

Supplementary information for:

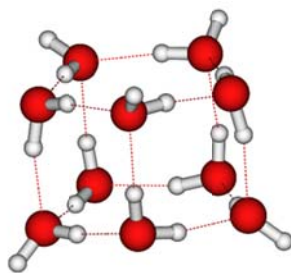
Are fragment-based quantum chemistry methods applicable to medium-sized water clusters?

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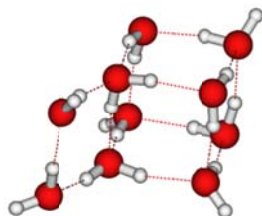
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Table S1. Isomer 1 of water cluster (H₂O)₁₀



O	1.687552	3.708965	11.875100	O	3.235018	7.328850	11.838391
H	1.246894	4.550559	11.992457	H	3.736160	8.017922	12.274589
H	2.619333	3.912609	11.956004	H	3.484616	7.397313	10.916845
O	0.691697	6.298916	11.858002	O	4.012403	7.307502	9.270585
H	1.550082	6.722072	11.876629	H	3.320260	7.167971	8.624287
H	0.186981	6.750098	12.534707	H	4.544708	6.513132	9.227452
O	0.075597	5.692279	9.222667	O	4.218938	4.725723	11.898119
H	0.255258	4.752098	9.226680	H	3.953592	5.641622	11.981497
H	0.197433	5.963776	10.132435	H	4.629803	4.672499	11.035222
O	1.980782	6.570036	7.543353	O	3.082310	4.040160	7.798033
H	1.257718	6.331024	8.123254	H	2.387069	3.604235	8.290821
H	1.558876	6.993127	6.795542	H	2.710678	4.889155	7.558596
O	5.177510	4.799444	9.301259	O	1.006214	3.087392	9.356643
H	4.470823	4.446460	8.760677	H	1.279658	3.221767	10.264059
H	5.973789	4.411093	8.938830	H	0.574883	2.232889	9.360007

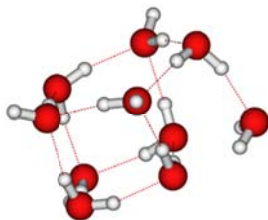
Table S2. Isomer 2 of water cluster (H₂O)₁₀



O	0.411589	0.369488	4.585053	O	3.675203	-3.193417	4.030674
H	0.076046	-0.492836	4.830087	H	4.479317	-3.685774	3.865695
H	-0.011029	0.973752	5.195374	H	3.914818	-2.281056	3.868144
O	-0.473417	2.028255	6.551284	O	2.347613	-2.502472	6.370068
H	-0.812148	2.907790	6.718351	H	1.442175	-2.526185	6.060469
H	0.273129	1.941980	7.144124	H	2.855739	-2.886267	5.655406
O	-0.102737	-2.296677	5.073438	O	1.805353	1.668991	8.005785
H	-0.884618	-2.842545	5.156648	H	2.128652	1.320747	8.836710
H	0.287248	-2.561444	4.240345	H	2.269857	1.165201	7.337456
O	1.221047	-2.833476	2.798632	O	2.758807	0.137393	5.959870
H	1.370575	-1.965471	2.423877	H	1.955852	0.298661	5.464403
H	2.079569	-3.106285	3.122279	H	2.692788	-0.777744	6.232631
O	1.687393	-0.149292	2.225294	O	4.049952	-0.563960	3.633107

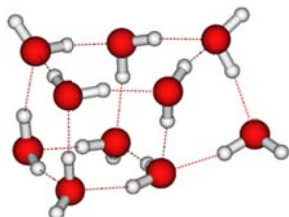
H	1.180260	0.144414	2.982120	H	3.770314	-0.202214	4.474044
H	1.440854	0.452569	1.523001	H	3.345243	-0.335036	3.027126

Table S3. Isomer 3 of water cluster (H₂O)₁₀



O	2.268246	-2.219030	-0.031609	O	0.538202	1.724439	-1.272748
H	1.910331	-1.773511	0.736273	H	1.104198	1.022033	-1.592915
H	1.663515	-2.943385	-0.192367	H	-0.314180	1.545652	-1.669878
O	0.096515	1.684240	1.374853	O	0.179073	-3.917639	-0.584205
H	0.314662	1.748783	0.445079	H	-0.442403	-3.629368	0.084301
H	0.244506	2.565549	1.717820	H	-0.110158	-3.480582	-1.385179
O	-1.327188	-1.875388	0.665983	O	-0.659636	-1.537373	-1.986133
H	-1.090193	-1.756799	-0.253801	H	-1.218645	-0.781721	-2.167055
H	-0.555141	-1.585651	1.152017	H	0.230898	-1.216774	-2.128953
O	-2.006272	0.880225	-2.019733	O	1.902007	-0.543474	-2.092521
H	-2.774079	1.249534	-2.455986	H	2.139511	-1.112312	-1.360232
H	-2.251913	0.839286	-1.095494	H	2.608044	-0.662640	-2.727773
O	0.881749	-0.875705	1.959752	O	-2.388525	0.654100	0.634173
H	1.015488	-0.949413	2.904693	H	-2.212280	-0.278748	0.756506
H	0.691637	0.051327	1.815868	H	-1.628884	1.093934	1.015913

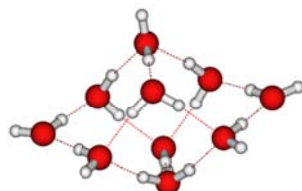
Table S4. Isomer 4 of water cluster (H₂O)₁₀



O	2.446909	-1.096282	0.484179	O	1.140412	-0.511404	-3.180347
H	1.584527	-0.687893	0.559992	H	1.858262	-0.145891	-3.697382
H	2.358713	-1.709573	-0.245429	H	1.521552	-1.274818	-2.746568
O	2.414822	-2.553457	-1.864389	O	3.511687	0.579429	-4.139971
H	3.277776	-2.237451	-2.132127	H	3.625110	1.207224	-3.426359
H	2.448915	-3.498588	-2.012031	H	3.833885	1.037614	-4.916172
O	-1.275230	-0.733546	-1.845563	O	3.758661	2.143240	-1.976246
H	-2.002002	-0.400164	-2.371768	H	2.831874	2.166795	-1.738038
H	-0.520139	-0.703841	-2.433090	H	4.160553	1.573275	-1.320612
O	4.707884	0.176842	-0.277735	O	4.713010	-1.373643	-2.576670
H	5.291074	0.235160	0.479048	H	4.418464	-0.737039	-3.227984

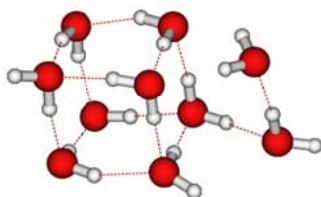
H	3.908898	-0.223404	0.065277	H	4.882820	-0.852830	-1.791717
O	1.113188	1.698382	-1.510362	O	-0.055359	0.098530	0.446845
H	1.074409	0.973973	-2.134830	H	-0.558513	-0.248370	-0.289856
H	0.730694	1.344000	-0.707652	H	-0.695934	0.192624	1.151857

Table S5. Isomer 5 of water cluster (H₂O)₁₀



O	-1.927685	1.087813	0.497243	O	1.544704	-0.054234	0.909457
H	-1.148322	1.446628	0.072887	H	0.749416	-0.523972	1.160647
H	-1.634147	0.259967	0.877690	H	1.235241	0.662690	0.355845
O	3.210058	-1.666149	-0.461970	O	0.114059	0.128998	-2.944905
H	4.045418	-1.691670	0.004672	H	0.642894	-0.661051	-2.833600
H	2.659661	-1.084883	0.062841	H	-0.786165	-0.191042	-3.003246
O	-3.884827	0.667314	-1.304217	O	1.422390	-2.254010	-2.407895
H	-4.651853	1.168807	-1.027798	H	2.084147	-2.072357	-1.740578
H	-3.224688	0.850441	-0.635702	H	1.856325	-2.847421	-3.020917
O	-0.873133	-1.344904	1.287485	O	-0.998552	-2.588630	-1.101790
H	-1.159127	-1.976139	1.947775	H	-1.572259	-2.111130	-1.701029
H	-0.931401	-1.821046	0.459157	H	-0.143200	-2.581139	-1.531383
O	-2.419554	-0.990419	-2.863980	O	0.403156	1.772522	-0.826776
H	-2.971828	-0.409479	-2.340782	H	0.313807	1.220462	-1.603616
H	-2.977064	-1.257750	-3.594698	H	0.718921	2.611123	-1.163339

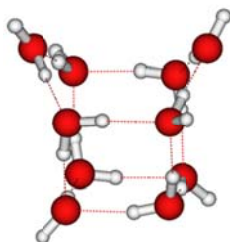
Table S6. Isomer 6 of water cluster (H₂O)₁₀



O	-0.910181	-0.787706	-1.700454	O	0.557554	1.861900	0.767802
H	-1.663140	-0.571179	-2.250364	H	1.147501	1.375160	1.343371
H	-1.164931	-0.504388	-0.822350	H	0.845188	1.636357	-0.116862
O	-0.036374	-1.837676	1.912718	O	0.948014	-2.546894	-0.589164
H	-0.681538	-1.192848	1.622558	H	0.615497	-2.490720	0.306665
H	-0.447502	-2.267890	2.662466	H	0.267464	-2.137990	-1.123843
O	-0.846296	3.071688	-1.435587	O	1.138092	1.028703	-1.770526
H	-0.145590	2.613531	-1.899629	H	0.450234	0.373124	-1.885855
H	-0.514649	3.177150	-0.543892	H	1.911317	0.523580	-1.519118

O	2.944521	-0.742716	-0.613119	O	-3.022097	1.475314	-1.138964
H	3.775437	-1.149718	-0.858396	H	-2.308662	2.088731	-1.314930
H	2.308223	-1.457012	-0.646852	H	-3.818713	1.987842	-1.276627
O	2.103505	-0.045311	1.949965	O	-1.545411	0.162177	0.774204
H	1.447054	-0.731509	2.070123	H	-0.858118	0.821527	0.869700
H	2.546893	-0.277582	1.134067	H	-2.246964	0.613107	0.304397

Table S7. Isomer 7 of water cluster (H₂O)₁₀



O	0.011617	-3.414151	-0.066897	O	0.701838	-0.813529	2.510687
H	0.833000	-2.934041	0.038261	H	0.031023	-1.493992	2.567355
H	-0.391414	-3.032317	-0.846641	H	0.213745	-0.009593	2.332687
O	-2.804028	-0.598213	1.330881	O	0.067932	2.123063	-0.587872
H	-2.360695	-1.369093	1.685046	H	0.171915	2.786686	-1.269799
H	-2.203426	0.126038	1.506864	H	0.385032	1.314255	-0.989754
O	-1.270920	-2.729565	2.198022	O	-3.364779	-1.014452	-1.278453
H	-0.867483	-3.038693	1.386905	H	-3.192080	-0.857393	-0.350154
H	-1.516818	-3.528952	2.663584	H	-4.239051	-0.653093	-1.424403
O	-0.886199	1.335913	1.820820	O	-1.044249	-2.045494	-2.218594
H	-0.997247	2.135029	2.335906	H	-1.872690	-1.673994	-1.915434
H	-0.565665	1.640256	0.971782	H	-1.249471	-2.423768	-3.073594
O	0.939422	-0.198981	-1.657889	O	2.107036	-1.661333	0.377600
H	1.438458	-0.682061	-0.999232	H	3.024488	-1.755548	0.633799
H	0.250184	-0.805289	-1.929134	H	1.674570	-1.313578	1.157518

