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

Supporting Information:

Water model for hydrophobic cavities: structure and energy from quantum-chemical calculations

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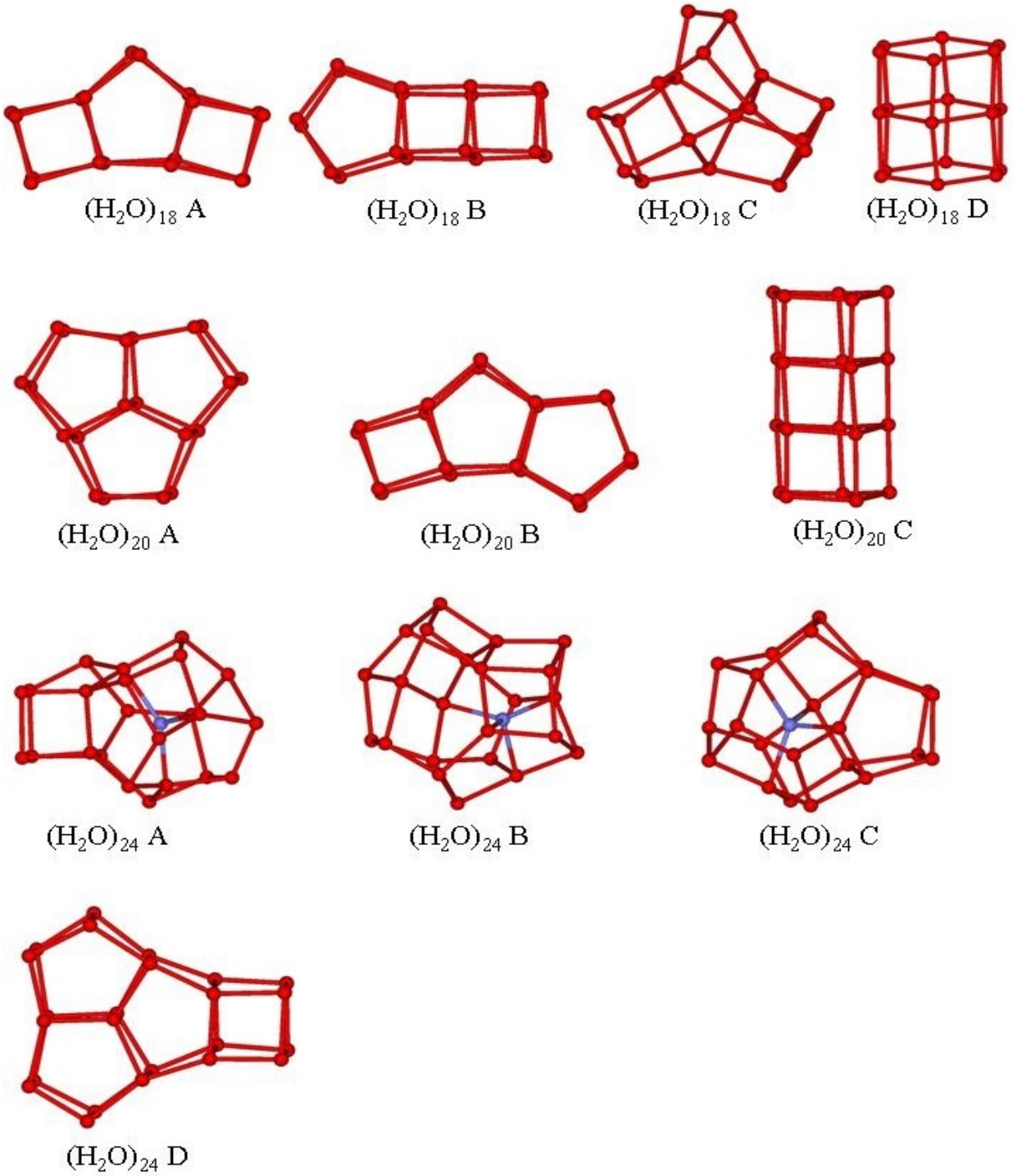

Fig. S1. Low-lying energy structures of the $(H_2O)_{18}$, $(H_2O)_{20}$ and $(H_2O)_{24}$ clusters. Hydrogen atoms have been omitted for clarity and the sticks represent the O–H bonds involved in hydrogen bonding. The full solvated molecules are indicated with blue oxygens.

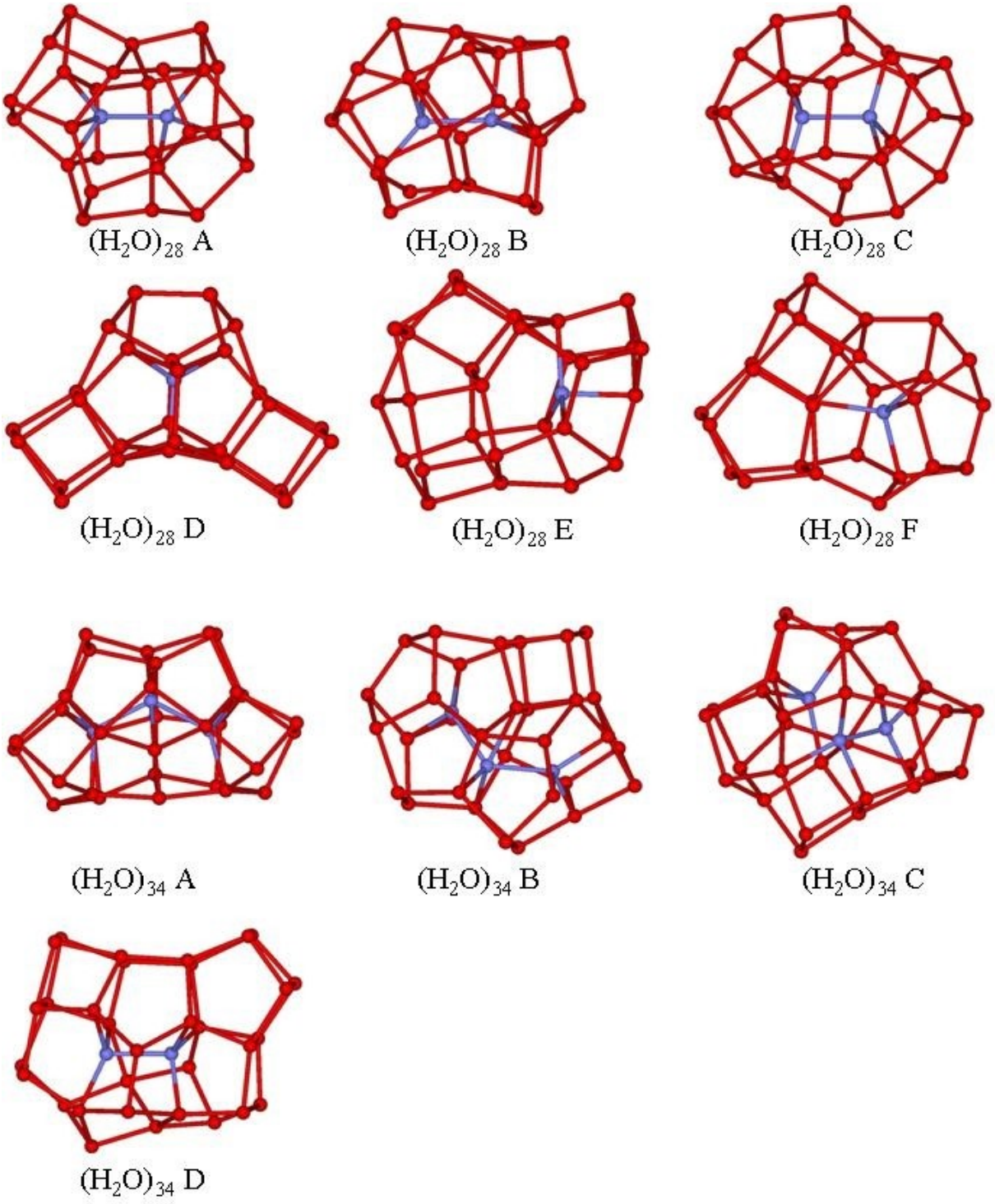

Fig. S2. Low-lying energy structures of the $(H_2O)_{28}$ and $(H_2O)_{34}$ clusters. Hydrogen atoms have been omitted for clarity and the sticks represent the O–H bonds involved in hydrogen bonding. The full solvated molecules are indicated with blue oxygens.

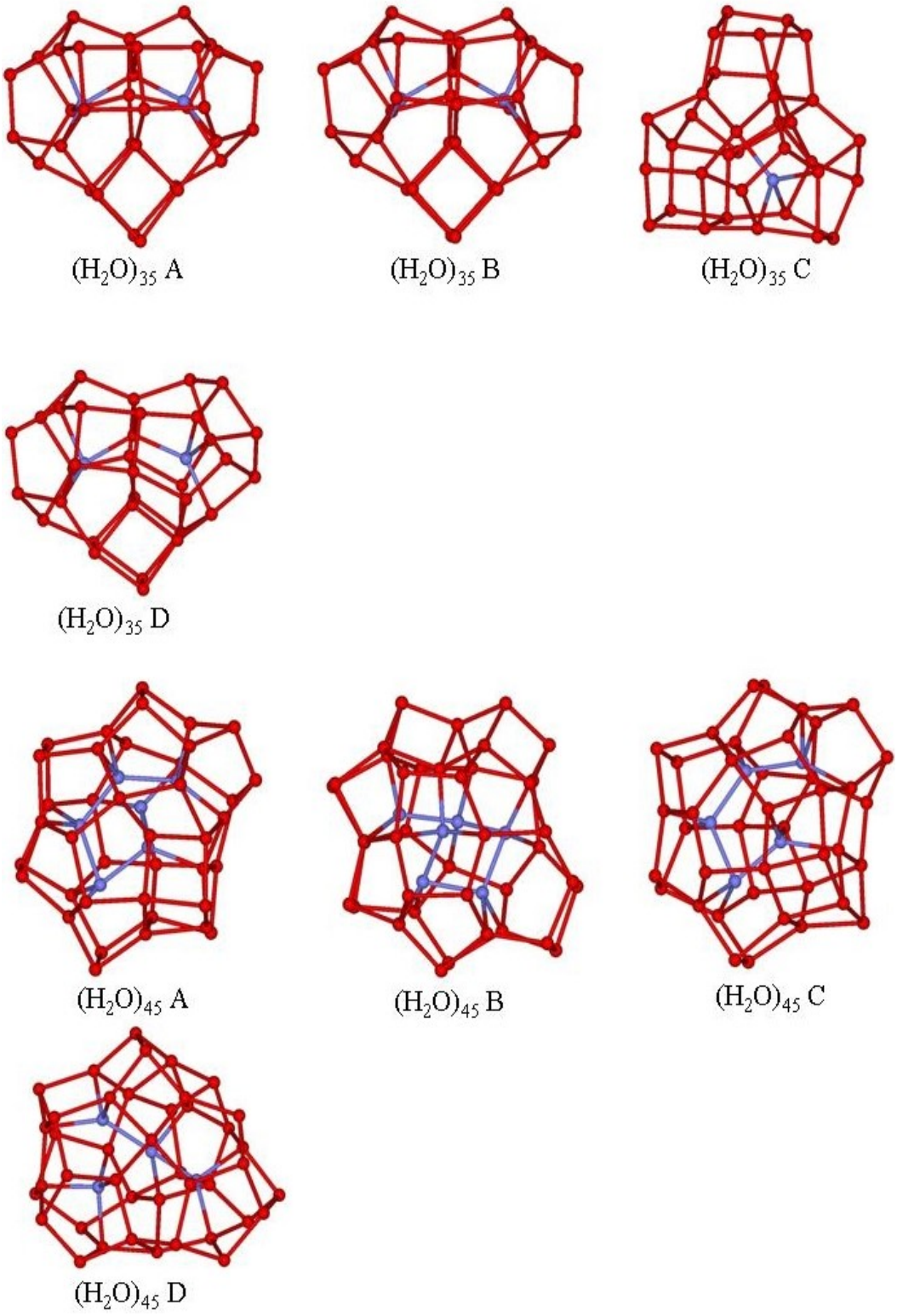

Fig. S3. Low-lying energy structures of the $(H_2O)_{35}$ and $(H_2O)_{45}$ clusters. Hydrogen atoms have been omitted for clarity and the sticks represent the O–H bonds involved in hydrogen bonding. The full solvated molecules are indicated with blue oxygens.

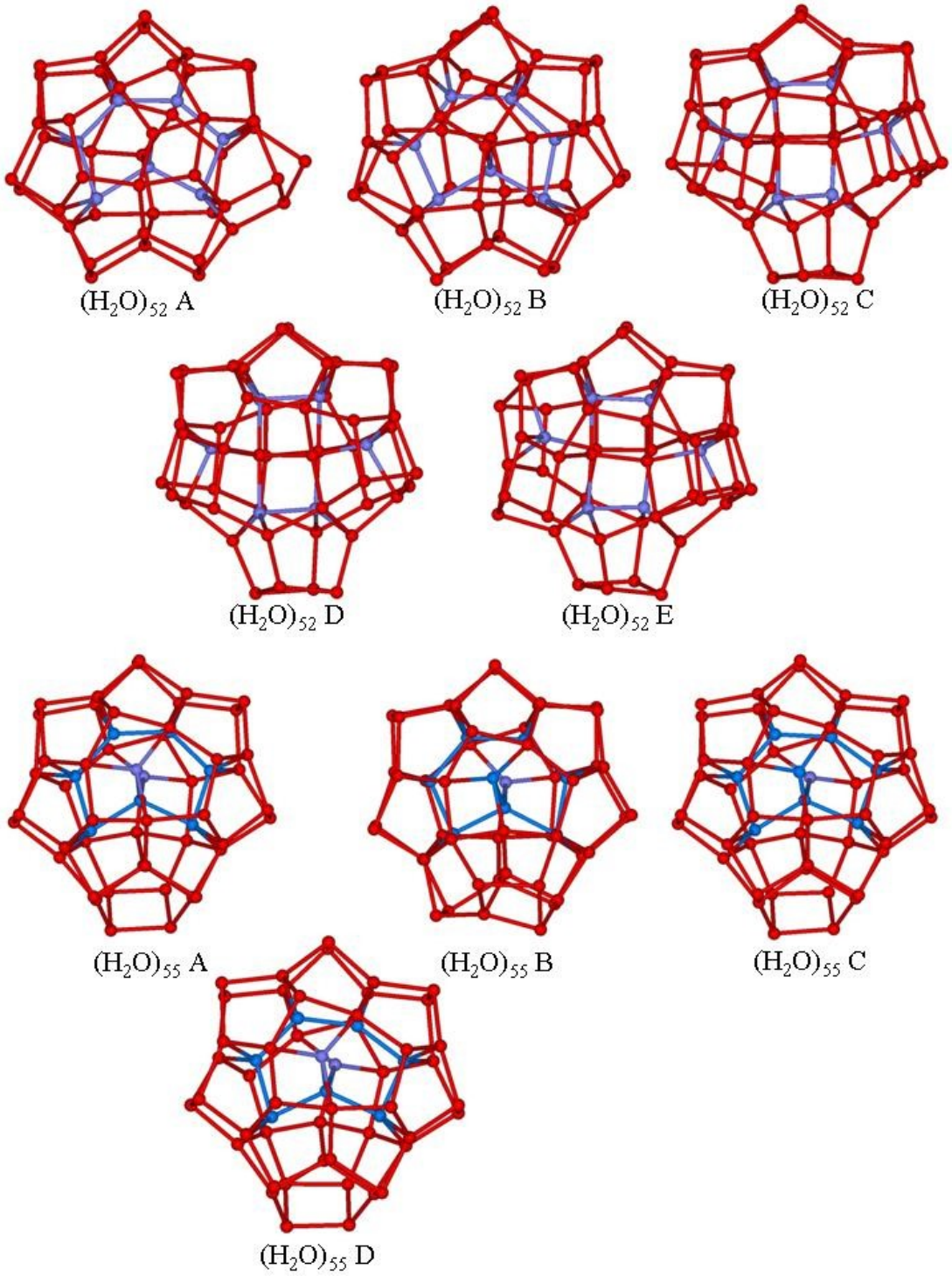

Fig. S4. Low-lying energy structures of the $(H_2O)_{52}$ and $(H_2O)_{55}$ clusters. Hydrogen atoms have been omitted for clarity and the sticks represent the O–H bonds involved in hydrogen bonding. The full solvated molecules are indicated with blue oxygens.

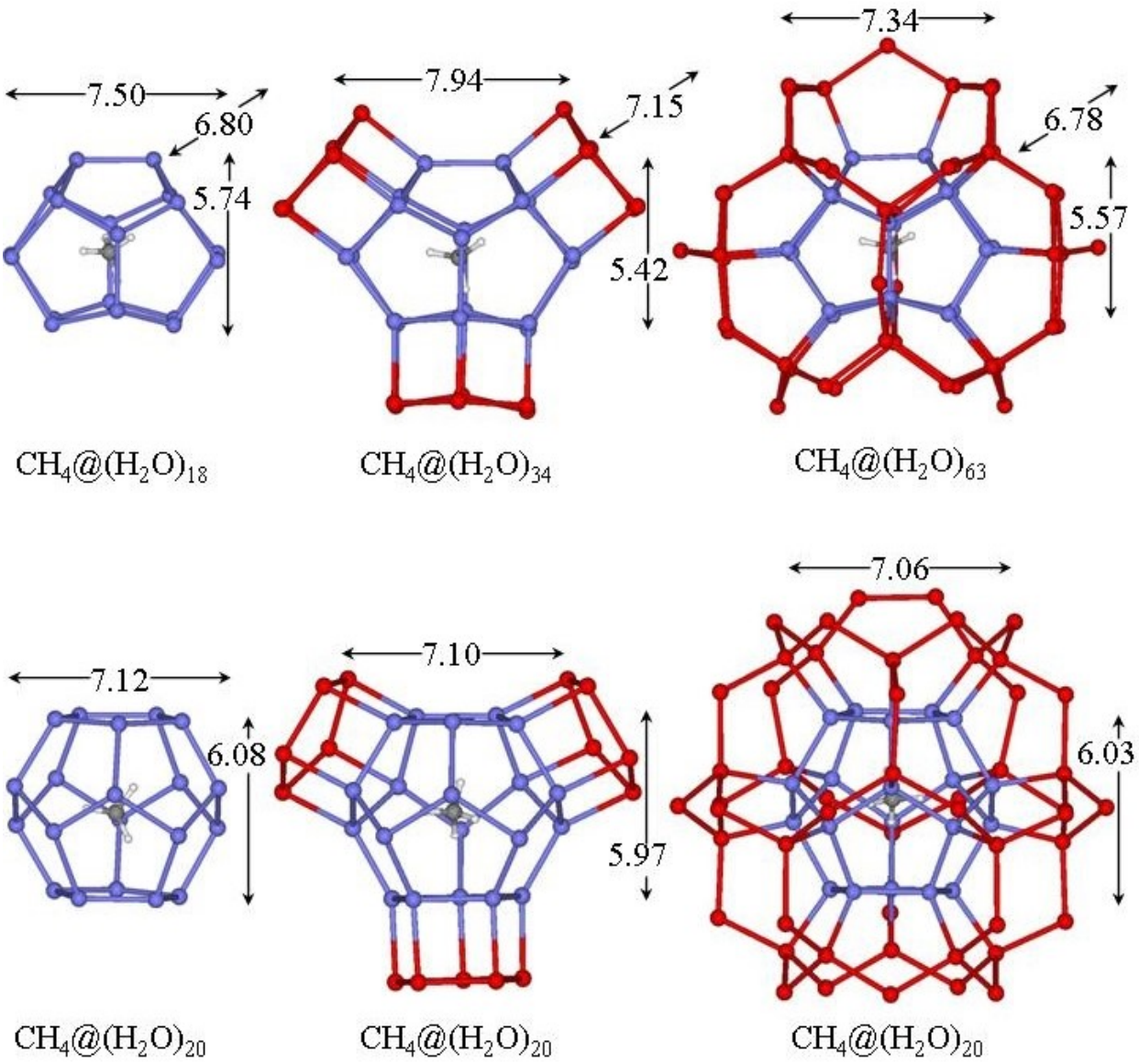

Fig. S5. Optimized structures of various clusters encapsulating methane. Water hydrogen atoms have been omitted for clarity and the sticks represent the O–H bonds involved in hydrogen bonding. The oxygen atoms in blue represent the cage.

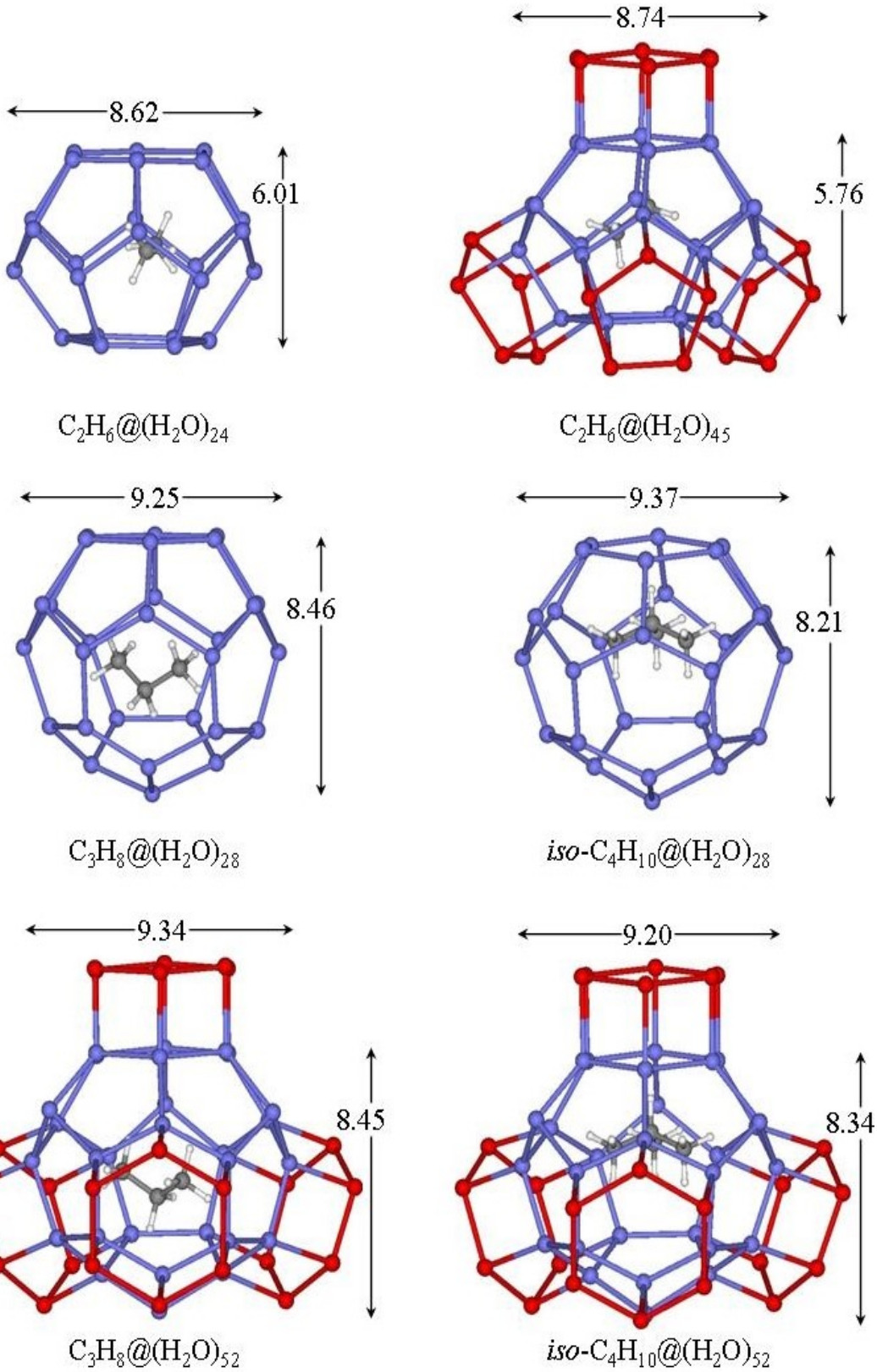

Fig. S6. Optimized structures of various clusters encapsulating ethane, propane and isobutane. Water hydrogen atoms have been omitted for clarity and the sticks represent the O–H bonds involved in hydrogen bonding. The oxygen atoms in blue represent the cage.

Table S1. Average coordination number of water molecules and relative electronic energy (kcal mol^{-1}) for low-lying minima of the $(H_2O)_n$ clusters.

	label	n_{HB}/n	E_r
$(H_2O)_{18}$			
Pentagonal prism with two cubes	18A	3.44	0.0
Pentagonal prism and two fused cubes	18B	3.44	1.6
Irregular prism and two cubes	18C	3.33	1.7
2-stacked hexagonal prisms	18D	3.33	3.3
$(H_2O)_{20}$			
3-edge-sharing pentagonal prisms	20A	3.40	0.0
2-edge-sharing pentagonal prisms with a cube	20C	3.40	0.5
3-stacked pentagonal prisms	20D	3.50	0.5
$(H_2O)_{24}$			
One internal water molecule	24A	3.33	0.0
One internal water molecule	24B	3.42	1.2
One internal water molecule	24C	3.42	1.4
3-edge-sharing pentagonal prisms with a cube	24D	3.50	2.0
$(H_2O)_{28}$			
Two internal water molecules	28A	3.43	0.0
Two internal water molecules	28B	3.50	2.1
Two internal water molecules	28C	3.29	3.6
One internal water molecole	28D	3.50	3.7
One internal water molecole	28E	3.50	4.0
One internal water molecole	28F	3.50	4.0
$(H_2O)_{34}$			
Three internal water molecules	34A	3.53	0.0
Three internal water molecules	34B	3.41	0.1
Three internal water molecules	34C	3.47	1.3
Two internal water molecules	34D	3.53	3.4
$(H_2O)_{35}$			
Two internal water molecules	35A	3.54	0.0
Two internal water molecules	35B	3.54	0.7
One internal water molecule	35C	3.49	0.8
Two internal water molecules	35D	3.54	1.5
$(H_2O)_{45}$			
Six internal water molecules	45A	3.60	0.0
Six internal water molecules	45B	3.51	0.5
Five internal water molecules	45C	3.60	2.1
Four internal water molecules	45D	3.56	3.2
$(H_2O)_{52}$			
Seven internal water molecules	52A	3.54	0.0
Seven internal water molecules	52B	3.58	1.1
Six internal water molecules	52C	3.58	4.3
Six internal water molecules	52D	3.58	4.4
Six internal water molecules	52E	3.58	4.9

Table S1 Continue

$(H_2O)_{55}$			
Nine internal water molecules	55A	3.60	0.0
Nine internal water molecules	55B	3.60	0.4
Nine internal water molecules	55C	3.60	2.3
Nine internal water molecules	55D	3.60	2.4
$(H_2O)_{123}$			
$(H_2O)_{123}$	123	3.67	

Table S2. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{18}$ cluster with one pentagonal prism and two cubes, 18A configuration

O	1.449411	-1.235226	-1.487230
O	-0.178995	3.140711	-1.296655
O	0.102181	3.043704	1.533448
O	1.309590	-1.465063	1.254934
O	2.148809	1.138208	1.516827
O	-1.298277	-1.377787	-1.334918
O	-2.124694	1.232885	-1.415334
O	-2.005861	1.315840	1.338914
O	-1.441642	-1.353252	1.415881
H	-1.283366	-1.443876	-0.349787
H	-0.368224	-1.491823	-1.622125
H	0.380408	-1.601776	1.534794
H	1.292759	-1.459031	0.267961
H	-1.290287	1.943997	1.601279
H	-2.033010	1.366119	0.354530
H	-0.956814	2.568470	-1.490830
H	-0.271150	3.939792	-1.836352
H	1.609883	-0.262015	-1.527589
H	2.311212	-1.660124	-1.688393
H	-1.610682	-0.386244	1.529715
H	-2.299883	-1.798795	1.583671
H	-1.785784	0.312619	-1.530153
H	-3.095068	1.187495	-1.562017
H	0.885547	2.468510	1.651522
H	0.075556	3.260298	0.579464
H	3.119067	1.076939	1.655653
H	1.807955	0.213653	1.566637
H	2.026618	1.416249	-0.218871
O	2.000404	1.430434	-1.205804
H	1.304379	2.080635	-1.441831
H	-3.067629	-1.923501	-1.576057
O	-4.020554	-2.002294	-1.369279
H	-4.391498	-1.104292	-1.501133
H	-5.598769	1.100386	-1.668028
O	-4.817176	0.677451	-1.283068
H	-4.904763	0.719732	-0.293908
H	-4.558068	-2.934764	1.703524
O	-4.073933	-2.188463	1.320697
H	-4.128636	-2.267580	0.332258
H	-3.796673	0.933625	1.589914
O	-4.675777	0.544544	1.401513
H	-4.567938	-0.420536	1.536597
H	5.627719	0.975687	1.755475
O	4.845101	0.581285	1.343327
H	4.925373	0.703005	0.360513
H	4.570355	-0.285199	-1.551708
O	4.678197	0.666611	-1.342930
H	3.798007	1.068297	-1.493696
H	3.080018	-2.024683	1.447480
O	4.031956	-2.091159	1.231700
H	4.408217	-1.207968	1.431307
H	4.137975	-2.221019	-0.485119
O	4.082026	-2.065822	-1.464505
H	4.561045	-2.783138	-1.904839

Table S3. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{18}$ cluster with one pentagonal prism and two fused cubes, 18B configuration.

O	-4.955513	-0.247981	-1.469963
H	-4.394670	-1.068767	-1.439455
H	-5.735328	-0.450377	-2.007320
O	-3.436606	2.084277	-1.651339
H	-3.478429	2.381222	-0.719381
H	-4.020757	1.298023	-1.699463
O	-4.911695	0.222210	1.281868
H	-5.100223	0.118437	0.325059
H	-4.349141	1.022081	1.350929
O	-3.391962	-2.393129	-1.054279
H	-3.433661	-2.447448	-0.075982
H	-2.451274	-2.219560	-1.263022
O	-3.274346	2.496202	1.142760
H	-2.321886	2.304147	1.306879
H	-3.487655	3.314539	1.615217
O	-0.903801	1.109881	-1.598334
H	-1.813156	1.466396	-1.761397
H	-0.973434	0.127843	-1.573097
O	-3.515377	-2.019881	1.723604
H	-3.906881	-2.606573	2.387281
H	-4.073682	-1.196456	1.685766
O	-0.712816	-1.593608	-1.126012
H	-0.693026	-1.513963	-0.140480
H	0.192819	-1.851426	-1.388305
O	-0.732921	1.535336	1.083093
H	-0.709260	1.445129	0.095893
H	0.169626	1.805037	1.346206
O	-0.905231	-1.164528	1.569017
H	-0.976934	-0.182488	1.539706
H	-1.796099	-1.512450	1.797505
O	1.852651	1.057803	-1.608505
H	1.860693	0.072531	-1.535679
H	0.931845	1.299278	-1.839907
O	2.067013	-1.630179	-1.102389
H	2.044568	-1.546700	-0.119067
H	3.000844	-1.826195	-1.328769
O	1.856089	-1.089527	1.582454
H	0.940841	-1.343516	1.820179
H	1.850870	-0.104256	1.509234
O	2.038166	1.599774	1.075661
H	2.027709	1.514581	0.091952
H	2.966339	1.810069	1.312397
O	4.821123	-1.520575	-1.256746
H	5.520070	-1.971690	-1.752575
H	4.871443	-0.553464	-1.474974
O	4.653786	1.159103	-1.517780
H	4.780174	1.446853	-0.588580
H	3.711994	1.323924	-1.720297
O	4.659647	-1.152294	1.513397
H	3.718836	-1.329725	1.709707

H	4.796062	-1.438270	0.585042
O	4.791198	1.529635	1.253960
H	4.853666	0.563185	1.472075
H	5.481859	1.989899	1.752992

Table S4. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{18}$ cluster with irregular prism and two cubes, 18C configuration.

O	-1.448195	1.174218	-1.865917
H	-0.606327	0.723141	-2.084915
H	-1.320696	2.137427	-2.043341
O	-1.990053	1.204497	0.825574
H	-2.940724	0.963660	0.882426
H	-1.754550	1.206146	-0.133633
O	-0.742168	-0.971860	1.884654
H	-1.204746	-0.192297	1.491536
H	0.122000	-0.604163	2.186651
O	0.871553	-0.329808	-1.929359
H	0.537028	-1.081964	-1.380509
H	1.729916	-0.630451	-2.298109
O	-0.022686	-2.348039	-0.337557
H	-0.286305	-1.883700	0.496560
H	-0.851870	-2.734189	-0.695523
O	1.906028	1.503344	-0.186185
H	1.507910	2.401016	-0.204802
H	1.428508	0.932031	-0.833030
O	0.653087	3.928429	0.226778
H	1.206773	4.706254	0.390692
H	0.342090	3.596230	1.109917
O	-2.613329	-2.992879	-1.013254
H	-2.983702	-2.165086	-1.421990
H	-2.958735	-3.745533	-1.515529
O	-4.422337	-0.075446	0.822630
H	-5.285144	0.134841	1.208986
H	-4.100924	-0.918567	1.236474
O	3.704608	-1.313407	1.772599
H	4.321300	-1.775645	2.359082
H	3.317786	-1.994425	1.160831
O	3.465271	-1.261157	-2.242587
H	3.956571	-0.633645	-1.648763
H	4.031102	-1.448553	-3.005803
O	1.583737	0.418917	2.298058
H	1.702651	0.786313	1.388062
H	2.342654	-0.192575	2.405533
O	-3.601705	-0.619377	-1.799441
H	-2.887952	0.035637	-1.948277
H	-4.049081	-0.342757	-0.972934
O	2.683803	-2.932557	-0.132300
H	1.705429	-2.883472	-0.173855
H	2.997758	-2.506350	-0.957129
O	4.424032	0.385224	-0.344520
H	3.645488	0.979578	-0.290615
H	4.361221	-0.170647	0.460764
O	-3.185624	-2.328507	1.643746

H	-3.012689	-2.736435	0.768480
H	-2.314114	-2.027207	1.966744
O	-0.229230	2.637017	2.416992
H	0.429294	1.961194	2.666586
H	-0.950221	2.150394	1.962491
O	-1.019570	3.865730	-1.977339
H	-1.823300	4.395436	-1.873898
H	-0.492183	4.003658	-1.159751

Table S5. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{18}$ cluster in the 3-stacked hexagonal prisms, 18D configuration.

O	-2.875586	0.014500	-2.734198
H	-2.922961	0.872173	-2.234317
H	-3.504925	0.078712	-3.467650
O	-2.699938	-2.398377	-1.327570
H	-1.756278	-2.602964	-1.476525
H	-2.860674	-1.543703	-1.782124
O	-2.871774	-2.374142	1.360908
H	-2.921552	-2.370212	0.368328
H	-3.501345	-3.040391	1.673771
O	-2.692421	0.049282	2.745861
H	-2.855256	-0.771531	2.233093
H	-1.747609	0.022581	2.993280
O	-2.695489	2.353586	-1.409887
H	-2.854856	2.320340	-0.442104
H	-1.751701	2.583819	-1.514099
H	-2.917005	1.503915	1.875992
O	-2.867771	2.365729	1.383152
H	-3.494238	2.970837	1.806848
H	-1.047330	-0.129721	-2.999712
O	-0.114655	-0.178879	-2.699739
H	-0.074121	-0.956328	-2.090213
H	0.067063	-2.292385	-0.217883
O	0.106872	-2.430451	-1.196131
H	1.039206	-2.666312	-1.389483
H	-1.042295	-2.535083	1.615583
O	-0.109690	-2.251648	1.505598
H	-0.067244	-1.334502	1.872670
H	0.074160	0.955347	2.088230
O	0.114376	0.178026	2.697932
H	1.046793	0.129266	2.998745
H	-1.039162	2.665415	1.388642
O	-0.106829	2.429885	1.194836
H	-0.067309	2.291825	0.216625
O	0.109958	2.250542	-1.506892
H	0.067347	1.333413	-1.873991
H	1.042886	2.533452	-1.615900
H	1.747682	-0.021737	-2.992577
O	2.692402	-0.048791	-2.744849
H	2.855698	0.772077	-2.232367
H	2.916942	-1.503603	-1.875117
O	2.868128	-2.365611	-1.382613
H	3.495838	-2.969761	-1.805846

H	1.751815	-2.583250	1.513426
O	2.695803	-2.353361	1.410194
H	2.855879	-2.319816	0.442531
H	2.922792	-0.872026	2.234585
O	2.875405	-0.014249	2.734353
H	3.503955	-0.078798	3.468453
O	2.699422	2.399067	1.328588
H	1.755482	2.602777	1.477123
H	2.860612	1.544339	1.782892
O	2.871842	2.374690	-1.359689
H	3.500098	3.042110	-1.672687
H	2.921164	2.371342	-0.367042

Table S6. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{20}$ cluster in the 3-edge-sharing pentagonal prisms, 20A configuration.

O	-0.096628	-0.119417	1.283332
H	-0.087844	-0.109557	0.293603
H	-0.938808	-0.577878	1.513176
O	0.057231	-0.013982	-1.435320
H	0.077272	0.965890	-1.552876
H	0.970346	-0.370978	-1.551797
O	-0.118610	2.693285	-1.313901
H	-0.135231	2.731305	-0.326704
H	-1.035268	2.903329	-1.595828
O	2.511978	-1.165933	-1.309234
H	2.538066	-1.217044	-0.323253
H	3.193143	-0.503239	-1.556344
O	2.639873	3.202700	-1.296144
H	2.652777	3.350573	-0.326334
H	1.695731	3.090673	-1.526051
O	4.194406	1.008859	-1.446827
H	3.634677	1.826767	-1.520816
H	4.998045	1.162237	-1.965057
O	2.319510	-1.338944	1.431204
H	2.189453	-2.299515	1.587148
H	1.423592	-0.937550	1.536690
O	4.074578	0.841787	1.353843
H	3.543815	0.036705	1.523085
H	4.277251	0.830237	0.394584
O	2.683877	3.143615	1.506525
H	3.131305	3.798798	2.062163
H	3.203889	2.298730	1.574060
O	-0.024053	2.590320	1.430993
H	-0.032866	1.609589	1.540543
H	0.894037	2.878961	1.628721
O	-2.265880	-1.435625	-1.396954
H	-2.052355	-2.375868	-1.584761
H	-1.422477	-0.945353	-1.532749
O	-1.239974	-3.994149	-1.458496
H	-0.254582	-3.911673	-1.558662
H	-1.516701	-4.760556	-1.982074
O	1.443879	-3.766478	-1.383281
H	1.845987	-2.896811	-1.579437

H	1.598018	-3.914446	-0.425784
O	-1.229857	-3.897710	1.342096
H	-1.698744	-3.072548	1.575596
H	-1.374728	-4.017150	0.379173
O	1.466745	-3.965463	1.412818
H	0.479137	-3.944179	1.517239
H	1.789251	-4.731472	1.910094
O	-2.511520	-1.388416	1.345609
H	-3.166079	-0.705040	1.606006
H	-2.533050	-1.407810	0.358798
O	-4.164147	0.825024	1.494877
H	-4.972719	0.955970	2.011762
H	-3.647693	1.673168	1.540980
O	-2.763573	3.118187	1.276433
H	-1.810025	3.046068	1.485098
H	-2.810163	3.250718	0.305833
O	-4.130461	0.648612	-1.305350
H	-4.293972	0.638360	-0.338286
H	-3.569926	-0.133284	-1.485459
O	-2.858535	3.013931	-1.528196
H	-3.333440	2.141755	-1.573741
H	-3.359851	3.640498	-2.070549

Table S7. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{20}$ cluster in the 4-fused cubes, 20B configuration.

O	5.597670	-0.277849	1.955556
H	6.280998	-0.277546	2.641854
H	5.661987	0.582635	1.464345
O	5.475287	-1.876410	-0.338529
H	4.536764	-2.146880	-0.370477
H	5.601440	-1.458756	0.539932
O	-2.844509	1.881450	0.461377
H	-2.820126	1.102616	1.067046
H	-3.776964	2.186708	0.459618
O	-2.676434	-0.467288	1.884017
H	-1.767919	-0.494775	2.245078
H	-2.677502	-1.070488	1.101764
O	-2.676776	0.465648	-1.881841
H	-1.769071	0.494810	-2.244745
H	-2.677178	1.068343	-1.099263
O	-2.845739	-1.882240	-0.459072
H	-2.820638	-1.103632	-1.065053
H	-3.778046	-2.187750	-0.458585
O	0.084869	-0.281577	1.923100
H	0.998955	-0.380309	2.257471
H	0.066881	0.572739	1.429030
O	-0.084822	-1.923510	-0.283049
H	-0.068474	-1.429326	0.571292
H	-0.997847	-2.260645	-0.381665
O	0.084399	0.283160	-1.925655
H	0.998409	0.381305	-2.260334
H	0.066281	-0.571336	-1.431959
O	-0.084321	1.925287	0.281000

H	-0.998197	2.260208	0.379772
H	-0.066682	1.431730	-0.573627
O	-5.475001	-0.336683	1.876341
H	-5.602194	0.541715	1.458890
H	-4.536140	-0.368244	2.145740
O	-5.595712	1.956627	0.277482
H	-5.661040	1.464712	-0.582553
H	-6.276472	2.645499	0.275458
O	-5.597622	-1.955859	-0.277665
H	-5.662520	-1.464219	0.582513
H	-6.280638	-2.642485	-0.276997
O	-5.475734	0.337721	-1.876675
H	-4.536811	0.369204	-2.145882
H	-5.602777	-0.540601	-1.458997
O	2.845445	-0.462658	1.881681
H	2.822134	-1.067860	1.102364
H	3.777564	-0.460608	2.187720
O	2.676365	1.881794	0.467849
H	2.677503	1.099054	1.070297
H	1.767985	2.243196	0.495938
O	2.676108	-1.884218	-0.467047
H	2.676880	-1.101828	-1.069968
H	1.767154	-2.244395	-0.493231
O	2.845194	0.459910	-1.881062
H	3.777363	0.459085	-2.187048
H	2.820876	1.065466	-1.102147
O	5.474680	1.877448	0.338318
H	5.601903	1.460469	-0.540267
H	4.535555	2.145944	0.370304
O	5.596671	0.279139	-1.955623
H	6.279041	0.278597	-2.642887
H	5.661423	-0.581500	-1.464770

Table S8. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{20}$ cluster in the 2-edge-sharing pentagonal prisms with a fused cube, 20C configuration.

O	5.284002	-0.873708	-1.290097
H	5.446073	-0.869758	-0.322768
H	4.988127	0.037031	-1.501771
O	5.199383	-0.883312	1.501958
H	5.889723	-1.151785	2.125855
H	4.453543	-1.536449	1.586413
O	4.361079	1.768900	-1.433939
H	4.877020	2.483928	-1.834520
H	4.406116	1.886864	-0.446629
O	4.244884	1.720293	1.243448
H	4.596583	0.830819	1.462952
H	3.287346	1.687251	1.450719
O	3.286094	-2.653644	-1.403978
H	3.473621	-3.410648	-1.978244
H	4.052490	-2.022677	-1.482802
O	3.142456	-2.604528	1.399577
H	3.145952	-2.806053	0.439993

H	2.285615	-2.157463	1.564912
O	0.963229	-1.181201	-1.390097
H	1.753950	-1.743922	-1.550848
H	1.243222	-0.244155	-1.523813
O	1.611718	1.473600	-1.317003
H	2.534812	1.665770	-1.590878
H	1.626057	1.509928	-0.329126
O	0.751619	-1.162833	1.347697
H	-0.169896	-1.361027	1.614837
H	0.755515	-1.205991	0.360122
O	1.479230	1.475873	1.422957
H	1.136768	0.562485	1.565818
H	0.746499	2.106483	1.599523
O	-1.774964	-1.370477	-1.266128
H	-1.783108	-1.397130	-0.279221
H	-0.830218	-1.435093	-1.524325
O	-0.666233	3.071514	-1.310525
H	-1.419212	2.480283	-1.516735
H	0.144295	2.553528	-1.504844
O	-2.006546	-1.244632	1.470736
H	-2.226610	-0.284662	1.544424
H	-2.846065	-1.723769	1.640509
O	-0.636816	3.244043	1.376591
H	-0.621853	4.136893	1.751697
H	-0.644962	3.335707	0.386020
O	-2.730757	1.185592	-1.451101
H	-3.687406	1.101582	-1.653459
H	-2.361929	0.271525	-1.519244
O	-2.696200	1.394317	1.277424
H	-2.061588	2.085095	1.563528
H	-2.679622	1.418848	0.289593
O	-4.465547	-2.125634	-1.365025
H	-4.554448	-2.305985	-0.404878
H	-3.504426	-2.030585	-1.521483
O	-4.632722	-2.118061	1.429219
H	-5.156650	-2.689769	2.009376
H	-5.011756	-1.201200	1.486875
O	-5.332065	0.473080	1.277369
H	-4.491689	0.943891	1.453284
H	-5.487970	0.576172	0.314569
O	-5.384386	0.398102	-1.520748
H	-5.166068	-0.568917	-1.583749
H	-6.117532	0.574695	-2.128359

Table S9. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{20}$ cluster in the 3-stacked pentagonal prisms, 20D configuration.

O	-1.280195	0.912363	2.146179
H	-0.367736	1.116145	2.433750
H	-1.274712	-0.054068	1.936800
O	1.481515	1.102061	2.019011
H	2.414457	1.216703	2.296198
H	1.415696	1.523160	1.127383
O	1.495506	-1.612464	1.639729

H	1.463766	-0.632419	1.765469
H	2.436003	-1.850467	1.784256
O	1.220940	2.281159	-0.434798
H	0.310878	2.638927	-0.432600
H	1.229605	1.564071	-1.116754
O	1.242636	-2.088527	-1.032541
H	0.337065	-2.407845	-1.216402
H	1.276298	-1.912177	-0.059377
O	1.401003	0.321233	-2.319055
H	1.370639	-0.547626	-1.849377
H	2.329281	0.427204	-2.618415
O	-1.541552	2.267119	-0.217808
H	-2.476084	2.556255	-0.293901
H	-1.486594	1.770547	0.635583
O	-1.362845	0.459468	-2.238801
H	-1.363032	1.116371	-1.498346
H	-0.468180	0.498080	-2.630888
O	-1.532386	-2.027032	-1.112393
H	-2.467185	-2.313237	-1.194664
H	-1.500463	-1.123982	-1.513738
O	-1.264484	-1.766740	1.581881
H	-0.358713	-2.033256	1.835175
H	-1.306477	-1.855576	0.596918
O	4.024452	2.322772	-0.378880
H	4.190906	1.878697	0.480075
H	3.080209	2.574448	-0.367855
O	4.263733	-1.695257	1.484029
H	4.285835	-1.825812	0.497100
H	4.914060	-2.302136	1.867868
O	4.155958	0.527538	-2.377602
H	4.218962	1.221850	-1.668746
H	4.801948	0.753229	-3.063031
O	4.045987	-1.985835	-1.175795
H	3.107147	-2.220620	-1.310715
H	4.173141	-1.123761	-1.628682
O	-4.308358	2.314720	-0.237895
H	-4.353858	1.889199	0.661472
H	-4.964204	3.027035	-0.255915
O	-4.073264	-1.640806	1.711447
H	-4.236232	-1.838078	0.764121
H	-3.135746	-1.867656	1.864533
O	-4.172150	0.334259	-2.197527
H	-4.303533	1.045954	-1.533160
H	-3.237856	0.407010	-2.474317
O	-4.301048	-2.088817	-1.042178
H	-4.963672	-2.678114	-1.431451
H	-4.383250	-1.208427	-1.496569
O	-4.088221	1.078376	2.124986
H	-4.167515	0.105254	1.975623
H	-3.151815	1.208761	2.370466
O	4.254929	0.981388	2.073431
H	4.391648	0.015360	1.922700
H	4.922039	1.265170	2.716048

Table S10. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{24}$ cluster with one internal water molecule, 24A configuration.

O	0.100644	4.350033	-0.400009
H	-0.598179	4.233796	0.300184
H	0.332211	5.290302	-0.420569
O	-1.932518	3.747139	1.231379
H	-2.348509	3.087409	0.630153
H	-1.754766	3.227750	2.042171
O	1.868782	2.316019	0.124328
H	1.354131	3.130201	-0.079345
H	1.433790	1.903905	0.908960
O	-1.347600	3.104084	-2.480042
H	-0.762777	3.610551	-1.878135
H	-1.956770	2.619513	-1.880864
O	-2.707822	1.754095	-0.483629
H	-2.078643	1.035850	-0.229586
H	-3.598313	1.357971	-0.369164
O	0.636172	0.872911	2.046241
H	-0.108587	1.195852	2.604536
H	1.219891	0.306975	2.601605
O	1.674740	0.354459	-1.777706
H	1.651085	1.105346	-1.137762
H	1.126761	0.625080	-2.547239
O	-0.090515	1.133959	-3.764987
H	-0.534034	1.939340	-3.380527
H	0.150416	1.338118	-4.680290
O	-0.936353	-0.259250	0.107228
H	-0.252774	0.090784	0.725592
H	-1.372900	-0.990188	0.606481
O	-1.672432	1.765415	3.194493
H	-2.358645	1.083097	2.954447
H	-1.763822	1.926768	4.145196
O	4.514199	1.746254	0.260029
H	3.604056	2.130465	0.251474
H	5.125198	2.461599	0.490359
O	-1.321344	-0.978741	-2.488341
H	-1.003813	-0.331896	-3.152492
H	-0.998504	-0.643860	-1.620454
O	-3.433776	-0.153120	2.542055
H	-3.980627	-0.009895	1.740845
H	-2.920963	-0.967873	2.353134
O	4.417116	0.083374	-2.000972
H	3.443801	0.192603	-2.096054
H	4.657202	0.735139	-1.310673
O	-4.798149	0.084586	0.101521
H	-4.519015	-0.656558	-0.502539
H	-5.759103	0.174120	0.023466
O	2.369670	-0.842063	3.283837
H	3.201508	-0.792435	2.737114
H	2.632056	-0.770072	4.213096
O	1.569108	-2.131762	-0.540278
H	1.445915	-1.228901	-0.914560
H	2.531168	-2.314006	-0.622304
O	4.509454	-0.669955	1.690650
H	4.537850	0.207474	1.252752
H	4.492815	-1.325564	0.962128

O	-1.889294	-2.292148	1.697756
H	-0.957394	-2.515127	1.952818
H	-2.189933	-3.000603	1.087320
O	0.745552	-2.735521	2.019958
H	1.258794	-2.159802	2.621958
H	1.046992	-2.485317	1.116770
O	-3.829020	-1.768500	-1.564477
H	-3.035157	-1.401727	-2.010631
H	-3.517080	-2.591321	-1.131954
O	4.341703	-2.215012	-0.644555
H	4.506596	-1.446962	-1.255035
H	4.917228	-2.942763	-0.922044
O	-0.404097	-3.517650	-1.913195
H	-0.723947	-2.700452	-2.353112
H	0.359307	-3.196329	-1.384624
O	-2.551525	-3.963945	-0.382395
H	-1.720559	-3.939141	-0.931578
H	-2.875526	-4.876504	-0.382146

Table S11. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{24}$ cluster with one internal water molecule, 24B configuration.

