

Supporting Information:

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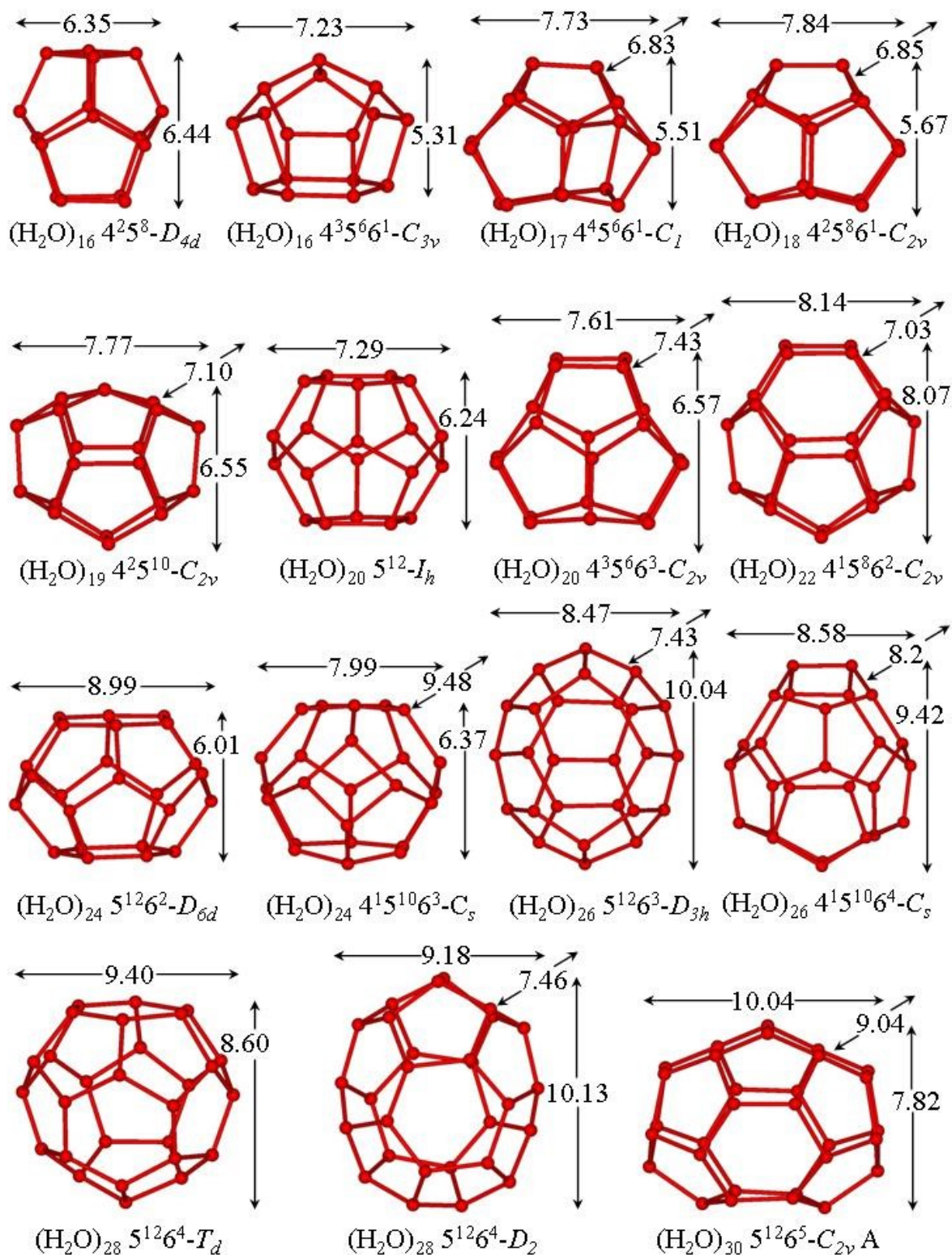


Fig. S1. MP2/6-31+G*/PCM optimized structure of the hollow $(\text{H}_2\text{O})_n$ cages, $n=16-30$. Water's hydrogen atoms have been removed for clarity and the sticks show the oxygen atoms hydrogen bonded.

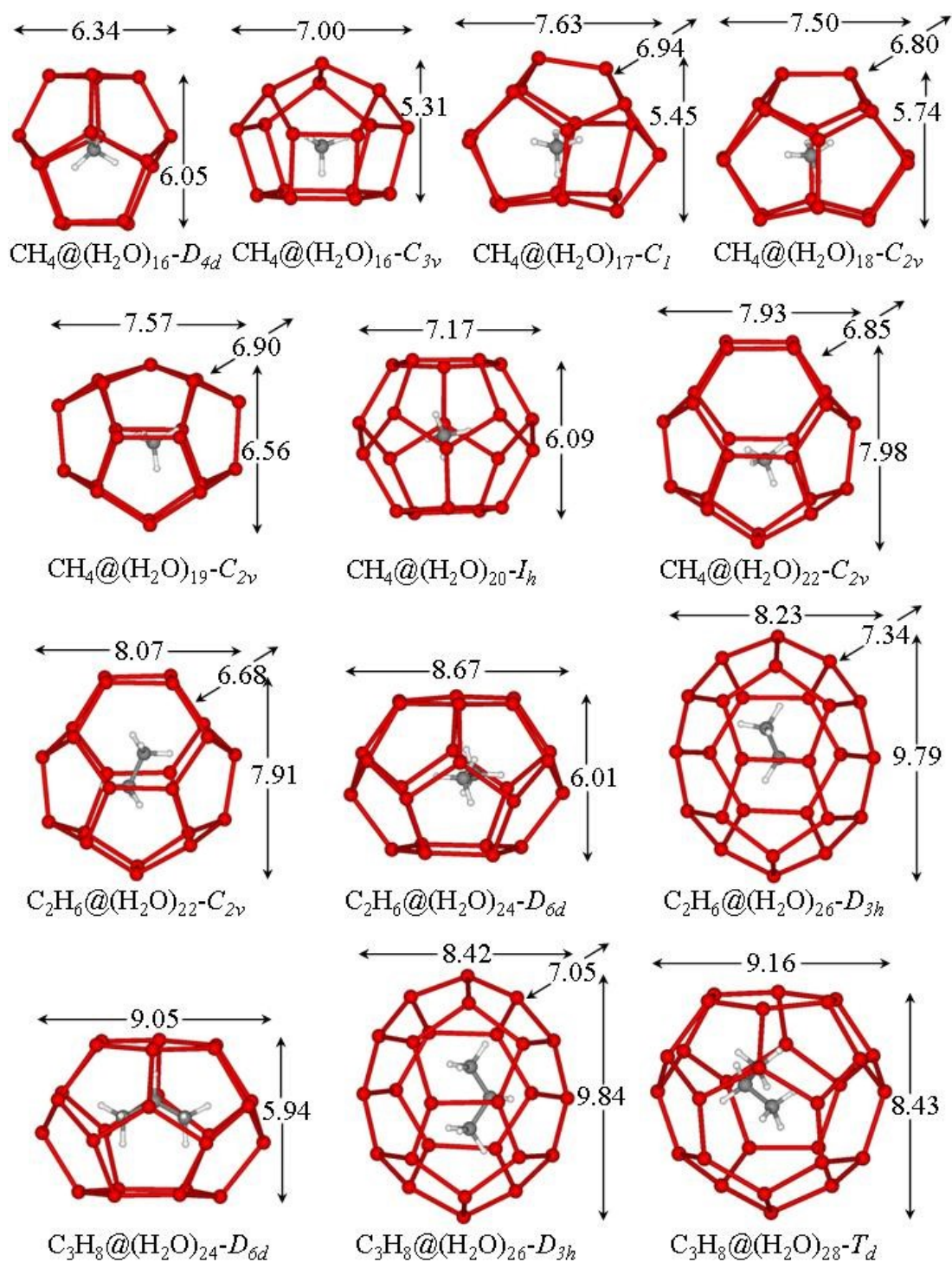


Fig. S2. M06-2X/6-31+G*/PCM optimized structure of the methane, ethane and propane clathrates. Water's hydrogen atoms have been removed for clarity and the sticks show the oxygen atoms hydrogen bonded.

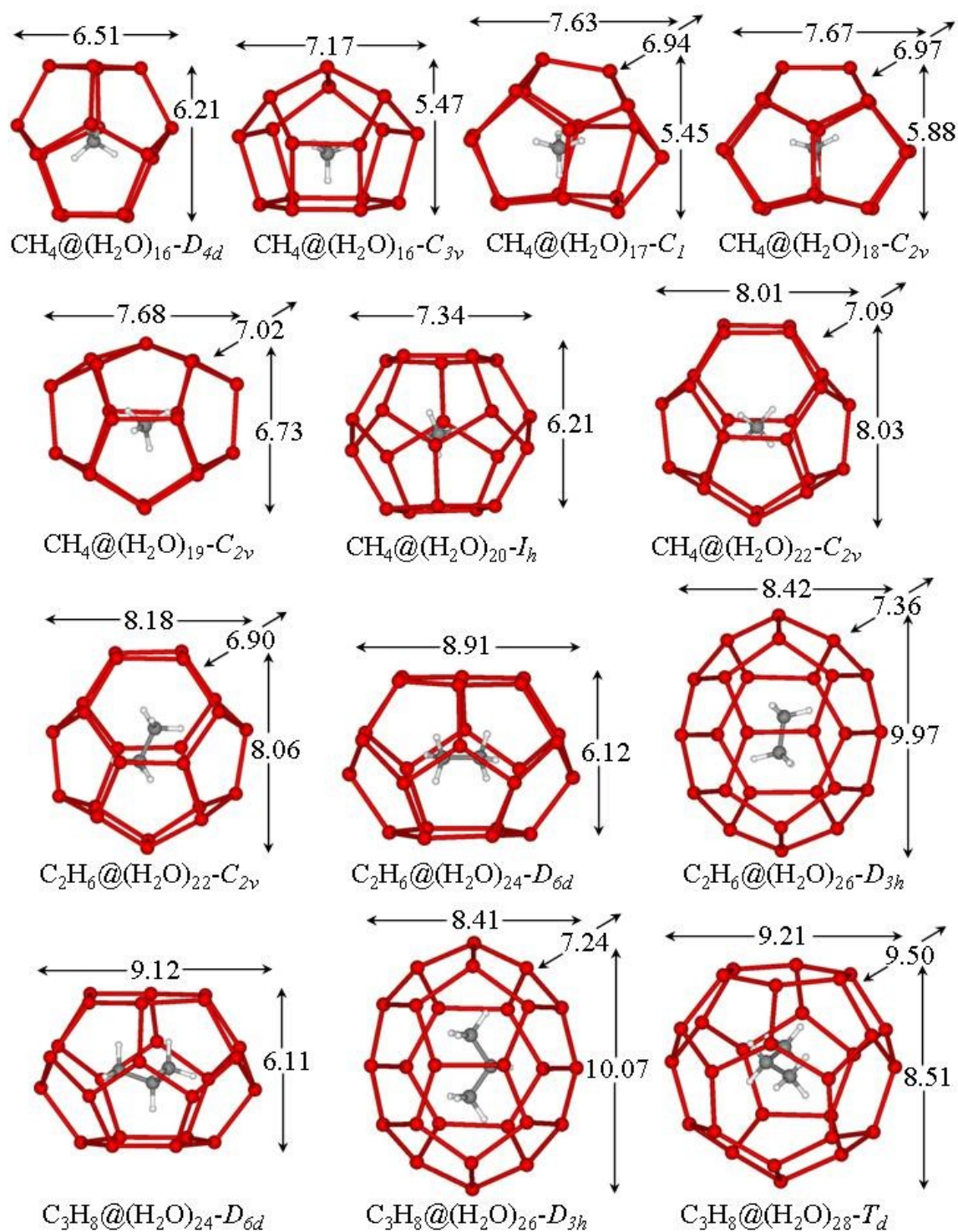


Fig. S3. MP2/6-31+G*/PCM optimized structure of the methane, ethane and propane clathrates. Water's hydrogen atoms have been removed for clarity and the sticks show the oxygen atoms hydrogen bonded.

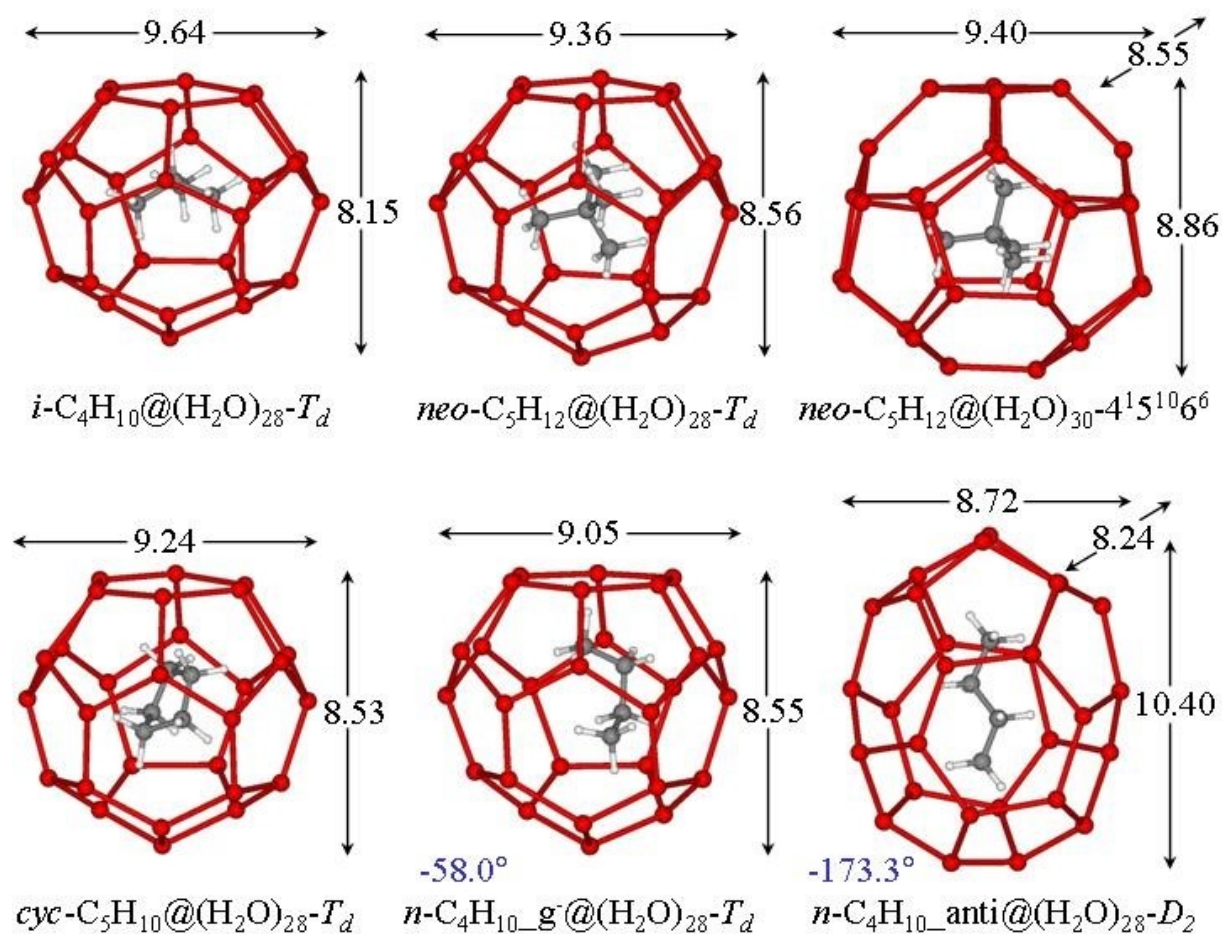


Fig. S4. MP2/6-31+G*/PCM optimized structure of the isobutane, neopentane, cyclopentane and *n*-butane clathrates. Water's hydrogen atoms have been removed for clarity and the sticks show the oxygen atoms hydrogen bonded.

Table S1. M06-2X Relative Electronic, Gibbs Energies (kcal mol⁻¹) and Entropy (cal mol⁻¹K⁻¹) of long chain alkane conformers in the gas-phase

			ΔE	ΔS°_{298}	ΔG°_{298}
<i>n</i> -butane_anti	180.0		0.0	0.0	0.0
<i>n</i> -butane_g ⁻	-61.4		0.5	-0.4	0.8
<i>n</i> -pentane_anti/anti	180.0	180.0	0.0	0.0	0.0
<i>n</i> -pentane_g ⁻ /anti	-61.5	-174.6	0.5	1.1	0.2
<i>n</i> -pentane_g ⁻ /g ⁺	-59.0	95.9	2.5	-0.2	2.7
<i>n</i> -pentane_g ⁻ /g ⁻	-56.9	56.9	0.6	-1.8	1.3
<i>n</i> -hexane_anti/anti/anti	180.0	180.0	180.0	0.0	0.0
<i>n</i> -hexane_g ⁻ /g ⁻ /anti	-56.7	-57.0	-174.4	0.6	-0.7
<i>n</i> -hexane_g ⁻ /anti/g ⁻	-60.8	-168.5	-60.8	1.0	0.1
<i>n</i> -hexane_g ⁻ /anti/g ⁺	-63.0	180.0	63.1	1.2	1.9
<i>n</i> -hexane_g ⁻ /anti/anti	-61.3	-174.2	-179.2	0.5	1.0
<i>n</i> -hexane_anti/g ⁻ /anti	-174.1	-61.5	-174.1	0.5	0.8
<i>n</i> -hexane_g ⁻ /g ⁻ /g ⁻	-57.8	-55.0	-57.8	0.7	-3.0

Table S2. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₆ hollow clathrate in the decahedron 4²5⁸ configuration.

O	0.651586	-2.007410	2.366411
H	0.187283	-1.182237	2.650336
H	1.559113	-1.737119	2.108775
O	0.646385	-2.463286	-1.971599
H	0.178327	-2.760264	-1.152037
H	0.693479	-3.236768	-2.553563
O	-3.142482	1.907468	-0.190174
H	-2.267919	2.352629	-0.222336
H	-3.171279	1.410422	0.655121
O	-0.671650	0.264782	3.123992
H	-0.237693	1.052231	2.734253
H	-1.578323	0.239813	2.750433
O	-3.200741	-0.110236	-1.945189
H	-3.226420	0.705666	-1.373416
H	-3.973085	-0.072949	-2.528485
O	3.164261	1.465963	1.229866
H	3.197485	1.531459	0.251355
H	2.298624	1.840600	1.500812
O	-3.197098	0.115141	1.946639
H	-3.971217	0.080816	2.527757
H	-3.224866	-0.700326	1.374205
O	3.157290	-1.469411	-1.233885
H	2.290832	-1.843047	-1.503411
H	3.191857	-1.534285	-0.255349
O	0.652375	2.005938	-2.366173
H	1.560027	1.734444	-2.110025
H	0.186306	1.181213	-2.648817

O	-3.145578	-1.901869	0.191548
H	-2.271879	-2.348683	0.223091
H	-3.174899	-1.405257	-0.653987
O	3.188634	-1.190366	1.537570
H	3.220134	-0.194152	1.527461
H	3.947479	-1.492467	2.058239
O	3.189689	1.186229	-1.541766
H	3.944997	1.484850	-2.069484
H	3.217358	0.189763	-1.531350
O	-0.637574	-3.116552	0.345414
H	-0.702311	-4.067432	0.521139
H	-0.139792	-2.717103	1.120077
O	-0.631613	3.116926	-0.342332
H	-0.693670	4.068177	-0.517293
H	-0.135478	2.716754	-1.117609
O	0.655391	2.460497	1.972276
H	0.186421	2.758803	1.153762
H	0.704608	3.233474	2.554728
O	-0.675251	-0.263673	-3.121754
H	-0.242674	-1.052457	-2.733148
H	-1.581803	-0.237688	-2.747993

Table S3. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₆ hollow clathrate in the decahedron 4³5⁶6¹ configuration.

O	-2.293669	-1.334512	2.122234
H	-2.861427	-1.688043	2.823435
H	-2.042758	-2.102505	1.552136
O	3.584323	0.359332	0.539404
H	3.163759	1.263629	0.639599
H	4.535327	0.470659	0.687722
O	-1.480620	-2.187924	-2.158500
H	-1.646181	-2.564342	-1.268721
H	-1.890574	-1.295584	-2.165410
O	-1.306509	2.543451	-1.932577
H	-0.330663	2.455301	-1.994804
H	-1.505694	2.815904	-1.011269
O	-2.729248	0.292796	-2.110393
H	-2.166862	1.115572	-2.146424
H	-3.416983	0.395796	-2.784871
O	2.264930	-1.468877	2.059707
H	2.810415	-0.814172	1.556893
H	2.843471	-1.840972	2.742217
O	1.184437	-2.306608	-2.276262
H	0.193436	-2.217943	-2.336558
H	1.455915	-2.896308	-2.995340
O	-3.509228	0.637534	0.550955
H	-3.107299	-0.065796	1.104717
H	-3.330206	0.391646	-0.381847
O	2.319185	2.683935	0.597887
H	1.534445	2.633474	1.199964
H	1.964887	2.724372	-0.315334

O	1.183459	-3.358737	0.308930
H	1.589165	-2.709879	0.923792
H	1.339413	-3.016782	-0.597661
O	0.175587	2.494022	2.263854
H	0.106587	1.561707	2.577610
H	-0.645748	2.670706	1.759186
O	2.708021	0.012233	-2.094566
H	3.090534	-0.010458	-1.191999
H	2.144494	-0.787159	-2.179699
O	-1.475851	-3.292409	0.415822
H	-1.846015	-4.180922	0.527450
H	-0.481801	-3.384093	0.457394
O	1.465386	2.377337	-2.055810
H	1.890736	1.483989	-2.174106
H	1.861101	2.963766	-2.717547
O	0.040002	-0.118095	3.122949
H	-0.764863	-0.562920	2.785008
H	0.802044	-0.619257	2.765039
O	-2.118957	2.919886	0.707612
H	-2.682887	3.675399	0.929643
H	-2.695754	2.108298	0.739827

Table S4. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₇ hollow clathrate in the undecahedron 4⁴5⁶6¹ configuration.