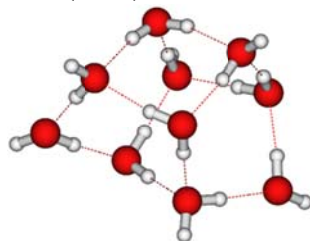
Table S8. Isomer 8 of water cluster (H₂O)₁₀



O	1.296083	-1.576406	-0.759450	O	0.267431	2.458003	-0.358385
H	0.397787	-1.904712	-0.798343	H	0.796148	2.254564	0.413174
H	1.300030	-0.818283	-1.343802	H	0.637956	1.914085	-1.053436
O	-1.397317	-2.208982	-0.858413	O	-0.234067	-0.149085	2.819383
H	-1.909507	-3.017616	-0.860627	H	0.494673	-0.719098	2.573913
H	-1.738358	-1.710920	-0.115542	H	0.107769	0.738228	2.709576
O	2.202491	-1.021975	1.706243	O	-2.307244	-0.631505	1.107082

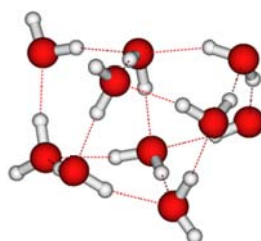
H	1.905842	-1.241852	0.823131	H	-2.405319	0.218799	0.678598
H	2.841254	-1.701737	1.921041	H	-1.654523	-0.481733	1.791009
O	0.980122	0.666429	-2.341205	O	-2.317393	1.699452	-0.387643
H	1.325979	0.839757	-3.216747	H	-2.865350	2.483321	-0.348588
H	0.058636	0.451272	-2.485434	H	-1.421087	2.029947	-0.327300
O	1.718683	1.700468	1.856735	O	-1.620236	0.019772	-2.479899
H	2.448796	2.147716	2.284680	H	-1.629657	-0.828761	-2.037025
H	2.005717	0.790438	1.781317	H	-2.006730	0.625073	-1.847075

Table S9. Isomer 9 of water cluster (H₂O)₁₀



O	-1.430432	0.871849	-2.767842	O	-3.085456	-2.506664	-2.399453
H	-2.296385	0.613811	-3.083712	H	-3.712500	-2.642042	-1.689015
H	-1.093949	0.092169	-2.326127	H	-3.422997	-1.748383	-2.876221
O	-3.265193	-2.884178	1.876408	O	-4.869709	-2.590364	-0.283721
H	-2.882896	-3.348485	2.621056	H	-5.611401	-3.184931	-0.171396
H	-2.630547	-2.198009	1.669940	H	-4.333241	-2.725656	0.497387
O	-1.564589	-0.928489	1.148391	O	-0.794233	-1.467139	-1.448454
H	-2.072569	-0.122417	1.056536	H	-1.579109	-1.905434	-1.777240
H	-1.216835	-1.094173	0.272122	H	-0.072421	-2.037875	-1.712049
O	-3.156390	1.293761	0.780145	O	-3.970375	-0.056280	-3.344924
H	-2.652170	1.869130	0.204867	H	-4.386603	0.079657	-2.493744
H	-3.431082	1.857945	1.502968	H	-4.616202	0.253191	-3.980037
O	-5.018443	0.109722	-0.876139	O	-1.713617	2.818999	-0.926240
H	-4.416643	0.541117	-0.269536	H	-1.050355	3.487158	-1.099099
H	-5.039243	-0.802122	-0.585725	H	-1.591627	2.173893	-1.622796

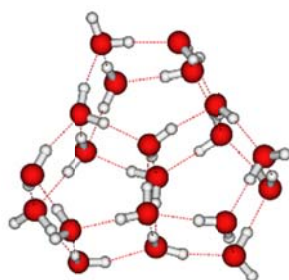
Table S10. Isomer 10 of water cluster (H₂O)₁₀



O	7.657649	9.024649	6.020089	O	5.772105	8.299297	3.042459
H	7.768529	9.415184	5.153244	H	5.327246	8.355951	3.888109
H	7.708607	8.081215	5.866568	H	6.430780	8.993254	3.070824
O	5.457573	5.951024	6.698883	O	10.643467	6.913457	5.341554

H	5.514480	5.543763	7.563251	H	11.499270	6.521143	5.514536
H	6.358453	5.954419	6.375409	H	10.611148	7.680544	5.913188
O	10.214213	9.075852	6.928471	O	7.947065	6.328831	5.565437
H	9.290368	9.166514	6.694968	H	8.903958	6.351544	5.573909
H	10.340979	9.692002	7.649944	H	7.718839	6.171823	4.649198
O	7.373671	6.156648	2.895709	O	4.966215	8.456894	5.648280
H	6.967654	5.468804	2.368211	H	4.941391	7.583345	6.038829
H	6.738309	6.872516	2.886757	H	5.798551	8.827434	5.941793
O	8.024123	9.885287	3.436070	O	9.627390	7.788487	2.900636
H	8.325915	10.676778	2.990316	H	8.948228	7.131390	2.748339
H	8.656780	9.212337	3.184839	H	10.089299	7.479982	3.680185

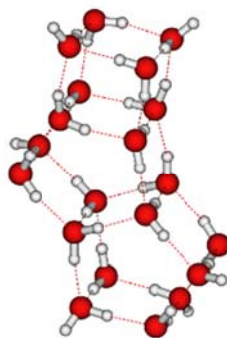
Table S11. Isomer 1 of water cluster (H₂O)₂₀



O	0.381332	-0.452904	-0.383074	O	-1.515748	1.634128	2.849702
H	-0.442954	-0.837023	-0.681798	H	-1.491521	2.199994	2.078053
H	1.058557	-1.012080	-0.763761	H	-1.381871	2.228825	3.587703
O	-0.213563	1.962040	-1.480915	O	-1.656622	3.108369	0.599132
H	0.132760	1.174110	-1.062036	H	-2.533916	2.929719	0.260498
H	0.240751	2.005981	-2.322284	H	-1.069656	2.875139	-0.120109
O	0.897605	1.681433	-3.982215	O	2.178725	-4.126691	0.415424
H	1.454794	2.252379	-4.511170	H	2.917618	-4.617650	0.774908
H	1.363248	0.845426	-3.959808	H	1.698151	-3.819272	1.184043
O	1.895693	-2.321916	-1.662489	O	1.987745	-0.787476	-3.994714
H	1.115740	-2.733178	-2.035006	H	1.320429	-1.299174	-4.451975
H	2.171286	-2.917322	-0.965515	H	2.171585	-1.288420	-3.200050
O	-2.620026	-1.889645	1.384590	O	-0.249781	-2.047082	-5.055476
H	-2.499671	-2.834326	1.481157	H	-0.752419	-1.240401	-4.942105
H	-1.823940	-1.507314	1.753780	H	-0.440592	-2.324828	-5.951401
O	-1.762163	-4.511057	1.586163	O	-3.884357	0.528610	1.907548
H	-1.293836	-4.770931	0.792835	H	-3.140620	0.905182	2.377953
H	-2.166416	-5.319247	1.901822	H	-3.643900	-0.388051	1.772846
O	-0.223879	-5.151849	-0.538580	O	-4.132959	2.146123	-0.234716
H	0.665929	-4.922888	-0.270154	H	-4.992252	2.566497	-0.201044
H	-0.354466	-4.682008	-1.362248	H	-4.130864	1.544327	0.509643
O	-2.622952	0.912874	-2.181538	O	-0.442302	-3.337103	-2.630476
H	-1.798614	1.346356	-1.960645	H	-1.073352	-2.766683	-2.191580
H	-3.274875	1.339202	-1.625235	H	-0.429359	-3.028422	-3.536446

O	-1.939692	-1.544895	-1.227256	O	0.613167	-3.371968	2.480275
H	-2.344205	-0.744648	-1.562227	H	-0.224819	-3.804537	2.316273
H	-2.338549	-1.673329	-0.366645	H	0.392459	-2.444095	2.561350
O	-1.442561	0.342603	-4.651701	O	-0.296506	-0.760564	2.233712
H	-0.690375	0.918256	-4.513599	H	0.068925	-0.580348	1.367563
				H	-0.608598	0.089428	2.544109

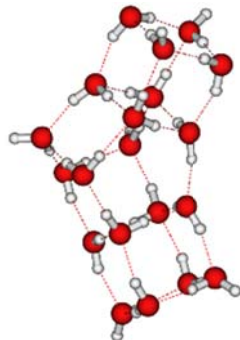
Table S12. Isomer 2 of water cluster (H₂O)₂₀



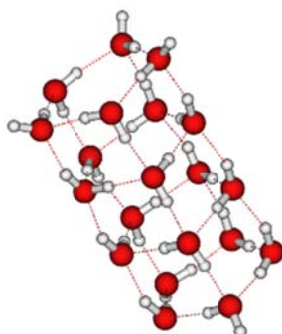
O	-4.029017	3.794182	-3.588565	O	-0.013637	6.178788	-1.726072
H	-3.479740	3.320797	-2.963717	H	-0.536351	6.948286	-1.951628
H	-3.420538	4.094099	-4.263869	H	0.618216	6.498285	-1.081931
O	-3.202656	7.311138	-4.345676	O	-0.358655	4.001776	-3.408930
H	-3.976396	7.011372	-3.868497	H	-0.072849	4.768262	-2.911892
H	-2.668543	7.751343	-3.684483	H	-0.878166	4.361897	-4.127716
O	-1.827962	8.185533	-2.115300	O	-2.163890	4.996527	-5.251377
H	-2.500749	7.772252	-1.574200	H	-2.475439	5.861768	-4.985807
H	-1.700193	9.048670	-1.721724	H	-2.086420	5.051277	-6.203865
O	1.349814	7.146778	0.474317	O	-2.146068	2.699969	-1.883323
H	0.998785	8.024993	0.621793	H	-1.907682	1.777068	-1.795808
H	2.109673	7.091615	1.053803	H	-1.455619	3.075404	-2.429731
O	3.141825	7.109289	2.580184	O	-1.878155	4.883815	-0.223349
H	4.004477	6.737640	2.764418	H	-2.051692	4.047568	-0.655564
H	2.549281	6.645153	3.171540	H	-1.200458	5.295139	-0.759792
O	1.985593	9.525561	3.333230	O	-1.556151	8.160102	2.836251
H	2.539292	8.791637	3.066760	H	-1.132034	8.283823	3.685398
H	1.466859	9.729721	2.555113	H	-1.314054	7.271865	2.574224
O	-1.690807	10.465873	-0.561150	O	0.180194	9.490360	1.217473
H	-2.000343	11.354760	-0.735223	H	-0.337818	9.951796	0.557948
H	-2.364538	10.082847	0.000642	H	-0.469142	9.088239	1.794444
O	-3.418767	9.138976	1.018583	O	0.171941	8.410878	4.982550
H	-3.676104	8.349646	0.542172	H	0.836233	8.880582	4.478242
H	-2.932867	8.814083	1.776593	H	0.170975	8.841192	5.837572
O	-3.681721	6.903390	-0.602151	O	1.251268	5.990690	4.136912
H	-3.166313	6.124514	-0.392531	H	0.592408	5.706190	3.503511
H	-4.296403	6.610504	-1.274919	H	0.847439	6.733230	4.586122

O	-5.153970	6.099459	-2.778937	O	-0.487426	5.802478	1.973075
H	-4.820140	5.238194	-3.029962	H	0.185263	6.206878	1.425187
H	-6.098979	6.040856	-2.919493	H	-1.038682	5.318413	1.358234

