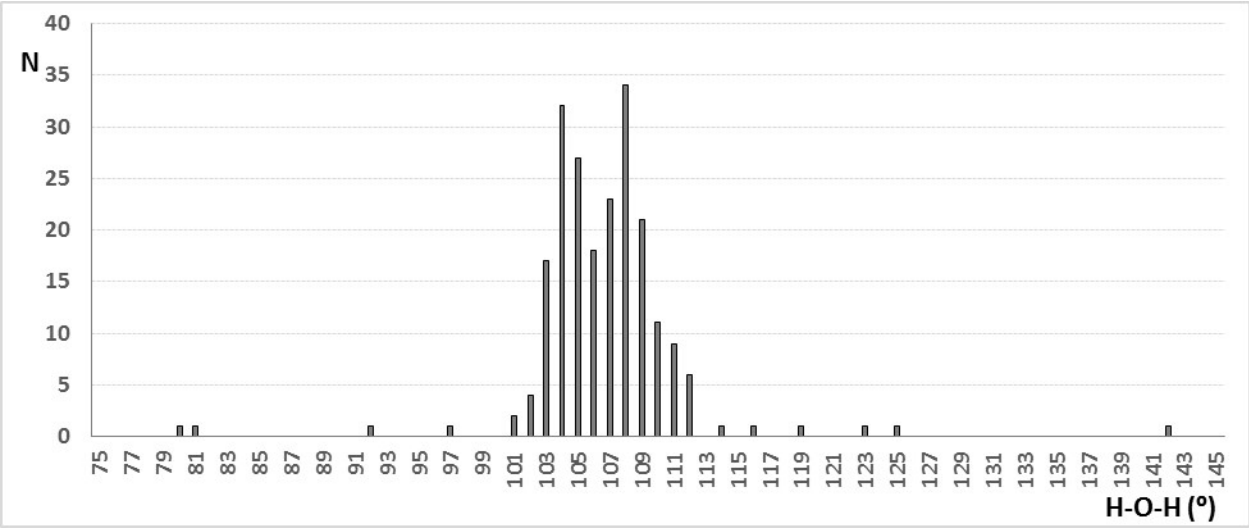

Figure ESI 3. Distribution of the bond angle of crystal structures that contain non-coordinated water molecule(s). The structures are solved by neutron diffraction analysis having R factor ≤ 0.1.