O	1.758781	1.536780	1.766932
H	1.751223	0.620158	2.126736
H	2.621017	1.618863	1.309015
O	-0.427830	-3.398843	0.031662
H	-1.200301	-3.045269	-0.457715
H	0.368465	-3.117823	-0.466833
O	-2.664100	-2.289999	-1.224581
H	-3.142837	-1.719137	-0.555997
H	-3.310663	-2.924962	-1.567410
O	1.875836	-2.558877	-1.333667
H	2.341245	-3.286611	-1.772488
H	2.520863	-2.160733	-0.685679
O	-3.314356	1.487357	-1.354030
H	-2.694807	1.016885	-1.948218
H	-2.795918	2.189986	-0.907405
O	2.330490	1.652320	-2.382517
H	1.865768	0.821687	-2.689553
H	2.686591	2.088766	-3.170399
O	-1.749669	-0.314556	-2.878891
H	-2.084018	-1.106708	-2.391283
H	-2.109900	-0.381352	-3.776554
O	-2.184190	-0.138058	2.662389
H	-2.676166	-0.138408	3.497163
H	-1.710346	0.734727	2.618675
O	3.521947	-1.445550	0.455862
H	3.719556	-0.515470	0.217082
H	3.022812	-1.396107	1.299978
O	-0.927350	2.243928	2.467582
H	-1.305195	2.704942	1.687957

H	0.028363	2.147642	2.290805
O	-3.807715	-0.544962	0.412750
H	-3.262211	-0.394899	1.214316
H	-3.695135	0.259147	-0.149531
O	1.942754	-1.054837	2.702215
H	2.304314	-1.151103	3.595577
H	1.071998	-1.551899	2.680606
O	0.760082	2.896964	-0.480834
H	1.206574	2.553940	-1.283380
H	1.014358	2.287063	0.240635
O	1.044568	-0.561882	-3.077533
H	0.072706	-0.464663	-2.983821
H	1.312844	-1.293722	-2.479208
O	-0.388260	-2.274580	2.522738
H	-0.432308	-2.684286	1.624154
H	-1.052592	-1.552754	2.538115
O	3.822701	1.288989	-0.109613
H	4.708486	1.680088	-0.138405
H	3.410293	1.449126	-0.991788
O	-1.796738	3.364892	0.043355
H	-2.055954	4.297283	0.003106
H	-0.874715	3.302918	-0.318791

Table S5. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₈ hollow clathrate in the undecahedron 4²5⁸6¹ configuration.

O	2.240367	-2.351233	1.624149
H	1.430551	-2.772812	1.236535
H	2.707121	-3.051151	2.105911
O	-2.388443	-1.232651	-2.556265
H	-2.965082	-1.398972	-1.781408
H	-2.301814	-0.256888	-2.601441
O	2.253041	1.550124	-2.493119
H	2.864570	1.621543	-1.730748
H	2.161933	0.587198	-2.654688
O	-2.185199	2.140477	1.988937
H	-1.400512	2.622152	1.626509
H	-2.614767	2.748519	2.609294
O	-2.122627	-2.370019	1.698713
H	-1.854655	-1.592458	2.246657
H	-2.777614	-2.036164	1.048129
O	2.199956	-1.239837	-2.733837
H	2.584050	-1.615524	-3.539688
H	1.345513	-1.731823	-2.567932
O	-2.342097	1.565669	-2.451169
H	-2.759409	2.035666	-3.188094
H	-1.479417	2.035073	-2.265119
O	2.195711	2.148125	1.877000
H	2.821602	1.899247	1.161708
H	1.972128	1.316008	2.346199
O	-0.001188	-3.382870	0.496683
H	-0.058030	-4.348167	0.563774
H	-0.817497	-3.018773	0.954063
O	-0.031034	-2.572821	-2.195094

H	-0.029571	-2.859630	-1.257350
H	-0.868748	-2.066949	-2.328742
O	-0.082715	2.829478	-1.861570
H	-0.037668	3.006821	-0.898282
H	0.746346	2.345593	-2.093456
O	-3.904942	-1.364889	-0.196060
H	-4.810479	-1.708563	-0.196081
H	-3.969370	-0.375458	-0.090988
O	3.876469	1.394987	-0.203469
H	3.939783	0.400066	-0.227734
H	4.782945	1.736291	-0.204514
O	0.019973	3.321837	0.903913
H	0.094308	4.270841	1.086366
H	0.845798	2.897912	1.277085
O	3.788226	-1.258604	-0.449642
H	3.251656	-1.361234	-1.266256
H	3.263009	-1.661986	0.273488
O	-3.831610	1.300815	-0.112564
H	-3.332038	1.503938	-0.933548
H	-3.274138	1.617985	0.630100
O	1.489685	-0.225181	3.184892
H	1.790438	-1.012518	2.669926
H	1.882063	-0.310906	4.066882
O	-1.320830	-0.236614	3.214118
H	-0.341558	-0.206045	3.229025
H	-1.613401	0.606804	2.809505

Table S6. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₉ hollow clathrate in the dodecahedron 4²⁵1⁰ configuration.

O	1.959524	-2.055486	-2.276536
H	2.715216	-1.543775	-1.897924
H	1.624854	-2.629027	-1.552200
O	2.283655	2.010984	2.124423
H	1.418364	1.794648	2.578280
H	2.773891	2.588157	2.729397
O	-0.942791	3.618138	-0.413753
H	0.053080	3.569348	-0.328821
H	-1.162341	4.542374	-0.605264
O	3.886369	-0.363848	-1.322215
H	3.471812	0.451115	-1.670038
H	3.811879	-0.312228	-0.345856
O	1.683181	3.317295	-0.263750
H	1.929371	2.846910	0.562368
H	1.915427	2.722553	-1.007730
O	-1.604517	1.904077	-2.523881
H	-0.909016	1.224844	-2.591125
H	-1.340073	2.505856	-1.795797
O	2.267193	1.653783	-2.439809
H	1.521974	1.095092	-2.754615
H	2.587772	2.142994	-3.212626
O	-3.757207	0.335228	-1.759534
H	-3.100948	1.015403	-2.031404
H	-3.320508	-0.503667	-2.035213

O	-2.154526	-1.759143	-2.559780
H	-1.330588	-1.262314	-2.720808
H	-1.975434	-2.344022	-1.784274
O	1.043773	-3.619998	-0.167295
H	1.362781	-3.204241	0.682013
H	1.378063	-4.529212	-0.172636
O	-2.119450	2.509484	1.776728
H	-1.726180	2.974875	0.997322
H	-2.619984	3.177603	2.268980
O	-3.712070	0.335573	0.967862
H	-3.172484	1.109131	1.234897
H	-3.745838	0.346246	-0.021870
O	-0.033612	1.414726	3.273463
H	-0.783444	1.795310	2.766827
H	-0.184822	0.445494	3.304321
O	-0.424047	-1.353795	3.328042
H	-1.249076	-1.583327	2.830821
H	-0.550226	-1.684071	4.230449
O	0.280734	-0.219364	-3.116256
H	0.888612	-0.960236	-2.800461
H	0.271241	-0.278745	-4.085249
O	3.569555	-0.303419	1.465862
H	3.155098	0.550121	1.745282
H	4.403977	-0.372239	1.954014
O	1.837650	-2.420394	2.077883
H	2.441875	-1.672281	1.883234
H	1.058780	-2.037630	2.535792
O	-1.727865	-3.357158	-0.380639
H	-2.037524	-2.878461	0.416876
H	-0.763202	-3.490686	-0.264102
O	-2.638580	-1.915341	1.846882
H	-3.325606	-2.397134	2.331834
H	-3.062521	-1.065515	1.523724

Table S7. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₀ hollow clathrate in the regular dodecahedron 5¹² configuration.

O	1.735362	-3.380394	0.306697
H	0.969207	-3.453298	-0.300243
H	1.369535	-3.101807	1.182554
O	-2.448009	0.436743	2.883033
H	-2.818392	0.851311	2.075015
H	-1.599485	0.908017	3.079466
O	3.591616	0.465608	1.323172
H	3.571062	-0.245028	0.646549
H	3.288532	1.285836	0.875092
O	-0.668796	2.630272	-2.732983
H	-1.074184	2.927639	-1.891838
H	-1.117035	1.790732	-2.971129
O	-0.463508	-3.551417	-1.439773
H	-1.289539	-3.321323	-0.949650
H	-0.591252	-4.449899	-1.779879
O	2.016944	2.217323	-2.414920
H	1.045710	2.350673	-2.539614

H	2.193204	1.269587	-2.593188
O	-2.003325	-2.133166	2.487766
H	-2.189755	-1.160187	2.652969
H	-2.495840	-2.624790	3.162406
O	0.062327	-1.666203	-3.436137
H	-0.107252	-2.341437	-2.744838
H	0.940242	-1.277091	-3.234111
O	1.990184	-0.165279	3.361272
H	2.613233	0.075296	2.619824
H	2.522956	-0.191031	4.169893
O	0.393080	3.566969	1.493498
H	-0.351241	3.560137	0.856374
H	1.193830	3.322245	0.982357
O	2.543204	-0.501567	-2.867008
H	2.935949	-0.915197	-2.058325
H	3.179505	-0.647497	-3.583244
O	-3.514068	1.548468	0.542015
H	-3.557467	0.825944	-0.148140
H	-4.423419	1.856830	0.673485
O	0.758671	-2.586985	2.727858
H	-0.204525	-2.413618	2.670261
H	1.176924	-1.736924	2.984190
O	-3.569264	-0.393515	-1.270123
H	-3.260430	-1.234757	-0.871926
H	-2.970739	-0.206637	-2.026746
O	-0.105944	1.701722	3.453108
H	0.095135	2.373537	2.759248
H	0.638445	1.064165	3.437626
O	3.487010	-1.599081	-0.557648
H	4.341908	-2.046704	-0.647256
H	2.836704	-2.291143	-0.234592
O	-1.775818	3.483048	-0.291393
H	-2.241836	4.328410	-0.375517
H	-2.447426	2.825661	0.016038
O	-2.697633	-2.767547	-0.055810
H	-3.409826	-3.424965	-0.036485
H	-2.474013	-2.571444	0.890462
O	2.690547	2.794138	0.088878
H	3.366833	3.487596	0.067758
H	2.457080	2.599033	-0.864077
O	-1.856194	0.185491	-3.385143
H	-2.302426	0.183909	-4.245102
H	-1.141004	-0.508810	-3.436550

Table S8. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₀ hollow clathrate in the irregular dodecahedron 4³⁵6³ configuration.

O	1.211201	-1.790752	-3.016156
H	0.512160	-2.365445	-2.639066
H	1.969203	-1.817281	-2.395199
O	1.843640	2.507312	-2.223615
H	1.278624	1.850489	-2.730424
H	2.295346	3.045340	-2.891687
O	-2.813885	-0.127761	2.512996

H	-1.929275	-0.365773	2.865386
H	-3.032600	-0.792639	1.824660
O	-1.251767	-3.793737	0.527668
H	-0.541177	-3.480885	1.127371
H	-2.035091	-3.231284	0.708855
O	-2.797699	2.398802	1.678194
H	-2.839871	1.448160	1.979751
H	-3.513798	2.866624	2.132595
O	3.212514	-2.090044	1.280311
H	3.330137	-1.171305	1.604561
H	2.337206	-2.388591	1.607415
O	-3.085796	-1.562290	-1.979796
H	-2.316318	-2.140161	-2.170988
H	-2.822991	-0.649847	-2.229853
O	3.786534	1.027777	-0.861998
H	3.092709	1.554470	-1.314461
H	3.695699	0.107054	-1.188904
O	1.271281	1.388757	3.179931
H	2.062860	1.181008	2.638973
H	0.786650	2.117496	2.722558
O	-2.332365	0.995782	-2.783962
H	-2.869354	1.273402	-3.541333
H	-2.404066	1.727275	-2.109515
O	3.451705	-1.697042	-1.353830
H	3.348280	-1.952573	-0.396583
H	4.213194	-2.190766	-1.692534
O	3.551721	0.635123	1.769555
H	4.372363	0.906030	2.207419
H	3.643132	0.890983	0.810593
O	0.355448	0.752314	-3.522113
H	-0.589626	0.816420	-3.265426
H	0.642542	-0.172785	-3.324473
O	-0.287829	-0.710806	3.561774
H	-0.357560	-0.832506	4.520943
H	0.310438	0.082639	3.423257
O	0.729813	-2.904550	2.298246
H	0.364544	-2.128785	2.793227
H	0.885594	-3.593479	2.962389
O	0.156609	4.004593	-0.691424
H	0.803562	3.499913	-1.244499
H	0.283577	4.941044	-0.904808
O	-0.923195	-3.325680	-2.084395
H	-0.957179	-3.568810	-1.118928
H	-1.057564	-4.145955	-2.581810
O	-0.201701	3.383445	2.027057
H	0.038837	3.618830	1.107627
H	-1.129494	3.068667	1.977929
O	-2.432686	2.990408	-1.014913
H	-2.655533	2.727653	-0.095775
H	-1.540935	3.395883	-0.961530
O	-3.439851	-2.063922	0.617721
H	-4.309757	-2.467096	0.756342
H	-3.394010	-1.805244	-0.344068

Table S9. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₂ hollow clathrate in the tridecahedron 4¹⁵106² configuration.

O	1.914345	-3.699245	0.402172
H	2.175890	-3.113756	1.145194
H	2.250462	-3.270159	-0.412116
O	-1.679642	-3.013128	-2.022230
H	-1.350657	-3.382717	-1.148795
H	-1.891267	-3.779813	-2.576575
O	-1.766204	2.983947	1.919642
H	-1.337912	3.343242	1.113020
H	-1.079780	2.478646	2.407161
O	2.609484	2.357129	2.134463
H	2.389752	2.846978	1.314696
H	1.754359	2.133123	2.559922
O	-3.929682	1.613076	1.201471
H	-3.125311	2.117642	1.509487
H	-4.701433	2.070907	1.566017
O	2.774426	1.899535	-2.284954
H	1.946501	1.596134	-2.718641
H	2.507310	2.539930	-1.590843
O	0.168946	-1.015055	3.526219
H	0.999376	-1.392501	3.161831
H	-0.573467	-1.495954	3.100894
O	0.447048	-1.674267	-3.252116
H	-0.308431	-2.111317	-2.803402
H	1.259266	-1.972266	-2.789364
O	-1.580619	2.572864	-2.452165
H	-0.910742	1.947232	-2.801786
H	-2.362984	2.040466	-2.169908
O	-1.921743	-2.474021	2.392253
H	-2.293081	-3.063450	3.065870
H	-2.690847	-1.958048	2.021986
O	2.799398	-2.435293	-1.949063
H	3.323821	-1.626098	-1.727004
H	3.371684	-2.987037	-2.503196
O	0.452444	0.980139	-3.519325
H	0.492862	1.141449	-4.474065
H	0.407723	-0.010198	-3.410310
O	-0.802934	-3.942826	0.290496
H	-1.179405	-3.434517	1.041071
H	0.179339	-3.846625	0.349133
O	-0.665470	4.012404	-0.433648
H	-0.957787	4.925812	-0.573476
H	-1.015395	3.480664	-1.208999
O	2.031614	3.691492	-0.271144
H	1.062039	3.877737	-0.339218
H	2.480098	4.546659	-0.352383
O	-3.898852	-1.536526	-1.458430
H	-3.112777	-2.081753	-1.711804
H	-4.670396	-1.961770	-1.861499
O	2.570898	-1.995068	2.516535
H	3.114720	-1.230835	2.168404
H	3.107522	-2.423070	3.200356
O	-3.814860	1.268402	-1.573878
H	-3.816834	0.292303	-1.650558
H	-3.900946	1.452978	-0.614385

O	-3.980764	-1.163530	1.313959
H	-3.944121	-0.185100	1.383376
H	-3.997523	-1.357517	0.352480
O	0.198001	1.645990	3.370735
H	0.183525	1.961110	4.286989
H	0.150567	0.650518	3.420635
O	3.956472	0.051620	1.546312
H	3.480290	0.895361	1.742042
H	4.018701	-0.009989	0.569630
O	4.107073	-0.149986	-1.250843
H	3.626707	0.630824	-1.652078
H	5.023572	-0.096450	-1.561473

Table S10. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₄ hollow clathrate in the regular tetradecahedron 5¹²6² configuration.

O	2.710830	0.338380	-2.995271
H	3.243890	0.432019	-3.799133
H	2.088987	1.118600	-2.985777
O	1.703148	4.111770	-0.750291
H	2.038835	4.978720	-1.023635
H	0.885315	4.284306	-0.220182
O	1.117980	2.474257	-2.945273
H	1.304177	3.055036	-2.176911
H	0.147360	2.325503	-2.954720
O	3.536195	2.613020	0.759682
H	3.055679	2.287215	1.550557
H	2.897722	3.160079	0.256120
O	2.203965	1.605434	3.007242
H	2.286273	0.611319	2.992244
H	2.642711	1.898223	3.820123
O	2.710166	-3.530748	-0.745701
H	3.294517	-4.254207	-1.018015
H	3.267355	-2.907328	-0.216076
O	1.586063	-2.207496	-2.942399
H	1.995142	-2.657961	-2.172954
H	1.942680	-1.292648	-2.952913
O	4.090137	-1.705247	0.723910
H	4.219234	-0.877542	0.170564
H	4.973452	-1.990901	1.002119
O	4.357379	0.478434	-0.732602
H	3.782792	0.437579	-1.527390
H	4.056604	1.262986	-0.211388
O	-0.356549	2.701304	2.932869
H	0.530059	2.279704	2.935333
H	-0.388832	3.295117	2.152214
O	2.514979	-1.040653	2.933837
H	1.706843	-1.598123	2.934757
H	3.046254	-1.308364	2.153340
O	-1.648663	2.174255	-2.996257
H	-1.997090	2.587829	-3.800446
H	-2.013113	1.245418	-2.985384
O	-1.060099	-2.518898	-2.994002
H	-1.244075	-3.027892	-3.797878

H	-0.073595	-2.369711	-2.983199
O	0.494430	-4.369418	0.761122
H	1.288160	-4.089659	0.258855
H	0.451498	-3.791016	1.552442
O	-1.764457	-4.013411	-0.731344
H	-1.512651	-3.495521	-1.526252
H	-0.934530	-4.145365	-0.210334
O	-3.522148	-2.687719	0.723320
H	-2.869249	-3.213872	0.171313
H	-4.210902	-3.309764	1.002517
O	-4.412418	-0.581509	-0.748847
H	-4.151391	-1.375042	-0.217990
H	-5.331055	-0.726449	-1.021196
O	-2.493245	1.109384	3.004780
H	-2.965184	1.343235	3.818201
H	-1.673362	1.677607	2.989558
O	-2.591425	3.533539	-0.735273
H	-2.268027	3.054718	-1.528771
H	-3.121948	2.882251	-0.213873
O	-0.566476	4.395738	0.720895
H	-1.347821	4.092261	0.168529
H	-0.761920	5.303430	0.998721
O	-4.033032	1.757754	0.757779
H	-4.187337	0.930453	0.255531
H	-3.511103	1.505657	1.549369
O	-2.160244	-1.655529	2.933585
H	-2.658098	-1.981708	2.153272
H	-2.239634	-0.676957	2.935053
O	0.285939	-2.710362	3.006732
H	0.320500	-3.234253	3.821235
H	-0.616019	-2.284083	2.991408
O	-2.702592	-0.272396	-2.943615
H	-2.088935	-1.038995	-2.952516
H	-3.299060	-0.400959	-2.175443

Table S11. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₄ hollow clathrate in the irregular tetradecahedron 4¹⁵10⁶3 configuration.

O	0.757840	-2.096568	-3.324025
H	0.902316	-2.517163	-4.184936
H	1.249341	-1.229282	-3.355348
O	4.318414	0.068298	-1.626703
H	5.161563	0.122060	-2.101436
H	4.298641	0.841971	-1.010078
O	2.147553	0.178332	-3.394860
H	2.905081	0.160543	-2.771841
H	1.660611	1.012792	-3.219317
O	4.005714	-2.345620	-0.217727
H	3.787811	-2.114705	0.709235
H	4.140072	-1.495793	-0.686711
O	3.306708	-1.713283	2.428841
H	2.395106	-2.034201	2.641621
H	3.896235	-2.118476	3.082569
O	-2.398444	-3.510136	-0.441171
H	-2.751549	-4.383087	-0.671160

H	-1.520716	-3.676056	0.015721
O	-1.967627	-2.032252	-2.779669
H	-2.094851	-2.551118	-1.956417
H	-1.001617	-2.015839	-2.956369
O	-0.053009	-3.964201	0.679468
H	0.656396	-3.839437	0.000182
H	0.189724	-3.408905	1.450227
O	1.833597	-3.674371	-1.257939
H	1.475728	-3.123628	-1.985482
H	2.624597	-3.195862	-0.914218
O	3.363070	1.077880	2.583653
H	3.367343	0.099738	2.507352
H	3.641830	1.431009	1.711061
O	0.747834	-2.516040	2.945307
H	0.218832	-1.709875	3.217510
H	0.713732	-3.124646	3.699006
O	0.861973	2.602812	-2.930867
H	0.986349	3.183725	-3.696479
H	-0.120521	2.580496	-2.758693
O	-3.251674	0.298078	-2.730939
H	-3.765064	0.341325	-3.551723
H	-2.743402	-0.560540	-2.766749
O	-4.170070	-2.029468	0.996957
H	-3.532082	-2.611110	0.513153
H	-4.872997	-2.608014	1.328288
O	-4.917586	0.209587	-0.498082
H	-4.350041	0.239475	-1.299916
H	-4.718664	-0.643463	-0.055953
O	-4.102151	1.991480	1.295384
H	-4.469365	1.391280	0.584961
H	-4.859957	2.446233	1.693207
O	-2.277587	3.642063	0.133933
H	-2.957033	3.083270	0.586972
H	-2.664780	4.527573	0.060427
O	0.927856	1.944580	3.255594
H	1.016369	2.408605	4.101926
H	1.845281	1.632730	3.017219
O	2.120524	3.695777	-0.679842
H	1.676236	3.316876	-1.468802
H	1.432899	3.749573	0.028477
O	4.104428	2.149871	0.116512
H	3.367628	2.758326	-0.191512
H	4.900446	2.697417	0.192856
O	0.259897	3.845318	1.313593
H	-0.648566	3.716951	0.970071
H	0.415834	3.151814	1.989493
O	-3.172017	-0.168779	2.849883
H	-3.439930	0.660149	2.402423
H	-3.468799	-0.887990	2.254485
O	-0.583958	-0.361959	3.710317
H	-1.500217	-0.261218	3.358408
H	-0.101255	0.469925	3.514755
O	-1.754258	2.626093	-2.424881
H	-2.248936	1.783961	-2.525550
H	-1.951870	2.962655	-1.524815

Table S12. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₆ hollow clathrate in the regular pentadecahedron 5¹²6³ configuration.