Table S13. Isomer 3 of water cluster (H₂O)₂₀

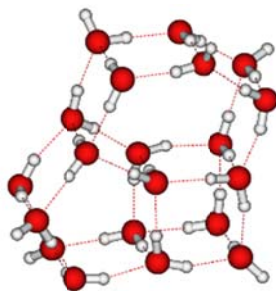


O	9.965301	1.518588	15.554349	O	17.317880	4.791749	18.542924
H	10.166481	0.799616	16.153379	H	16.998862	5.050942	17.678471
H	9.383053	1.130823	14.901006	H	16.660410	5.127799	19.152052
O	16.951778	2.161982	19.102853	O	19.174436	4.836402	20.611914
H	17.112430	3.058568	18.808645	H	18.728753	4.906255	19.767687
H	17.618691	2.005668	19.771453	H	19.192860	3.897366	20.796591
O	16.815720	3.117985	22.861598	O	18.717490	2.159500	21.224672
H	16.027244	2.973502	22.338469	H	18.074020	2.434009	21.877990
H	16.937588	4.067372	22.854823	H	19.294709	1.557570	21.694492
O	15.420896	5.530971	20.327562	O	13.916111	6.025959	18.030915
H	15.962273	5.798724	21.070160	H	14.372943	6.019477	18.872043
H	15.124039	4.649222	20.552565	H	14.607629	5.899529	17.381260
O	12.642434	2.127580	19.554383	O	10.007642	1.294921	19.591597
H	11.756989	1.827206	19.759311	H	9.313847	1.221734	20.246979
H	12.936606	1.546576	18.852863	H	9.699380	1.973063	18.990489
O	10.685837	-0.296104	17.411847	O	16.017212	0.834974	16.913722
H	10.403498	0.094380	18.238914	H	16.387346	1.249778	17.692934
H	11.639351	-0.212601	17.420180	H	16.681725	0.202826	16.639782
O	15.966717	5.437904	16.243187	O	15.228970	3.003628	15.352635
H	16.132541	5.976937	15.469767	H	14.279767	2.888445	15.308141
H	15.713411	4.584585	15.891171	H	15.543219	2.228507	15.818109
O	17.325504	5.799222	22.321475	O	14.946607	2.893496	20.825692
H	17.678645	6.512779	22.852851	H	15.576932	2.535925	20.200341
H	18.051659	5.540478	21.754038	H	14.095228	2.595869	20.505061
O	9.377206	3.139381	17.740700	O	12.503246	2.620761	15.700936
H	9.446539	2.678410	16.904679	H	11.642586	2.293361	15.439580
H	10.148424	3.705734	17.767153	H	12.317097	3.271218	16.378053
O	11.948089	4.166537	17.859409	O	13.305500	0.644831	17.372497
H	12.556702	4.902562	17.923380	H	13.038153	1.299620	16.727510
H	12.233008	3.559472	18.542436	H	14.249050	0.550583	17.241871

Table S14. Isomer 4 of water cluster (H₂O)₂₀

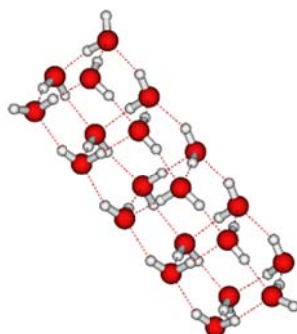
O	3.509582	-1.662908	3.191029	O	1.309792	-2.064418	-0.555776
H	4.277336	-1.111568	3.039996	H	0.636506	-2.733631	-0.433005
H	3.446377	-2.206649	2.405801	H	0.954361	-1.285156	-0.128398
O	1.531750	-4.768826	2.175537	O	0.393003	0.161234	0.716299
H	2.305708	-4.452452	1.709566	H	0.782041	0.215197	1.589208
H	1.531417	-4.281061	2.999137	H	0.838275	0.842572	0.212569
O	5.459215	0.074235	2.230577	O	1.549323	0.225850	3.174787
H	4.796628	0.749041	2.082764	H	2.230670	-0.444946	3.219874
H	6.136822	0.512008	2.745783	H	0.841989	-0.113286	3.723328
O	-0.491805	-3.854340	0.602646	O	-0.524695	-6.397324	3.169001
H	0.208761	-4.211922	1.148150	H	0.295399	-6.083325	2.788102
H	-1.236776	-4.435064	0.757602	H	-0.529822	-6.038878	4.056539
O	5.377885	-1.453941	-0.057808	O	1.528872	-3.225579	4.422613
H	5.487608	-0.893481	0.710358	H	2.338203	-2.740148	4.262698
H	6.267824	-1.595756	-0.380499	H	0.838862	-2.563821	4.375760
O	3.362609	-3.097448	0.888407	O	-3.370530	-3.231124	3.053764
H	4.150514	-2.713330	0.503841	H	-3.185084	-4.043066	2.581969
H	2.644669	-2.757593	0.354278	H	-2.944663	-2.549135	2.534378
O	3.309163	-0.405284	-1.597042	O	2.186043	1.822596	-0.579112
H	4.077658	-0.753880	-1.145237	H	2.627432	1.086144	-1.002251
H	2.633916	-1.071967	-1.471314	H	2.124825	2.490317	-1.262219
O	3.446233	1.824965	1.891984	O	-0.377737	-4.983717	5.504104
H	2.735023	1.498595	2.443252	H	-1.082710	-4.343678	5.602067
H	3.046525	1.944753	1.030522	H	0.401979	-4.456948	5.328635
O	-2.301934	-2.985157	5.518351	O	-0.463341	-1.379911	4.227218
H	-2.751232	-3.118308	4.683704	H	-1.094940	-1.784997	4.821542
H	-3.007321	-2.902013	6.160028	H	-0.869848	-1.446669	3.363199
O	-2.508396	-5.445514	1.629468	O	-1.520933	-1.602506	1.729751
H	-1.857328	-5.842002	2.208381	H	-1.168142	-2.384175	1.304586
H	-3.031391	-6.183212	1.315605	H	-1.101649	-0.872025	1.274965

Table S15. Isomer 5 of water cluster (H₂O)₂₀



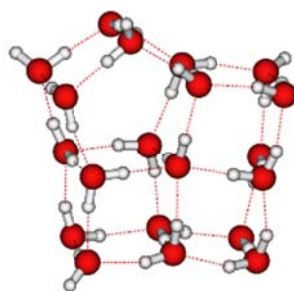
O -1.955489	-5.741183	7.482835	O -0.371532	1.249384	6.783737
H -2.207236	-5.845466	6.565240	H -1.147412	0.725847	6.984117
H -2.472476	-6.397732	7.949634	H -0.469027	2.037303	7.318444
O 4.233926	-4.155742	3.330617	O 0.239032	-5.778864	4.186993
H 4.534734	-4.195527	4.238452	H 0.436757	-5.773901	5.123536
H 3.713981	-4.951056	3.215008	H 1.042128	-6.096003	3.773842
O 4.865535	-4.090071	6.025055	O -2.711362	-3.032821	4.659165
H 4.627764	-3.162999	6.040432	H -3.030483	-2.156605	4.443200
H 5.740545	-4.119856	6.411970	H -2.568693	-3.009808	5.605393
O 3.280477	-6.364453	6.074034	O 0.564782	-2.827309	6.510646
H 3.818758	-5.581332	6.188963	H 1.048040	-2.004486	6.585844
H 2.457517	-6.157090	6.516719	H 0.377215	-2.910886	5.575731
O 0.749383	-5.532179	6.861594	O 1.269810	-0.743565	3.575829
H -0.113153	-5.722616	7.230374	H 2.147397	-0.944928	3.250982
H 0.812943	-4.577278	6.880454	H 0.803848	-1.579012	3.542036
O 4.293776	-1.460185	5.753932	O -2.475916	-5.820216	4.842130
H 4.230893	-1.356168	4.804480	H -1.621018	-5.944985	4.430045
H 3.516456	-1.018413	6.095758	H -2.732027	-4.930567	4.598895
O 3.857795	-1.497203	3.009629	O -3.282480	-0.349042	4.394980
H 3.945841	-2.450180	3.027400	H -2.459956	0.096654	4.192389
H 4.458671	-1.213485	2.320655	H -3.949185	0.152783	3.926036
O -2.600864	-0.242941	7.091111	O -0.102550	-3.090640	3.900062
H -2.982621	-0.263185	6.213567	H 0.073706	-4.028524	3.825638
H -2.513636	-1.164116	7.336186	H -1.049428	-3.033827	4.028234
O 2.780783	-6.519444	3.437686	O -2.032557	-2.965781	7.296411
H 2.995479	-6.552659	4.369907	H -2.122661	-3.884155	7.550780
H 3.102133	-7.350374	3.087653	H -1.094272	-2.848986	7.147373
O 1.771496	-0.404046	6.235808	O -0.915213	0.906780	4.079555
H 1.126258	0.229116	6.550461	H -0.675158	1.163089	4.970012
H 1.621717	-0.450224	5.291527	H -0.147857	0.439605	3.749184

Table S16. Isomer 6 of water cluster (H₂O)₂₀



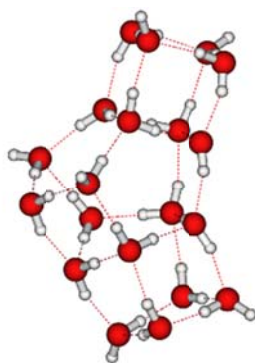
O	10.249888	2.728160	19.748004	O	14.749688	6.250549	13.677904
H	10.641234	3.294000	20.413516	H	14.024127	5.874852	14.176548
H	9.322977	2.686573	19.983250	H	15.168904	6.859438	14.285970
O	16.653348	4.306460	13.816559	O	16.332211	7.251370	11.601451
H	15.940413	4.931027	13.682872	H	16.688595	7.992623	12.091112
H	17.234714	4.442124	13.068333	H	15.595058	6.946427	12.130458
O	19.364490	7.043490	13.663556	O	18.222338	5.340916	11.783542
H	19.149674	6.412246	12.976812	H	18.519254	5.062560	10.917175
H	19.135737	6.597860	14.479227	H	17.555936	6.004962	11.606953
O	16.191205	7.772091	15.419042	O	16.478797	4.731103	17.837901
H	16.585828	8.394835	14.808554	H	16.243635	4.292083	18.655331
H	16.880710	7.129318	15.585347	H	15.862380	5.460360	17.771210
O	15.018366	3.440413	19.833389	O	13.623573	2.379254	21.976630
H	14.738958	3.093684	20.680704	H	13.823910	1.856245	22.752877
H	14.623276	2.851111	19.190847	H	13.178333	1.771534	21.386147
O	12.328499	0.917705	20.121305	O	15.304338	3.136536	15.959493
H	11.507218	1.386507	19.973130	H	15.804075	3.618489	16.618444
H	12.818599	1.028796	19.306631	H	15.801105	3.252250	15.149514
O	14.580562	6.642167	17.396367	O	13.292341	4.959199	15.676332
H	14.056483	6.141299	16.771302	H	13.933099	4.248857	15.709136
H	15.051803	7.278660	16.858741	H	12.559495	4.646012	16.206506
O	17.560238	9.020675	13.361915	O	17.981962	5.740269	15.714875
H	18.280535	8.398508	13.463476	H	17.740985	5.364902	16.561788
H	17.989894	9.863626	13.216789	H	17.588636	5.151498	15.070766
O	11.630837	4.256439	21.483779	O	11.793119	3.950041	17.801101
H	12.310549	3.677629	21.829037	H	12.211638	4.557549	18.411026
H	12.106643	4.895921	20.953776	H	11.096538	3.538362	18.312500
O	13.230397	5.475753	19.541522	O	13.693991	2.002434	17.935791
H	13.918925	4.832495	19.709986	H	12.979572	2.625574	17.803370
H	13.641644	6.123039	18.968697	H	14.249281	2.106213	17.163058