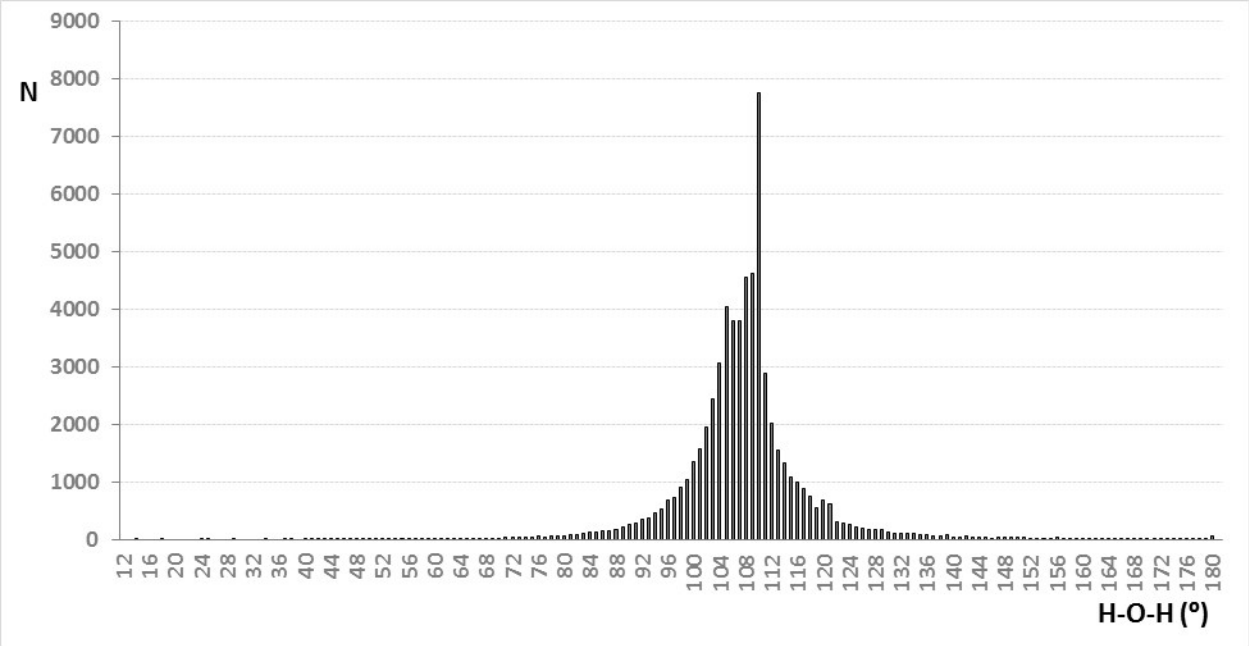

Figure ESI 4. Full distribution of the bond angle of crystal structures that contain non-coordinated water molecule(s). The structures are solved by X-ray diffraction analysis having R factor ≤ 0.1.

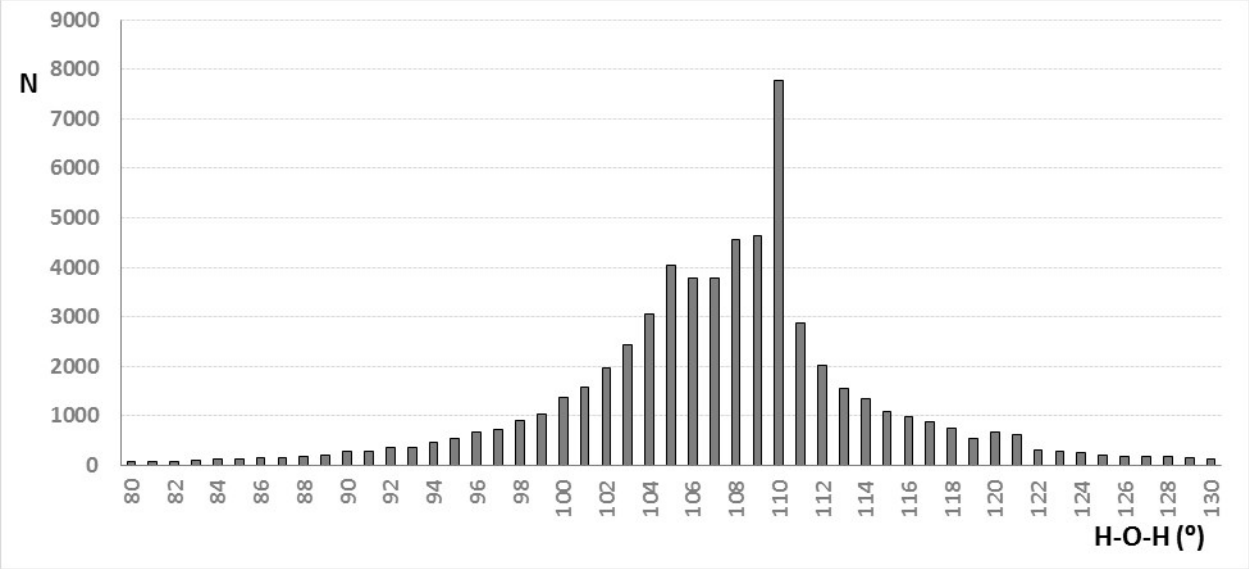

Figure ESI 5. Zoomed distribution of the bond angle of crystal structures that contain non-coordinated water molecule(s). The structures are solved by X-ray diffraction analysis having R factor ≤ 0.1.