O	3.985024	-2.439288	0.801311
H	4.700649	-3.074640	0.952381
H	3.415327	-2.824186	0.078556
O	2.322282	-1.656776	-3.291969
H	2.725331	-2.099702	-4.054201
H	1.441859	-1.330739	-3.603532
O	2.429486	-3.424257	-1.130118
H	2.303366	-2.801515	-1.877265
H	1.539264	-3.670805	-0.800666
O	3.919393	0.523013	-2.497935
H	3.350228	1.322036	-2.485661
H	3.348260	-0.218493	-2.788295
O	2.337173	2.827890	-2.387300
H	2.309304	3.142778	-1.440742
H	2.742417	3.544935	-2.897796
O	2.438465	0.768175	3.578248
H	2.866699	0.900855	4.437654
H	3.027589	1.201036	2.911648
O	2.396957	-1.996512	3.055638
H	2.385929	-1.031029	3.222252
H	2.983243	-2.136058	2.281446
O	3.975531	1.930461	1.645533
H	4.347190	1.228036	1.032454
H	4.736853	2.416929	1.996468
O	4.906308	0.075815	0.012178
H	4.601189	-0.816613	0.284443
H	4.554053	0.221963	-0.899775
O	-0.065569	2.102341	-3.587644
H	0.764169	2.347103	-3.123284
H	-0.019435	1.139092	-3.769142
O	2.345847	3.637118	0.150083
H	1.476305	3.722086	0.598063
H	2.893583	3.039940	0.703900
O	-2.341052	-3.484368	-1.138810
H	-2.819663	-4.257444	-1.475619
H	-2.910738	-3.104922	-0.408653
O	-2.282757	-2.036785	3.086666
H	-2.677524	-2.481867	3.851615
H	-1.395912	-2.474542	2.940584
O	-0.042082	2.091353	3.589997
H	0.813226	1.613762	3.569188
H	-0.016030	2.741416	2.855939
O	-2.397603	0.716684	3.541189
H	-2.269431	-0.240988	3.370731
H	-1.505346	1.139881	3.552824
O	-3.952615	1.874446	1.747594
H	-3.373288	1.435443	2.439438
H	-4.625865	2.375029	2.232927
O	-4.956197	-0.019856	0.072546
H	-4.652699	0.683948	0.698889
H	-5.924055	-0.028082	0.119304
O	-2.372164	2.768309	-2.431503
H	-2.757640	3.462233	-2.987231
H	-1.491391	2.542805	-2.842400

O	-2.319065	-1.617037	-3.237830
H	-2.278715	-2.254441	-2.493989
H	-2.914219	-0.882636	-2.948260
O	-0.050586	-0.634837	-4.171537
H	-0.889953	-1.035723	-3.798118
H	-0.115611	-0.729815	-5.134128
O	-3.941945	0.453127	-2.502056
H	-4.314347	0.317044	-1.605831
H	-3.416052	1.280288	-2.458770
O	-2.378238	3.610060	0.223565
H	-2.945159	2.981561	0.720182
H	-2.341892	3.291408	-0.704386
O	-0.066566	3.956485	1.502127
H	-0.101634	4.855962	1.860975
H	-0.913972	3.831125	0.990434
O	-3.827227	-2.466599	0.812987
H	-3.296882	-2.302321	1.624143
H	-4.230953	-1.606949	0.565774
O	0.015170	-4.255360	0.000723
H	0.009929	-5.224351	0.026437
H	-0.829888	-3.991397	-0.441513
O	0.020255	-3.276123	2.634636
H	0.858311	-2.774951	2.782630
H	0.048224	-3.604311	1.711441

Table S13. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₆ hollow clathrate in the irregular pentadecahedron 4¹⁵10⁶4 configuration.

O	-2.538079	-3.855829	-0.298343
H	-2.937490	-4.734789	-0.379222
H	-1.625183	-3.994719	0.080134
O	0.129453	-2.710343	3.097223
H	0.171942	-3.381199	3.795989
H	0.949610	-2.146797	3.212621
O	-0.094132	-4.163730	0.720655
H	0.056297	-3.602542	1.511399
H	0.609839	-3.955134	0.070553
O	-2.216339	-1.330158	3.374383
H	-2.565229	-1.577629	4.244212
H	-1.350778	-1.801061	3.287662
O	-2.263540	1.489468	3.245924
H	-2.920696	1.719648	2.547449
H	-2.197482	0.513080	3.256309
O	-3.740840	-0.093506	-2.518298
H	-4.443735	-0.115563	-3.185452
H	-4.199526	-0.093560	-1.641962
O	-2.300145	-2.503993	-2.732822
H	-2.773302	-1.650286	-2.648100
H	-2.422869	-2.974362	-1.880810
O	-4.895581	-0.089276	-0.042785
H	-4.567036	-0.871308	0.487943
H	-5.862224	-0.156989	-0.059093
O	-3.977688	-2.148367	1.358243
H	-3.475924	-2.770728	0.786878

H	-3.358923	-1.867536	2.066535
O	2.265564	1.534168	3.524443
H	1.433883	2.032143	3.284294
H	2.557136	1.891892	4.376134
O	-4.047313	2.228638	1.288623
H	-3.565785	2.791471	0.647577
H	-4.357319	1.444046	0.789473
O	4.016679	-2.287682	-0.871902
H	4.810921	-2.776155	-1.137152
H	3.980750	-1.478181	-1.458427
O	1.559960	-0.165094	-3.932721
H	1.774168	-0.199380	-4.877179
H	1.070568	-1.013040	-3.729192
O	-2.306648	2.304021	-2.829125
H	-2.786921	1.458720	-2.705234
H	-2.446727	2.825698	-2.011670
O	0.360892	2.292112	-3.395897
H	0.709954	1.388653	-3.554298
H	-0.603449	2.211753	-3.197908
O	1.662988	3.662877	-1.567728
H	1.165594	3.132415	-2.263124
H	1.922281	4.490826	-2.001535
O	3.929837	2.255318	-0.934956
H	3.119358	2.783810	-1.136391
H	4.678774	2.796278	-1.228452
O	0.055484	2.874601	2.916063
H	0.036074	3.299506	2.034788
H	-0.780084	2.353119	3.004644
O	4.427986	-1.333764	1.748539
H	4.260351	-1.685678	0.850122
H	4.507058	-0.355898	1.649545
O	2.307299	-1.259440	3.470203
H	3.045517	-1.390817	2.826416
H	2.188013	-0.287354	3.531211
O	4.388727	1.414858	1.706938
H	4.158758	1.759929	0.819805
H	3.615610	1.579533	2.286928
O	-0.059265	4.274050	0.465854
H	0.589691	4.048851	-0.246675
H	0.095971	5.206419	0.682223
O	-2.595613	3.842247	-0.497471
H	-3.014871	4.698109	-0.672923
H	-1.696026	4.043179	-0.143794
O	3.887483	-0.126530	-2.412463
H	3.067075	-0.117640	-2.953761
H	3.889276	0.707242	-1.895250
O	1.765480	-3.758450	-1.323945
H	2.052538	-4.631541	-1.631943
H	2.594109	-3.249203	-1.140572
O	0.355181	-2.463412	-3.379474
H	-0.601412	-2.436511	-3.135592
H	0.819226	-2.922972	-2.648428

Table S14. M06-2X/6-31+G*/PCM optimized Cartesian

coordinates of the $(\text{H}_2\text{O})_{28}$ hollow clathrate in the hexadecahedron $5^{12}6^4$ - T_d configuration.

O	-0.370239	4.726595	0.563571
H	-1.175710	4.322228	0.971216
H	-0.455038	5.683750	0.689720
O	-0.030333	-2.063809	4.249783
H	-0.002470	-2.759574	3.560308
H	-0.875812	-1.583756	4.119628
O	-3.748180	-1.548847	-2.539061
H	-4.514854	-1.846413	-3.051813
H	-4.110635	-1.094176	-1.738796
O	4.092754	-1.069871	-2.222516
H	3.588807	-1.892507	-2.045069
H	3.532722	-0.517153	-2.807200
O	0.328015	-3.250865	-3.049380
H	1.147800	-3.307882	-2.513840
H	0.364812	-2.394791	-3.524302
O	0.319838	-0.817936	-4.469886
H	0.382993	-1.012637	-5.417410
H	1.107258	-0.258184	-4.256670
O	-1.642404	2.009175	3.670311
H	-0.663035	2.020048	3.746198
H	-1.920128	1.067778	3.703244
O	-3.858984	2.262470	-0.472335
H	-3.327265	2.423771	-1.282401
H	-3.361061	2.645451	0.281314
O	-2.438388	2.652679	-2.835878
H	-2.323795	1.770374	-3.286840
H	-2.959284	3.198479	-3.443945
O	3.829390	-1.339782	2.151484
H	4.119740	-0.734236	1.410098
H	4.641360	-1.620463	2.599871
O	3.631713	2.799372	-0.070385
H	3.011122	3.124675	0.639493
H	4.380829	3.414161	-0.070247
O	2.354709	2.903174	-2.560133
H	2.788303	2.866380	-1.680420
H	1.450803	3.273040	-2.413208
O	-2.190310	-3.956346	0.806988
H	-2.103449	-3.859353	-0.187033
H	-2.703595	-4.765950	0.951568
O	-0.102631	4.025168	-2.145477
H	-0.225920	4.273204	-1.205607
H	-0.898525	3.511738	-2.399704
O	0.120727	-4.046980	2.259563
H	0.152364	-4.930113	2.657686
H	-0.691458	-4.033086	1.695180
O	-4.629011	-0.268485	-0.292983
H	-4.331444	0.685852	-0.327389
H	-5.596377	-0.246357	-0.235080
O	4.628020	0.198429	0.143151
H	4.244669	1.100555	0.102748
H	4.425205	-0.233920	-0.721626
O	-2.540221	3.486826	1.663977
H	-2.219904	2.902920	2.411020
H	-3.161875	4.114848	2.062504
O	2.716626	-3.430309	-1.616556

H	3.223377	-4.203181	-1.907427
H	2.646815	-3.501635	-0.624147
O	2.084521	-0.337124	4.085601
H	1.334914	-0.979456	4.121529
H	2.685622	-0.645996	3.374283
O	-2.212355	0.268919	-4.007686
H	-2.719044	-0.401347	-3.501440
H	-1.307161	-0.089386	-4.128677
O	1.954548	3.741500	1.775921
H	1.127504	4.080514	1.371982
H	1.684046	3.137243	2.501453
O	-2.070939	-3.673986	-1.816733
H	-2.649371	-2.929928	-2.086895
H	-1.188032	-3.507455	-2.227309
O	2.561125	0.614495	-3.864322
H	3.068593	0.820437	-4.663961
H	2.447632	1.482592	-3.376644
O	-2.423129	-0.651992	3.874566
H	-3.007443	-0.763200	4.639560
H	-2.904624	-1.053388	3.098814
O	1.135807	2.128200	3.887623
H	1.372358	2.564340	4.720141
H	1.522331	1.206409	3.939920
O	-3.675475	-1.814725	1.829564
H	-3.149896	-2.546229	1.439713
H	-3.969674	-1.247012	1.085572
O	2.595466	-3.577030	1.042322
H	2.992000	-2.782264	1.462060
H	1.707618	-3.701074	1.439519

Table S15. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₈ hollow clathrate in the hexadecahedron 5¹²6⁴-D₂ configuration.

O	2.926258	3.417084	1.531378
O	0.268141	4.293089	1.489582
O	-1.639644	2.980643	2.814444
O	3.419395	1.006619	2.860192
O	1.273131	-0.588929	3.646280
O	-1.195456	0.409444	3.809344
O	3.900703	-2.983380	1.034299
O	4.981002	-0.404007	1.239867
O	-3.862812	2.987077	1.120861
O	-4.952559	0.411710	1.337272
O	-3.295734	-1.164958	2.834708
O	-3.021488	3.327170	-1.456038
O	-0.407623	4.287540	-1.216090
O	1.516611	3.211039	-2.716986
O	-3.417375	1.046146	-2.755953
O	-1.277808	-0.436754	-3.769700
O	1.304195	0.621822	-3.708040
O	-4.998862	-0.696875	-1.240362
O	4.988337	0.695974	-1.252821
O	3.798910	3.156478	-1.063744
O	3.394762	-0.864497	-2.975523

O	-1.551171	-2.903883	-2.784643
O	-3.738245	-3.118704	-1.035003
O	1.717067	-3.170433	2.661465
O	-0.197780	-4.281957	1.201340
O	-2.827539	-3.399161	1.511552
O	0.523922	-4.227421	-1.489293
O	2.992404	-3.243957	-1.597566
H	-4.601776	1.322549	1.248427
H	-4.999748	0.048983	0.428164
H	-3.872180	-0.563898	2.302812
H	-2.525379	-0.634010	3.129821
H	-3.587518	3.155445	0.185940
H	-4.489378	3.689545	1.351117
H	-1.342055	0.468901	4.765707
H	-0.275114	0.043129	3.703319
H	-1.454847	2.066035	3.119585
H	-2.433522	2.936179	2.240146
H	-0.413760	3.783813	2.009216
H	0.248142	5.197060	1.838259
H	1.976770	3.656793	1.572053
H	3.031067	2.572058	2.018034
H	3.941183	1.203524	3.652818
H	4.021136	0.479930	2.258425
H	3.005883	3.186471	-1.638560
H	3.470638	3.262060	-0.139754
H	4.983108	-0.019951	0.327395
H	4.627703	-1.314427	1.156940
H	4.560656	1.585303	-1.208056
H	4.438146	0.162105	-1.863049
H	2.589624	-0.338665	-3.237343
H	3.873052	-1.046172	-3.798426
H	3.337182	-3.114904	-0.688362
H	3.101527	-2.389249	-2.069260
H	0.390720	0.267793	-3.655608
H	1.295932	1.526028	-3.325954
H	3.134801	-3.086664	1.651714
H	4.528992	-3.685496	1.260904
H	0.772301	3.595266	-2.176077
H	1.656284	3.824957	-3.453546
H	0.969876	-3.574838	2.133683
H	1.864655	-3.760053	3.416561
H	-0.188164	4.281711	-0.258712
H	-1.308197	3.908552	-1.301538
H	-3.538402	3.989376	-1.939711
H	-3.139489	2.467672	-1.952699
H	-2.638265	0.544456	-3.081452
H	-3.961995	0.413513	-2.240749
H	-3.303589	-4.088366	1.999654
H	-2.970811	-2.548127	2.023305
H	-4.601174	-1.599460	-1.189357
H	-5.888861	-0.811521	-1.606258
H	-4.289762	-3.884706	-1.255921
H	-3.436888	-3.252962	-0.100280
H	-1.103696	-3.919310	1.304029
H	0.018188	-4.251506	0.243582
H	-1.459085	-0.536621	-4.716927
H	-1.343878	-1.355306	-3.387303
H	0.584933	-5.131206	-1.833735

H	1.443329	-3.843201	-1.557600
H	-2.302992	-2.986118	-2.161260
H	-0.782764	-3.330088	-2.346246
H	1.406495	-1.481179	3.262205
H	2.015035	-0.026550	3.333373

Table S16. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₀ hollow clathrate in the heptadecahedron 5¹²6⁵-C_{2v} A configuration.

O	4.854189	2.116422	-0.555167
O	2.748829	3.718090	-1.289993
O	4.853815	-0.061765	-2.179941
O	-1.305386	2.447625	-3.291700
O	1.338303	2.497004	-3.396218
O	2.569277	0.095643	-3.812127
O	-2.617909	3.800263	-1.222812
O	4.769148	-2.225809	-0.676092
O	-1.452336	-2.373036	-3.394475
O	1.212262	-2.301551	-3.339565
O	2.619476	-3.734964	-1.386791
O	-2.691004	0.122373	-3.689809
O	4.368576	-1.470104	1.986257
O	4.422731	1.304736	2.105574
O	2.295156	2.645623	2.983856
O	2.287056	-2.780692	2.995310
O	0.092000	-1.362993	3.959493
O	0.109762	1.304260	4.087948
O	-1.374440	-4.385285	0.975030
O	1.275582	-4.410760	0.973471
O	-2.796791	-3.630395	-1.306240
O	-1.248616	4.475615	1.124082
O	1.400112	4.439559	1.046176
O	-2.067645	2.747136	3.072727
O	-2.164904	-2.725421	2.995182
O	-4.388622	-1.289649	2.077773
O	-4.335948	1.375263	2.186328
O	-4.870963	-2.170675	-0.532262
O	-4.988554	0.077955	-2.067556
O	-4.686126	2.316616	-0.418576
H	1.644757	-3.832618	1.676962
H	1.725825	-4.157900	0.139043
H	2.935663	-4.547421	-1.810922
H	3.431193	-3.222320	-1.143541
H	3.058289	-2.258323	2.634864
H	2.645230	-3.324399	3.713186
H	1.657326	-1.436022	-3.459546
H	1.691306	-2.774799	-2.626656
H	0.878014	-1.824490	3.595074
H	-0.695818	-1.810307	3.584842
H	-0.458215	-2.332840	-3.342009
H	-1.651299	-2.884026	-4.193686
H	-1.887512	-3.350565	2.279768
H	-2.467048	-3.282430	3.729058
H	-2.208262	-3.853367	-0.553665

H	-2.249245	-3.187937	-1.991052
H	-0.374459	-4.392177	0.941328
H	-1.641155	-5.300758	1.150378
H	-4.099838	-2.733651	-0.832646
H	-5.656664	-2.736391	-0.577454
H	-3.591643	-1.764296	2.397090
H	-4.555150	-1.612396	1.166047
H	-2.229136	-0.733561	-3.564290
H	-3.494962	0.084714	-3.131138
H	-5.806808	0.088014	-2.586568
H	-5.007533	-0.754965	-1.534347
H	-4.333042	0.378196	2.168182
H	-5.087617	1.630078	2.742302
H	-4.812911	1.525828	-0.985352
H	-4.568452	1.983368	0.497970
H	-2.816035	2.178623	2.794007
H	-1.353771	2.157202	3.393775
H	-2.988863	4.613570	-1.597500
H	-3.399804	3.252631	-0.931638
H	-1.739203	2.905590	-2.540308
H	-1.774248	1.587044	-3.409438
H	-1.698691	4.227316	0.288379
H	-1.559540	3.836860	1.810898
H	0.129967	1.483914	5.040109
H	0.104268	0.312073	4.002267
H	1.522118	3.071985	-4.154925
H	0.340918	2.454774	-3.326493
H	1.947585	3.264632	2.304931
H	1.528225	2.139930	3.329526
H	2.187779	3.948893	-0.519493
H	2.171976	3.285328	-1.952759
H	1.688782	5.332999	1.286031
H	0.399901	4.464631	1.043131
H	4.700921	1.842817	0.373390
H	4.095933	2.698776	-0.798703
H	3.613162	1.774352	2.451325
H	5.158780	1.595097	2.664880
H	2.089357	0.949140	-3.667656
H	2.832150	0.094976	-4.745130
H	4.852318	0.739516	-1.597469
H	4.056796	0.007995	-2.746660
H	4.515763	-1.705063	1.044771
H	4.350006	-0.489144	2.033091
H	5.617188	-2.685166	-0.771816
H	4.819180	-1.412222	-1.262796

Table S17. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₀ hollow clathrate in the heptadecahedron 5¹²6⁵-D_{5h} configuration.

O	4.963279	-2.110965	0.909093
H	5.755159	-2.644836	1.076891
H	4.958456	-1.914242	-0.075687
O	2.664372	-3.454814	1.570710
H	3.511420	-2.999871	1.342552
H	2.917996	-4.304167	1.963658

O	-1.328951	-1.991695	3.609101
H	-1.535030	-2.440365	4.443168
H	-0.335290	-1.967530	3.556809
O	1.344113	-1.963573	3.544792
H	1.787547	-1.090302	3.590317
H	1.789001	-2.467916	2.831153
O	4.982489	0.251018	2.273686
H	5.793921	0.301535	2.801876
H	5.012469	-0.618845	1.802069
O	2.678486	0.496086	3.746208
H	3.532093	0.410217	3.257479
H	2.917890	0.621803	4.677289
O	4.928333	2.302876	0.361944
H	4.116252	2.838547	0.501361
H	4.928683	1.605932	1.051513
O	-1.342461	2.808222	2.975373
H	-0.347744	2.785792	2.926680
H	-1.555115	3.454305	3.665917
O	1.326650	2.811612	2.911047
H	1.791558	1.986919	3.165260
H	1.760114	3.145155	2.096007
O	2.622884	3.827016	0.665118
H	2.847967	4.757780	0.813871
H	2.118661	3.797760	-0.195900
O	-2.672364	0.464534	3.755656
H	-2.128073	-0.345586	3.664832
H	-2.121657	1.220674	3.463711
O	4.915709	1.193431	-2.046786
H	4.941118	1.629091	-1.145930
H	5.713764	1.483075	-2.514475
O	-1.416479	3.689941	-1.698822
H	-1.661336	4.543684	-2.087580
H	-1.842395	3.675098	-0.796614
O	1.361961	3.736435	-1.675875
H	1.718542	3.038509	-2.265158
H	0.383947	3.647193	-1.668711
O	2.595878	1.847070	-3.332865
H	3.458408	1.630895	-2.899419
H	2.821607	2.294570	-4.162831
O	-2.646548	3.685052	0.667642
H	-2.163512	3.345491	1.451892
H	-3.489203	3.183018	0.610789
O	4.911448	-1.568873	-1.672572
H	4.101607	-1.933695	-2.093371
H	4.900334	-0.599641	-1.830153
O	-1.397376	-0.538639	-4.033489
H	-0.402182	-0.532975	-3.987605
H	-1.614194	-0.665575	-4.969600
O	1.270994	-0.533557	-4.002624
H	1.723445	-1.275345	-3.546209
H	1.726644	0.290869	-3.730547
O	2.616838	-2.657157	-2.803923
H	2.851128	-3.312627	-3.478174
H	2.123216	-3.154308	-2.093143
O	-2.745603	1.800251	-3.283866
H	-2.205635	2.402524	-2.729868
H	-2.190584	1.020672	-3.496239
O	-1.391480	-3.999093	-0.771788

H	-1.626217	-4.920239	-0.962218
H	-1.836865	-3.457455	-1.481529
O	1.386090	-3.995920	-0.861781
H	1.755892	-3.786391	0.021665
H	0.408463	-3.927135	-0.798448
O	-2.705233	-3.431841	1.639652
H	-2.172295	-3.584895	0.831383
H	-2.145772	-2.927706	2.267231
O	-2.670792	-2.603190	-2.650165
H	-3.506721	-2.231064	-2.292281
H	-2.198177	-1.867816	-3.096671
O	-5.036667	-2.115866	1.025226
H	-4.197864	-2.577196	1.264623
H	-5.032369	-1.257290	1.515003
O	-5.045195	-1.639611	-1.572531
H	-5.065744	-1.834458	-0.588256
H	-5.818484	-2.079544	-1.955997
O	-5.052632	1.117364	-1.979858
H	-5.054325	0.143136	-1.857761
H	-4.217346	1.338457	-2.458628
O	-5.038411	2.295043	0.398891
H	-5.808253	2.880652	0.452576
H	-5.070287	1.866686	-0.504815
O	-5.029888	0.279691	2.348231
H	-4.183211	0.368681	2.845461
H	-5.036986	1.003517	1.687380

Table S18. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₀ hollow clathrate in the heptadecahedron 5¹²6⁵-C_{2v} B inverted_inverted configuration.