O	1.009506	-3.070653	1.164135
H	0.470667	-3.526685	0.466518
H	0.424172	-3.007413	1.951934
O	-1.399710	-0.243064	-0.135460
H	-0.433808	-0.245141	0.089992
H	-1.426904	-0.220189	-1.118068
O	1.191816	-0.420725	0.486675
H	1.242324	0.068319	1.342785
H	1.205377	-1.384167	0.703501
O	-0.156465	2.775174	0.697311
H	-1.031418	3.196377	0.847842
H	-0.225685	2.301610	-0.162388
O	-0.196881	1.996980	-1.955887
H	-0.330734	1.159594	-2.444860
H	0.614584	2.430528	-2.296487
O	-1.297012	-0.351986	-2.888026
H	-0.889280	-1.240110	-3.006602
H	-2.270296	-0.441563	-2.923186
O	1.052853	1.256712	2.609158
H	1.989071	1.549428	2.654350
H	0.584943	1.897927	2.024166
O	2.828620	0.417387	-1.542548
H	2.118364	0.300986	-0.872139
H	2.729954	1.312852	-1.930747
O	3.666470	1.876073	2.016874
H	4.042778	1.086523	1.541105
H	4.368498	2.218943	2.589550
O	0.105766	-2.735111	-2.942604
H	1.059136	-2.554483	-2.714166
H	0.115505	-3.231343	-3.774973
O	-0.972416	-2.674489	3.056110
H	-1.115386	-3.217940	3.844931

H	-1.036436	-1.721268	3.341786
O	-2.934002	0.936242	1.728612
H	-2.342150	0.692229	0.977131
H	-3.052398	1.905334	1.655051
O	-3.905051	0.053236	-2.039871
H	-4.696384	0.061415	-2.599404
H	-4.192242	-0.322547	-1.164319
O	-1.177367	-0.074494	3.645294
H	-0.333141	0.372610	3.432431
H	-1.847230	0.329463	3.048916
O	2.327498	3.033493	-2.275947
H	2.767861	3.607307	-2.919614
H	2.472585	3.417590	-1.370047
O	2.659592	-2.218549	-2.288112
H	2.762868	-1.244433	-2.227341
H	2.965788	-2.546888	-1.416866
O	-2.477962	-2.603266	0.707359
H	-2.022218	-1.780554	0.402721
H	-2.127341	-2.754230	1.611452
O	-2.808810	3.547530	0.831332
H	-2.987221	3.320382	-0.120067
H	-3.189496	4.420718	1.005313
O	-2.904540	2.651743	-1.685033
H	-3.301006	1.757446	-1.773773
H	-1.953461	2.540636	-1.892536
O	4.591257	-0.142797	0.495835
H	4.142902	0.125029	-0.336270
H	4.256408	-1.049291	0.653217
O	2.428714	3.745985	0.300697
H	1.489990	3.573607	0.524639
H	2.948590	3.117833	0.846390
O	-4.629226	-0.855875	0.409424
H	-4.067420	-1.640411	0.585257
H	-4.251086	-0.160566	0.988963
O	-0.652815	-4.177446	-0.678464
H	-1.451834	-3.745427	-0.306280
H	-0.467100	-3.719330	-1.526052
O	3.565302	-2.780663	0.343139
H	4.203011	-3.499655	0.466257
H	2.745226	-3.042540	0.819980

Table S12. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{24}$ cluster with one internal water molecule, 24C configuration.

O	1.871809	0.244263	3.369304
H	1.603176	-0.691358	3.482886
H	1.086652	0.690010	3.003328
O	0.931182	-2.378523	3.266108
H	1.063290	-3.091049	3.908656
H	1.409711	-2.627245	2.436906
O	-1.365302	-1.308170	2.155820
H	-0.690113	-1.796084	2.677456
H	-1.005141	-0.401359	2.053612
O	1.249270	3.609485	1.616890

H	1.302041	4.087354	2.458227
H	0.775960	2.764206	1.798018
O	4.046461	0.494338	1.645394
H	3.265149	0.383468	2.233210
H	3.914831	1.347776	1.167599
O	-4.165575	-1.060872	2.072583
H	-4.347454	-1.590925	1.268579
H	-3.208359	-1.171385	2.249924
O	-0.185429	1.242508	1.681994
H	-0.987057	1.656463	1.267388
H	0.284760	0.779250	0.938594
O	2.009382	-2.573558	0.821421
H	2.948372	-2.470529	0.548357
H	1.573592	-3.203631	0.190484
O	-4.698416	1.365104	1.054251
H	-5.428925	1.829151	1.488899
H	-4.541233	0.517376	1.550721
O	4.366021	-1.531886	-0.033517
H	4.301271	-0.750608	0.589370
H	5.269985	-1.872899	0.034757
O	3.594261	2.834405	0.274004
H	3.223000	2.497188	-0.570499
H	2.827392	3.208697	0.754515
O	1.049204	-0.207821	-0.182935
H	0.396557	-0.541366	-0.848015
H	1.440660	-1.013513	0.235366
O	-1.752425	-2.742100	-0.197768
H	-2.726615	-2.713679	-0.327258
H	-1.572355	-2.232938	0.627021
O	-2.242122	2.340890	0.319611
H	-2.189830	1.883917	-0.555234
H	-3.133620	2.140195	0.682996
O	0.615724	-4.079337	-0.927232
H	-0.296674	-3.791035	-0.722314
H	0.850851	-3.663453	-1.783620
O	-0.529395	4.412907	-0.395976
H	-1.279015	3.871413	-0.071436
H	0.166365	4.300372	0.284659
O	-4.425345	-2.163634	-0.487035
H	-5.129854	-2.745958	-0.807378
H	-4.493409	-1.311156	-0.991741
O	2.329265	1.543081	-1.830467
H	1.612256	2.081561	-2.231681
H	1.879118	0.954185	-1.180728
O	-4.590107	0.322018	-1.539957
H	-3.777807	0.704219	-1.926491
H	-4.750996	0.813741	-0.707257
O	-0.695769	-1.100477	-2.055144
H	-0.094445	-1.599895	-2.652192
H	-1.163144	-1.757903	-1.483145
O	3.404817	-0.940881	-2.598642
H	3.083588	-0.017527	-2.534578
H	3.776955	-1.148612	-1.713349
O	-2.000343	1.282470	-2.198622
H	-1.358850	1.939543	-2.549036
H	-1.525857	0.420143	-2.223878
O	1.334340	-2.547884	-3.160470
H	2.131861	-1.976653	-2.978799

H	1.429691	-2.891303	-4.061008
O	0.097010	3.058399	-2.637514
H	-0.070877	3.649656	-1.855037
H	0.166421	3.634389	-3.413670

Table S13. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{24}$ cluster in the 3-edge-sharing pentagonal prisms with a fused cube configuration, 24D configuration.

O	-4.184349	2.645639	-1.387929
H	-4.385900	2.695956	-0.429176
H	-4.092188	1.691344	-1.583322
O	0.184547	2.408198	-1.393819
H	-0.286156	1.554211	-1.531793
H	-0.476481	3.109696	-1.585118
O	-1.904426	4.071695	1.334877
H	-1.837892	4.244245	0.371450
H	-1.095610	3.574416	1.567431
O	-4.317471	-2.637558	1.341828
H	-4.193940	-1.680384	1.508408
H	-4.495770	-2.718617	0.381062
O	5.552639	1.302532	-1.332152
H	5.661399	0.346553	-1.520745
H	4.609261	1.496626	-1.508492
O	-3.713482	0.093165	1.417391
H	-4.058511	0.998516	1.578214
H	-2.734852	0.162449	1.526622
O	0.111631	-2.320037	1.454334
H	-0.585798	-2.985807	1.644761
H	-0.309725	-1.435231	1.564277
O	0.278930	-2.371444	-1.294077
H	0.303083	-2.393645	-0.306606
H	1.194213	-2.159122	-1.573790
O	-4.277534	2.794879	1.410455
H	-3.411125	3.270541	1.511992
H	-4.936869	3.290681	1.917894
O	-2.037435	-4.053561	1.508499
H	-2.888324	-3.541658	1.568447
H	-2.136414	-4.838473	2.067321
O	2.909579	1.273812	1.477374
H	2.777445	0.300090	1.560647
H	3.867201	1.428138	1.632051
O	2.771541	1.454397	-1.266320
H	1.961825	1.930001	-1.545335
H	2.767538	1.473822	-0.279296
O	0.430665	2.496145	1.350391
H	0.441296	2.517971	0.363359
H	1.339796	2.246716	1.617871
O	2.730153	-1.467083	1.288252
H	2.705048	-1.484402	0.301566
H	1.910021	-1.915049	1.581857
O	5.517508	-1.469154	1.287945
H	5.681615	-0.520412	1.472613
H	4.568581	-1.610478	1.484472

O	-1.079486	-0.012146	-1.434265
H	-2.054279	-0.119783	-1.550302
H	-0.648549	-0.892488	-1.547662
O	5.572734	-1.493001	-1.404910
H	5.661955	-1.609930	-0.422300
H	6.195285	-2.099221	-1.832528
O	2.819052	-1.288872	-1.458150
H	2.740705	-0.308835	-1.537480
H	3.761641	-1.499066	-1.636796
O	-4.323816	-2.834045	-1.460462
H	-3.455434	-3.312664	-1.528954
H	-4.968820	-3.330355	-1.985399
O	-1.952038	4.145208	-1.466165
H	-2.071673	4.943617	-2.001202
H	-2.777731	3.599815	-1.563423
O	-1.945582	-4.084417	-1.293328
H	-1.156739	-3.549869	-1.514224
H	-1.898124	-4.225050	-0.323559
O	5.669516	1.323250	1.358561
H	6.329066	1.900480	1.770573
H	5.741902	1.435199	0.373990
O	-1.000408	0.161029	1.286987
H	-0.502359	0.978013	1.522304
H	-0.991713	0.145774	0.297633
O	-3.791287	-0.134538	-1.321960
H	-3.839140	-0.103464	-0.335791
H	-4.098211	-1.033592	-1.570390

Table S14. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{28}$ cluster with two internal water molecules, 28A configuration.

O	-4.722360	0.461898	-1.102285
H	-4.501947	-0.039437	-0.286001
H	-4.144690	1.252494	-1.046582
O	-3.824211	-1.362138	-2.852724
H	-4.225281	-0.653535	-2.279080
H	-4.446272	-1.537461	-3.573879
O	-3.550045	-0.803702	1.041678
H	-2.657212	-0.617991	0.665037
H	-3.584845	-1.771488	1.193108
O	-2.759281	2.411247	-0.548868
H	-2.119251	1.694375	-0.316781
H	-2.912880	2.901454	0.288220
O	-1.319938	0.145481	-0.217512
H	-1.329325	-0.153186	-1.159854
H	-0.383043	0.041790	0.073641
O	-1.191083	-0.676440	-2.812721
H	-2.115021	-0.850926	-3.093452
H	-0.850054	0.130935	-3.279682
O	-2.645713	-3.540820	-1.506050
H	-3.102993	-2.799402	-1.957336
H	-1.691016	-3.317320	-1.506309
O	-3.335972	0.968004	3.145285
H	-3.658940	0.374847	2.433003

H	-2.415928	0.648180	3.260414
O	-3.135447	-3.533241	1.113251
H	-3.072363	-3.672451	0.130435
H	-3.557850	-4.312842	1.502240
O	-2.871357	3.367084	2.048793
H	-3.172576	2.549640	2.530100
H	-3.306873	4.129468	2.457109
O	-1.201598	3.631079	-2.374870
H	-1.902733	3.286966	-1.765026
H	-1.552418	4.426389	-2.801827
O	0.021477	1.516079	-3.739117
H	-0.416681	2.292762	-3.332872
H	0.828777	1.348144	-3.202451
O	-0.627253	-2.397133	1.424852
H	-1.455116	-2.924126	1.456694
H	-0.361843	-2.373535	0.475984
O	-0.006932	-2.586656	-1.275069
H	-0.203432	-1.873919	-1.920903
H	0.850931	-2.985944	-1.540562
O	-0.765218	0.005274	2.762645
H	-0.762116	-0.818741	2.219706
H	-0.046338	-0.108775	3.421288
O	-0.248275	2.490142	1.745878
H	-1.048621	3.016441	1.953915
H	-0.496743	1.555844	1.943758
O	1.354251	-0.096463	0.312075
H	1.690054	0.465971	1.048573
H	1.814802	-0.963744	0.406854
O	0.828240	3.781608	-0.455330
H	0.166028	3.787760	-1.177846
H	0.453716	3.218654	0.256860
O	2.183275	0.807521	-2.163224
H	1.844868	0.525661	-1.279977
H	2.705508	1.621137	-1.984983
O	2.242126	1.505893	2.399600
H	1.493058	2.135899	2.404568
H	2.118976	0.913601	3.174710
O	1.636009	-2.766388	2.997238
H	0.772448	-2.768527	2.529478
H	2.283380	-2.698005	2.263467
O	2.547723	-3.461798	-1.834730
H	3.081703	-2.722160	-2.236346
H	2.803457	-4.286501	-2.272901
O	2.963685	-2.322752	0.635699
H	2.860585	-2.936393	-0.122569
H	3.813626	-1.847411	0.487624
O	1.551925	-0.411665	4.238245
H	1.683595	-1.330890	3.873562
H	1.662419	-0.456105	5.199246
O	3.290638	3.149890	-1.249708
H	2.399008	3.476635	-0.947056
H	3.709947	3.866538	-1.747826
O	3.937366	-1.292650	-2.541643
H	3.296927	-0.545398	-2.538228
H	4.499755	-1.120878	-1.757518
O	4.512840	1.717555	0.792944
H	3.784617	1.681585	1.447061
H	4.170319	2.274968	0.061433

O	5.106334	-0.751849	-0.046475
H	4.915344	0.177321	0.262915
H	6.020925	-0.948839	0.203988

Table S15. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{28}$ cluster with two internal water molecules, 28B configuration.

O	2.666668	-3.319978	-2.214105
H	2.363954	-3.733907	-1.361012
H	3.019059	-4.024699	-2.776825
O	1.549409	-4.150324	0.076785
H	1.863578	-3.645432	0.856963
H	0.636300	-3.820757	-0.068924
O	3.415731	-0.859838	-1.302846
H	3.352255	-1.686580	-1.826018
H	3.648852	-0.112898	-1.896442
O	0.455835	-1.672949	-2.482490
H	1.197193	-2.309232	-2.575804
H	-0.047796	-1.968691	-1.686177
O	4.459986	-0.990366	1.256754
H	3.727741	-1.444810	1.725284
H	4.196552	-1.003744	0.310519
O	3.656628	1.538137	-2.617037
H	3.640106	2.176504	-1.854791
H	4.354645	1.831743	-3.220746
O	2.091893	-2.268970	2.074787
H	1.592523	-1.637704	1.505819
H	1.640720	-2.248004	2.944035
O	-0.836968	-2.764566	-0.340632
H	-1.731269	-3.067076	-0.611628
H	-0.966413	-2.280251	0.507730
O	-1.320577	-0.577375	-4.262956
H	-0.877424	0.286865	-4.302584
H	-0.668191	-1.144401	-3.796177
O	1.045096	0.898590	-3.285017
H	0.968226	0.022007	-2.847141
H	1.986687	1.162572	-3.199558
O	1.224424	-0.461842	0.270798
H	1.867396	-0.590782	-0.464400
H	0.330378	-0.289561	-0.108420
O	-3.514493	-3.113003	-0.975295
H	-3.871707	-2.824107	-0.091716
H	-3.998769	-3.907178	-1.244682
O	4.475934	1.636761	1.746594
H	4.591075	0.655624	1.617477
H	5.171604	1.937865	2.349113
O	3.578972	3.145104	-0.457394
H	3.927588	2.653393	0.316591
H	2.696203	3.474412	-0.202344
O	-3.090109	-0.677889	-2.166760
H	-2.578672	-0.661325	-3.010391
H	-3.299628	-1.611695	-1.946054
O	0.356216	-1.825981	4.214516
H	0.230502	-2.224044	5.088324

H	0.245519	-0.843613	4.310905
O	-1.419413	-1.667776	2.115319
H	-0.874894	-1.940655	2.886237
H	-1.516210	-0.695565	2.188845
O	-1.236676	0.367862	-0.469444
H	-1.001966	1.195366	-0.959878
H	-1.902662	-0.107216	-1.024999
O	1.761076	1.495759	2.055883
H	2.730954	1.608666	2.163932
H	1.642900	0.771764	1.391856
O	-0.337250	2.591644	-1.710225
H	0.208800	2.075997	-2.356086
H	0.261732	2.922815	-0.998010
O	-4.090063	-2.176528	1.457347
H	-4.415978	-1.250657	1.447166
H	-3.186643	-2.120446	1.833630
O	0.917336	3.566199	0.512955
H	1.160337	2.831006	1.125894
H	0.041964	3.879629	0.843607
O	-0.035622	0.827187	4.009171
H	0.693819	1.108485	3.410925
H	-0.843600	1.002537	3.489354
O	-2.040891	1.103444	1.984126
H	-3.020525	1.001482	1.996227
H	-1.783861	0.908865	1.045126
O	-4.559127	1.401916	-1.053523
H	-4.118210	0.674980	-1.542608
H	-3.958401	2.174528	-1.122127
O	-2.800938	3.580797	-1.214718
H	-1.941358	3.316911	-1.617817
H	-3.129505	4.339991	-1.719083
O	-4.689220	0.553307	1.470330
H	-5.465557	0.896733	1.936890
H	-4.722314	0.909240	0.538388
O	-1.689770	3.883870	1.352205
H	-2.194358	3.878995	0.512355
H	-1.825939	2.990513	1.728231

Table S16. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{28}$ cluster with two internal water molecules, 28C configuration.

O	-2.530608	-2.362613	-2.873556
H	-2.346173	-1.398373	-2.922649
H	-1.663899	-2.785739	-2.692245
O	-4.124030	-2.503646	-0.744467
H	-3.581010	-2.514691	-1.582385
H	-4.857887	-3.122766	-0.871619
O	-2.025986	0.323150	-2.626329
H	-2.779730	0.948400	-2.542927
H	-1.279765	0.813678	-3.059149
O	-0.011652	-3.475126	-2.347983
H	0.687271	-2.770938	-2.351312
H	0.268905	-4.144729	-2.989667
O	-1.403306	-0.064782	-0.003773

H	-1.661239	0.020738	-0.954920
H	-1.678304	-0.958287	0.320369
O	-2.060190	-2.485840	1.036458
H	-2.847962	-2.731297	0.503700
H	-1.335025	-3.130500	0.827068
O	-0.061720	-4.170137	0.351885
H	0.010646	-4.023116	-0.615305
H	0.817967	-3.954409	0.728504
O	-4.936366	0.071810	0.033705
H	-4.631560	-0.808022	-0.275263
H	-4.612472	0.733365	-0.614221
O	1.885559	-1.578094	-2.074308
H	1.639620	-1.002521	-1.307196
H	2.111222	-0.954247	-2.800833
O	-4.023157	1.996042	-1.794195
H	-3.472910	2.713854	-1.371013
H	-4.708911	2.433125	-2.320191
O	-0.010869	1.750763	-3.730045
H	0.871558	1.323358	-3.754311
H	0.073683	2.522980	-3.131160
O	1.274179	0.003901	0.052255
H	0.282601	-0.022193	0.065908
H	1.563957	-0.363343	0.922570
O	2.510715	0.510472	-3.750391
H	3.148561	0.978333	-3.141606
H	2.947580	0.425780	-4.610642
O	-1.929397	2.080532	1.587823
H	-1.734078	1.290323	1.027260
H	-2.758964	1.833828	2.051607
O	-2.424362	-1.222122	3.453652
H	-2.307986	-1.763005	2.641243
H	-3.051620	-0.511436	3.200379
O	-2.417435	3.733348	-0.564793
H	-2.240491	3.254076	0.276145
H	-1.551983	3.784615	-1.024555
O	2.461799	-3.523773	1.412710
H	3.085061	-3.223640	0.693203
H	2.904369	-4.243668	1.886139
O	-4.158865	0.755110	2.499152
H	-4.501045	0.475960	1.605252
H	-4.923598	1.041488	3.019584
O	3.980448	-2.572088	-0.572992
H	3.311948	-2.310337	-1.243875
H	4.414236	-1.728061	-0.319293
O	2.004645	-1.048359	2.475931
H	2.127235	-2.006040	2.288782
H	1.277450	-0.941741	3.130898
O	0.092572	3.787777	-1.821682
H	0.796247	3.438814	-1.215363
H	0.388397	4.663517	-2.112045
O	1.987229	2.596434	-0.312021
H	1.697850	1.662239	-0.153645
H	2.201434	2.945914	0.582057
O	-0.012161	-0.385597	4.213038
H	-0.928983	-0.690178	3.958089
H	0.100686	-0.597813	5.151463
O	4.046700	1.725935	-1.936035
H	3.387106	2.185010	-1.369934

H	4.461590	1.066266	-1.338405
O	0.153480	2.285476	3.397710
H	-0.577295	2.278106	2.738348
H	0.164171	1.376152	3.765232
O	5.065910	-0.053560	-0.027956
H	4.730709	0.296234	0.843891
H	6.033172	-0.045270	0.030385
O	4.079504	0.754981	2.324333
H	3.387716	0.082729	2.509269
H	3.608250	1.615214	2.334185
O	2.479680	3.053853	2.346636
H	1.616659	2.797589	2.778534
H	2.776491	3.873889	2.767580

Table S17. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{28}$ cluster with one internal water molecule, 28D configuration.

O	-0.115319	-1.511158	0.001165
H	-0.823574	-1.804902	0.631971
H	-0.044119	-0.532192	0.151320
O	0.054615	1.157399	0.289466
H	0.833536	1.473781	0.806825
H	-0.711894	1.498426	0.808887
O	3.603226	0.183729	1.431749
H	4.510154	-0.211525	1.421306
H	2.990756	-0.576387	1.582551
O	3.290156	0.702920	-1.220864
H	3.043986	1.632151	-1.432526
H	3.351398	0.624530	-0.236886
O	-2.080887	-1.917792	1.805865
H	-2.715514	-2.632915	1.578623
H	-2.590904	-1.078387	1.677655
O	-3.510344	0.359731	1.366259
H	-3.474890	0.523472	0.391431
H	-3.019131	1.108193	1.769676
O	-1.875341	-1.283843	-2.175045
H	-1.301155	-1.002224	-2.931980
H	-1.253312	-1.432946	-1.429896
O	-3.540513	0.718539	-1.333252
H	-4.443074	0.386446	-1.531593
H	-2.918843	0.038491	-1.690893
O	1.914940	2.199187	2.040121
H	1.412186	1.970153	2.853504
H	2.690380	1.597648	1.998686
O	-1.717885	2.289202	2.071991
H	-1.140474	2.179027	2.858432
H	-1.640699	3.207479	1.731965
O	1.992664	-2.014051	1.739141
H	2.678825	-2.687532	1.527434
H	1.350455	-2.004254	0.997446
O	0.055802	1.946374	-2.358934
H	0.862420	2.499947	-2.432606
H	0.081194	1.613305	-1.431594
O	0.099292	1.402608	3.936251

H	0.044582	0.412713	3.843034
H	0.128341	1.596126	4.884854
O	2.411397	3.260133	-1.834274
H	2.082292	3.755033	-1.032741
H	2.978847	3.863877	-2.335663
O	-1.391560	4.434429	0.423072
H	-1.804271	4.022683	-0.386135
H	-1.769595	5.322149	0.509580
O	4.203657	-3.444659	0.941288
H	4.147838	-3.407675	-0.052914
H	4.406954	-4.360467	1.182820
O	-2.328898	3.210581	-1.770650
H	-1.493053	2.854005	-2.144914
H	-2.875638	2.414844	-1.596669
O	1.412186	4.364188	0.378791
H	0.431744	4.407740	0.346741
H	1.627552	3.701322	1.067664
O	-4.161716	-3.451664	0.835802
H	-4.385703	-4.376233	1.017681
H	-4.114949	-3.346447	-0.152642
O	1.822807	-1.448090	-2.066616
H	1.159765	-1.665238	-1.383424
H	2.256170	-0.613768	-1.760862
O	0.000535	-1.263996	3.576496
H	-0.781822	-1.568883	3.071398
H	0.778888	-1.585617	3.076903
O	-5.908419	-0.710267	-1.436588
H	-6.039314	-0.857344	-0.462966
H	-6.776376	-0.534878	-1.828710
O	4.100413	-3.001423	-1.694648
H	3.233894	-2.574063	-1.875677
H	4.753670	-2.281426	-1.816984
O	-4.138757	-2.850558	-1.783894
H	-4.833268	-2.160740	-1.830897
H	-3.302858	-2.395129	-2.020890
O	-5.798040	-1.204327	1.209319
H	-5.108355	-0.562866	1.477918
H	-5.345716	-2.074218	1.215001
O	5.620026	-0.645258	-1.669025
H	6.265245	-0.327175	-2.317537
H	4.869173	-0.005147	-1.661911
O	0.001800	-0.353553	-3.899079
H	0.032764	0.538278	-3.485821
H	0.743871	-0.826581	-3.467930
O	5.915630	-1.207649	1.072245
H	6.018825	-1.031816	0.114412
H	5.491050	-2.088698	1.128349

Table S18. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{28}$ cluster with one internal water molecule, 28E configuration.

O	-4.449645	-1.792670	-2.136202
H	-4.682451	-0.893246	-1.778859
H	-5.096716	-2.007193	-2.824111

O	-4.868712	0.586861	-0.993629
H	-4.414085	1.349736	-1.396234
H	-4.501050	0.526596	-0.081681
O	-1.718262	-1.477740	-2.232653
H	-2.670876	-1.624297	-2.421611
H	-1.636341	-0.561569	-1.872332
O	-3.228826	2.854646	-1.195936
H	-2.625999	3.568176	-1.496453
H	-3.472693	3.090118	-0.273216
O	-1.215631	0.963364	-1.178449
H	-1.964691	1.606152	-1.164372
H	-0.455399	1.442775	-1.590918
O	-3.964526	-3.498507	0.026884
H	-4.223517	-2.937472	-0.736219
H	-3.020412	-3.709616	-0.116303
O	-1.176664	-3.373662	-0.341367
H	-1.312101	-2.645328	-0.995258
H	-0.316189	-3.786393	-0.575432
O	-3.820706	0.497039	1.574095
H	-2.832167	0.480376	1.550513
H	-4.074522	-0.365563	1.969803
O	0.805373	2.517387	-2.180417
H	0.270595	3.339002	-2.137152
H	1.384686	2.534812	-1.378514
O	0.986881	-1.740500	-2.546638
H	0.017465	-1.731588	-2.690259
H	1.215793	-2.654327	-2.265285
O	-1.003889	4.477662	-1.408955
H	-0.929796	4.404820	-0.421181
H	-0.963210	5.421411	-1.623231
O	-1.095613	0.397583	1.461945
H	-0.993867	0.500336	0.484817
H	-1.018564	-0.564067	1.670205
O	-3.744549	3.196206	1.506708
H	-3.982223	2.277794	1.766528
H	-4.432816	3.782078	1.855313
O	2.425870	0.530183	-3.365208
H	1.843063	1.268783	-3.097499
H	1.928750	-0.291473	-3.174533
O	-1.208248	-2.248995	2.129060
H	-1.198959	-2.713215	1.255092
H	-2.136384	-2.287837	2.444739
O	-3.988496	-2.154765	2.361411
H	-4.106914	-2.671835	1.520732
H	-4.554793	-2.565000	3.031595
O	1.778903	-0.627394	-0.144120
H	1.355806	-0.953882	-0.971516
H	2.718237	-0.935800	-0.184828
O	1.368116	-4.115249	-1.187528
H	2.032969	-3.986371	-0.456673
H	1.540576	-4.986551	-1.574447
O	-1.068839	4.105568	1.276946
H	-1.954237	3.757568	1.504141
H	-0.415072	3.508021	1.701524
O	2.244148	2.051096	0.018742
H	2.109472	1.076410	-0.070510
H	3.224384	2.201209	0.007051
O	0.768683	2.221557	2.290588

H	0.128810	1.498534	2.088418
H	1.348884	2.269107	1.493377
O	1.501918	-1.820768	2.278293
H	0.599215	-2.093759	2.538008
H	1.391876	-1.369078	1.408052
O	3.083206	-3.623685	0.822478
H	2.545409	-3.138118	1.484583
H	3.719151	-2.959557	0.487799
O	4.835251	0.384366	-2.152485
H	3.955461	0.471083	-2.608582
H	5.500483	0.284269	-2.849371
O	4.418529	-1.306295	-0.016557
H	4.734041	-0.839874	-0.822566
H	4.703461	-0.761611	0.753087
O	2.638312	0.437233	3.441308
H	2.016712	1.146494	3.169728
H	2.205540	-0.401206	3.166188
O	4.938078	2.221224	-0.047352
H	5.080037	1.645639	-0.827737
H	5.128662	1.666977	0.737675
O	4.948028	0.413869	2.074003
H	4.109208	0.473658	2.609996
H	5.667773	0.238968	2.698211

Table S19. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{28}$ cluster with one internal water molecule, 28F configuration.

O	1.124391	-0.030653	0.887748
H	1.253609	-0.082480	-0.099031
H	1.321855	-0.935103	1.244172
O	1.372084	-0.136171	-1.760048
H	0.697789	0.537265	-2.030365
H	2.252973	0.295550	-1.875703
O	1.173666	-2.823922	-1.157023
H	1.124375	-1.907477	-1.504996
H	0.336699	-3.274499	-1.410790
O	1.497454	-2.595314	1.573057
H	1.338169	-2.851863	0.634221
H	2.454228	-2.751848	1.740731
O	-0.402489	1.828243	-2.336825
H	-1.219642	1.331669	-2.566942
H	-0.604111	2.264252	-1.473387
O	-1.621144	-0.411811	0.281054
H	-1.817672	-1.363751	0.467432
H	-0.693123	-0.257756	0.557194
O	-0.877466	3.235861	-0.028000
H	-0.223240	3.958875	-0.151454
H	-0.635977	2.802413	0.824540
O	-2.313741	-2.994698	0.815427
H	-3.270203	-2.963099	0.582347
H	-1.887284	-3.525862	0.107489
O	3.708726	1.263012	-1.695717
H	3.714667	1.431072	-0.723153
H	4.411968	0.595349	-1.853200

O	3.488847	1.454842	1.043087
H	3.210236	2.341497	1.382918
H	2.684689	0.898607	1.125881
O	0.032523	2.051749	2.283695
H	0.469307	1.280045	1.863480
H	-0.571377	1.650796	2.946355
O	-2.581462	0.159025	-2.232930
H	-3.402797	0.685788	-2.106371
H	-2.240579	-0.018763	-1.325566
O	-3.403838	0.958086	1.827853
H	-2.733335	0.503033	1.263635
H	-3.036223	0.865210	2.729960
O	-1.287447	-3.998511	-1.553451
H	-1.985575	-3.480516	-2.042004
H	-1.344000	-4.914715	-1.862773
O	-4.833881	-2.615691	-0.207299
H	-5.154911	-1.703620	0.038891
H	-5.578468	-3.222124	-0.080846
O	1.347488	4.806456	-0.489069
H	1.372375	5.752108	-0.697102
H	1.670268	4.320684	-1.293245
O	4.238008	-2.854305	1.610227
H	4.709480	-1.979079	1.558327
H	4.754888	-3.425942	2.196928
O	-4.796540	1.677452	-1.562573
H	-5.384911	2.116817	-2.194032
H	-4.405112	2.381000	-0.975728
O	-1.569173	0.369255	3.814756
H	-1.587792	0.388127	4.782894
H	-1.279307	-0.544217	3.556694
O	-0.857870	-2.149505	3.056661
H	-1.477717	-2.534469	2.404679
H	0.029128	-2.326016	2.682835
O	5.399678	-0.916196	-1.638013
H	4.859354	-1.748843	-1.595254
H	6.177702	-1.108431	-2.181909
O	-3.640513	3.235122	0.273213
H	-3.601012	2.551352	0.977904
H	-2.698323	3.403692	0.058099
O	-3.283012	-2.517202	-2.542987
H	-3.937654	-2.576782	-1.814895
H	-3.030769	-1.567615	-2.575847
O	-5.551193	-0.127075	0.442102
H	-5.435131	0.462902	-0.332690
H	-4.903588	0.204747	1.100743
O	5.457173	-0.508923	1.139141
H	4.851829	0.253601	1.252777
H	5.601405	-0.582551	0.172149
O	3.964409	-3.154480	-1.161160
H	2.994748	-3.135703	-1.297194
H	4.089640	-3.226476	-0.191547
O	1.994413	3.290899	-2.628798
H	1.171006	2.785517	-2.777522
H	2.687356	2.629754	-2.426111
O	2.274794	3.730465	1.925925
H	1.458118	3.305465	2.256759
H	2.010895	4.204348	1.109186

Table S20. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{34}$ cluster with three internal water molecules, 34A configuration.

O	2.831806	3.975056	1.484993
H	3.279082	3.114600	1.687433
H	3.282686	4.667777	1.989848
O	2.491769	3.862147	-1.291619
H	2.662129	4.010886	-0.337612
H	1.604897	3.441780	-1.334142
O	3.713110	1.437741	1.694491
H	3.097863	1.052085	1.028409
H	3.519258	0.959375	2.531221
O	0.219854	3.069152	1.629445
H	1.086240	3.527002	1.689724
H	0.272272	2.291596	2.235696
O	-0.017106	2.629974	-1.073674
H	0.032144	2.598174	-0.089236
H	-0.786461	3.211327	-1.272715
O	2.241466	0.170255	-0.206548
H	1.319254	-0.042470	0.041777
H	2.314859	0.205710	-1.193293
O	0.270692	0.774873	3.082838
H	1.112409	0.597848	3.559047
H	0.279173	0.174034	2.303625
O	5.700232	0.915231	-0.235090
H	5.151638	1.076890	0.560293
H	5.271444	1.422257	-0.958717
O	2.780238	-0.013434	3.892129
H	2.677444	-0.976722	3.654956
H	3.161541	0.024014	4.781744
O	4.382772	2.269051	-2.301072
H	3.702709	2.904510	-1.941538
H	4.929537	2.767350	-2.926402
O	-2.325985	4.162410	1.425652
H	-1.401838	3.883833	1.604486
H	-2.356080	4.326237	0.459332
O	-0.087629	-0.797438	0.865350
H	-0.997630	-0.456462	0.657032
H	-0.174722	-1.672095	1.338716
O	2.712436	0.181733	-2.884747
H	3.401176	0.883501	-2.885805
H	3.172963	-0.689810	-2.988834
O	-2.294835	4.184974	-1.357242
H	-3.055664	3.620349	-1.670097
H	-2.289097	4.983510	-1.905503
O	0.000188	0.583472	-2.887238
H	-0.012945	1.271368	-2.178245
H	0.938857	0.522717	-3.167918
O	2.421141	-2.521130	3.031654
H	2.840500	-2.508015	2.142288
H	1.487482	-2.765877	2.864916
O	-2.467278	0.039279	0.056933
H	-2.861113	0.799335	0.555288
H	-2.560179	0.191506	-0.913620

O	3.360605	-2.245804	0.460305
H	3.013545	-1.350668	0.229634
H	4.299058	-2.229474	0.170700
O	-2.403677	0.157064	3.625410
H	-1.466490	0.436822	3.557522
H	-2.904814	0.717876	2.996964
O	5.725063	-1.698789	-0.827854
H	5.786540	-0.725369	-0.624608
H	6.615675	-2.067657	-0.735302
O	-3.631036	1.808422	1.692489
H	-3.243408	2.718661	1.613380
H	-4.502253	1.801901	1.241164
O	-0.134182	-1.859527	-1.691881
H	-0.061269	-1.548559	-0.763570
H	-0.128991	-1.024173	-2.219776
O	3.956144	-2.239699	-2.937828
H	4.655929	-2.118413	-2.261340
H	3.311969	-2.864104	-2.544006
O	-0.182107	-3.136564	2.127499
H	-1.036470	-3.110393	2.613195
H	-0.246911	-3.818467	1.411757
O	-4.234986	2.538528	-2.156816
H	-3.747863	1.750281	-2.477824
H	-4.796051	2.208810	-1.421802
O	-2.736425	0.264953	-2.665089
H	-1.843062	0.297395	-3.060843
H	-3.169759	-0.574906	-2.939247
O	1.947992	-3.628857	-1.462835
H	2.418188	-3.241777	-0.688213
H	1.273917	-2.955352	-1.707705
O	-2.598200	-2.500811	3.282535
H	-2.547627	-1.522926	3.464380
H	-3.010778	-2.913061	4.055761
O	-3.615444	-2.320689	0.720942
H	-3.212774	-1.432210	0.564768
H	-3.392272	-2.548883	1.649507
O	-5.702468	1.357859	-0.081820
H	-5.727584	0.392484	-0.321643
H	-6.624805	1.640225	0.008716
O	-0.215070	-4.818113	-0.029466
H	0.577375	-4.564520	-0.549416
H	-0.984351	-4.545658	-0.570837
O	-2.330202	-3.470732	-1.406884
H	-1.608941	-2.822503	-1.584975
H	-2.762552	-3.166387	-0.573070
O	-5.726464	-1.267406	-0.728653
H	-5.183900	-1.748928	-0.070016
H	-5.300113	-1.480793	-1.584101
O	-4.121323	-2.085243	-2.917121
H	-3.528710	-2.759218	-2.500937
H	-4.471019	-2.471651	-3.733854

Table S21. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{34}$ cluster with three internal water molecules, 34B configuration.

O	-3.734548	3.246427	1.544313
H	-4.117940	3.124295	0.649036
H	-3.676376	2.341860	1.916931
O	-4.706787	2.694449	-1.028754
H	-5.087377	1.772857	-0.998287
H	-5.408901	3.269739	-1.367812
O	-3.119961	0.588267	2.087348
H	-2.714529	0.518961	1.189032
H	-2.426839	0.312948	2.723737
O	-1.044980	3.487781	1.258149
H	-2.029842	3.505633	1.365219
H	-0.760378	2.552737	1.379982
O	-2.182923	0.323478	-0.453849
H	-2.028204	1.126917	-1.003417
H	-2.760940	-0.245111	-1.021073
O	-2.274178	2.386169	-2.267665
H	-3.159035	2.671722	-1.944803
H	-1.646559	3.123400	-2.128976
O	0.256306	1.088891	1.470093
H	-0.149781	0.410879	2.058731
H	1.074277	1.386714	1.936007
O	-0.188768	3.835428	-1.284934
H	-0.530845	3.828215	-0.355727
H	0.633365	4.368246	-1.258957
O	-5.637988	0.177019	-0.991362
H	-5.531834	-0.259926	-0.119450
H	-5.037045	-0.316912	-1.588915
O	-0.921776	-0.456942	3.427851
H	-0.967368	-1.419785	3.224881
H	-0.169451	-0.323104	4.045165
O	-5.057036	-1.164419	1.408885
H	-4.414184	-0.544485	1.835329
H	-5.778866	-1.300035	2.041051
O	1.487380	4.423516	1.973945
H	0.530842	4.236856	1.875017
H	1.874290	3.619536	2.377658
O	0.803520	1.256123	-1.201845
H	0.613367	1.043858	-0.258162
H	0.358784	2.122642	-1.358230
O	-3.589400	-1.099795	-2.326263
H	-3.034588	-0.738285	-3.062664
H	-3.392470	-2.058532	-2.235723
O	-0.259122	-1.458389	0.159834
H	-0.886824	-0.737498	-0.093934
H	-0.263268	-2.105958	-0.587235
O	2.467478	1.937843	2.871625
H	2.320637	1.314129	3.617154
H	3.234698	1.606959	2.352472
O	-1.162602	-2.896152	2.242772
H	-0.830722	-2.383961	1.462030
H	-0.472278	-3.580101	2.380752
O	2.292321	4.869537	-0.559984
H	2.091692	4.777229	0.409131
H	2.699175	5.738944	-0.688931
O	-1.956082	0.231815	-4.030164
H	-2.018614	1.085751	-3.553794
H	-1.055205	-0.108066	-3.843141

O	-3.524517	-3.480200	0.901233
H	-4.090891	-2.696076	1.064014
H	-2.723615	-3.356803	1.457508
O	1.576909	-0.083724	4.557906
H	1.954157	-0.893059	4.114465
H	1.800363	-0.145921	5.498607
O	0.473830	-0.743658	-3.063030
H	0.553854	-0.084051	-2.333693
H	1.387829	-0.851912	-3.408181
O	-2.904065	-3.685786	-1.691370
H	-3.133909	-3.666809	-0.719934
H	-3.352161	-4.454470	-2.074131
O	2.361234	-1.024728	0.560567
H	1.382391	-1.037359	0.423491
H	2.755391	-1.587432	-0.145959
O	3.315953	2.388989	-1.212476
H	2.439081	1.936891	-1.237743
H	3.112705	3.338719	-1.061508
O	4.164048	0.922959	0.939238
H	3.438183	0.265511	0.796416
H	3.996519	1.599451	0.242050
O	-0.212464	-3.152166	-1.952136
H	-0.054557	-2.377189	-2.539980
H	-1.156914	-3.416684	-2.019121
O	2.531164	-2.096591	3.084718
H	2.541402	-1.715189	2.176951
H	2.045664	-2.940952	2.980041
O	1.168309	-4.386196	2.199206
H	1.422293	-4.395860	1.238998
H	1.333376	-5.278350	2.537973
O	3.157965	-1.162558	-3.659727
H	3.770112	-0.403506	-3.454991
H	3.432074	-1.522723	-4.516383
O	1.820093	-4.346210	-0.432398
H	1.101814	-4.007992	-1.006844
H	2.610897	-3.824476	-0.673650
O	4.853536	0.721558	-2.798095
H	4.360628	1.433441	-2.335668
H	5.340151	0.248024	-2.091942
O	3.759497	-2.480942	-1.292575
H	3.535790	-2.141337	-2.188490
H	4.608179	-2.053106	-1.048241
O	5.788899	-0.703416	-0.551460
H	5.388434	-0.116494	0.134669
H	6.709942	-0.860587	-0.295562

Table S22. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{34}$ cluster with three internal water molecules, 34C configuration.

O	4.354349	-1.612751	2.708153
H	3.872767	-2.237118	2.115189
H	5.003919	-2.138026	3.198631
O	2.953210	-2.948459	0.792312
H	3.425695	-2.721121	-0.053011

H	2.480579	-3.792333	0.622227
O	5.255708	0.649125	1.281853
H	5.042829	-0.192411	1.737178
H	4.531992	1.266476	1.534566
O	2.814667	0.304636	4.100020
H	3.347485	-0.412573	3.697987
H	2.891882	1.059430	3.479317
O	0.742631	-1.351242	1.099274
H	1.584795	-1.857867	0.999005
H	0.039186	-1.969880	0.792943
O	3.022588	2.112967	1.966986
H	2.371184	1.722478	1.333440
H	2.983322	3.075087	1.783780
O	4.103187	-2.281985	-1.546290
H	4.554516	-1.413190	-1.490869
H	3.272238	-2.106125	-2.041893
O	0.241281	-0.419694	3.621677
H	1.143250	-0.181807	3.953302
H	0.405318	-0.829461	2.737555
O	5.051240	0.321180	-1.354091
H	5.180010	0.473925	-0.375714
H	5.861481	0.614964	-1.796129
O	1.187631	1.179675	0.186113
H	0.924759	0.259713	0.428751
H	1.595817	1.129611	-0.709568
O	1.223024	-5.008005	0.027015
H	1.064015	-4.911148	-0.949524
H	1.329599	-5.953863	0.206645
O	-0.988816	-3.389165	0.429539
H	-0.321464	-4.108735	0.438969
H	-1.324366	-3.317108	-0.497600
O	2.603979	1.340491	-2.150146
H	3.497691	0.971003	-1.968047
H	2.278652	0.963394	-2.995530
O	1.639002	-1.881257	-2.676247
H	1.031350	-1.417792	-2.056474
H	1.595611	-1.327761	-3.483651
O	-0.479662	-0.540572	-1.608340
H	-0.889079	-0.284730	-0.749564
H	-0.647929	0.206178	-2.231129
O	-1.241197	1.679775	2.765356
H	-0.578592	1.077649	3.178848
H	-0.764647	2.438270	2.359358
O	-2.255483	-1.244848	4.351916
H	-1.303908	-0.997173	4.266083
H	-2.346298	-1.739749	5.179698
O	-1.921466	0.085722	0.640275
H	-1.620102	0.657308	1.387710
H	-2.338693	-0.704644	1.059249
O	-0.110631	3.426404	1.047946
H	0.282356	2.649688	0.584696
H	0.637878	4.049540	1.164179
O	0.563310	-4.415969	-2.520680
H	1.042224	-3.575308	-2.694517
H	-0.374265	-4.138329	-2.516975
O	2.368358	4.608041	0.904663
H	2.340639	4.469947	-0.080560
H	2.690508	5.507381	1.062198

O	-2.930782	-2.174522	1.854951
H	-2.253638	-2.802653	1.519017
H	-2.734059	-2.005828	2.802916
O	2.052367	4.019832	-1.692574
H	2.350516	3.106971	-1.895237
H	1.112716	4.045618	-1.974420
O	-1.756647	-2.886237	-2.132334
H	-1.328998	-1.996705	-2.091521
H	-2.715358	-2.696876	-2.239781
O	1.321498	0.268719	-4.390366
H	0.414030	0.642936	-4.296231
H	1.608434	0.436292	-5.300111
O	-3.797912	0.980646	3.509931
H	-2.969825	1.437768	3.251442
H	-3.472511	0.138842	3.886023
O	-1.024863	1.316443	-3.529557
H	-0.900982	2.253268	-3.251158
H	-1.998848	1.131561	-3.526896
O	-2.230518	4.114842	-0.575672
H	-1.542505	3.939149	0.104082
H	-2.820259	3.327555	-0.564138
O	-3.696726	1.758931	-0.580686
H	-3.056342	1.121849	-0.179099
H	-4.485577	1.677910	-0.004096
O	-0.590085	3.903233	-2.652551
H	-1.262588	4.044647	-1.926161
H	-0.762608	4.577923	-3.326641
O	-5.132455	-1.612594	0.256387
H	-4.423626	-1.927612	0.855333
H	-5.344379	-0.711082	0.580418
O	-4.315442	-1.863415	-2.293646
H	-4.650291	-1.747245	-1.362947
H	-5.023451	-2.304731	-2.786044
O	-3.657703	0.749801	-3.155578
H	-3.784440	1.175521	-2.278384
H	-3.848208	-0.196757	-2.987555
O	-5.453697	0.924232	1.380808
H	-4.882788	0.923901	2.194850
H	-6.330163	1.232159	1.654251

Table S23. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{34}$ cluster with two internal water molecules, 34D configuration.