Table S17. Isomer 7 of water cluster (H₂O)₂₀



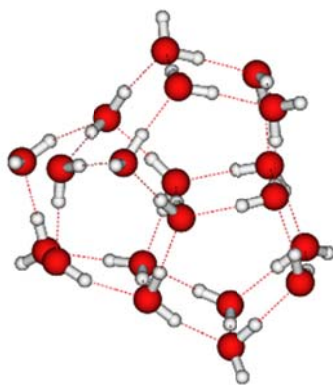
O	-7.830012	-0.654877	2.277550	O	-1.151374	-2.790665	4.198043
H	-7.638512	0.278645	2.367530	H	-1.999849	-2.612663	4.603797
H	-8.745113	-0.739046	2.545392	H	-0.789223	-3.515752	4.707284
O	-2.384742	0.980422	-1.990377	O	-5.654987	1.815361	-0.030586
H	-2.706724	0.079523	-1.959710	H	-6.017034	0.934963	-0.130849
H	-3.144329	1.497776	-2.257969	H	-5.422297	2.081884	-0.919998
O	-3.257959	-1.587251	-1.712150	O	-4.719717	1.142943	3.865268
H	-2.373705	-1.953567	-1.700276	H	-4.084944	1.129261	4.581584
H	-3.544289	-1.621744	-0.799430	H	-4.999980	0.232100	3.775539
O	-5.621587	-0.558972	-2.793007	O	-3.998191	-1.474907	0.959941
H	-4.819690	-1.063000	-2.654621	H	-3.181554	-1.923390	1.179485
H	-6.153000	-0.735535	-2.016696	H	-3.806320	-0.546979	1.095471
O	-6.493228	-0.791471	-0.135771	O	-0.821584	0.391962	1.617477
H	-7.113753	-0.835148	0.591742	H	-0.395784	0.517037	0.769372
H	-5.708405	-1.230999	0.191493	H	-1.679754	0.804195	1.518277
O	-0.670996	-2.236382	-1.169238	O	-6.995461	1.898976	2.430769
H	-0.261462	-1.371269	-1.159561	H	-6.603527	2.119904	1.585896
H	-0.801592	-2.450425	-0.245461	H	-6.256590	1.873508	3.038762
O	0.068358	0.452321	-0.983526	O	-2.787098	0.621529	5.756408
H	-0.755015	0.741837	-1.376552	H	-1.975163	0.462436	5.275073
H	0.746224	0.902834	-1.487280	H	-2.506402	1.047444	6.566370
O	-3.491879	-2.032164	5.300886	O	-3.468201	1.119721	1.460405
H	-3.328273	-1.136481	5.596212	H	-4.105055	1.524839	0.871737
H	-4.250882	-1.959204	4.722247	H	-3.834353	1.248495	2.335380
O	-4.870667	2.029758	-2.669717	O	-5.396688	-1.444418	3.348406
H	-5.175781	1.134883	-2.819170	H	-6.308210	-1.331147	3.079092
H	-5.144391	2.510271	-3.451008	H	-4.923538	-1.605715	2.532107
O	-1.456058	-2.248360	1.515271	O	-0.594272	-0.066470	4.350288
H	-1.308746	-2.595325	2.395127	H	-0.622528	-1.022774	4.319977
H	-1.167198	-1.337149	1.565154	H	-0.528543	0.200858	3.433529

Table S18. Isomer 8 of water cluster (H₂O)₂₀



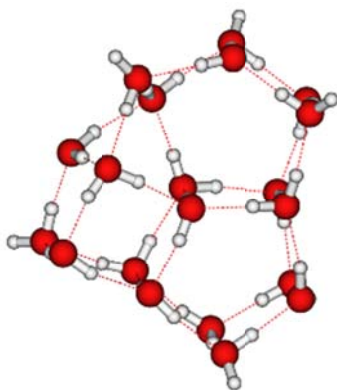
O	2.796722	5.995731	4.041732	O	-1.198456	-0.726927	5.640954
H	3.281891	5.291844	4.472298	H	-2.002064	-0.687709	5.122390
H	2.134114	5.545105	3.518167	H	-0.497704	-0.560010	5.010622
O	-3.378755	2.132267	5.679972	O	0.693024	-0.000997	3.738073
H	-2.788067	1.881107	6.390070	H	1.078451	0.820950	4.041524
H	-3.417688	1.360036	5.115724	H	1.444325	-0.549139	3.511534
O	-0.825266	5.412484	5.299932	O	1.644551	2.414719	4.593974
H	-0.256313	6.126783	5.586816	H	2.480216	2.767911	4.899184
H	-0.612901	4.686263	5.886223	H	1.297296	3.089776	4.010927
O	3.772628	3.883753	5.572711	O	-5.455297	0.752225	2.399916
H	3.302413	4.245896	6.323699	H	-5.375302	1.705887	2.418969
H	4.669156	3.763940	5.885944	H	-6.397746	0.589608	2.439644
O	1.283571	7.078097	5.992205	O	-3.022217	4.229184	4.029401
H	1.852322	6.799382	5.274520	H	-3.191712	3.529716	4.660470
H	1.426224	8.022272	6.058660	H	-2.431597	4.827433	4.487112
O	-1.484209	1.220695	7.476436	O	-3.602998	0.644299	0.323989
H	-1.331435	0.482135	6.887010	H	-4.307577	0.538712	0.963248
H	-1.715699	0.816480	8.312651	H	-2.804420	0.441968	0.811399
O	0.156646	3.286734	6.720410	O	2.226771	4.939636	7.499825
H	-0.401019	2.591146	7.068834	H	1.906997	5.769491	7.145823
H	0.650200	2.868043	6.015191	H	1.473678	4.350985	7.449094
O	0.618377	4.498474	3.189829	O	-5.047321	3.422133	2.266928
H	0.086518	4.882921	3.886650	H	-4.579836	3.541248	1.440186
H	-0.018696	4.153175	2.564418	H	-4.488681	3.841845	2.921142
O	-3.457761	3.307919	-0.016753	O	-1.524966	3.340770	1.943846
H	-3.523488	2.353027	-0.007140	H	-2.082964	3.447164	1.173423
H	-3.602572	3.549244	-0.931643	H	-2.065682	3.639732	2.674928
O	-3.314453	0.000886	3.971052	O	-1.446770	0.630195	2.108937
H	-4.153720	0.120737	3.526643	H	-0.643994	0.375379	2.563747
H	-2.658540	0.200423	3.303073	H	-1.400694	1.584897	2.057418

Table S19. Isomer 9 of water cluster (H₂O)₂₀



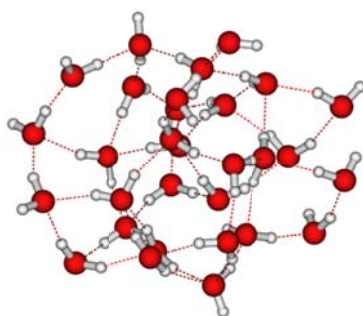
O	4.455390	-5.701857	9.930097	O	-0.087591	-3.767059	4.542143
H	3.966489	-5.512256	10.730885	H	0.721441	-4.246127	4.721570
H	4.970629	-6.480202	10.142088	H	-0.542714	-4.300257	3.890379
O	-2.323365	-1.378593	8.960935	O	3.352922	-2.054322	11.494891
H	-2.099506	-0.483861	8.704862	H	3.197626	-1.141435	11.252500
H	-2.022092	-1.919613	8.231028	H	4.057759	-2.340340	10.913831
O	-1.124695	-1.616022	11.367118	O	4.453415	-2.525286	7.159054
H	-1.586398	-1.623314	10.528661	H	4.399535	-2.516439	6.203412
H	-1.819092	-1.667614	12.023916	H	3.826451	-1.859190	7.440948
O	0.981429	-3.391107	11.260824	O	1.131126	-3.262364	8.577101
H	0.238435	-2.803337	11.397642	H	1.033711	-3.405368	9.518532
H	1.751900	-2.839675	11.396950	H	1.764317	-3.923790	8.298143
O	3.148242	-4.921390	12.160747	O	0.342612	-0.251474	6.482315
H	2.233813	-4.722417	11.959598	H	-0.150281	-1.065484	6.585644
H	3.536280	-4.073603	12.377350	H	1.134173	-0.382301	7.004377
O	-1.229918	1.067505	8.251225	O	5.230136	-3.042701	9.793223
H	-0.656832	0.699080	7.578866	H	5.112977	-3.992491	9.813367
H	-1.631796	1.829001	7.833073	H	5.171728	-2.813307	8.865753
O	0.073983	0.775484	10.683443	O	3.843885	-2.632971	4.467553
H	-0.351294	-0.014786	11.016379	H	3.031787	-2.134945	4.374287
H	-0.390174	0.973252	9.870007	H	4.347676	-2.419825	3.682061
O	2.318431	-4.889258	5.010057	O	2.440635	-0.936251	8.069189
H	2.935293	-4.211350	4.734096	H	2.591742	-0.440176	8.873744
H	2.564938	-5.084390	5.914154	H	1.981361	-1.725397	8.356503
O	2.722187	0.412135	10.448529	O	3.126762	-4.853852	7.662270
H	1.791395	0.589305	10.584429	H	3.559100	-5.286135	8.398780
H	3.156790	1.239217	10.656585	H	3.670990	-4.087660	7.480610
O	-0.912232	-2.623562	6.912401	O	1.422910	-1.456083	4.243390
H	-0.766080	-3.094233	6.091828	H	0.821545	-2.200471	4.221519
H	-0.245421	-2.966112	7.507595	H	1.070372	-0.882678	4.923946

Table S20. Isomer 10 of water cluster (H₂O)₂₀



O	-8.089741	1.074241	2.604597	O	-1.389892	-1.590569	3.650173
H	-7.897586	1.105451	1.667401	H	-2.196111	-1.394621	4.127507
H	-9.008893	0.811379	2.652497	H	-1.047858	-2.379591	4.070518
O	-2.491594	2.366302	-2.808838	O	-5.801948	3.625424	0.455744
H	-2.718975	1.472741	-3.065899	H	-6.312883	3.844757	1.234892
H	-3.328855	2.771379	-2.582698	H	-4.954089	3.340956	0.796987
O	-3.082319	-0.326799	-3.164350	O	-4.689817	2.555205	3.989712
H	-2.323032	-0.537229	-2.620810	H	-4.004954	2.424357	4.645513
H	-2.991242	-0.890624	-3.932490	H	-5.058943	1.683019	3.850891
O	-5.194877	0.470375	-1.575989	O	-4.318944	0.013724	0.981553
H	-4.558935	0.051769	-2.156144	H	-4.612322	0.061371	0.071668
H	-5.179072	1.393463	-1.828755	H	-3.458064	-0.402114	0.934667
O	-7.332604	1.373512	0.032896	O	-0.951752	1.791811	1.371249
H	-6.791426	0.852078	-0.559950	H	-0.636520	1.984060	0.488128
H	-6.850002	2.193183	0.139982	H	-1.812694	2.207898	1.414631
O	-0.920626	-0.668417	-1.601304	O	-7.031548	3.642818	2.893596
H	-0.541948	0.207821	-1.530297	H	-7.525843	2.823130	2.897654
H	-1.140526	-0.908490	-0.701170	H	-6.261517	3.461384	3.432453
O	-0.280166	2.020978	-1.293948	O	-2.642510	1.744428	5.647782
H	-1.055471	2.241180	-1.810326	H	-1.879822	1.579657	5.093353
H	0.430020	2.513559	-1.705326	H	-2.276311	2.079030	6.466423
O	-3.572237	-0.802506	5.022436	O	-3.560354	2.547371	1.518088
H	-3.321891	0.049699	5.379237	H	-3.855196	2.670109	2.420438
H	-4.381171	-0.632367	4.539827	H	-3.832542	1.657045	1.295678
O	-5.078067	3.166854	-2.145261	O	-5.640478	0.078334	3.384568
H	-5.323061	3.490346	-1.278333	H	-6.555918	0.291259	3.203281
H	-5.650501	3.640509	-2.748752	H	-5.251520	-0.063107	2.521470
O	-1.723783	-0.790061	1.035897	O	-0.598806	1.049974	4.030335
H	-1.587361	-1.220268	1.880020	H	-0.719459	0.108082	3.909857
H	-1.390298	0.098183	1.162560	H	-0.566550	1.403438	3.141371