O	-0.865508	-2.358188	-3.494277
H	-0.888484	-2.351428	-4.462653
H	-0.495670	-1.473524	-3.209746
O	-3.869959	2.125611	2.067314
H	-4.091258	1.205533	1.809997
H	-2.992689	2.101994	2.507222
O	-1.275341	-2.358351	3.450515
H	-1.457188	-2.432998	4.398980
H	-2.143241	-2.509887	2.979249
O	5.268565	0.490549	0.184023
H	4.927684	0.898844	-0.645013
H	4.979213	-0.450187	0.165589
O	2.539546	-0.283891	3.561685
H	2.613688	-0.284222	4.527680
H	2.796056	-1.190793	3.261273
O	3.084213	-2.757697	2.557929
H	3.662869	-3.308307	3.106896
H	2.213911	-3.244501	2.496376
O	-4.594722	-0.387648	-1.524234
H	-5.482852	-0.438163	-1.909896
H	-4.213775	0.484253	-1.833025
O	-2.865973	-4.297852	-0.133449
H	-3.439384	-5.074898	-0.216952
H	-3.041912	-3.731836	-0.940410

O	-0.217489	-4.982084	0.020423
H	-0.170478	-5.950304	0.040212
H	-1.180153	-4.761409	-0.037852
O	2.704081	3.842971	-1.376819
H	3.215417	4.627139	-1.628382
H	2.677388	3.846696	-0.377615
O	2.848590	-0.389510	-3.386182
H	3.066280	-1.286967	-3.031588
H	2.952544	-0.444216	-4.347849
O	3.303013	-2.839515	-2.273230
H	3.936605	-3.388842	-2.759204
H	2.438416	-3.340395	-2.278867
O	-1.364177	2.206327	3.297703
H	-0.864316	1.362293	3.095469
H	-1.448701	2.249278	4.262145
O	0.971611	-4.122541	-2.374203
H	0.300460	-3.543584	-2.797865
H	0.586233	-4.404887	-1.517492
O	0.029944	4.303500	2.233277
H	0.057675	5.017200	2.888285
H	-0.461566	3.559348	2.660421
O	-3.531843	-2.778457	2.112201
H	-3.324922	-3.314591	1.316021
H	-3.932386	-1.943711	1.787127
O	4.295465	1.657306	-2.124069
H	3.681091	2.386573	-1.894919
H	3.767888	0.980024	-2.594942
O	-3.307219	-2.766864	-2.252963
H	-3.694872	-1.896637	-2.018315
H	-2.464716	-2.586418	-2.725600
O	4.037770	1.738530	2.281844
H	4.490363	1.281971	1.530388
H	3.520118	1.046480	2.740800
O	0.090315	4.297059	-2.277264
H	-0.415863	4.588049	-1.479974
H	1.002680	4.106017	-1.969200
O	0.741499	-4.018122	2.474821
H	0.017274	-3.460785	2.834187
H	0.434439	-4.334456	1.598470
O	0.194378	-0.113142	-2.581253
H	1.127153	-0.091672	-2.883340
H	-0.229732	0.720192	-2.884010
O	-0.070909	0.002601	2.633425
H	-0.521401	-0.815929	2.937207
H	0.847743	-0.054052	2.974421
O	4.481712	-2.164127	0.189532
H	3.923405	-2.401820	0.958025
H	3.995561	-2.436088	-0.615757
O	-3.677617	1.984535	-2.293260
H	-3.706934	2.609778	-1.536006
H	-2.770783	2.041371	-2.666030
O	-1.106211	2.197552	-3.359514
H	-1.134859	2.333747	-4.318293
H	-0.642503	2.997067	-2.973293
O	-4.723289	-0.406014	1.208443
H	-4.701105	-0.395920	0.219171
H	-5.661653	-0.446690	1.449297
O	2.639055	3.854278	1.283144

H	1.735125	3.911686	1.655550
H	3.081522	3.064588	1.681363
O	-3.780008	3.684276	-0.095553
H	-4.554978	4.265640	-0.087057
H	-3.841871	3.118241	0.723938
O	-1.352017	5.082862	-0.088272
H	-2.212038	4.611342	-0.072807
H	-0.886337	4.823132	0.734294

Table S19. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₀ hollow clathrate in the heptadecahedron 5¹²6⁵-C_{2v} B inverted configuration.

O	0.562760	2.448417	-3.583011
H	0.579080	2.459128	-4.551483
H	0.294760	1.524480	-3.310345
O	4.066103	-1.668443	1.962303
H	4.184324	-0.730221	1.702307
H	3.217013	-1.736129	2.449075
O	1.037771	2.601096	3.586942
H	1.242027	3.011774	4.440685
H	1.841401	2.746388	3.013087
O	-5.168993	-1.053603	0.185330
H	-4.802624	-1.427243	-0.649107
H	-4.990420	-0.085851	0.153215
O	-2.562082	-0.027981	3.690647
H	-2.943182	-0.038631	4.582020
H	-2.847142	0.829666	3.288053
O	-3.301746	2.332450	2.525501
H	-3.942196	2.809434	3.075071
H	-2.500586	2.926259	2.459239
O	4.500916	0.888095	-1.647356
H	5.374160	1.036329	-2.041825
H	4.214351	-0.020053	-1.953800
O	2.364304	4.555384	-0.207411
H	2.864837	5.382893	-0.272937
H	2.595424	4.022230	-1.022949
O	-0.335083	4.953299	-0.029798
H	-0.495616	5.908956	0.002657
H	0.646109	4.847325	-0.101865
O	-2.287042	-4.109752	-1.424098
H	-2.714451	-4.946664	-1.661946
H	-2.241481	-4.103373	-0.425423
O	-2.922138	0.075943	-3.434393
H	-3.229936	0.944903	-3.075647
H	-3.055068	0.115002	-4.393272
O	-3.620866	2.463302	-2.311831
H	-4.316265	2.942725	-2.787176
H	-2.815778	3.055013	-2.324612
O	1.726548	-2.114117	3.431285
H	1.148994	-1.321876	3.618486
H	2.037314	-2.418863	4.297756
O	-1.442413	3.989416	-2.422540
H	-0.716552	3.492180	-2.859548
H	-1.081813	4.303549	-1.566055

O	0.469433	-4.213479	2.187912
H	0.506131	-4.942116	2.826014
H	0.885015	-3.439392	2.640207
O	3.145499	3.085967	2.035753
H	2.883646	3.603181	1.243581
H	3.648809	2.311368	1.705486
O	-4.118876	-2.111016	-2.142415
H	-3.426889	-2.771329	-1.925778
H	-3.674407	-1.382325	-2.622163
O	2.952674	3.111873	-2.351207
H	3.436674	2.288035	-2.128173
H	2.132017	2.843569	-2.820585
O	-3.771055	-2.149226	2.262661
H	-4.281106	-1.734449	1.523954
H	-3.327545	-1.415828	2.735280
O	0.351746	-4.278642	-2.344675
H	0.888940	-4.503561	-1.546288
H	-0.575654	-4.189062	-2.035206
O	-1.151006	3.887274	2.431589
H	-0.366168	3.442998	2.821008
H	-0.874694	4.228122	1.554210
O	-0.236583	0.089687	-2.690341
H	-1.166284	-0.033680	-2.977104
H	0.271405	-0.694080	-2.996075
O	0.214169	-0.018195	4.047645
H	0.527906	0.888761	3.841377
H	-0.751095	-0.032270	3.873541
O	-4.678827	1.666802	0.169131
H	-4.122807	1.938953	0.928043
H	-4.237870	1.988292	-0.643875
O	3.839902	-1.570324	-2.405899
H	3.942369	-2.184194	-1.645732
H	2.943983	-1.730465	-2.775067
O	1.303389	-2.072893	-3.459674
H	1.344150	-2.217590	-4.416786
H	0.932418	-2.913823	-3.061548
O	4.644159	0.921632	1.083876
H	4.617526	0.911579	0.094742
H	5.571503	1.075938	1.321055
O	-2.170932	-4.090922	1.232597
H	-1.263089	-4.037196	1.595707
H	-2.698568	-3.358553	1.637703
O	4.142653	-3.230815	-0.196682
H	4.978139	-3.721128	-0.184630
H	4.136998	-2.661361	0.622668
O	1.880344	-4.876019	-0.154459
H	2.689261	-4.321051	-0.160069
H	1.404782	-4.648338	0.671792

Table S20. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₀ hollow clathrate in the heptadecahedron 5¹²6⁵-C_{2v} B configuration.

O	-1.276637	-2.396818	-3.713549
H	-1.483771	-2.764838	-4.585869
H	-0.754520	-1.563902	-3.884237

O	-3.479646	2.701415	1.995496
H	-3.846451	1.823038	1.759577
H	-2.642871	2.551624	2.485184
O	-1.663486	-2.179073	3.702632
H	-1.964607	-2.508542	4.562903
H	-2.479007	-2.120450	3.130082
O	5.259749	-0.325510	0.234262
H	4.988838	0.110046	-0.606667
H	4.838986	-1.215830	0.227421
O	2.499173	-0.573392	3.765684
H	2.875866	-0.649464	4.655823
H	2.546577	-1.481855	3.376601
O	2.589804	-3.061503	2.635802
H	3.090864	-3.679163	3.190024
H	1.662071	-3.429698	2.583034
O	-4.582831	0.283046	-1.555919
H	-5.463851	0.348840	-1.955295
H	-4.073653	1.080125	-1.883066
O	-3.452680	-3.768110	-0.072494
H	-4.152881	-4.435110	-0.138184
H	-3.522813	-3.204864	-0.897177
O	-0.947427	-4.833281	0.109762
H	-1.021786	-5.799821	0.129353
H	-1.874304	-4.492313	0.045331
O	3.290957	3.352597	-1.388043
H	3.900046	4.059135	-1.650957
H	3.251033	3.383158	-0.389424
O	2.848173	-0.837942	-3.553140
H	2.848039	-1.708363	-3.083089
H	3.290596	-0.997888	-4.400816
O	2.814169	-3.227789	-2.218626
H	3.358245	-3.883415	-2.681149
H	1.884263	-3.593885	-2.218632
O	-1.103360	2.543535	3.464648
H	-0.750487	1.632578	3.669792
H	-1.321731	2.936568	4.323783
O	0.332779	-4.173728	-2.297141
H	-0.261442	-3.555210	-2.776055
H	-0.098106	-4.372511	-1.438692
O	0.656683	4.220300	2.192118
H	0.800158	4.951962	2.811507
H	0.054199	3.589289	2.656351
O	-3.827971	-2.124946	2.154653
H	-3.710373	-2.700002	1.367838
H	-4.117837	-1.250853	1.816421
O	4.486152	0.930993	-2.101113
H	4.011691	1.762754	-1.888612
H	3.863681	0.367151	-2.604607
O	-3.623511	-2.247433	-2.235190
H	-3.883201	-1.323520	-2.030694
H	-2.790479	-2.211719	-2.753909
O	4.221556	1.128880	2.302533
H	4.595090	0.585760	1.565312
H	3.603327	0.545410	2.787582
O	0.756303	4.039324	-2.340835
H	0.305803	4.438448	-1.557411
H	1.642968	3.754499	-2.031119
O	0.110826	-4.009144	2.570159

H	-0.529565	-3.370315	2.953266
H	-0.244524	-4.272891	1.694577
O	0.197277	-0.237270	-4.208785
H	1.127967	-0.356089	-3.923854
H	-0.099461	0.649894	-3.911034
O	-0.183853	0.140329	4.127055
H	-0.722862	-0.656878	3.933246
H	0.751535	-0.098387	3.952881
O	4.070941	-2.818531	0.261371
H	3.468105	-2.921044	1.026372
H	3.544274	-2.980323	-0.548328
O	-3.302879	2.455141	-2.372034
H	-3.218257	3.090043	-1.627212
H	-2.410101	2.362610	-2.770968
O	-0.797101	2.291701	-3.598568
H	-0.931476	2.686373	-4.473968
H	-0.183144	2.916824	-3.116395
O	-4.725465	0.338093	1.173782
H	-4.702523	0.323858	0.184542
H	-5.659914	0.430823	1.414995
O	3.185519	3.418508	1.266845
H	2.292402	3.601123	1.624723
H	3.505190	2.576912	1.677235
O	-3.142984	4.178563	-0.197802
H	-3.821060	4.870425	-0.204019
H	-3.288640	3.646322	0.633489
O	-0.522287	5.148011	-0.188821
H	-1.453849	4.840844	-0.176769
H	-0.125810	4.834988	0.651035

Table S21. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₀ hollow clathrate in the heptadecahedron 4¹5¹⁰6⁶-C_{2v} configuration.

O	-1.380456	4.381248	-1.058193
H	-0.401108	4.362115	-1.027327
H	-1.694180	4.195568	-0.147040
O	-4.050183	-0.533665	2.421717
H	-4.088266	-1.219421	1.719632
H	-4.111605	0.338258	1.976300
O	4.015495	-0.531085	2.649864
H	4.843392	-0.617760	3.147015
H	4.062112	-1.218316	1.922491
O	4.208723	1.975141	1.408407
H	3.418867	2.539054	1.542201
H	4.047614	1.125905	1.870403
O	1.936767	-0.855337	4.385892
H	2.681988	-0.753068	3.743207
H	2.347660	-1.001711	5.251276
O	1.493192	-3.767459	-2.530652
H	1.814725	-4.526884	-3.039734
H	1.978826	-2.982396	-2.881592
O	2.195458	-4.075524	0.175439
H	1.892707	-3.981504	-0.751470
H	1.391381	-4.098783	0.736293
O	-4.338602	1.978212	1.218390

H	-5.168149	2.337910	1.568622
H	-4.489992	1.842626	0.235222
O	-0.055812	3.355204	3.024809
H	-0.886929	3.433072	2.511809
H	-0.095340	2.505456	3.525642
O	-0.083458	-4.285915	1.788206
H	-0.078261	-5.181583	2.158396
H	-0.103617	-3.669705	2.571002
O	4.813361	-1.009142	-1.708980
H	4.828631	-0.020130	-1.538184
H	5.704597	-1.250452	-2.003797
O	-2.360198	3.837937	1.501200
H	-2.789715	4.629979	1.858752
H	-3.072073	3.153860	1.430020
O	-2.249552	-4.158961	0.022312
H	-1.496723	-4.148564	0.650912
H	-1.874568	-3.998981	-0.877306
O	2.127670	3.844608	1.615321
H	2.529424	4.614044	2.047270
H	1.306866	3.630425	2.148312
O	-4.265958	-2.492280	0.462221
H	-5.035718	-3.049662	0.651247
H	-3.495222	-3.117431	0.339407
O	-2.160213	-0.816039	4.271393
H	-2.853827	-0.706563	3.562960
H	-2.641294	-0.946826	5.102021
O	1.427540	4.461262	-0.941261
H	1.668191	5.390283	-1.081322
H	1.699154	4.249089	-0.011440
O	-0.108313	1.070512	4.518302
H	-0.887025	0.483802	4.415206
H	0.671653	0.482447	4.449294
O	-0.127358	-2.688175	3.926315
H	0.659079	-2.113870	4.039485
H	-0.903329	-2.092366	4.006417
O	4.218571	-2.311000	0.701469
H	4.408103	-1.871070	-0.154417
H	3.458702	-2.921187	0.542989
O	-1.310687	-3.743001	-2.511198
H	-1.688627	-2.947088	-2.941874
H	-0.336041	-3.671478	-2.573104
O	4.796147	1.585103	-1.226840
H	4.572134	1.740777	-0.276474
H	4.098555	2.033119	-1.750309
O	-4.701655	-1.072493	-1.914947
H	-4.528770	-1.589367	-1.099351
H	-3.977873	-1.288965	-2.541102
O	-4.710373	1.600683	-1.369074
H	-4.696062	0.634877	-1.581325
H	-3.990296	2.013584	-1.893139
O	-2.651700	2.820724	-2.812833
H	-3.021437	3.418161	-3.480192
H	-2.137461	3.396869	-2.183019
O	-2.616510	-1.584664	-3.706656
H	-2.122805	-0.730453	-3.861235
H	-2.957772	-1.856712	-4.571721
O	2.865339	-1.600185	-3.503507
H	3.611273	-1.392047	-2.884631

H	3.275846	-1.815679	-4.355149
O	2.775846	2.851557	-2.711510
H	2.272981	3.442389	-2.100572
H	3.153383	3.429873	-3.391530
O	-1.363689	0.721796	-4.135965
H	-1.741938	1.472196	-3.630639
H	-0.386728	0.743806	-4.009183
O	1.367681	0.755803	-3.941993
H	1.832167	1.484771	-3.481642
H	1.866145	-0.063212	-3.745158

Table S22. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₂ hollow clathrate in the octadecahedron 5¹²6⁶-D₃ configuration.

O	5.570445	-0.036995	-0.012477
H	6.539282	-0.060774	-0.011936
H	5.271522	-0.950435	-0.247656
O	4.560220	0.736145	2.475820
H	4.010832	1.541839	2.372420
H	4.902708	0.506862	1.585582
O	3.244615	3.722459	-0.526612
H	3.157496	3.517667	0.427608
H	2.348620	3.962786	-0.841184
O	4.578319	1.776757	-1.906825
H	4.070023	2.465564	-1.414723
H	4.932510	1.159190	-1.232960
O	-0.565783	1.247402	4.276973
H	-1.490155	1.024477	4.035141
H	-0.067749	0.395966	4.321740
O	0.547648	3.351886	3.131202
H	0.536632	4.017140	3.836434
H	0.129824	2.532723	3.527592
O	3.117357	3.120867	2.219329
H	2.193727	3.157546	2.570880
H	3.610000	3.800077	2.704905
O	3.226564	0.414558	-3.740156
H	3.713031	0.952165	-3.051352
H	3.730546	0.515793	-4.561730
O	0.695756	4.543035	-1.360912
H	0.762901	5.454013	-1.685254
H	0.241116	4.033545	-2.076499
O	-0.641344	3.175212	-3.315791
H	-0.178980	2.354757	-3.656014
H	-0.747741	3.753530	-4.086699
O	0.569561	1.050143	-4.315975
H	0.090116	0.187541	-4.304649
H	1.497220	0.861370	-4.058637
O	-0.804696	4.551237	0.999260
H	-0.337697	4.069636	1.715255
H	-0.234902	4.512592	0.201864
O	3.309736	-2.257641	-2.964217
H	2.407523	-2.640860	-2.994421
H	3.234333	-1.318513	-3.243602
O	4.624120	-2.509740	-0.673048

H	4.112868	-2.434911	-1.529201
H	5.332429	-3.150751	-0.837266
O	3.139055	-3.365212	1.550572
H	3.240569	-2.664983	2.229911
H	3.621434	-3.054181	0.756523
O	0.779950	-3.420667	-3.210421
H	0.864144	-4.151313	-3.841819
H	0.334936	-3.802535	-2.413874
O	-0.562523	-4.478731	-1.076720
H	-0.646129	-5.436535	-1.201957
H	-0.132353	-4.360684	-0.180032
O	0.574034	-4.278123	1.299337
H	0.059824	-3.874803	2.031118
H	1.489823	-3.914687	1.359391
O	-0.721901	-1.359842	-4.393609
H	-1.635985	-1.407591	-4.044401
H	-0.224729	-2.083478	-3.958533
O	0.765578	-1.128350	4.510352
H	0.255438	-1.877132	4.134764
H	1.672569	-1.195738	4.143804
O	3.370262	-1.403072	3.535543
H	3.797629	-0.583283	3.162271
H	3.948198	-1.704536	4.252438
O	-3.225930	-2.167168	3.163146
H	-3.236298	-1.200350	3.336137
H	-3.654870	-2.305125	2.290927
O	-0.798626	-3.211777	3.481610
H	-1.711976	-2.837474	3.334227
H	-0.899633	-3.906342	4.149712
O	-4.532239	-2.578215	0.740474
H	-5.267065	-3.196488	0.869787
H	-3.994311	-2.942509	-0.015709
O	-3.165716	-3.494221	-1.358407
H	-3.175287	-2.838113	-2.087373
H	-2.234912	-3.778382	-1.234569
O	-5.501372	-0.040746	0.045655
H	-5.161711	-0.934497	0.264444
H	-5.196574	0.155849	-0.864944
O	-4.615093	0.618432	-2.536621
H	-4.060426	1.446447	-2.463342
H	-5.369682	0.850128	-3.099102
O	-3.343511	-1.624826	-3.434424
H	-3.791837	-0.795378	-3.135805
H	-3.897547	-1.987248	-4.142372
O	-3.222393	2.864190	-2.283836
H	-3.205532	3.194170	-1.358883
H	-2.302576	2.911599	-2.621848
O	-3.218841	0.563831	3.738866
H	-3.702423	1.063187	3.019668
H	-3.726987	0.709171	4.551193
O	-4.565004	1.814206	1.825752
H	-4.892582	1.158050	1.163808
H	-4.073075	2.497877	1.322957
O	-3.274616	3.799392	0.342786
H	-3.810110	4.606146	0.382901
H	-2.357057	4.064788	0.629933

Table S23. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₂ hollow clathrate in the octadecahedron 5¹²6⁶-C₂ A configuration.

O	-5.227663	-2.334339	-0.189554
O	-3.086676	-3.456374	-1.590235
O	-4.459652	-2.065708	2.351415
O	1.279860	-4.511813	-0.397196
O	-1.278319	-4.349744	0.246457
O	-1.994420	-3.327816	2.759720
O	1.996653	-3.383275	-2.774941
O	-4.168438	0.658309	2.915663
O	-4.989882	2.096182	0.749384
O	-3.312590	3.810414	-0.357529
O	-1.551095	0.947995	3.865347
O	-0.175487	3.142669	3.227899
O	-1.024079	4.531610	0.950305
O	2.574792	2.872369	2.888678
O	2.197115	-1.795385	3.515721
O	-0.372209	-1.578362	4.084102
O	3.746389	0.521196	3.336748
O	3.040759	-3.491028	1.543889
O	0.186679	3.111699	-3.103777
O	-2.583734	2.938249	-2.908802
O	1.597040	1.027244	-3.983077
O	1.086695	4.606427	-0.913025
O	-5.562495	0.224113	-1.265047
O	-3.802363	0.618749	-3.319763
O	0.343439	-1.464167	-3.959461
O	-2.294399	-1.714647	-3.639396
O	3.383008	3.842581	0.378194
O	4.991928	1.986845	-0.790940
O	4.140357	0.632225	-2.888859
O	5.531214	0.125565	1.227655
O	5.222823	-2.330582	0.240086
O	4.441864	-2.042977	-2.423214
H	-5.385302	0.868051	-0.547362
H	-5.467897	-0.666965	-0.865730
H	-4.964091	-2.261801	0.769759
H	-6.032912	-2.872482	-0.213608
H	-5.785103	2.608560	0.960746
H	-4.334392	2.748733	0.362548
H	-3.855961	-3.045991	-1.141028
H	-2.789584	-2.822355	-2.276702
H	-4.427371	0.442586	-2.575070
H	-3.234498	-0.176456	-3.406281
H	-2.585146	-2.117074	-4.471743
H	-1.309010	-1.600283	-3.726367
H	-3.009663	2.049070	-3.078069
H	-2.954686	3.540910	-3.570924
H	-3.036288	3.505940	-1.249001
H	-2.485582	4.030645	0.134951
H	-1.908270	-3.983703	-0.420647
H	-1.494756	-3.933803	1.106599
H	-2.109846	-4.089635	3.347987
H	-1.370785	-2.717584	3.226438
H	-4.754532	0.915567	3.643746

H	-4.441163	1.209987	2.140523
H	-4.346345	-1.113573	2.559978
H	-3.589047	-2.490411	2.508355
H	-2.442033	0.833836	3.472830
H	-1.120769	0.066632	3.875725
H	-0.413825	-1.782206	5.031099
H	0.596102	-1.644306	3.835662
H	-0.676467	2.307345	3.435440
H	-0.306924	3.724257	3.991990
H	0.311900	-4.420102	-0.158823
H	1.455457	-5.464834	-0.423580
H	-0.263778	4.547129	0.332791
H	-0.740580	4.007094	1.728742
H	2.089599	-4.109114	-3.410454
H	1.696735	-3.799203	-1.928664
H	1.226266	5.516790	-1.215296
H	1.936510	4.326451	-0.495878
H	-0.784602	3.007229	-3.004331
H	0.507049	3.593111	-2.312367
H	0.774277	-0.583977	-3.906983
H	0.918712	-2.101700	-3.486772
H	1.747935	1.235874	-4.917563
H	1.062637	1.786849	-3.621759
H	4.216726	-0.340548	-2.731071
H	3.230431	0.795389	-3.217216
H	3.599170	-2.532148	-2.528422
H	4.723782	-2.179120	-1.493293
H	4.633473	1.496717	-1.589526
H	5.823973	2.392999	-1.078577
H	3.951922	4.611421	0.537788
H	3.951436	3.175336	-0.083736
H	6.052108	-2.816813	0.359743
H	5.370477	-1.419678	0.620275
H	5.328953	0.794001	0.538027
H	4.901081	0.283086	1.964465
H	3.804932	-3.113118	1.058617
H	2.403911	-3.800061	0.866313
H	1.598412	2.928124	2.976739
H	2.803428	3.207866	1.996721
H	3.273064	1.387286	3.193321
H	4.239984	0.619870	4.164883
H	2.468086	-2.389054	2.774866
H	2.705758	-0.962453	3.417590

Table S24. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₂ hollow clathrate in the octadecahedron 5¹²6⁶-C₂ B configuration.