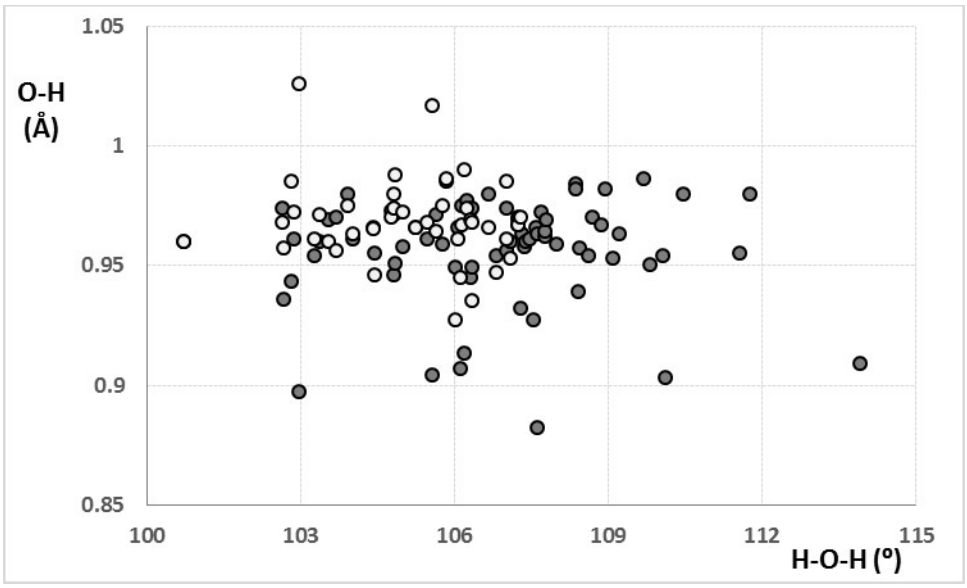

Figure ESI 6. Distribution of the bond lengths and corresponding bond angle of crystal structures that contain non-coordinated water molecule(s). The structures are solved by **neutron** diffraction analysis having *R* factor ≤ 0.05.

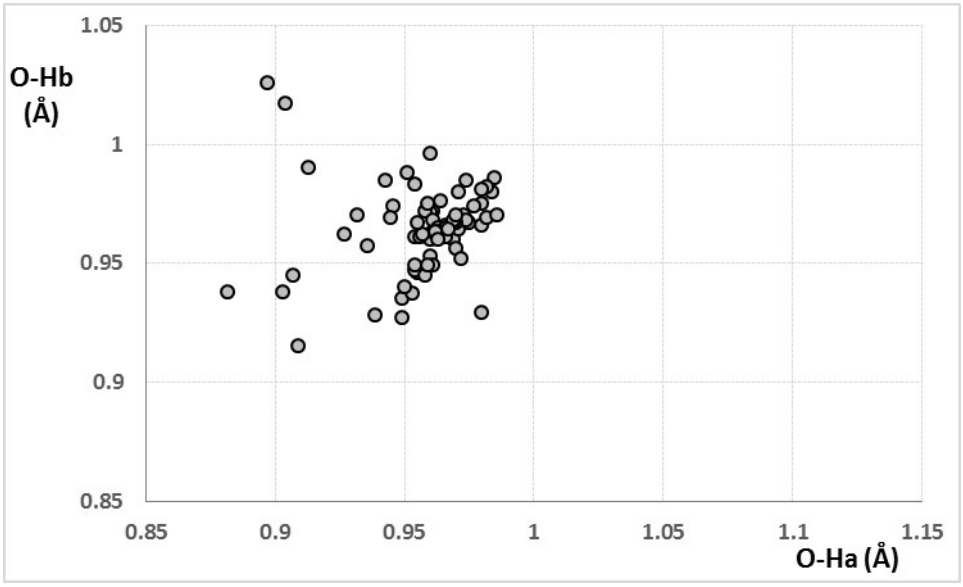

Figure ESI 7. Distribution of corresponding bond lengths of crystal structures that contain non-coordinated water molecule(s). The structures are solved by **neutron** diffraction analysis having *R* factor ≤ 0.05.