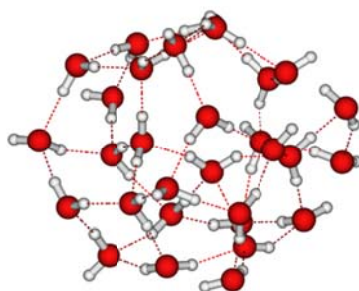
Table S21. Isomer 1 of water cluster (H₂O)₃₀



O	-0.017101	0.050647	-0.345591	O	-0.020192	-3.674536	1.559387
H	-0.045692	0.327530	0.586042	H	-0.813573	-3.125035	1.795477
H	-0.925304	0.091592	-0.671906	H	-0.295409	-4.594069	1.573765
O	0.494518	2.137789	-2.081502	O	3.757348	-1.749024	2.611553
H	0.458089	1.387721	-1.450153	H	3.561768	-0.785201	2.577272
H	0.392808	2.948103	-1.538253	H	4.645734	-1.837416	2.965767
O	0.093376	0.925466	2.250440	O	-0.450306	-0.800483	4.346213
H	-0.068413	0.342822	3.013551	H	-0.624116	-0.658494	5.278675
H	0.240161	1.819771	2.592255	H	0.277603	-1.471724	4.268308
O	-2.455499	0.368020	-1.711786	O	3.971645	-0.121507	-3.117816
H	-2.787541	1.123685	-1.195141	H	3.445107	-0.763302	-3.620526
H	-2.511402	0.630455	-2.645425	H	3.737624	-0.312027	-2.198566
O	2.937933	-0.295014	-0.408682	O	0.459101	4.510156	-0.393215
H	2.132279	-0.830745	-0.485776	H	1.342548	4.534228	0.055840
H	3.548864	-0.844278	0.096108	H	0.383430	5.269856	-0.978304
O	-0.540559	-1.659437	-2.710795	O	-4.640017	-3.674983	-0.017341
H	-0.863733	-1.980710	-3.556459	H	-3.825912	-3.171381	0.082090
H	-1.176789	-0.988825	-2.430194	H	-4.538809	-4.176154	-0.826998
O	2.922178	0.781570	2.288578	O	2.194840	-2.137391	-3.948220
H	2.853251	1.515668	2.913780	H	1.370936	-1.987218	-3.473681
H	2.003924	0.671943	1.993164	H	2.538986	-2.974293	-3.592412
O	1.199665	-2.736115	-0.752045	O	-5.555104	0.197348	-1.546625
H	0.771714	-3.041791	0.068880	H	-5.827014	1.120364	-1.451256
H	0.512575	-2.304350	-1.283523	H	-5.978930	-0.260127	-0.810786
O	-3.584419	-0.885739	0.501033	O	1.629999	3.142091	3.164404
H	-4.521638	-1.101150	0.624924	H	2.052760	3.673305	2.454562
H	-3.485278	-0.643377	-0.437735	H	1.436077	3.743844	3.886008
O	-3.247495	1.988605	0.345749	O	1.363315	-2.645919	3.793828
H	-2.616128	2.565965	0.818649	H	2.249700	-2.397768	3.482766
H	-3.374240	1.184922	0.869098	H	0.949696	-3.133160	3.061150
O	3.255891	2.450477	-2.622545	O	2.741612	4.350515	1.002540
H	2.312825	2.244361	-2.508282	H	3.240029	3.559837	0.540303
H	3.624754	1.634806	-3.013873	H	3.381641	5.060936	1.092787
O	-1.954267	-2.091860	2.345594	O	-5.687536	2.947516	-0.664299
H	-2.455200	-1.548917	1.714017	H	-4.812843	2.691951	-0.325768
H	-1.657375	-1.526126	3.074834	H	-5.580418	3.801123	-1.075027

O	-1.465861	3.742387	1.464664	O	-6.347797	-1.620321	0.513097
H	-1.721742	4.543714	1.921991	H	-6.982128	-1.618000	1.232209
H	-0.790308	4.011831	0.812653	H	-6.077733	-2.536526	0.342301
O	3.870873	2.437414	-0.064783	O	3.918476	-3.131734	0.043063
H	3.738549	2.432118	-1.051147	H	3.824052	-2.881494	0.970856
H	3.531975	1.588678	0.256263	H	3.083766	-2.874684	-0.367480
O	-1.350104	1.295632	-3.978844	O	2.826867	-4.424146	-2.385872
H	-0.950085	1.239306	-4.844923	H	2.145157	-4.085838	-1.786283
H	-0.682413	1.689373	-3.383949	H	3.630746	-4.415027	-1.853990

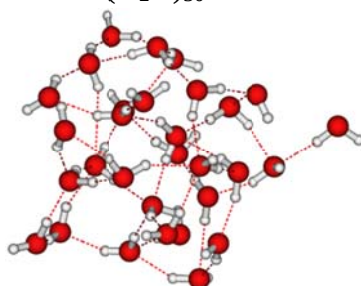
Table S22. Isomer 2 of water cluster (H₂O)₃₀



O	0.125191	-0.204148	0.231681	O	0.446112	-1.215397	-3.306178
H	0.903554	-0.142055	0.815477	H	1.140846	-1.636736	-2.772721
H	-0.682733	-0.095529	0.754899	H	-0.002398	-1.964086	-3.715815
O	0.326470	1.267440	-2.058538	O	-2.729144	3.987766	-0.244275
H	0.195745	0.884554	-1.166458	H	-2.838593	3.316234	0.454896
H	0.446168	0.483019	-2.618703	H	-2.737476	3.471187	-1.067670
O	2.424374	-0.472092	1.736987	O	-2.244033	-0.296924	-3.833638
H	3.285905	-0.049505	1.559891	H	-1.345495	-0.157771	-4.146236
H	2.505139	-1.372735	1.372159	H	-2.122858	-0.711880	-2.967909
O	-2.030511	-1.504225	2.004300	O	0.874530	3.647538	1.384477
H	-1.797044	-2.145550	1.325165	H	1.035217	3.346786	0.468515
H	-1.586502	-1.795703	2.816791	H	0.372696	4.464097	1.207219
O	-0.559753	-2.861821	-0.572716	O	2.655958	-3.054608	0.690870
H	-0.522747	-1.885831	-0.634787	H	2.187478	-3.664995	1.281042
H	-0.019422	-3.119706	0.192826	H	3.619386	-3.076150	0.807943
O	0.823559	-0.207558	3.904653	O	0.430795	-4.019316	1.859436
H	1.554412	-0.275406	3.259348	H	0.153471	-3.504093	2.648235
H	0.323710	0.583753	3.623661	H	0.039508	-4.890414	1.967053
O	-2.370003	-0.517254	-0.861789	O	-0.300736	-2.494010	3.985642
H	-2.474647	0.382746	-1.217919	H	0.161006	-1.593833	3.992334
H	-3.278510	-0.860545	-0.768705	H	-0.415056	-2.762118	4.899840
O	3.473052	2.718952	0.244862	O	-5.191301	1.282564	-1.075091
H	3.909102	2.968720	-0.583724	H	-4.565148	1.369737	-0.350519
H	2.969163	3.467589	0.579587	H	-5.313872	0.334778	-1.190547
O	-4.485352	-0.340946	1.865239	O	-4.931513	-1.581091	-0.600623

H	-3.663549	-0.865513	1.942235	H	-4.621089	-2.497585	-0.572310
H	-4.927164	-0.375113	2.716964	H	-5.103014	-1.311210	0.310175
O	-2.992908	2.114376	1.751984	O	-3.227544	-3.761732	-0.382087
H	-3.516850	1.296494	1.763928	H	-3.140052	-4.694886	-0.592215
H	-2.158631	1.930611	2.211745	H	-2.346668	-3.371457	-0.518315
O	3.345920	0.181999	-1.486756	O	0.475773	-4.049460	-2.878598
H	3.004217	-0.657070	-1.828413	H	0.070606	-4.862359	-3.186570
H	2.584161	0.762221	-1.371106	H	-0.020642	-3.750457	-2.095022
O	-2.353653	2.046511	-2.180204	O	4.962987	-1.909070	0.117504
H	-2.766348	1.645172	-2.956441	H	4.755675	-1.888186	-0.821645
H	-1.397471	1.905774	-2.306267	H	4.971288	-0.975298	0.382341
O	4.889099	0.738201	1.230366	O	5.329088	2.084272	-1.708739
H	5.429612	1.009951	1.976495	H	5.975942	1.752076	-1.079912
H	4.421246	1.548557	0.908238	H	4.743097	1.323064	-1.856834
O	-0.462388	2.113057	3.088885	O	-0.630587	5.518462	-0.016848
H	0.045311	2.668418	2.438530	H	-1.475999	4.992708	-0.086050
H	-0.641384	2.684998	3.840017	H	-0.872688	6.445239	-0.062069
O	2.618953	-2.477841	-2.008123	O	1.212268	3.807850	-1.292929
H	2.580330	-2.736605	-1.068801	H	0.912387	3.081523	-1.856180
H	2.294434	-3.251235	-2.491891	H	0.525636	4.489659	-1.283822

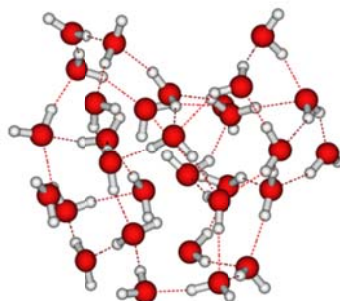
Table S23. Isomer 3 of water cluster (H₂O)₃₀



O	0.612704	-0.736806	-0.003974	O	-0.674952	-3.970137	0.196249
H	-0.215811	-1.232938	-0.149047	H	-1.465204	-3.557224	0.576566
H	0.324686	0.190913	-0.060161	H	-0.572420	-3.583144	-0.691024
O	-2.033192	-1.392779	-0.465977	O	-2.599877	-2.355298	-3.018121
H	-2.360403	-1.720991	-1.320943	H	-1.894022	-3.008892	-3.130281
H	-2.835450	-1.209391	0.048558	H	-3.395935	-2.689515	-3.455685
O	3.009428	-1.927422	0.713538	O	-0.080834	-2.863359	-2.322404
H	3.746508	-1.378136	0.390055	H	-0.183662	-1.911563	-2.469547
H	2.196119	-1.419838	0.526895	H	0.888950	-3.000506	-2.288005
O	-0.135963	1.926785	-0.469196	O	1.065747	-3.312110	2.068959
H	-0.581332	2.160560	-1.309117	H	0.525710	-3.615837	1.292980
H	0.810707	2.079330	-0.667913	H	1.971086	-3.168770	1.753188
O	-1.662803	0.946017	1.753187	O	-4.442405	-1.573641	0.997646
H	-1.143892	0.264010	2.209648	H	-3.960580	-2.163175	1.608256
H	-1.080075	1.296668	1.060792	H	-4.935301	-0.953161	1.545141