O	1.083937	4.227021	-2.360888
H	0.742427	4.557294	-1.493031
H	1.081749	4.991148	-2.957212
O	3.693601	3.226065	-2.041715
H	2.789588	3.593571	-2.129661
H	3.888148	3.196196	-1.080443
O	0.265314	5.101986	0.085478

H	0.309799	6.067918	0.152219
H	-0.666465	4.848314	0.345783
O	-2.183710	4.435030	0.848256
H	-2.175411	3.882730	1.661049
H	-2.745198	3.970033	0.192281
O	-3.904493	3.200490	-0.977595
H	-4.513320	3.871393	-1.322242
H	-3.518793	2.751824	-1.769706
O	4.288511	3.060134	0.685110
H	5.043959	3.621777	0.914453
H	4.567109	2.123710	0.887237
O	5.050526	0.550660	1.151744
H	4.539832	0.060337	1.830011
H	5.020435	0.019134	0.326160
O	3.745882	-0.884828	3.168429
H	2.878223	-0.565136	3.519764
H	4.343879	-0.919808	3.930504
O	1.995190	3.974769	1.993102
H	1.423843	4.359741	1.296193
H	2.788156	3.618137	1.539366
O	0.583363	2.361704	3.692780
H	-0.364270	2.521263	3.495082
H	1.103832	2.905600	3.054215
O	1.319826	-0.129769	4.176998
H	1.036066	0.804144	3.953139
H	1.381713	-0.157544	5.144282
O	3.458643	-3.438556	2.024486
H	2.531103	-3.724542	2.168869
H	3.541624	-2.556227	2.442331
O	0.812873	-4.276919	2.349172
H	0.480694	-4.575630	1.453874
H	0.766081	-5.053629	2.926674
O	0.009435	-5.080936	-0.046195
H	-0.888046	-4.770869	-0.316327
H	0.631808	-4.772949	-0.740057
O	-0.508288	-2.162750	3.576175
H	0.131469	-1.431940	3.711396
H	-0.041865	-2.881472	3.096592
O	3.965709	-3.361342	-0.664483
H	4.297429	-2.466900	-0.893575
H	3.795806	-3.360240	0.308621
O	5.028015	-0.850180	-1.254001
H	4.574412	-0.293163	-1.949723
H	5.939398	-0.970617	-1.560534
O	3.875160	0.700461	-3.073556
H	2.990170	0.428775	-3.397496
H	3.776823	1.615539	-2.714219
O	1.824017	-4.203315	-1.982032
H	2.124977	-4.951859	-2.518843
H	2.635864	-3.859314	-1.509495
O	0.459055	-2.433636	-3.645483
H	-0.497953	-2.540130	-3.456429
H	0.943830	-3.022190	-3.027180
O	1.374030	0.021421	-4.135102
H	1.028336	-0.885959	-3.910231
H	1.497133	0.021117	-5.096576
O	-3.911286	-0.731315	-3.001602
H	-3.526017	0.170660	-3.014036

H	-4.426235	-0.813795	-2.171099
O	-2.924810	1.883417	-3.167808
H	-3.330980	2.250521	-3.968067
H	-1.939584	1.968030	-3.304093
O	-0.324968	2.171625	-3.624030
H	0.172857	2.855548	-3.128340
H	0.267466	1.397276	-3.738007
O	-2.268305	-2.820691	-3.217897
H	-2.850376	-2.013088	-3.162000
H	-2.612823	-3.347000	-3.955110
O	-5.399180	-1.091941	-0.659509
H	-6.300229	-1.392893	-0.850810
H	-4.997500	-1.776056	-0.071366
O	-4.172851	-2.935338	0.961762
H	-3.753156	-2.502987	1.747658
H	-4.790417	-3.592483	1.317879
O	-2.482383	-4.290433	-0.845468
H	-2.437659	-3.750922	-1.663596
H	-3.021807	-3.784140	-0.204839
O	-2.101746	2.945835	3.200139
H	-2.415903	3.503376	3.928000
H	-2.746833	2.184262	3.140792
O	-3.887269	0.994862	2.987226
H	-4.384417	1.103938	2.140540
H	-3.554633	0.073280	3.004191
O	-3.084192	-1.695290	3.133553
H	-3.510468	-2.034085	3.935842
H	-2.107046	-1.852868	3.261856
O	-5.278163	1.376176	0.663603
H	-4.806572	1.996926	0.069738
H	-5.353616	0.531578	0.172576

Table S25. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₂ hollow clathrate in the octadecahedron 5¹²6⁶-D₂ configuration.

O	2.393282	4.099785	0.880261
O	-2.340186	3.949268	-1.297542
O	-0.201339	3.257013	-2.974075
O	2.205154	3.504272	-1.847491
O	4.555136	2.556647	1.799285
O	5.729926	1.256306	-0.295789
O	4.185451	1.689651	-2.584403
O	3.553721	0.614653	3.546441
O	0.876239	1.258307	3.954106
O	-0.858315	-0.751880	4.197256
O	4.186258	-1.753685	2.498804
O	2.182068	-3.596774	1.898059
O	-0.263955	-3.118146	2.853064
O	5.754312	-1.331500	0.226742
O	-3.515224	-0.188974	3.563057
O	-4.509128	-2.386771	2.133905
O	-2.429886	-3.953836	1.269163
O	-4.132172	2.108780	2.351531
O	-2.094612	3.776804	1.420208
O	0.288920	3.603709	2.542565

O	-5.703148	1.483720	0.113097
O	-5.737842	-1.244613	-0.118345
O	-4.559131	2.448699	-2.079865
O	-3.480130	0.341621	-3.560235
O	0.124498	-3.453844	-2.443358
O	-2.283756	-3.842271	-1.458341
O	-4.206577	-2.081703	-2.328058
O	2.280079	-4.005656	-0.866137
O	4.543040	-2.644915	-1.828763
O	-0.853083	0.810517	-4.155426
O	0.788004	-1.271537	-4.054918
O	3.462216	-0.699287	-3.518465
H	-5.158787	1.700065	0.900177
H	-5.717238	0.498305	0.048633
H	-5.015850	2.107095	-1.257908
H	-5.221225	2.959033	-2.569397
H	-3.886173	1.062014	-3.031746
H	-3.699775	-0.497139	-3.105231
H	-3.110568	3.427991	-1.610002
H	-1.579093	3.681481	-1.854642
H	-2.524438	-4.716588	-1.802664
H	-1.363682	-3.656228	-1.814921
H	-2.551322	-4.892631	1.479376
H	-2.340419	-3.906769	0.284577
H	-2.778429	3.146460	1.732212
H	-2.153536	3.804238	0.434876
H	-4.652342	2.608359	2.998630
H	-3.869652	1.262082	2.807664
H	-5.111753	-2.926677	2.667326
H	-3.786104	-2.991107	1.839081
H	-2.567829	-0.357217	3.757787
H	-3.841616	-0.970620	3.069127
H	-3.490142	-2.698021	-2.040858
H	-4.756221	-2.585399	-2.947377
H	-5.330209	-1.667651	0.666064
H	-5.204850	-1.535895	-0.887439
H	-1.790834	0.626217	-3.908367
H	-0.597182	1.641310	-3.700756
H	0.691242	3.320233	-2.536570
H	-0.189925	3.913375	-3.687088
H	0.321909	-2.646078	-2.963779
H	0.894733	-3.611150	-1.845109
H	0.174854	-0.482288	-4.052932
H	0.776256	-1.607364	-4.964188
H	2.506637	-0.876765	-3.659498
H	3.804053	-1.411864	-2.937330
H	5.033474	-2.195197	-1.096237
H	5.188353	-3.207409	-2.282690
H	4.718618	2.094734	-3.284950
H	3.878271	0.811871	-2.945581
H	2.217363	-3.837409	0.098184
H	3.087162	-3.544251	-1.175032
H	2.251507	3.655851	-0.880190
H	2.880614	2.828484	-2.071564
H	1.271636	-3.384562	2.241637
H	2.435823	-4.428464	2.326406
H	1.601497	3.936720	1.451308
H	2.585354	5.046716	0.956110

H	-0.467019	-2.256061	3.276340
H	-1.012091	-3.336659	2.260346
H	-0.609625	3.637361	2.100310
H	0.272256	4.296915	3.220347
H	-0.833777	-0.955559	5.144627
H	-0.215513	-0.001418	4.067015
H	1.807945	1.016984	3.760934
H	0.659576	2.042157	3.406113
H	4.007234	0.652761	4.402001
H	3.757677	-0.284969	3.166706
H	4.192799	1.893411	2.424915
H	3.793620	3.097967	1.502687
H	3.452448	-2.367013	2.277255
H	4.717534	-1.638079	1.681820
H	5.188384	1.427751	-1.096368
H	5.295360	1.744228	0.446418
H	6.672095	-1.595308	0.392234
H	5.772374	-0.347236	0.030506

Table S26. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₂ hollow clathrate in the octadecahedron 5¹²6⁶-D_{3d} configuration.

O	-1.213985	-4.186864	-0.721795
H	-2.056060	-3.852771	-1.114839
H	-1.288395	-5.153610	-0.739583
O	1.177140	-3.705732	-2.149764
H	1.119870	-2.885644	-2.701770
H	0.334900	-3.783657	-1.656064
O	3.433293	-3.182589	1.885297
H	3.403450	-3.388375	0.918500
H	3.791121	-3.974285	2.314796
O	-1.297941	-3.590990	2.020815
H	-1.195052	-3.731679	1.056520
H	-0.464742	-3.179993	2.354731
O	0.979493	-2.565565	3.099436
H	1.009222	-1.639649	3.420461
H	1.829371	-2.740718	2.645131
O	3.449991	-3.692080	-0.799247
H	3.867592	-4.547138	-0.984315
H	2.563536	-3.711116	-1.266381
O	-3.424734	3.218022	-2.130357
H	-3.404230	3.343101	-1.150583
H	-3.974193	2.423361	-2.296440
O	-1.038850	2.733622	-3.166435
H	-1.098965	2.896163	-4.119814
H	-1.931928	2.972287	-2.779287
O	1.200049	4.134848	0.687348
H	1.201794	3.974102	-0.279856
H	2.025313	3.745164	1.049681
O	-3.434646	3.606185	0.575138
H	-3.986450	2.947315	1.045426
H	-2.575234	3.630672	1.046828
O	-1.054527	3.723213	2.049128
H	-1.124548	4.509461	2.611554

H	-0.213105	3.840363	1.527698
O	1.214455	3.824984	-2.094791
H	0.376862	3.459164	-2.472342
H	1.310718	4.711414	-2.474868
O	-3.614463	-3.286925	-1.735215
H	-4.086791	-4.022156	-2.155445
H	-4.189953	-2.985017	-0.967302
O	-0.904187	0.019692	-2.508003
H	-0.920204	0.964793	-2.767879
H	-1.750278	-0.359998	-2.822382
O	3.529340	-0.099497	-3.633874
H	3.914893	-0.056752	-4.521678
H	3.506622	0.839939	-3.295516
O	1.073846	-1.458997	-3.679007
H	1.917402	-0.960742	-3.654430
H	0.391341	-0.870312	-3.277959
O	3.567395	2.394665	-2.702826
H	2.718722	2.839179	-2.498502
H	4.112714	2.434848	-1.879412
O	-3.314527	-1.135015	-3.371239
H	-3.299176	-1.415903	-4.298472
H	-3.446248	-1.953013	-2.829083
O	-3.557422	0.144801	3.531072
H	-3.911457	0.115536	4.433242
H	-3.531684	-0.794817	3.218078
O	-3.585780	-2.422174	2.626750
H	-2.698398	-2.838593	2.415982
H	-4.009245	-3.007714	3.272957
O	3.583921	3.177464	1.751969
H	4.007404	3.899461	2.240152
H	3.529466	2.408118	2.388512
O	1.060003	0.021671	4.162325
H	0.256109	0.577028	3.970120
H	1.086270	-0.075398	5.126261
O	-1.114050	1.515622	3.746838
H	-1.948458	1.026930	3.591780
H	-1.085586	2.259161	3.106342
O	3.525562	1.112163	3.417682
H	2.639851	0.753853	3.639842
H	4.049924	0.360124	3.049510
O	5.036166	-0.927621	2.394396
H	4.496320	-1.723386	2.205476
H	5.434968	-0.661960	1.538197
O	5.135072	2.455276	-0.464534
H	4.612039	2.693309	0.330669
H	5.495482	1.557985	-0.298969
O	5.056148	-1.696675	-1.945142
H	4.500556	-1.154451	-2.547507
H	4.468445	-2.380326	-1.557678
O	6.111088	-0.133664	-0.060577
H	5.747499	-0.729409	-0.774048
H	7.076028	-0.203660	-0.109050
O	-6.039714	0.068342	-0.198888
H	-5.679946	0.407968	-1.044727
H	-5.717141	0.674053	0.500962
O	-5.098941	-2.455238	0.272461
H	-5.434330	-1.539229	0.111321
H	-4.578508	-2.420460	1.103745

O	-4.968143	0.924006	-2.649000
H	-5.652958	1.079072	-3.316914
H	-4.419841	0.173969	-2.981731
O	-5.069470	1.708938	1.857165
H	-5.776833	2.123874	2.373473
H	-4.558516	1.149051	2.489881

Table S27. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₂ hollow clathrate in the octadecahedron 5¹²6⁶-D_{3h} inverted configuration.

O	2.129848	3.968632	-2.268163
O	-0.233219	4.974416	-1.556868
O	-2.579149	3.659550	-2.274616
O	2.206963	1.332006	-3.208550
O	0.102539	-2.534769	-3.209464
O	0.001157	-0.063948	-2.205083
O	-2.311900	1.156001	-3.149668
O	2.416247	-3.856051	-2.317257
O	-5.461789	1.254648	0.029958
O	-4.198854	3.670930	0.025150
O	-4.267897	-2.753634	-1.492344
O	-4.566412	-0.196370	-2.209338
O	-1.972836	-4.159961	-2.281451
O	-2.494351	3.781701	2.134123
O	-0.314919	4.981449	1.230295
O	2.139327	3.988613	2.132764
O	-4.511043	-0.177263	2.165418
O	-2.239502	1.170576	3.114316
O	3.801695	3.997750	-0.028494
O	5.214068	1.759601	-0.061859
O	0.064033	-0.045751	3.738801
O	2.383931	1.446627	3.280681
O	4.557219	0.316880	2.221647
O	4.472985	-2.243169	-1.526215
O	4.539897	0.256960	-2.320492
O	2.437268	-3.906799	2.179033
O	4.498326	-2.292399	1.214642
O	-4.162167	-2.820000	1.293946
O	-1.992378	-4.103159	2.170415
O	0.233694	-2.789505	3.196689
O	-1.042958	-5.518341	-0.077441
O	1.696939	-5.344293	-0.128267
H	0.030317	-0.049433	4.707905
H	-0.777368	0.399518	3.452312
H	0.131395	-1.818808	3.290036
H	-0.597885	-3.146573	2.817240
H	-2.305621	-4.725584	2.843823
H	-2.797348	-3.598976	1.867312
H	-4.204772	-2.796265	0.312798
H	-4.263163	-1.893030	1.597327
H	2.189193	2.310873	2.861155
H	1.541370	0.948315	3.348104
H	-4.902016	0.344647	1.423861
H	-5.169276	-0.162758	2.876996

H	-2.280427	2.076004	2.740641
H	-3.005859	0.679154	2.751397
H	-1.652250	4.220134	1.815575
H	-2.826890	4.331732	2.859929
H	-5.066761	2.161623	0.032700
H	-6.423738	1.374554	0.020262
H	-3.612366	3.746536	0.821176
H	-4.780998	4.446016	0.040439
H	2.772110	4.017633	1.372364
H	2.492635	4.603275	2.794108
H	-0.273893	4.981407	0.248686
H	0.537440	4.610440	1.545105
H	-1.733801	4.098530	-2.035235
H	-3.138081	3.681508	-1.469745
H	0.633986	4.577040	-1.851249
H	-0.245320	5.878431	-1.905851
H	-3.761563	0.256106	-2.544058
H	-4.877088	0.329106	-1.442702
H	4.361443	3.166813	-0.041716
H	4.418575	4.745080	-0.048820
H	-2.391053	2.102742	-2.843745
H	-2.317368	1.182923	-4.118311
H	2.730793	3.977559	-1.491969
H	2.136270	3.048204	-2.608039
H	2.200668	1.288029	-4.176695
H	3.056204	0.911009	-2.920902
H	0.766905	0.452666	-2.535495
H	-0.803563	0.398509	-2.526649
H	4.491147	-0.711725	-2.050709
H	5.252879	0.321452	-2.973905
H	0.061455	-1.603875	-2.853832
H	0.096592	-2.454939	-4.174845
H	4.979844	1.213411	-0.843818
H	4.995224	1.223467	0.732194
H	-5.051791	-3.215728	-1.825568
H	-4.362041	-1.805316	-1.785133
H	5.244434	0.394406	2.900227
H	3.729640	0.702808	2.620617
H	-1.282138	-3.548076	-2.613862
H	-2.749992	-3.609879	-2.049177
H	4.463983	-2.268764	-0.539339
H	3.709366	-2.794260	-1.827220
H	2.139405	-4.397286	-1.538893
H	1.612981	-3.385107	-2.622168
H	4.452732	-1.396378	1.608842
H	3.754150	-2.807557	1.592430
H	1.955151	-4.859902	0.683336
H	0.713414	-5.423376	-0.094122
H	-1.389566	-5.030576	-0.861410
H	-1.376077	-5.035309	0.707282
H	2.761925	-4.494042	2.877835
H	1.632341	-3.455539	2.552708

Table S28. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₂ hollow clathrate in the

octadecahedron $5^{12}6^6-D_{3h}$ configuration.

O	-3.681968	2.684507	2.228743
O	-1.972126	4.556917	1.472046
O	0.697447	4.289756	2.182047
O	-2.659091	0.397598	3.317873
O	1.171080	-2.457877	3.467438
O	0.077976	0.037188	3.935126
O	1.731304	2.154469	3.385295
O	-0.418688	-4.475799	2.274113
O	4.303911	3.509320	-0.155752
O	2.089387	5.090074	-0.127587
O	5.054353	-0.584866	1.326965
O	4.203118	1.826012	2.091194
O	3.631370	-2.842430	2.152632
O	0.511736	4.472906	-2.244600
O	-1.959562	4.595453	-1.312168
O	-3.726680	2.612306	-2.185884
O	4.074231	1.835428	-2.314663
O	1.430596	2.022616	-3.240488
O	-5.190570	1.906138	-0.001102
O	-5.444684	-0.725001	0.081871
O	-0.103777	-0.090763	-3.840443
O	-2.837145	0.216410	-3.328059
O	-4.268740	-1.747604	-2.223735
O	-2.996467	-3.989101	1.513027
O	-4.126617	-1.744737	2.312645
O	-0.492635	-4.584856	-2.240542
O	-3.039764	-4.055648	-1.230255
O	4.948059	-0.687213	-1.459088
O	3.562717	-2.803271	-2.309642
O	0.974006	-2.623746	-3.311996
O	3.376346	-4.474996	-0.046603
O	0.837320	-5.500639	0.067878
H	-0.090545	-0.080056	-4.809997
H	0.458217	0.681568	-3.565055
H	0.633669	-1.708933	-3.405516
H	1.882264	-2.572314	-2.943892
H	4.113528	-3.227664	-2.984585
H	4.063696	-1.992228	-2.017507
H	4.989690	-0.644937	-0.478615
H	4.624522	0.188113	-1.760244
H	-3.038425	1.081959	-2.914279
H	-1.862683	0.144255	-3.416401
H	4.196880	2.465350	-1.564076
H	4.652865	2.152279	-3.025107
H	1.068430	2.852527	-2.864783
H	2.340245	1.926400	-2.888767
H	-0.434990	4.498023	-1.918016
H	0.567397	5.122940	-2.961701
H	3.545804	4.144896	-0.153677
H	5.111364	4.045797	-0.146998
H	1.529194	4.911987	-0.926276
H	2.247223	6.046401	-0.111666
H	-4.298012	2.363942	-1.416342
H	-4.322573	3.005554	-2.841854
H	-1.977507	4.578953	-0.329598
H	-2.563204	3.883336	-1.615188

H	-0.258391	4.333136	1.958883
H	1.180381	4.560642	1.373511
H	-2.604304	3.844817	1.781842
H	-2.312055	5.391605	1.828205
H	3.317392	1.893086	2.507526
H	4.201559	2.437100	1.324919
H	-5.316073	0.912348	0.031812
H	-6.077630	2.295907	0.023104
H	1.296613	2.926892	2.924673
H	1.995068	2.489951	4.256389
H	-4.215465	2.398353	1.457023
H	-3.274136	1.867734	2.603774
H	-1.699717	0.232968	3.411940
H	-3.068961	-0.416320	2.954679
H	0.010295	0.092147	4.901379
H	0.656981	0.795538	3.673985
H	-3.673729	-2.597730	2.040482
H	-4.780055	-1.991055	2.984533
H	0.790961	-1.554264	3.574925
H	1.322968	-2.781703	4.368562
H	-4.972784	-1.098102	0.859633
H	-5.028604	-1.117985	-0.716690
H	5.966671	-0.656885	1.645541
H	4.722693	0.301662	1.639187
H	-4.934257	-1.984338	-2.886941
H	-3.704094	-1.039695	-2.639291
H	2.779083	-2.609012	2.573863
H	4.075592	-2.001710	1.913997
H	-2.990106	-4.013594	0.526548
H	-2.061816	-4.124682	1.802235
H	0.069402	-4.824273	1.489146
H	0.108062	-3.731362	2.627530
H	-3.406324	-3.235258	-1.621228
H	-2.152158	-4.186631	-1.625927
H	0.377616	-5.195355	-0.741725
H	1.758614	-5.151211	0.003909
H	3.470966	-3.880213	0.733891
H	3.448483	-3.898271	-0.835520
H	-0.530780	-5.269895	-2.924486
H	0.023447	-3.830915	-2.635966

Table S29. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₄ hollow clathrate in the nonadecahedron 5¹²6⁷-C_{3v} configuration.