O	1.429036	-4.476099	-2.127229
H	2.244571	-4.284401	-1.587884
H	1.571212	-5.336847	-2.548266
O	0.542500	-3.130840	1.732364
H	0.669649	-2.241427	1.311141
H	-0.073145	-2.961786	2.480826
O	-1.869320	0.585214	-1.808222
H	-1.745672	-0.285364	-2.250241
H	-1.928265	0.341218	-0.852444
O	-4.481948	-2.464052	-2.080113
H	-4.943919	-1.647955	-1.746395

H	-5.066404	-2.864326	-2.740848
O	-5.721625	-0.283263	-1.100498
H	-5.336094	0.566188	-1.394194
H	-5.669843	-0.271197	-0.121191
O	4.942359	3.523148	0.927115
H	5.361309	2.660968	1.189622
H	5.431565	4.231338	1.371015
O	-0.674118	3.035809	-1.894710
H	-1.031274	2.117924	-1.944390
H	-1.409709	3.624544	-2.170064
O	4.061258	-0.905541	1.684783
H	3.872368	-1.804190	2.029298
H	4.008170	-0.997538	0.701289
O	-3.515063	-4.004084	0.049425
H	-3.941640	-3.547683	-0.706865
H	-2.582560	-4.140353	-0.217378
O	0.646945	-0.766140	0.480110
H	1.098521	-0.150408	1.111110
H	-0.319744	-0.569125	0.562041
O	0.733766	-2.240328	-3.669121
H	1.035784	-3.068172	-3.237549
H	-0.229110	-2.206552	-3.498518
O	-3.053434	4.480514	-2.086142
H	-3.085085	4.782228	-1.142989
H	-3.294361	5.236311	-2.641909
O	-3.001361	4.893960	0.594068
H	-3.563960	4.195171	0.977655
H	-2.078503	4.660404	0.820562
O	-0.431846	3.747274	0.747342
H	-0.486304	3.440428	-0.190662
H	0.523621	3.728889	0.969081
O	-4.169665	1.991367	-1.597068
H	-3.366430	1.466402	-1.827014
H	-4.001371	2.893009	-1.944286
O	4.748324	3.017745	-1.825022
H	3.790934	2.848852	-1.949573
H	4.840098	3.380027	-0.919051
O	-1.277247	-2.226208	3.624908
H	-0.935707	-1.296748	3.740900
H	-1.314269	-2.617582	4.510561
O	-0.792476	-3.861588	-0.577985
H	-0.371349	-3.662603	0.289838
H	-0.071105	-4.236980	-1.130567
O	1.960782	0.728169	2.304190
H	2.792163	0.207312	2.194933
H	2.101244	1.597194	1.855877
O	2.022488	2.355222	-1.806366
H	1.171090	2.778441	-2.042690
H	1.892056	1.389150	-1.963362
O	-1.766419	-2.067885	-2.466328
H	-1.428654	-2.561946	-1.684355
H	-2.734414	-2.236179	-2.487879
O	6.086440	0.713877	-1.474675
H	5.630841	1.561270	-1.727931
H	6.863034	0.619123	-2.045572
O	1.716699	-0.351161	-1.969753
H	1.226489	-0.540510	-1.132814
H	1.366277	-0.978775	-2.651346

O	3.624050	-3.869284	-0.699284
H	3.907720	-2.955039	-0.915546
H	3.497595	-3.873406	0.272776
O	-4.301511	2.393302	1.142669
H	-4.201170	2.208430	0.178432
H	-4.783135	1.615695	1.496403
O	-0.319297	0.271887	3.859059
H	-0.930442	0.923679	3.459855
H	0.535841	0.405859	3.397270
O	4.120243	-1.162644	-1.033818
H	3.294513	-0.822718	-1.459837
H	4.859033	-0.584317	-1.326806
O	2.238894	3.026941	0.864871
H	3.152442	3.361721	1.003631
H	2.207102	2.719468	-0.072766
O	-3.464018	-2.067207	1.944453
H	-2.799618	-2.263379	2.642416
H	-3.489618	-2.836848	1.318231
O	-5.396767	-0.141381	1.690382
H	-4.764407	-0.861397	1.922509
H	-6.191789	-0.288470	2.224384
O	6.025285	1.084033	1.299370
H	5.424021	0.386322	1.629857
H	6.199285	0.857261	0.361215
O	3.194648	-3.542188	2.065482
H	2.206891	-3.504617	2.110746
H	3.487695	-4.203160	2.710023
O	-1.950988	-0.166399	0.760482
H	-1.934422	0.587709	1.398160
H	-2.533466	-0.871942	1.136340
O	-1.855521	2.039264	2.327373
H	-2.771306	2.263274	2.040680
H	-1.263605	2.626653	1.797633

Table S24. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{35}$ cluster with two internal water molecules, 35A configuration.

O	2.021683	3.204471	-1.563627
H	2.900384	2.863045	-1.866340
H	1.397224	2.443322	-1.616906
O	4.277077	1.960731	-2.412561
H	3.788211	1.178423	-2.740701
H	4.805378	1.635121	-1.652496
O	1.972231	3.526047	1.124068
H	2.031755	3.502648	0.135609
H	1.450788	4.327210	1.341452
O	0.037057	1.344111	-1.377057
H	0.057256	1.153139	-0.412473
H	0.019598	0.487906	-1.862841
O	0.076865	5.204945	-1.539841
H	0.861801	4.640724	-1.700302
H	-0.689412	4.604413	-1.663420
O	0.134689	1.496248	1.331728
H	0.906838	2.102667	1.417024

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H      0.089434     0.935005     2.144872
O      2.628781    -0.242211    -2.844257
H      1.711591    -0.359489    -3.165668
H      3.107130    -1.087955    -3.011262
O     -1.942042     3.233543    -1.483716
H     -1.308847     2.480555    -1.567939
H     -2.027933     3.354714    -0.507920
O      3.629835     1.413320     1.553556
H      3.294964     2.332492     1.515415
H      4.485200     1.371582     1.069444
O      2.390469    -0.351253    -0.111041
H      2.511705    -0.201380    -1.078314
H      2.756884     0.412102     0.391807
O      0.069034     5.565553     1.130711
H      0.070191     5.605479     0.138165
H      0.082650     6.475827     1.460978
O      5.659531     0.887531    -0.212134
H      5.679360    -0.096161    -0.374051
H      6.581951     1.168046    -0.116001
O     -1.745332     3.474442     1.247427
H     -1.059331     2.769667     1.346710
H     -1.272330     4.323022     1.385869
O     -0.097139    -0.801290    -3.081529
H     -1.039652    -0.573365    -3.237795
H     -0.108635    -1.690185    -2.650525
O      0.059325    -1.499084     0.520396
H      0.854570    -0.940498     0.342258
H     -0.737308    -0.921562     0.431331
O     -2.301177    -0.314133     0.030717
H     -2.662517     0.409202     0.595549
H     -2.814350    -1.123625     0.275085
O     -2.746926    -0.175879    -2.675108
H     -2.591112    -0.144947    -1.699772
H     -3.293228     0.615779    -2.866407
O      5.645120    -1.762321    -0.666460
H      5.237993    -1.978433    -1.531814
H      5.043591    -2.179994    -0.013087
O     -0.081311     0.089815     3.651302
H     -0.068980    -0.885335     3.492214
H     -0.996693     0.292684     3.941635
O      2.730619     0.020078     3.808635
H      3.090725     0.509714     3.038497
H      1.781759     0.246991     3.864123
O     -4.197841     2.164355    -2.485265
H     -3.431724     2.699997    -2.153722
H     -4.679976     2.710856    -3.123149
O      4.086733    -2.543119    -2.879705
H      3.502817    -3.216907    -2.430674
H      4.452094    -2.959993    -3.674031
O      3.467927    -2.701945     0.765008
H      3.054715    -1.841442     0.516644
H      3.312156    -2.808911     1.728881
O     -3.564360     1.488361     1.685386
H     -3.108066     2.355117     1.686194
H     -3.395416     1.075012     2.563746
O     -0.063330    -3.119794    -1.632450
H     -0.058123    -2.605318    -0.786939
H     -0.921876    -3.598653    -1.645482
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O	2.525232	-4.127686	-1.412850
H	2.781804	-3.772765	-0.533132
H	1.583809	-3.877278	-1.539882
O	0.079605	-2.559414	2.999157
H	0.143822	-2.305240	2.046705
H	0.985102	-2.820620	3.272358
O	-5.492995	0.989266	-0.286920
H	-5.087379	1.416665	-1.071168
H	-4.900259	1.193095	0.466016
O	2.806866	-2.649449	3.467557
H	2.869635	-1.675242	3.656913
H	3.318634	-3.108069	4.150099
O	-2.846696	0.136222	3.973027
H	-2.889099	-0.837504	3.764372
H	-3.331547	0.268375	4.801315
O	-4.269760	-2.473705	-2.754249
H	-3.728819	-1.655131	-2.838767
H	-4.947151	-2.244955	-2.083545
O	-3.585475	-2.645048	0.675385
H	-3.222081	-3.308223	0.046914
H	-4.493901	-2.436300	0.359277
O	-2.703499	-2.457169	3.308961
H	-1.749414	-2.672081	3.276492
H	-3.045128	-2.597289	2.399598
O	-2.637452	-4.142174	-1.459713
H	-3.247287	-3.621449	-2.052773
H	-2.842905	-5.080187	-1.587737
O	-5.819525	-1.656965	-0.561813
H	-5.734751	-0.668258	-0.467395
H	-6.748815	-1.877043	-0.400952

Table S25. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{35}$ cluster with two internal water molecules, 35B configuration.

O	2.735338	-0.014848	4.029965
H	2.752044	-0.978852	3.775958
H	3.238689	0.068655	4.853633
O	-2.822218	-0.026594	3.889015
H	-3.141437	0.504621	3.128056
H	-1.872028	0.181242	3.984960
O	-2.340748	-0.311917	-0.053967
H	-2.648980	0.396204	0.557421
H	-1.425469	-0.574657	0.213147
O	3.520523	1.378019	1.785513
H	3.070320	2.248337	1.771229
H	3.315788	0.954941	2.651573
O	0.030324	5.524126	1.127918
H	0.045349	5.573636	0.135728
H	0.044369	6.431831	1.465391
O	-1.894060	3.211042	-1.621102
H	-2.772958	2.889453	-1.947016
H	-1.279673	2.441319	-1.658634
O	-0.011028	0.252600	3.692907
H	0.002846	0.700886	2.811714

H	0.914763	0.294133	4.017415
O	0.099091	1.342163	-1.405098
H	0.061773	1.177530	-0.435540
H	0.057850	0.476956	-1.874154
O	2.056052	3.219059	-1.572597
H	1.457547	2.437043	-1.638345
H	2.925159	2.938980	-1.931870
O	-2.603011	-4.041557	-1.480664
H	-1.655224	-3.813572	-1.594941
H	-2.864695	-3.682408	-0.604021
O	2.628468	-4.166250	-1.527061
H	3.240780	-3.619897	-2.092793
H	2.835471	-5.097658	-1.694703
O	-0.043331	-0.819238	-3.064411
H	-1.002525	-0.649407	-3.208704
H	0.002925	-1.706300	-2.632250
O	-0.028037	-1.503382	0.515485
H	-0.091355	-1.890938	1.422559
H	0.806904	-0.977104	0.474410
O	-0.216570	-2.381991	3.080189
H	-1.118533	-2.729710	3.248960
H	-0.216203	-1.452658	3.418462
O	-3.567815	-2.630139	0.695779
H	-3.113450	-1.777637	0.488772
H	-3.437285	-2.774323	1.658492
O	2.651670	-0.173344	-2.659873
H	1.776256	-0.264877	-3.085622
H	2.476512	-0.188507	-1.685942
O	-1.926069	3.546743	1.064466
H	-1.974496	3.519817	0.075344
H	-1.396886	4.341610	1.288212
O	4.336938	1.919919	-2.469505
H	3.801139	1.155422	-2.788553
H	4.904976	2.202097	-3.201826
O	-4.254745	-2.524078	-2.936868
H	-3.637277	-3.176459	-2.505779
H	-4.602647	-2.937890	-3.740295
O	2.355372	-0.375552	0.036293
H	2.718825	0.324632	0.629990
H	2.853637	-1.201716	0.254753
O	1.935852	3.505330	1.134149
H	2.068460	3.490406	0.154700
H	1.407164	4.310066	1.324599
O	-5.707844	-1.600710	-0.710898
H	-5.354565	-1.864290	-1.586125
H	-5.110666	-2.049245	-0.073195
O	5.537480	0.921032	-0.126247
H	5.146409	1.317698	-0.933312
H	4.918703	1.122521	0.605335
O	-4.207925	2.069096	-2.465841
H	-3.778986	1.235257	-2.759226
H	-4.734014	1.806893	-1.680777
O	-2.720037	-0.243023	-2.770187
H	-3.284100	-1.024038	-2.969032
H	-2.595972	-0.258675	-1.790509
O	-3.572439	1.450028	1.636663
H	-4.392366	1.421040	1.092202
H	-3.192277	2.349911	1.560523

O	4.262543	-2.430696	-2.733541
H	3.695865	-1.632940	-2.825345
H	4.915950	-2.196963	-2.040470
O	3.559491	-2.748940	0.661867
H	3.204492	-3.391681	0.007691
H	4.482091	-2.552562	0.383286
O	-0.020944	1.575831	1.309754
H	0.751264	2.192721	1.325459
H	-0.787795	2.199630	1.311425
O	0.070732	5.190383	-1.541742
H	-0.702111	4.615932	-1.724935
H	0.852594	4.622882	-1.704486
O	0.048069	-3.139276	-1.622429
H	0.905843	-3.616020	-1.672580
H	0.065926	-2.645344	-0.765939
O	5.814897	-1.723447	-0.499156
H	5.756778	-0.740408	-0.347868
H	6.744946	-1.971480	-0.392286
O	2.558681	-2.575184	3.254087
H	1.595413	-2.735220	3.188860
H	2.926069	-2.704599	2.353626
O	-5.562822	1.042205	-0.216748
H	-5.634675	0.066555	-0.407770
H	-6.468089	1.358620	-0.077566
O	-2.951577	-2.669610	3.403774
H	-3.018048	-1.706836	3.642898
H	-3.439493	-3.166988	4.076539

Table S26. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{35}$ cluster with one internal water molecule, 35C configuration.

O	0.195708	0.309279	-1.670211
H	0.100715	-0.477772	-2.260133
H	0.699659	0.001003	-0.882205
O	2.010092	2.142765	-2.493545
H	1.306956	1.489987	-2.251752
H	2.674708	1.627051	-2.999693
O	-0.083830	-1.976968	-3.148466
H	-0.172298	-2.585731	-2.376053
H	-0.967853	-1.972228	-3.579691
O	2.014777	-0.605523	0.155770
H	2.849162	-0.167853	-0.138677
H	2.040158	-0.583960	1.141227
O	-2.201913	1.554078	-1.378101
H	-1.325083	1.097782	-1.375081
H	-2.025549	2.494913	-1.600028
O	-0.332782	1.342717	1.124735
H	0.583663	1.622344	1.363681
H	-0.804579	2.162658	0.853861
O	-0.938593	-1.303923	0.920517
H	-0.702246	-0.351891	0.826580
H	-1.904654	-1.321618	1.134329
O	2.659955	-2.060755	-3.557859
H	1.685645	-1.990331	-3.634491

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H      2.799682    -2.472201    -2.675219
O     -0.538639    -3.339170    -0.836465
H     -0.601642    -2.583725    -0.204819
H      0.078999    -3.991299    -0.438287
O      3.874447     0.308508    -3.406730
H      3.422348    -0.572499    -3.537392
H      4.542585     0.392613    -4.102907
O      2.888125    -2.949918    -0.951024
H      2.401499    -2.219279    -0.502020
H      2.473798    -3.781387    -0.634430
O      3.413546     2.886547    -0.261046
H      2.845227     2.634154    -1.029426
H      3.310321     3.858542    -0.175698
O      4.451446     0.386504    -0.714001
H      4.386361     0.362811    -1.696933
H      4.453141     1.332725    -0.467511
O     -3.908122     0.202006    -3.102673
H     -3.257813     0.721112    -2.578905
H     -4.623276    -0.013464    -2.458940
O      2.105227     2.168785     2.022710
H      2.681690     2.299713     1.232852
H      2.379061     1.344772     2.477598
O     -2.733908    -2.034787    -3.928076
H     -3.194448    -1.185060    -3.670497
H     -3.026318    -2.257070    -4.824273
O     -1.673444     4.259013    -1.743259
H     -0.731632     4.460250    -2.002561
H     -2.247476     4.817161    -2.287876
O      0.899008     4.691673    -2.337439
H      1.315454     3.827365    -2.539366
H      1.383313     5.042499    -1.559271
O     -1.521288     3.825658     0.946915
H     -1.762398     4.140299     0.048941
H     -2.334998     3.747158     1.489013
O     -4.030958     1.162911     0.619640
H     -3.300690     1.354136    -0.017369
H     -3.996364     1.854362     1.316141
O      2.303789    -0.428653     2.903661
H      1.511820    -0.880215     3.274414
H      3.058847    -1.047273     3.025071
O     -3.112436    -3.789342    -1.787243
H     -2.219534    -3.737823    -1.381145
H     -3.058751    -3.231463    -2.593143
O     -3.541566    -1.283932     1.693370
H     -3.777961    -0.378013     1.372253
H     -4.073723    -1.915363     1.156683
O      0.110672    -2.000502     3.323028
H     -0.248078    -1.797463     2.423097
H     -0.665555    -1.899576     3.909577
O      0.879910     4.670628     2.049032
H      1.296184     3.811052     2.263141
H     -0.012884     4.449418     1.704497
O      5.193892    -2.105880     0.330296
H      4.485781    -2.549011    -0.188110
H      5.132196    -1.167257     0.059349
O      1.424315    -4.921863     0.301953
H      1.599334    -4.670507     1.250825
H      1.462740    -5.887640     0.243596
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O	-1.604910	1.313482	3.604261
H	-1.100053	1.199980	2.768708
H	-1.905864	0.420250	3.873282
O	2.355540	5.433548	-0.059074
H	1.800957	5.268731	0.751005
H	2.752844	6.311703	0.035768
O	-5.732828	-0.277875	-1.086410
H	-5.331145	0.309873	-0.414914
H	-5.564317	-1.190279	-0.770607
O	-4.942552	-2.791746	-0.120613
H	-4.284506	-3.208900	-0.744759
H	-5.579312	-3.479101	0.124635
O	-3.488195	2.947523	2.646419
H	-2.870656	2.359526	3.160236
H	-4.066653	3.400052	3.277314
O	1.931613	-4.037799	2.771732
H	1.239853	-3.401214	3.053469
H	2.775156	-3.537308	2.779970
O	-2.454735	-1.297190	4.177026
H	-3.017863	-1.423815	3.377606
H	-3.012540	-1.464782	4.950808
O	4.212679	-2.395973	2.804129
H	4.655652	-2.284760	1.917792
H	4.910868	-2.567462	3.453199

Table S27. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{35}$ cluster with two internal water molecules, 35D configuration.

O	1.776385	3.915980	0.023002
H	1.118506	4.612201	-0.191988
H	2.038216	3.511895	-0.839618
O	-0.007143	-1.312990	0.665335
H	-0.776366	-0.890067	0.211979
H	0.795767	-0.770241	0.470734
O	2.191685	1.472169	4.027371
H	2.206303	0.479183	4.113165
H	2.626459	1.830228	4.815670
O	0.727289	-1.814603	-2.774796
H	0.555717	-2.555017	-2.147924
H	1.699488	-1.659475	-2.749499
O	-3.551739	1.738524	-1.185332
H	-3.085078	0.962223	-0.787397
H	-3.216076	2.517890	-0.685670
O	-0.484138	1.550121	3.273782
H	-0.265562	1.619815	2.313530
H	0.369051	1.711346	3.730185
O	2.220452	2.461513	-2.230635
H	1.668459	1.666775	-2.041946
H	3.137657	2.148293	-2.390749
O	4.778570	-3.084773	-1.203700
H	4.108846	-3.631092	-0.743142
H	5.268645	-2.609713	-0.499882
O	-3.255489	-1.401886	2.211900
H	-2.430719	-1.377171	2.749484

H	-3.837541	-0.674092	2.529227
O	-2.993171	2.784213	2.935366
H	-2.818590	3.226893	2.077810
H	-2.130069	2.410077	3.212203
O	5.823259	-1.496069	0.857465
H	5.736248	-0.527733	0.639040
H	6.702687	-1.618526	1.244370
O	-1.757778	1.653257	-3.271702
H	-1.821672	0.777105	-3.724215
H	-2.522708	1.720981	-2.654459
O	0.249646	0.643982	-1.684904
H	0.357225	-0.293788	-1.976366
H	-0.496268	1.010750	-2.217845
O	3.215854	2.109256	1.543025
H	2.901001	1.962396	2.465400
H	2.791958	2.928283	1.217526
O	0.277724	-3.599485	-0.721301
H	0.131257	-2.819762	-0.128016
H	-0.585108	-4.067804	-0.762973
O	-2.222443	3.582224	0.366327
H	-1.447157	2.971448	0.427450
H	-1.840702	4.387660	-0.041426
O	2.708414	-4.317623	0.261641
H	1.799252	-4.210091	-0.113943
H	2.769889	-5.225691	0.593740
O	-0.703371	-1.186621	3.283706
H	-0.396112	-1.293785	2.350069
H	-0.712834	-0.207814	3.406066
O	-0.026333	3.852703	-3.178304
H	-0.662919	3.117943	-3.304453
H	0.844546	3.428985	-3.037612
O	-0.450494	5.295488	-0.935682
H	-0.371435	4.838573	-1.814343
H	-0.514183	6.244766	-1.117524
O	3.294021	-1.028281	-2.162592
H	3.861454	-1.805337	-1.921569
H	2.970719	-0.689170	-1.292108
O	-4.190728	-3.593296	0.801534
H	-3.843804	-2.921276	1.426083
H	-4.800408	-3.091966	0.218911
O	5.515792	1.107163	0.254525
H	5.281206	1.210413	-0.691986
H	4.784361	1.516893	0.760446
O	-2.344221	-4.521122	-0.910770
H	-2.981049	-4.278741	-0.184638
H	-2.556326	-5.427346	-1.179445
O	-5.765178	0.563166	0.012327
H	-5.498675	0.640729	0.953042
H	-5.108877	1.102804	-0.480404
O	4.698740	1.234825	-2.432460
H	4.323553	0.323338	-2.531080
H	5.321840	1.376952	-3.160467
O	-4.798210	0.813902	2.650023
H	-4.158387	1.568943	2.767802
H	-5.446990	0.884385	3.366003
O	2.396765	-0.195958	0.282892
H	2.599957	0.692828	0.658657
H	2.811902	-0.850703	0.897100

O	-5.612755	-1.938310	-0.964232
H	-5.694168	-1.018091	-0.589271
H	-6.490521	-2.181778	-1.293604
O	3.379594	-2.168300	1.893549
H	4.339845	-2.044444	1.721232
H	3.113448	-2.992247	1.426980
O	-2.399184	-0.527917	-0.253876
H	-2.817153	-0.847254	0.582530
H	-2.637774	-1.177426	-0.959757
O	-3.189684	-2.245521	-2.237975
H	-2.888133	-3.137850	-1.957216
H	-4.143625	-2.190325	-2.006942
O	1.997559	-1.202183	4.124936
H	1.048149	-1.353125	3.929396
H	2.497390	-1.605275	3.383298
O	-0.052059	1.967351	0.634201
H	0.024011	1.339256	-0.123184
H	0.656546	2.639692	0.488375
O	-1.608261	-0.942556	-4.130581
H	-0.731989	-1.259586	-3.832314
H	-2.247508	-1.424870	-3.565021

Table S28. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{45}$ cluster with six internal water molecules, 45A. configuration

O	2.516855	1.749329	-4.452726
H	1.547204	1.830729	-4.560798
H	2.704381	0.795785	-4.349551
O	-1.571845	4.022540	1.953153
H	-1.453527	3.611583	2.839546
H	-0.794610	4.606861	1.798738
O	0.682159	0.034694	-2.353356
H	0.408831	0.816569	-2.889868
H	1.582041	-0.237968	-2.655024
O	-0.443670	-0.879750	-0.092876
H	0.061742	-0.453247	-0.825514
H	-1.376044	-0.572260	-0.181688
O	4.940536	2.300157	1.801161
H	4.794401	1.346887	1.998741
H	4.095120	2.747147	2.022661
O	-2.414783	-5.188563	-1.560710
H	-2.272483	-5.372281	-0.612226
H	-1.530417	-5.155928	-1.971680
O	0.044251	-4.181496	-2.751237
H	1.006871	-4.091601	-2.929003
H	-0.367512	-3.361002	-3.107432
O	2.989799	-0.623327	4.536855
H	2.424075	-1.409298	4.398728
H	2.392547	0.152853	4.497239
O	-6.000416	-1.117191	0.771288
H	-5.927819	-1.111395	-0.221508
H	-6.869228	-1.484441	0.990898
O	4.385596	-0.402177	2.185554
H	3.972911	-0.523263	3.076353

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H      3.644922    -0.471390     1.539354
O     -2.039641    -4.703005     1.305781
H     -1.300307    -4.253019     0.826543
H     -2.767811    -4.044821     1.307846
O      2.788712    -3.580076    -3.106880
H      3.358096    -3.711529    -2.302082
H      3.211050    -4.088419    -3.816241
O     -0.234342     1.968955    -4.062171
H     -0.995420     1.466236    -4.425114
H     -0.611365     2.696609    -3.510291
O     -4.096172     3.649490     0.724741
H     -4.331756     2.754341     1.050382
H     -3.265201     3.894995     1.179823
O     -1.043304    -4.067671     3.787941
H     -1.399830    -4.460479     2.952091
H     -1.231565    -4.697936     4.499313
O      5.249465     2.417787    -0.836444
H      5.174695     2.434583     0.160996
H      6.059765     2.893996    -1.070975
O     -4.538759     1.045204     1.647669
H     -5.258992     0.389124     1.540257
H     -4.163005     0.947157     2.561156
O      2.651235    -0.721899     0.089408
H      2.119610     0.115089     0.103706
H      3.369804    -0.563559    -0.564964
O      2.345393     3.220459     2.176277
H      2.040516     2.695401     1.392075
H      1.918464     4.095221     2.056504
O     -3.947263     3.729533    -1.958836
H     -4.015371     3.721983    -0.965113
H     -4.630529     4.338227    -2.276804
O     -1.075246     2.276279    -0.059124
H     -1.770510     1.576853    -0.126846
H     -1.291034     2.842166     0.722714
O     -2.870243     0.281863    -0.347327
H     -3.323965     0.505861    -1.195719
H     -3.500396     0.466661     0.392072
O      2.352639    -3.276563     1.032398
H      2.444487    -2.341147     0.737692
H      1.489620    -3.543645     0.630958
O      0.259431    -0.557064     2.471142
H      0.120885    -0.619020     1.494708
H      0.767304    -1.353785     2.755436
O      4.249867    -3.925804    -0.845597
H      4.927848    -3.280322    -0.565484
H      3.578460    -3.875161    -0.128816
O     -2.113609    -1.519385     3.405450
H     -1.279367    -1.112364     3.067186
H     -1.843544    -2.394966     3.756769
O     -1.191579     3.797756    -2.280171
H     -1.163100     3.226760    -1.470926
H     -2.144190     4.009543    -2.372863
O      5.878407    -1.941800     0.450976
H      5.475438    -1.505335     1.238316
H      6.800135    -2.134271     0.678370
O     -0.073043    -3.532651    -0.112645
H     -0.008710    -3.822834    -1.055180
H     -0.265779    -2.561631    -0.150411
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O	-3.401527	0.820146	4.096467
H	-2.670455	1.464153	4.204749
H	-2.973594	-0.060559	4.052928
O	-3.079751	-2.503837	-1.442653
H	-3.076037	-2.278518	-0.484033
H	-2.946021	-3.480074	-1.494393
O	2.784128	2.898719	-1.981189
H	3.713243	2.836453	-1.665646
H	2.747671	2.483836	-2.878400
O	0.767831	5.348061	1.296197
H	0.905268	5.267801	0.312400
H	0.887485	6.284197	1.514865
O	-3.572592	-2.391565	1.261478
H	-3.103882	-1.942717	2.003669
H	-4.484022	-2.027882	1.226130
O	-1.270158	2.669933	4.351613
H	-0.366696	2.259755	4.326602
H	-1.314139	3.194489	5.165342
O	-5.500190	-1.207915	-1.869527
H	-5.213382	-0.339259	-2.216260
H	-4.679844	-1.749385	-1.849492
O	-4.076585	1.063863	-2.669116
H	-3.503713	0.867353	-3.443000
H	-4.083490	2.039683	-2.538070
O	-1.202770	-1.748205	-3.237662
H	-0.491669	-1.164971	-2.879631
H	-1.853540	-1.889426	-2.505636
O	1.115149	5.061652	-1.357262
H	1.761285	4.363406	-1.599371
H	0.267359	4.782726	-1.762592
O	1.447627	-2.775036	3.547594
H	0.657788	-3.335889	3.707314
H	1.878580	-3.122438	2.731084
O	3.052908	-0.815056	-3.408733
H	2.944289	-1.792816	-3.426424
H	3.817662	-0.643679	-2.816561
O	1.533704	1.701986	0.111918
H	0.552846	1.804622	0.034284
H	1.913673	2.073598	-0.722684
O	-2.334876	0.252099	-4.672337
H	-1.977366	-0.586394	-4.283646
H	-2.663919	0.041544	-5.558993
O	4.898965	-0.231837	-1.462473
H	5.129727	0.707668	-1.277037
H	5.476765	-0.790232	-0.898777
O	1.152001	1.498791	3.957369
H	0.822500	0.843590	3.295583
H	1.633420	2.179090	3.429669

Table S29. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{45}$ cluster with six internal water molecules, 45B configuration.

O	-2.555787	-0.997288	-0.452175
H	-3.352000	-0.437441	-0.604415

H	-1.789291	-0.451436	-0.751704
O	-1.224358	-1.551800	3.602685
H	-0.472630	-2.059603	3.984257
H	-1.708584	-2.150739	2.984222
O	0.300088	5.724671	-1.095885
H	0.326887	5.130527	-1.896456
H	0.739595	6.551976	-1.341860
O	-5.556725	2.435995	0.319248
H	-4.845525	3.043355	-0.001719
H	-6.395090	2.919118	0.275708
O	-3.849801	0.810031	-3.864820
H	-3.419742	-0.061507	-4.100660
H	-4.456120	1.030029	-4.587598
O	1.055442	-2.885569	4.346742
H	1.782949	-2.198556	4.310978
H	1.150648	-3.363410	5.183888
O	2.431115	-0.095270	-4.290533
H	3.046469	-0.617760	-3.711702
H	2.806735	-0.095238	-5.183582
O	-3.255864	-3.019903	-2.122086
H	-2.840265	-2.373675	-1.501825
H	-2.780638	-3.871847	-2.006731
O	-1.650562	-5.245777	-1.720116
H	-1.514030	-5.322975	-0.735001
H	-1.846788	-6.131502	-2.058684
O	3.611880	-4.268790	0.829480
H	3.451427	-4.182530	-0.152035
H	4.157979	-5.059269	0.953247
O	5.413849	2.489433	0.791054
H	4.639029	2.739574	1.367987
H	6.129920	3.096898	1.030796
O	0.285905	-2.243124	0.110800
H	0.227171	-2.727867	-0.749623
H	0.533584	-2.916683	0.790523
O	-4.485250	0.647947	2.190121
H	-5.067160	1.261511	1.694812
H	-4.762113	-0.266641	1.953527
O	-0.609445	0.549390	-1.508630
H	-1.102506	1.276588	-1.962950
H	0.112968	0.993671	-0.999603
O	-1.963460	2.526731	-2.838333
H	-2.609045	2.006193	-3.367311
H	-2.493767	2.978200	-2.138634
O	3.861742	-1.368163	-2.413138
H	3.396474	-1.044233	-1.602118
H	4.791788	-1.057124	-2.323926
O	1.587256	1.257851	3.173074
H	0.892419	1.639740	3.754978
H	1.087295	0.864520	2.422788
O	-1.169300	3.865372	2.362461
H	-0.942748	3.578857	3.273216
H	-1.605840	3.072542	1.965334
O	-2.057856	5.687384	0.417930
H	-1.753704	5.277529	1.252005
H	-1.254745	5.809194	-0.131163
O	-5.692409	-2.264396	-0.993846
H	-4.933214	-2.726061	-1.411314
H	-5.559950	-1.320856	-1.231197

O	-2.218936	1.696476	1.093447
H	-1.467873	1.053111	1.113514
H	-2.991767	1.216654	1.474223
O	0.375946	4.028464	-3.165966
H	-0.417728	3.453018	-3.154766
H	1.158963	3.442559	-3.099714
O	2.922961	-1.024890	4.071323
H	2.467432	-0.189411	3.824710
H	3.452483	-1.282268	3.282588
O	-1.350816	-5.180722	0.931936
H	-1.850202	-4.370794	1.183669
H	-0.441143	-5.015081	1.253807
O	1.159691	4.100059	0.950276
H	0.341562	4.024637	1.499500
H	0.963068	4.760999	0.248733
O	5.142050	2.333628	-1.996412
H	5.161955	2.476377	-1.025469
H	5.584610	1.469139	-2.124755
O	3.365754	3.212188	2.347877
H	2.826955	2.460710	2.682174
H	2.714633	3.737698	1.838312
O	-2.551991	-2.791659	1.605394
H	-3.518220	-2.689094	1.755382
H	-2.370107	-2.141485	0.886758
O	-5.179705	-1.987786	1.614169
H	-5.440756	-2.157729	0.666086
H	-5.893624	-2.333646	2.170540
O	1.522193	1.757326	-0.388251
H	1.380810	2.583751	0.136334
H	1.926668	2.022001	-1.251233
O	1.075725	-4.158706	1.894583
H	1.104308	-3.795831	2.808654
H	2.007512	-4.293889	1.606536
O	-2.636702	-1.508465	-4.358344
H	-2.898485	-2.132375	-3.643774
H	-1.675259	-1.362226	-4.223196
O	6.347543	-0.144687	0.755201
H	5.688969	-0.763539	1.140959
H	5.991608	0.758692	0.900722
O	-4.814600	0.328958	-1.313236
H	-4.570527	0.620051	-2.220688
H	-5.199758	1.094522	-0.834942
O	2.539331	-0.721180	-0.135284
H	1.733514	-1.291786	-0.087567
H	2.228299	0.212794	-0.069964
O	-0.592487	2.336583	4.578966
H	-1.387155	1.738691	4.547700
H	-0.487644	2.609393	5.502599
O	-2.683488	0.638890	4.417783
H	-2.238203	-0.210205	4.206306
H	-3.359632	0.763864	3.722693
O	-3.254632	3.480364	-0.637114
H	-2.783578	2.804899	-0.091050
H	-2.899972	4.349766	-0.322156
O	-0.005462	-1.162317	-3.546083
H	0.811836	-0.838357	-3.984789
H	-0.149829	-0.546869	-2.786590
O	2.562891	2.288119	-2.845659

H	2.471652	1.487277	-3.408053
H	3.525158	2.350331	-2.614133
O	3.121516	-3.967554	-1.784208
H	2.160076	-3.902779	-1.970271
H	3.496416	-3.110761	-2.084442
O	-0.222419	-0.025039	1.573712
H	-0.575963	-0.507073	2.363250
H	-0.112220	-0.733947	0.902452
O	0.406444	-3.525190	-2.264297
H	0.197113	-2.772685	-2.867731
H	-0.317710	-4.186834	-2.303751
O	4.247036	-1.698750	1.722001
H	3.606627	-1.295298	1.085893
H	4.201237	-2.657743	1.516552
O	6.308907	-0.230623	-1.911798
H	6.416086	-0.281766	-0.921345
H	7.154269	-0.486234	-2.309123

Table S30. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{45}$ cluster with five internal water molecules, 45C configuration.

O	-2.411726	-1.988789	-4.597600
H	-1.433838	-2.126503	-4.553894
H	-2.740440	-2.495149	-5.355073
O	1.465723	-3.885894	1.949286
H	1.245490	-3.224794	1.247079
H	0.774361	-4.574680	1.848893
O	-0.490699	0.074769	-2.381182
H	0.140591	0.725105	-2.783960
H	-0.343983	0.201699	-1.416355
O	0.483793	0.901818	-0.004989
H	0.135675	0.615482	0.874554
H	1.429081	0.631866	-0.048211
O	-4.943613	-2.279133	1.769305
H	-4.831054	-1.328444	1.998539
H	-4.073251	-2.693529	1.956212
O	2.294118	5.176621	-1.779613
H	1.450551	5.055730	-2.263047
H	2.833420	5.770684	-2.323629
O	-0.138665	4.055125	-2.658527
H	-1.080220	3.911175	-2.912418
H	-0.111560	3.856758	-1.690977
O	-2.970290	0.748906	4.646260
H	-2.476644	1.566945	4.411316
H	-3.409297	0.921677	5.492674
O	5.973420	1.090019	0.834725
H	5.927212	1.067168	-0.160318
H	6.847026	1.435824	1.070208
O	-4.436404	0.411664	2.269106
H	-3.676399	0.516978	1.649769
H	-4.066927	0.538700	3.168774
O	2.276660	4.846592	1.069262
H	2.436194	5.289371	0.213042
H	2.950001	4.132324	1.139923

O	-2.806518	3.368374	-3.080504
H	-2.918035	2.429790	-3.329565
H	-3.401690	3.528667	-2.319839
O	0.191047	-2.065605	-3.873354
H	0.569512	-2.841624	-3.397680
H	-0.033984	-1.409345	-3.169655
O	4.072779	-3.682173	0.871983
H	4.312347	-2.790514	1.200372
H	3.215074	-3.903734	1.291192
O	0.921853	3.904068	3.493694
H	1.245191	4.421743	2.733984
H	1.466560	3.088355	3.510598
O	-5.224277	-2.401036	-0.867865
H	-5.170154	-2.398583	0.131332
H	-6.065110	-2.817223	-1.108685
O	4.547463	-1.059061	1.787422
H	5.246319	-0.386231	1.638836
H	4.196511	-0.936843	2.698494
O	-2.717206	0.865273	0.211216
H	-3.435137	0.773241	-0.457734
H	-2.549160	1.828021	0.361981
O	-2.308653	-3.079792	2.081572
H	-2.000916	-2.537247	1.314369
H	-1.879020	-3.956321	1.965065
O	4.006693	-3.750572	-1.824692
H	4.049509	-3.744694	-0.830406
H	4.720089	-4.332316	-2.126391
O	1.038475	-2.221625	-0.119644
H	0.135085	-1.819434	-0.104441
H	1.702431	-1.493097	-0.180179
O	2.908938	-0.260806	-0.251423
H	3.368441	-0.495500	-1.095289
H	3.502127	-0.503479	0.498345
O	-2.381190	3.477344	0.871744
H	-3.049886	3.928327	0.310961
H	-1.482211	3.686915	0.519964
O	-0.360372	0.461122	2.474742
H	-0.696108	-0.316096	2.984667
H	-0.893939	1.243512	2.754975
O	-4.436674	4.020079	-0.819358
H	-5.030467	3.358739	-0.377415
H	-4.948236	4.836322	-0.920785
O	2.083898	1.392553	3.220360
H	1.240509	0.949192	2.962365
H	2.587904	0.727216	3.739635
O	1.255380	-3.943321	-2.178528
H	1.210295	-3.314467	-1.414345
H	2.214159	-4.121757	-2.271262
O	-5.835612	2.007102	0.333586
H	-5.653722	1.340202	-0.360619
H	-5.458550	1.625294	1.152321
O	0.135037	3.538434	-0.023400
H	0.874680	4.006722	0.427199
H	0.340526	2.568175	0.006534
O	3.335595	-0.809833	4.268233
H	2.579096	-1.456680	4.348638
H	3.854547	-0.875022	5.083408
O	3.162673	2.518720	-1.462979

H	3.147442	2.322360	-0.497067
H	3.002808	3.483243	-1.551562
O	-2.776661	-2.907742	-2.002558
H	-2.771468	-2.607645	-2.938905
H	-3.706942	-2.863795	-1.685578
O	-0.853246	-5.329454	1.352903
H	-0.968056	-5.291312	0.364463
H	-1.083970	-6.229504	1.626370
O	3.591224	2.463562	1.237693
H	3.062097	1.968451	1.908507
H	4.489434	2.065230	1.227124
O	1.281627	-2.513835	4.332555
H	1.309774	-3.031506	3.493860
H	0.391450	-2.110595	4.370199
O	5.564696	1.157672	-1.819144
H	5.245502	0.294868	-2.155154
H	4.768928	1.733312	-1.832361
O	4.079153	-1.075016	-2.567587
H	3.472974	-0.897313	-3.330309
H	4.101405	-2.047383	-2.420564
O	1.321492	1.835182	-3.348968
H	0.795446	2.668974	-3.291537
H	1.985504	1.925983	-2.625014
O	-1.131941	-5.085444	-1.313100
H	-1.743137	-4.362238	-1.571451
H	-0.261640	-4.848248	-1.695869
O	-1.576078	2.742498	3.365896
H	-0.742856	3.265807	3.458018
H	-2.041134	3.111553	2.582762
O	-2.913450	0.543053	-3.481891
H	-2.929390	-0.194389	-4.124770
H	-2.068592	0.393275	-2.987849
O	-1.535488	-1.528997	-0.019639
H	-1.971926	-1.894759	-0.827223
H	-1.864813	-0.607997	0.106148
O	2.358633	-0.463575	-4.600523
H	1.605775	-1.083638	-4.481823
H	2.003437	0.416766	-4.365387
O	-4.764139	0.242653	-1.516907
H	-4.963281	-0.707504	-1.358401
H	-4.214155	0.297490	-2.335117
O	-1.351144	-1.491581	4.065425
H	-2.026085	-0.892403	4.445599
H	-1.805687	-2.121058	3.454889

Table S31. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{45}$ cluster with four internal water molecules, 45D configuration.

O	-2.279244	-3.982130	2.654819
H	-1.922788	-4.664881	3.242552
H	-2.785823	-3.340016	3.226201
O	-0.538577	-2.410212	1.225801
H	0.014021	-1.846029	1.820693

H	-1.097885	-2.975937	1.807689
O	-1.039545	5.039798	-2.506172
H	-0.711464	4.339369	-3.110468
H	-1.691746	4.623663	-1.910398
O	-5.385825	1.193922	-1.351745
H	-4.400974	1.216569	-1.357759
H	-5.614370	0.371739	-1.833549
O	4.483022	1.429497	3.018376
H	4.440171	1.711438	2.078524
H	3.545518	1.386597	3.302677
O	-2.036115	-1.456324	-0.818019
H	-1.703181	-1.918981	-1.622301
H	-1.482097	-1.762286	-0.058107
O	-1.530869	-5.218448	-1.511840
H	-2.264446	-5.133319	-0.838885
H	-1.586425	-6.114237	-1.876485
O	3.345923	-2.267204	2.139715
H	3.217934	-1.616401	1.407872
H	4.190017	-1.996891	2.561790
O	-2.629733	1.156755	-1.416215
H	-2.339914	0.284488	-1.062015
H	-2.348284	1.150985	-2.361104
O	-3.479567	-4.858159	0.274066
H	-3.996474	-4.085940	-0.042995
H	-3.106003	-4.588668	1.140215
O	-1.559982	0.871615	-3.922669
H	-1.178109	1.712293	-4.251229
H	-0.806139	0.427003	-3.462110
O	2.746078	-0.464632	0.165520
H	1.782132	-0.303846	0.276809
H	3.191317	0.414128	0.236147
O	0.022266	3.158226	-4.303540
H	0.886925	2.800500	-3.989329
H	0.186621	3.554864	-5.172334
O	-5.584362	-1.212842	-2.782797
H	-4.787324	-1.216792	-3.378407
H	-6.341366	-1.485486	-3.321736
O	-3.669563	2.698520	1.816944
H	-4.603591	2.404607	1.751801
H	-3.137636	1.868961	1.756245
O	1.012257	-1.186715	3.092755
H	1.843295	-1.701257	2.984871
H	1.284810	-0.238724	3.024441
O	-0.614387	4.876268	1.097733
H	-0.058747	5.488119	0.570040
H	-1.273227	4.499082	0.464420
O	6.576749	-1.330446	0.245511
H	6.270750	-1.214717	1.170425
H	6.131095	-2.128009	-0.109848
O	1.704739	1.434371	3.282123
H	1.526204	1.957537	2.464167
H	1.057932	1.762316	3.944971
O	-4.699649	-0.972231	1.726731
H	-4.828697	-1.531539	0.923933
H	-5.309193	-0.205244	1.645964
O	-1.439994	-2.942493	-3.063387
H	-0.492053	-2.854832	-3.286487
H	-1.538660	-3.830398	-2.647995

O	0.103340	0.354352	0.295809
H	-0.771809	0.196348	0.719466
H	0.333357	1.291918	0.505492
O	-6.039732	1.381005	1.221871
H	-5.925618	1.335596	0.232219
H	-6.966975	1.594819	1.401445
O	-2.270734	0.318440	1.664093
H	-3.063375	-0.255134	1.540289
H	-1.941677	0.103708	2.570061
O	-3.334440	-1.263161	-4.258516
H	-2.814715	-0.433295	-4.270493
H	-2.716570	-1.940818	-3.913027
O	-4.543410	-2.441876	-0.544529
H	-3.639252	-2.068182	-0.696440
H	-5.074129	-2.149149	-1.317768
O	3.353032	-4.520772	0.546690
H	3.341378	-3.807635	1.224547
H	2.466245	-4.489892	0.129000
O	1.279924	-2.635427	-2.745506
H	2.229773	-2.374492	-2.756166
H	1.163969	-3.140156	-1.902799
O	-0.475802	2.185114	4.853299
H	-0.988330	2.883139	4.361404
H	-0.401825	2.489928	5.769920
O	3.709847	-1.575897	-2.182923
H	3.354750	-1.181580	-1.351546
H	4.350124	-2.263831	-1.892698
O	6.323910	0.942540	-1.147629
H	6.454963	0.071850	-0.680871
H	7.173662	1.406147	-1.115083
O	2.616633	3.707272	-1.001227
H	2.175473	4.581692	-1.087281
H	2.363641	3.157336	-1.782653
O	0.417468	-0.076512	-2.352664
H	0.172460	0.046662	-1.402439
H	0.710320	-1.014403	-2.454111
O	-1.372941	-0.340497	4.183939
H	-1.120331	0.529651	4.568906
H	-0.532654	-0.815171	4.012380
O	5.279679	-3.485010	-0.980970
H	4.585194	-3.975398	-0.458854
H	5.822868	-4.146030	-1.434714
O	0.781146	-4.072269	-0.489193
H	0.045376	-4.647139	-0.796818
H	0.368287	-3.459226	0.166327
O	1.069895	2.763760	1.015115
H	1.678554	3.071115	0.299317
H	0.436515	3.510423	1.151545
O	2.127032	1.956871	-3.023618
H	3.035959	1.611621	-3.213947
H	1.603652	1.176590	-2.719993
O	-3.571212	-2.071249	3.998435
H	-4.094763	-1.660009	3.276417
H	-2.868989	-1.426238	4.221696
O	-1.872540	4.033692	3.475359
H	-2.631535	3.622107	3.009563
H	-1.352856	4.470478	2.771160
O	5.657456	-0.967966	2.868555

H	5.261179	-0.063496	3.006245
H	6.283251	-1.121331	3.591509
O	0.958727	5.926871	-0.947986
H	0.251368	5.692689	-1.606603
H	1.232925	6.836770	-1.135781
O	4.563386	0.760991	-3.356069
H	5.239777	1.008289	-2.694589
H	4.303737	-0.144891	-3.074940
O	-2.506839	3.693531	-0.459232
H	-3.129184	3.556463	0.290388
H	-2.350801	2.770619	-0.768886
O	4.211970	1.873375	0.297165
H	5.019715	1.648651	-0.222872
H	3.809493	2.658539	-0.128674

Table S32. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{52}$ cluster with seven internal water molecules, 52A configuration.

O	1.159367	2.224429	0.336147
H	1.258603	2.752987	1.163540
H	1.907728	1.575484	0.300835
O	1.756771	3.970351	-1.663181
H	1.551555	3.348648	-0.920908
H	2.708907	4.186126	-1.551197
O	4.517378	1.059427	2.531898
H	3.755940	0.953482	3.151168
H	5.046669	0.232160	2.571823
O	-2.439015	0.550290	-4.037555
H	-2.193773	1.354793	-4.541397
H	-1.705925	0.455591	-3.381026
O	2.370804	-1.928379	0.214457
H	2.650619	-2.295409	1.087772
H	2.886095	-2.394563	-0.489878
O	-0.033910	-0.723567	-0.050309
H	-0.786146	-1.355481	0.008643
H	0.787040	-1.269060	-0.001035
O	3.090310	-1.969062	-4.107193
H	3.210200	-0.979226	-4.152498
H	3.478468	-2.331076	-4.917583
O	-4.045858	-3.131930	1.864885
H	-4.866701	-2.670339	1.575663
H	-3.805467	-2.760099	2.743713
O	0.721219	3.052812	4.830629
H	-0.204495	2.784561	4.600496
H	0.680334	3.579745	5.642252
O	3.313926	-2.837811	2.613246
H	4.202699	-2.414643	2.604667
H	2.817709	-2.472298	3.392208
O	-0.194739	-3.962813	1.285824
H	-0.171658	-3.730243	0.329232
H	0.647806	-4.436001	1.465393
O	-0.552579	-2.143399	3.292404
H	-1.466582	-2.194105	3.653051
H	-0.483601	-2.774437	2.536237

O	-2.189563	3.892532	-2.302022
H	-3.163348	3.912082	-2.168461
H	-1.869506	3.215788	-1.655381
O	-0.333126	5.743532	-1.289282
H	-1.085331	5.232452	-1.657226
H	0.463725	5.202562	-1.488283
O	-5.026796	3.459862	0.985888
H	-4.132933	3.692410	1.320537
H	-5.195083	2.543482	1.293015
O	-5.067490	0.760519	1.751663
H	-4.336367	0.570281	1.112489
H	-5.693637	0.024132	1.589396
O	-1.349890	3.012507	-4.713414
H	-1.711699	3.438379	-3.893679
H	-1.500407	3.627584	-5.446337
O	-6.160212	-1.657834	0.873521
H	-6.000094	-1.651647	-0.110569
H	-7.057774	-1.998578	1.003235
O	2.204383	0.850714	3.964021
H	1.886507	1.612530	4.491026
H	1.497121	0.725995	3.283828
O	-2.565486	-5.395195	1.139829
H	-3.244687	-4.749393	1.421349
H	-1.706209	-4.948230	1.311517
O	-3.212984	0.283993	-0.151585
H	-3.722957	0.428220	-0.987149
H	-2.915239	-0.659338	-0.144492
O	5.665954	-1.453238	2.234534
H	5.834554	-1.658379	1.271336
H	6.459261	-1.733661	2.715030
O	-2.150247	-2.181266	-4.614960
H	-2.314067	-1.214750	-4.607116
H	-1.195710	-2.281884	-4.412390
O	-0.198651	0.216426	-2.552186
H	0.374449	0.977005	-2.810429
H	-0.113925	0.046358	-1.583149
O	-2.363866	3.835185	1.715616
H	-1.816128	4.650373	1.709182
H	-2.005146	3.286305	0.972909
O	1.133521	2.282186	-3.709192
H	0.358344	2.626860	-4.204654
H	1.386691	2.973134	-3.050705
O	0.024426	0.356871	2.445008
H	-0.240699	-0.547362	2.753121
H	0.060530	0.262234	1.467195
O	3.277368	0.601506	0.165759
H	3.767584	0.757073	1.011066
H	2.993015	-0.347347	0.178222
O	-1.567493	2.142353	3.717599
H	-1.049682	1.506874	3.164692
H	-1.891099	2.824933	3.081056
O	1.852269	-1.842678	4.654738
H	0.944778	-1.994193	4.312758
H	1.993933	-0.873632	4.605867
O	6.090074	-2.081990	-0.323490
H	5.340611	-2.474563	-0.818521
H	6.426331	-1.331440	-0.864667
O	-0.423483	5.789694	1.381554

H	-0.395266	5.837238	0.384583
H	-0.455442	6.702084	1.705644
O	-3.803557	0.541617	4.202146
H	-3.015033	1.121658	4.109345
H	-4.303641	0.645929	3.360092
O	2.413527	-5.321033	-1.127679
H	2.484633	-5.361232	-0.152196
H	1.518495	-4.949264	-1.297658
O	-3.137361	-2.027742	4.221199
H	-3.383903	-1.058904	4.278734
H	-3.371279	-2.433444	5.069179
O	4.435983	4.126478	-0.999450
H	4.394048	4.008530	-0.011990
H	5.034519	4.868374	-1.170950
O	7.036818	0.065314	-1.785047
H	6.278445	0.692536	-1.850317
H	7.736780	0.537904	-1.311898
O	3.874013	-3.120573	-1.701855
H	3.440925	-4.008326	-1.627533
H	3.642077	-2.746376	-2.581339
O	-2.295516	-2.243115	-0.037730
H	-2.874610	-2.616065	0.670375
H	-2.605128	-2.614264	-0.899624
O	0.395752	-2.238817	-3.501501
H	0.273908	-1.317270	-3.163423
H	1.324237	-2.274967	-3.820682
O	-0.012393	-4.026826	-1.462282
H	0.087216	-3.360883	-2.184394
H	-0.808483	-4.566262	-1.658086
O	-4.881326	3.513639	-1.688683
H	-4.976652	3.517616	-0.695102
H	-5.593794	4.068053	-2.040210
O	-5.649705	-1.642777	-1.757480
H	-5.400733	-0.744892	-2.059274
H	-4.891909	-2.223221	-1.988207
O	4.735466	1.529482	-1.926126
H	4.206678	1.142203	-1.185856
H	4.748826	2.493541	-1.737288
O	1.481869	4.020275	2.358952
H	1.233056	3.784665	3.280514
H	0.862915	4.727223	2.064646
O	-4.598876	0.861378	-2.418902
H	-4.803804	1.809470	-2.254452
H	-3.875761	0.828859	-3.091554
O	-2.371435	-5.528649	-1.533853
H	-2.525412	-5.564309	-0.550700
H	-2.405837	-6.438886	-1.862522
O	-1.433204	2.260243	-0.284260
H	-1.954794	1.422717	-0.222389
H	-0.485711	2.064770	-0.097455
O	3.385197	0.692642	-4.191802
H	3.901946	1.014089	-3.418385
H	2.553234	1.210110	-4.167511
O	2.299160	-5.153692	1.682975
H	2.814653	-4.431846	2.116774
H	2.372498	-5.936399	2.249011
O	4.181773	3.732206	1.646901
H	4.424840	2.838319	1.960334

H	3.256376	3.884695	1.935323
O	-3.368754	-3.127298	-2.382075
H	-3.188603	-4.087213	-2.293564
H	-2.924758	-2.816017	-3.213152

Table S33. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{52}$ cluster with seven internal water molecules, 52B configuration.