O	2.545036	1.484129	0.343325	O	-0.092216	-0.203981	-3.556760
H	2.377007	1.064010	1.211181	H	-0.074028	-0.607368	-4.430118
H	2.716583	2.409487	0.584385	H	0.842394	-0.128376	-3.243604
O	2.324435	0.347393	2.836287	O	-2.787107	0.617453	-2.766333
H	2.906030	-0.425003	2.793537	H	-3.522975	-0.016922	-2.753508
H	1.441092	-0.014767	3.024626	H	-2.000276	0.064682	-2.872899
O	1.947276	2.814780	-2.185619	O	-0.746749	2.527430	-3.117305
H	2.286477	3.514368	-1.595767	H	-1.690846	2.632201	-3.286928
H	1.219498	3.192396	-2.700838	H	-0.552665	1.632433	-3.453644
O	-3.668578	1.316663	-0.221172	O	2.802588	3.316618	2.510676
H	-3.156112	1.162216	-1.038146	H	2.857972	2.511639	3.037783
H	-3.102895	1.011593	0.507821	H	1.852376	3.505316	2.419779
O	2.222626	0.068913	-2.299382	O	-4.124400	3.902357	0.650974
H	1.866188	-0.236372	-1.448148	H	-4.080692	3.025160	0.227422
H	2.324323	1.037168	-2.202214	H	-5.040313	4.184548	0.619840
O	2.622603	-2.876469	-2.014335	O	-0.523315	-3.608909	4.228624
H	3.029583	-2.108658	-2.429458	H	0.208445	-3.787904	3.608196
H	2.886267	-2.826509	-1.080979	H	-0.476226	-4.263434	4.929633
O	-0.091451	-1.054392	3.047068	O	-2.166152	3.679766	2.633973
H	0.347000	-1.767512	2.523645	H	-2.123269	2.714227	2.594310
H	-0.303519	-1.489782	3.884839	H	-2.898108	3.915310	2.036259
O	4.625062	-0.016549	-0.575229	O	-5.006833	-0.785564	-1.690209
H	4.025475	0.681259	-0.239277	H	-4.867404	-0.053028	-1.067713
H	4.353299	-0.121130	-1.495999	H	-5.000499	-1.558369	-1.108478
O	0.293497	3.968208	1.503066	O	6.727945	-1.851075	-1.006606
H	0.017496	3.341134	0.813959	H	6.204458	-1.134372	-0.614658
H	-0.539441	4.130050	1.993714	H	7.569444	-1.443990	-1.237613
O	-2.356410	-2.797317	2.251859	O	2.536563	4.523182	-0.057414
H	-1.984830	-3.279109	3.009256	H	1.717322	4.669920	0.446203
H	-1.842845	-1.978615	2.228046	H	3.230347	4.552582	0.612036

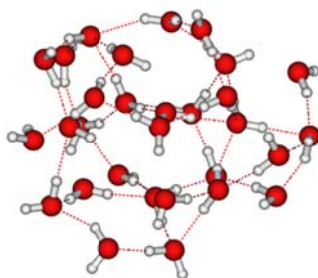
Table S24. Isomer 4 of water cluster (H₂O)₃₀



O	0.248262	-0.275430	-0.418453	O	2.187900	-1.317739	4.254989
H	-0.435112	0.253529	0.041456	H	2.321227	-0.353963	4.305482
H	0.902571	-0.495237	0.265982	H	2.905658	-1.736003	4.737005
O	-1.470441	1.245166	1.082719	O	-5.174454	-0.375220	-0.776553

H	-1.328826	0.788762	1.940254	H	-6.072840	-0.354660	-1.117033
H	-2.412220	1.450572	0.994803	H	-4.624687	-0.751055	-1.491001
O	-0.186805	-2.542166	-1.737574	O	2.794731	-0.020811	-4.099951
H	-0.078551	-1.655232	-1.301386	H	3.241349	0.604390	-4.678023
H	-1.039635	-2.884431	-1.445349	H	2.119126	0.493914	-3.624567
O	0.225362	3.463982	0.873447	O	-2.608430	-3.590951	-0.511255
H	-0.352506	2.682052	0.963768	H	-3.118078	-3.160562	0.208752
H	-0.235065	4.062632	0.257680	H	-2.662375	-4.538407	-0.356015
O	2.172870	-1.388102	1.421477	O	0.275350	-1.642757	-4.372210
H	2.082226	-1.425454	2.389895	H	1.207957	-1.397085	-4.478445
H	2.813036	-0.656748	1.267533	H	0.218456	-2.125561	-3.531995
O	2.094117	1.253234	3.435850	O	3.972640	-2.679315	-0.438822
H	1.832162	2.184234	3.571179	H	3.403514	-3.170229	-1.055235
H	2.750356	1.255133	2.713694	H	3.400214	-2.477746	0.311067
O	-0.389418	0.006155	3.186595	O	-4.298850	-2.252056	1.132287
H	0.501494	0.398022	3.242438	H	-5.006024	-2.578837	1.695039
H	-0.720436	-0.078795	4.084784	H	-4.655685	-1.501833	0.628750
O	-0.022566	-3.286635	1.341022	O	-2.838834	-1.611410	3.650017
H	0.721857	-2.703294	1.139190	H	-1.901204	-1.855242	3.683449
H	-0.595227	-3.251304	0.571988	H	-3.112835	-1.815590	2.752523
O	0.832156	1.474421	-2.719002	O	-0.292214	-2.905391	4.176262
H	0.141642	0.838275	-2.450469	H	0.453153	-2.298326	4.265012
H	0.392817	2.074470	-3.329360	H	-0.246843	-3.197868	3.254458
O	-1.487355	0.035150	-3.194122	O	2.086365	-4.066503	-1.988618
H	-2.077151	-0.630966	-2.811981	H	1.234320	-3.626721	-1.807378
H	-0.915209	-0.469400	-3.814666	H	1.989666	-4.981711	-1.722232
O	2.396666	2.401126	-0.544750	O	-3.689155	4.245884	-0.672139
H	1.711705	2.814969	0.008124	H	-3.720826	3.650796	0.087510
H	1.905441	2.008333	-1.281382	H	-3.500999	3.641137	-1.412119
O	3.701040	0.824825	1.207673	O	-1.143362	4.953659	-1.029135
H	3.312000	1.371027	0.488277	H	-2.115432	4.965863	-0.866227
H	4.650009	0.896330	1.035198	H	-0.873807	5.839362	-1.280646
O	-3.524952	-1.861311	-2.447469	O	4.647778	-0.379617	-1.851261
H	-3.276920	-2.617750	-1.880219	H	4.094286	-0.492968	-2.630815
H	-3.713125	-2.218874	-3.319900	H	4.530341	-1.183659	-1.310961
O	-4.245275	1.776401	0.846500	O	1.316203	3.874387	3.351827
H	-4.618865	1.202402	0.160249	H	0.953096	4.563401	3.909130
H	-4.975866	2.013716	1.422912	H	0.862290	3.922344	2.489018
O	-2.263131	2.589663	-2.282376	O	5.366637	2.065122	-0.754723
H	-1.442886	3.032987	-2.033072	H	5.201993	1.239180	-1.240082
H	-2.052644	1.747013	-2.711127	H	4.565258	2.580570	-0.882924

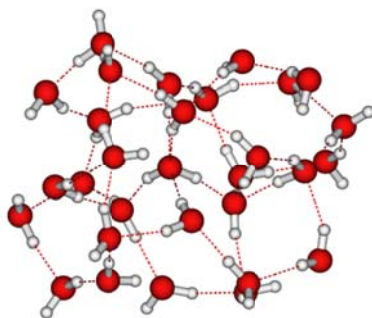
Table S25. Isomer 5 of water cluster (H₂O)₃₀



O	0.229779	-0.490385	-0.621442	O	1.357585	-3.119024	-2.842975
H	1.171641	-0.429372	-0.440283	H	1.814182	-2.248278	-2.894105
H	0.045759	0.144192	-1.345806	H	1.168435	-3.360321	-3.741825
O	-1.376667	2.007982	-0.300213	O	0.412296	3.405562	-1.962569
H	-0.810312	1.816250	0.472734	H	0.223049	4.328739	-1.778155
H	-0.813146	2.417956	-0.977407	H	1.228707	3.169105	-1.492553
O	-1.275596	-1.455823	1.370618	O	-4.415906	-1.973203	-1.520009
H	-1.701455	-2.220668	0.938830	H	-3.933327	-1.225970	-1.129197
H	-0.729413	-1.036610	0.675115	H	-4.201565	-1.955994	-2.459756
O	-1.503170	-2.146575	-2.101891	O	-4.633550	1.409761	-2.002937
H	-0.635967	-1.902508	-1.768929	H	-4.855119	0.766834	-1.317773
H	-1.923985	-2.624854	-1.360951	H	-5.408126	1.503039	-2.562567
O	2.924315	-0.476088	-0.034470	O	-3.812149	3.074157	0.631612
H	3.891602	-0.376148	0.018481	H	-3.685035	2.267031	0.121596
H	2.731842	-1.399757	0.271392	H	-4.744189	3.308803	0.499660
O	0.032699	0.896913	-3.019863	O	-2.979017	-1.100161	3.508661
H	0.070774	1.862972	-3.042992	H	-2.233823	-1.080145	2.894306
H	-0.866414	0.643569	-3.329286	H	-3.228853	-0.164706	3.567487
O	2.385275	2.292246	-0.208453	O	-2.668980	1.588910	2.840808
H	1.897491	2.873689	0.399709	H	-3.130259	2.209251	2.252593
H	2.297530	1.381324	0.115823	H	-1.727347	1.758378	2.724439
O	-3.332233	0.127526	-0.059280	O	0.874586	4.386641	0.975530
H	-3.054910	-0.260232	0.783903	H	1.250905	5.193417	1.321618
H	-2.539605	0.611187	-0.364544	H	-0.033066	4.602002	0.647623
O	2.283176	0.687932	3.060968	O	4.584575	1.729099	1.776194
H	1.907346	-0.230445	2.918698	H	4.171686	2.294127	1.120402
H	2.408159	0.761912	4.009275	H	3.835335	1.285610	2.217708
O	2.344866	-3.015074	0.713800	O	-3.700568	-3.587657	2.691504
H	3.230917	-3.402340	0.588895	H	-3.455112	-4.183291	3.390612
H	1.654974	-3.538699	0.270667	H	-3.628147	-2.677545	3.063373
O	1.192726	-1.658154	2.778060	O	5.678929	-0.178673	0.094376
H	1.679684	-2.248684	2.150697	H	5.561529	0.484941	0.803178
H	0.275484	-1.713719	2.500578	H	5.640270	0.327033	-0.732145
O	0.060820	1.980039	2.107025	O	5.096789	-2.859015	0.679912
H	0.344019	2.904290	2.055154	H	5.458474	-2.003493	0.434228
H	0.817963	1.494503	2.490961	H	5.667661	-3.191455	1.403058
O	2.469611	-0.524025	-2.890930	O	0.224594	-4.110969	-0.533170