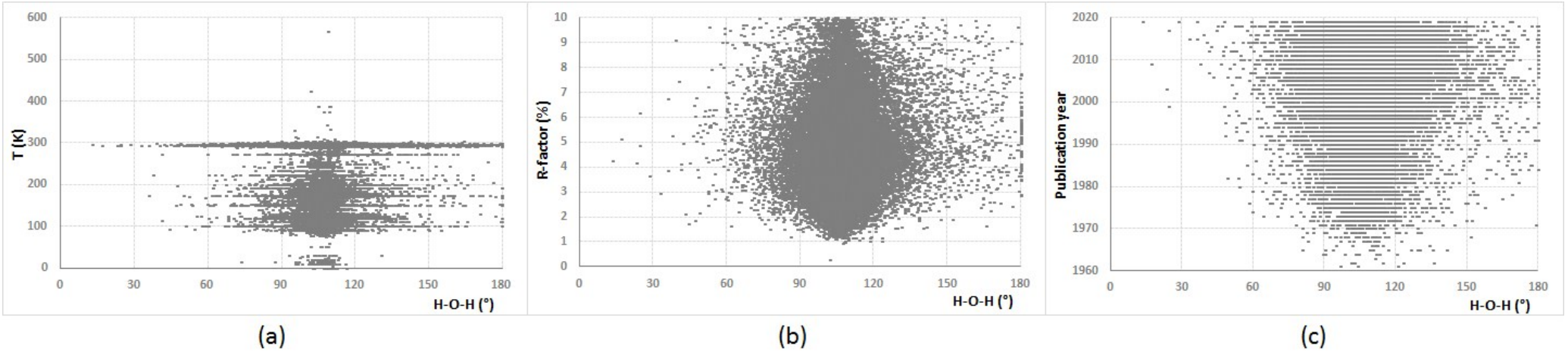

Figure ESI 8. Distribution of the of bond angle and (a) used temperature; (b) *R*-factor and (c) publication year of corresponding crystal structures that contain non-coordinated water molecule(s). The structures are solved by **X-Ray** diffraction analysis having *R* factor ≤ 0.10.

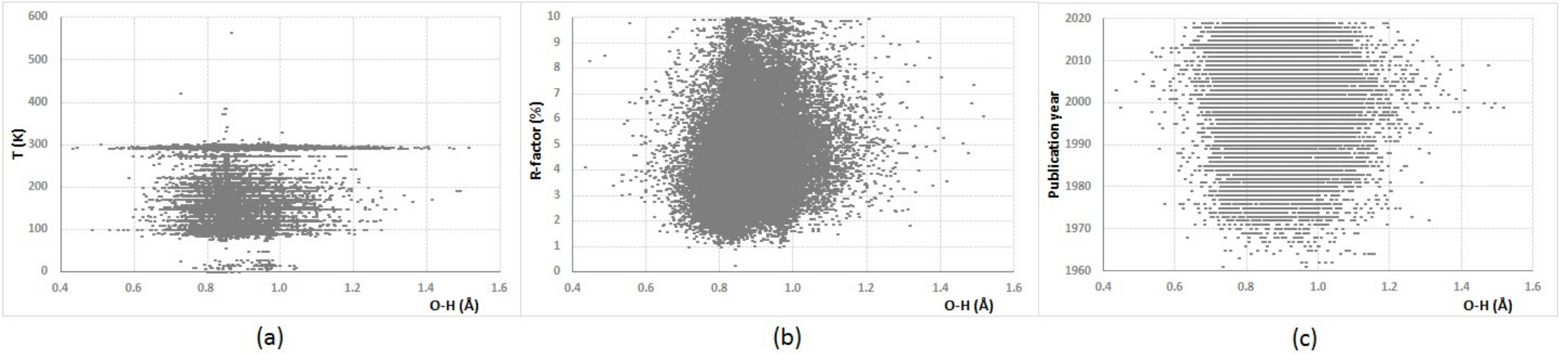

Figure ESI 9. Distribution of the of average value of bond lengths and (a) used temperature; (b) *R*-factor and (c) publication year of corresponding crystal structures that contain non-coordinated water molecule(s). The structures are solved by **X-Ray** diffraction analysis having *R* factor ≤ 0.10.

3. References.

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