O	5.713736	-2.272302	-0.833071
H	4.998720	-2.779934	-1.274076
H	5.637170	-1.353416	-1.161267
O	2.015302	-2.424788	0.066550
H	1.100895	-2.055670	0.086320
H	2.223382	-2.858475	0.929731
O	-4.321398	1.550969	-2.192388
H	-3.838335	1.210134	-1.397427
H	-5.039824	0.897851	-2.330511
O	0.417251	5.448879	2.034915
H	-0.454226	5.020770	2.174714
H	0.412740	5.742130	1.101010
O	1.991945	2.023063	-3.366906
H	2.657545	1.429150	-3.784249
H	2.469337	2.568835	-2.695717
O	3.204051	-0.021067	0.081680
H	2.809312	-0.927675	0.027613
H	3.850066	0.075894	-0.659454
O	0.023485	6.293077	-0.633155
H	0.625804	6.197681	-1.415281
H	-0.363837	7.179904	-0.681274
O	1.715374	2.177892	0.498523
H	1.939369	2.538360	1.390874
H	2.201559	1.325765	0.381548
O	-2.223395	-1.210274	-4.716695
H	-1.356787	-1.550159	-4.372971
H	-2.294732	-1.496337	-5.639679
O	-3.205912	-5.239931	0.468838
H	-3.195825	-5.155023	-0.523711
H	-3.361340	-6.174669	0.669676
O	2.738255	-2.124966	-4.235144
H	3.068302	-2.640789	-3.464216
H	1.776350	-2.020975	-4.060749
O	2.937508	3.646266	-1.429345
H	3.891301	3.512430	-1.230049
H	2.456116	3.216301	-0.679672
O	-3.595518	0.376788	4.267491
H	-2.739310	0.852874	4.301536
H	-4.046746	0.707207	3.455998
O	5.164132	0.351473	-1.749078
H	4.815634	0.408265	-2.667139
H	5.399590	1.258235	-1.451824
O	-4.298188	-2.952032	1.506195
H	-4.114207	-3.896648	1.313747
H	-3.976995	-2.767481	2.418717
O	-2.658746	-2.008853	-0.466142

H	-3.223676	-2.388386	0.248364
H	-3.106107	-2.166522	-1.332447
O	-0.942057	2.280833	0.317545
H	0.036607	2.140714	0.381323
H	-1.071490	2.884733	-0.455378
O	-3.943048	-2.335957	-2.851097
H	-4.739723	-1.782835	-2.683001
H	-3.427805	-1.904103	-3.568733
O	-2.128156	1.438505	-3.838995
H	-2.969312	1.534504	-3.331778
H	-2.210241	0.586459	-4.320293
O	1.345495	2.219856	4.995296
H	1.769209	1.346857	4.791761
H	1.603540	2.464290	5.896382
O	1.544834	-5.718618	1.049303
H	2.208731	-5.146305	1.487178
H	0.704946	-5.208106	1.105656
O	1.473482	5.566748	-2.778192
H	2.067857	4.906173	-2.358634
H	0.881946	5.067009	-3.368734
O	-2.911484	-4.861648	-2.172890
H	-1.976097	-4.558824	-2.145105
H	-3.421732	-4.091045	-2.493098
O	-1.241190	1.876317	4.008046
H	-0.421698	2.081249	4.508024
H	-1.497549	2.695148	3.520486
O	0.076672	-1.848935	-3.460384
H	-0.068729	-2.558554	-2.787824
H	0.109151	-0.994781	-2.967209
O	3.455372	-3.490383	-1.946182
H	3.151859	-4.419538	-2.008821
H	2.844488	-3.105234	-1.272537
O	1.737838	-2.805045	4.488410
H	0.805092	-2.837577	4.184850
H	1.967391	-1.850438	4.468099
O	-0.221330	-0.947223	-0.039586
H	-0.132127	-0.306814	-0.784908
H	-1.049808	-1.454663	-0.202367
O	-0.034302	-0.028326	2.475425
H	-0.573763	0.718623	2.823494
H	-0.169286	-0.128353	1.505342
O	2.228980	-0.104649	3.971287
H	1.526205	-0.076997	3.279708
H	3.089841	-0.044197	3.490870
O	-0.737052	-2.540577	3.228181
H	-0.564218	-1.599147	2.982796
H	-1.641445	-2.547077	3.614605
O	2.274303	3.576229	2.747737
H	1.952550	3.198246	3.595321
H	1.657997	4.315641	2.513160
O	-4.549804	3.955046	1.484334
H	-4.463272	4.054947	0.496443
H	-5.169300	4.638343	1.780325
O	4.493374	0.042794	2.440760
H	5.025802	-0.780169	2.468021
H	4.052395	0.002450	1.553970
O	-0.032905	0.595259	-2.252881
H	0.750931	1.112368	-2.559822

H	-0.823702	0.980781	-2.699385
O	5.440838	2.860515	-0.580154
H	5.271491	2.831360	0.401635
H	6.233321	3.403460	-0.706774
O	1.835935	-5.690533	-1.605827
H	1.806906	-5.805175	-0.615849
H	1.758372	-6.573208	-1.996858
O	-4.195863	4.115241	-1.174830
H	-4.451620	3.261116	-1.584288
H	-3.236053	4.194812	-1.364679
O	-0.702194	-4.102386	0.987115
H	-0.734787	-3.499723	1.770036
H	-1.581037	-4.538746	0.930343
O	3.910375	0.255141	-4.213205
H	3.489057	-0.651954	-4.267021
H	4.396517	0.391557	-5.039927
O	3.007756	-3.678923	2.252866
H	3.922588	-3.321252	2.205489
H	2.611654	-3.385483	3.112641
O	-3.362755	-2.260599	4.013182
H	-3.461069	-1.275399	4.155339
H	-3.751219	-2.697372	4.785646
O	5.484253	-2.482949	1.843685
H	5.595927	-2.410288	0.856930
H	6.278516	-2.925837	2.177573
O	4.897362	2.769511	2.054509
H	4.864720	1.827576	2.325257
H	4.031887	3.153872	2.306480
O	-1.430856	4.138595	-1.582313
H	-1.011040	4.947453	-1.210661
H	-0.971684	3.947472	-2.433187
O	-4.768103	1.199860	1.908884
H	-4.901154	2.170986	1.859934
H	-4.052177	1.021752	1.249715
O	-2.996105	0.638647	-0.031809
H	-2.848608	-0.327106	-0.173603
H	-2.118548	1.080795	0.083268
O	-5.988681	-0.673396	-2.037185
H	-6.052201	-0.778400	-1.048621
H	-6.887506	-0.773752	-2.384279
O	-0.329855	-3.927361	-1.736167
H	-0.436476	-3.757556	-0.771885
H	0.415260	-4.567381	-1.802237
O	-1.875757	3.872774	2.283674
H	-2.832728	4.025157	2.120507
H	-1.574010	3.282855	1.547467
O	-6.084355	-0.948016	0.638120
H	-5.527670	-1.692766	0.946635
H	-5.770550	-0.154566	1.121044
O	-0.237601	3.496746	-4.001928
H	-0.966958	2.883106	-4.232591
H	0.564022	2.930943	-3.937837

Table S34. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{52}$ cluster with six internal water molecules, 52C configuration.

O	-0.123340	-5.709735	1.320693
H	0.551704	-5.256021	1.867976
H	0.214637	-5.690348	0.400475
O	-0.970066	-4.165857	-2.810767
H	-1.926419	-4.256576	-3.015651
H	-0.547760	-3.603060	-3.513542
O	2.868254	-3.797798	-1.158520
H	2.338327	-3.258563	-0.518818
H	2.302393	-4.583768	-1.318934
O	1.844141	0.161236	-1.514890
H	2.358628	0.028091	-0.682988
H	0.888765	0.032842	-1.304605
O	-0.475443	6.145827	-1.947414
H	0.289326	6.270061	-1.345529
H	-0.324541	5.287305	-2.399301
O	-3.290379	3.596644	0.149210
H	-3.188926	4.570300	0.063350
H	-2.460205	3.214686	-0.234137
O	1.499893	6.360942	0.019342
H	2.106583	5.586873	-0.103245
H	2.055763	7.151621	0.084297
O	-2.858915	2.311200	2.520024
H	-3.708216	1.913914	2.836565
H	-3.096604	2.852427	1.729656
O	5.844387	-1.175043	-0.911164
H	6.345663	-0.340500	-0.786735
H	5.649836	-1.217287	-1.874640
O	4.142731	1.916973	3.576805
H	3.252674	2.180720	3.887217
H	4.163289	0.939594	3.596144
O	1.257470	-2.461464	0.517777
H	0.346931	-2.586631	0.146189
H	1.296537	-1.508754	0.775548
O	-4.808688	-1.723419	3.542142
H	-3.849280	-1.968630	3.573302
H	-5.252644	-2.198252	4.260165
O	-1.038737	2.463472	-0.760165
H	-1.109524	1.488515	-0.907064
H	-0.345433	2.582386	-0.062993
O	-2.410049	-4.222748	1.317478
H	-2.355008	-3.571575	2.057338
H	-1.620422	-4.816420	1.389294
O	-4.970334	1.803190	-1.007812
H	-4.808871	1.780580	-1.983293
H	-4.464690	2.566280	-0.641442
O	-1.216837	-2.660450	-0.556740
H	-1.763892	-3.192319	0.070576
H	-1.128095	-3.196491	-1.382665
O	2.520447	2.600626	-2.554920
H	2.216852	1.740281	-2.175821
H	3.444191	2.407802	-2.847218
O	1.599684	-3.998318	2.716975
H	1.494737	-3.382571	1.950251
H	2.566099	-4.021652	2.884378
O	-1.306816	-0.376422	-4.091516
H	-2.199148	-0.749502	-3.890538
H	-1.443239	0.529367	-4.446912

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O      6.610499     1.489102    -0.710420
H      6.054391     1.894393    -0.003137
H      7.494539     1.878104    -0.636921
O      3.859973    -0.862059     3.102267
H      3.749995    -0.710463     2.132005
H      4.120875    -1.805707     3.189447
O      0.824024     0.036181     1.397565
H      0.994810    -0.091151     2.364905
H     -0.164120    -0.003260     1.320221
O      3.663217    -0.174937     0.461804
H      3.971107     0.758775     0.568926
H      4.379969    -0.619644    -0.049865
O      5.089599     1.771062    -3.094269
H      5.062980     0.832111    -3.372450
H      5.643217     1.777643    -2.286678
O      5.085080    -1.001099    -3.565413
H      4.171569    -1.390309    -3.544788
H      5.560291    -1.414808    -4.301053
O     -3.736851    -4.063597    -2.894414
H     -4.081566    -4.153002    -1.963837
H     -4.302406    -4.616442    -3.453890
O      0.892501     2.675090     1.110248
H      1.035445     1.701119     1.226884
H      0.426845     2.988811     1.923390
O     -4.367312     1.377570    -3.631732
H     -4.231010     0.409264    -3.623884
H     -3.521735     1.770683    -3.930630
O      0.788300    -5.660810    -1.356387
H      0.118458    -5.234072    -1.943028
H      0.915251    -6.559932    -1.694869
O     -0.074601     3.575795    -3.015768
H      0.873480     3.333623    -3.088336
H     -0.386054     3.139189    -2.181955
O     -0.832586    -0.126542    -1.412010
H     -1.180362    -0.965046    -1.029999
H     -0.961550    -0.195535    -2.389282
O      1.396965    -0.270815     4.042703
H      2.335386    -0.521931     3.860114
H      1.402338     0.643025     4.402698
O     -2.205773    -2.198732     3.140186
H     -1.412147    -2.354031     3.718120
H     -2.010356    -1.404917     2.587447
O     -1.851783     2.275499    -4.635999
H     -1.178522     2.807448    -4.141331
H     -1.889535     2.638444    -5.533453
O     -5.197137     1.025274     3.112532
H     -5.035932     0.092117     3.363547
H     -5.751763     0.981773     2.306382
O     -3.643027    -1.301981    -3.089902
H     -3.753311    -2.275230    -3.172940
H     -3.577561    -1.123527    -2.120688
O      0.042188    -2.627898     4.567273
H      0.601380    -3.191955     3.986618
H      0.484628    -1.752906     4.548667
O     -2.463307     6.204781    -0.143380
H     -1.811458     6.201130    -0.896097
H     -3.011065     6.996859    -0.245831
O     -0.562398     5.981495     1.923537
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H	0.232808	6.094154	1.361699
H	-1.316773	6.087429	1.306852
O	-1.853812	-0.024741	1.495084
H	-2.166774	0.836483	1.867830
H	-2.442682	-0.214695	0.722860
O	-5.627867	-1.900151	0.901495
H	-5.385391	-1.942428	1.854126
H	-6.241306	-1.139223	0.817519
O	0.308708	-2.561642	-4.561306
H	-0.209225	-1.728988	-4.537466
H	1.156379	-2.349597	-4.110570
O	-6.705770	0.658599	0.734630
H	-6.244330	1.147090	0.012593
H	-7.633299	0.937587	0.717799
O	5.220786	-3.648162	0.304904
H	5.586047	-2.801840	-0.023359
H	4.433937	-3.820564	-0.258298
O	2.794073	4.006931	-0.214720
H	2.721495	3.611575	-1.118488
H	2.090251	3.542859	0.304694
O	2.602906	-1.910084	-3.125318
H	2.294314	-1.159377	-2.557841
H	2.736186	-2.661826	-2.498304
O	-4.617430	-4.217849	-0.357025
H	-3.866292	-4.315492	0.267677
H	-5.110287	-3.435166	-0.038827
O	-0.506439	3.607131	3.246135
H	-0.598718	4.514996	2.858682
H	-1.379261	3.163347	3.157207
O	4.651026	2.343457	0.938669
H	4.075377	3.038359	0.541485
H	4.490073	2.339686	1.914611
O	-3.654753	-0.539973	-0.454922
H	-4.307569	-1.092839	0.037205
H	-4.098341	0.333834	-0.588650
O	4.370746	-3.579611	2.862518
H	4.732387	-3.629846	1.936227
H	4.981968	-4.074993	3.427550
O	1.548950	2.434011	4.652290
H	0.801691	2.927407	4.239477
H	1.592072	2.725477	5.575464

Table S35. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{52}$ cluster with six internal water molecules, 52D configuration.

O	-6.224930	-2.558398	1.407542
H	-5.630167	-3.059191	0.811356
H	-6.311838	-1.665432	1.015485
O	-4.196301	-3.780292	-0.088156
H	-3.480714	-4.156360	0.474328
H	-3.993083	-4.056529	-1.008492
O	-4.925510	-2.056615	3.716899
H	-5.431578	-2.335947	2.907796
H	-5.367578	-2.458306	4.479470

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O     -5.803327     0.074716     0.533582
H     -4.940766    -0.264765     0.189655
H     -6.045602     0.803765    -0.074986
O     -3.529556    -1.112427    -0.342599
H     -2.783603    -0.791242     0.221151
H     -3.673438    -2.063851    -0.129032
O     -5.196493     0.700312     3.171236
H     -5.487724     0.545427     2.243924
H     -5.053750    -0.198014     3.533422
O     -2.220453    -2.326619     3.211705
H     -2.096543    -1.529193     2.642400
H     -3.159614    -2.299549     3.502147
O     -1.887681    -4.270707     1.303211
H     -2.001262    -3.690572     2.092846
H     -1.531583    -3.663242     0.610587
O     -1.810017    -0.203003     1.512673
H     -2.153509     0.660344     1.850026
H     -0.828996    -0.114914     1.430181
O     -3.405756    -4.202489    -2.744865
H     -2.445378    -4.403117    -2.846471
H     -3.881593    -4.833336    -3.305735
O     -5.828538     2.161604    -1.320352
H     -5.377889     1.827986    -2.139987
H     -6.581994     2.694418    -1.614506
O     -3.579871    -1.423433    -3.034085
H     -3.436049    -1.240036    -2.073324
H     -3.636769    -2.401401    -3.095747
O     -0.876682    -2.785035    -0.694163
H     -0.819895    -3.333736    -1.514681
H     -1.031569    -1.854219    -0.993284
O     -2.955636     2.084477     2.506546
H     -3.738121     1.624457     2.902200
H     -3.307906     2.550740     1.713151
O     -4.540376     1.191193    -3.494506
H     -3.711269     1.620122    -3.790214
H     -4.346275     0.234837    -3.433445
O     -3.724475     3.253803     0.120878
H     -2.982613     2.838409    -0.386207
H     -4.550296     2.963296    -0.326944
O     -0.818376    -0.264749    -1.579143
H     -0.919201    -0.325632    -2.561054
H      0.148770    -0.100139    -1.435151
O     -0.670872    -4.367616    -2.889359
H      0.020580    -4.956262    -2.510920
H     -0.231497    -3.771167    -3.551668
O      0.243488    -2.665111     4.495648
H     -0.661063    -2.588228     4.123878
H      0.591127    -1.748852     4.527396
O      0.491267    -5.708255     1.146665
H     -0.396529    -5.304406     1.270011
H      1.087994    -5.172647     1.710634
O      0.877722     0.013830     1.516199
H      1.276557    -0.776497     1.078349
H      1.059843    -0.070427     2.483172
O     -1.517979     2.249347    -1.008685
H     -1.122514     2.692894    -1.798617
H     -1.430619     1.278139    -1.181692
O     -1.355863    -0.485691    -4.247237
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H	-2.224288	-0.870574	-3.977299
H	-1.538810	0.432253	-4.544160
O	1.565043	-2.361668	0.421336
H	0.682560	-2.586214	0.033297
H	1.642230	-2.891574	1.256320
O	1.279502	-5.696557	-1.429674
H	0.974141	-5.717476	-0.480838
H	1.519660	-6.607685	-1.655896
O	1.882544	-3.833385	2.667180
H	1.331249	-3.434582	3.388732
H	2.831864	-3.693449	2.876373
O	1.460960	-0.211596	4.175367
H	1.401960	0.703151	4.529139
H	2.409248	-0.381791	3.959708
O	-2.100437	2.166929	-4.595581
H	-1.440572	2.744857	-4.143515
H	-2.237251	2.543950	-5.477744
O	-0.575011	3.411464	3.071224
H	-1.456801	2.980717	3.115444
H	-0.184643	3.070392	2.226156
O	0.501722	2.545440	0.762915
H	-0.245149	2.468760	0.117118
H	0.803718	1.621209	0.938597
O	0.452296	-2.578494	-4.578623
H	1.269629	-2.258953	-4.135443
H	-0.154419	-1.809205	-4.591685
O	1.806277	0.258641	-1.466531
H	1.949684	1.178526	-1.801857
H	2.403047	0.161222	-0.683600
O	-2.797564	5.785083	-0.013332
H	-3.268565	4.914153	0.028376
H	-3.478945	6.472315	-0.055349
O	-0.284744	3.533750	-3.074220
H	-0.357245	4.450413	-2.700720
H	0.659767	3.268675	-3.015900
O	3.173822	-3.640222	-1.297155
H	2.613803	-3.161779	-0.632074
H	2.679835	-4.473668	-1.457837
O	1.413820	2.498401	4.701225
H	0.648004	2.874413	4.196743
H	1.372028	2.873378	5.593502
O	-0.843365	5.990592	1.983940
H	-0.767118	5.126224	2.443700
H	-1.608909	5.908919	1.375935
O	2.691062	-1.707640	-3.173817
H	2.892635	-2.466082	-2.572515
H	2.341377	-0.994934	-2.584620
O	3.695751	0.125515	0.470245
H	3.916056	1.081568	0.593890
H	4.450958	-0.252753	-0.039109
O	3.930139	-0.572965	3.114350
H	3.794213	-0.412254	2.149208
H	4.268751	-1.493194	3.175093
O	-0.678600	5.924415	-1.864997
H	-1.482670	5.859715	-1.307263
H	0.029705	6.199845	-1.246146
O	4.594572	-3.238513	2.798977
H	4.943748	-3.263823	1.866596

H	5.219417	-3.739194	3.344092
O	2.320510	2.769619	-2.440494
H	3.234394	2.583431	-2.772255
H	2.436823	3.366951	-1.664161
O	2.440535	4.172009	-0.101678
H	1.698145	3.623714	0.258700
H	2.146984	5.104676	-0.006641
O	1.101071	6.554910	0.221404
H	0.455438	6.388564	0.960956
H	1.461664	7.444238	0.351350
O	4.051135	2.194665	3.664422
H	3.144948	2.384836	3.983641
H	4.138484	1.220657	3.656645
O	5.460083	-3.246148	0.244936
H	4.722373	-3.499819	-0.352014
H	5.760719	-2.371627	-0.074652
O	4.438578	2.709726	1.018598
H	3.790146	3.365870	0.670875
H	4.317265	2.659162	1.999106
O	5.926530	-0.716103	-0.925605
H	5.718855	-0.774341	-1.885555
H	6.358102	0.156348	-0.803000
O	5.120710	-0.638924	-3.571303
H	4.234013	-1.085196	-3.566746
H	5.629206	-1.008223	-4.308371
O	4.892258	2.108303	-3.082267
H	4.953421	1.172036	-3.364696
H	5.440213	2.166516	-2.272248
O	6.418312	2.012489	-0.692579
H	5.839674	2.371807	0.021750
H	7.260386	2.488690	-0.641712

Table S36. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{52}$ cluster with six internal water molecules, 52E configuration.

O	-0.349764	-5.743430	1.241809
H	0.320478	-5.293627	1.795944
H	-0.010458	-5.720549	0.322548
O	-1.184052	-4.010595	-2.790487
H	-2.148681	-4.065671	-2.970810
H	-0.751500	-3.491371	-3.519639
O	2.681547	-3.934748	-1.265053
H	2.214031	-3.402914	-0.573024
H	2.067522	-4.681128	-1.437448
O	1.834328	0.110658	-1.516644
H	2.327311	-0.026250	-0.673005
H	0.866547	0.065608	-1.328173
O	-0.240952	6.210446	-1.881809
H	0.527314	6.285927	-1.276163
H	-0.121784	5.360637	-2.358160
O	-3.122498	3.738093	0.214438
H	-3.011739	4.711478	0.145230
H	-2.295716	3.356436	-0.177444
O	1.736314	6.282021	0.090343

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H      2.304848     5.481525    -0.046925
H      2.330803     7.041875     0.177797
O     -2.742467     2.328084     2.525040
H     -3.612642     1.974894     2.837760
H     -2.954156     2.909060     1.756250
O      5.769422    -1.386976    -0.944045
H      6.319920    -0.584946    -0.815017
H      5.566997    -1.409632    -1.906667
O      4.240870     1.746136     3.572205
H      3.363378     2.038380     3.892682
H      4.223667     0.768694     3.577406
O      1.293569    -2.605685     0.597618
H      1.342574    -1.655211     0.862430
H      1.301609    -3.137570     1.433852
O     -4.924234    -1.567595     3.527654
H     -3.975836    -1.862109     3.520830
H     -5.366296    -2.027764     4.256360
O     -0.904870     2.578327    -0.724189
H     -1.037287     1.616065    -0.909225
H     -0.199590     2.620211    -0.030366
O     -2.524796    -4.076887     1.160498
H     -1.849040    -4.789773     1.272075
H     -2.093542    -3.468127     0.508274
O     -4.838452     1.980427    -0.947488
H     -4.693533     1.974038    -1.925948
H     -4.313187     2.727071    -0.574854
O     -1.167078    -2.495333    -0.534457
H     -0.265296    -2.600580    -0.138884
H     -1.151618    -3.014100    -1.377587
O      2.621009     2.526388    -2.545084
H      2.283717     1.674018    -2.176782
H      3.537198     2.301725    -2.838472
O      1.399773    -4.172830     2.790534
H      0.944714    -3.669470     3.514885
H      2.368173    -4.135542     2.948795
O     -1.353206    -0.256458    -4.139470
H     -2.254101    -0.600633    -3.927792
H     -1.459687     0.658057    -4.482036
O      6.677368     1.232692    -0.728339
H      6.156163     1.671942    -0.015196
H      7.582415     1.573141    -0.671267
O      3.839438    -1.010616     3.060991
H      3.728262    -0.827641     2.095762
H      4.038360    -1.971229     3.123711
O      0.855275    -0.084956     1.422346
H      1.013529    -0.185097     2.395034
H     -0.132908    -0.103079     1.337178
O      3.665770    -0.252791     0.443618
H      4.026299     0.660812     0.554266
H      4.350615    -0.734377    -0.078065
O      5.153280     1.600584    -3.099233
H      5.077969     0.666285    -3.383982
H      5.710836     1.574036    -2.294791
O      5.002894    -1.163667    -3.591908
H      4.074014    -1.515032    -3.573169
H      5.461053    -1.594490    -4.328528
O     -3.950738    -3.867439    -2.888887
H     -4.308977    -3.974040    -1.965002
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H	-4.498859	-4.420544	-3.465137
O	1.038065	2.559607	1.147289
H	1.123506	1.576778	1.240837
H	0.579494	2.880602	1.961704
O	-4.311655	1.603068	-3.592924
H	-4.217325	0.629753	-3.605083
H	-3.453593	1.966821	-3.893403
O	0.506542	-5.678350	-1.455709
H	-0.154706	-5.191213	-2.004426
H	0.566572	-6.571744	-1.826108
O	0.075492	3.640753	-2.993201
H	1.010479	3.355029	-3.074532
H	-0.242638	3.226128	-2.150572
O	-0.857791	0.017373	-1.465090
H	-1.144053	-0.845879	-1.078846
H	-0.987029	-0.060783	-2.441090
O	1.422568	-0.360188	4.070526
H	2.349525	-0.633756	3.862656
H	1.460843	0.551677	4.433568
O	-2.347544	-2.206941	3.140544
H	-2.118982	-1.418885	2.589879
H	-2.421268	-2.955854	2.497665
O	-1.775558	2.430615	-4.607013
H	-1.074778	2.921084	-4.107554
H	-1.815427	2.825731	-5.490664
O	-5.157885	1.192395	3.113969
H	-5.054528	0.251368	3.366896
H	-5.714210	1.179597	2.307785
O	-3.704772	-1.113209	-3.099729
H	-3.880856	-2.075328	-3.192255
H	-3.620652	-0.956385	-2.127981
O	0.003038	-2.681424	4.568224
H	-0.859423	-2.540232	4.118538
H	0.454356	-1.811578	4.532985
O	-2.220850	6.323018	-0.064869
H	-1.574614	6.301727	-0.821442
H	-2.726456	7.144949	-0.146161
O	-0.331880	5.935415	1.988947
H	0.464448	6.031786	1.425448
H	-1.083620	6.099042	1.381906
O	-1.822378	-0.052741	1.505892
H	-2.102701	0.824106	1.867615
H	-2.410439	-0.220874	0.727882
O	-5.727668	-1.707442	0.883673
H	-5.506735	-1.759244	1.841057
H	-6.299463	-0.915946	0.788758
O	0.157144	-2.516033	-4.592874
H	-0.316533	-1.657413	-4.581362
H	1.014784	-2.341358	-4.144904
O	-6.671251	0.906071	0.730419
H	-6.168009	1.381983	0.027564
H	-7.580884	1.238002	0.702778
O	5.016534	-3.843252	0.239766
H	5.410241	-3.006968	-0.081784
H	4.249884	-4.009583	-0.351117
O	2.942072	3.888430	-0.186362
H	2.855660	3.506581	-1.094883
H	2.242133	3.422120	0.335386

O	2.484456	-1.973919	-3.161448
H	2.215402	-1.222161	-2.576199
H	2.584713	-2.746049	-2.552561
O	-4.842912	-4.090446	-0.357643
H	-4.069441	-4.220799	0.235304
H	-5.289671	-3.287696	-0.021302
O	-0.350004	3.537871	3.269172
H	-0.416308	4.450086	2.886227
H	-1.234876	3.119144	3.177558
O	4.791771	2.205330	0.945723
H	4.228962	2.914017	0.555214
H	4.621937	2.188583	1.919809
O	-3.660399	-0.446907	-0.440843
H	-4.346382	-0.968914	0.039016
H	-4.046695	0.456915	-0.549127
O	4.155184	-3.753362	2.795921
H	4.494713	-3.812427	1.861508
H	4.765766	-4.268892	3.343660
O	1.677065	2.334809	4.682208
H	0.938140	2.844392	4.273926
H	1.735776	2.627438	5.604126

Table S37. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{55}$ cluster with nine internal water molecules, 55A configuration.

O	1.565473	-3.511813	-4.011234
H	0.825464	-2.863742	-4.148942
H	1.717982	-3.944755	-4.864638
O	2.586363	4.033614	-0.838069
H	1.971152	3.444833	-0.332688
H	2.094246	4.876727	-0.947892
O	0.397655	-4.971288	-1.969958
H	1.067730	-5.388719	-1.383261
H	0.882233	-4.554877	-2.718228
O	3.512657	3.115480	3.413214
H	3.992624	3.151783	2.552326
H	4.168288	3.296120	4.103143
O	-0.489552	5.934832	1.428544
H	0.016927	5.360848	2.041754
H	-1.402202	5.583141	1.405254
O	-1.641910	-4.694058	1.724563
H	-2.440313	-5.072229	1.296134
H	-1.229835	-4.130935	1.022061
O	2.315893	0.578393	3.351589
H	2.715666	1.463431	3.508417
H	2.430866	0.436148	2.383763
O	4.999194	-1.469668	1.402961
H	4.357221	-0.751311	1.172624
H	4.674910	-2.265252	0.929148
O	7.004303	-0.581838	-0.195683
H	6.362950	-0.954894	0.460903
H	7.882753	-0.906466	0.052354
O	0.966991	2.560413	0.728961
H	0.977526	1.578785	0.776281

H	0.044675	2.755276	0.415536
O	6.624303	2.174151	-0.576652
H	6.813707	1.237611	-0.355400
H	6.362103	2.157821	-1.521107
O	3.236761	0.533407	0.796215
H	2.942942	0.343952	-0.129601
H	3.670341	1.420390	0.773887
O	-1.958666	-0.386961	2.246252
H	-2.148089	-1.298745	2.574070
H	-2.816789	0.102980	2.236176
O	-4.950560	-1.788847	3.073017
H	-4.839299	-0.816980	3.018895
H	-4.117332	-2.139480	3.449525
O	-3.600984	3.948712	-2.987902
H	-3.561910	3.028280	-3.324646
H	-2.670821	4.243750	-2.901229
O	1.757331	-3.264309	3.736002
H	2.597400	-2.792976	3.965331
H	1.060864	-2.904292	4.329282
O	-3.300293	1.267883	-3.782683
H	-2.542422	1.053149	-4.384236
H	-3.970056	0.554979	-3.886814
O	-5.186173	1.513116	-0.039729
H	-4.309579	1.342794	-0.471244
H	-5.344908	2.469141	-0.192701
O	-4.925382	4.227097	-0.651100
H	-4.441748	4.142969	-1.517374
H	-5.666132	4.830805	-0.811025
O	-1.483308	3.064783	-0.151275
H	-1.964329	2.254325	-0.457857
H	-2.080417	3.572257	0.451069
O	0.379418	2.321760	-3.522959
H	-0.008129	3.167656	-3.190294
H	1.353590	2.421004	-3.512547
O	0.943151	-5.564712	2.350724
H	-0.012436	-5.395247	2.212138
H	1.277396	-4.815098	2.886944
O	-1.094870	0.761545	-5.290495
H	-0.472993	1.351356	-4.813186
H	-0.833598	-0.150705	-5.044182
O	0.137283	-0.011261	0.590556
H	0.763867	-0.729250	0.832318
H	-0.679450	-0.160101	1.124336
O	-0.251394	0.355172	4.245968
H	-0.853411	0.173079	3.484651
H	0.657194	0.456803	3.869294
O	-4.351054	0.894496	2.486795
H	-4.126801	1.719340	2.973489
H	-4.728732	1.171998	1.617131
O	-6.080622	-0.866206	-1.224146
H	-5.650276	-1.529116	-0.642221
H	-5.924070	0.004354	-0.801399
O	-0.467831	-1.727142	-4.111150
H	-0.320648	-1.190429	-3.297653
H	-1.353822	-2.135133	-3.963300
O	6.104421	-0.897367	-2.837278
H	5.312462	-1.473716	-2.867492
H	6.429359	-0.920741	-1.912273

O	-0.305129	-2.155115	5.225955
H	-0.260612	-1.184623	5.022800
H	-0.335904	-2.247442	6.189890
O	-1.032574	2.990128	4.652343
H	-0.362824	3.438319	4.087985
H	-0.776351	2.041590	4.624091
O	3.669937	-2.273039	-2.617563
H	3.239968	-1.414865	-2.377875
H	3.035314	-2.732906	-3.209178
O	-0.391571	-3.159160	-0.112172
H	0.409030	-2.823640	0.360649
H	-0.082062	-3.739974	-0.849220
O	1.700764	-2.141086	1.246645
H	2.471586	-2.536297	0.772264
H	1.680916	-2.528938	2.155411
O	3.701447	-3.389091	-0.125445
H	3.698189	-3.072500	-1.062290
H	3.299080	-4.287144	-0.119447
O	3.129023	2.439504	-2.971973
H	3.056256	3.098047	-2.239987
H	4.082061	2.337558	-3.191578
O	-2.800992	0.981298	-1.140717
H	-2.587509	0.032273	-0.949616
H	-2.876287	1.058293	-2.124798
O	-4.681781	-2.593120	0.483438
H	-4.814904	-2.369632	1.438821
H	-4.520702	-3.559690	0.409735
O	4.474908	2.994458	0.851592
H	3.952692	3.569864	0.250617
H	5.312622	2.764091	0.372091
O	-2.911991	-2.614247	-3.245132
H	-2.799532	-2.220727	-2.342400
H	-3.698411	-2.156967	-3.612409
O	-0.081302	0.033574	-2.087797
H	-0.217427	0.055969	-1.110106
H	-0.105086	0.954860	-2.432670
O	-3.051155	4.674219	1.342954
H	-3.320768	4.225092	2.176591
H	-3.819725	4.655081	0.729466
O	-2.424028	-5.169908	-2.254668
H	-1.449736	-5.195515	-2.163520
H	-2.634979	-4.332539	-2.721101
O	-2.488892	-1.627853	-0.767828
H	-1.662343	-2.083495	-0.476670
H	-3.223954	-1.954367	-0.192372
O	-3.498475	3.260400	3.670122
H	-2.584303	3.166277	4.064695
H	-4.053763	3.665157	4.353276
O	-3.796773	-5.201314	0.063703
H	-3.311909	-5.224230	-0.805504
H	-4.391654	-5.965797	0.070052
O	5.781402	1.745531	-3.237852
H	5.858163	0.754207	-3.196641
H	6.359201	2.039384	-3.957739
O	-2.388424	-2.774568	3.502303
H	-1.710048	-2.702110	4.208268
H	-2.130108	-3.530763	2.920608
O	3.912490	-1.634450	4.010226

H	3.399174	-0.801368	3.930545
H	4.409587	-1.687849	3.166452
O	0.909566	4.044894	2.972060
H	0.964661	3.408469	2.215756
H	1.811834	4.023382	3.347847
O	0.762855	6.139795	-0.957342
H	0.299612	6.108927	-0.078062
H	0.997927	7.066063	-1.115114
O	2.205995	-5.716790	-0.007836
H	1.735901	-5.675479	0.871581
H	2.655103	-6.575063	-0.036168
O	-0.904635	4.437368	-2.386566
H	-1.097923	3.977132	-1.530587
H	-0.342860	5.197586	-2.125892
O	2.593753	0.052829	-1.783629
H	2.837554	0.898210	-2.238798
H	1.616793	-0.031272	-1.913866
O	-5.044969	-0.883592	-3.703345
H	-5.464810	-0.878951	-2.799475
H	-5.765014	-0.984743	-4.343374

Table S38. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{55}$ cluster with nine internal water molecules, 55B configuration.

O	-1.482797	3.479712	-3.979442
H	-2.312111	3.047832	-3.656831
H	-1.702882	3.908978	-4.819988
O	-2.553974	-4.038783	-0.833579
H	-2.008503	-3.398373	-0.311427
H	-1.974470	-4.826714	-0.946277
O	-0.294893	4.999964	-1.980714
H	-0.765548	4.549964	-2.717472
H	-0.975932	5.454338	-1.435878
O	-3.633611	-3.419786	3.264160
H	-4.098928	-3.639276	2.411014
H	-4.237215	-3.661183	3.982112
O	0.521300	-5.934618	1.375253
H	-0.027028	-5.363725	1.956205
H	1.423992	-5.557146	1.388701
O	1.481771	4.719183	1.915484
H	1.126257	4.173646	1.169407
H	2.303829	5.112871	1.551819
O	-2.685261	-0.802268	3.023702
H	-2.845645	-0.687511	2.058021
H	-3.032557	-1.700501	3.224872
O	-5.110772	1.675329	1.094109
H	-4.462249	0.975027	0.829555
H	-4.787636	2.493573	0.661881
O	-7.053655	0.605443	-0.452696
H	-6.482555	1.102745	0.184951
H	-7.976035	0.792785	-0.223813
O	-0.939729	-2.488059	0.675125
H	-0.930132	-1.503879	0.707365
H	-0.033206	-2.707456	0.334548

O	-5.737500	-1.832200	-0.528110
H	-6.369975	-1.087846	-0.423897
H	-5.624335	-1.938271	-1.498561
O	-3.534328	-0.457915	0.450872
H	-3.013874	-0.294518	-0.373827
H	-4.250644	-1.071181	0.163768
O	1.750491	0.404596	2.290892
H	1.917189	1.296566	2.680093
H	2.609343	-0.082774	2.311731
O	4.698699	1.804395	3.357882
H	3.841714	2.138110	3.694365
H	4.595521	0.833589	3.268771
O	3.879482	-3.858458	-2.864567
H	3.816474	-2.937185	-3.195251
H	2.964162	-4.206024	-2.852689
O	-2.057090	3.215396	3.657439
H	-1.375478	2.847236	4.262568
H	-2.879651	2.686415	3.817439
O	3.534328	-1.176986	-3.653648
H	2.805530	-0.959552	-4.288646
H	4.196049	-0.451377	-3.705783
O	5.253220	-1.433234	0.224310
H	5.440963	-2.384496	0.078037
H	4.409045	-1.277828	-0.273831
O	5.041360	-4.138897	-0.438532
H	4.619372	-4.048644	-1.335354
H	5.777716	-4.759260	-0.546029
O	1.507156	-3.028173	-0.222030
H	2.003966	-2.211357	-0.488780
H	2.067354	-3.516380	0.429494
O	-0.121702	-2.383283	-3.676505
H	0.064643	-1.710587	-2.983991
H	0.332252	-3.203288	-3.367691
O	-1.157745	5.548148	2.346723
H	-0.192375	5.386123	2.294459
H	-1.535346	4.791296	2.841235
O	1.407630	-0.671918	-5.280122
H	1.074287	0.198720	-4.977778
H	0.795631	-1.337562	-4.900637
O	-0.253004	0.114300	0.509217
H	0.533419	0.256204	1.088903
H	-0.900615	0.818687	0.736845
O	-0.166769	-0.431817	4.050867
H	0.495475	-0.224673	3.349669
H	-1.036640	-0.569907	3.602746
O	4.149608	-0.846468	2.655698
H	3.920542	-1.675372	3.133251
H	4.619267	-1.113010	1.828720
O	6.133730	0.985929	-0.879113
H	5.641742	1.621197	-0.315102
H	5.992254	0.104599	-0.473887
O	0.724921	1.735170	-4.018553
H	-0.015949	2.376994	-4.066480
H	1.551090	2.224116	-3.793471
O	-5.967248	0.945073	-3.041879
H	-5.732789	0.017078	-3.245722
H	-6.406977	0.909718	-2.167271
O	-0.096154	2.008231	5.200767

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H     -0.168699     1.059541     4.918806
H     -0.138173     2.025885     6.168391
O      0.775178    -2.975708     4.665404
H      0.173103    -3.473218     4.066175
H      0.469571    -2.046125     4.575977
O     -3.553936     2.199276    -2.744925
H     -4.475744     1.914241    -2.958984
H     -3.119170     1.349300    -2.487257
O      0.375200     3.228508    -0.040925
H      0.125032     3.808524    -0.801203
H     -0.463383     2.900628     0.368177
O     -1.836176     2.227158     1.122758
H     -2.558631     2.668605     0.612512
H     -1.875832     2.565883     2.050183
O     -3.688158     3.536130    -0.368265
H     -3.626906     3.152229    -1.276934
H     -3.267163     4.424963    -0.379197
O     -2.812835    -2.632502    -3.151112
H     -1.899528    -2.626670    -3.522791
H     -2.761716    -3.212377    -2.351065
O      2.946519    -0.942582    -1.025471
H      2.655027    -0.019560    -0.824313
H      3.040431    -0.996810    -2.009211
O      4.565444     2.624134     0.765151
H      4.645899     2.391195     1.724616
H      4.400117     3.590853     0.696806
O     -4.729895    -4.026723     0.884495
H     -3.977642    -4.155254     0.263957
H     -5.250228    -3.298159     0.488973
O      3.063005     2.707127    -3.021620
H      2.892493     2.290360    -2.138818
H      3.867839     2.255184    -3.355092
O      0.222886    -0.145556    -2.129405
H      0.486348     0.632180    -2.675621
H      0.286928     0.078447    -1.172775
O      3.018139    -4.573062     1.408351
H      3.218027    -4.133395     2.265941
H      3.831379    -4.543361     0.855949
O      2.529968     5.252430    -2.048216
H      2.783466     4.419174    -2.501292
H      1.551181     5.268144    -2.042571
O      2.455225     1.649538    -0.615700
H      1.629240     2.127453    -0.357713
H      3.166076     1.962764    -0.002014
O      3.286241    -3.215432     3.801630
H      2.354849    -3.126033     4.155887
H      3.812785    -3.622606     4.505696
O      3.718017     5.246904     0.369169
H      3.290194     5.285586    -0.529115
H      4.333969     5.993157     0.414592
O     -5.387335    -1.823335    -3.300847
H     -4.482479    -2.172395    -3.472459
H     -5.997299    -2.348515    -3.840224
O      2.100717     2.734889     3.674419
H      1.877985     3.514050     3.108968
H      1.375944     2.624354     4.327199
O     -4.159280     1.501717     3.738483
H     -3.682121     0.651941     3.618840
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H	-4.610070	1.652585	2.880333
O	-0.976692	-4.086481	2.845082
H	-0.990914	-3.406200	2.126520
H	-1.901766	-4.100595	3.168512
O	-0.642747	-6.056830	-1.050948
H	-0.197833	-6.058508	-0.160580
H	-0.929073	-6.967293	-1.216937
O	-2.171067	5.831411	-0.125727
H	-1.795503	5.738488	0.793442
H	-2.593596	6.702685	-0.161603
O	1.173034	-4.476235	-2.457362
H	1.281064	-3.982681	-1.604309
H	0.568235	-5.210684	-2.222780
O	-2.452471	-0.158570	-1.995171
H	-2.711316	-1.002757	-2.434798
H	-1.465349	-0.124699	-2.074590
O	5.229971	1.004124	-3.410495
H	5.600457	0.993068	-2.485267
H	5.979354	1.148203	-4.007238

Table S39. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{55}$ cluster with nine internal water molecules, 55C configuration.