H	2.664721	-0.476414	-1.938752	H	0.379307	-3.866108	-1.447022
H	1.650333	-0.021956	-3.025059	H	-0.747453	-4.209516	-0.395078
O	-2.784403	-3.556118	0.125445	O	4.570868	1.371622	-1.957942
H	-3.558964	-3.229491	-0.390846	H	3.864097	1.881742	-1.549989
H	-3.126666	-3.735448	1.017863	H	4.153811	0.914283	-2.707992
O	-2.482646	0.034448	-3.381396	O	-1.589873	4.816326	0.012126
H	-2.279577	-0.765460	-2.864362	H	-2.133803	4.016927	0.087219
H	-3.154436	0.547586	-2.899078	H	-2.167453	5.543182	0.295791

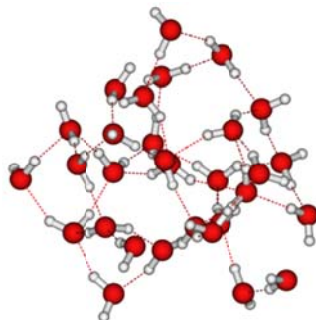
Table S26. Isomer 6 of water cluster (H₂O)₃₀



O	-0.672825	0.542568	0.055070	O	-0.537304	3.043694	-1.974942
H	-1.169339	-0.053213	-0.538581	H	-1.293771	3.319356	-1.440984
H	0.066323	-0.006385	0.360182	H	-0.880525	2.308037	-2.516327
O	-2.556580	1.382701	1.927521	O	-4.503089	-1.029760	-3.167016
H	-2.703346	2.334497	2.050160	H	-4.149501	-0.240703	-2.720622
H	-1.898134	1.253335	1.214951	H	-4.615087	-0.826768	-4.099179
O	-1.463768	-1.803973	-1.261667	O	2.737242	3.900108	-0.650485
H	-2.362060	-2.154998	-1.129260	H	3.383032	3.319716	-1.150357
H	-0.899341	-2.208149	-0.577226	H	2.567157	4.667295	-1.203424
O	0.714476	2.851145	0.757741	O	-0.474854	4.841868	2.165770
H	1.408978	3.225567	0.166816	H	0.098130	5.053073	2.906678
H	0.135979	2.332941	0.170432	H	-0.023170	4.134584	1.647689
O	1.530543	1.168355	-2.252865	O	-4.138592	-2.648020	-1.019599
H	1.174393	2.062578	-2.088687	H	-4.509524	-2.006984	-0.392817
H	1.694434	0.799043	-1.364664	H	-4.378935	-2.322618	-1.908559
O	-3.306402	0.576824	-1.310169	O	3.939489	1.942080	0.909602
H	-3.327021	1.503419	-1.020623	H	3.575005	2.828302	1.038112
H	-3.519048	0.034129	-0.521497	H	4.158040	1.613126	1.788436
O	2.424234	-0.303350	-0.071236	O	1.673176	-1.251074	4.293094
H	3.374286	-0.093409	-0.175261	H	0.801221	-1.130499	4.707319
H	2.265689	-1.137002	-0.541055	H	1.775887	-0.469425	3.725415
O	0.136652	-2.089506	0.947962	O	-3.017037	4.164658	1.998333
H	0.713193	-2.735067	1.397093	H	-3.652574	4.611496	2.562841
H	-0.371828	-1.675592	1.662502	H	-2.125440	4.551219	2.170499
O	-1.156947	0.567152	-3.193988	O	-2.712098	-4.544521	0.407681
H	-1.796128	0.247621	-2.539284	H	-3.196888	-5.347030	0.613737

H	-0.280918	0.365989	-2.831480	H	-3.275294	-4.055713	-0.219181
O	1.444423	0.607080	2.266418	O	1.808854	-3.474001	2.765729
H	1.290048	1.502205	1.914052	H	1.509912	-4.239044	3.268084
H	1.868639	0.146688	1.509898	H	1.819622	-2.709630	3.394379
O	-0.363391	-2.210138	-3.789389	O	4.409775	-2.652241	-1.570688
H	-0.879448	-2.105035	-2.969184	H	3.587185	-2.536336	-2.072332
H	-0.680842	-1.501389	-4.362958	H	4.176267	-3.115131	-0.751069
O	-0.932014	-0.561664	3.135183	O	4.201388	2.231764	-2.092404
H	-0.137881	-0.072086	2.847394	H	4.620542	1.532985	-1.564250
H	-1.658669	0.062025	2.969503	H	3.444630	1.784299	-2.509733
O	-4.143400	-0.691925	1.004921	O	3.983511	-3.698263	1.002315
H	-3.907326	0.136632	1.460446	H	4.723223	-4.069446	1.485788
H	-3.715389	-1.389301	1.546536	H	3.240989	-3.648731	1.625883
O	2.025684	-1.665463	-2.577698	O	-2.862364	-2.610339	2.415467
H	2.098236	-0.745783	-2.867707	H	-2.631781	-3.334790	1.804149
H	1.245935	-2.003223	-3.064410	H	-2.045531	-2.245570	2.776742
O	-3.115781	3.370797	-0.646667	O	5.082738	-0.195881	-0.869267
H	-3.195598	3.716115	0.261183	H	4.980787	-1.124164	-1.197872
H	-3.651518	3.945217	-1.200590	H	5.888177	-0.173656	-0.345558

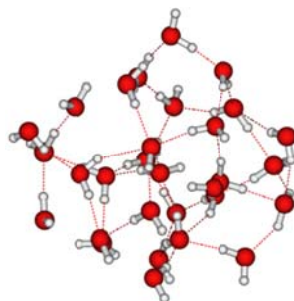
Table S27. Isomer 7 of water cluster (H₂O)₃₀



O	-0.386742	0.351459	-0.069013	O	-5.011045	-2.014735	-2.449223
H	-0.833499	0.083305	-0.894148	H	-4.860077	-1.530889	-1.620796
H	0.556420	0.273589	-0.179205	H	-5.491524	-1.410123	-3.025823
O	-2.223141	0.029197	-2.065937	O	1.077001	2.579381	-3.097711
H	-2.145974	0.883470	-2.511568	H	0.147464	2.644315	-3.028360
H	-3.000896	0.082566	-1.478479	H	1.489423	3.166478	-2.433697
O	-2.534425	1.955155	0.553806	O	5.547410	-1.092119	-0.730021
H	-2.989054	1.142684	0.835157	H	5.126479	-1.714150	-0.133906
H	-1.628614	1.656629	0.387960	H	5.125377	-1.233868	-1.611223
O	1.805682	-1.986444	0.817309	O	2.937337	3.373617	-1.000028
H	1.634347	-2.364041	-0.059433	H	3.680857	2.722128	-0.985400
H	2.134050	-2.676323	1.438174	H	3.359633	4.235205	-1.147315
O	-0.346587	-1.052265	2.362914	O	0.073569	-3.391523	-3.959189
H	-0.920161	-0.661945	1.679451	H	-0.873357	-3.288182	-3.790241
H	0.346874	-1.501979	1.837793	H	0.209577	-4.304810	-4.232892

O	2.668181	0.524705	0.689400	O	-2.327955	-2.051835	3.839012
H	2.522999	-0.441932	0.791852	H	-1.436427	-1.838681	3.508633
H	2.286837	0.883418	1.514348	H	-2.245056	-2.575389	4.655216
O	2.180842	0.402008	-2.056051	O	-1.701701	2.594279	-3.128892
H	2.474295	0.709190	-1.187214	H	-1.936596	2.912305	-3.992380
H	1.724147	1.163146	-2.503763	H	-2.043541	3.267466	-2.458396
O	0.952008	-2.027776	-1.751384	O	4.887364	1.642524	-0.466371
H	0.829116	-2.540276	-2.578302	H	4.326957	1.152060	0.162577
H	1.351132	-1.171233	-1.988070	H	5.424591	0.942749	-0.839010
O	-2.355375	-2.632643	-2.913641	O	3.092082	-0.592151	4.140357
H	-2.192703	-1.679644	-2.764386	H	3.983324	-0.265223	4.003398
H	-3.320491	-2.667289	-2.958442	H	2.501731	0.124613	3.876631
O	-1.150555	-3.168267	-0.458062	O	0.397580	-4.428970	1.525002
H	-0.438990	-2.562513	-0.755314	H	0.464926	-5.407721	1.467767
H	-1.666988	-3.269858	-1.266787	H	-0.205529	-4.189349	0.814587
O	1.226489	1.176502	2.989511	O	4.208411	-1.053298	-3.133785
H	0.974930	2.039482	2.618941	H	3.477353	-0.446635	-2.925628
H	0.522855	0.543884	2.824171	H	4.542156	-0.807531	-4.003820
O	-3.295873	0.320110	2.683192	O	2.692970	-3.145621	3.060382
H	-3.131982	-0.451482	3.236948	H	1.902685	-3.578416	3.429694
H	-3.220833	1.093392	3.274268	H	2.814752	-2.317188	3.544217
O	-4.260677	-0.484007	-0.159173	O	-3.158764	-2.423055	1.193756
H	-3.849723	-1.167505	0.441283	H	-2.985312	-2.509292	2.140662
H	-4.964077	-0.078983	0.345168	H	-2.351429	-2.700822	0.717604
O	-2.585162	4.115466	-1.186518	O	-2.816414	3.827915	2.550202
H	-2.839233	3.369658	-0.611924	H	-3.665674	4.235258	2.401185
H	-1.926082	4.597118	-0.642521	H	-2.740194	3.105838	1.880686
O	1.499170	3.539053	1.395263	O	-0.902204	5.045596	0.802888
H	2.070986	4.125717	1.874112	H	-0.085945	4.548676	0.973030
H	1.951089	3.351547	0.553765	H	-1.483202	4.839321	1.555223

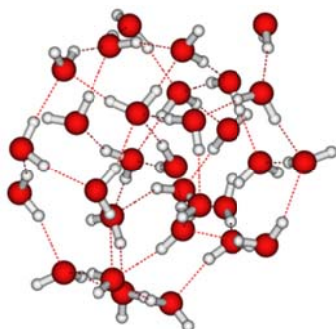
Table S28. Isomer 8 of water cluster (H₂O)₃₀



O	0.426226	0.325720	-0.334459	O	-1.244827	-2.769337	-3.562967
H	1.096592	-0.138520	0.213467	H	-0.695564	-1.973631	-3.407763
H	-0.373032	-0.249346	-0.200347	H	-1.059294	-3.071897	-4.456354
O	-0.114108	2.376227	1.552349	O	2.118449	4.497748	-1.640143