O	-5.535504	-0.849111	0.868052
O	-4.016290	-2.857059	1.914899
O	-5.028439	-0.776193	-1.875811
O	-4.148269	1.632927	-2.534101
O	-1.516105	1.892364	-3.457455
O	-3.404221	-2.949662	-2.503525
O	-0.837636	-2.698849	-3.551878
O	0.132610	-0.126423	-4.056884
O	-0.586395	-5.391242	-0.111607
O	-3.183684	-4.387523	-0.269413

O	1.048571	-4.782952	2.093094
O	1.832601	4.749289	-1.884125
O	-0.698212	4.406987	-2.581945
O	1.965690	5.287208	0.784248
O	4.979575	2.207464	-0.141840
O	3.596291	3.425872	1.977691
O	2.820391	0.380179	-3.485572
O	3.648292	2.695555	-2.480620
O	-2.215913	4.963569	-0.316199
O	-4.381596	3.189201	-0.305648
O	-4.752235	1.476690	1.867244
O	-0.625910	4.987417	1.824098
O	-0.549979	2.755964	3.487236
O	-2.631643	1.099850	3.632746
O	2.070779	1.816668	3.690288
O	-2.115611	-1.641516	3.586370
O	0.358480	-2.633695	3.752393
O	2.478118	-0.820257	3.623395
O	4.529799	-1.887851	2.071456
O	5.423687	-0.554131	-0.057509
O	0.663559	-4.562423	-2.399398
O	3.306024	-3.995734	-1.652069
O	4.336658	-1.663690	-2.367895
O	3.544310	-4.308455	1.045019
H	-5.255682	0.027906	1.261709
H	-6.482918	-0.941411	1.050614
H	-4.577163	-3.403747	2.486290
H	-4.605237	-2.147181	1.556722
H	-3.416998	-3.861993	0.525644
H	-2.266858	-4.714096	-0.144263
H	-3.893991	-3.495275	-3.137722
H	-3.322548	-3.500531	-1.674648
H	-2.755674	-2.050064	2.966532
H	-2.262619	-0.671639	3.555585
H	-5.207182	-0.829152	-0.912019
H	-4.432376	-1.526424	-2.092689
H	-3.953924	1.398194	2.433867
H	-4.539141	2.099364	1.139657
H	-2.992774	1.281534	4.513845
H	-1.842396	1.701326	3.539116
H	-4.723343	1.942571	-3.250481
H	-4.459961	0.708977	-2.308164
H	-4.329135	2.638562	-1.126574
H	-5.196931	3.707652	-0.385836
H	0.365950	2.404040	3.495587
H	-0.570780	3.510514	2.859934
H	-1.700509	4.763673	-1.128528
H	-2.961622	4.326876	-0.296619
H	-0.884162	5.759167	2.349983
H	-1.249110	4.961811	1.045709
H	-0.872200	5.052413	-3.283488
H	0.266942	4.515285	-2.338804
H	-1.195161	2.757065	-3.121875
H	-2.417364	1.760169	-3.095457
H	2.356941	2.059369	4.583991
H	2.199739	0.831241	3.628058
H	1.068648	5.198007	1.169010
H	2.530234	4.619983	1.241232

H	2.425920	3.994152	-2.079321
H	1.903599	4.926373	-0.912986
H	3.093597	2.782494	2.520139
H	4.051637	2.919860	1.273573
H	4.245315	3.047776	-3.158296
H	3.296153	1.835973	-2.847639
H	4.519563	2.410389	-0.993692
H	5.842385	2.646307	-0.195295
H	1.867155	0.176868	-3.597618
H	3.251451	-0.400793	-3.075978
H	5.246072	0.410429	-0.074119
H	5.043680	-0.922680	-0.885309
H	3.922007	-2.540122	-2.119339
H	5.040391	-1.871621	-3.000887
H	5.300932	-2.047228	2.636049
H	4.860387	-1.355433	1.295460
H	-0.472266	0.613825	-3.781892
H	0.132100	-0.107032	-5.026382
H	1.720790	-1.443835	3.606664
H	3.172914	-1.184298	3.033691
H	-0.529495	-1.771426	-3.639578
H	-1.743279	-2.681869	-3.173570
H	-0.552678	-2.245395	3.652549
H	0.389333	-2.993207	4.652054
H	-0.640356	-6.358761	-0.141006
H	-0.126479	-5.120670	-0.944553
H	0.720923	-4.018408	2.611795
H	0.421195	-4.925068	1.354748
H	0.132137	-3.832076	-2.826121
H	0.709136	-5.274964	-3.055091
H	2.657806	-4.464263	1.448079
H	3.879374	-3.472481	1.431821
H	2.369347	-4.142644	-1.899902
H	3.366237	-4.117838	-0.671848

Table S30. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{H}_2\text{O})_{36}$ hollow clathrate in the icosahedron $5^{12}6^8-D_{6h}$ configuration.

O	-2.865497	-3.564446	2.367846
H	-3.619679	-2.997874	2.060774
H	-3.263986	-4.247993	2.929191
O	2.710667	0.155259	4.499898
H	3.071972	0.206805	5.397758
H	2.178312	-0.676926	4.469219
O	2.466060	-4.181693	-1.902713
H	2.740078	-5.019330	-2.306577
H	1.941605	-4.427154	-1.103872
O	2.965884	3.698586	-2.500655
H	2.414360	4.037378	-1.767865
H	2.381984	3.159315	-3.085392
O	4.862027	-0.374771	-2.738968
H	5.660060	-0.451207	-3.284188
H	4.102509	-0.378936	-3.373045

O	2.710354	-0.409327	-4.426360
H	2.993474	-0.501063	-5.348914
H	2.159211	-1.216593	-4.229407
O	-1.468856	-1.996611	4.243684
H	-1.848641	-2.548327	3.529681
H	-0.491968	-2.065608	4.189066
O	-1.649918	-4.807147	0.265047
H	-1.925919	-5.734187	0.345254
H	-2.071174	-4.339730	1.030858
O	-1.470895	-2.607874	-4.038263
H	-1.678024	-3.124819	-4.832121
H	-1.926813	-3.070650	-3.296264
O	2.905470	3.928724	1.930934
H	3.289058	4.681166	2.407269
H	3.682830	3.352647	1.656448
O	-1.105307	4.968302	-0.249077
H	-1.288006	5.918161	-0.313811
H	-0.121425	4.890459	-0.242243
O	-1.182350	2.253814	-4.322465
H	-1.604375	2.800694	-3.621975
H	-1.680257	1.405797	-4.347177
O	4.790797	-2.467153	1.467788
H	4.788370	-2.517806	0.471563
H	5.572234	-2.960987	1.758680
O	-2.661849	-0.077942	-4.456868
H	-3.451649	-0.045165	-3.877840
H	-2.227127	-0.936559	-4.278037
O	4.831340	0.069788	2.649905
H	4.083165	0.068508	3.282150
H	4.809761	-0.798198	2.194880
O	1.103603	-4.896415	0.382848
H	0.121894	-4.800272	0.346584
H	1.264679	-5.839701	0.542148
O	1.645962	4.881856	-0.288811
H	2.080495	4.525783	0.527651
H	1.947553	5.800759	-0.361648
O	-2.663783	0.381378	4.494060
H	-2.992619	0.405621	5.405236
H	-2.179746	-0.483165	4.401391
O	4.998341	2.163400	-1.490200
H	4.262476	2.699329	-1.872698
H	4.927670	1.273240	-1.890466
O	1.417339	2.574212	3.896813
H	1.849966	1.713661	4.072775
H	1.921804	3.003692	3.174911
O	1.320954	-2.625430	-3.923227
H	1.635576	-3.162638	-3.166421
H	0.341437	-2.606134	-3.884616
O	-2.615784	4.148938	1.993714
H	-2.007409	4.369116	1.260114
H	-2.090151	3.663832	2.673348
O	4.733912	-2.697657	-1.186204
H	3.933197	-3.191982	-1.461991
H	4.750421	-1.868573	-1.711197
O	1.544507	2.156722	-4.247990
H	1.852071	1.228705	-4.273046
H	0.557565	2.141181	-4.248956
O	1.311730	-2.198414	4.363570

H	1.457417	-2.690552	5.186369
H	1.731982	-2.748100	3.642976
O	-1.320021	2.794904	3.985311
H	-1.712083	1.911895	4.144683
H	-0.345188	2.672038	3.927887
O	2.501783	-3.667949	2.497514
H	3.296312	-3.245065	2.103021
H	1.969135	-4.021812	1.755913
O	4.937775	2.409930	1.225283
H	4.895668	1.532042	1.672054
H	4.956868	2.247915	0.250814
O	-2.868093	-3.875786	-2.027793
H	-3.310217	-4.656665	-2.395818
H	-2.381005	-4.195385	-1.230908
O	-2.458009	3.816487	-2.433944
H	-1.964115	4.159210	-1.661025
H	-3.258336	3.372088	-2.085490
O	-4.819314	0.344509	2.721714
H	-4.055358	0.392903	3.336290
H	-4.780394	1.152377	2.151877
O	-4.909907	-2.096180	-1.261671
H	-4.891716	-1.999957	-0.284911
H	-4.177415	-2.702953	-1.496971
O	-4.923002	-1.995927	1.522937
H	-5.766844	-2.382546	1.803398
H	-4.879817	-1.088627	1.952754
O	-4.935491	0.071658	-2.802638
H	-5.736839	-0.006778	-3.342285
H	-4.936640	-0.717613	-2.191561
O	-4.801137	2.514273	-1.577370
H	-5.571481	3.015829	-1.884494
H	-4.871959	1.623481	-1.999519
O	-4.761381	2.623793	1.236975
H	-3.979493	3.179969	1.470540
H	-4.758595	2.535560	0.262216

Table S31. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $\text{CH}_4@(\text{H}_2\text{O})_{16}$ 4²⁵ methane-clathrate.

O	-0.773735	3.267718	-0.713957
H	-0.328398	3.151645	0.160055
H	-1.651178	2.838177	-0.616409
O	-0.432937	-0.673227	-3.104012
H	-0.077158	0.233773	-2.943207
H	-0.512866	-0.762734	-4.065944
O	3.055000	-0.938163	1.619646
H	2.198639	-1.238330	1.995611
H	3.014259	0.041713	1.585597
O	0.452975	2.901383	1.735335
H	0.035280	2.152633	2.207774
H	1.361709	2.590581	1.533634
O	3.125356	-1.571083	-0.974114
H	3.129587	-1.425878	0.013235
H	3.975437	-1.978447	-1.198545
O	-3.094178	0.358241	1.803440

H	-3.073449	-0.554854	1.443969
H	-2.246992	0.479011	2.284163
O	2.931034	1.800155	1.086195
H	3.717368	2.313289	1.325697
H	2.971567	1.655745	0.099231
O	-2.927500	-0.599307	-1.853916
H	-2.058135	-0.655085	-2.305781
H	-2.993333	0.312372	-1.495943
O	-0.482246	-3.286350	0.651313
H	-1.391089	-2.932342	0.538980
H	-0.030895	-3.140311	-0.214302
O	2.963085	1.163574	-1.502256
H	2.102445	1.402782	-1.910055
H	2.998266	0.183447	-1.470308
O	-3.121577	1.798216	-0.447059
H	-3.135540	1.343571	0.441046
H	-3.962205	2.273325	-0.528498
O	-2.959910	-2.043909	0.386250
H	-3.740762	-2.617094	0.414363
H	-2.971487	-1.587012	-0.501268
O	0.511350	1.874773	-2.591168
H	0.602338	2.434995	-3.376919
H	0.029880	2.422274	-1.904774
O	0.599290	-1.798115	2.581769
H	0.681289	-2.366293	3.362884
H	0.199682	-2.366503	1.860285
O	-0.627265	0.629913	3.077493
H	-0.176169	-0.235133	2.923454
H	-0.695289	0.730759	4.039134
O	0.797697	-2.874958	-1.772599
H	0.349360	-2.164105	-2.274140
H	1.669474	-2.496302	-1.527985
C	-0.012124	-0.010887	0.024567
H	-0.727270	-0.649649	0.548123
H	-0.556624	0.768321	-0.512382
H	0.563653	-0.615700	-0.678624
H	0.669841	0.451777	0.741579

Table S32. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $\text{CH}_4@(\text{H}_2\text{O})_{16}$ 4³5⁶1 methane-clathrate.

O	-2.408861	0.983279	-2.197501
H	-3.024340	1.226155	-2.905619
H	-2.283635	1.792672	-1.643264
O	3.580960	0.107678	-0.501017
H	3.263897	-0.840532	-0.589557
H	4.539335	0.100510	-0.644876
O	-1.827585	2.065131	2.140430
H	-2.010096	2.386191	1.232317
H	-2.078134	1.115540	2.148988
O	-0.986310	-2.696019	2.015338
H	-0.040012	-2.440381	2.075486
H	-1.130593	-2.990155	1.090255
O	-2.627042	-0.591855	2.094282
H	-1.982497	-1.351825	2.154554
H	-3.336982	-0.783308	2.725667

O	2.071658	1.679217	-2.114950
H	2.707094	1.131544	-1.589903
H	2.592810	2.133318	-2.794217
O	0.816469	2.444030	2.230150
H	-0.162415	2.260438	2.289348
H	1.010690	3.120794	2.896138
O	-3.321043	-1.080968	-0.558938
H	-3.008072	-0.355058	-1.140692
H	-3.160620	-0.785677	0.363435
O	2.576873	-2.332277	-0.538205
H	1.819338	-2.394613	-1.173776
H	2.192937	-2.370779	0.363532
O	0.735553	3.404699	-0.379502
H	1.210883	2.801845	-0.991588
H	0.914489	3.077905	0.529069
O	0.515980	-2.508763	-2.302537
H	0.325120	-1.593461	-2.618333
H	-0.266864	-2.782751	-1.780532
O	2.716623	0.418973	2.147667
H	3.078660	0.460339	1.237208
H	2.023729	1.112670	2.199209
O	-1.890998	3.039032	-0.494665
H	-2.366736	3.871571	-0.635662
H	-0.914130	3.251125	-0.530880
O	1.710385	-2.058207	2.105117
H	2.042491	-1.123720	2.210432
H	2.211861	-2.599700	2.733179
O	0.053230	0.051060	-3.187347
H	-0.797346	0.385856	-2.834827
H	0.748425	0.630202	-2.811219
O	-1.659173	-3.168162	-0.656766
H	-2.120994	-3.993541	-0.866946
H	-2.335905	-2.437478	-0.708481
C	-0.011851	-0.007024	0.159992
H	1.011943	0.128825	-0.199945
H	-0.638752	0.812386	-0.202967
H	-0.016657	-0.010919	1.253144
H	-0.401565	-0.958630	-0.211072

Table S33. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₁₇ 4⁴5⁶6¹ methane-clathrate.

O	2.285027	1.916838	1.168277
H	2.011802	1.176804	1.757952
H	3.060155	1.559827	0.686016
O	-1.043876	-3.139555	1.302770
H	-1.784331	-2.873998	0.717569
H	-0.247571	-3.178232	0.730556
O	-3.082270	-2.120586	-0.300898
H	-3.348173	-1.245172	0.107648
H	-3.887224	-2.657181	-0.360640
O	1.245211	-3.188533	-0.305117
H	1.578312	-4.087527	-0.447367
H	1.975555	-2.688976	0.156594
O	-2.924289	1.386085	-1.851292

H	-2.487273	0.600587	-2.238874
H	-2.224320	2.047175	-1.661886
O	2.237422	0.270614	-2.712663
H	1.643266	-0.536093	-2.712998
H	2.622047	0.332668	-3.599924
O	-2.019179	-1.165699	-2.637251
H	-2.436153	-1.620924	-1.865446
H	-2.486674	-1.485339	-3.424150
O	-1.974898	1.288998	2.557053
H	-2.446493	1.647225	3.323914
H	-1.342975	1.994519	2.259030
O	3.135031	-1.792985	0.960440
H	3.502504	-1.084360	0.390749
H	2.693610	-1.319419	1.699869
O	-0.306994	3.176936	1.570806
H	-0.648046	3.324765	0.661218
H	0.623010	2.902095	1.465514
O	-3.667973	0.319176	0.542998
H	-3.076014	0.667709	1.242604
H	-3.428173	0.800185	-0.286744
O	1.794092	-0.243177	2.808911
H	2.181253	-0.135577	3.690560
H	0.859732	-0.585646	2.942384
O	1.450729	2.599112	-1.443054
H	1.618115	1.813201	-2.006036
H	1.650535	2.305789	-0.529764
O	0.685122	-1.877554	-2.686602
H	-0.262453	-1.621929	-2.670561
H	0.853869	-2.359998	-1.846897
O	-0.668576	-1.111121	3.095768
H	-0.840352	-1.816045	2.424396
H	-1.209660	-0.329572	2.856305
O	3.912913	0.419636	-0.555462
H	4.845574	0.538433	-0.789384
H	3.414352	0.338175	-1.403978
O	-1.072087	3.320224	-1.111285
H	-1.263976	4.194129	-1.483824
H	-0.146773	3.082771	-1.395156
C	-0.145435	-0.016653	-0.161573
H	-0.842133	-0.853922	-0.066905
H	0.877916	-0.371941	0.001486
H	-0.387097	0.747000	0.582463
H	-0.226368	0.411459	-1.164065

Table S34. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₁₈ 4⁴5⁶6¹ methane-clathrate.

O	2.021200	-2.586127	1.553284
H	1.181260	-2.949159	1.167032
H	2.456757	-3.323199	2.008188
O	-2.432371	-0.988896	-2.653634
H	-3.007125	-1.132720	-1.872350
H	-2.189781	-0.039302	-2.617221
O	2.363316	1.501962	-2.430382
H	2.967313	1.474879	-1.658618

H	2.141145	0.564262	-2.611333
O	-1.982588	2.248014	2.065500
H	-1.176643	2.721374	1.740210
H	-2.412570	2.840085	2.700860
O	-2.316763	-2.302431	1.679110
H	-1.978139	-1.545872	2.219228
H	-2.920983	-1.909351	1.012046
O	1.984800	-1.249532	-2.743937
H	2.358740	-1.618844	-3.557810
H	1.122757	-1.734771	-2.581924
O	-2.025777	1.762092	-2.380329
H	-2.439638	2.281688	-3.085715
H	-1.165745	2.224879	-2.158216
O	2.314667	1.927832	1.951443
H	2.911811	1.657487	1.219013
H	2.010809	1.095267	2.372729
O	-0.283740	-3.398482	0.418853
H	-0.417904	-4.358414	0.445068
H	-1.066707	-2.990796	0.901619
O	-0.250787	-2.567708	-2.258628
H	-0.268092	-2.830917	-1.313802
H	-1.035874	-1.982982	-2.397698
O	0.211254	3.025728	-1.747920
H	0.243052	3.140427	-0.774614
H	0.990082	2.465782	-1.986603
O	-3.894501	-1.107431	-0.266697
H	-4.829507	-1.359679	-0.291627
H	-3.863609	-0.119268	-0.124367
O	3.924536	1.108383	-0.143273
H	3.893457	0.112658	-0.202339
H	4.858596	1.363746	-0.123775
O	0.280771	3.352928	1.044060
H	0.428413	4.281847	1.278617
H	1.065934	2.841004	1.398905
O	3.587797	-1.502926	-0.497539
H	3.025323	-1.515286	-1.303825
H	3.051121	-1.903999	0.218332
O	-3.576244	1.520719	-0.098601
H	-3.028252	1.700023	-0.894921
H	-3.029258	1.783732	0.672640
O	1.447332	-0.441499	3.145280
H	1.692266	-1.241346	2.619898
H	1.817682	-0.573031	4.031314
O	-1.339410	-0.244885	3.175390
H	-0.360789	-0.299536	3.171447
H	-1.560451	0.625757	2.783692
C	-0.173475	-0.020670	-0.090031
H	-1.174398	-0.462310	-0.064819
H	0.127068	0.144446	-1.128471
H	0.536450	-0.700832	0.391224
H	-0.181653	0.934353	0.442321

Table S35. M06-2X/6-31+G*/PC M optimized Cartesian coordinates of the CH₄@(H₂O)₁₉ 4⁴5⁶6¹ methane-clathrate.

C	0.163400	0.002718	0.070310
H	-0.455905	0.747315	-0.439892
H	1.175564	0.012649	-0.347354
H	-0.275420	-0.991357	-0.063181
H	0.207454	0.240897	1.136424
O	2.056578	-2.378132	-1.839118
H	2.781252	-1.768154	-1.556529
H	1.711800	-2.793420	-1.016993
O	3.882596	-0.451523	-1.208217
H	3.452896	0.264012	-1.718406
H	3.782613	-0.211601	-0.262301
O	2.191839	1.232036	-2.685874
H	1.486284	0.582456	-2.905498
H	2.485449	1.613824	-3.527146
O	1.536863	3.198449	-0.828121
H	1.746651	2.891743	0.081239
H	1.798381	2.480714	-1.442868
O	1.136453	-3.510297	0.510205
H	1.412956	-2.920524	1.268951
H	1.518908	-4.383117	0.685438
O	2.081736	2.430063	1.778284
H	1.230821	2.296227	2.290138
H	2.569784	3.132138	2.235241
O	-0.193897	2.055109	3.075478
H	-0.924775	2.290260	2.462700
H	-0.309178	1.104205	3.290339
O	-0.430227	-0.682050	3.542112
H	-1.224902	-1.035284	3.065390
H	-0.554949	-0.902001	4.477983
O	3.478954	0.122303	1.493745
H	3.006068	0.981920	1.626078
H	4.301041	0.184712	2.003732
O	1.846097	-1.898813	2.491778
H	2.420004	-1.182196	2.144431
H	1.055133	-1.460553	2.873343
O	0.336001	-0.822710	-3.041410
H	0.967919	-1.457680	-2.570576
H	0.362402	-1.072088	-3.979733
O	-1.582287	1.335715	-2.959819
H	-0.876024	0.668814	-2.877660
H	-1.360986	2.059344	-2.335198
O	-3.650102	-0.115345	-1.826999
H	-3.021597	0.514759	-2.245542
H	-3.193177	-0.981876	-1.937432
O	-3.666871	0.388602	0.838802
H	-3.163397	1.217736	0.981829
H	-3.664804	0.222251	-0.138308
O	-2.198555	2.725851	1.273040
H	-1.811386	3.016599	0.409381
H	-2.754760	3.456922	1.582371
O	-2.035513	-2.299581	-2.224668
H	-1.221391	-1.821695	-2.472327
H	-1.857601	-2.716618	-1.346623
O	-1.619677	-3.426953	0.222655
H	-1.946317	-2.807592	0.909611
H	-0.652692	-3.508640	0.368333
O	-2.545410	-1.608298	2.125960
H	-3.233793	-2.002995	2.682777

H	-2.981254	-0.845595	1.636649
O	-1.071211	3.363193	-1.112299
H	-0.075285	3.373764	-0.993726
H	-1.321119	4.232450	-1.461226

Table S36. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₂₀ 5¹² methane-clathrate.