O	7.021298	-1.135693	-0.456552
H	6.387913	-1.512694	0.205805
H	7.885772	-1.537724	-0.284930
O	5.007915	-1.959453	1.149720
H	4.440200	-1.162224	1.001007
H	4.576075	-2.673212	0.627887
O	6.765704	1.658832	-0.600264
H	6.916956	0.701212	-0.452429
H	6.461636	1.719493	-1.530416
O	5.879400	-1.220303	-3.021831
H	6.279894	-1.328306	-2.133309
H	5.016108	-1.686027	-2.999472
O	3.382552	0.209984	0.881187
H	3.844080	1.083904	0.901081
H	2.845042	0.174234	1.706679
O	5.782231	1.453110	-3.236612
H	5.782349	0.457280	-3.260285
H	6.341169	1.750241	-3.969909
O	3.329451	-2.327200	-2.710997
H	2.955006	-1.477164	-2.367854
H	2.654099	-2.691896	-3.323443
O	3.339010	-3.635762	-0.299250
H	3.367991	-3.247927	-1.207867
H	2.653468	-3.110053	0.187644
O	2.438590	-0.029270	-1.628687
H	2.705787	0.037797	-0.679453
H	2.757039	0.797318	-2.068524
O	4.747630	2.588427	0.953023
H	5.547237	2.301589	0.439779
H	4.255617	3.215813	0.378596
O	3.832514	-2.118467	3.714497

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H      4.324302    -2.188228     2.868661
H      3.129124    -2.799738     3.679891
O      3.186816     2.292923    -2.865327
H      4.124801     2.118359    -3.104131
H      3.186463     2.932431    -2.112574
O      1.484727    -2.267678     1.105632
H      1.488395    -2.620815     2.027217
H      0.676438    -2.655872     0.681850
O      2.417661     0.184255     3.430360
H      2.967954    -0.609980     3.656506
H      2.938583     0.981756     3.668281
O      3.799312     2.621668     3.534171
H      4.274651     2.681901     2.672441
H      4.444532     2.844179     4.221863
O      2.915572     3.847306    -0.646795
H      2.238672     3.337201    -0.130175
H      2.511346     4.734726    -0.757472
O      1.748682    -5.825634    -0.415147
H      2.440762    -5.114799    -0.402211
H      2.211016    -6.661358    -0.579671
O      1.498045    -3.614130     3.493277
H      1.163989    -4.450985     3.082777
H      0.823642    -3.314226     4.140983
O      1.100272     2.551231     0.852784
H      1.181551     2.926804     1.763749
H      0.250845     2.921056     0.500012
O     -0.131111     0.344603    -2.235598
H      0.733457     0.114496    -1.812849
H     -0.763517     0.429660    -1.496972
O      1.151245    -3.292898    -4.199744
H      0.474409    -2.574874    -4.320619
H      1.293914    -3.690486    -5.071824
O      0.136327     0.036516     0.544255
H      0.772769    -0.669141     0.792873
H      0.584200     0.892895     0.738190
O     -0.692290    -3.144387    -0.172676
H     -0.493728    -3.624786    -1.012330
H     -1.348854    -2.431300    -0.369727
O      0.536591     2.572093    -3.653223
H      1.516962     2.551204    -3.624300
H      0.260697     1.842146    -3.046572
O     -0.081275    -4.799308    -2.232248
H      0.577046    -5.303591    -1.703602
H      0.407990    -4.359898    -2.964170
O      0.540784    -5.785954     2.141333
H      0.960766    -5.819806     1.255634
H     -0.409864    -5.619871     1.975458
O     -0.709923    -1.331095    -4.275432
H     -0.478636    -0.792959    -3.478259
H     -1.595965    -1.701640    -4.050552
O      1.283999     3.810977     3.253374
H      2.186502     3.544971     3.527994
H      0.640032     3.428485     3.904896
O     -0.112364     0.059149     4.447090
H      0.803809     0.109169     4.079869
H     -0.712230    -0.028104     3.665179
O      1.202889     6.041140    -0.740761
H      0.780280     5.988535     0.158314
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H      1.483839     6.960922    -0.857803
O     -0.427775    -2.518558     5.171187
H     -0.279493    -1.542131     5.075943
H     -0.478132    -2.713615     6.118657
O     -1.219497     3.383502    -0.168048
H     -1.039984     3.943728    -0.964376
H     -1.726891     3.926743     0.485266
O     -1.799272    -0.327642     2.340334
H     -1.163821    -0.228576     1.582962
H     -1.990155    -1.285828     2.467697
O     -1.238199     1.214809    -5.368092
H     -0.507143     1.744418    -4.987819
H     -1.011157     0.279951    -5.177454
O     -2.690686    -1.431164    -0.638734
H     -2.606848    -0.454297    -0.585783
H     -3.510886    -1.697262    -0.151111
O     -0.576323     4.743675    -2.413345
H     -0.090944     4.039684    -2.908544
H      0.094636     5.327342    -1.994532
O     -1.998787    -4.789598     1.513418
H     -1.545847    -4.209365     0.850792
H     -2.837994    -5.049733     1.076056
O     -0.587234     2.762878     4.902769
H     -0.462117     1.789912     4.845453
H     -1.476756     2.941232     4.531380
O      0.085299     5.842091     1.710017
H      0.538800     5.191488     2.286227
H     -0.863006     5.605111     1.711712
O     -2.512767     1.232770    -1.012806
H     -2.029767     2.035829    -0.680500
H     -2.713927     1.392875    -1.971758
O     -2.464706    -2.795792     3.304545
H     -1.825242    -2.844680     4.047327
H     -2.318462    -3.587095     2.731306
O     -3.114872    -2.155104    -3.228397
H     -2.971889    -1.838252    -2.302614
H     -3.887282    -1.638664    -3.545533
O     -2.901611    -4.824357    -2.476991
H     -1.932104    -4.936823    -2.399021
H     -3.036612    -3.927248    -2.853066
O     -3.237606     1.683073    -3.572175
H     -2.547730     1.497140    -4.259146
H     -3.965816     1.033552    -3.699105
O     -2.607966     4.878989     1.603454
H     -2.837901     4.339336     2.394992
H     -3.414544     4.916444     1.041943
O     -4.224027    -4.954501    -0.135928
H     -3.758493    -4.938604    -1.016419
H     -4.873116    -5.672338    -0.178951
O     -3.140079     3.279391     3.792688
H     -3.571157     2.451806     3.450786
H     -3.749187     3.659776     4.443596
O     -3.359212     4.339857    -2.684427
H     -2.415244     4.595220    -2.658354
H     -3.383515     3.431237    -3.054146
O     -4.111548     1.017266     2.670141
H     -3.244959     0.596647     2.444199
H     -4.495326     1.309933     1.809820
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O	-4.985961	-2.340924	0.442501
H	-4.854253	-3.305999	0.307697
H	-5.044239	-2.166568	1.416436
O	-4.921981	1.780772	0.151912
H	-4.062166	1.578176	-0.289291
H	-5.016543	2.753984	0.055159
O	-4.981500	-1.652798	3.069942
H	-4.131533	-2.064054	3.336567
H	-4.808224	-0.688453	3.029671
O	-5.157516	-0.313384	-3.594592
H	-5.588345	-0.331421	-2.695183
H	-5.871857	-0.337227	-4.248366
O	-4.589854	4.516892	-0.294286
H	-4.134818	4.479890	-1.179409
H	-5.342536	5.117800	-0.400854
O	-6.189828	-0.354198	-1.122468
H	-5.850597	-1.113804	-0.602619
H	-5.879235	0.449274	-0.652534

Table S40. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{55}$ cluster with nine internal water molecules, 55D configuration.

O	-7.014066	1.334644	-0.307582
H	-6.340962	1.704528	0.317864
H	-7.860615	1.755815	-0.097232
O	-4.915764	2.136367	1.209735
H	-4.496489	2.873039	0.715977
H	-4.357416	1.340984	1.022706
O	-5.897104	1.404827	-2.888998
H	-5.839445	0.444018	-3.074546
H	-6.341506	1.469107	-2.017662
O	-6.864050	-1.464001	-0.524687
H	-6.969276	-0.504050	-0.355581
H	-6.566509	-1.526817	-1.457107
O	-3.379757	-0.100502	0.908471
H	-3.892861	-0.945452	0.911145
H	-2.863721	-0.105951	1.750737
O	-5.840900	-1.404238	-3.138722
H	-4.925524	-1.786228	-3.137021
H	-6.317549	-1.811518	-3.877163
O	-3.391438	2.430435	-2.615036
H	-4.324037	2.139575	-2.782140
H	-3.401925	2.990271	-1.799872
O	-3.223270	3.772768	-0.255432
H	-2.529961	3.259524	0.235408
H	-2.838331	4.671694	-0.339179
O	-4.814548	-2.443873	0.952304
H	-4.345039	-3.080744	0.369591
H	-5.625242	-2.146940	0.462842
O	-2.451267	0.083878	-1.616106
H	-2.768072	0.945460	-1.982839
H	-2.710938	0.058950	-0.663791
O	-3.752471	2.191012	3.806907
H	-4.240355	2.285966	2.962211

H	-3.360540	1.291619	3.775752
O	-3.270266	-2.197295	-2.864376
H	-2.996851	-1.347959	-2.435967
H	-3.248130	-2.855879	-2.128776
O	-2.446697	-0.254191	3.436295
H	-2.848410	-1.123338	3.650500
H	-1.488544	-0.278853	3.674359
O	-1.376973	2.391073	1.125094
H	-0.551974	2.742887	0.699317
H	-1.359966	2.733466	2.050213
O	-3.871201	-2.662582	3.524669
H	-4.350796	-2.645239	2.663527
H	-4.541315	-2.786978	4.212961
O	-3.016582	-3.773596	-0.639814
H	-2.336430	-3.237009	-0.156777
H	-2.618158	-4.668588	-0.699120
O	-0.251371	-0.003939	0.472571
H	-0.799648	0.758998	0.760433
H	0.585989	0.078850	0.979820
O	-1.173464	-2.464925	0.806654
H	-0.994933	-1.490511	0.734680
H	-0.331482	-2.873306	0.481013
O	-1.516610	5.967933	-0.345263
H	-1.089476	5.895597	0.551422
H	-1.797111	6.890560	-0.439212
O	-1.420129	3.576294	3.596098
H	-0.765560	3.184632	4.214838
H	-2.304311	3.186965	3.809254
O	-1.277423	3.276628	-4.104371
H	-2.113836	2.965042	-3.677066
H	-1.539635	3.746514	-4.910414
O	0.075052	-0.444051	-2.271462
H	-0.782417	-0.176540	-1.853517
H	0.706730	-0.514527	-1.530754
O	-0.619470	-2.675522	-3.647947
H	-0.315875	-1.944113	-3.054932
H	-1.599096	-2.625444	-3.591108
O	0.818178	3.198838	-0.138536
H	1.439679	2.459872	-0.362435
H	0.585974	3.664125	-0.978560
O	-0.384799	5.728246	2.090387
H	0.568984	5.522616	2.010098
H	-0.778733	5.021489	2.643667
O	-1.323884	-3.750291	3.155729
H	-1.294596	-3.168947	2.353658
H	-2.241123	-3.650713	3.480295
O	0.136226	4.772947	-2.230897
H	-0.478862	5.315442	-1.687696
H	-0.400884	4.311519	-2.913517
O	0.184821	-0.130623	4.126695
H	0.295627	0.696449	4.645520
H	0.788203	-0.021202	3.352400
O	0.665688	1.239928	-4.291750
H	0.001032	1.959948	-4.344859
H	0.425203	0.712377	-3.490437
O	0.640899	2.433198	5.075524
H	1.447490	2.628974	4.534661
H	0.833256	2.703275	5.985624

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O      1.927527     0.365133     2.063455
H      2.146717     1.286414     2.336671
H      2.741012    -0.174650     2.220894
O     -1.348395    -6.022232    -0.633944
H     -0.897262    -5.994792     0.252478
H     -1.671205    -6.928643    -0.747569
O      1.140339    -3.436657    -0.119606
H      0.954753    -3.998293    -0.912997
H      1.641224    -3.981349     0.537013
O      2.717351     1.430713    -0.726802
H      2.863560     1.561158    -1.698363
H      2.551216     0.473050    -0.594768
O      1.128793    -1.301595    -5.370200
H      0.395996    -1.833440    -4.996627
H      0.874838    -0.366662    -5.226830
O      0.651073    -2.761117     4.830756
H      0.518226    -1.793628     4.727880
H     -0.057666    -3.166757     4.281447
O      0.460410    -4.821923    -2.345915
H     -0.014143    -4.124570    -2.861175
H     -0.221270    -5.377274    -1.906252
O      2.205490     4.781449     1.520769
H      1.733947     4.224172     0.850138
H      3.031074     5.058229     1.068402
O     -0.146180    -5.896457     1.785538
H     -0.579190    -5.216235     2.345721
H      0.804997    -5.673425     1.762868
O      2.419641    -1.269257    -0.965497
H      1.953767    -2.077861    -0.622801
H      2.616231    -1.443970    -1.923010
O      2.607166     2.740364     3.268189
H      3.550886     2.448359     3.323213
H      2.564881     3.538351     2.686291
O      3.093937     2.025157    -3.341176
H      2.270007     1.750453    -3.812493
H      3.826444     1.437268    -3.630949
O      2.963247     4.679297    -2.483122
H      3.066886     3.774416    -2.847384
H      1.998860     4.828349    -2.408966
O      3.099050    -1.758267    -3.533102
H      2.417791    -1.561799    -4.225684
H      3.859106    -1.152385    -3.682652
O      2.554035    -4.927501     1.635934
H      2.785272    -4.385601     2.425799
H      3.350963    -4.947540     1.059976
O      4.164407    -1.080306     2.648613
H      3.837160    -1.865075     3.143543
H      4.516499    -1.417833     1.790742
O      3.054127    -3.334358     3.841258
H      2.159499    -3.133017     4.242425
H      3.573683    -3.769335     4.534191
O      4.379225     4.949416    -0.201384
H      3.879346     4.885788    -1.058882
H      5.015670     5.672176    -0.305530
O      3.234403    -4.419440    -2.671057
H      2.293835    -4.683710    -2.622455
H      3.240582    -3.508262    -3.036169
O      5.046325     2.282824     0.364377
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H	4.159290	1.969974	0.062090
H	5.020232	3.251945	0.209211
O	5.053665	1.574127	3.046060
H	4.855770	0.615638	3.055303
H	5.165361	1.805422	2.096041
O	4.873603	-1.818357	0.117457
H	3.999290	-1.592287	-0.281324
H	4.944795	-2.792086	0.002178
O	5.098123	0.160461	-3.621780
H	5.554490	0.205243	-2.735539
H	5.793233	0.164446	-4.296363
O	6.220948	0.250862	-1.188167
H	5.937360	1.039588	-0.677871
H	5.873411	-0.523848	-0.695656
O	4.502210	-4.551059	-0.300768
H	4.031296	-4.532611	-1.178526
H	5.254579	-5.152104	-0.409191

Table S41. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{123}$ cluster.

O	6.866643	-4.671765	-4.013780
H	6.902564	-4.824520	-3.038830
H	7.443163	-5.331213	-4.427648
O	7.455684	-1.909098	-3.865069
H	7.297104	-2.843012	-4.110740
H	7.330472	-1.887789	-2.892170
O	3.877960	-4.774286	-1.722048
H	3.560584	-4.042974	-1.142911
H	3.811571	-4.457844	-2.647571
O	5.480538	-0.072113	-4.189866
H	6.187008	-0.766122	-4.206804
H	5.922249	0.735698	-3.846141
O	6.979819	1.812924	-0.347659
H	7.059881	0.924338	0.051631
H	7.484749	2.424279	0.250899
O	6.800831	2.134694	-3.073872
H	6.950814	2.006014	-2.106588
H	7.673987	2.276186	-3.469718
O	4.640246	3.832754	-3.571860
H	5.500015	3.371528	-3.469574
H	3.958798	3.125122	-3.498219
O	6.962381	-5.188178	1.329188
H	6.918830	-5.096360	0.343004
H	7.495474	-5.974130	1.520469
O	6.789180	-0.640143	1.148565
H	7.078198	-1.432454	1.681472
H	5.800685	-0.611399	1.221163
O	6.501841	-1.927227	-1.274323
H	6.760719	-1.472556	-0.443099
H	5.572686	-1.643242	-1.454172
O	7.147577	1.268130	3.143392
H	7.184278	0.569568	2.454125
H	6.234158	1.638237	3.046980
O	4.460111	2.813936	0.209151

H	5.334550	2.439747	-0.049078
H	4.433685	2.710071	1.190026
O	3.129930	5.410832	-5.381137
H	3.800345	5.018437	-4.786019
H	2.599402	4.639286	-5.683338
O	8.187341	3.314310	1.561520
H	7.984971	2.666036	2.269994
H	7.710616	4.132307	1.816475
O	7.585129	-2.754549	2.595956
H	7.401623	-3.622995	2.179718
H	7.228476	-2.796059	3.508139
O	6.495068	-2.769675	5.199266
H	5.592374	-3.156870	5.091539
H	6.949715	-3.289562	5.878680
O	5.996994	-0.052182	5.250968
H	6.594301	0.371150	4.592264
H	6.319786	-0.969575	5.387625
O	3.777765	4.014137	6.449050
H	3.992364	3.052501	6.600509
H	3.979507	4.482001	7.272913
O	3.448477	-2.967450	-6.789920
H	2.483286	-2.931075	-7.040756
H	3.906415	-3.367753	-7.544522
O	3.751687	-0.303737	-6.279249
H	4.480743	-0.126313	-5.640094
H	3.814964	-1.252921	-6.531341
O	2.012193	1.320582	-7.692150
H	2.703084	0.749716	-7.294771
H	1.209641	0.760635	-7.761377
O	1.582190	3.161528	-5.759558
H	1.739275	2.510341	-6.492449
H	1.892244	2.729391	-4.927490
O	6.552349	-4.643744	-1.291057
H	5.581320	-4.813419	-1.379175
H	6.600937	-3.657844	-1.221156
O	1.538986	-5.072496	-3.998282
H	2.470168	-5.220361	-4.257684
H	1.239310	-5.841847	-3.455002
O	1.913008	-2.626510	-2.737123
H	1.714957	-3.504355	-3.138394
H	1.166775	-2.403073	-2.134423
O	4.044579	-0.981432	-2.018788
H	4.383679	-0.653243	-2.885813
H	3.390592	-1.687445	-2.214128
O	1.898139	-0.382146	-4.271217
H	2.481444	-0.391115	-5.067656
H	1.956247	-1.270150	-3.845667
O	2.504777	2.132451	-3.394402
H	2.345001	1.166025	-3.479907
H	1.940059	2.480118	-2.661997
O	1.002373	3.394463	-1.507420
H	1.283270	3.089677	-0.616330
H	1.221629	4.360438	-1.509881
O	1.244876	6.828295	-4.022913
H	1.945412	6.361838	-4.548137
H	0.371537	6.511755	-4.345876
O	0.836001	9.462597	-3.428081
H	1.101814	8.557738	-3.714997

H	1.618174	9.853971	-3.012425
O	2.809163	-7.243067	-0.879027
H	3.197224	-6.396986	-1.189359
H	1.965528	-7.320482	-1.372409
O	-2.391640	-3.329959	-1.808631
H	-1.970855	-4.112407	-1.368966
H	-3.134921	-3.036948	-1.224133
O	3.296625	-3.097429	0.317740
H	3.614010	-2.199511	0.579263
H	2.350875	-3.148210	0.597332
O	4.085208	-0.662157	1.259615
H	3.526301	-0.014875	0.770462
H	3.837083	-0.632909	2.217694
O	2.680061	0.888477	-0.494725
H	3.231411	1.695957	-0.358708
H	3.123330	0.342642	-1.182843
O	1.680158	3.126917	1.176509
H	2.110061	3.992670	1.380709
H	0.708506	3.263237	1.309065
O	2.862892	5.459630	2.095588
H	3.513961	6.000244	1.581730
H	2.130540	6.071361	2.369438
O	6.817908	5.608492	2.489476
H	6.164122	5.350868	3.181174
H	7.435917	6.223504	2.912806
O	4.183654	5.137415	-1.205938
H	4.395538	4.778529	-2.100283
H	4.195705	4.344038	-0.619525
O	2.417603	-6.868036	1.808182
H	2.572727	-7.144914	0.870217
H	3.093233	-6.167264	1.965064
O	4.311237	-4.878775	2.078965
H	5.243114	-5.111298	1.869536
H	4.029088	-4.219257	1.395981
O	4.023867	-3.496065	4.403317
H	4.144874	-4.019781	3.573096
H	3.162247	-3.791661	4.789838
O	3.706608	-0.834742	3.905057
H	4.519196	-0.462205	4.323332
H	3.789327	-1.812543	4.039057
O	2.090875	1.814564	3.527134
H	1.951710	2.294144	2.671563
H	1.823486	2.453553	4.230661
O	4.684017	2.319773	2.906928
H	3.856827	1.915969	3.257410
H	4.730582	3.210453	3.338640
O	4.186063	1.389480	6.823335
H	4.910975	0.946264	6.334711
H	3.383257	0.859727	6.629457
O	4.683930	4.790891	3.976783
H	4.404429	4.653753	4.910102
H	3.902053	5.102105	3.456493
O	2.007533	-0.136060	5.932633
H	2.449239	-0.330517	5.073066
H	1.654275	-0.986584	6.287612
O	4.134937	-4.371422	-4.464811
H	5.101092	-4.541750	-4.475794
H	3.927847	-3.812888	-5.246393

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O      0.872370    -2.821565    -7.497885
H      0.438869    -1.943554    -7.499799
H      0.321447    -3.418115    -6.942397
O     -0.310770    -0.255361    -7.843870
H     -1.007114     0.201338    -7.307389
H     -0.642231    -0.269828    -8.754665
O     -2.015843     1.070909    -6.168274
H     -2.992399     0.902038    -6.146785
H     -1.653940     0.658207    -5.347102
O     -4.671089     0.515545    -5.901298
H     -4.629905    -0.398636    -5.548019
H     -4.995715     1.020000    -5.125287
O     -1.056180     3.477071    -5.295677
H     -0.094368     3.357572    -5.507434
H     -1.523639     2.716922    -5.715363
O     -1.783528    -8.310892    -3.327229
H     -1.995021    -7.684496    -4.071966
H     -1.851804    -9.208138    -3.685944
O      0.482661    -7.001870    -2.400949
H     -0.122972    -7.654224    -2.814384
H     -0.123832    -6.443279    -1.856773
O     -0.485255    -4.501330    -5.757714
H      0.286463    -4.750131    -5.198251
H     -0.944275    -3.790010    -5.247488
O     -1.802562    -2.589395    -4.359726
H     -1.901659    -2.875243    -3.425493
H     -1.373098    -1.699234    -4.306065
O     -0.777971    -0.105549    -4.071693
H      0.200863    -0.113977    -4.200162
H     -0.964660     0.184930    -3.148230
O     -3.977108    -0.614513    -1.974263
H     -3.125221    -0.141803    -1.815069
H     -4.499159    -0.504510    -1.144729
O     -1.516975     3.398380    -2.600120
H     -0.664773     3.498438    -2.116038
H     -1.290038     3.366361    -3.561178
O     -7.402570     5.985052    -0.783028
H     -6.621174     6.151609    -1.375001
H     -8.140779     6.499643    -1.140788
O     -1.168914     9.041498    -1.659096
H     -0.457060     9.273589    -2.310615
H     -1.666030     9.854231    -1.483953
O      1.628759     6.031324    -1.441351
H      1.507140     6.348347    -2.370350
H      2.594194     5.854157    -1.321993
O     -0.065788    -5.844542     1.486993
H      0.835231    -6.245373     1.590533
H     -0.619457    -6.176994     2.229284
O     -1.537970    -6.872476     3.589383
H     -2.332596    -6.282991     3.605707
H     -1.868530    -7.759636     3.381607
O      0.697713    -3.281047     1.099584
H      0.354995    -4.202566     1.174344
H      0.253811    -2.842714     0.332687
O     -0.122974    -1.878301    -1.053117
H     -1.045940    -2.133992    -1.255483
H     -0.158765    -1.023752    -0.559799
O      0.097154     0.489168     0.306169
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H      1.030140     0.726942     0.103072
H      0.022616     0.366558     1.280928
O     -1.709746     0.837309    -1.680759
H     -1.765344     1.775294    -1.979646
H     -1.152910     0.830400    -0.868004
O     -0.981822     3.420461     1.500495
H     -1.498823     2.582734     1.442276
H     -1.367086     4.038948     0.837017
O     -2.588881     6.727385    -2.363415
H     -2.146613     7.580195    -2.158227
H     -2.193277     6.421347    -3.208538
O     -0.069315     7.360416     0.241406
H     -0.429439     8.095757    -0.301199
H      0.617612     6.928015    -0.320815
O      4.885251     6.799170     0.835351
H      5.663168     6.445953     1.314998
H      4.866879     6.344214    -0.031623
O      1.177425    -6.830153     4.429232
H      1.621466    -7.021367     3.580636
H      0.218689    -6.921310     4.264012
O     -1.930205    -1.446123     6.770967
H     -1.849557    -0.706681     6.119411
H     -1.696428    -1.048061     7.637990
O      1.526233    -4.211296     5.204783
H      1.402067    -5.161514     4.966257
H      0.978452    -3.688148     4.573263
O      0.089461    -2.509490     3.589612
H      0.316405    -2.765612     2.659005
H     -0.886652    -2.610240     3.647161
O      0.025698     0.153323     3.055536
H      0.819667     0.672624     3.338630
H      0.196311    -0.787934     3.296246
O     -1.757026     0.629331     5.033906
H     -1.167295     0.489411     4.252089
H     -2.561687     1.089153     4.696674
O      1.245099     3.596981     5.461091
H      2.069764     3.912833     5.893593
H      0.801371     2.987124     6.098564
O     -0.625552     4.798821     3.847073
H     -0.696405     4.223647     3.049717
H      0.046930     4.392998     4.441469
O      0.764481     6.995920     2.845954
H      0.380892     7.249549     1.979591
H      0.175396     6.302868     3.215698
O     -0.415285    -0.345438     8.834281
H     -0.194155     0.432884     8.278360
H      0.260810    -1.011154     8.614042
O      0.098748     1.544302     6.809462
H      0.789882     0.966056     6.402363
H     -0.691148     1.387655     6.242401
O     -4.422677    -1.832361    -4.406840
H     -3.528682    -2.199651    -4.599731
H     -4.317955    -1.447090    -3.506496
O     -5.376863     1.378708    -3.349492
H     -4.894710     0.669828    -2.866383
H     -6.318820     1.321394    -3.043136
O     -1.313919    -5.621128    -0.888359
H     -0.933984    -5.760750     0.012234
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H     -2.099552    -6.213201    -0.976453
O     -3.522931    -7.086787    -1.496380
H     -3.044045    -7.760659    -2.026236
H     -3.881110    -6.451667    -2.160011
O     -2.432176    -6.413746    -5.109747
H     -1.707978    -5.815293    -5.399208
H     -3.038246    -5.861023    -4.571499
O     -5.454187     0.032579     0.199763
H     -5.343616     0.994764     0.340791
H     -5.251811    -0.430889     1.053184
O     -4.229780     3.576945    -2.262370
H     -3.257414     3.590673    -2.406005
H     -4.604017     2.814116    -2.771610
O     -1.337776     6.097107    -4.783522
H     -1.363512     5.160844    -5.100662
H     -1.673099     6.645583    -5.508845
O     -5.306722     6.101206    -2.455033
H     -4.463499     6.591063    -2.365806
H     -5.009374     5.164457    -2.466362
O     -7.934032     1.311130    -2.396109
H     -8.112403     0.530409    -1.833012
H     -7.895535     2.061512    -1.761383
O     -3.608486    -5.154742     3.230800
H     -3.973122    -5.389176     2.343705
H     -4.375354    -5.029974     3.834665
O     -4.550859    -5.623884     0.708557
H     -4.223956    -6.295119     0.077834
H     -5.541483    -5.585136     0.624537
O     -4.368262    -2.931427    -0.007418
H     -4.346425    -3.861293     0.314277
H     -5.227068    -2.849145    -0.489390
O     -2.309227    -1.242506     0.818016
H     -3.114959    -1.711507     0.510826
H     -2.143996    -1.628411     1.699412
O     -2.771559     1.370238     1.376545
H     -2.609394     0.423924     1.132663
H     -3.417913     1.731449     0.735989
O     -4.860266     2.774906     0.201374
H     -4.544035     3.094279    -0.687054
H     -4.652948     3.503853     0.839541
O     -2.030049     5.466527     0.024748
H     -2.275958     5.654474    -0.909827
H     -1.356621     6.162527     0.222508
O     -6.838915     5.576229     1.950636
H     -7.114110     5.838796     1.048916
H     -5.872129     5.436255     1.878472
O     -2.700098    -2.575769     3.346947
H     -2.953542    -3.524639     3.221092
H     -3.130413    -2.317001     4.196686
O     -4.280837    -2.004571     5.549705
H     -3.604418    -1.830229     6.244121
H     -4.816195    -1.190169     5.435616
O      0.721988    -2.300535     7.041766
H     -0.209444    -2.189017     6.751791
H      1.043212    -3.120470     6.610128
O     -5.730719     0.170854     4.599896
H     -5.149554     0.942211     4.405025
H     -6.651507     0.453896     4.393951
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O	-3.823297	1.924194	3.845018
H	-3.509530	1.747140	2.926041
H	-3.672304	2.877207	4.032830
O	-3.249891	4.579341	4.292419
H	-2.270030	4.731202	4.321258
H	-3.655046	5.113809	4.991306
O	-4.067175	-5.092286	-3.277546
H	-3.567496	-4.367719	-2.846319
H	-4.943589	-4.723437	-3.527378
O	-7.155502	-5.033344	0.563863
H	-7.155529	-4.405775	-0.191038
H	-7.190376	-4.451523	1.357287
O	-6.318016	-3.653420	-3.946678
H	-5.729284	-2.938235	-4.297786
H	-6.967661	-3.870329	-4.631585
O	-6.783669	-3.013436	-1.300527
H	-6.755127	-3.170173	-2.268987
H	-7.333460	-2.212289	-1.122211
O	-8.229919	0.952698	3.708946
H	-8.194138	1.801725	3.191323
H	-8.915048	1.081543	4.382242
O	-7.043057	-3.266831	2.685890
H	-6.300848	-2.647392	2.489568
H	-6.771998	-3.695927	3.524463
O	-8.927230	-1.256664	2.073768
H	-8.694082	-0.490319	2.638926
H	-8.379978	-2.003277	2.394274
O	-5.109209	-1.354998	2.450015
H	-4.230347	-1.761293	2.592257
H	-5.306892	-0.807205	3.251542
O	-7.976433	-0.729012	-0.455033
H	-7.097143	-0.385385	-0.168501
H	-8.450552	-0.915339	0.391590
O	-7.548716	3.229185	-0.459625
H	-7.608090	4.188983	-0.666389
H	-6.607825	3.077440	-0.220513
O	-4.135766	4.927147	1.702509
H	-3.407248	5.273043	1.135073
H	-3.779367	4.851952	2.615554
O	-5.636591	-4.279720	4.897807
H	-5.202029	-3.489766	5.299005
H	-5.992305	-4.806731	5.628949
O	-8.263687	3.205934	2.231294
H	-7.725631	4.022510	2.341104
H	-8.203168	3.045884	1.266384

Table S42. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{34}$ cluster with the undecahedral $(H_2O)_{18}$ hollow cage.

O	2.010115	1.863731	2.313111
H	1.261047	1.482828	2.820927
H	1.625471	2.244976	1.485804

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O     -2.249128    -2.648472     1.233196
H     -2.384345    -3.608783     1.383287
H     -2.131715    -2.555980     0.254962
O      2.459237    -2.109238    -1.214423
H      3.136204    -1.428299    -1.412710
H      2.347020    -2.090009    -0.232158
O     -2.139525     1.765632    -2.317213
H     -1.362396     1.386583    -2.800558
H     -1.799114     2.148926    -1.475763
O     -2.402384     1.593588     2.225978
H     -3.096006     2.224257     2.517359
H     -2.901932     0.816942     1.863872
O      2.370164    -2.319284     1.490454
H      2.576455    -3.275920     1.576434
H      1.480185    -2.187305     1.902179
O     -2.231416    -2.380291    -1.465097
H     -2.892948    -1.685656    -1.670816
H     -1.375905    -2.119194    -1.884081
O      2.214852     1.823921    -2.175684
H      2.817440     1.139128    -1.795016
H      2.831797     2.530748    -2.460732
O     -0.207769     0.664570     3.574688
H     -0.271799     0.802960     4.531812
H     -1.031092     1.048358     3.184293
O     -0.048781    -2.012069     2.706009
H     -0.106493    -1.118360     3.109105
H     -0.840384    -2.111158     2.124604
O      0.176746    -2.042790    -2.703148
H      0.209605    -2.960285    -3.049674
H      0.961875    -1.987779    -2.105980
O     -3.857548    -0.434157     1.178157
H     -3.453382    -1.303672     1.392567
H     -3.787747    -0.346685     0.195202
O      4.071180     0.110208    -1.143537
H      4.015731     0.140647    -0.154923
H      4.918708     0.545241    -1.376191
O      0.041011     0.671019    -3.547344
H      0.087236    -0.291449    -3.374588
H      0.843367     1.062172    -3.140130
O      3.853537    -0.003345     1.564857
H      3.458679    -0.894434     1.688995
H      3.160569     0.639340     1.857047
O     -3.860520    -0.166270    -1.537473
H     -4.763201     0.186100    -1.690524
H     -3.234771     0.542624    -1.837086
O      1.160511     3.070533     0.025500
H      1.423454     2.557826    -0.775473
H      0.180294     3.166012     0.003653
O     -1.554787     3.013704     0.043784
H     -2.178588     3.771976     0.058516
H     -1.810511     2.452389     0.815905
O     -2.068948    -5.407659     1.200769
H     -2.723961    -6.065805     1.475736
H     -2.011387    -5.447378     0.207968
O      2.547646    -4.871236    -1.384019
H      2.707182    -3.902605    -1.396240
H      2.449752    -5.095843    -0.435388
O      2.448118    -5.085276     1.426002
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H	3.097967	-5.641074	1.881029
H	1.601705	-5.143705	1.943637
O	-2.025952	-5.149477	-1.470614
H	-2.291238	-4.210847	-1.569416
H	-1.170168	-5.202364	-1.948263
O	0.154311	-4.856821	2.798042
H	0.065843	-3.901953	2.987518
H	-0.618602	-5.100288	2.244765
O	0.340029	-4.843205	-2.914347
H	0.468531	-5.368715	-3.717866
H	1.152337	-4.972096	-2.354973
O	-4.444563	3.367953	-2.229169
H	-3.615231	2.898578	-2.455024
H	-4.241949	3.899904	-1.430973
O	-4.625886	3.272970	2.283590
H	-5.058263	3.693600	3.041829
H	-5.255822	2.584230	1.931711
O	-6.062388	1.261459	1.266681
H	-5.437830	0.513972	1.368013
H	-6.187357	1.360365	0.297709
O	-6.136776	1.410364	-1.524762
H	-6.956765	1.380894	-2.039305
H	-5.621700	2.204462	-1.830159
O	-3.736155	4.703728	0.138956
H	-3.755871	5.668395	0.224947
H	-4.150363	4.328127	0.953353
O	4.223247	3.626483	2.261197
H	3.449564	3.077550	2.499536
H	3.940055	4.129545	1.461250
O	4.360054	3.626856	-2.285240
H	5.114836	3.064885	-1.988716
H	4.683729	4.158883	-3.027357
O	6.202189	1.866768	-1.266579
H	6.243839	1.894399	-0.269781
H	7.110555	1.785723	-1.592765
O	6.022604	1.757081	1.396381
H	5.478580	0.961051	1.559451
H	5.448412	2.497023	1.714667
O	3.254296	4.870075	-0.005383
H	3.717898	4.540736	-0.802768
H	2.394326	4.396857	-0.010807

Table S43. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{63}$ cluster with the undecahedral $(H_2O)_{18}$ hollow cage.

O	2.091018	-2.186228	1.873404
H	1.288126	-2.644975	1.515268
H	2.594496	-2.845215	2.412773
O	-2.361621	-1.354909	-2.353396
H	-2.916908	-1.363206	-1.533266
H	-2.204322	-0.395172	-2.532423
O	2.337521	1.201522	-2.455976
H	2.906807	1.263355	-1.648063
H	2.180099	0.231785	-2.571283

O	-2.013893	2.384994	1.695683
H	-1.199446	2.800364	1.313193
H	-2.493293	3.073625	2.219158
O	-2.236613	-2.028030	1.814004
H	-1.921975	-1.221928	2.296883
H	-2.839833	-1.699291	1.100303
O	2.164540	-1.490313	-2.522594
H	2.660428	-1.949216	-3.244028
H	1.310785	-1.969642	-2.374382
O	-2.194686	1.329778	-2.584972
H	-2.706891	1.751037	-3.317642
H	-1.342571	1.820650	-2.470472
O	2.322133	2.108355	1.696747
H	2.904938	1.715846	0.998587
H	1.984957	1.355292	2.244373
O	-0.098669	-3.283229	0.763766
H	-0.183014	-4.248749	0.960950
H	-0.898428	-2.843561	1.151660
O	-0.115098	-2.775623	-1.905054
H	-0.099742	-2.975787	-0.935872
H	-0.924637	-2.227605	-2.063919
O	0.096188	2.646564	-2.068701
H	0.124128	2.915779	-1.116725
H	0.901958	2.090236	-2.217626
O	-3.851215	-1.112362	-0.120246
H	-4.787291	-1.431231	-0.157663
H	-3.868517	-0.122484	-0.091719
O	3.873083	1.087335	-0.238442
H	3.893479	0.099532	-0.166203
H	4.807180	1.401489	-0.326993
O	0.222315	3.346004	0.550547
H	0.322487	4.320043	0.689484
H	1.007351	2.910685	0.970861
O	3.618481	-1.576595	-0.250263
H	3.065269	-1.646853	-1.068192
H	3.047218	-1.829228	0.519474
O	-3.605589	1.548608	-0.294931
H	-3.079992	1.566214	-1.133681
H	-3.015306	1.883986	0.427558
O	1.337119	0.060248	3.156945
H	1.631840	-0.786325	2.735050
H	1.703358	0.067284	4.075485
O	-1.354584	0.173530	3.102966
H	-0.364779	0.146109	3.134412
H	-1.596846	0.993630	2.604337
O	2.401539	0.108553	5.651373
H	2.938369	-0.716903	5.665405
H	3.015878	0.878840	5.627151
O	-2.335083	0.253486	5.615727
H	-1.977752	0.220424	4.692196
H	-1.534492	0.251513	6.189674
O	0.023262	0.201296	7.098200
H	0.881361	0.190191	6.617203
H	0.117644	0.868417	7.793064
O	3.911599	2.423997	5.494048
H	3.936255	2.951627	4.661623
H	4.821243	2.405090	5.824153
O	3.916522	3.785680	3.070527

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H      3.323735     3.165662     2.573972
H      3.472373     4.661415     2.996969
O      0.359287     6.026985     0.912502
H     -0.492369     6.222754     1.366402
H      0.311886     6.378305    -0.007138
O      2.582410     6.184351     2.596093
H      1.808492     6.156644     1.989661
H      2.304423     6.720810     3.352287
O     -3.699373    -2.175595     5.756078
H     -3.214429    -1.317139     5.734566
H     -3.340032    -2.661200     6.512410
O     -0.324047    -5.938352     1.286905
H     -0.467535    -6.331424     0.394637
H     -1.162529    -6.023568     1.798902
O     -3.470084     4.151016     3.141003
H     -3.521984     3.704955     4.018865
H     -4.369684     4.123041     2.737356
O     -1.907205     6.355714     2.458252
H     -2.503875     7.106000     2.325354
H     -2.476807     5.601498     2.730195
O     -3.506440     2.778262     5.540993
H     -3.086923     1.887505     5.601908
H     -3.179466     3.278157     6.302688
O      6.269416     3.783893     1.592709
H      6.536222     4.706743     1.474852
H      5.431557     3.807600     2.113461
O      6.395465     2.011129    -0.509663
H      6.377733     2.423304    -1.405407
H      6.416622     2.726870     0.167760
O      7.704942    -0.424949    -0.253442
H      8.277949    -0.387267     0.525718
H      7.279292     0.459802    -0.318428
O      6.068166    -2.661623    -0.425258
H      5.160957    -2.270434    -0.356468
H      6.682915    -1.894267    -0.356655
O      3.934394     2.052956    -4.457832
H      4.073931     1.258066    -5.020727
H      3.339785     1.737270    -3.731195
O      6.211671     2.871647    -3.114670
H      6.328646     3.810239    -3.319937
H      5.408278     2.583530    -3.610142
O     -4.037278    -2.315484    -4.241358
H     -3.415071    -1.958894    -3.558177
H     -4.203722    -1.553253    -4.840722
O     -3.762209     2.448141    -4.500496
H     -4.524759     2.823964    -4.000485
H     -3.218246     3.205295    -4.821021
O     -6.373731    -2.059241    -0.247639
H     -6.375930    -2.544099    -1.106548
H     -6.386404    -2.713679     0.489889
O     -6.074191     2.596536    -0.432619
H     -6.681611     1.827195    -0.328026
H     -5.161621     2.214979    -0.380533
O     -7.699628     0.371179    -0.098027
H     -8.477436     0.332675    -0.672842
H     -7.272768    -0.513300    -0.161980
O     -2.559752    -4.550655    -4.982827
H     -3.098133    -3.745957    -4.800144
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H     -2.324780    -4.504229    -5.920764
O      4.141261    -0.361059    -5.858928
H      4.907527    -0.513163    -6.430181
H      3.985657    -1.210108    -5.388114
O      3.661450    -2.716979    -4.428084
H      4.442108    -3.065737    -3.936130
H      3.104313    -3.489583    -4.681678
O     -4.314448     0.015927    -5.764977
H     -5.100518     0.140772    -6.315484
H     -4.131700     0.891141    -5.355807
O     -0.325719    -5.030782    -3.380780
H     -0.256784    -4.204346    -2.839234
H     -1.126233    -4.902561    -3.941078
O      0.220516     4.812748    -3.680299
H      0.182723     4.017716    -3.090582
H      1.019883     4.674965    -4.239528
O      1.909797    -4.776310    -5.010753
H      2.281957    -5.658229    -5.154095
H      1.124468    -4.903962    -4.427265
O     -2.035143     4.466101    -5.260570
H     -2.410510     5.340158    -5.439372
H     -1.241279     4.621462    -4.695423
O     -5.955458     3.354666    -3.086495
H     -6.144695     4.301776    -3.150405
H     -6.042658     3.122799    -2.131323
O      0.332247     6.812671    -1.742363
H      0.333314     6.131407    -2.455087
H      1.021446     7.448738    -1.981694
O     -5.915461     4.147541     1.859727
H     -6.691769     3.984894     2.414476
H     -6.035753     3.592382     1.053311
O      3.553464    -3.974060     3.293479
H      3.041348    -4.807633     3.175014
H      4.397194    -4.075901     2.792123
O     -3.812660    -3.583563     3.349466
H     -3.229164    -2.997665     2.803202
H     -3.817650    -3.165075     4.240878
O      3.725620    -2.322486     5.539792
H      3.640429    -2.944580     4.782992
H      3.681696    -2.867553     6.338344
O      5.916099    -4.186246     1.883403
H      6.701275    -4.033852     2.428573
H      6.039656    -3.642478     1.069822
O      5.896285    -3.545074    -3.035814
H      6.088247    -4.493565    -3.054639
H      5.999965    -3.264294    -2.095438
O      2.458857     4.272020    -5.262413
H      2.988920     3.467357    -5.057260
H      2.234653     4.208544    -6.201979
O     -6.212233    -3.178533    -2.753369
H     -5.469961    -2.845328    -3.311450
H     -7.011109    -3.093203    -3.293242
O      2.007886    -6.206543     2.785213
H      1.184505    -6.139385     2.250460
H      1.804640    -6.813347     3.511264
O     -2.555517    -6.010242     2.909669
H     -3.248644    -6.653063     2.701722
H     -3.022437    -5.165638     3.113128
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O	-6.212257	-3.700723	1.958364
H	-6.938294	-3.590121	2.588990
H	-5.382217	-3.631842	2.486978
O	-0.583851	-6.875165	-1.308923
H	-0.531192	-6.249316	-2.069066
H	-1.328171	-7.463654	-1.499669

Table S44. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{90}$ cluster with the undecahedral $(H_2O)_{18}$ hollow cage.

O	2.261911	-1.436380	2.362429
H	1.472652	-1.993429	2.145507
H	2.777506	-1.912815	3.056762
O	-2.390800	-2.190687	-1.834410
H	-2.970619	-2.051024	-1.045715
H	-2.322506	-1.298473	-2.254571
O	2.470051	0.686058	-2.714330
H	2.999575	1.042451	-1.959641
H	2.401745	-0.282332	-2.533568
O	-2.347023	2.505698	0.994081
H	-1.555905	2.833291	0.497405
H	-2.874137	3.294786	1.264762
O	-2.244518	-1.631261	2.328617
H	-1.992706	-0.705321	2.567224
H	-2.868165	-1.572723	1.564643
O	2.418978	-1.922148	-1.953641
H	2.953979	-2.571675	-2.466669
H	1.559971	-2.336523	-1.699879
O	-2.359385	0.349323	-2.769886
H	-2.869891	0.550116	-3.589784
H	-1.499716	0.835214	-2.798482
O	2.133025	2.670125	0.994201
H	2.794340	2.189135	0.439941
H	1.877365	2.062351	1.732798
O	0.070399	-2.882702	1.675968
H	0.076412	-3.752637	2.149723
H	-0.776023	-2.435478	1.929084
O	0.081466	-2.991091	-1.034020
H	0.082640	-2.977482	-0.043658
H	-0.804327	-2.653559	-1.319837
O	-0.039960	1.755211	-2.628349
H	-0.074282	2.325139	-1.821164
H	0.851523	1.327540	-2.633233
O	-3.997065	-1.505153	0.251083
H	-4.917943	-1.862290	0.281778
H	-4.071744	-0.551819	-0.004951
O	3.965974	1.379071	-0.545803
H	4.040292	0.457903	-0.189791
H	4.886301	1.698605	-0.700631
O	-0.127724	3.270460	-0.368568
H	-0.126381	4.250243	-0.487901
H	0.698143	3.056384	0.135121
O	3.886426	-1.200679	0.207144
H	3.351950	-1.545148	-0.549785

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H      3.314000   -1.297975    1.008727
O     -3.910954    1.027557   -0.658892
H     -3.341594    0.866595   -1.451269
H     -3.370186    1.586518   -0.047856
O      1.290452    1.017782    2.974060
H      1.671263    0.118999    2.813744
H      1.602381    1.302527    3.869407
O     -1.430784    0.889441    2.968128
H     -0.441975    0.934740    2.956161
H     -1.754437    1.505182    2.264491
O      3.811687   -2.711818    4.202285
H      4.024472   -3.600458    3.838502
H      3.246350   -2.834483    5.002919
O     -3.812375   -3.792362   -3.526618
H     -3.380623   -3.164936   -2.899620
H     -4.705454   -3.424194   -3.743767
O      4.072126    1.049935   -4.905473
H      3.573659    0.890471   -4.069921
H      4.959186    0.620941   -4.811238
O     -3.944636    4.608832    1.675125
H     -4.151470    5.092255    0.842395
H     -3.425502    5.212115    2.253831
O     -3.927622   -2.820582    4.120211
H     -4.696591   -2.205837    4.225198
H     -3.312287   -2.366946    3.496920
O      4.085621   -3.559457   -3.371551
H      3.544968   -3.702283   -4.181797
H      4.178047   -4.409103   -2.883654
O     -3.899999    0.810112   -4.968919
H     -3.990227    1.786864   -5.067686
H     -3.291545    0.459897   -5.660686
O      3.685864    4.747241    1.821782
H      3.108593    3.993417    1.549964
H      4.450235    4.332571    2.298268
O      0.091866   -5.227377    3.028214
H      0.876621   -5.728889    2.720179
H     -0.701462   -5.728865    2.695867
O      0.171625   -5.470024   -2.029288
H      0.148474   -4.561666   -1.625681
H      0.157339   -5.315127   -3.000009
O      0.023015    3.263467   -4.878869
H     -0.011351    2.754174   -4.032886
H      0.804449    3.863918   -4.782097
O     -6.571380   -2.405407    0.339440
H     -7.071917   -2.306019   -0.503547
H     -7.035150   -1.854686    1.011504
O      6.548711    2.221213   -0.918890
H      6.962601    2.206081   -0.023500
H      7.100992    1.642351   -1.496958
O     -0.129755    5.989320   -0.587080
H      0.705357    6.243588   -1.050878
H     -0.095535    6.350114    0.328426
O      6.439782   -2.151969    0.389652
H      5.518109   -1.814572    0.288891
H      6.340933   -3.127722    0.525866
O     -6.447353    1.872853   -1.217489
H     -5.530810    1.551104   -1.044701
H     -6.329263    2.738833   -1.683939
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O      2.124937     1.793340     5.429632
H      1.764312     1.130246     6.071966
H      1.732544     2.672163     5.624486
O     -2.410140     1.727628     5.332520
H     -2.030021     1.436749     4.464213
H     -2.134120     2.662209     5.448184
O      1.215903    -0.184787     7.044359
H      1.521701    -1.071339     6.758090
H      0.235661    -0.222537     7.062520
O     -1.579038    -0.195054     7.061965
H     -1.944578    -0.029132     7.943879
H     -1.899097     0.544775     6.485623
O      1.127847     4.387213     5.631648
H      1.409332     4.843586     6.439541
H      0.141346     4.408745     5.639680
O     -1.626318     4.423658     5.538578
H     -2.009307     4.839676     6.326555
H     -1.907336     4.983319     4.775018
O      2.110298    -2.777712     6.331687
H      1.329669    -3.354190     6.081236
H      2.485833    -3.169433     7.134844
O     -2.216695    -2.850901     6.285469
H     -2.023354    -1.915479     6.500132
H     -2.885455    -2.837371     5.563163
O      0.034473    -4.282691     5.667748
H     -0.799313    -3.774340     5.816833
H      0.025558    -4.609856     4.742259
O      4.438432    -5.138972     2.971893
H      4.919796    -5.732478     3.569031
H      3.661156    -5.655036     2.651252
O      2.303982    -6.578518     1.973253
H      2.334234    -7.502792     2.265148
H      2.244740    -6.609314     0.988777
O     -4.521886     5.809772    -0.763754
H     -3.701310     6.068488    -1.252217
H     -5.031247     6.626931    -0.649051
O     -4.393069     3.510651    -4.835475
H     -4.868190     3.858064    -5.605795
H     -3.553917     4.049787    -4.764069
O     -2.159379     4.929743    -4.603308
H     -2.105813     5.377497    -3.734041
H     -1.362877     4.354446    -4.691586
O     -2.260407     6.412088    -2.181216
H     -2.264050     7.338892    -2.466434
H     -1.475010     6.313719    -1.582823
O     -5.959271     4.173957    -2.566363
H     -5.389928     3.951062    -3.333317
H     -5.429927     4.750813    -1.977588
O     -1.978442    -3.279261    -5.525258
H     -2.709629    -3.427305    -4.882449
H     -1.957999    -2.323542    -5.738971
O      2.354502    -0.581563    -6.350895
H      3.048857    -0.068439    -5.880937
H      2.336345    -1.476459    -5.958324
O      2.417651    -3.353688    -5.529327
H      2.705739    -3.766457    -6.357999
H      1.577474    -3.811541    -5.280864
O     -2.069918    -0.566955    -6.456411
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H     -2.300517    -0.704253    -7.387999
H     -1.246487    -0.001820    -6.465144
O      0.149668    -4.709449    -4.759125
H      0.090518    -5.492984    -5.328027
H     -0.631642    -4.142018    -5.011944
O      0.098875     0.982283    -6.550604
H      0.149146     1.787858    -5.991569
H      0.916878     0.452715    -6.404137
O      6.556493    -0.038147    -4.835227
H      7.108932     0.332686    -4.115451
H      6.544884    -1.004774    -4.672853
O      6.569012    -2.731709    -4.078580
H      6.958530    -3.400320    -4.661214
H      5.662439    -3.054478    -3.844231
O      8.063057     0.676429    -2.585859
H      8.128712    -0.264596    -2.250359
H      8.968602     0.997536    -2.710312
O      8.001417    -1.859663    -1.843942
H      7.520559    -2.283604    -2.585922
H      7.422869    -1.956464    -1.050604
O     -4.376345    -5.774334    -1.619337
H     -3.504094    -6.124219    -1.343167
H     -4.191013    -5.113017    -2.321469
O     -4.340541    -5.302953     2.881596
H     -4.241651    -4.422200     3.304521
H     -4.905905    -5.178756     2.082470
O     -2.044666    -6.523710     2.060853
H     -2.018597    -6.532320     1.082585
H     -2.875301    -6.058855     2.330684
O     -1.887581    -6.772441    -0.767311
H     -1.158871    -6.330899    -1.267829
H     -1.811436    -7.718443    -0.963275
O     -5.867962    -5.081324     0.613158
H     -5.334681    -5.269884    -0.192876
H     -6.169089    -4.151772     0.533623
O      4.573457    -5.677293    -1.665174
H      5.112088    -6.375244    -2.069036
H      3.739247    -6.115896    -1.370141
O      6.009327    -4.820195     0.645991
H      5.480125    -5.109266    -0.125944
H      5.449028    -4.954335     1.438374
O      2.206384    -6.766026    -0.799678
H      2.132670    -7.705927    -1.027834
H      1.470605    -6.308377    -1.285851
O     -5.995965     3.375636     2.992253
H     -5.275914     3.853971     2.512115
H     -6.544311     4.061909     3.401632
O     -5.981639    -1.048348     4.417147
H     -5.667074    -0.134075     4.609947
H     -6.582979    -0.964028     3.648523
O     -7.701494    -0.730798     2.206117
H     -8.628186    -0.900634     2.432030
H     -7.662331     0.207299     1.866056
O     -7.571271     1.781009     1.302143
H     -7.201751     1.855678     0.392345
H     -7.008141     2.345642     1.872991
O     -5.163610     1.528373     4.969112
H     -4.195710     1.622764     5.104941
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H	-5.407345	2.172758	4.273342
O	5.786453	-0.875499	4.619447
H	5.097837	-1.572154	4.481714
H	6.310397	-1.166540	5.381048
O	5.720459	3.545257	3.164951
H	6.354469	3.043617	2.611902
H	5.399729	2.907692	3.845861
O	7.536985	2.035281	1.627119
H	7.507411	1.076780	1.907612
H	8.451620	2.328411	1.754689
O	7.440547	-0.523892	2.383704
H	7.118364	-1.141626	1.687951
H	6.855074	-0.659450	3.159023
O	4.880662	1.764935	5.091200
H	5.137009	0.836418	4.915897
H	3.909531	1.763329	5.236192
O	-6.299754	-2.936435	-4.201329
H	-6.883244	-2.823053	-3.421775
H	-6.294704	-2.060205	-4.640934
O	-6.349011	-0.316144	-5.180445
H	-6.705467	-0.127411	-6.061126
H	-5.450840	0.101289	-5.142955
O	-7.928148	-2.214125	-2.037821
H	-8.827957	-2.571929	-2.007421
H	-8.003459	-1.258007	-2.322908
O	-7.887219	0.279335	-2.925038
H	-7.365379	0.193439	-3.750800
H	-7.351022	0.840362	-2.315984
O	4.561343	3.786248	-4.646933
H	5.043071	3.930796	-3.806692
H	4.428028	2.816738	-4.741893
O	4.267926	6.005495	-0.582312
H	4.865548	5.433247	-1.109886
H	4.104190	5.546256	0.273467
O	2.102180	4.985854	-4.474882
H	2.077972	5.462033	-3.619907
H	2.992922	4.563987	-4.529395
O	5.909381	4.475482	-2.247555
H	6.228943	3.687506	-1.739119
H	6.700174	4.985045	-2.480499
O	2.105336	6.496181	-2.049576
H	2.170169	7.424675	-2.320411
H	2.917064	6.314331	-1.494060
O	-2.354918	6.047637	3.415414
H	-1.554485	6.368077	2.926049
H	-2.786281	6.841413	3.768645
O	1.930785	6.049821	3.479000
H	2.606627	5.590966	2.925454
H	1.679729	5.428710	4.194199
O	-0.140928	6.880153	2.049656
H	-0.099290	7.849000	2.070440
H	0.652502	6.561024	2.573828

Table S45. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the dodecahedral $(H_2O)_{20}$ hollow

cage. This structure has the C_i symmetry.