H	0.084738	1.726775	0.853569	H	2.103895	4.598520	-0.660268
H	0.475416	3.134077	1.394131	H	2.177931	5.375776	-2.023102
O	1.972523	-1.434634	1.067014	O	-3.781931	-2.981396	-2.115807
H	1.659856	-2.300527	0.752766	H	-3.126869	-2.765810	-2.793635
H	2.048912	-1.497086	2.033619	H	-4.078756	-2.112962	-1.803319
O	-1.528664	-1.430910	0.011583	O	2.797356	-1.397123	3.767196
H	-1.390530	-2.317367	-0.361921	H	2.751320	-1.810111	4.629262
H	-1.749776	-1.551241	0.983452	H	3.717347	-1.476400	3.431327
O	0.274189	-0.522979	-3.051441	O	-2.143614	-1.586248	2.513041
H	0.408925	-0.271830	-2.119017	H	-1.846191	-0.735735	2.908315
H	1.163437	-0.567270	-3.435438	H	-3.088554	-1.667271	2.715555
O	-0.061850	2.737272	-1.753056	O	4.202387	-3.528196	0.555554
H	0.312904	1.987308	-1.259872	H	4.871763	-4.133979	0.222937
H	0.599801	3.448964	-1.745178	H	3.850977	-3.077104	-0.240921
O	4.127371	0.122231	0.140337	O	1.929609	4.361774	1.019983
H	3.814237	0.475133	-0.700297	H	2.717954	3.807883	1.300902
H	3.413128	-0.472241	0.441265	H	1.880417	5.110990	1.620035
O	-3.784548	-0.310668	-1.030251	O	5.064672	-1.544136	2.317177
H	-2.978026	-0.687780	-0.619759	H	5.140412	-0.776115	1.734990
H	-3.429868	0.369651	-1.629250	H	4.840295	-2.277071	1.712931
O	-1.423406	-4.066495	-1.100838	O	-4.974991	-1.727033	2.948683
H	-2.393249	-4.033638	-1.095044	H	-5.418517	-2.576495	2.981525
H	-1.210214	-3.856872	-2.026270	H	-5.368813	-1.216536	2.213560
O	-2.138927	1.159619	-2.779575	O	3.827546	2.763752	1.714480
H	-1.537956	0.548395	-3.224028	H	3.331106	1.999601	2.089447
H	-1.568520	1.895690	-2.510495	H	4.471192	2.383893	1.105495
O	-1.484905	0.876247	3.525422	O	3.045071	-0.438700	-3.525423
H	-1.104939	1.555418	2.950849	H	3.667818	-0.649984	-4.224660
H	-2.414771	1.127354	3.670388	H	3.087220	0.527137	-3.368774
O	1.117130	-3.820208	-0.116571	O	2.511098	2.099645	-3.011454
H	1.647339	-4.561511	0.198582	H	1.598643	2.177132	-3.319204
H	0.201962	-4.131604	-0.239794	H	2.674084	2.924612	-2.526231
O	2.120489	1.075473	2.802882	O	-5.455321	0.167296	1.027033
H	2.216208	0.287884	3.359424	H	-4.891217	0.089984	0.217090
H	1.188840	1.323653	2.755439	H	-6.257503	0.630701	0.765867
O	3.025120	-2.601740	-1.709425	O	-4.116439	3.337008	-2.374906
H	2.997508	-1.801590	-2.254296	H	-3.736120	3.326197	-1.485040
H	2.119337	-2.868286	-1.495978	H	-3.750967	2.561005	-2.807784
O	-2.336186	3.416116	-0.112126	O	-4.246693	0.947142	3.546626
H	-1.941474	2.986073	0.659406	H	-4.574784	0.911041	2.631166
H	-1.602427	3.417310	-0.743840	H	-4.526173	0.091918	3.903787

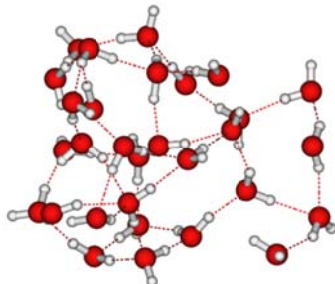
Table S29. Isomer 9 of water cluster (H₂O)₃₀



O	0.358810	-0.794396	0.107482	O	5.238882	-0.521628	1.146925
H	0.081945	-0.039578	0.664274	H	4.730410	-0.625513	1.984562
H	1.330970	-0.784486	0.102630	H	5.971599	-1.141574	1.180403
O	2.989386	-1.167904	-0.426605	O	-2.732351	-2.094224	1.558120
H	3.848559	-0.885985	-0.065914	H	-2.122425	-1.661399	2.209575
H	2.972778	-0.995949	-1.393693	H	-2.192673	-2.793639	1.156515
O	-1.817176	1.273963	-2.318789	O	-3.028940	-2.273975	-1.633464
H	-1.087917	0.666437	-2.477069	H	-3.856425	-2.241971	-1.133186
H	-2.585288	0.865078	-2.797114	H	-2.426949	-2.840149	-1.124177
O	0.157003	1.457775	1.965307	O	2.640101	-0.639346	-3.056148
H	-0.641903	1.987333	1.701427	H	1.886741	-0.023721	-3.028178
H	0.246698	1.758105	2.893120	H	3.391182	-0.040385	-3.226724
O	2.098683	-3.437113	0.822714	O	1.332013	-3.123761	-3.124533
H	2.506260	-2.744498	0.271944	H	0.527279	-2.572989	-3.114976
H	1.860020	-4.167391	0.213872	H	2.040239	-2.471005	-3.236501
O	-2.728338	0.471857	0.254059	O	1.450040	-2.508295	3.180486
H	-2.671809	-0.474390	0.458108	H	1.610910	-2.917226	2.286413
H	-2.261932	0.640984	-0.585891	H	1.504371	-3.232627	3.810963
O	-0.840784	-0.908794	3.151947	O	-0.484797	2.551675	4.350189
H	-0.513667	-0.114597	2.687057	H	-1.140712	1.939003	4.735797
H	-0.061205	-1.495098	3.234417	H	-1.022432	3.200080	3.873271
O	1.300125	1.753814	-2.464394	O	-2.207704	0.501512	5.142571
H	1.447762	1.840451	-1.500068	H	-1.805971	-0.153881	4.547422
H	0.664535	2.446373	-2.697388	H	-3.152442	0.497930	4.952516
O	-0.933277	-3.333459	-0.083857	O	-3.888845	-0.059912	-3.343293
H	-0.341970	-2.585016	0.089198	H	-3.641315	-0.978673	-3.197214
H	-0.365005	-4.051368	-0.432040	H	-4.544617	0.108054	-2.640390
O	-0.583159	-1.181133	-2.490740	O	-5.283991	0.314010	-0.984460
H	-0.199667	-1.055070	-1.597680	H	-5.636644	-0.491851	-0.594714
H	-1.490032	-1.475429	-2.315336	H	-4.513814	0.512931	-0.433947
O	0.906689	4.797309	-0.586721	O	4.159325	1.638142	-2.821191
H	0.548638	4.468479	-1.418950	H	4.496806	1.758259	-1.922304
H	1.422857	4.055866	-0.243587	H	3.264487	2.012369	-2.800976
O	2.043161	2.285489	0.129740	O	3.646479	-0.777296	3.277246
H	2.983731	2.100331	0.260994	H	3.700253	-0.362747	4.143717
H	1.531992	1.963333	0.895354	H	2.863164	-1.358820	3.283637

O	-2.089656	2.820711	1.689207	O	-1.842490	4.886202	-0.078952
H	-2.610521	2.100617	1.303733	H	-1.838041	4.581078	-1.000909
H	-2.129398	3.571091	1.057808	H	-0.898016	5.081396	0.063165
O	-0.877966	3.703054	-2.653941	O	1.054971	-4.943272	-1.264154
H	-1.130099	4.108080	-3.483613	H	1.233051	-4.322376	-2.020094
H	-1.361975	2.841924	-2.586532	H	1.125553	-5.839265	-1.606196
O	4.840386	1.908604	-0.011000	O	-5.127817	-2.210486	0.351766
H	5.433004	2.633343	0.212096	H	-4.415501	-2.141772	1.017816
H	5.179375	1.112041	0.435280	H	-5.734923	-2.883510	0.664158

Table S30. Isomer 10 of water cluster (H₂O)₃₀



O	-0.647612	0.386355	-0.680971	O	-4.076684	1.157045	-1.851808
H	0.200411	0.168014	-0.236166	H	-3.546306	0.833723	-2.599200
H	-1.386148	0.034306	-0.151361	H	-4.866896	0.596382	-1.845447
O	0.125159	0.506350	-3.297326	O	0.782239	3.643192	-1.719183
H	-0.115406	0.561336	-2.349748	H	-0.133693	3.371712	-1.886649
H	0.771538	1.206284	-3.495296	H	1.307827	3.333022	-2.475014
O	-3.039312	0.317296	0.615744	O	2.308050	2.206918	-3.560520
H	-3.705050	-0.341233	0.897325	H	2.852957	2.635702	-4.223889
H	-3.433630	0.736792	-0.168318	H	2.959086	1.857904	-2.895559
O	1.909676	-0.050708	0.041263	O	0.138844	-2.601449	3.557007
H	2.082920	-0.553051	0.864091	H	0.641228	-2.217656	4.291139
H	2.171954	0.877565	0.199200	H	-0.706232	-2.118883	3.516404
O	-1.835165	2.808785	-1.327598	O	-0.370262	-4.218182	1.289325
H	-1.447981	1.995391	-0.953690	H	0.436405	-4.250512	0.731255
H	-2.753416	2.599193	-1.538824	H	-0.082121	-3.958594	2.175083
O	-1.889881	1.581411	2.819244	O	-0.999347	5.112025	0.050638
H	-2.224767	1.173371	1.992913	H	-0.165466	5.170210	-0.429280
H	-2.384424	1.130664	3.506146	H	-1.472363	4.399207	-0.408371
O	-2.815542	-2.034073	-2.189004	O	4.130119	1.679810	-1.739850
H	-2.379750	-2.820444	-2.535209	H	4.587160	0.844512	-1.570541
H	-2.579942	-1.310725	-2.799938	H	3.819179	2.035587	-0.894875
O	2.451867	2.612111	0.264142	O	-4.947312	-1.644471	0.952464
H	2.357519	2.992969	1.157739	H	-5.415558	-1.569063	0.107065
H	1.788364	3.046731	-0.302741	H	-4.306243	-2.366889	0.829291
O	2.337409	-1.102519	-2.469348	O	-5.483412	-1.318734	-1.875088
H	1.606528	-0.688755	-2.964731	H	-4.609650	-1.732702	-2.028405

H	2.193803	-0.823379	-1.538748	H	-6.108518	-1.769007	-2.450348
O	2.400243	-1.567981	2.229811	O	1.908194	-0.853070	4.878112
H	1.607142	-2.113201	2.364680	H	1.426445	-0.024434	4.639820
H	2.569135	-1.228017	3.125642	H	2.337323	-0.707513	5.722368
O	-2.428094	-2.708510	0.648179	O	1.845128	-4.192961	-0.262344
H	-1.664557	-3.329417	0.800060	H	2.688567	-3.748822	-0.064073
H	-2.294069	-2.274340	-0.202588	H	1.814229	-4.252764	-1.227906
O	-2.387700	-1.401111	3.079264	O	4.959396	-1.002087	-1.877782
H	-2.414347	-1.765908	2.171033	H	5.665231	-1.335273	-2.438207
H	-3.132560	-1.805856	3.532660	H	4.122852	-1.042069	-2.387711
O	0.665989	1.305083	4.013652	O	1.857250	3.563343	2.789681
H	-0.167005	1.297734	3.506798	H	0.905211	3.874216	2.739618
H	1.203061	2.023852	3.642399	H	2.335619	4.203960	3.320456
O	-2.433587	0.152367	-3.889396	O	2.059196	-3.813789	-3.040305
H	-1.475365	0.384721	-3.839004	H	2.211919	-2.866079	-2.875243
H	-2.744920	0.371407	-4.770429	H	2.829906	-4.140616	-3.507088
O	4.143060	-2.716031	0.321629	O	-0.659507	4.162599	2.609389
H	3.768593	-2.220608	1.059358	H	-1.228380	3.383679	2.711990
H	4.479620	-2.077789	-0.323142	H	-0.864171	4.561354	1.741026