C	-0.104310	-0.013275	0.033174
H	-0.560868	0.980404	-0.009326
H	-0.111705	-0.462087	-0.965048
H	-0.670341	-0.644884	0.724359
H	0.927879	0.075590	0.386874
O	1.490437	-3.383671	0.543091
H	0.729618	-3.435533	-0.072945
H	1.136608	-3.032822	1.398502
O	-2.426716	0.768416	2.816666
H	-2.755255	1.133771	1.967322
H	-1.537507	1.178350	2.973271
O	3.648940	0.338579	1.318565
H	3.579376	-0.411668	0.688901
H	3.384128	1.144551	0.821870
O	-0.499393	2.480265	-2.887870
H	-0.891030	2.846621	-2.067606
H	-0.976147	1.642423	-3.071236
O	-0.674297	-3.553964	-1.219795
H	-1.483122	-3.243959	-0.744291
H	-0.841619	-4.476210	-1.466775
O	2.133197	1.908096	-2.501078
H	1.173950	2.102942	-2.641702
H	2.243267	0.940709	-2.617252
O	-2.146533	-1.828300	2.614428
H	-2.279100	-0.834442	2.712703
H	-2.668364	-2.247910	3.315351
O	-0.000439	-1.917431	-3.364236
H	-0.229625	-2.519596	-2.623841
H	0.896053	-1.567728	-3.169280
O	1.979589	-0.069925	3.344086
H	2.629215	0.084649	2.601050
H	2.493636	-0.065683	4.165157
O	0.591113	3.613966	1.254230
H	-0.151159	3.608554	0.614694
H	1.373822	3.272779	0.770431
O	2.501867	-0.844288	-2.792132
H	2.859449	-1.216796	-1.946712
H	3.156257	-1.048568	-3.477305
O	-3.388953	1.768035	0.398424
H	-3.446644	1.005504	-0.249712
H	-4.289321	2.112834	0.498281
O	0.572123	-2.421439	2.909728
H	-0.378517	-2.194225	2.833283
H	1.045545	-1.580059	3.088443
O	-3.504987	-0.263847	-1.279540
H	-3.252845	-1.087637	-0.810832
H	-2.881120	-0.164220	-2.032457

O	-0.011151	1.888491	3.293934
H	0.220077	2.506350	2.559867
H	0.694404	1.208064	3.310040
O	3.367175	-1.815183	-0.412732
H	4.178166	-2.342036	-0.477474
H	2.658693	-2.426015	-0.043951
O	-1.565286	3.547246	-0.527483
H	-1.971378	4.414705	-0.674890
H	-2.281882	2.957052	-0.184149
O	-2.843474	-2.581842	0.119135
H	-3.601867	-3.184619	0.157064
H	-2.624504	-2.344865	1.057869
O	2.837760	2.605867	-0.051966
H	3.539150	3.270622	-0.122712
H	2.589346	2.355943	-0.989951
O	-1.769221	0.061927	-3.411612
H	-2.229156	0.043958	-4.264226
H	-1.103712	-0.683139	-3.431455

Table S37. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₂₂ 4¹⁵1⁰6² methane-clathrate.

O	1.927800	-3.611577	0.525200
H	2.150383	-2.954879	1.220966
H	2.260452	-3.233713	-0.315213
O	-1.655270	-3.062020	-1.882618
H	-1.327314	-3.395203	-0.992695
H	-1.845192	-3.851918	-2.411928
O	-1.843113	3.012303	1.772146
H	-1.417178	3.341005	0.951379
H	-1.153259	2.536175	2.283857
O	2.529058	2.497898	2.088476
H	2.291990	2.930452	1.241306
H	1.681047	2.262061	2.522054
O	-4.003703	1.619630	1.106184
H	-3.197601	2.132874	1.395972
H	-4.774633	2.092515	1.452806
O	2.725057	1.817012	-2.317986
H	1.903113	1.473168	-2.733493
H	2.440873	2.464308	-1.636807
O	0.113630	-0.857548	3.572311
H	0.943512	-1.204902	3.175951
H	-0.626359	-1.340479	3.144789
O	0.477366	-1.807257	-3.158951
H	-0.274048	-2.210840	-2.673025
H	1.295819	-2.061694	-2.681511
O	-1.639558	2.430825	-2.574420
H	-0.957073	1.793686	-2.876032
H	-2.419267	1.907447	-2.268142
O	-1.942145	-2.359785	2.458335
H	-2.305906	-2.928247	3.153879
H	-2.720151	-1.877029	2.060769
O	2.854857	-2.468420	-1.865042
H	3.380068	-1.652222	-1.670982
H	3.423690	-3.042187	-2.400144

O	0.428823	0.818782	-3.508183
H	0.485784	0.945615	-4.467510
H	0.405835	-0.170034	-3.362888
O	-0.775486	-3.901215	0.450349
H	-1.159931	-3.362824	1.175742
H	0.205925	-3.781596	0.492477
O	-0.754004	3.952286	-0.613889
H	-1.046773	4.858485	-0.793868
H	-1.094184	3.386685	-1.370807
O	1.931632	3.656608	-0.383828
H	0.960621	3.826073	-0.479336
H	2.371062	4.511058	-0.510561
O	-3.919951	-1.630554	-1.419621
H	-3.112845	-2.161970	-1.634584
H	-4.671060	-2.094695	-1.818263
O	2.502954	-1.772047	2.522633
H	3.052594	-1.015221	2.161955
H	3.035161	-2.182230	3.221130
O	-3.870326	1.162719	-1.650226
H	-3.864833	0.184166	-1.685180
H	-3.963690	1.387623	-0.700078
O	-4.024962	-1.146274	1.329621
H	-4.003758	-0.165209	1.358676
H	-4.036968	-1.380126	0.376913
O	0.118867	1.778033	3.301115
H	0.076479	2.137667	4.200134
H	0.075736	0.783585	3.398596
O	3.940844	0.225979	1.559480
H	3.436596	1.060560	1.724404
H	3.999886	0.122564	0.585858
O	4.101536	-0.146062	-1.212148
H	3.598161	0.605137	-1.645835
H	5.019273	-0.072419	-1.515627
C	0.767680	-0.227330	0.055203
H	0.083022	-1.038333	0.321394
H	1.712981	-0.652238	-0.293226
H	0.957194	0.395636	0.934021
H	0.327434	0.381111	-0.740008

Table S38. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_2H_6@(H_2O)_{22}$ $4^15^{10}6^2$ ethane-clathrate.

O	1.336381	-3.843045	0.472947
H	1.671761	-3.290411	1.211731
H	1.758141	-3.491814	-0.338520
O	-2.041549	-2.832131	-1.966536
H	-1.805671	-3.250630	-1.083148
H	-2.357841	-3.552468	-2.533266
O	-1.313963	3.177527	1.830001
H	-0.830249	3.468118	1.026434
H	-0.712586	2.578208	2.324993
O	2.889153	2.044992	2.153470
H	2.753824	2.528077	1.311345
H	1.998137	1.908726	2.541236
O	-3.639971	2.113874	1.162708

H	-2.767466	2.510829	1.448658
H	-4.336541	2.683168	1.521956
O	3.072278	1.496220	-2.279573
H	2.192849	1.264525	-2.654227
H	2.905439	2.167763	-1.583140
O	-0.072267	-0.999251	3.438468
H	0.714482	-1.480399	3.099570
H	-0.862164	-1.378790	2.995616
O	0.263165	-1.807726	-3.118810
H	-0.544671	-2.136831	-2.667736
H	1.033207	-2.202295	-2.656099
O	-1.155121	2.687786	-2.422634
H	-0.576581	1.948751	-2.711341
H	-2.017510	2.298205	-2.135405
O	-2.325704	-2.185387	2.347114
H	-2.778918	-2.666385	3.055987
H	-3.004542	-1.567424	1.951261
O	2.514970	-2.799630	-1.841091
H	3.136578	-2.056960	-1.634656
H	3.015506	-3.441175	-2.367185
O	0.624734	0.798387	-3.366633
H	0.657275	0.932223	-4.326431
H	0.450474	-0.177842	-3.235986
O	-1.379094	-3.874269	0.354815
H	-1.718035	-3.306693	1.081159
H	-0.392082	-3.850690	0.417719
O	-0.040811	4.037935	-0.478765
H	-0.218471	4.978743	-0.630156
H	-0.472486	3.537955	-1.238663
O	2.576050	3.379415	-0.286788
H	1.641346	3.695822	-0.373225
H	3.139102	4.164867	-0.361016
O	-3.975041	-0.988321	-1.515886
H	-3.271435	-1.655046	-1.720047
H	-4.785951	-1.307802	-1.939612
O	2.230556	-2.230928	2.545037
H	2.876349	-1.548218	2.195671
H	2.692153	-2.713984	3.246561
O	-3.578858	1.776662	-1.603570
H	-3.674995	0.805613	-1.686196
H	-3.634242	1.959778	-0.641105
O	-4.144627	-0.610928	1.233762
H	-3.942500	0.345407	1.321967
H	-4.131010	-0.793777	0.269365
O	0.391452	1.597389	3.306886
H	0.383231	1.907468	4.225052
H	0.176635	0.621247	3.341242
O	3.896365	-0.419666	1.589230
H	3.538923	0.483802	1.774531
H	3.953479	-0.500446	0.613293
O	4.079591	-0.684473	-1.185665
H	3.724298	0.150537	-1.612989
H	5.005196	-0.763465	-1.462356
C	-0.856713	-0.125800	-0.191009
C	0.607400	0.294120	-0.067846
H	-1.208534	-0.047379	-1.226786
H	-1.503780	0.507782	0.428332
H	-1.000846	-1.164716	0.129749

H	0.964183	0.194417	0.964038
H	0.746489	1.340369	-0.368116
H	1.254414	-0.322148	-0.704817

Table S39. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_2H_6@(H_2O)_{24}$ $5^{12}6^2$ ethane-clathrate.

O	-4.117188	-2.302408	-0.993265
H	-4.857082	-2.892363	-1.200688
H	-3.504524	-2.816749	-0.396556
O	-2.113232	-2.249626	3.008445
H	-2.469256	-2.806868	3.717323
H	-1.197631	-2.005084	3.292257
O	-2.448962	-3.625057	0.608541
H	-2.256411	-3.134540	1.435975
H	-1.588105	-3.815631	0.178631
O	-3.711555	0.046284	2.746438
H	-3.135705	0.838396	2.809380
H	-3.126219	-0.732900	2.849310
O	-2.130655	2.337705	2.885125
H	-2.168029	2.821471	2.011160
H	-2.486699	2.949556	3.546955
O	-2.646735	1.336766	-3.240936
H	-3.128357	1.614823	-4.035020
H	-3.191853	1.641166	-2.472555
O	-2.667269	-1.473556	-3.225759
H	-2.626436	-0.494685	-3.212302
H	-3.210100	-1.739418	-2.452969
O	-4.042237	2.138294	-1.051406
H	-4.380794	1.340657	-0.542621
H	-4.820363	2.674940	-1.265844
O	-4.899137	0.042724	0.293632
H	-4.641889	-0.792456	-0.153870
H	-4.474126	0.022250	1.186404
O	0.269981	1.330923	3.814142
H	-0.567721	1.662633	3.423031
H	0.236733	0.350262	3.792182
O	-2.336314	3.623132	0.573864
H	-1.490941	3.784905	0.100822
H	-2.902997	3.094955	-0.028951
O	2.296941	-3.654827	0.351264
H	2.785769	-4.480391	0.492462
H	2.813139	-3.146406	-0.341179
O	1.935685	-1.486231	-3.507593
H	2.291500	-1.759374	-4.366611
H	1.065343	-1.969532	-3.402548
O	-0.219243	2.733136	-3.186856
H	-1.063407	2.235110	-3.178759
H	-0.187047	3.249204	-2.352911
O	2.064504	1.286981	-3.435498
H	1.909238	0.318268	-3.429311
H	1.191421	1.739201	-3.334949
O	3.787123	2.094244	-1.628850
H	3.137837	1.782768	-2.330812
H	4.430773	2.660115	-2.081776

O	4.868322	-0.061109	-0.391735
H	4.537578	0.746923	-0.859224
H	5.829075	-0.076399	-0.518073
O	2.476792	2.197078	2.642307
H	2.884306	2.795614	3.286939
H	1.622537	1.886000	3.059917
O	2.574321	-2.255848	2.758712
H	2.441457	-2.715340	1.902190
H	3.140100	-1.466263	2.570970
O	0.335872	-1.448261	3.884065
H	1.171801	-1.778704	3.435940
H	0.423608	-1.686969	4.819767
O	4.103136	-0.043735	2.300292
H	4.386609	-0.039764	1.361942
H	3.535620	0.750019	2.409397
O	2.348998	3.564531	0.239775
H	2.869620	3.035884	-0.403043
H	2.340506	3.054154	1.079456
O	-0.006471	4.187730	-0.818485
H	0.048334	5.138564	-0.997820
H	0.861536	3.936358	-0.392173
O	3.641566	-2.306326	-1.482889
H	3.047218	-1.994261	-2.201231
H	4.072090	-1.508012	-1.107518
O	-0.112999	-4.249925	-0.774588
H	-0.098601	-5.202203	-0.954830
H	0.751557	-4.042591	-0.339434
O	-0.311668	-2.844809	-3.191813
H	-1.146503	-2.316402	-3.186923
H	-0.276553	-3.326942	-2.339061
C	1.142644	0.162016	0.441603
C	-0.070637	1.089682	0.413011
H	2.035043	0.660854	0.043614
H	0.972205	-0.739948	-0.157826
H	1.372860	-0.156625	1.464013
H	-0.961157	0.595954	0.821476
H	-0.303121	1.412932	-0.608533
H	0.107555	1.990227	1.011290

Table S40. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_2H_6@(H_2O)_{26}$ $5^{12}6^3$ ethane-clathrate.

O	-4.117188	-2.302408	-0.993265
H	-4.857082	-2.892363	-1.200688
H	-3.504524	-2.816749	-0.396556
O	-2.113232	-2.249626	3.008445
H	-2.469256	-2.806868	3.717323
H	-1.197631	-2.005084	3.292257
O	-2.448962	-3.625057	0.608541
H	-2.256411	-3.134540	1.435975
H	-1.588105	-3.815631	0.178631
O	-3.711555	0.046284	2.746438
H	-3.135705	0.838396	2.809380
H	-3.126219	-0.732900	2.849310
O	-2.130655	2.337705	2.885125

H	-2.168029	2.821471	2.011160
H	-2.486699	2.949556	3.546955
O	-2.646735	1.336766	-3.240936
H	-3.128357	1.614823	-4.035020
H	-3.191853	1.641166	-2.472555
O	-2.667269	-1.473556	-3.225759
H	-2.626436	-0.494685	-3.212302
H	-3.210100	-1.739418	-2.452969
O	-4.042237	2.138294	-1.051406
H	-4.380794	1.340657	-0.542621
H	-4.820363	2.674940	-1.265844
O	-4.899137	0.042724	0.293632
H	-4.641889	-0.792456	-0.153870
H	-4.474126	0.022250	1.186404
O	0.269981	1.330923	3.814142
H	-0.567721	1.662633	3.423031
H	0.236733	0.350262	3.792182
O	-2.336314	3.623132	0.573864
H	-1.490941	3.784905	0.100822
H	-2.902997	3.094955	-0.028951
O	2.296941	-3.654827	0.351264
H	2.785769	-4.480391	0.492462
H	2.813139	-3.146406	-0.341179
O	1.935685	-1.486231	-3.507593
H	2.291500	-1.759374	-4.366611
H	1.065343	-1.969532	-3.402548
O	-0.219243	2.733136	-3.186856
H	-1.063407	2.235110	-3.178759
H	-0.187047	3.249204	-2.352911
O	2.064504	1.286981	-3.435498
H	1.909238	0.318268	-3.429311
H	1.191421	1.739201	-3.334949
O	3.787123	2.094244	-1.628850
H	3.137837	1.782768	-2.330812
H	4.430773	2.660115	-2.081776
O	4.868322	-0.061109	-0.391735
H	4.537578	0.746923	-0.859224
H	5.829075	-0.076399	-0.518073
O	2.476792	2.197078	2.642307
H	2.884306	2.795614	3.286939
H	1.622537	1.886000	3.059917
O	2.574321	-2.255848	2.758712
H	2.441457	-2.715340	1.902190
H	3.140100	-1.466263	2.570970
O	0.335872	-1.448261	3.884065
H	1.171801	-1.778704	3.435940
H	0.423608	-1.686969	4.819767
O	4.103136	-0.043735	2.300292
H	4.386609	-0.039764	1.361942
H	3.535620	0.750019	2.409397
O	2.348998	3.564531	0.239775
H	2.869620	3.035884	-0.403043
H	2.340506	3.054154	1.079456
O	-0.006471	4.187730	-0.818485
H	0.048334	5.138564	-0.997820
H	0.861536	3.936358	-0.392173
O	3.641566	-2.306326	-1.482889
H	3.047218	-1.994261	-2.201231

H	4.072090	-1.508012	-1.107518
O	-0.112999	-4.249925	-0.774588
H	-0.098601	-5.202203	-0.954830
H	0.751557	-4.042591	-0.339434
O	-0.311668	-2.844809	-3.191813
H	-1.146503	-2.316402	-3.186923
H	-0.276553	-3.326942	-2.339061
C	1.142644	0.162016	0.441603
C	-0.070637	1.089682	0.413011
H	2.035043	0.660854	0.043614
H	0.972205	-0.739948	-0.157826
H	1.372860	-0.156625	1.464013
H	-0.961157	0.595954	0.821476
H	-0.303121	1.412932	-0.608533
H	0.107555	1.990227	1.011290

Table S41. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_3H_8@(H_2O)_{24}$ $5^{12}6^2$ propane-clathrate.

C	1.278522	-0.327707	0.083082
C	0.038890	0.346586	0.661880
C	-1.238465	-0.238133	0.067180
H	2.200270	0.082024	0.505335
H	1.319245	-0.194483	-1.004709
H	1.262125	-1.407875	0.285180
H	0.078841	1.427301	0.464811
H	0.029622	0.232102	1.755366
H	-2.135661	0.244547	0.469340
H	-1.307804	-1.313726	0.277509
H	-1.247903	-0.111138	-1.022630
O	-1.530678	-2.528992	-2.790542
H	-1.739832	-3.114354	-3.534315
H	-0.534823	-2.482016	-2.756580
O	2.228207	-3.807575	-0.477296
H	2.688257	-4.632710	-0.693231
H	2.885486	-3.233617	-0.008838
O	1.133978	-2.577958	-2.731868
H	1.509318	-2.999721	-1.929894
H	1.666151	-1.766021	-2.880849
O	-0.107175	-4.122322	1.024290
H	-0.049762	-3.453275	1.740851
H	0.716701	-4.033119	0.501269
O	-0.007861	-2.269007	3.081600
H	-0.863242	-1.749686	3.071512
H	-0.019662	-2.775194	3.908640
O	-4.543488	0.013564	-0.617464
H	-5.491844	-0.025425	-0.814627
H	-4.351538	-0.759066	-0.027908
O	-3.042905	-0.214041	-2.969282
H	-3.562811	-0.155014	-2.138657
H	-2.498372	-1.028720	-2.898254
O	-3.861454	-2.052329	1.004283
H	-3.311354	-2.701782	0.470047
H	-4.613637	-2.553136	1.355304

O	-2.377736	-3.710058	-0.408273
H	-2.107496	-3.286067	-1.251530
H	-1.539281	-3.873759	0.090982
O	2.498703	-1.097304	3.003172
H	1.589110	-1.467589	2.979784
H	2.971754	-1.468496	2.227233
O	-2.326825	-0.996803	3.082414
H	-2.239027	-0.025518	2.963034
H	-2.867804	-1.328220	2.332936
O	2.745969	-0.351725	-3.099379
H	3.228815	-0.399015	-3.938374
H	2.196931	0.481753	-3.138293
O	-1.470011	1.920653	-3.142722
H	-1.727102	2.382648	-3.955177
H	-2.049153	1.107578	-3.093469
O	-3.792364	2.380506	0.683607
H	-4.088442	1.545818	0.262893
H	-3.241823	2.126490	1.455489
O	-2.052786	3.610452	-1.002486
H	-1.842148	2.991081	-1.734417
H	-2.699599	3.148142	-0.414017
O	0.073099	4.393107	0.329306
H	-0.748046	4.106111	-0.174337
H	0.000393	5.351973	0.451174
O	2.196979	3.616881	-1.161718
H	1.444165	3.961066	-0.617822
H	2.615762	4.390836	-1.567851
O	2.512498	1.549033	2.760442
H	3.022850	1.871127	3.519426
H	2.472073	0.555456	2.862872
O	4.502219	-0.193493	-0.914556
H	3.883463	-0.246950	-1.674863
H	4.304502	0.660264	-0.457177
O	3.914484	-2.110988	0.808397
H	4.156863	-1.386968	0.156259
H	4.748684	-2.519164	1.086424
O	3.945727	2.125846	0.426810
H	3.342913	2.670099	-0.122507
H	3.450910	1.933314	1.252091
O	0.158653	3.037124	2.755211
H	0.165201	3.532606	1.907553
H	0.949608	2.455096	2.737989
O	-2.170508	1.755056	2.862642
H	-2.589598	2.113341	3.660310
H	-1.273954	2.194473	2.809259
O	1.306323	1.873745	-3.138566
H	0.327908	1.804855	-3.103265
H	1.575735	2.490259	-2.424315

Table S42. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_3H_8@(H_2O)_{26}$ $5^{12}6^3$ propane-clathrate.

O	4.021664	1.899676	-1.650444
H	4.754684	2.405028	-2.032668
H	3.446595	2.558930	-1.167765

O	2.319762	2.882606	2.326417
H	2.708301	3.596302	2.855188
H	1.403041	2.754318	2.675428
O	2.479963	3.622554	-0.345019
H	2.353943	3.350516	0.589338
H	1.589497	3.696751	-0.749507
O	3.892682	0.559608	2.571917
H	3.290184	-0.184083	2.790106
H	3.326858	1.356091	2.497515
O	2.229100	-1.586378	3.178044
H	2.208612	-2.275235	2.452829
H	2.540733	-2.044459	3.973451
O	2.401489	-2.108600	-2.862625
H	2.847525	-2.566001	-3.592132
H	2.994217	-2.217282	-2.076991
O	2.482705	0.601161	-3.564558
H	2.411845	-0.338443	-3.295348
H	3.052420	1.036943	-2.894588
O	3.971175	-2.379019	-0.662619
H	4.345017	-1.494722	-0.362313
H	4.730646	-2.962565	-0.811676
O	4.908310	-0.050528	0.117988
H	4.602923	0.647685	-0.501655
H	4.545565	0.190698	1.006164
O	-0.112821	-0.328367	3.882220
H	0.709552	-0.753549	3.553171
H	-0.071688	0.623736	3.647729
O	2.276289	-3.418345	1.272591
H	1.408898	-3.667758	0.884351
H	2.839079	-3.083013	0.541715
O	-2.325744	3.670301	-0.465830
H	-2.797625	4.515604	-0.521879
H	-2.872524	3.014277	-0.991494
O	-2.115066	0.607631	-3.646718
H	-2.487179	0.655857	-4.540255
H	-1.238965	1.091733	-3.684884
O	-0.000020	-3.481865	-2.450637
H	0.837205	-2.984659	-2.564333
H	-0.013376	-3.792582	-1.519750
O	-2.267841	-2.055830	-2.892502
H	-2.095200	-1.117455	-3.121081
H	-1.399616	-2.501913	-2.737123
O	-3.930872	-2.370453	-0.891865
H	-3.301620	-2.249667	-1.667514
H	-4.602832	-3.007172	-1.179556
O	-4.930681	0.048657	-0.184335
H	-4.625907	-0.855771	-0.448898
H	-5.896044	0.047449	-0.270490
O	-2.392217	-1.430835	3.141795
H	-2.741460	-1.828815	3.953937
H	-1.508875	-1.032832	3.391384
O	-2.448306	2.913321	2.215108
H	-2.377736	3.154734	1.266642
H	-3.027546	2.112320	2.258547
O	-0.143690	2.394395	3.368756
H	-1.002330	2.611641	2.893676
H	-0.209949	2.814612	4.240247
O	-4.025347	0.693993	2.384401

H	-4.362480	0.472934	1.490919
H	-3.456729	-0.063167	2.644586
O	-2.408454	-3.387336	1.193891
H	-2.964390	-3.029072	0.468296
H	-2.345673	-2.677148	1.870443
O	-0.121393	-4.292031	0.206198
H	-0.174855	-5.254893	0.302111
H	-0.964330	-3.926286	0.600546
O	-3.752765	1.933983	-1.853362
H	-3.183387	1.444869	-2.488669
H	-4.162934	1.259712	-1.269481
O	0.077397	3.907819	-1.716679
H	0.076190	4.784936	-2.129452
H	-0.783905	3.834419	-1.233845
O	0.142939	1.970599	-3.731695
H	0.977433	1.447124	-3.647835
H	0.154067	2.638756	-3.014422
C	-1.314411	-0.067735	0.344185
C	-0.054241	-0.929758	0.404092
C	1.217063	-0.082014	0.422013
H	-2.224951	-0.678111	0.319065
H	-1.313620	0.569115	-0.550676
H	-1.377424	0.589236	1.221366
H	-0.032219	-1.614794	-0.454470
H	-0.085320	-1.562560	1.302170
H	2.119424	-0.700535	0.484477
H	1.218418	0.598213	1.284439
H	1.293285	0.533312	-0.484312

Table S42. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $C_3H_8@(H_2O)_{28}$ propane-clathrate.