O	-0.749937	3.179639	2.000703
H	0.198104	3.150268	1.749596
H	-1.259993	3.198393	1.162598
O	0.749937	-3.179639	-2.000703
H	-0.198104	-3.150268	-1.749596
H	1.259993	-3.198393	-1.162598
O	1.968027	3.042363	1.345974
H	2.105133	3.023237	0.366186
H	2.466078	3.805809	1.675116
O	-1.968027	-3.042363	-1.345974
H	-2.105133	-3.023237	-0.366186
H	-2.466078	-3.805809	-1.675116
O	-0.340900	2.974204	-2.441626
H	0.552502	2.963185	-2.038620
H	-0.977693	3.067352	-1.703103
O	0.340900	-2.974204	2.441626
H	-0.552502	-2.963185	2.038620
H	0.977693	-3.067352	1.703103
O	2.245290	2.857386	-1.358569
H	2.638200	1.966030	-1.588283
H	2.828895	3.523957	-1.751401
O	-2.245290	-2.857386	1.358569
H	-2.638200	-1.966030	1.588283
H	-2.828895	-3.523957	1.751401
O	-0.827982	0.588911	-3.726391
H	-0.630116	1.443753	-3.276396
H	-0.018544	0.042145	-3.644565
O	0.827982	-0.588911	3.726391
H	0.630116	-1.443753	3.276396
H	0.018544	-0.042145	3.644565
O	2.893325	0.626831	2.434631
H	2.560728	1.477950	2.079346
H	2.134098	0.201901	2.907519
O	-2.893325	-0.626831	-2.434631
H	-2.560728	-1.477950	-2.079346
H	-2.134098	-0.201901	-2.907519
O	2.230623	-3.169892	0.368249
H	2.825684	-2.380306	0.407475
H	2.801063	-3.946779	0.468781
O	-2.230623	3.169892	-0.368249
H	-2.825684	2.380306	-0.407475
H	-2.801063	3.946779	-0.468781
O	3.741054	-0.900486	0.454754
H	3.438877	-0.323887	1.218949
H	4.688284	-1.057441	0.587009
O	-3.741054	0.900486	-0.454754
H	-3.438877	0.323887	-1.218949
H	-4.688284	1.057441	-0.587009
O	1.442051	-1.032215	-3.425374
H	1.185515	-1.853426	-2.920118
H	1.815954	-1.334050	-4.266658
O	-1.442051	1.032215	3.425374
H	-1.185515	1.853426	2.920118
H	-1.815954	1.334050	4.266658
O	3.247270	0.467117	-1.926592
H	2.622326	-0.076088	-2.455617

H	3.427009	-0.036385	-1.102935
O	-3.247270	-0.467117	1.926592
H	-2.622326	0.076088	2.455617
H	-3.427009	0.036385	1.102935

Table S46. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{35}$ cluster with the dodecahedral $(H_2O)_{20}$ hollow cage.

O	2.338522	-0.538333	-2.449475
H	1.512477	-0.312753	-2.931631
H	2.562775	0.234225	-1.877041
O	-2.485782	0.637325	3.482168
H	-1.594198	0.379114	3.797256
H	-2.803188	-0.106901	2.926225
O	-0.104372	0.115750	-3.625103
H	-0.375418	1.006466	-3.286516
H	-0.136140	0.164615	-4.592305
O	0.117978	-0.022873	4.380880
H	0.386697	-0.929675	4.097890
H	0.134737	-0.031668	5.350132
O	1.326914	3.352004	-0.886945
H	0.613286	2.913322	-1.406838
H	2.123924	2.780450	-0.963975
O	-1.196043	-3.228241	1.730324
H	-0.504674	-3.039519	2.402878
H	-1.847659	-2.488313	1.772564
O	-0.792646	2.434106	-2.388793
H	-1.547067	2.212202	-1.784276
H	-1.056273	3.281312	-2.811249
O	0.849171	-2.513447	3.455840
H	1.623806	-2.417960	2.836929
H	1.110346	-3.153520	4.134982
O	0.495238	3.502621	1.727741
H	0.824157	3.389121	0.803480
H	-0.413926	3.118442	1.732286
O	-0.314501	-3.564415	-0.841796
H	-0.559555	-3.390904	0.099196
H	0.659816	-3.446777	-0.902176
O	-1.706273	-1.843434	-2.439935
H	-1.141357	-1.187778	-2.904939
H	-1.115439	-2.401757	-1.876980
O	1.978601	1.868117	3.398496
H	1.331968	1.223262	3.754939
H	1.457793	2.485140	2.834193
O	-3.236598	-1.407190	1.736961
H	-3.289394	-1.072713	0.808685
H	-4.008378	-2.008510	1.812852
O	3.309695	1.465288	-0.877848
H	3.314081	1.135393	0.055207
H	4.256045	1.494849	-1.135480
O	-3.580399	-0.664154	-0.872082
H	-2.879704	-1.080114	-1.435921
H	-4.413884	-1.137204	-1.085432
O	3.492496	0.509376	1.660107

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H      3.032463     1.044915     2.361936
H      4.460495     0.514868     1.811731
O     -2.109498     2.653338     1.734779
H     -2.321109     1.994742     2.446724
H     -2.609779     3.483041     1.886696
O      2.322299    -2.798382    -0.919495
H      2.284241    -1.974527    -1.466135
H      3.168874    -3.233143    -1.161396
O     -2.913527     1.974734    -0.771063
H     -2.621952     2.101228     0.164677
H     -3.280471     1.063643    -0.839189
O      2.824902    -2.121379     1.692778
H      2.534266    -2.346258     0.776010
H      2.993804    -1.146358     1.686517
O      0.414652     5.956813    -1.313184
H     -0.320490     5.738702    -1.923894
H      0.921481     5.122534    -1.227499
O     -1.685742     5.011358    -2.909127
H     -2.490862     4.960975    -2.325167
H     -1.960585     5.419167    -3.743474
O     -0.486898     6.078080     1.294109
H     -0.225300     6.152798     0.345885
H     -0.043214     5.254119     1.594251
O     -3.023013     5.240380     1.412524
H     -2.118097     5.659609     1.391173
H     -3.587520     5.807680     1.957952
O     -3.718114     4.580207    -1.214151
H     -3.529394     4.927141    -0.315209
H     -3.633523     3.606741    -1.122072
O      5.017823    -1.169677    -2.929928
H      4.066517    -0.936034    -2.968668
H      5.440384    -0.456798    -2.405531
O      5.990365     0.900687    -1.300212
H      6.203504     0.589666    -0.386782
H      6.716037     1.477217    -1.581962
O      6.164698    -0.051244     1.253074
H      6.031811    -1.039134     1.218822
H      6.951953     0.110551     1.794055
O      4.971487    -3.417351    -1.477330
H      5.100675    -2.634172    -2.077755
H      5.354134    -4.188969    -1.920224
O      5.517562    -2.646953     1.149971
H      5.454079    -2.962236     0.222712
H      4.587844    -2.603146     1.462760
O     -3.126764    -5.195411     1.284553
H     -2.396295    -4.620493     1.595750
H     -3.922294    -4.624529     1.304211
O     -2.279932    -5.489284    -1.332768
H     -2.652663    -5.470484    -0.420560
H     -1.455729    -4.963964    -1.262157
O     -3.732101    -3.734285    -2.848390
H     -3.050357    -3.037508    -2.944192
H     -3.280021    -4.440176    -2.322866
O     -5.224158    -3.309730     1.288033
H     -5.480021    -3.093061     0.359640
H     -6.045391    -3.463245     1.778329
O     -5.555958    -2.548965    -1.320080
H     -4.965845    -3.071883    -1.934644
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H	-6.417994	-2.458568	-1.752449

Table S47. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{71}$ cluster with the dodecahedral $(H_2O)_{20}$ hollow cage.

O	-1.116773	0.031761	-3.539948
H	-1.383772	0.869311	-3.085466
H	-1.530603	-0.708771	-3.028800
O	-2.437852	-1.833643	2.140809
H	-2.063349	-1.064719	2.639606
H	-1.665603	-2.401962	1.892359
O	2.082179	-2.463738	-2.028952
H	1.905925	-1.648650	-2.562984
H	2.594304	-2.175211	-1.231787
O	2.395063	2.043398	2.167744
H	1.984568	1.313910	2.696578
H	1.649515	2.610235	1.845493
O	-1.818324	2.333258	-2.288214
H	-2.437562	2.133198	-1.543314
H	-2.284042	2.945987	-2.909637
O	3.741418	0.979958	0.078122
H	3.241391	1.377723	0.835164
H	3.317743	1.322785	-0.748868
O	-3.720212	-1.001581	-0.108728
H	-3.283605	-1.302265	0.727165
H	-4.616338	-1.418375	-0.124479
O	0.490702	3.467129	-1.446624
H	-0.348224	3.048763	-1.764370
H	1.233841	2.877224	-1.729439
O	-0.241674	-3.565542	-1.212275
H	0.615418	-3.184981	-1.532533
H	-0.280996	-4.499285	-1.536291
O	1.958779	-2.282218	2.342521
H	1.739468	-1.430165	2.796642
H	2.523035	-2.055329	1.561211
O	2.565873	1.890880	-2.175958
H	2.231846	1.117450	-2.696962
H	3.218464	2.365247	-2.748435
O	-1.394759	0.274907	3.481456
H	-1.625105	1.090481	2.968863
H	-1.794717	0.371626	4.381000
O	-2.243536	-2.012220	-2.164875
H	-2.774321	-1.661899	-1.406639
H	-1.531794	-2.585603	-1.784690
O	-1.986086	2.452051	1.994611
H	-2.499604	2.188565	1.191470
H	-1.142319	2.865116	1.682187
O	-0.343218	-3.422584	1.485759
H	0.502695	-3.006280	1.789287
H	-0.285305	-3.484857	0.499050
O	1.568751	-0.246934	-3.486523
H	1.917652	-0.338079	-4.407874
H	0.585863	-0.141147	-3.549695
O	1.298213	0.022224	3.588697

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H      1.600520     0.030975     4.530605
H      0.312426     0.115473     3.596215
O     -3.431693     1.710714    -0.188865
H     -4.277395     2.221142    -0.223699
H     -3.646287     0.746552    -0.170596
O      3.461656    -1.701365     0.167263
H      3.608020    -0.721806     0.133938
H      4.352206    -2.128978     0.217795
O      0.364302     3.568565     1.242306
H      0.472474     4.504179     1.544468
H      0.428375     3.573657     0.253395
O      5.887298    -2.919241     0.346153
H      6.551081    -2.191719     0.410658
H      5.874045    -3.391636     1.212928
O      6.362573     1.649140     0.175296
H      6.471287     2.213515     0.977368
H      5.401128     1.412724     0.151306
O      4.103827     3.453717     3.723756
H      4.056065     3.031564     4.613605
H      3.478143     2.935183     3.157595
O      3.290095    -3.930024     4.022479
H      2.796736    -3.331380     3.406544
H      2.758111    -4.760184     4.061562
O      2.165215     0.008138     6.164615
H      1.343983     0.074490     6.707034
H      2.543262    -0.893321     6.300702
O      0.349609    -0.462511    -7.555341
H     -0.490707    -0.292678    -7.065415
H      0.373827     0.183975    -8.275356
O     -2.967086     4.020548    -4.078480
H     -3.017385     3.516575    -4.925456
H     -2.329774     4.763364    -4.207247
O      0.897011     5.933223    -2.492328
H      0.748866     5.029381    -2.116354
H      1.761660     5.881399    -2.964758
O      4.402247     3.170325    -3.718079
H      4.452685     2.630729    -4.542297
H      5.259621     3.071980    -3.239125
O      2.601941    -0.515515    -5.983174
H      3.015872    -1.411414    -6.006792
H      1.829513    -0.522495    -6.597717
O     -4.043995    -3.270560     3.786329
H     -3.445125    -2.755278     3.188819
H     -3.595978    -4.138580     3.928060
O     -6.141862    -2.270883    -0.169587
H     -6.203996    -2.782626     0.672673
H     -6.909682    -1.649855    -0.183657
O     -0.380534    -6.133752    -2.104744
H      0.456075    -6.297078    -2.602924
H     -1.118213    -6.126972    -2.760630
O     -3.745034    -3.532049    -3.839794
H     -4.622079    -3.626055    -3.396522
H     -3.204389    -2.974996    -3.225666
O     -0.538081    -5.918288     2.524054
H     -0.463003    -5.008725     2.139199
H     -0.598220    -6.524658     1.748597
O      5.715552    -4.247261     2.746584
H      4.848838    -4.173376     3.213843
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H      5.896206    -5.195190     2.669727
O      3.917521     2.150327     6.159851
H      3.717335     2.703962     6.928063
H      3.288526     1.393101     6.200822
O      0.725801     6.122656     2.105190
H      1.574968     6.120077     2.608551
H      0.857221     6.668391     1.293300
O     -2.782975    -5.707621     4.108673
H     -3.371081    -6.458667     3.943940
H     -2.000244    -5.841582     3.522475
O     -1.955442     0.001722    -6.117207
H     -1.658037     0.005658    -5.172844
H     -2.611376    -0.733014    -6.179953
O      3.292225     5.697701    -3.851846
H      3.972990     6.337467    -3.598344
H      3.725344     4.813438    -3.814624
O      7.629399    -0.793236     0.372660
H      7.202321     0.096271     0.338693
H      8.262932    -0.758557     1.103655
O      6.544544     3.198658     2.458409
H      7.188976     2.870781     3.102040
H      5.692005     3.283020     2.948734
O     -1.209734     6.125692    -4.261396
H     -0.855257     6.313746    -5.142305
H     -0.430016     6.084158    -3.657137
O     -3.165890     2.469053    -6.340885
H     -2.730367     1.583948    -6.302308
H     -2.884205     2.870377    -7.175485
O      4.385918     1.598088    -5.975906
H      3.737619     0.857249    -6.018731
H      4.305564     2.072598    -6.815625
O     -0.673882    -7.518235     0.270515
H     -0.593995    -7.052705    -0.594478
H     -1.460399    -8.077844     0.199416
O     -6.143037    -3.736623    -2.500256
H     -6.149803    -3.252417    -1.640336
H     -6.411528    -4.644211    -2.297473
O     -6.257980    -3.659502     2.196725
H     -5.473697    -3.544585     2.785887
H     -6.367474    -4.614670     2.083264
O      3.302964    -2.488093     6.375605
H      2.976857    -3.054114     7.089857
H      3.287086    -3.042674     5.558964
O      6.699597     2.971303    -2.218401
H      7.475672     2.591541    -2.654752
H      6.616055     2.501471    -1.354072
O      3.568013    -4.226643    -3.448482
H      3.032625    -3.575663    -2.928334
H      4.412492    -4.326450    -2.948639
O     -3.779867    -2.074566    -6.184100
H     -3.810264    -2.604664    -5.351987
H     -4.686138    -1.770095    -6.336277
O      5.873949    -4.471238    -1.941194
H      6.707869    -4.323616    -2.409777
H      5.919189    -3.918049    -1.126825
O      2.031574    -6.506118    -3.366099
H      2.000515    -6.879187    -4.258703
H      2.603630    -5.703241    -3.425191
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O	3.802741	-2.986926	-5.902585
H	4.737959	-2.956943	-6.150694
H	3.768117	-3.442606	-5.027647
O	-5.597489	3.351464	-0.318557
H	-5.468525	3.873902	-1.146213
H	-5.514223	3.975752	0.442577
O	-8.043433	2.123774	-0.203369
H	-7.162455	2.564345	-0.268977
H	-8.614292	2.572847	-0.843233
O	-5.232180	4.714525	-2.674514
H	-4.455072	4.465453	-3.227312
H	-5.998949	4.694157	-3.264940
O	-4.144800	-1.707469	6.054230
H	-4.136981	-2.286106	5.254352
H	-5.077087	-1.545195	6.257642
O	1.744488	-6.221628	4.035922
H	0.918400	-6.144429	3.500776
H	1.463751	-6.509963	4.916306
O	-2.472840	0.475124	5.969358
H	-2.966610	1.329257	5.984124
H	-3.129804	-0.258958	6.026283
O	-0.195446	0.364936	7.526600
H	-1.030850	0.376006	7.003755
H	-0.376056	-0.172128	8.311135
O	3.044839	5.995024	3.575234
H	3.433358	5.093381	3.678642
H	2.936901	6.343174	4.472008
O	-1.577167	6.444272	3.594534
H	-0.740966	6.362968	3.079299
H	-1.316732	6.737436	4.479464
O	-3.294050	4.284888	3.507995
H	-2.819464	3.618225	2.950984
H	-2.680739	5.055134	3.575879
O	1.016740	7.524958	-0.242918
H	0.970259	6.981367	-1.065711
H	0.364443	8.231578	-0.353785
O	-3.649533	2.960270	5.901659
H	-3.546020	3.457974	5.055520
H	-4.585125	3.028850	6.139943
O	-5.394412	4.980001	1.877555
H	-6.207838	4.975542	2.402476
H	-4.665858	4.743596	2.501052
O	-2.512270	-5.991768	-3.832443
H	-2.329509	-6.235785	-4.751197
H	-2.951824	-5.107943	-3.867406
O	-8.300355	-0.597260	-0.315918
H	-8.169170	0.379852	-0.273668
H	-8.989151	-0.800167	0.333247

Table S48. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{100}$ cluster with the dodecahedral $(H_2O)_{20}$ hollow cage. This structure has the C_i symmetry.

O	0.055463	-0.036577	7.737937

O	5.164891	-0.002241	3.961131
O	-5.689167	3.731202	3.829973
O	-0.770963	2.073050	3.100439
O	-2.342685	-3.743237	6.424625
O	-1.148190	-0.580392	3.594628
O	6.344783	-2.519272	3.790095
O	-3.975963	2.992360	5.935828
O	2.995605	0.001790	2.317290
O	1.193866	-1.872963	3.115929
O	0.098899	-5.035431	5.895471
O	-6.223370	-0.540520	4.615213
O	7.006470	-3.081248	1.287897
O	2.095074	-3.195632	5.325424
O	2.343984	-1.292200	7.299582
O	3.064645	3.011092	6.480848
O	3.123415	4.157069	3.976680
O	-5.105180	-2.582925	3.116412
O	0.392746	2.636732	7.270039
O	-4.155751	-4.708265	4.625797
O	-6.428462	0.982423	0.404817
O	-7.025299	1.468858	3.082559
O	3.743063	-0.578217	-0.233766
O	4.516936	-4.357623	4.649165
O	-4.355954	0.414179	6.458382
O	4.217618	0.613723	6.479736
O	-2.986550	-1.500121	1.815771
O	-2.011976	-1.008225	6.145517
O	-1.733606	-7.469967	-1.287479
O	4.133928	-4.751297	-1.775996
O	-6.868205	-1.975581	-3.026633
O	-1.804963	-2.447414	-2.314262
O	-2.955666	-6.480649	3.073624
O	-1.790986	-3.372645	0.243758
O	5.619776	-5.365055	0.468174
O	-5.704824	-4.350521	-3.044545
O	2.386464	-2.790423	-1.039334
O	0.800376	-3.571881	1.034123
O	-0.296773	-6.741050	3.888385
O	-6.853864	-3.465015	1.248880
O	1.398243	-6.121855	1.781530
O	0.951481	-7.670116	-0.480817
O	0.933500	-6.197424	-4.602946
O	1.351537	-3.552066	-5.312896
O	-1.714695	-6.539471	-3.782860
O	-7.621648	-1.368079	-0.466481
O	4.060124	-6.103832	2.490694
O	-5.615325	-5.335871	-0.424366
O	2.511846	-6.870800	-2.582076
O	-3.079780	-5.757643	0.412640
O	1.733606	7.469967	1.287479
O	-4.133928	4.751297	1.775996
O	6.868205	1.975581	3.026633
O	1.804963	2.447414	2.314262
O	2.955666	6.480649	-3.073624
O	1.790986	3.372645	-0.243758
O	-5.619776	5.365055	-0.468174
O	5.704824	4.350521	3.044545
O	-2.386464	2.790423	1.039334

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O     -0.800376     3.571881    -1.034123
O      0.296773     6.741050    -3.888385
O      6.853864     3.465015    -1.248880
O     -7.006470     3.081248    -1.287897
O     -1.398243     6.121855    -1.781530
O     -0.951481     7.670116     0.480817
O     -0.933500     6.197424     4.602946
O     -1.351537     3.552066     5.312896
O      5.105180     2.582925    -3.116412
O      1.714695     6.539471     3.782860
O      4.155751     4.708265    -4.625797
O      6.428462    -0.982423    -0.404817
O      7.621648     1.368079     0.466481
O     -3.743063     0.578217     0.233766
O     -4.060124     6.103832    -2.490694
O      5.615325     5.335871     0.424366
O     -2.511846     6.870800     2.582076
O      2.986550     1.500121    -1.815771
O      3.079780     5.757643    -0.412640
O     -0.055463     0.036577    -7.737937
O     -5.164891     0.002241    -3.961131
O      5.689167    -3.731202    -3.829973
O      0.770963    -2.073050    -3.100439
O      2.342685     3.743237    -6.424625
O      1.148190     0.580392    -3.594628
O     -6.344783     2.519272    -3.790095
O      3.975963    -2.992360    -5.935828
O     -2.995605    -0.001790    -2.317290
O     -1.193866     1.872963    -3.115929
O     -0.098899     5.035431    -5.895471
O      6.223370     0.540520    -4.615213
O     -2.095074     3.195632    -5.325424
O     -2.343984     1.292200    -7.299582
O     -3.064645    -3.011092    -6.480848
O     -3.123415    -4.157069    -3.976680
O     -0.392746    -2.636732    -7.270039
O      7.025299    -1.468858    -3.082559
O     -4.516936     4.357623    -4.649165
O      4.355954    -0.414179    -6.458382
O     -4.217618    -0.613723    -6.479736
O      2.011976     1.008225    -6.145517
H      2.326318    -0.658864     2.624049
H      2.554909     0.887350     2.331383
H      2.253083     2.719539    -0.825863
H      2.272642     4.233327    -0.328748
H      1.820137    -2.555171    -1.816197
H      3.007070    -3.501452    -1.332316
H      0.299754     1.073551    -3.469210
H      1.446402     0.746816    -4.522167
H     -0.299754    -1.073551     3.469210
H     -1.446402    -0.746816     4.522167
H     -1.820137     2.555171     1.816197
H     -3.007070     3.501452     1.332316
H     -2.253083    -2.719539     0.825863
H     -2.272642    -4.233327     0.328748
H     -2.326318     0.658864    -2.624049
H     -2.554909    -0.887350    -2.331383
H     -1.061316     2.520789    -2.379419
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H	-1.527511	2.378988	-3.896279
H	-1.825763	-2.820620	-1.398194
H	-2.288577	-3.081423	-2.898880
H	-3.252603	1.392958	0.507916
H	-3.470427	0.382803	-0.697191
H	1.367042	-3.303026	0.269406
H	-0.139008	-3.507168	0.729455
H	-0.884423	1.109667	3.292910
H	0.171533	2.201575	2.828393
H	2.323579	1.151789	-2.462958
H	3.261296	0.734668	-1.251558
H	0.139008	3.507168	-0.729455
H	-1.367042	3.303026	-0.269406
H	0.884423	-1.109667	-3.292910
H	-0.171533	-2.201575	-2.828393
H	-2.323579	-1.151789	2.462958
H	-3.261296	-0.734668	1.251558
H	1.061316	-2.520789	2.379419
H	1.527511	-2.378988	3.896279
H	1.825763	2.820620	1.398194
H	2.288577	3.081423	2.898880
H	3.470427	-0.382803	0.697191
H	3.252603	-1.392958	-0.507916
H	-1.084103	7.137138	-0.334388
H	-0.005265	7.581782	0.720917
H	-1.130432	3.031266	4.502687
H	-1.212871	4.497994	5.077878
H	4.894019	5.165930	-5.056361
H	3.714037	5.385297	-4.031550
H	-3.101096	6.107917	-2.264697
H	-4.170793	5.490345	-3.247059
H	-4.534206	3.273611	5.180896
H	-3.045144	3.214734	5.700639
H	2.009112	6.571594	-3.318507
H	2.983816	6.241284	-2.118915
H	-6.233146	6.098310	-0.308355
H	-5.026047	5.657785	-1.217941
H	0.723017	4.532288	-6.075261
H	-0.803294	4.375516	-5.707271
H	-4.702026	0.362431	7.362168
H	-4.199935	1.385205	6.275429
H	-4.733142	4.411058	2.478163
H	-4.696143	4.978236	0.999267
H	-3.088909	6.131435	2.291105
H	-1.966987	7.132005	1.800007
H	0.794319	6.377912	4.084487
H	2.201106	5.690218	3.877052
H	3.140106	3.763151	4.880128
H	4.061177	4.236105	3.682226
H	-2.976727	3.590623	-5.138672
H	-2.218358	2.535518	-6.047568
H	2.128768	8.354127	1.318214
H	1.742147	7.127397	2.226245
H	-4.912217	4.860979	-5.377288
H	-5.199730	3.697777	-4.369344
H	2.187652	1.967728	-6.272876
H	2.863785	0.533145	-6.285833
H	3.021155	4.104524	-5.801208

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H      2.631526     3.999694    -7.313822
H     -6.204133     2.929860     3.561562
H     -6.339071     4.368701     4.163197
H      0.138078     7.633282    -4.231985
H      0.132470     6.115045    -4.649476
H     -1.543544     6.455607     3.851357
H     -1.130841     6.803900     5.332674
H     -0.806318     6.357288    -2.531602
H     -1.161312     5.198420    -1.521029
H     -7.123888    -1.730749    -2.104098
H     -6.272251    -1.263456    -3.351212
H     -4.763198    -3.332364     3.655582
H     -4.323841    -2.195188     2.647143
H     -1.308156    -2.797695    -6.958794
H      0.206151    -2.992586    -6.576363
H     -7.163342     2.540725    -4.309035
H     -6.607431     2.722060    -2.843975
H     -5.812705    -1.276682     4.107731
H     -5.551677    -0.234512     5.262767
H     -3.512694    -2.117104    -6.482718
H     -3.525884    -3.546732    -7.143482
H     -6.803789     2.348428    -0.661471
H     -6.516163     3.869534    -0.968566
H     -2.609285     1.677074    -8.148596
H     -1.469408     0.830326    -7.464619
H     -6.639635     1.158007     1.348825
H     -5.451033     0.840358     0.359468
H     -7.209307    -0.538504    -0.137374
H     -7.346201    -2.075350     0.153170
H     -5.653716    -4.971835    -1.334963
H     -6.061189    -4.681362     0.154752
H     -2.641557    -6.390370    -0.201860
H     -4.008100    -5.628410     0.085535
H     -6.149032    -3.451236    -3.054157
H     -6.256678    -4.930667    -3.590580
H     -0.146353    -0.928453    -7.544144
H      0.682818     0.369461    -7.182582
H     -6.733911     0.700014     3.655348
H     -7.983987     1.548151     3.203081
H     -3.570588     0.076340    -6.741742
H     -4.557122    -0.361568    -5.590440
H     -7.622448    -3.831114     1.711783
H     -6.227685    -3.155866     1.954122
H     -4.380530     0.021399    -3.359535
H     -5.583472     0.889847    -3.900166
H      6.272251     1.263456     3.351212
H      7.123888     1.730749     2.104098
H      4.763198     3.332364    -3.655582
H      4.323841     2.195188    -2.647143
H      1.308156     2.797695     6.958794
H     -0.206151     2.992586     6.576363
H      7.163342    -2.540725     4.309035
H      6.607431    -2.722060     2.843975
H      5.812705     1.276682    -4.107731
H      5.551677     0.234512    -5.262767
H      3.525884     3.546732     7.143482
H      3.512694     2.117104     6.482718
H      6.803789    -2.348428     0.661471
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H      6.516163    -3.869534     0.968566
H      1.469408    -0.830326     7.464619
H      2.609285    -1.677074     8.148596
H      4.199935    -1.385205    -6.275429
H      4.702026    -0.362431    -7.362168
H      5.451033    -0.840358    -0.359468
H      6.639635    -1.158007    -1.348825
H      7.346201     2.075350    -0.153170
H      7.209307     0.538504     0.137374
H      5.653716     4.971835     1.334963
H      6.061189     4.681362    -0.154752
H      2.641557     6.390370     0.201860
H      4.008100     5.628410    -0.085535
H      2.218358    -2.535518     6.047568
H      2.976727    -3.590623     5.138672
H      6.256678     4.930667     3.590580
H      6.149032     3.451236     3.054157
H      4.912217    -4.860979     5.377288
H      5.199730    -3.697777     4.369344
H     -2.187652    -1.967728     6.272876
H     -2.863785    -0.533145     6.285833
H      0.146353     0.928453     7.544144
H     -0.682818    -0.369461     7.182582
H      6.733911    -0.700014    -3.655348
H      7.983987    -1.548151    -3.203081
H      4.557122     0.361568     5.590440
H      3.570588    -0.076340     6.741742
H      7.622448     3.831114    -1.711783
H      6.227685     3.155866    -1.954122
H      5.583472    -0.889847     3.900166
H      4.380530    -0.021399     3.359535
H      1.084103    -7.137138     0.334388
H      0.005265    -7.581782    -0.720917
H      1.212871    -4.497994    -5.077878
H      1.130432    -3.031266    -4.502687
H     -3.714037    -5.385297     4.031550
H     -4.894019    -5.165930     5.056361
H      4.170793    -5.490345     3.247059
H      3.101096    -6.107917     2.264697
H      4.534206    -3.273611    -5.180896
H      3.045144    -3.214734    -5.700639
H     -2.983816    -6.241284     2.118915
H     -2.009112    -6.571594     3.318507
H      5.026047    -5.657785     1.217941
H      6.233146    -6.098310     0.308355
H     -0.723017    -4.532288     6.075261
H      0.803294    -4.375516     5.707271
H      4.696143    -4.978236    -0.999267
H      4.733142    -4.411058    -2.478163
H      3.088909    -6.131435    -2.291105
H      1.966987    -7.132005    -1.800007
H     -0.794319    -6.377912    -4.084487
H     -2.201106    -5.690218    -3.877052
H     -4.061177    -4.236105    -3.682226
H     -3.140106    -3.763151    -4.880128
H     -2.128768    -8.354127    -1.318214
H     -1.742147    -7.127397    -2.226245
H     -3.021155    -4.104524     5.801208
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H	-2.631526	-3.999694	7.313822
H	6.339071	-4.368701	-4.163197
H	6.204133	-2.929860	-3.561562
H	-0.138078	-7.633282	4.231985
H	-0.132470	-6.115045	4.649476
H	1.130841	-6.803900	-5.332674
H	1.543544	-6.455607	-3.851357
H	0.806318	-6.357288	2.531602
H	1.161312	-5.198420	1.521029

Table S49. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the tetradecahedral $(H_2O)_{24}$ hollow cage. This structure has the C_3 symmetry.

O	-1.6519945411	2.1795351427	-2.9961715645
O	-1.0615355315	-2.5204368109	-2.9961715645
O	2.7135300726	0.3409016681	-2.9961715645
H	-2.0007232282	2.5929832034	-3.8002621144
H	-1.2452277116	-3.0291687433	-3.8002621144
H	3.2459509399	0.4361855399	-3.8002621144
H	-2.0149045609	1.2502021470	-2.9856799324
H	-0.0752545387	-2.3700596094	-2.9856799324
H	2.0901590996	1.1198574624	-2.9856799324
O	-2.7016245466	-0.2694287492	-2.9447873962
O	1.5841444146	-2.2049611143	-2.9447873962
O	1.1174801320	2.4743898634	-2.9447873962
H	-3.2972635007	-0.3993358757	-2.1762606397
H	1.9944667633	-2.6558460168	-2.1762606397
H	1.3027967374	3.0551818924	-2.1762606397
H	-2.0864093345	-1.0347676232	-2.9541452561
H	1.9393397160	-1.2894996748	-2.9541452561
H	0.1470696185	2.3242672980	-2.9541452561
O	-2.4913685063	1.1054592276	3.0061704835
O	0.2883284792	-2.7103180304	3.0061704835
O	2.2030400271	1.6048588029	3.0061704835
H	-1.6712144119	1.6733228077	2.9899638656
H	-0.6135328542	-2.2839755398	2.9899638656
H	2.2847472662	0.6106527320	2.9899638656
H	-2.9631735212	1.3403717974	3.8193240221
H	0.3207907335	-3.2363694439	3.8193240221
H	2.6423827877	1.8959976464	3.8193240221
O	-0.3561409658	2.6985840443	2.9318435292
O	-2.1589718537	-1.6577191458	2.9318435292
O	2.5151128195	-1.0408648985	2.9318435292
H	0.5311890576	2.2783682600	2.9332800885
H	-2.2387193211	-0.6791609119	2.9332800885
H	1.7075302636	-1.5992073481	2.9332800885
H	-0.3903626234	3.2924800040	2.1513267181
H	-2.6561900133	-1.9843039506	2.1513267181
H	3.0465526367	-1.3081760535	2.1513267181
O	-4.4117306718	-0.5825090008	-0.7496492312
O	2.7103329285	-3.5294163360	-0.7496492312
O	1.7013977433	4.1119253368	-0.7496492312
H	-5.3302239275	-0.7266934798	-1.0228524542
H	3.2944469780	-4.2527625892	-1.0228524542

H	2.0357769495	4.9794560690	-1.0228524542
H	-4.1514454372	-1.3763806700	-0.2193382614
H	3.2677033441	-2.9070668761	-0.2193382614
H	0.8837420931	4.2834475461	-0.2193382614
O	-2.5961731748	3.5346366908	-0.7334118023
O	-1.7629985800	-4.0156702674	-0.7334118023
O	4.3591717548	0.4810335766	-0.7334118023
H	-2.2741289838	3.0583078007	-1.5289003613
H	-1.5115077561	-3.4986073718	-1.5289003613
H	3.7856367399	0.4402995711	-1.5289003613
H	-3.1245426203	2.8812261136	-0.2123129628
H	-0.9329436983	-4.1465463412	-0.2123129628
H	4.0574863186	1.2653202276	-0.2123129628
O	-4.0320575668	1.7550240675	0.7598328653
O	0.4961333566	-4.3693763161	0.7598328653
O	3.5359242101	2.6143522486	0.7598328653
H	-3.5087226082	1.5020514188	1.5502037516
H	0.4535466176	-3.7896686230	1.5502037516
H	3.0551759906	2.2876172042	1.5502037516
H	-4.1868485219	0.9283787238	0.2566463187
H	1.2894247018	-4.0901065437	0.2566463187
H	2.8974238201	3.1617278199	0.2566463187
O	-0.5699582891	4.3946905497	0.7221976620
O	-3.5209345133	-2.6909436323	0.7221976620
O	4.0908928024	-1.7037469174	0.7221976620
H	-1.3511873701	4.0917066111	0.1692893685
H	-2.8679281849	-3.2160158934	0.1692893685
H	4.2191155551	-0.8756907177	0.1692893685
H	-0.7653328625	5.3021624434	1.0007643725
H	-4.2091409398	-3.3138789230	1.0007643725
H	4.9744738022	-1.9882835205	1.0007643725

Table S50. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{45}$ cluster with the tetradecahedral $(H_2O)_{24}$ hollow cage. This structure has the C_3 symmetry.

O	-2.635140	-0.597178	3.032615
O	0.800399	2.580687	3.032615
O	1.834741	-1.983509	3.032615
H	-2.842045	-0.664532	3.990755
H	0.845521	2.793549	3.990755
H	1.996524	-2.129017	3.990755
H	-2.307378	0.327018	2.911125
H	1.436894	1.834739	2.911125
H	0.870483	-2.161757	2.911125
O	-0.825985	4.227611	-0.566676
O	4.074211	-1.398481	-0.566676
O	-3.248226	-2.829130	-0.566676
H	0.000000	4.301768	-0.019556
H	3.725440	-2.150884	-0.019556
H	-3.725440	-2.150884	-0.019556
H	-0.655945	3.591611	-1.299228
H	3.438399	-1.227741	-1.299228
H	-2.782454	-2.363871	-1.299228

O	-2.987682	3.382242	0.805432
O	4.422948	0.896287	0.805432
O	-1.435267	-4.278529	0.805432
H	-2.177252	3.678939	0.315486
H	4.274681	0.046086	0.315486
H	-2.097428	-3.725025	0.315486
H	-3.663657	4.069431	0.625527
H	5.356059	1.138104	0.625527
H	-1.692402	-5.207536	0.625527
O	-2.617881	0.742864	-2.755089
O	1.952280	1.895719	-2.755089
O	0.665601	-2.638583	-2.755089
H	-3.098501	0.822454	-1.896797
H	2.261517	2.272154	-1.896797
H	0.836985	-3.094608	-1.896797
H	-2.395655	-0.208901	-2.876377
H	1.016914	2.179148	-2.876377
H	1.378741	-1.970247	-2.876377
O	-4.485764	-0.996659	0.980351
O	1.379750	4.383115	0.980351
O	3.106014	-3.386456	0.980351
H	-3.904579	-0.868693	1.761461
H	1.199979	3.815811	1.761461
H	2.704600	-2.947118	1.761461
H	-4.441732	-0.154167	0.477105
H	2.087353	3.923736	0.477105
H	2.354379	-3.769569	0.477105
O	-4.128591	1.296387	-0.545055
O	3.187000	2.927272	-0.545055
O	0.941592	-4.223659	-0.545055
H	-3.652474	1.994120	-0.031298
H	3.553196	2.166075	-0.031298
H	0.099278	-4.160196	-0.031298
H	-4.881719	1.772918	-0.956982
H	3.976251	3.341234	-0.956982
H	0.905468	-5.114152	-0.956982
O	-0.683222	2.668722	-2.830227
O	2.652792	-0.742673	-2.830227
O	-1.969570	-1.926049	-2.830227
H	-1.089325	3.307765	-3.456086
H	3.409271	-0.710499	-3.456086
H	-2.319946	-2.597266	-3.456086
H	-1.321368	1.915367	-2.777284
H	2.319440	0.186654	-2.777284
H	-0.998073	-2.102021	-2.777284
O	-1.873824	2.024629	2.932177
O	2.690292	0.610465	2.932177
O	-0.816468	-2.635094	2.932177
H	-0.909348	2.201216	2.819325
H	2.360983	-0.313089	2.819325
H	-1.451635	-1.888127	2.819325
H	-2.348853	2.578519	2.273856
H	3.407490	0.744907	2.273856
H	-1.058636	-3.323426	2.273856
O	-2.559555	5.921403	-1.891805
O	6.407863	-0.744062	-1.891805
O	-3.848308	-5.177341	-1.891805
H	-1.839567	5.480560	-1.389374

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H      5.666088    -1.147169    -1.389374
H     -3.826521    -4.333392    -1.389374
H     -2.538239     5.498761    -2.777273
H      6.031187    -0.551201    -2.777273
H     -3.492947    -4.947560    -2.777273
O     -4.698136     5.167808    -0.483405
O      6.824521     1.484801    -0.483405
O     -2.126385    -6.652609    -0.483405
H     -3.965989     5.539167    -1.051066
H      6.780054     0.665064    -1.051066
H     -2.814065    -6.204231    -1.051066
H     -5.208270     5.918855    -0.145512
H      7.730014     1.551066    -0.145512
H     -2.521744    -7.469921    -0.145512
O     -4.236774     2.558836    -4.094429
O      4.334404     2.389736    -4.094429
O     -0.097630    -4.948572    -4.094429
H     -4.860128     2.787882    -3.373204
H      4.844441     2.815053    -3.373204
H      0.015688    -5.602935    -3.373204
H     -3.718266     1.796852    -3.755388
H      3.415253     2.321687    -3.755388
H      0.303013    -4.118539    -3.755388
O     -5.822104     3.084208    -1.835544
O      5.582055     3.499986    -1.835544
O      0.240049    -6.584194    -1.835544
H     -5.557044     3.913521    -1.368567
H      6.167730     2.855781    -1.368567
H     -0.610686    -6.769302    -1.368567
H     -6.790037     3.074296    -1.872297
H      6.057437     4.343196    -1.872297
H      0.732600    -7.417493    -1.872297
O     -2.324465     4.420432    -4.233120
O      4.990439    -0.197170    -4.233120
O     -2.665974    -4.223262    -4.233120
H     -2.194328     4.793795    -5.117253
H      5.248713    -0.496553    -5.117253
H     -3.054384    -4.297242    -5.117253
H     -3.096469     3.793154    -4.284832
H      4.833202     0.785044    -4.284832
H     -1.736733    -4.578198    -4.284832
O     -2.659185    -0.579917     5.819469
O      0.827370     2.592880     5.819469
O      1.831815    -2.012963     5.819469
H     -3.445487    -0.689547     6.374344
H      1.125579     3.328653     6.374344
H      2.319909    -2.639106     6.374344
H     -2.367435     0.368046     5.910917
H      1.502455     1.866236     5.910917
H      0.864981    -2.234282     5.910917
O     -1.896448     1.981200     5.709984
O      2.663993     0.651773     5.709984
O     -0.767545    -2.632972     5.709984
H     -0.947275     2.157132     5.883874
H      2.341769    -0.258201     5.883874
H     -1.394493    -1.898931     5.883874
H     -2.007713     2.138869     4.747182
H      2.856171     0.669296     4.747182
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H	-0.848459	-2.808165	4.747182

Table S51. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{84}$ cluster with the tetradecahedral $(H_2O)_{24}$ hollow cage. This structure has the C_3 symmetry.

O	1.1647695187	-4.1645735884	-0.7473501735
O	3.0242417642	3.0910067870	-0.7473501735
O	-4.1890112829	1.0735668015	-0.7473501735
H	1.4518843686	-5.0845212470	-0.9700617071
H	3.6773823816	3.7996293701	-0.9700617071
H	-5.1292667503	1.2848918769	-0.9700617071
H	1.8841196636	-3.7664254196	-0.1948143991
H	2.3197602631	3.5149082022	-0.1948143991
H	-4.2038799266	0.2515172174	-0.1948143991
O	0.7353833535	-2.6360127792	-2.9666270616
O	1.9151623548	1.9548670552	-2.9666270616
O	-2.6505457082	0.6811457240	-2.9666270616
H	0.9088938177	-3.1700185697	-2.1524377083
H	2.2908697030	2.3721344204	-2.1524377083
H	-3.1997635207	0.7978841494	-2.1524377083
H	1.3938082808	-1.8990730624	-2.9676320242
H	0.9477413753	2.1566099103	-2.9676320242
H	-2.3415496561	-0.2575368479	-2.9676320242
O	-1.9096380813	-1.9521883389	-2.9861641136
O	2.6454637351	-0.6777009210	-2.9861641136
O	-0.7358256538	2.6298892598	-2.9861641136
H	-2.3124026707	-2.4144587980	-3.7617882475
H	3.2471839908	-0.7953700576	-3.7617882475
H	-0.9347813201	3.2098288556	-3.7617882475
H	-0.9424655104	-2.1559485424	-3.0037482772
H	2.3383389621	0.2617751970	-3.0037482772
H	-1.3958734518	1.8941733453	-3.0037482772
O	-1.0681320933	-4.1922885786	0.7769523761
O	4.1646944557	1.1711147619	0.7769523761
O	-3.0965623624	3.0211738167	0.7769523761
H	-0.2426758004	-4.2240441002	0.2299627439
H	3.7794673977	1.9018586421	0.2299627439
H	-3.5367915973	2.3221854582	0.2299627439
H	-1.3050672371	-5.1290275736	0.9880700211
H	5.0944017940	1.4342924058	0.9880700211
H	-3.7893345569	3.6947351678	0.9880700211
O	-3.0077499658	-3.0894312421	-0.7569702661
O	4.1794009218	-1.0600722576	-0.7569702661
O	-1.1716509560	4.1495034996	-0.7569702661
H	-2.5900947906	-2.6892562011	-1.5591566634
H	3.6240115827	-0.8984597863	-1.5591566634
H	-1.0339167921	3.5877159874	-1.5591566634
H	-2.2811507384	-3.5045997170	-0.2272171819
H	4.1756477542	-0.2232346308	-0.2272171819
H	-1.8944970158	3.7278343478	-0.2272171819
O	-4.1441100112	-1.1631847024	0.7661363507
O	3.0794025072	-3.0073121945	0.7661363507
O	1.0647075040	4.1704968970	0.7661363507

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H  -3.7092444650  -1.8729167569   0.2296443358
H   3.4766157232  -2.2758415571   0.2296443358
H   0.2326287419   4.1487583140   0.2296443358
H  -3.5808680342  -1.0181005518   1.5664591637
H   2.6721349585  -2.5920724093   1.5664591637
H   0.9087330756   3.6101729611   1.5664591637
O  -2.6357243191  -0.7366982838   2.9957606926
O   1.9558615882  -1.9142550758   2.9957606926
O   0.6798627309   2.6509533596   2.9957606926
H  -3.2357289714  -0.8752992895   3.7695367941
H   2.3758959064  -2.3645738442   3.7695367941
H   0.8598330651   3.2398731338   3.7695367941
H  -2.3474491147   0.2084063964   3.0188804271
H   0.9932393237  -2.1371537656   3.0188804271
H   1.3542097909   1.9287473692   3.0188804271
O  -0.6764756775  -2.6466241191   2.9861708202
O   2.6302815602   0.7374669378   2.9861708202
O  -1.9538058827   1.9091571813   2.9861708202
H  -0.8364616842  -3.1872258938   2.1734159052
H   3.1784494338   0.8692158791   2.1734159052
H  -2.3419877495   2.3180100148   2.1734159052
H  -1.3529952967  -1.9266186445   2.9870786889
H   2.3449983379  -0.2084189759   2.9870786889
H  -0.9920030412   2.1350376204   2.9870786889
O   1.9081131508  -6.7186902892  -1.3444986143
O   4.8644998952   5.0118196065  -1.3444986143
O  -6.7726130460   1.7068706827  -1.3444986143
H   1.9832086638  -6.7818456257  -2.3274859015
H   4.8816462645   5.1084318967  -2.3274859015
H  -6.8648549283   1.6734137290  -2.3274859015
H   2.8015181862  -6.8869862629  -0.9581025118
H   4.5635459661   5.8696790498  -0.9581025118
H  -7.3650641523   1.0173072131  -0.9581025118
O  -1.7529295007  -6.7812328433   1.3114146831
O   6.7491846617   1.8725349430   1.3114146831
O  -4.9962551610   4.9086979003   1.3114146831
H  -1.1048775997  -7.3503216564   0.8294965529
H   6.9180040803   2.7183087588   0.8294965529
H  -5.8131264806   4.6320128977   0.8294965529
H  -2.6332725695  -6.9444886875   0.8933329046
H   7.3307399044   1.1917634035   0.8933329046
H  -4.6974673349   5.7527252840   0.8933329046
O  -1.0902159964  -4.3282097801   5.0993461428
O   4.2934476207   1.2199501416   5.0993461428
O  -3.2032316243   3.1082596386   5.0993461428
H  -1.3095760228  -5.2113603700   4.7148337650
H   5.1679584801   1.4715540811   4.7148337650
H  -3.8583824573   3.7398062890   4.7148337650
H  -0.9430003158  -3.7217857022   4.3319672818
H   3.6946611234   1.0442306218   4.3319672818
H  -2.7516608076   2.6775550803   4.3319672818
O  -6.7137144747  -1.8438405874   1.3356807327
O   4.9536700266  -4.8923269952   1.3356807327
O   1.7600444481   6.7361675826   1.3356807327
H  -5.7730762578  -1.5978730701   1.1528194490
H   4.2703367997  -4.2006941622   1.1528194490
H   1.5027394581   5.7985672323   1.1528194490
H  -6.7934737788  -1.8921632672   2.3186801864
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H   5.0353983469  -4.9372392388   2.3186801864
H   1.7580754319   6.8294025060   2.3186801864
O  -4.3351392617  -1.2167606957   5.0839773674
O   3.2213153037  -3.1459603817   5.0839773674
O   1.1138239580   4.3627210775   5.0839773674
H  -3.9328462568  -1.9353652885   5.6298907508
H   3.6424986338  -2.4382621234   5.6298907508
H   0.2903476230   4.3736274118   5.6298907508
H  -4.3765688903  -0.4070508675   5.6484481425
H   2.5408008371  -3.5866944067   5.6484481425
H   1.8357680532   3.9937452742   5.6484481425
O   1.2360696357  -4.3048726321  -5.0750678817
O   3.1100942416   3.2229040214  -5.0750678817
O  -4.3461638773   1.0819686107  -5.0750678817
H   1.0641247267  -3.6905706250  -4.3192964951
H   2.6640655524   2.7668443586  -4.3192964951
H  -3.7281902790   0.9237262664  -4.3192964951
H   1.9725105611  -3.8990504462  -5.5940610737
H   2.3904214565   3.6577694782  -5.5940610737
H  -4.3629320176   0.2412809680  -5.5940610737
O  -3.1038825765  -3.2425958726  -5.0822838937
O   4.3601116882  -1.0667432253  -5.0822838937
O  -1.2562291117   4.3093390980  -5.0822838937
H  -3.7299205174  -3.9185786473  -4.7260427461
H   5.2585489140  -1.2709165985  -4.7260427461
H  -1.5286283966   5.1894952458  -4.7260427461
H  -2.4132611248  -3.7241076529  -5.5995228103
H   4.4318023962  -0.2278916136  -5.5995228103
H  -2.0185412714   3.9519992665  -5.5995228103
O  -1.7309361875  -6.7860232687   4.0543588417
O   6.7423366351   1.8939769237   4.0543588417
O  -5.0114004476   4.8920463450   4.0543588417
H  -1.1546794094  -7.4999390554   4.3630299648
H   7.0724774535   2.7499878259   4.3630299648
H  -5.9177980441   4.7499512295   4.3630299648
H  -1.7257254148  -6.8382628622   3.0689794901
H   6.7849720638   1.9246093819   3.0689794901
H  -5.0592466490   4.9136534803   3.0689794901
O   0.0264079377  -8.2876710149  -0.1154189038
O   7.1641296682   4.1667054524  -0.1154189038
O  -7.1905376060   4.1209655625  -0.1154189038
H   0.7161513818  -7.7512511973  -0.5747307019
H   6.3547047570   4.4958308883  -0.5747307019
H  -7.0708561389   3.2554203090  -0.5747307019
H   0.5032189630  -8.9681799220   0.3810973770
H   7.5150621567   4.9198903666   0.3810973770
H  -8.0182811197   4.0482895554   0.3810973770
O   4.3022643794  -7.1359073773  -0.0902556632
O   4.0287448781   7.2938239350  -0.0902556632
O  -8.3310092575  -0.1579165577  -0.0902556632
H   4.5264240398  -6.3689783921   0.4898649177
H   3.2524850638   7.1044874028   0.4898649177
H  -7.7789091036  -0.7355090108   0.4898649177
H   4.2671135097  -7.9100826700   0.4899678728
H   4.7167757834   7.6504700353   0.4899678728
H  -8.9838892931   0.2596126348   0.4899678728
O   3.2591674324  -3.1326289846  -6.5080612658
O   1.0833525651   4.3888362840  -6.5080612658
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O  -4.3425199975  -1.2562072993  -6.5080612658
H   3.6966768386  -2.3985553928  -6.0135045907
H   0.2288714832   4.4006937482  -6.0135045907
H  -3.9255483218  -2.0021383554  -6.0135045907
H   3.9669371736  -3.7400744834  -6.7671330933
H   1.2555309279   5.3055056093  -6.7671330933
H  -5.2224681015  -1.5654311258  -6.7671330933
O  -1.1098088184  -4.4843577260  -6.4848084750
O   4.4384721196   1.2810562329  -6.4848084750
O  -3.3286633011   3.2033014931  -6.4848084750
H  -0.9756541594  -4.0821447443  -7.3551529029
H   4.0230681303   1.1961310848  -7.3551529029
H  -3.0474139708   2.8860136596  -7.3551529029
H  -0.2440807871  -4.4108630940  -6.0148954375
H   3.9419598856   1.9940513848  -6.0148954375
H  -3.6978790985   2.4168117092  -6.0148954375
O  -6.8019413857  -1.8977341604   4.0783488081
O   5.0444566854  -4.9417869549   4.0783488081
O   1.7574847003  6.83952111530   4.0783488081
H  -5.9211916303  -1.6755369280   4.4652613423
H   4.4116533598  -4.2901339085   4.4652613423
H   1.5095382705  5.96567083650   4.4652613423
H  -7.0567661119  -2.7470374216   4.4666653826
H   5.9073872482  -4.7378200106   4.4666653826
H   1.1493788637   7.4848574322   4.4666653826
O  -4.4702715423   1.1237825087   6.4999716257
O   1.2619115703  -4.4332599718   6.4999716257
O   3.2083599720   3.3094774631   6.4999716257
H  -4.0899948477   1.0987773073   7.3898107600
H   1.0934283626  -4.0914280931   7.3898107600
H   2.9965664851   2.9926507858   7.3898107600
H  -4.0044077130   1.8532947907   6.0238510352
H   0.3972034871  -4.3945662019   6.0238510352
H   3.6072042260   2.5412714112   6.0238510352
O  -3.1902490767  -3.2573930009   6.5043632565
O   4.4161096272  -1.1341402444   6.5043632565
O  -1.2258605505   4.3915332453   6.5043632565
H  -2.4493523860  -3.6820446638   6.0080122410
H   4.4134204097  -0.2801790572   6.0080122410
H  -1.9640680238   3.9622237210   6.0080122410
H  -3.8155760880  -3.9673699497   6.7095659847
H   5.3436312067  -1.3207008474   6.7095659847
H  -1.5280551187   5.2880707971   6.7095659847
O  -4.9096710003  -4.9521148234  -1.3171258461
O   6.7434927396  -1.7758423988  -1.3171258461
O  -1.8338217393   6.7279572222  -1.3171258461
H  -4.2287993062  -4.2634937823  -1.1147417764
H   5.8066935774  -1.5305007355  -1.1147417764
H  -1.5778942712   5.7939945178  -1.1147417764
H  -5.7551078722  -4.6283223484  -0.9212109645
H   6.8857986667  -2.6699084446  -0.9212109645
H  -1.1306907945   7.2982307930  -0.9212109645
O  -4.1951102546  -7.1603162383   0.1344360997
O   8.2985708888  -0.0529139330   0.1344360997
O  -4.1034606342   7.2132301713   0.1344360997
H  -4.2318528938  -7.9388352106  -0.4397674431
H   8.9911594158   0.3045254942  -0.4397674431
H  -4.7593065219   7.6343097164  -0.4397674431
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H	-4.4564285509	-6.3913953834	-0.4284333458
H	7.7633250431	-0.6636826435	-0.4284333458
H	-3.3068964922	7.0550780269	-0.4284333458
O	-7.2264498641	-4.1041230117	-0.1213484028
O	7.1674997204	-4.2062276556	-0.1213484028
O	0.0589501437	8.3103506673	-0.1213484028
H	-7.0692065652	-3.3036356361	0.4351651453
H	6.3956356683	-4.4702946520	0.4351651453
H	0.6735708969	7.7739302881	0.4351651453
H	-7.9338759549	-3.8638133432	-0.7370414824
H	7.3130984881	-4.9390314558	-0.7370414824
H	0.6207774668	8.8028447990	-0.7370414824
O	2.0023206416	-6.7434837317	-4.0761898779
O	4.8388679009	5.1058024080	-4.0761898779
O	-6.8411885425	1.6376813237	-4.0761898779
H	1.4235470335	-7.4091029490	-4.4751599684
H	5.7046978563	4.9373793690	-4.4751599684
H	-7.1282448899	2.4717235800	-4.4751599684
H	1.7139822680	-5.8747134416	-4.4475327269
H	4.2306599464	4.4217089065	-4.4475327269
H	-5.9446422144	1.4530045351	-4.4475327269
O	-4.8802271333	-5.0619350164	-4.0576945166
O	6.8238778831	-1.6954331655	-4.0576945166
O	-1.9436507498	6.7573681819	-4.0576945166
H	-4.9494463013	-5.0319977183	-3.0729941243
H	6.8325610065	-1.7703473724	-3.0729941243
H	-1.8831147052	6.8023450907	-3.0729941243
H	-5.7780778273	-4.9269914182	-4.3935637013
H	7.1559386460	-2.5404664744	-4.3935637013
H	-1.3778608187	7.4674578926	-4.3935637013

Table S52. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{120}$ cluster with the tetradecahedral $(H_2O)_{24}$ hollow cage. This structure has the C_3 symmetry.

O	0.827247	4.378403	-0.720174
O	-4.205431	-1.472784	-0.720174
O	3.378184	-2.905618	-0.720174
H	1.000014	5.333280	-0.896779
H	-5.118763	-1.800602	-0.896779
H	4.118749	-3.532677	-0.896779
H	0.000000	4.337682	-0.177042
H	-3.756543	-2.168841	-0.177042
H	3.756543	-2.168841	-0.177042
O	0.557119	2.709469	-2.883688
O	-2.625028	-0.872255	-2.883688
O	2.067909	-1.837214	-2.883688
H	0.634196	3.295284	-2.092299
H	-3.170897	-1.098412	-2.092299
H	2.536701	-2.196872	-2.092299
H	-0.364116	2.355823	-2.887585
H	-1.858144	-1.493245	-2.887585
H	2.222260	-0.862578	-2.887585
O	2.609223	0.871804	-2.923176

O	-2.059616	1.823751	-2.923176
O	-0.549607	-2.695555	-2.923176
H	3.169870	1.095658	-3.703554
H	-2.533802	2.197359	-3.703554
H	-0.636067	-3.293017	-3.703554
H	1.846169	1.498686	-2.931318
H	-2.220984	0.849486	-2.931318
H	0.374816	-2.348172	-2.931318
O	2.898993	3.352930	0.719662
O	-4.353219	0.834137	0.719662
O	1.454226	-4.187066	0.719662
H	2.156697	3.748137	0.198458
H	-4.324330	-0.006314	0.198458
H	2.167633	-3.741823	0.198458
H	3.537314	4.085426	0.898741
H	-5.306739	1.020691	0.898741
H	1.769426	-5.106116	0.898741
O	4.153577	1.419153	-0.726684
O	-3.305811	2.887526	-0.726684
O	-0.847766	-4.306679	-0.726684
H	3.601553	1.238794	-1.526188
H	-2.873603	2.499639	-1.526188
H	-0.727949	-3.738433	-1.526188
H	3.688026	2.129883	-0.219480
H	-3.688546	2.128983	-0.219480
H	0.000520	-4.258865	-0.219480
O	-1.439104	4.186571	0.756892
O	-2.906125	-3.339586	0.756892
O	4.345229	-0.846985	0.756892
H	-2.115649	3.691207	0.231099
H	-2.138854	-3.677809	0.231099
H	4.254503	-0.013398	0.231099
H	-1.238874	3.628809	1.547678
H	-2.523204	-2.887301	1.547678
H	3.762077	-0.741508	1.547678
O	-0.871513	2.611713	2.924733
O	-1.826053	-2.060609	2.924733
O	2.697566	-0.551104	2.924733
H	-1.031054	3.184747	3.712262
H	-2.242545	-2.485292	3.712262
H	3.273599	-0.699454	3.712262
H	0.087939	2.378659	2.931031
H	-2.103948	-1.113172	2.931031
H	2.016009	-1.265487	2.931031
O	1.832514	2.075160	2.894738
O	-2.713398	0.549424	2.894738
O	0.880884	-2.624583	2.894738
H	2.233780	2.498483	2.097491
H	-3.280639	0.685269	2.097491
H	1.046860	-3.183751	2.097491
H	2.105438	1.127099	2.888552
H	-2.028815	1.259813	2.888552
H	-0.076623	-2.386912	2.888552
O	1.367713	7.047201	-1.131897
O	-6.786912	-2.339127	-1.131897
O	5.419199	-4.708075	-1.131897
H	0.641375	7.480443	-1.643303
H	-6.798942	-3.184775	-1.643303

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H      6.157567    -4.295669    -1.643303
H      1.451165     7.540508    -0.282821
H     -7.255854    -2.513509    -0.282821
H      5.804689    -5.027000    -0.282821
O      4.712000     5.362635     1.149821
O     -7.000178     1.399394     1.149821
O      2.288178    -6.762029     1.149821
H      4.308816     6.105662     1.654766
H     -7.442066     0.678713     1.654766
H      3.133250    -6.784375     1.654766
H      5.045538     5.745473     0.292388
H     -7.498494     1.496827     0.292388
H      2.452956    -7.242300     0.292388
O      2.953627     3.385260     5.037874
O     -4.408534     0.865286     5.037874
O      1.454908    -4.250546     5.037874
H      3.941283     3.312864     4.990919
H     -4.839666     1.756819     4.990919
H      0.898383    -5.069683     4.990919
H      2.590485     2.916370     4.249780
H     -3.820893     0.785241     4.249780
H      1.230408    -3.701611     4.249780
O     -2.314709     6.771344     1.116288
O     -4.706802    -5.390269     1.116288
O      7.021511    -1.381076     1.116288
H     -2.021863     5.835123     1.018824
H     -4.042433    -4.668546     1.018824
H      6.064296    -1.166577     1.018824
H     -3.118366     6.761028     1.702374
H     -4.296040    -6.081098     1.702374
H      7.414405    -0.679930     1.702374
O     -1.422289     4.239535     5.065183
O     -2.960400    -3.351506     5.065183
O      4.382689    -0.888029     5.065183
H     -1.205201     3.721791     5.876336
H     -2.620565    -2.904630     5.876336
H      3.825766    -0.817161     5.876336
H     -0.849399     5.043201     5.066258
H     -3.942840    -3.257201     5.066258
H      4.792239    -1.785999     5.066258
O      0.893583     4.404481    -5.023387
O     -4.261184    -1.428375    -5.023387
O      3.367601    -2.976106    -5.023387
H      0.755450     3.824999    -4.237302
H     -3.690271    -1.258261    -4.237302
H      2.934821    -2.566738    -4.237302
H      0.235205     5.142168    -4.959002
H     -4.570850    -2.367390    -4.959002
H      4.335645    -2.774777    -4.959002
O      4.246903     1.439156    -5.059498
O     -3.369797     2.958348    -5.059498
O     -0.877106    -4.397504    -5.059498
H      3.693955     1.302347    -5.865328
H     -2.974843     2.547885    -5.865328
H     -0.719112    -3.850232    -5.865328
H      4.528069     2.385954    -5.054124
H     -4.330331     2.728446    -5.054124
H     -0.197738    -5.114399    -5.054124
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O      1.643731     8.452135     1.239039
O     -8.141629    -2.802555     1.239039
O      6.497898    -5.649580     1.239039
H      0.810676     8.360517     1.795841
H     -7.645758    -3.478193     1.795841
H      6.835082    -4.882325     1.795841
H      1.753273     9.398493     1.059446
H     -9.015970    -3.180868     1.059446
H      7.262698    -6.217625     1.059446
O      6.752245     2.207250    -1.105487
O     -5.287657     4.743991    -1.105487
O     -1.464588    -6.951241    -1.105487
H      5.822371     1.893744    -1.000955
H     -4.551216     4.095449    -1.000955
H     -1.271155    -5.989193    -1.000955
H      7.207043     1.569243    -1.697525
H     -4.962526     5.456861    -1.697525
H     -2.244518    -7.026104    -1.697525
O      0.563034     2.665031    -7.139695
O     -2.589501    -0.844914    -7.139695
O      2.026467    -1.820117    -7.139695
H      0.641019     3.311873    -6.400738
H     -3.188675    -1.100798    -6.400738
H      2.547656    -2.211075    -6.400738
H     -0.351437     2.312102    -7.114681
H     -1.826620    -1.460404    -7.114681
H      2.178057    -0.851698    -7.114681
O      2.587645     0.934585    -7.197516
O     -2.103197     1.773674    -7.197516
O     -0.484448    -2.708259    -7.197516
H      3.022980     1.093139    -8.048991
H     -2.458176     2.071408    -8.048991
H     -0.564804    -3.164547    -8.048991
H      1.805826     1.556350    -7.171198
H     -2.250751     0.785716    -7.171198
H      0.444926    -2.342066    -7.171198
O      6.613729     0.138193    -5.122604
O     -3.426543     5.658561    -5.122604
O     -3.187186    -5.796754    -5.122604
H      7.048060     0.381372    -5.954293
H     -3.854308     5.913113    -5.954293
H     -3.193752    -6.294485    -5.954293
H      5.735211     0.602147    -5.122082
H     -3.389080     4.665765    -5.122082
H     -2.346131    -5.267912    -5.122082
O      8.133162     0.595545    -2.886441
O     -4.582338     6.745753    -2.886441
O     -3.550824    -7.341298    -2.886441
H      7.612862     0.459321    -3.714982
H     -4.204215     6.363272    -3.714982
H     -3.408648    -6.822593    -3.714982
H      8.954033     1.039685    -3.147129
H     -5.377410     7.234578    -3.147129
H     -3.576623    -8.274263    -3.147129
O      8.427278    -1.643337    -1.238992
O     -2.790468     8.119906    -1.238992
O     -5.636811    -6.476569    -1.238992
H      8.342240    -0.828677    -1.776455
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H     -3.453465     7.638931    -1.776455
H     -4.888775    -6.810254    -1.776455
H      7.904176    -1.503359    -0.414871
H     -2.650141     7.596897    -0.414871
H     -5.254035    -6.093538    -0.414871
O     -0.834940     2.620831     7.214497
O     -1.852236    -2.033495     7.214497
O      2.687176    -0.587336     7.214497
H     -0.974498     3.065042     8.064691
H     -2.167155    -2.376461     8.064691
H      3.141653    -0.688581     8.064691
H      0.134057     2.378483     7.189147
H     -2.126855    -1.073145     7.189147
H      1.992798    -1.305338     7.189147
O      1.770803     2.068406     7.155257
O     -2.676693     0.499357     7.155257
O      0.905891    -2.567763     7.155257
H      2.234796     2.523475     6.414830
H     -3.302791     0.673653     6.414830
H      1.067995    -3.197127     6.414830
H      2.048936     1.128418     7.131084
H     -2.001707     1.210222     7.131084
H     -0.047229    -2.338639     7.131084
O      6.748086     4.587069     2.723617
O     -7.346561     3.550480     2.723617
O      0.598475    -8.137549     2.723617
H      6.012957     4.894745     2.129594
H     -7.245451     2.760001     2.129594
H      1.232495    -7.654745     2.129594
H      7.266544     5.375953     2.942259
H     -8.288984     3.605036     2.942259
H      1.022439    -8.980988     2.942259
O      8.177566     2.698710     1.237373
O     -6.425934     5.732625     1.237373
O     -1.751632    -8.431335     1.237373
H      7.655126     2.525657     0.423516
H     -6.014846     5.366706     0.423516
H     -1.640280    -7.892362     0.423516
H      7.697735     3.398669     1.728232
H     -6.792201     4.967100     1.728232
H     -0.905534    -8.365769     1.728232
O      8.155328     0.425887     2.740831
O     -4.446493     6.849778     2.740831
O     -3.708835    -7.275665     2.740831
H      8.168415     1.282379     2.247788
H     -5.194780     6.432866     2.247788
H     -2.973635    -7.715245     2.247788
H      7.594776     0.558342     3.533107
H     -4.280927     6.298098     3.533107
H     -3.313850    -6.856440     3.533107
O      6.565859     0.728851     5.051643
O     -3.914133     5.321776     5.051643
O     -2.651726    -6.050627     5.051643
H      7.073057     0.519008     5.850142
H     -3.986003     5.865943     5.850142
H     -3.087055    -6.384951     5.850142
H      5.758762     0.154635     5.080326
H     -3.013299     4.909916     5.080326
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H	-2.745463	-5.064551	5.080326
O	5.660361	3.359550	4.994330
O	-5.739636	3.222241	4.994330
O	0.079275	-6.581791	4.994330
H	6.044009	3.792636	4.202148
H	-6.306523	3.337947	4.202148
H	0.262515	-7.130583	4.202148
H	6.026733	2.449896	5.016195
H	-5.135038	3.994356	5.016195
H	-0.891694	-6.444251	5.016195
O	3.633492	7.351473	2.711660
O	-8.183309	-0.529041	2.711660
O	4.549817	-6.822433	2.711660
H	2.935288	7.826088	2.193618
H	-8.245235	-1.371010	2.193618
H	5.309947	-6.455078	2.193618
H	4.291421	8.017566	2.962359
H	-9.089127	-0.292304	2.962359
H	4.797706	-7.725263	2.962359
O	-0.527097	8.122297	2.675503
O	-6.770567	-4.517628	2.675503
O	7.297664	-3.604669	2.675503
H	-1.167923	7.620408	2.116362
H	-6.015506	-4.821655	2.116362
H	7.183429	-2.798753	2.116362
H	-0.365429	7.574201	3.474046
H	-6.376736	-4.103571	3.474046
H	6.742165	-3.470630	3.474046
O	-0.026936	6.600595	4.971837
O	-5.702815	-3.323625	4.971837
O	5.729751	-3.276970	4.971837
H	-0.243143	7.133302	5.752311
H	-6.056050	-3.777219	5.752311
H	6.299193	-3.356083	5.752311
H	0.961302	6.436688	5.007432
H	-6.054986	-2.385832	5.007432
H	5.093684	-4.050856	5.007432
O	2.564205	6.106356	4.988703
O	-6.570361	-0.832511	4.988703
O	4.006157	-5.273844	4.988703
H	2.968548	6.484605	4.179978
H	-7.100106	-0.671464	4.179978
H	4.131558	-5.813140	4.179978
H	2.699664	5.130040	4.956156
H	-5.792577	-0.227042	4.956156
H	3.092913	-4.902997	4.956156
O	3.541168	7.357495	-2.692266
O	-8.142362	-0.612007	-2.692266
O	4.601194	-6.745489	-2.692266
H	3.608898	8.294889	-2.928277
H	-8.988034	-1.022048	-2.928277
H	5.379136	-7.272842	-2.928277
H	2.744689	7.276324	-2.105692
H	-7.673826	-1.261192	-2.105692
H	4.929137	-6.015132	-2.105692
O	3.293877	5.751014	-4.971012
O	-6.627462	-0.022926	-4.971012
O	3.333585	-5.728088	-4.971012

H	3.329041	6.310090	-4.165505
H	-7.129218	-0.272011	-4.165505
H	3.800177	-6.038079	-4.165505
H	2.436090	5.265462	-4.949235
H	-5.778068	-0.523015	-4.949235
H	3.341979	-4.742446	-4.949235
O	5.255528	3.984382	-4.965807
O	-6.078340	2.559230	-4.965807
O	0.822812	-6.543611	-4.965807
H	5.800764	4.139764	-5.752010
H	-6.485522	2.953727	-5.752010
H	0.684759	-7.093490	-5.752010
H	4.528773	4.674121	-4.987534
H	-6.312294	1.584972	-4.987534
H	1.783521	-6.259092	-4.987534
O	5.659088	6.412173	-1.136027
O	-8.382648	1.694827	-1.136027
O	2.723561	-8.107000	-1.136027
H	4.936052	6.783380	-1.684434
H	-8.342606	0.883056	-1.684434
H	3.406554	-7.666436	-1.684434
H	6.092454	5.726498	-1.701070
H	-8.005519	2.412971	-1.701070
H	1.913066	-8.139468	-1.701070
O	6.815384	4.476035	-2.673840
O	-7.284052	3.664279	-2.673840
O	0.468667	-8.140313	-2.673840
H	6.776390	3.666094	-2.117178
H	-6.563126	4.035479	-2.117178
H	-0.213265	-7.701573	-2.117178
H	6.271122	4.286127	-3.466666
H	-6.847455	3.287887	-3.466666
H	0.576334	-7.574014	-3.466666
O	-5.266738	-3.942478	-4.939818
O	6.047655	-2.589890	-4.939818
O	-0.780917	6.532367	-4.939818
H	-5.791471	-4.164807	-4.141686
H	6.502564	-2.933157	-4.141686
H	-0.711093	7.097964	-4.141686
H	-4.571491	-4.629410	-5.012044
H	6.294932	-1.644322	-5.012044
H	-1.723441	6.273732	-5.012044
O	-6.790248	-4.581936	-2.670160
O	7.363197	-3.589560	-2.670160
O	-0.572948	8.171496	-2.670160
H	-7.684354	-4.866392	-2.912465
H	8.056596	-4.221650	-2.912465
H	-0.372242	9.088042	-2.912465
H	-6.387430	-5.327221	-2.134231
H	7.807223	-2.868066	-2.134231
H	-1.419794	8.195287	-2.134231

Table S53. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{52}$ cluster with the hexadecahedral $(H_2O)_{28}$ hollow cage.

O	2.072036	-3.897667	2.328983
H	2.480914	-4.660547	2.764278
H	2.006633	-4.117678	1.364014
O	-4.141800	-1.586249	-2.239880
H	-4.932656	-1.913633	-2.693816
H	-3.378700	-2.131762	-2.562428
O	-1.129566	3.543780	3.290773
H	-1.354650	4.220153	3.946936
H	-1.614706	2.718516	3.551680
O	3.164231	1.637267	-3.405660
H	2.942475	0.690940	-3.544229
H	3.571187	1.697248	-2.514078
O	0.467749	4.426207	-0.976415
H	-0.308783	4.214748	-0.402665
H	0.251264	5.288925	-1.393466
O	2.614392	3.680314	0.565650
H	1.908076	4.070444	0.001563
H	2.167609	3.348965	1.381471
O	-2.375074	-3.611145	1.391054
H	-2.953668	-4.163095	1.962539
H	-2.950069	-2.868622	1.079914
O	-0.400199	-0.617121	4.458659
H	0.504769	-0.230676	4.427491
H	-0.364429	-1.452193	3.932363
O	2.099811	0.428816	3.994817
H	2.810156	0.673219	4.628157
H	2.511442	-0.240818	3.394822
O	-0.315549	-1.092747	-4.303710
H	-0.878790	-1.629805	-3.699491
H	-0.717146	-0.194999	-4.355288
O	3.366659	-2.430921	-1.623606
H	3.880439	-1.847234	-1.019729
H	2.929999	-1.842409	-2.285565
O	4.484053	-0.661541	0.155357
H	5.415038	-0.555700	0.449068
H	4.225198	0.238209	-0.162984
O	-3.797819	2.580182	-0.277292
H	-4.368294	3.308310	-0.608518
H	-3.618855	2.011452	-1.066123
O	3.391236	-1.459726	2.523303
H	2.971386	-2.347237	2.474099
H	3.647535	-1.200224	1.606627
O	-3.501548	1.098455	-2.538939
H	-2.633689	1.142229	-3.006627
H	-3.759163	0.151414	-2.483081
O	-2.322817	1.167160	3.759173
H	-1.602472	0.506539	3.921837
H	-2.952575	1.045466	4.505695
O	2.351067	-1.015713	-3.722844
H	1.369864	-1.016852	-3.842196
H	2.692905	-1.588946	-4.443776
O	-0.422432	-3.049608	3.221671
H	0.445900	-3.407196	2.932168
H	-1.050576	-3.163960	2.469935
O	0.794961	2.950086	-3.262489
H	1.676333	2.497845	-3.320942
H	0.718755	3.344270	-2.362807

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O     -1.886975    -2.890161    -2.949645
H     -1.886100    -3.592043    -3.639028
H     -1.508219    -3.322752    -2.143272
O      1.563677     2.906962     2.968632
H      0.629689     3.160516     3.138493
H      1.661201     1.963275     3.238466
O      1.764834    -4.199475    -0.333908
H      2.289305    -3.486004    -0.778338
H      2.014676    -5.027927    -0.802002
O     -1.708551     4.083500     0.626876
H     -1.535827     3.938505     1.583742
H     -2.386758     3.423866     0.346481
O      4.119708     1.866779    -0.796940
H      3.507154     2.465849    -0.301670
H      5.020718     2.206329    -0.603797
O     -4.141084    -1.728685     0.536196
H     -4.198571    -1.665158    -0.442728
H     -4.055506    -0.810687     0.891173
O     -0.928272    -4.299747    -0.833288
H     -1.469932    -4.177211    -0.019532
H      0.009895    -4.125684    -0.586046
O     -4.116663     0.728266     1.723075
H     -4.115293     1.463183     1.068706
H     -3.363982     0.889088     2.337970
O     -1.298377     1.456578    -4.107125
H     -1.698757     2.053835    -4.776285
H     -0.537597     1.965392    -3.727174
O     -0.672654     6.583998    -2.309391
H     -0.356661     7.499287    -2.287441
H     -1.525549     6.557396    -1.796263
O     -4.955182     4.705966    -1.643793
H     -4.898266     4.270399    -2.537492
H     -5.863904     5.025150    -1.541315
O     -4.682471     3.241085    -3.866229
H     -3.949880     3.483911    -4.471590
H     -4.407042     2.386327    -3.469671
O     -0.384973     5.054430    -4.634986
H      0.180667     4.349551    -4.249725
H     -0.569223     5.666317    -3.891197
O     -2.808436     6.249715    -0.732057
H     -2.448875     5.589168    -0.101025
H     -3.587877     5.813107    -1.136798
O     -2.439036     3.576048    -5.500463
H     -2.544880     3.649207    -6.460453
H     -1.735185     4.228740    -5.234478
O      0.310041    -3.118080    -6.102613
H     -0.200820    -3.852318    -5.700798
H      0.014388    -2.314256    -5.623058
O      3.938696    -4.506546    -3.387398
H      3.936809    -3.770505    -2.738306
H      3.584551    -4.113213    -4.213397
O      2.925791    -3.045821    -5.542401
H      1.980663    -3.176467    -5.827453
H      3.453543    -2.948182    -6.348710
O     -1.337335    -4.928771    -4.744963
H     -2.005146    -5.429889    -5.236043
H     -0.953702    -5.544768    -4.062688
O      2.341678    -6.235968    -2.121756
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H	2.813246	-7.052716	-1.900782
H	2.953899	-5.689279	-2.686449
O	-0.399459	-6.328589	-2.669560
H	0.577158	-6.367598	-2.588600
H	-0.692175	-5.755076	-1.929245
O	5.028196	4.449618	1.722116
H	4.183368	4.383086	1.227905
H	4.784630	4.190598	2.642589
O	4.441948	1.223672	5.258280
H	4.657982	1.126498	6.197367
H	5.033809	0.600720	4.756438
O	6.876842	0.180271	1.303083
H	7.761596	-0.158954	1.101072
H	6.864460	1.126038	1.019210
O	5.727090	-0.582572	3.753490
H	4.953679	-1.058913	3.380898
H	6.212239	-0.238566	2.974764
O	3.951444	3.758581	4.154878
H	3.037178	3.585330	3.844940
H	4.239276	2.918566	4.568755
O	6.508919	2.718393	0.356854
H	6.058344	3.391505	0.942671
H	7.232636	3.175937	-0.096335
O	-4.131321	-4.630808	3.285035
H	-4.531930	-5.512562	3.283956
H	-4.857156	-3.979606	3.076326
O	-2.195188	-1.476781	6.412096
H	-1.440604	-1.119274	5.897403
H	-2.324806	-2.383320	6.045352
O	-4.067094	0.291660	5.722743
H	-3.455853	-0.416758	6.068802
H	-4.354972	0.815834	6.484604
O	-2.190887	-3.945650	5.194856
H	-2.954107	-4.196366	4.634126
H	-1.464671	-3.764236	4.561077
O	-5.860589	-2.772789	2.462801
H	-5.398650	-2.475971	1.649635
H	-5.908120	-1.957977	3.016355
O	-5.872551	-0.288031	3.650981
H	-5.397237	0.191546	2.940176
H	-5.320856	-0.160149	4.450223

Table S54. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{98}$ cluster with the hexadecahedral $(H_2O)_{28}$ hollow cage.

O	-1.536467	3.931392	-2.072501
H	-1.867082	4.751661	-2.514834
H	-2.138274	3.754883	-1.307976
O	-3.443305	-3.208832	-0.014831
H	-4.176134	-3.873170	-0.007489
H	-3.766665	-2.421813	0.488878
O	3.715247	-1.662755	-2.350027
H	4.488462	-2.022601	-2.850548
H	2.951410	-1.646772	-2.977832

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O      1.226126     0.964033     4.405530
H      0.278319     1.202333     4.256237
H      1.767673     1.512611     3.786060
O      3.617459    -1.847543     2.070261
H      3.428526    -2.394061     1.269010
H      4.395778    -2.260290     2.518459
O      4.327861     0.695087     1.290870
H      4.063678    -0.224781     1.537070
H      4.258580     0.760753     0.307167
O     -3.512750     0.117698    -2.901648
H     -4.275748     0.131576    -3.529810
H     -3.239454    -0.827690    -2.812321
O      0.975848     1.091863    -4.301637
H      1.533521     1.642651    -3.699984
H      0.035830     1.330573    -4.112270
O      2.589095     2.627054    -2.680242
H      3.129450     3.222648    -3.254770
H      2.048859     3.218865    -2.102178
O     -2.670230    -0.835210     3.570045
H     -3.224951    -0.865685     2.753058
H     -2.008951    -1.565856     3.495728
O     -1.545609     3.606250     2.274427
H     -0.608974     3.785487     2.015772
H     -1.524251     2.831682     2.887477
O      1.041812     4.183092     1.535611
H      1.268524     5.071344     1.905741
H      1.691276     3.549420     1.925198
O      0.761761    -4.436040    -0.761682
H      0.917408    -5.398369    -0.925015
H      0.078826    -4.374529    -0.050173
O      1.026782     4.329617    -1.201902
H      0.090409     4.178680    -1.481160
H      1.047787     4.235420    -0.218479
O     -1.207835    -4.283818     1.135449
H     -1.013815    -3.761958     1.951736
H     -2.013213    -3.875775     0.732243
O      1.570717    -1.569695    -4.045143
H      1.319980    -0.619257    -4.145011
H      1.872976    -1.884258    -4.932421
O     -1.424353     1.551364     4.078559
H     -1.898643     0.709176     3.873715
H     -1.761941     1.867909     4.952152
O     -1.618005     1.858946    -3.851495
H     -1.606716     2.597863    -3.194083
H     -2.259229     1.191026    -3.506332
O      1.617316    -1.703101     3.937865
H      1.478365    -0.734950     4.082111
H      2.305601    -1.781387     3.232904
O     -4.294540    -1.008862     1.372086
H     -5.220986    -1.177377     1.673550
H     -4.329339    -0.247394     0.743554
O      4.279528     0.853414    -1.445455
H      4.044582    -0.040235    -1.797985
H      3.642835     1.493369    -1.846999
O     -3.152967     3.388183     0.066363
H     -2.597549     3.442046     0.881641
H     -3.825129     4.110915     0.124052
O      3.191040    -3.290975    -0.217374
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H      3.361280    -2.700461    -0.992124
H      2.297345    -3.686465    -0.363985
O      2.803061     2.450327     2.740197
H      3.340715     1.841945     2.177159
H      3.443110     2.948001     3.305896
O     -2.852542    -2.521949    -2.588480
H     -3.045562    -2.769662    -1.650500
H     -1.911854    -2.771951    -2.756771
O     -4.417312     1.019472    -0.466102
H     -4.070962     0.707724    -1.337556
H     -3.928152     1.849235    -0.245868
O     -0.272867    -3.338342    -3.059034
H      0.119495    -3.714427    -2.233566
H      0.361648    -2.657587    -3.390483
O     -0.817111    -2.862706     3.448169
H     -0.983627    -3.481761     4.200542
H      0.079160    -2.473314     3.594282
O      5.762415    -2.936200     3.393333
H      6.513614    -2.293532     3.382338
H      6.072899    -3.753789     2.932117
O      1.268249    -7.081775    -1.281078
H      0.719551    -7.663045    -0.699519
H      1.022372    -7.286490    -2.216399
O     -1.857254    -6.876342     1.755434
H     -1.613338    -5.940226     1.551999
H     -1.831297    -6.966732     2.740188
O      2.493094    -2.759722     6.313077
H      2.194232    -2.388423     5.446902
H      3.430329    -3.049744     6.187463
O      5.122626    -5.237132    -0.239637
H      4.411800    -4.550059    -0.229529
H      4.681171    -6.097129    -0.449040
O     -1.355955    -4.617704     5.488574
H     -0.600706    -4.655925     6.125358
H     -2.146309    -4.303825     5.992682
O     -4.255946    -1.309031     5.760819
H     -5.198114    -1.264642     5.462391
H     -3.698189    -1.134291     4.963917
O     -2.536886     5.769930     3.646635
H     -2.185261     4.985527     3.159257
H     -2.923592     5.427757     4.490430
O     -2.285533     2.507377     6.499425
H     -2.821722     1.822475     6.968998
H     -1.500135     2.697941     7.068996
O     -6.825394    -1.581385     2.252712
H     -7.028526    -2.528538     2.053479
H     -7.495219    -1.038708     1.768553
O     -5.032887     5.381170     0.092278
H     -4.853219     6.012992     0.830917
H     -4.960910     5.893615    -0.750212
O     -7.089083     1.609953    -0.708942
H     -7.214286     2.544547    -0.409818
H     -6.126106     1.408729    -0.614956
O      6.945679     1.094769     2.009808
H      6.009410     0.949584     1.727910
H      7.484598     1.177825     1.184466
O      4.106669     4.257336    -4.290028
H      3.865722     4.108283    -5.236903
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H      3.923943     5.208913    -4.093838
O      1.640813     6.659103     2.557011
H      0.888822     6.985756     3.108962
H      2.429277     6.602039     3.151039
O      1.627667     6.931643    -1.834169
H      1.416394     5.997842    -1.587284
H      1.868358     7.401064    -0.997077
O      6.802826     1.394113    -2.376511
H      5.886369     1.221752    -2.047894
H      6.775942     2.259264    -2.855616
O      4.530533     3.847100     4.346819
H      5.464680     3.683948     4.066293
H      4.452864     3.531975     5.280584
O     -5.632702     0.235110    -4.641523
H     -6.445742     0.532016    -4.164035
H     -5.823786    -0.658125    -5.019724
O      1.611855     1.717573    -6.899162
H      1.366774     1.493762    -5.968347
H      0.769014     1.936863    -7.368106
O      2.468136    -2.537478    -6.446220
H      3.348450    -2.962196    -6.296588
H      2.612379    -1.793757    -7.081199
O     -2.507454     2.885300    -6.231542
H     -3.421511     2.542432    -6.391513
H     -2.205174     2.498204    -5.373411
O     -4.577829    -3.952595    -4.165004
H     -3.935779    -3.446078    -3.609493
H     -4.052871    -4.637391    -4.648491
O     -0.492111    -5.328268    -4.937879
H     -0.410114    -4.601491    -4.272947
H     -0.055748    -5.005982    -5.765163
O      8.477001     1.376439    -0.228525
H      7.903364     1.386246    -1.033402
H      9.094506     0.640519    -0.349235
O      3.680476     6.867522    -3.622585
H      3.459683     7.453368    -4.360943
H      2.930609     6.936112    -2.982404
O      3.903690     6.480674     4.061437
H      3.875957     6.903059     4.931934
H      4.147983     5.536032     4.219747
O      2.209768     8.292083     0.450217
H      2.018133     7.732108     1.242133
H      3.138009     8.556031     0.527360
O      6.733142     3.722853    -3.783770
H      5.793376     3.952854    -3.986926
H      7.100315     4.486340    -3.315221
O      7.078557     3.370480     3.507294
H      7.064732     2.564552     2.935328
H      7.418387     4.087208     2.952128
O      5.090801    -3.509326     5.974133
H      5.362355    -3.333425     5.039817
H      5.244160    -4.453383     6.124405
O      6.460311    -5.250286     2.133451
H      5.993232    -5.277008     1.262908
H      7.403278    -5.343105     1.934876
O      3.916817    -7.596445    -0.875222
H      2.949537    -7.447292    -1.014806
H      3.986302    -8.269296    -0.182558
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O	-0.164834	-8.591574	0.477814
H	-0.793259	-7.998573	0.957112
H	-0.702134	-9.300279	0.095447
O	-1.834906	-7.103456	4.469866
H	-1.149597	-7.700467	4.803376
H	-1.647168	-6.220009	4.871957
O	0.832705	-4.769464	7.106564
H	0.660454	-4.644927	8.051072
H	1.457345	-4.049688	6.845116
O	-5.017570	1.930538	-6.687121
H	-5.686191	2.629704	-6.723795
H	-5.285671	1.333337	-5.946358
O	-6.032258	-2.241916	-5.711303
H	-5.722018	-2.279545	-6.627636
H	-5.480595	-2.888841	-5.208060
O	-3.113779	-5.834945	-5.485192
H	-2.157484	-5.689274	-5.281540
H	-3.316512	-6.735390	-5.192876
O	0.710593	-4.465375	-7.227394
H	1.340825	-3.735549	-7.009759
H	0.080469	-4.096916	-7.863302
O	-0.709026	2.321733	-8.197419
H	-1.407816	2.491977	-7.519507
H	-1.027917	1.579889	-8.731603
O	2.751164	-0.423992	-8.146283
H	2.369907	0.371151	-7.700159
H	3.667590	-0.197808	-8.361330
O	-7.474950	4.175731	0.128723
H	-7.845476	4.213121	1.022367
H	-6.609911	4.652444	0.169663
O	-4.502664	7.006355	2.216881
H	-4.196854	7.895397	1.986078
H	-3.771470	6.590675	2.735775
O	-3.589306	4.843929	5.984616
H	-3.168505	3.977697	6.207622
H	-4.540819	4.674317	5.928779
O	-3.833405	0.590875	7.669590
H	-3.979580	-0.123478	7.002459
H	-3.439598	0.160323	8.442087
O	-8.585123	0.018215	0.921682
H	-9.232062	-0.454506	0.378328
H	-8.064200	0.583038	0.300033
O	-6.856878	-1.221211	4.953495
H	-7.293627	-0.381706	5.157839
H	-6.897528	-1.319989	3.970674
O	-0.492047	7.542263	4.021799
H	-0.305268	7.614325	4.969017
H	-1.239488	6.901617	3.938934
O	-3.583872	-3.743941	6.798381
H	-4.328122	-4.350725	6.674350
H	-3.872047	-2.877936	6.419880
O	0.655671	-7.576583	-3.894257
H	1.452264	-7.787986	-4.402311
H	0.271918	-6.768215	-4.312991
O	-7.825898	1.148032	-3.297988
H	-8.157717	1.971470	-3.684247
H	-7.581303	1.363101	-2.365262
O	3.444398	3.743929	-6.891016

H	2.751464	3.040718	-6.924758
H	3.079974	4.502940	-7.368829
O	7.779962	-1.102239	3.393533
H	7.493476	-0.284019	2.918993
H	8.020957	-0.823334	4.288743
O	-2.409367	6.185570	-3.352658
H	-2.444999	6.009964	-4.324811
H	-1.756250	6.914747	-3.214071
O	-0.591829	8.148702	-2.848028
H	-0.326805	8.676097	-3.615324
H	0.233845	7.728559	-2.503634
O	-2.589209	5.601201	-6.010839
H	-2.540478	4.620146	-6.120380
H	-1.883876	5.968567	-6.562864
O	-4.873283	6.669634	-2.303053
H	-3.979044	6.556670	-2.708163
H	-5.046752	7.621801	-2.289560
O	1.931245	1.520689	6.984304
H	1.677195	1.301174	6.053918
H	2.036971	0.660055	7.459073
O	2.231965	-0.870679	8.270183
H	2.364990	-1.568843	7.583717
H	3.021612	-0.892696	8.830082
O	4.221315	2.999638	6.923968
H	3.416091	2.428990	6.977066
H	4.956273	2.456441	7.243451
O	-0.066813	3.093688	7.970045
H	-0.152762	2.963069	8.925342
H	0.674973	2.510770	7.676185
O	-5.436952	-5.074604	-0.019868
H	-5.066507	-5.955127	0.234521
H	-5.796648	-5.161611	-0.936857
O	-4.359454	-7.433133	0.820520
H	-3.444689	-7.255896	1.149681
H	-4.272679	-8.116195	0.140004
O	-7.353330	-4.198697	1.710023
H	-6.666937	-4.564119	1.100148
H	-7.337531	-4.759011	2.499402
O	-6.389276	-5.217866	-2.566235
H	-7.245189	-4.777762	-2.671444
H	-5.760289	-4.740869	-3.160914
O	5.880470	-2.664272	-3.687336
H	6.531179	-1.936161	-3.841157
H	6.326976	-3.342786	-3.123628
O	4.836380	-3.782531	-5.937098
H	5.278360	-3.377416	-5.151543
H	5.488004	-3.768695	-6.652671
O	7.002586	-4.580224	-2.108909
H	6.326973	-4.855514	-1.442369
H	7.223691	-5.378490	-2.610188
O	7.550670	-0.559488	-4.129140
H	7.312129	0.157312	-3.492034
H	8.492481	-0.737808	-3.993595

Table S55. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(H_2O)_{140}$ cluster with the hexadecahedral $(H_2O)_{28}$ hollow cage.

O	-3.740473	0.348840	-2.923808
H	-4.527829	0.419991	-3.512853
H	-4.068578	0.023940	-2.049930
O	0.472997	-4.481875	1.425643
H	0.573036	-5.411617	1.749067
H	-0.426189	-4.178746	1.699089
O	3.952127	1.317817	-2.311588
H	4.767522	1.577822	-2.805079
H	3.558294	0.552689	-2.798712
O	-0.669973	2.797113	3.716932
H	-1.402526	2.136218	3.668404
H	-0.702218	3.328622	2.884254
O	3.372326	2.420616	1.935270
H	3.797265	1.736859	1.362013
H	4.109553	2.921579	2.357556
O	1.851973	4.128092	0.390121
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H	1.936699	3.843441	-0.552165
O	-1.722307	-3.534903	-2.265300
H	-2.085972	-4.321898	-2.738397
H	-0.823764	-3.794593	-1.947703
O	0.383057	0.081919	-4.551231
H	0.215420	1.001259	-4.232885
H	-0.407290	-0.453753	-4.299397
O	-0.033818	2.682186	-3.710231
H	-0.060778	3.262952	-4.507176
H	-0.921604	2.757522	-3.284249
O	-1.506824	-1.532155	3.978144
H	-1.681065	-2.225537	3.297898
H	-0.527250	-1.413128	4.030127
O	-4.094993	1.470962	1.323318
H	-3.624020	2.213534	0.874187
H	-3.571331	1.244112	2.128166
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O	2.822623	-0.797301	-3.628246
H	1.932202	-0.525319	-3.957178
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O	-0.668178	4.355644	1.467076
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H	2.890849	-2.144395	-2.470576
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H	1.434255	-0.198825	4.100282
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O	3.890543	-4.761359	4.087513
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O	-1.036324	6.916950	2.431096
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O	1.088940	-6.974494	-2.124798
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O	4.689585	-4.739958	-3.061416
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H	1.304689	4.310649	-6.969863
O	4.874223	0.776757	-7.576400
H	3.994485	1.106054	-7.935245
H	5.375266	0.439610	-8.334627
O	4.254334	4.996122	-6.058709
H	4.895501	4.259879	-6.144109
H	3.508504	4.769797	-6.655026
O	8.300893	0.306740	-3.732479
H	9.069583	0.730291	-4.142814
H	8.580042	0.040712	-2.807186
O	8.356706	-3.098531	-1.046721
H	9.106025	-3.653260	-0.782632
H	7.691048	-3.165917	-0.313906
O	7.182560	-1.786871	-5.205100
H	6.234389	-1.585070	-5.361210
H	7.557835	-1.022627	-4.719229
O	8.948200	-0.396006	-1.271809
H	8.781710	-1.358020	-1.169727
H	8.342739	0.058053	-0.639944

O	7.207090	-3.905005	-3.482215
H	7.626478	-3.614090	-2.645965
H	7.242306	-3.135322	-4.100148
O	-7.961488	2.202242	-3.870584
H	-8.679276	2.172043	-4.520973
H	-8.341526	1.885599	-3.012099
O	-8.294276	3.265185	0.248553
H	-7.856968	4.034217	-0.176365
H	-7.651177	2.901699	0.902739
O	-7.062613	5.438042	-1.007523
H	-7.529760	6.274178	-0.860643
H	-6.139860	5.571882	-0.668102
O	-6.694107	4.689762	-3.652790
H	-7.161947	3.834120	-3.745590
H	-6.876461	4.993752	-2.738012
O	-8.795705	1.334851	-1.447772
H	-8.641883	2.089716	-0.799859
H	-9.738331	1.114097	-1.396714

Table S56. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $CH_4@(H_2O)_{34}$ methane-clathrate. The methane is inside the $(H_2O)_{18}$ $4^2 5^8 6^1$ cage.

O	2.010115	1.863731	2.313111
H	1.261047	1.482828	2.820927
H	1.625471	2.244976	1.485804
O	-2.249128	-2.648472	1.233196
H	-2.384345	-3.608783	1.383287
H	-2.131715	-2.555980	0.254962
O	2.459237	-2.109238	-1.214423
H	3.136204	-1.428299	-1.412710
H	2.347020	-2.090009	-0.232158
O	-2.139525	1.765632	-2.317213
H	-1.362396	1.386583	-2.800558
H	-1.799114	2.148926	-1.475763
O	-2.402384	1.593588	2.225978
H	-3.096006	2.224257	2.517359
H	-2.901932	0.816942	1.863872
O	2.370164	-2.319284	1.490454
H	2.576455	-3.275920	1.576434
H	1.480185	-2.187305	1.902179
O	-2.231416	-2.380291	-1.465097
H	-2.892948	-1.685656	-1.670816
H	-1.375905	-2.119194	-1.884081
O	2.214852	1.823921	-2.175684
H	2.817440	1.139128	-1.795016
H	2.831797	2.530748	-2.460732
O	-0.207769	0.664570	3.574688
H	-0.271799	0.802960	4.531812
H	-1.031092	1.048358	3.184293
O	-0.048781	-2.012069	2.706009
H	-0.106493	-1.118360	3.109105
H	-0.840384	-2.111158	2.124604
O	0.176746	-2.042790	-2.703148
H	0.209605	-2.960285	-3.049674

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H      0.961875    -1.987779    -2.105980
O     -3.857548    -0.434157     1.178157
H     -3.453382    -1.303672     1.392567
H     -3.787747    -0.346685     0.195202
O      4.071180     0.110208    -1.143537
H      4.015731     0.140647    -0.154923
H      4.918708     0.545241    -1.376191
O      0.041011     0.671019    -3.547344
H      0.087236    -0.291449    -3.374588
H      0.843367     1.062172    -3.140130
O      3.853537    -0.003345     1.564857
H      3.458679    -0.894434     1.688995
H      3.160569     0.639340     1.857047
O     -3.860520    -0.166270    -1.537473
H     -4.763201     0.186100    -1.690524
H     -3.234771     0.542624    -1.837086
O      1.160511     3.070533     0.025500
H      1.423454     2.557826    -0.775473
H      0.180294     3.166012     0.003653
O     -1.554787     3.013704     0.043784
H     -2.178588     3.771976     0.058516
H     -1.810511     2.452389     0.815905
O     -2.068948    -5.407659     1.200769
H     -2.723961    -6.065805     1.475736
H     -2.011387    -5.447378     0.207968
O      2.547646    -4.871236    -1.384019
H      2.707182    -3.902605    -1.396240
H      2.449752    -5.095843    -0.435388
O      2.448118    -5.085276     1.426002
H      3.097967    -5.641074     1.881029
H      1.601705    -5.143705     1.943637
O     -2.025952    -5.149477    -1.470614
H     -2.291238    -4.210847    -1.569416
H     -1.170168    -5.202364    -1.948263
O      0.154311    -4.856821     2.798042
H      0.065843    -3.901953     2.987518
H     -0.618602    -5.100288     2.244765
O      0.340029    -4.843205    -2.914347
H      0.468531    -5.368715    -3.717866
H      1.152337    -4.972096    -2.354973
O     -4.444563     3.367953    -2.229169
H     -3.615231     2.898578    -2.455024
H     -4.241949     3.899904    -1.430973
O     -4.625886     3.272970     2.283590
H     -5.058263     3.693600     3.041829
H     -5.255822     2.584230     1.931711
O     -6.062388     1.261459     1.266681
H     -5.437830     0.513972     1.368013
H     -6.187357     1.360365     0.297709
O     -6.136776     1.410364    -1.524762
H     -6.956765     1.380894    -2.039305
H     -5.621700     2.204462    -1.830159
O     -3.736155     4.703728     0.138956
H     -3.755871     5.668395     0.224947
H     -4.150363     4.328127     0.953353
O      4.223247     3.626483     2.261197
H      3.449564     3.077550     2.499536
H      3.940055     4.129545     1.461250
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O	4.360054	3.626856	-2.285240
H	5.114836	3.064885	-1.988716
H	4.683729	4.158883	-3.027357
O	6.202189	1.866768	-1.266579
H	6.243839	1.894399	-0.269781
H	7.110555	1.785723	-1.592765
O	6.022604	1.757081	1.396381
H	5.478580	0.961051	1.559451
H	5.448412	2.497023	1.714667
O	3.254296	4.870075	-0.005383
H	3.717898	4.540736	-0.802768
H	2.394326	4.396857	-0.010807

Table S57. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $CH_4@(H_2O)_{63}$ methane-clathrate. The methane is inside the $(H_2O)_{18}$ $4^2 5^8 6^1$ cage.

O	-1.940950	2.290919	1.896446
H	-1.128023	2.746135	1.556570
H	-2.445425	2.950374	2.434888
O	2.372485	1.296418	-2.314865
H	2.923824	1.258207	-1.492593
H	2.139457	0.352572	-2.494763
O	-2.354128	-1.094054	-2.503023
H	-2.913677	-1.135838	-1.686379
H	-2.115490	-0.139091	-2.592912
O	1.878392	-2.489812	1.663816
H	1.042807	-2.871385	1.289703
H	2.330138	-3.196678	2.188186
O	2.293832	1.936761	1.841218
H	1.921663	1.138917	2.297559
H	2.870524	1.582308	1.117537
O	-1.981267	1.582014	-2.526117
H	-2.475505	2.070924	-3.229053
H	-1.138652	2.071289	-2.344322
O	2.051476	-1.369003	-2.571892
H	2.544020	-1.804180	-3.309816
H	1.196004	-1.851635	-2.438285
O	-2.440288	-2.077534	1.719456
H	-2.986507	-1.666983	1.000703
H	-2.068928	-1.327937	2.250772
O	0.267416	3.364384	0.818904
H	0.393412	4.322557	1.030591
H	1.045054	2.879041	1.200022
O	0.263530	2.891811	-1.857820
H	0.243342	3.075330	-0.885788
H	1.032531	2.284502	-2.008794
O	-0.231784	-2.680894	-2.061626
H	-0.274979	-2.931532	-1.105206
H	-0.998737	-2.073866	-2.220495
O	3.844791	0.939869	-0.094546
H	4.795376	1.213615	-0.131142
H	3.813165	-0.050299	-0.079543
O	-3.842832	-0.967397	-0.262080
H	-3.795097	0.018627	-0.168993

H	-4.795870	-1.216951	-0.359736
O	-0.395579	-3.377354	0.553689
H	-0.529172	-4.349230	0.681406
H	-1.160618	-2.921391	0.989337
O	-3.422323	1.665789	-0.247813
H	-2.862516	1.719564	-1.062808
H	-2.854691	1.914129	0.526088
O	3.488276	-1.699824	-0.318391
H	2.951332	-1.670664	-1.150441
H	2.892743	-2.028761	0.403310
O	-1.363751	-0.039889	3.110534
H	-1.594586	0.829014	2.693781
H	-1.723023	-0.021995	4.032032
O	1.313398	-0.251864	3.069072
H	0.324451	-0.188868	3.084211
H	1.529368	-1.070719	2.557103
O	-2.419160	-0.041902	5.609901
H	-2.917110	0.807450	5.638627
H	-3.068804	-0.782670	5.589880
O	2.279313	-0.406759	5.587236
H	1.925165	-0.347167	4.663991
H	1.479317	-0.378108	6.161741
O	-0.066734	-0.274737	7.078272
H	-0.917486	-0.210095	6.588104
H	-0.195804	-0.967371	7.741988
O	-4.046957	-2.281878	5.480948
H	-4.100538	-2.824213	4.659691
H	-4.955006	-2.202234	5.806428
O	-4.122758	-3.675974	3.074741
H	-3.496938	-3.082186	2.586882
H	-3.718599	-4.570321	2.998042
O	-0.646956	-6.052321	0.890712
H	0.196288	-6.286805	1.341836
H	-0.617074	-6.400401	-0.030852
O	-2.882443	-6.121137	2.568767
H	-2.105119	-6.122168	1.966248
H	-2.641765	-6.695883	3.309437
O	3.758753	1.948422	5.783726
H	3.231643	1.116008	5.739335
H	3.408908	2.440429	6.540395
O	0.615968	5.995476	1.374108
H	0.785941	6.385711	0.485433
H	1.456553	6.022311	1.888924
O	3.259870	-4.322669	3.098447
H	3.333287	-3.886617	3.979904
H	4.158590	-4.329490	2.691858
O	1.606171	-6.465115	2.432826
H	2.165871	-7.246763	2.321972
H	2.209426	-5.734225	2.695921
O	3.356695	-2.970913	5.506510
H	2.969261	-2.065597	5.566685
H	3.006079	-3.460451	6.264411
O	-6.431394	-3.541763	1.533709
H	-6.738426	-4.448381	1.390425
H	-5.612775	-3.615212	2.079717
O	-6.412947	-1.738233	-0.548052
H	-6.423588	-2.140860	-1.448419
H	-6.484049	-2.457862	0.121904

O	-7.597076	0.754465	-0.282943
H	-8.175715	0.747688	0.492927
H	-7.220667	-0.152559	-0.347902
O	-5.821694	2.877509	-0.425971
H	-4.936394	2.440016	-0.357770
H	-6.478129	2.144199	-0.366227
O	-3.997631	-1.835433	-4.508989
H	-4.095245	-1.030622	-5.066431
H	-3.387487	-1.555236	-3.780969
O	-6.299149	-2.574621	-3.163578
H	-6.454466	-3.505793	-3.377051
H	-5.488505	-2.313241	-3.662088
O	4.100918	2.175220	-4.198737
H	3.460012	1.846606	-3.519231
H	4.220241	1.414116	-4.810890
O	3.568541	-2.542912	-4.501373
H	4.320789	-2.954942	-4.014307
H	2.997222	-3.276016	-4.830350
O	6.409200	1.764878	-0.217095
H	6.439086	2.259186	-1.070220
H	6.460548	2.408881	0.528089
O	5.910805	-2.852763	-0.476112
H	6.554084	-2.113903	-0.364755
H	5.017332	-2.429770	-0.419862
O	7.640835	-0.715117	-0.118733
H	8.408660	-0.698474	-0.707878
H	7.248079	0.186436	-0.161826
O	2.807185	4.528782	-4.915687
H	3.274891	3.679720	-4.739003
H	2.577191	4.513051	-5.855869
O	-4.063956	0.605167	-5.878267
H	-4.820546	0.813788	-6.444474
H	-3.855837	1.434408	-5.392477
O	-3.442967	2.899548	-4.401723
H	-4.209420	3.277939	-3.908705
H	-2.855829	3.651332	-4.650025
O	4.231023	-0.139272	-5.761980
H	5.002723	-0.299834	-6.323436
H	4.008992	-1.006900	-5.355738
O	0.596177	5.132705	-3.322899
H	0.487488	4.309390	-2.782831
H	1.391736	4.967206	-3.880365
O	-0.463166	-4.819743	-3.693651
H	-0.387854	-4.036385	-3.091881
H	-1.252369	-4.634591	-4.253526
O	-1.630301	4.913027	-4.971865
H	-1.986226	5.799831	-5.125947
H	-0.847722	5.032554	-4.383037
O	1.788911	-4.506482	-5.284687
H	2.150239	-5.384647	-5.472169
H	0.996398	-4.654187	-4.715589
O	5.738933	-3.571945	-3.136229
H	5.867901	-4.528334	-3.211797
H	5.846289	-3.357128	-2.179123
O	-0.668235	-6.826010	-1.768771
H	-0.638108	-6.142368	-2.478451
H	-1.394824	-7.420841	-2.003520
O	5.697998	-4.410375	1.807403

H	6.481775	-4.276589	2.359395
H	5.834221	-3.856199	1.002810
O	-3.363481	4.107451	3.317763
H	-2.815550	4.920058	3.217023
H	-4.194744	4.250425	2.805012
O	3.953921	3.380476	3.398364
H	3.341139	2.832240	2.845332
H	3.936277	2.951335	4.284621
O	-3.633613	2.444842	5.543938
H	-3.513162	3.070662	4.794986
H	-3.554850	2.975548	6.349471
O	-5.680610	4.423097	1.864090
H	-6.484411	4.296125	2.388234
H	-5.792976	3.870691	1.054377
O	-5.636712	3.820416	-3.009712
H	-5.754184	4.781075	-2.993802
H	-5.740477	3.517612	-2.076006
O	-2.656033	-4.146777	-5.291444
H	-3.135178	-3.308453	-5.096893
H	-2.418385	-4.103898	-6.228879
O	6.316290	2.918093	-2.709280
H	5.559094	2.624324	-3.269545
H	7.110863	2.794176	-3.248005
O	-1.724518	6.287608	2.860852
H	-0.898116	6.214622	2.332230
H	-1.520092	6.886887	3.592780
O	2.839226	5.884879	3.004412
H	3.570656	6.494355	2.830043
H	3.254506	5.009362	3.188282
O	6.354871	3.387064	2.006957
H	7.075107	3.220283	2.631890
H	5.523736	3.356517	2.537523
O	0.936438	6.930274	-1.217765
H	0.857043	6.322299	-1.989861
H	1.698103	7.497952	-1.402894
C	-0.000997	-0.031476	-0.120172
H	-0.826585	-0.655633	0.234330
H	-0.101749	0.128406	-1.196542
H	0.950451	-0.532449	0.085524
H	-0.024033	0.931508	0.396249

Table S58. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $CH_4@(H_2O)_{20}$ methane-clathrate.

O	-0.668168	2.815286	2.545075
H	0.274859	2.811764	2.272802
H	-1.192989	2.984177	1.732854
O	0.646111	-2.728975	-2.476391
H	-0.295105	-2.721925	-2.198541
H	1.177074	-2.891499	-1.667017
O	2.014779	2.720016	1.811960
H	2.131042	2.859880	0.838317
H	2.544467	3.403132	2.250262
O	-2.044419	-2.692788	-1.780880
H	-2.176487	-2.854058	-0.812982
H	-2.540170	-3.385149	-2.243772

O	-0.337832	3.353394	-1.867739
H	0.561322	3.237086	-1.494664
H	-0.958568	3.317628	-1.110470
O	0.319588	-3.392016	1.857860
H	-0.583003	-3.288165	1.490265
H	0.939991	-3.329466	1.101964
O	2.246308	2.987366	-0.875119
H	2.632720	2.146534	-1.261360
H	2.829297	3.710110	-1.152816
O	-2.279982	-3.009592	0.901905
H	-2.651399	-2.165045	1.296019
H	-2.872007	-3.726595	1.175519
O	-0.884520	1.270501	-3.563041
H	-0.673046	2.023549	-2.961359
H	-0.083560	0.704974	-3.584550
O	0.856974	-1.248511	3.478692
H	0.637727	-2.012142	2.893915
H	0.062213	-0.674899	3.498681
O	2.926357	0.157058	2.444833
H	2.592781	1.056650	2.241261
H	2.160543	-0.349181	2.819102
O	-2.926857	-0.136752	-2.467056
H	-2.593010	-1.033983	-2.253766
H	-2.171854	0.360629	-2.872646
O	2.188147	-3.177713	-0.212575
H	2.803817	-2.421481	-0.041937
H	2.740528	-3.970576	-0.286625
O	-2.171951	3.208268	0.242137
H	-2.765367	2.433671	0.072972
H	-2.744440	3.989588	0.273574
O	3.737547	-0.994292	0.233032
H	3.455211	-0.553829	1.093195
H	4.683486	-1.188091	0.318124
O	-3.683413	1.004679	-0.226333
H	-3.405362	0.577185	-1.093468
H	-4.630386	1.195636	-0.305890
O	1.346555	-0.402079	-3.533392
H	1.076502	-1.286674	-3.153173
H	1.705263	-0.581878	-4.415444
O	-1.354794	0.451766	3.546476
H	-1.097867	1.351719	3.197339
H	-1.690519	0.590738	4.444636
O	3.233373	0.751651	-1.869780
H	2.571277	0.322569	-2.456771
H	3.420360	0.116020	-1.144831
O	-3.211382	-0.744305	1.875878
H	-2.559708	-0.309931	2.469971
H	-3.376652	-0.116070	1.138823
C	0.043916	-0.187456	-0.063687
H	1.105060	-0.453375	-0.038019
H	-0.139596	0.640701	0.628454
H	-0.554376	-1.052345	0.238559
H	-0.232940	0.113467	-1.078729

Table S59. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $CH_4@(H_2O)_{35}$ methane-clathrate. The methane is inside the $(H_2O)_{20}$ 5^{12} cage.

O	2.270845	-0.565296	-2.412994
H	1.447045	-0.315413	-2.887429
H	2.514581	0.191747	-1.827868
O	-2.469909	0.665718	3.466848
H	-1.579084	0.396323	3.776308
H	-2.798570	-0.072349	2.908394
O	-0.128790	0.138247	-3.610086
H	-0.392760	1.036409	-3.284823
H	-0.145602	0.174230	-4.578322
O	0.116261	-0.027323	4.329817
H	0.367648	-0.936303	4.035195
H	0.141332	-0.046301	5.298821
O	1.383474	3.306856	-0.931089
H	0.655794	2.891467	-1.450042
H	2.156254	2.699405	-0.983667
O	-1.253632	-3.220317	1.717350
H	-0.543432	-3.029125	2.369819
H	-1.881658	-2.459324	1.748547
O	-0.779648	2.466624	-2.401507
H	-1.537234	2.264360	-1.791219
H	-1.020825	3.322289	-2.820723
O	0.806465	-2.512879	3.407352
H	1.587685	-2.425940	2.793159
H	1.057455	-3.150012	4.093228
O	0.554677	3.419066	1.673052
H	0.875522	3.304242	0.745849
H	-0.361107	3.050196	1.684872
O	-0.383605	-3.588027	-0.840975
H	-0.634464	-3.412331	0.098947
H	0.591534	-3.470159	-0.895553
O	-1.710129	-1.825118	-2.433641
H	-1.134327	-1.168473	-2.883770
H	-1.135900	-2.397197	-1.866872
O	2.009340	1.817905	3.372114
H	1.353051	1.177142	3.719603
H	1.501380	2.420839	2.779852
O	-3.232152	-1.346258	1.717170
H	-3.270222	-1.005492	0.789748
H	-4.018755	-1.929617	1.785832
O	3.316987	1.390184	-0.849918
H	3.334843	1.067575	0.085843
H	4.258087	1.402840	-1.128796
O	-3.541146	-0.595785	-0.879420
H	-2.846846	-1.032297	-1.437389
H	-4.385975	-1.046988	-1.096711
O	3.528688	0.445631	1.677820
H	3.074021	0.988559	2.379813
H	4.497812	0.438903	1.821153
O	-2.062343	2.660416	1.724028
H	-2.282416	2.001954	2.435112
H	-2.534740	3.503865	1.889214
O	2.237475	-2.821008	-0.912051
H	2.198755	-1.992233	-1.453466
H	3.075489	-3.263831	-1.170429

O	-2.878215	2.030825	-0.776155
H	-2.573110	2.143793	0.157834
H	-3.231300	1.114152	-0.852833
O	2.798226	-2.160968	1.677539
H	2.488903	-2.370066	0.762487
H	2.991953	-1.190571	1.680728
O	0.525153	5.938309	-1.319406
H	-0.221332	5.741990	-1.923768
H	1.015846	5.093515	-1.247696
O	-1.615772	5.063162	-2.900589
H	-2.416335	5.024089	-2.309638
H	-1.888660	5.486889	-3.727609
O	-0.350175	6.027519	1.297762
H	-0.095493	6.117805	0.349143
H	0.065781	5.179719	1.570785
O	-2.908816	5.272979	1.434604
H	-1.991820	5.665210	1.407823
H	-3.451195	5.851358	1.990714
O	-3.640867	4.655992	-1.190393
H	-3.436940	4.989604	-0.289624
H	-3.577746	3.680343	-1.108400
O	4.927514	-1.229790	-2.965339
H	3.980306	-0.976708	-2.975006
H	5.378959	-0.532314	-2.444588
O	5.977869	0.800256	-1.332617
H	6.203559	0.483963	-0.423885
H	6.700775	1.376178	-1.622583
O	6.179916	-0.158415	1.215008
H	6.023203	-1.142534	1.174117
H	6.985047	-0.021077	1.736108
O	4.862910	-3.482118	-1.522506
H	4.996346	-2.699680	-2.123132
H	5.216581	-4.260737	-1.977154
O	5.472554	-2.737899	1.097813
H	5.390080	-3.045634	0.169568
H	4.548045	-2.677110	1.422546
O	-3.228375	-5.143693	1.273541
H	-2.485034	-4.586712	1.586338
H	-4.009017	-4.552670	1.290555
O	-2.390789	-5.466568	-1.343815
H	-2.762551	-5.436124	-0.431538
H	-1.551942	-4.965448	-1.273183
O	-3.782190	-3.662807	-2.859301
H	-3.080022	-2.986051	-2.949476
H	-3.354347	-4.383581	-2.333711
O	-5.267908	-3.195705	1.270178
H	-5.517050	-2.970735	0.341909
H	-6.093449	-3.315332	1.762665
O	-5.569851	-2.419944	-1.335828
H	-4.995770	-2.962107	-1.949006
H	-6.427677	-2.301715	-1.769883
C	0.079991	0.072712	0.437165
H	1.032576	0.373329	0.884243
H	-0.130770	0.705371	-0.430593
H	-0.720101	0.189563	1.175142
H	0.137039	-0.973354	0.120454

Table S60. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $CH_4@(H_2O)_{71}$ methane-clathrate. The methane is inside the $(H_2O)_{20}$ 5^{12} cage.

O	1.140528	0.095698	-3.466925
H	1.438163	-0.737377	-3.023348
H	1.509767	0.846804	-2.936066
O	2.295453	1.864939	2.168996
H	1.948947	1.065766	2.640033
H	1.501894	2.402426	1.916975
O	-2.171168	2.423187	-1.993093
H	-1.945913	1.625284	-2.535851
H	-2.667918	2.092682	-1.201849
O	-2.321416	-2.178002	2.090662
H	-1.951461	-1.442977	2.641338
H	-1.544886	-2.691971	1.751210
O	1.949197	-2.199237	-2.286005
H	2.554596	-1.990436	-1.531777
H	2.448768	-2.767572	-2.923528
O	-3.678187	-1.137930	0.011096
H	-3.168900	-1.523740	0.769125
H	-3.227939	-1.446189	-0.815633
O	3.655055	1.152906	-0.053717
H	3.183425	1.409828	0.779562
H	4.527095	1.618993	-0.042234
O	-0.317266	-3.453957	-1.545231
H	0.508770	-2.984608	-1.825143
H	-1.081892	-2.889109	-1.823321
O	0.081159	3.606385	-1.138759
H	-0.756957	3.199633	-1.479843
H	0.087756	4.549812	-1.437264
O	-2.075324	2.131824	2.368807
H	-1.816623	1.282491	2.807090
H	-2.614470	1.892946	1.572938
O	-2.442493	-1.950228	-2.239628
H	-2.143458	-1.145269	-2.735546
H	-3.068783	-2.439368	-2.829641
O	1.356991	-0.310698	3.460401
H	1.629322	-1.101107	2.926770
H	1.761217	-0.408247	4.358348
O	2.164264	2.169927	-2.081842
H	2.693918	1.813039	-1.325203
H	1.420136	2.698164	-1.698298
O	2.071016	-2.409655	1.942940
H	2.588703	-2.096114	1.160801
H	1.242238	-2.829598	1.599272
O	0.161992	3.395023	1.547472
H	-0.662402	2.924739	1.833029
H	0.109345	3.479836	0.562141
O	-1.538761	0.260588	-3.463513
H	-1.869596	0.357071	-4.391206
H	-0.549601	0.197049	-3.501672
O	-1.327340	-0.158782	3.574707
H	-1.640895	-0.204001	4.512328
H	-0.338201	-0.219355	3.589996
O	3.526787	-1.551433	-0.179436

H	4.393324	-2.026568	-0.215389
H	3.698070	-0.578204	-0.143403
O	-3.514392	1.538354	0.166760
H	-3.612539	0.553301	0.103994
H	-4.425283	1.921416	0.216450
O	-0.225646	-3.567465	1.132217
H	-0.294793	-4.513643	1.412837
H	-0.279308	-3.555195	0.141752
O	-5.997744	2.634763	0.338712
H	-6.629828	1.877558	0.374588
H	-6.022024	3.087433	1.215823
O	-6.265598	-1.937971	0.058366
H	-6.359490	-2.522747	0.847733
H	-5.316414	-1.655957	0.053176
O	-3.976800	-3.708385	3.592986
H	-3.958438	-3.307026	4.493599
H	-3.369716	-3.148171	3.047018
O	-3.511158	3.669840	4.070028
H	-2.980975	3.112184	3.446572
H	-3.021735	4.524184	4.137067
O	-2.221458	-0.248237	6.137073
H	-1.402951	-0.290505	6.686181
H	-2.642533	0.631083	6.291206
O	-0.272251	0.610620	-7.514578
H	0.562927	0.468962	-7.007111
H	-0.256220	-0.030621	-8.239472
O	3.195928	-3.777339	-4.110115
H	3.234897	-3.251071	-4.944307
H	2.600359	-4.548514	-4.268743
O	-0.593387	-5.910018	-2.656739
H	-0.491142	-5.009920	-2.257768
H	-1.454728	-5.886269	-3.137602
O	-4.199170	-3.273823	-3.832762
H	-4.263887	-2.718134	-4.645371
H	-5.067320	-3.227337	-3.365237
O	-2.540217	0.537791	-5.971005
H	-2.995865	1.413425	-5.986798
H	-1.762536	0.590009	-6.576972
O	3.802137	3.340188	3.879170
H	3.236559	2.812404	3.260888
H	3.313353	4.183097	4.037864
O	6.010129	2.541178	-0.042527
H	6.035428	3.037804	0.810881
H	6.806455	1.957098	-0.056570
O	0.119573	6.199451	-1.962028
H	-0.717124	6.335389	-2.468308
H	0.866018	6.244993	-2.606522
O	3.618017	3.799662	-3.695650
H	4.487264	3.918764	-3.242876
H	3.096605	3.204247	-3.101417
O	0.214111	5.870041	2.652447
H	0.189072	4.968692	2.242832
H	0.252475	6.500124	1.894607
O	-5.932452	3.909622	2.771544
H	-5.069003	3.862651	3.248320
H	-6.153985	4.850252	2.714469
O	-3.880741	-2.461114	6.062015
H	-3.668853	-3.024085	6.820240

H	-3.283396	-1.680444	6.129061
O	-0.478749	-6.157219	1.930635
H	-1.329996	-6.212619	2.427602
H	-0.574196	-6.694666	1.108135
O	2.448278	5.716731	4.254991
H	3.013495	6.488501	4.106717
H	1.666412	5.834647	3.664113
O	2.017654	0.226613	-6.032790
H	1.709344	0.185593	-5.093094
H	2.634176	0.996484	-6.074034
O	-2.986676	-5.749238	-4.028928
H	-3.640104	-6.421553	-3.787984
H	-3.454878	-4.884228	-3.969082
O	-7.647238	0.437695	0.282950
H	-7.179527	-0.430621	0.237803
H	-8.293083	0.357331	0.999456
O	-6.412663	-3.539139	2.306409
H	-7.077397	-3.249130	2.947561
H	-5.562544	-3.594912	2.805038
O	1.554647	-5.964814	-4.383124
H	1.232732	-6.150707	-5.276865
H	0.758789	-5.974348	-3.798966
O	3.351423	-2.165462	-6.330049
H	2.871325	-1.305342	-6.263073
H	3.083506	-2.557066	-7.173768
O	-4.229312	-1.648979	-6.050832
H	-3.613458	-0.879689	-6.062443
H	-4.114913	-2.096262	-6.901487
O	0.290555	7.539040	0.449005
H	0.258144	7.094086	-0.429809
H	1.037204	8.153627	0.409507
O	5.995523	4.064773	-2.334343
H	6.006945	3.559423	-1.486643
H	6.226837	4.976246	-2.104969
O	6.022016	3.886521	2.348298
H	5.233134	3.714487	2.917123
H	6.074618	4.848221	2.250486
O	-3.480593	2.183081	6.394148
H	-3.182824	2.749431	7.120430
H	-3.483077	2.752546	5.587607
O	-6.524611	-3.216752	-2.367208
H	-7.307242	-2.852840	-2.805401
H	-6.468328	-2.764832	-1.491154
O	-3.723270	4.144837	-3.392259
H	-3.165372	3.507250	-2.879480
H	-4.577680	4.194748	-2.901686
O	3.721900	2.399157	-6.069004
H	3.731484	2.912629	-5.225925
H	4.642829	2.155280	-6.240959
O	-6.056401	4.239395	-1.911387
H	-6.870098	4.041609	-2.396806
H	-6.073589	3.666089	-1.109843
O	-2.292745	6.488936	-3.244008
H	-2.269883	6.883399	-4.127608
H	-2.826401	5.662123	-3.327326
O	-3.859920	2.946921	-5.873663
H	-4.788110	2.874846	-6.138925
H	-3.863036	3.386492	-4.989864

O	5.759360	-3.093552	-0.318946
H	5.664182	-3.599108	-1.161731
H	5.693103	-3.740935	0.424459
O	8.140110	-1.751914	-0.134507
H	7.283587	-2.234219	-0.225287
H	8.743525	-2.157613	-0.773472
O	5.481221	-4.409036	-2.711484
H	4.696546	-4.178598	-3.261894
H	6.250092	-4.331753	-3.294433
O	3.980778	1.740567	6.114013
H	3.944832	2.332895	5.324913
H	4.919550	1.625171	6.319526
O	-2.083483	6.032834	4.160765
H	-1.253753	6.005226	3.626309
H	-1.816532	6.306298	5.050136
O	2.424146	-0.518270	5.950955
H	2.956429	-1.349175	5.956439
H	3.045517	0.243754	6.036031
O	0.143217	-0.532797	7.506843
H	0.977192	-0.501437	6.982414
H	0.302034	0.004091	8.296221
O	-2.808002	-6.195105	3.387392
H	-3.237295	-5.314966	3.512825
H	-2.683620	-6.560208	4.275254
O	1.808518	-6.457510	3.444135
H	0.977654	-6.383979	2.918736
H	1.542724	-6.774675	4.319159
O	3.431399	-4.228498	3.429115
H	2.934548	-3.570927	2.881178
H	2.852242	-5.026678	3.472510
O	-0.676798	-7.542083	-0.436581
H	-0.641107	-6.985703	-1.251377
H	0.007985	-8.217661	-0.545212
O	3.713954	-2.944309	5.853040
H	3.636979	-3.427630	4.995769
H	4.651172	-2.972272	6.093135
O	5.592424	-4.788022	1.828610
H	6.393692	-4.758902	2.371161
H	4.840696	-4.600068	2.441161
O	2.281365	6.203051	-3.655329
H	2.103141	6.460796	-4.571213
H	2.759140	5.339862	-3.702852
O	8.251581	0.980446	-0.187930
H	8.173083	-0.003046	-0.168015
H	8.920050	1.206175	0.474809
C	0.144620	-0.014788	0.015786
H	1.205959	-0.257832	-0.093972
H	-0.453647	-0.713234	-0.577851
H	-0.031196	1.006812	-0.334560
H	-0.140153	-0.093081	1.069580

Table S62. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_2H_6@(H_2O)_{45}$ ethane-clathrate. The ethane is inside the $(H_2O)_{24}$ $5^{12}6^2$ cage.

O	-1.177675	-2.971091	2.658188
H	-1.372604	-3.263502	3.575438
H	-1.864505	-2.289094	2.455508
O	-4.356578	-1.441454	-0.216192
H	-5.183540	-1.771175	-0.627834
H	-4.223649	-0.531375	-0.590265
O	-3.237969	-1.219530	2.289524
H	-3.744518	-1.367132	1.460352
H	-2.994188	-0.262696	2.305626
O	-2.596270	-3.147001	-1.404905
H	-3.213373	-3.608708	-2.013389
H	-3.164895	-2.490811	-0.930876
O	-1.061127	-1.773274	-3.188101
H	-0.087687	-1.905484	-3.117656
H	-1.484556	-2.268881	-2.447359
O	3.162861	-3.010511	1.153267
H	3.916597	-3.635688	1.099983
H	2.508510	-3.332724	0.477270
O	1.381842	-2.110530	3.035326
H	2.056875	-2.524368	2.452308
H	0.489568	-2.396258	2.725665
O	1.423936	-3.900081	-0.667416
H	0.521552	-4.112996	-0.307194
H	1.337317	-3.213567	-1.367898
O	-0.978392	-4.515492	0.358127
H	-1.073112	-4.051491	1.218197
H	-1.629802	-4.094069	-0.245230
O	-2.108875	0.727873	-3.233793
H	-1.667160	-0.155366	-3.170529
H	-2.695805	0.670460	-4.019531
O	1.616645	-2.174918	-2.784594
H	2.168535	-1.383126	-2.565849
H	2.188369	-2.738604	-3.351320
O	-2.738589	1.428650	2.693976
H	-3.070379	1.500288	3.616099
H	-1.791584	1.707983	2.740518
O	1.787489	0.542880	3.401057
H	1.814869	0.549147	4.383816
H	1.598897	-0.398668	3.161624
O	4.379169	-0.771646	0.191237
H	3.879316	-1.547826	0.547044
H	5.249346	-1.142131	-0.071342
O	3.984303	1.357314	1.912080
H	3.238631	1.064674	2.481399
H	4.202134	0.587849	1.341839
O	2.959508	3.217618	0.272788
H	3.365087	2.529306	0.865490
H	2.704489	2.778404	-0.571843
O	0.733132	4.280211	1.348634
H	1.547684	3.865101	0.960646
H	0.886765	5.247637	1.299942
O	-0.405766	2.768631	-2.606062
H	-0.800494	3.119436	-1.772105
H	-0.999319	2.049095	-2.923251
O	-3.670083	2.911827	0.536950
H	-3.412456	2.429507	1.352798
H	-2.865470	3.396850	0.249545
O	-4.050694	0.997006	-1.313003

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H     -3.919339     1.727081    -0.651277
H     -3.257391     0.966120    -1.896212
O     -1.340125     4.080537    -0.409105
H     -0.601342     4.065895     0.247959
H     -1.343812     5.003729    -0.743760
O      2.264027     2.390196    -2.245911
H      2.613787     3.164415    -2.739828
H      1.281909     2.431307    -2.356331
O      3.330950    -0.130842    -2.244791
H      3.617451    -0.249884    -1.307944
H      2.978101     0.785228    -2.326311
O     -0.204511     2.345321     3.065870
H      0.524144     1.678037     3.044474
H      0.103021     3.122902     2.550021
O     -6.315445    -2.181694    -2.056556
H     -7.252874    -2.391967    -1.932125
H     -6.269486    -1.310872    -2.542457
O     -4.550194    -3.889410    -3.236606
H     -4.883447    -4.779177    -3.425490
H     -5.304955    -3.367365    -2.870537
O     -3.003729    -2.425603    -5.067153
H     -2.200733    -2.278794    -4.521552
H     -3.593419    -2.980561    -4.514577
O     -3.983310     0.058482    -5.173195
H     -3.679794    -0.886470    -5.256278
H     -4.083308     0.410955    -6.069746
O     -5.930473     0.207461    -3.178587
H     -5.379231     0.646159    -2.494083
H     -5.347997     0.148283    -3.966247
O      5.253089    -4.568214     0.168718
H      5.750277    -5.304100     0.555702
H      4.690498    -4.945412    -0.564191
O      3.526647    -5.359611    -1.708322
H      2.684645    -5.007071    -1.345287
H      3.651899    -4.875168    -2.552434
O      3.631329    -3.698620    -3.945913
H      4.347215    -3.020699    -3.804573
H      3.696927    -4.003160    -4.862958
O      6.457075    -2.323282    -0.807419
H      6.166993    -3.198408    -0.452289
H      7.409754    -2.252406    -0.646858
O      5.331310    -1.736746    -3.313630
H      5.805325    -1.975303    -2.489050
H      4.699492    -1.031933    -3.054593
O      3.464477     5.747794    -0.720195
H      3.473471     4.862599    -0.295220
H      3.310060     5.563183    -1.671658
O      1.319339     6.843256     0.430733
H      2.157628     6.546863    -0.022612
H      1.523741     7.661911     0.906630
O      0.243905     5.269310    -3.619040
H     -0.089554     5.833932    -2.890245
H     -0.085457     4.366253    -3.416297
O     -0.726422     6.622038    -1.357499
H     -0.008623     6.860197    -0.721859
H     -1.311133     7.391154    -1.428175
O      2.867682     4.888340    -3.305931
H      3.397477     5.091777    -4.090741
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H	1.923330	5.129373	-3.512487
O	-1.715991	-3.198855	5.382129
H	-2.025269	-3.994038	5.840521
H	-2.472581	-2.551145	5.377836
O	-3.703998	-1.448266	5.018971
H	-3.723795	-1.424063	4.037948
H	-3.523658	-0.523285	5.291109
O	0.898127	-2.291939	5.764662
H	1.186832	-2.358967	4.828622
H	-0.039556	-2.579520	5.761368
O	-3.215942	1.272371	5.432961
H	-3.853432	1.806059	5.929831
H	-2.306908	1.580297	5.699347
O	1.352572	0.313016	6.143185
H	2.021825	0.457214	6.828331
H	1.151581	-0.662641	6.132224
O	-0.718514	2.152556	5.790268
H	-0.048704	1.481737	6.041863
H	-0.499601	2.389396	4.862462
C	0.907076	0.147138	0.239414
C	-0.465792	-0.291277	0.744754
H	1.163779	1.151232	0.598849
H	0.938852	0.166859	-0.855645
H	1.692257	-0.538031	0.582938
H	-0.712549	-1.303370	0.399552
H	-1.255195	0.385026	0.393517
H	-0.502226	-0.299149	1.840339

Table S63. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_3H_8@(H_2O)_{52}$ propane-clathrate. The propane is inside the $(H_2O)_{28}$ $5^{12}6^4$ cage.

O	-1.286990	-4.135978	2.502567
H	-1.554088	-4.927648	2.993062
H	-1.268356	-4.381061	1.540979
O	-3.698429	0.966564	-3.126678
H	-4.355192	1.144855	-3.816578
H	-3.369539	0.041200	-3.274953
O	0.609410	3.750073	3.046614
H	0.717338	4.476113	3.679234
H	-0.325312	3.425567	3.134486
O	4.135341	-0.993684	-2.480824
H	3.412712	-1.616309	-2.713018
H	4.289451	-1.091681	-1.515887
O	3.396625	3.145067	-0.666094
H	2.533771	3.454366	-0.294352
H	3.794457	3.934316	-1.094841
O	4.292402	1.444862	1.287235
H	4.122402	2.115453	0.587209
H	3.549312	1.528598	1.933293
O	-4.365541	-1.246016	0.613111
H	-5.247506	-1.298641	1.044246
H	-4.325475	-0.339001	0.219029
O	-1.536158	0.170905	4.054476
H	-0.592315	-0.059629	4.216513

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H     -1.917869    -0.565574     3.517465
O      1.099892    -0.545778     4.213169
H      1.630234    -0.694867     5.027030
H      1.108508    -1.413712     3.737234
O     -0.004270    -1.139109    -4.230321
H     -0.884488    -1.158573    -3.788309
H      0.266719    -0.195058    -4.307032
O      1.425770    -4.139184    -0.935961
H      2.052816    -3.924342    -0.208480
H      1.597928    -3.485749    -1.657211
O      3.009101    -3.222872     1.109080
H      3.730384    -3.662483     1.610491
H      3.404997    -2.369558     0.806647
O     -1.234130     4.122639    -0.970331
H     -1.181451     5.012277    -1.385477
H     -1.295177     3.490842    -1.730731
O      1.174939    -3.010830     3.102714
H      0.317149    -3.452484     2.914023
H      1.723470    -3.053239     2.283726
O     -1.472587     2.595180    -3.175073
H     -0.675372     2.063942    -3.410664
H     -2.258461     2.004250    -3.206616
O     -1.850025     2.661629     3.082527
H     -1.707278     1.715882     3.347858
H     -2.536805     3.000204     3.701411
O      1.975789    -2.633564    -3.124720
H      1.238998    -2.055845    -3.443937
H      2.036923    -3.355472    -3.788276
O     -2.821860    -1.847151     2.781106
H     -2.328730    -2.690295     2.670996
H     -3.236900    -1.622391     1.915633
O      3.175548     1.507141    -2.841625
H      3.551161     0.598268    -2.706596
H      3.191589     1.971440    -1.972473
O     -2.579506    -1.463998    -3.359057
H     -2.862152    -2.078459    -4.074005
H     -2.735809    -1.962177    -2.516649
O      2.400982     1.638123     3.231203
H      1.777496     2.397092     3.204899
H      1.863671     0.837128     3.435982
O     -1.149192    -4.446941    -0.157839
H     -0.219235    -4.237281    -0.428640
H     -1.361764    -5.295609    -0.608118
O      1.127585     4.219034     0.371279
H      0.970202     4.111465     1.335480
H      0.267932     4.036983    -0.078839
O      4.468377    -1.076208     0.273694
H      4.313258    -0.161284     0.617606
H      5.322477    -1.354813     0.670746
O     -4.542799     1.236296    -0.497171
H     -4.291944     1.181969    -1.445866
H     -3.968890     1.926712    -0.083669
O     -3.196028    -2.949129    -1.184255
H     -3.694872    -2.412985    -0.525419
H     -2.420487    -3.345521    -0.723839
O     -3.166265     3.242703     0.753741
H     -2.537722     3.675146     0.130411
H     -2.617069     2.931865     1.510879
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O      0.803844     1.462717    -4.122170
H      0.984299     2.100800    -4.847471
H      1.627373     1.456507    -3.569185
O      3.978112     5.414826    -2.161495
H      4.748178     5.991823    -2.051147
H      3.183027     5.924687    -1.845731
O     -0.643262     6.390535    -2.470442
H     -0.674898     5.929930    -3.352913
H     -1.197870     7.181286    -2.542915
O     -0.832130     4.860354    -4.655039
H      0.008784     4.568091    -5.066440
H     -1.204798     4.050865    -4.243405
O      3.768577     3.734075    -4.388304
H      3.717850     2.879475    -3.906771
H      3.837787     4.418134    -3.688972
O      1.780287     6.495731    -1.089485
H      1.558063     5.803405    -0.429669
H      0.988401     6.554015    -1.665325
O      1.451065     3.645917    -5.715082
H      1.593899     3.629608    -6.672944
H      2.340469     3.789922    -5.289815
O     -0.396674    -3.257679    -5.985500
H     -1.318148    -3.492686    -5.746499
H     -0.229635    -2.405653    -5.527652
O      0.983613    -6.296425    -2.639169
H      1.289055    -5.651059    -1.965883
H      1.129128    -5.850429    -3.500774
O      1.542416    -4.741446    -4.891367
H      0.794044    -4.296675    -5.374880
H      2.165889    -5.056482    -5.562338
O     -3.040324    -3.553524    -5.117376
H     -3.756383    -3.574710    -5.769357
H     -3.272758    -4.211944    -4.407004
O     -1.560839    -6.580357    -1.873180
H     -1.740181    -7.488461    -1.587733
H     -0.639150    -6.569923    -2.251627
O     -3.620019    -5.046304    -2.978049
H     -2.907564    -5.656770    -2.692341
H     -3.656375    -4.353055    -2.285381
O      6.288400     0.623819     3.043186
H      5.748925     1.060665     2.350463
H      5.714787     0.664707     3.845058
O      3.029338    -1.173593     6.105364
H      2.901903    -1.269883     7.060577
H      3.209575    -2.081767     5.740867
O      5.104250    -3.895973     2.810232
H      5.603047    -4.726300     2.789445
H      5.741398    -3.176465     2.583196
O      3.241484    -3.551080     4.888719
H      2.438450    -3.519484     4.325308
H      3.987431    -3.651033     4.261332
O      4.445059     1.003230     5.046206
H      3.720682     1.379958     4.503420
H      4.054381     0.213892     5.475302
O      6.588424    -1.774029     1.941121
H      6.553395    -0.914096     2.449732
H      7.508698    -1.904700     1.668043
O     -6.688628    -0.868858     2.087270
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H	-7.523944	-1.346550	1.977988
H	-6.842935	0.066022	1.776373
O	-3.778728	0.719570	5.620591
H	-2.892429	0.508622	5.256925
H	-4.372672	0.050368	5.204902
O	-4.058775	3.188365	4.665292
H	-4.066251	2.287268	5.094141
H	-4.086190	3.843297	5.378265
O	-5.083520	-1.332816	4.339618
H	-5.734948	-1.117375	3.640349
H	-4.300276	-1.670955	3.855476
O	-6.825228	1.584070	1.045224
H	-6.166162	1.476457	0.326871
H	-6.442720	2.299541	1.605699
O	-5.479049	3.643342	2.287900
H	-4.707079	3.691908	1.686850
H	-5.095789	3.477581	3.174247
C	-0.051385	0.814555	0.835431
C	0.992227	0.803381	-0.280116
H	0.253512	0.134342	1.642197
C	-1.436252	0.417822	0.329472
H	-0.095418	1.818487	1.280069
H	0.736007	1.534969	-1.058210
H	1.050904	-0.183329	-0.758061
H	1.989168	1.053704	0.097856
H	-2.194263	0.500770	1.117144
H	-1.441930	-0.618349	-0.033697
H	-1.745767	1.064348	-0.501846

Table S64. M06-2 X/6-31+G*/PC M optimized Cartesian coordinates of the iso-C_4H_{10}@$(H_2O)_{52}$ isobutane-clathrate. The isobutane is inside the $(H_2O)_{28}$ $5^{12}6^4$ cage.

O	-4.514595	-1.576632	1.294918
H	-5.377573	-1.877130	1.618913
H	-4.019640	-1.237234	2.085486
O	3.349082	-2.607257	2.461534
H	3.972405	-3.105308	3.012306
H	2.723524	-2.152231	3.083887
O	0.641533	-0.719703	-4.769124
H	0.750064	-0.861408	-5.721421
H	0.441037	-1.604551	-4.365728
O	0.455483	4.829565	1.185859
H	0.253595	4.244508	1.948570
H	-0.273078	4.687720	0.542520
O	2.310197	2.982732	-2.553640
H	2.426069	2.023986	-2.764727
H	3.089248	3.431035	-2.950624
O	-0.361406	3.399297	-2.961470
H	0.619235	3.349310	-2.886898
H	-0.665171	2.502569	-3.241021
O	-0.781515	-4.121593	1.476282
H	-0.962820	-5.087301	1.523136
H	0.151011	-4.055988	1.149768
O	-2.503183	-2.811642	-2.585312

H	-2.918450	-1.945178	-2.800012
H	-2.667263	-2.970408	-1.623710
O	-3.487942	-0.269319	-2.930514
H	-4.175129	0.050299	-3.555823
H	-3.824541	-0.014949	-2.035105
O	2.051748	1.376376	3.552995
H	1.853246	0.410645	3.540193
H	2.770452	1.539453	2.899405
O	-2.558191	2.032326	2.886649
H	-2.972940	2.363934	2.057262
H	-1.622565	2.351082	2.893031
O	-3.505475	2.754520	0.416020
H	-4.255508	3.354140	0.207593
H	-2.728164	3.183048	-0.022297
O	4.035209	-1.382633	-1.811550
H	4.940014	-1.277005	-2.179551
H	4.119374	-1.141952	-0.855072
O	-4.619300	0.468199	-0.578673
H	-4.639175	-0.252961	0.089693
H	-4.112219	1.216432	-0.184357
O	4.498420	-0.732637	0.778545
H	4.113988	0.143975	1.013637
H	4.136039	-1.392434	1.411881
O	0.075310	-2.966547	-3.404846
H	-0.831704	-2.852222	-3.022110
H	0.050281	-3.837513	-3.863322
O	-0.071775	3.050163	3.264810
H	0.672025	2.398204	3.286100
H	-0.171258	3.355032	4.193664
O	-3.006525	-3.513760	-0.006642
H	-3.569424	-2.868882	0.477004
H	-2.164483	-3.596851	0.498246
O	2.676549	3.780430	0.029949
H	1.874281	4.189641	0.446936
H	2.403894	3.433870	-0.851474
O	1.550500	-1.272615	3.957520
H	1.593212	-1.283817	4.940533
H	0.648674	-1.617009	3.731006
O	-1.332999	1.055060	-3.955063
H	-0.666119	0.415769	-4.290138
H	-2.015411	0.537788	-3.465990
O	-2.985203	-0.602107	3.293597
H	-2.762571	0.340610	3.079943
H	-3.297987	-0.587821	4.226406
O	2.743051	0.430969	-3.375826
H	2.029998	0.010017	-3.905835
H	3.080438	-0.245791	-2.741915
O	-1.536683	4.271079	-0.684019
H	-1.078736	3.884290	-1.473190
H	-2.104730	4.986977	-1.043902
O	1.834974	-4.171207	0.732382
H	2.404775	-3.651784	1.341935
H	1.998383	-3.827039	-0.179997
O	-0.901851	-2.334408	3.551703
H	-0.909261	-3.048244	2.872200
H	-1.612840	-1.693217	3.313443
O	2.281965	-3.488228	-1.858940
H	2.973287	-2.791622	-1.932614

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H      1.480567   -3.153499   -2.322649
O      3.818447    1.817275    1.507532
H      4.743784    2.146211    1.548560
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H      7.002267    3.144402    1.557978
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O      1.692098    1.706626    6.298692
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O	1.926226	-6.193509	-2.498166
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