O	2.792497	-2.139914	-3.242987
H	1.853131	-2.338370	-3.482091
H	3.339506	-2.581546	-3.910145
O	-2.810323	3.022840	-2.215907
H	-3.021535	3.029499	-1.258923
H	-2.994957	2.111913	-2.529724
O	-2.597716	-3.188996	2.188138
H	-3.152354	-3.860517	2.613906
H	-2.786293	-3.250972	1.218070
O	2.744457	2.379970	3.049877
H	1.793627	2.484838	3.266816
H	2.948580	1.422176	3.094436
O	-0.936611	0.337253	4.168518
H	-0.614337	1.231531	3.925369
H	-0.177359	-0.271863	4.055892
O	1.164203	-1.503915	3.978851
H	1.365215	-1.773889	4.888385
H	2.002098	-1.113571	3.623192
O	-0.968075	-0.283779	-4.388633
H	-0.347182	0.470118	-4.280646
H	-1.785213	-0.056843	-3.893697
O	-0.811576	-3.995866	-1.632676
H	-0.086330	-4.058786	-0.972186

H	-0.478077	-3.450842	-2.377726
O	1.157800	-4.265583	0.293401
H	0.782404	-4.024781	1.188298
H	1.374451	-5.209235	0.344501
O	0.906045	4.515947	-0.341779
H	1.744429	4.062496	-0.035402
H	1.116935	5.460304	-0.394549
O	4.296943	1.333384	-0.955270
H	3.865926	1.089913	-1.822397
H	5.199011	1.610496	-1.175805
O	4.459377	-0.885212	0.732336
H	4.374747	-0.110278	0.135926
H	4.054479	-1.649334	0.253892
O	-4.478666	0.666055	1.174169
H	-3.991583	0.195778	1.917129
H	-5.392844	0.776794	1.477727
O	3.456331	-3.009762	-0.653928
H	3.210294	-2.712351	-1.554635
H	2.642326	-3.401139	-0.271658
O	-3.402594	3.079203	0.519587
H	-4.106784	3.724869	0.684234
H	-3.769037	2.202926	0.798517
O	-3.081179	-3.298476	-0.485003
H	-2.226240	-3.526745	-0.955284
H	-3.697094	-4.019379	-0.688244
O	3.119554	3.362239	0.532472
H	3.489664	2.643757	-0.024152
H	2.995862	2.982603	1.436322
O	0.168467	-2.596406	-3.820318
H	-0.283009	-1.725100	-4.022836
H	0.049023	-3.151806	-4.605738
O	0.054480	2.859883	3.607380
H	-0.032936	3.432386	4.384171
H	-0.380989	3.345350	2.850722
O	-0.235894	3.736536	-2.752960
H	-1.163737	3.483058	-2.526147
H	0.205885	3.968022	-1.907869
O	0.099539	-3.696647	2.656174
H	-0.848825	-3.488923	2.510982
H	0.493872	-2.909011	3.089893
O	3.215164	0.616505	-3.273220
H	3.042992	-0.349317	-3.282557
H	2.377665	1.053491	-3.542578
O	-3.233426	-0.630055	3.087208
H	-3.003270	-1.530772	2.774017
H	-2.396178	-0.234314	3.432772
O	3.449913	-0.330625	3.099978
H	4.183958	-0.465403	3.718481
H	3.803870	-0.569197	2.190750
O	-3.334674	0.438810	-3.131613
H	-4.029493	0.474266	-3.806270
H	-3.711152	-0.097407	-2.378141
O	0.865115	1.794408	-4.161726
H	1.023700	2.167400	-5.042093
H	0.481326	2.538494	-3.611134
O	-4.400042	-0.933221	-1.117119
H	-4.443385	-0.388980	-0.301379
H	-3.893485	-1.742679	-0.890181

O	-1.061421	4.158151	1.581541
H	-0.406613	4.259937	0.856150
H	-1.851228	3.717813	1.202732
C	-1.126448	0.264338	0.208495
C	-0.415819	-0.950847	0.803766
C	1.101659	-0.780522	0.814689
H	-2.212458	0.126583	0.185342
H	-0.790515	0.452924	-0.819229
H	-0.914631	1.165211	0.799549
H	-0.680954	-1.854285	0.236676
H	-0.772832	-1.111933	1.828698
H	1.607225	-1.648433	1.253453
H	1.390389	0.105939	1.395941
H	1.492469	-0.652512	-0.203148

Table S43. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the iso-C₄H₁₀@(H₂O)₂₆ isobutane-clathrate.

O	-3.892600	-0.612890	-2.452745
H	-4.578127	-0.757237	-3.122155
H	-3.363602	-1.459025	-2.405926
O	-2.416926	-3.847940	0.298666
H	-2.803981	-4.736587	0.319502
H	-1.492458	-3.945750	0.632021
O	-2.490673	-2.868351	-2.306363
H	-2.431409	-3.197870	-1.383895
H	-1.571790	-2.709075	-2.610741
O	-3.999625	-1.969839	1.726329
H	-3.377019	-1.500007	2.322510
H	-3.455439	-2.615669	1.230782
O	-2.266634	-0.574827	3.399800
H	-2.188553	0.390874	3.154918
H	-2.589811	-0.590999	4.313591
O	-2.355945	3.644029	-1.223419
H	-2.874517	4.362639	-1.616955
H	-2.938620	3.237637	-0.536053
O	-2.338472	1.590130	-3.135999
H	-2.300169	2.275397	-2.436907
H	-2.911759	0.864039	-2.809918
O	-3.900773	2.388248	0.654366
H	-4.272028	1.486031	0.415567
H	-4.657547	2.924267	0.937172
O	-4.883812	0.012180	0.048613
H	-4.564115	-0.235290	-0.846859
H	-4.575950	-0.706980	0.652312
O	0.011977	-2.112693	3.370244
H	-0.795619	-1.557141	3.299213
H	-0.008050	-2.762986	2.635731
O	-2.213307	2.005452	2.808059
H	-1.375092	2.493748	2.651377
H	-2.789140	2.174098	2.030926
O	2.415944	-2.863757	-2.349894
H	2.882683	-3.494548	-2.919581
H	2.944646	-2.012636	-2.386997
O	2.229188	1.589329	-3.090972

H	2.621529	1.956639	-3.898111
H	1.355591	1.188794	-3.374779
O	0.044449	4.689088	-0.116087
H	-0.766822	4.328715	-0.530573
H	0.061120	4.305935	0.787141
O	2.335551	3.695004	-1.288012
H	2.131911	2.973532	-1.921831
H	1.479994	4.021867	-0.919461
O	3.828477	2.521978	0.556402
H	3.268600	2.977566	-0.140913
H	4.510298	3.161089	0.814678
O	4.894051	0.060466	0.013536
H	4.540190	0.963563	0.204754
H	5.858830	0.148800	-0.014561
O	2.247740	-0.704294	3.375544
H	2.565438	-0.751125	4.290347
H	1.385184	-1.210465	3.360357
O	2.487255	-3.849270	0.257450
H	2.439024	-3.498374	-0.657884
H	3.040602	-3.204116	0.762040
O	0.097234	-4.057525	1.384727
H	0.978720	-3.972290	0.913518
H	0.140504	-4.897984	1.866991
O	3.997755	-2.041259	1.671845
H	4.327914	-1.335554	1.078654
H	3.387530	-1.583028	2.290127
O	2.245848	1.996183	2.763619
H	2.825990	2.123775	1.982444
H	2.171810	1.028504	2.915306
O	0.085116	3.505285	2.441126
H	0.124653	4.154548	3.159852
H	0.879648	2.912807	2.563361
O	3.795976	-0.611037	-2.444681
H	3.232737	0.167058	-2.656055
H	4.208581	-0.411855	-1.576517
O	-0.013912	-2.289845	-3.416983
H	-0.010196	-2.694298	-4.298275
H	0.851211	-2.538828	-3.004540
O	-0.006765	0.463463	-3.898892
H	-0.845560	0.878744	-3.579342
H	-0.046348	-0.488206	-3.667951
C	1.258735	-0.623284	0.277796
C	-0.002767	0.149850	0.653743
C	-1.256962	-0.638949	0.286031
C	-0.014100	1.513262	-0.025475
H	2.165281	-0.055080	0.525552
H	1.276155	-0.826016	-0.803352
H	1.310271	-1.584102	0.801429
H	-0.000070	0.308736	1.744155
H	-2.167132	-0.096426	0.571518
H	-1.275619	-1.617208	0.781434
H	-1.295596	-0.811800	-0.799682
H	-0.906316	2.086043	0.252391
H	-0.013755	1.402487	-1.120008
H	0.869184	2.096890	0.255363

Table S44. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the iso-C₄H₁₀@(H₂O)₂₈ isobutane-clathrate.

O	-0.120106	-0.267274	4.717493
H	-0.736630	-0.964576	4.381253
H	-0.146720	-0.323294	5.684601
O	1.495405	-4.324545	-1.673391
H	1.277893	-3.678577	-2.378017
H	0.669756	-4.426464	-1.153814
O	-4.474729	0.991092	-1.515134
H	-5.375600	1.138519	-1.841350
H	-4.505424	0.153286	-0.989338
O	3.167422	3.489683	-1.342627
H	2.722832	3.023325	-2.083161
H	2.445305	3.853907	-0.788015
O	-0.776906	2.692776	-3.289653
H	0.172412	2.442209	-3.300478
H	-0.924715	3.192734	-2.460021
O	-1.291859	4.173433	-0.971387
H	-1.537743	5.061176	-1.274823
H	-0.449510	4.290310	-0.462932
O	-0.229782	-3.853809	2.357306
H	0.713172	-3.578081	2.339765
H	-0.475650	-4.079289	1.433032
O	-3.785752	-0.683149	2.410081
H	-3.562840	0.271863	2.471657
H	-3.029464	-1.183931	2.784037
O	-3.280484	2.037068	2.535438
H	-3.395164	2.443588	1.630080
H	-3.941169	2.459510	3.104895
O	4.275587	-0.796977	-1.112343
H	4.324768	0.074223	-0.619788
H	5.176802	-0.970851	-1.424985
O	3.425126	1.563805	2.683237
H	3.074111	0.701784	3.044190
H	4.123118	1.843733	3.294419
O	1.386278	3.457659	2.645636
H	2.097676	2.781264	2.656371
H	0.578019	3.020208	3.007690
O	-1.764359	-1.762122	-3.520201
H	-2.040766	-0.794383	-3.529398
H	-2.183454	-2.157828	-4.300762
O	-0.795003	2.279423	3.767736
H	-0.592886	1.379523	4.098346
H	-1.643576	2.211316	3.281195
O	0.863746	-2.430794	-3.652305
H	0.974221	-2.781453	-4.549529
H	-0.081247	-2.141995	-3.589886
O	-4.461923	-1.321040	-0.057147
H	-4.187328	-1.098916	0.881117
H	-5.351040	-1.702578	0.007019
O	4.456831	1.547717	0.105709
H	4.061801	1.533706	1.004210
H	3.982545	2.252628	-0.398827
O	-1.771197	-2.147835	3.651499
H	-1.207809	-2.787276	3.124311
H	-2.213432	-2.679284	4.331089

O	1.929478	2.124967	-3.442765
H	2.242864	2.452679	-4.299454
H	2.190033	1.160942	-3.406118
O	3.425492	-3.242295	-0.057109
H	2.730857	-3.603859	-0.660017
H	3.671983	-2.356444	-0.397852
O	-3.620460	3.088357	0.119483
H	-3.904465	2.370802	-0.486904
H	-2.774649	3.438469	-0.232908
O	2.464008	-0.675184	3.739348
H	1.549259	-0.557721	4.073259
H	2.466586	-1.502305	3.209666
O	-2.609934	0.719751	-3.588132
H	-3.255463	0.838759	-2.859378
H	-1.910244	1.406708	-3.454973
O	1.105454	4.524160	0.261132
H	1.264137	5.471374	0.394448
H	1.189039	4.101332	1.168834
O	-0.896882	-4.589428	-0.220664
H	-1.209359	-5.506803	-0.228792
H	-1.632175	-4.042915	-0.615396
O	2.437815	-3.092850	2.387807
H	2.940836	-3.734214	2.912177
H	2.822096	-3.129869	1.463067
O	-2.819691	-3.148612	-1.366644
H	-2.458777	-2.625219	-2.115557
H	-3.363988	-2.528117	-0.835792
O	2.721807	-0.400737	-3.362966
H	3.244622	-0.577689	-2.549987
H	2.028584	-1.093507	-3.416410
C	-0.014049	0.066627	-1.046838
C	0.968906	1.113547	-0.526247
C	-1.426456	0.351553	-0.539592
C	0.435329	-1.338707	-0.652030
H	-0.025898	0.128412	-2.147300
H	1.980278	0.933117	-0.908529
H	1.016185	1.090640	0.572226
H	0.670717	2.125538	-0.826387
H	-2.143065	-0.387239	-0.918271
H	-1.763439	1.345377	-0.856554
H	-1.457627	0.318417	0.559017
H	-0.245019	-2.100093	-1.052024
H	0.455774	-1.448286	0.441933
H	1.442620	-1.552348	-1.027425

Table S45. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the iso-C₄H₁₀@(H₂O)₃₀-C_{2v} B isobutane-clathrate.

O	-2.249781	-1.923280	-3.484652
H	-2.620819	-2.186063	-4.340684
H	-1.430758	-1.389665	-3.692092
O	-1.959521	4.156504	1.695562
H	-2.650988	3.484079	1.517955

H	-1.240162	3.722576	2.202685
O	-2.261556	-0.792697	3.622354
H	-2.621573	-0.930197	4.512388
H	-3.024567	-0.448518	3.073899
O	4.627137	-2.490436	0.269955
H	4.547550	-2.028479	-0.597035
H	3.850527	-3.093771	0.320824
O	2.103027	-1.054779	3.653718
H	2.379944	-1.274895	4.557072
H	1.713543	-1.889545	3.289016
O	1.054670	-3.376986	2.707117
H	1.277111	-4.069204	3.349582
H	0.052682	-3.359628	2.666450
O	-3.992779	2.126712	-1.665606
H	-4.780526	2.494774	-2.094653
H	-3.212755	2.627945	-2.047421
O	-4.698822	-1.911966	0.181984
H	-5.633457	-2.168525	0.154629
H	-4.516835	-1.427398	-0.677291
O	-3.009671	-4.032322	0.434748
H	-3.508027	-4.846910	0.602079
H	-3.682702	-3.313390	0.334438
O	4.359390	1.525466	-1.650632
H	5.200001	1.872933	-1.985344
H	4.389994	1.644701	-0.656995
O	2.068768	-2.222649	-3.360757
H	1.680195	-2.969574	-2.840168
H	2.364821	-2.614171	-4.197005
O	0.998164	-4.282923	-1.938562
H	1.228412	-5.126647	-2.357190
H	-0.002572	-4.248529	-1.922491
O	0.199931	3.191745	3.159230
H	0.125106	2.244685	3.479110
H	0.215697	3.739994	3.959201
O	-1.647810	-4.195081	-2.008129
H	-1.887389	-3.378436	-2.499564
H	-2.087637	-4.133065	-1.133407
O	2.506763	3.683751	1.785495
H	2.977505	4.333064	2.330187
H	1.685367	3.458747	2.288406
O	-4.335587	-0.017061	2.186353
H	-4.470615	-0.669525	1.464891
H	-4.251299	0.863965	1.761562
O	4.375081	-1.206811	-2.145685
H	4.304147	-0.239017	-2.001689
H	3.534783	-1.498380	-2.555364
O	-4.206651	-0.617675	-2.056406
H	-4.024588	0.339407	-1.940582
H	-3.463483	-1.006000	-2.568799
O	4.474501	-0.579555	2.214260
H	4.512983	-1.279452	1.516069
H	3.632830	-0.725307	2.693215
O	2.349898	3.154973	-2.672895
H	2.134356	3.772911	-1.932366
H	3.030707	2.538490	-2.326163
O	-1.574910	-3.321711	2.724174
H	-1.860974	-2.415729	2.976477
H	-2.037108	-3.551454	1.889595

O	-0.046896	-0.587609	-4.085513
H	0.751876	-1.063780	-3.774039
H	0.058728	0.363686	-3.866500
O	0.009630	0.726633	4.046960
H	-0.808703	0.234323	3.816034
H	0.761925	0.129876	3.841085
O	2.449505	-4.175157	0.446778
H	1.880613	-3.880010	1.188414
H	1.888520	-4.179089	-0.356317
O	-1.979900	3.530644	-2.632771
H	-1.617010	4.113488	-1.929839
H	-1.223678	3.019010	-2.996142
O	0.156534	2.155935	-3.757319
H	0.190309	2.462542	-4.676591
H	0.999373	2.491667	-3.332960
O	-4.089210	2.491891	1.024401
H	-4.072409	2.383708	0.039741
H	-4.883024	3.012987	1.220646
O	4.452759	1.834592	0.976950
H	3.711771	2.381189	1.310060
H	4.420482	0.964216	1.448533
O	-1.036898	5.149974	-0.590516
H	-1.333769	6.069521	-0.660480
H	-1.394802	4.801200	0.274085
O	1.739891	4.870612	-0.639571
H	0.767351	4.992910	-0.599455
H	1.999195	4.468645	0.216050
C	-0.063174	-0.641002	0.792396
C	1.434676	-0.469525	0.538656
C	-0.648046	-1.726896	-0.109726
C	-0.804866	0.682597	0.596942
H	-0.201790	-0.958799	1.836870
H	1.865792	0.288598	1.203505
H	1.613864	-0.151302	-0.498452
H	1.979846	-1.408690	0.698932
H	-1.732626	-1.818695	0.031061
H	-0.199419	-2.706657	0.097890
H	-0.466051	-1.490856	-1.168003
H	-1.868837	0.582607	0.846497
H	-0.733419	1.011300	-0.449409
H	-0.380324	1.472704	1.227556

Table S46. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the neo-C₅H₁₂@(H₂O)₂₈ neopentane-clathrate.

O	-3.292592	-1.876585	2.763582
H	-3.680660	-1.624184	1.888130
H	-4.033856	-2.188774	3.304890
O	0.499956	-2.713501	-3.961449
H	1.115353	-1.950947	-3.995423
H	-0.400332	-2.327301	-3.907693
O	-1.331267	4.311186	-1.286725
H	-1.568730	5.215728	-1.541242
H	-2.081321	3.732659	-1.575289

O	4.220506	0.143918	2.322462
H	4.304378	0.521276	1.420449
H	3.571027	0.703236	2.799519
O	3.030056	3.480774	-0.316582
H	3.524218	2.632586	-0.316549
H	2.599911	3.545636	0.561960
O	1.694207	3.689765	2.137647
H	1.974469	4.480863	2.622981
H	1.888783	2.923323	2.733410
O	-3.163867	-2.732102	-1.409895
H	-2.506263	-3.339664	-1.004921
H	-2.733613	-2.320592	-2.192023
O	-4.452952	1.641470	0.160300
H	-3.959835	1.998393	0.931561
H	-4.349100	0.666219	0.200888
O	-2.997212	2.625447	2.321945
H	-2.215743	3.169477	2.019773
H	-3.526337	3.205270	2.890524
O	3.214239	-3.036648	-0.483647
H	3.182349	-2.785023	0.486096
H	3.873687	-3.743997	-0.551731
O	0.870593	-2.739669	3.510848
H	0.065854	-3.158839	3.093040
H	1.080178	-3.281662	4.286485
O	0.430930	-0.128600	4.381511
H	0.573403	-1.033997	4.030129
H	-0.492536	0.123313	4.137380
O	0.776936	1.725509	-4.099182
H	0.985385	2.415812	-3.401554
H	0.846903	2.177939	-4.953931
O	-2.168661	0.442520	3.836395
H	-2.588962	-0.353265	3.447685
H	-2.431222	1.202287	3.274290
O	2.279031	-0.543892	-4.067257
H	2.771012	-0.561438	-4.902542
H	1.762384	0.300118	-4.073627
O	-3.309414	2.605176	-2.028682
H	-3.741719	2.218120	-1.211708
H	-4.018534	3.030930	-2.534492
O	3.214744	-2.377852	2.064627
H	2.358710	-2.466462	2.535484
H	3.533952	-1.450909	2.189669
O	-4.318210	-1.141742	0.351512
H	-3.850167	-1.694798	-0.340484
H	-5.246706	-1.421126	0.319777
O	4.516001	1.135389	-0.269543
H	5.447329	1.364308	-0.409681
H	4.312356	0.410968	-0.926351
O	0.906562	-4.070039	-1.623637
H	0.762539	-3.550100	-2.451539
H	1.675807	-3.663815	-1.169495
O	-0.974567	4.106108	1.458889
H	-1.034965	4.164472	0.481747
H	-0.049635	3.865547	1.680615
O	-1.331425	-3.851166	2.494600
H	-2.036386	-3.173012	2.573876
H	-1.264271	-4.052932	1.535396
O	1.167922	3.589915	-2.294586

H	0.306156	3.831310	-1.895519
H	1.825165	3.507636	-1.560445
O	2.319703	1.593344	3.750097
H	2.682499	1.888607	4.599170
H	1.584379	0.946716	3.970039
O	-2.064045	-1.644539	-3.693415
H	-2.629047	-1.898606	-4.438940
H	-2.020676	-0.645690	-3.707245
O	-1.305460	-4.426980	-0.225909
H	-1.539600	-5.355359	-0.376828
H	-0.448334	-4.274901	-0.721738
O	-1.892656	0.990752	-3.809024
H	-0.953267	1.274850	-3.831102
H	-2.344781	1.510157	-3.110762
O	4.076190	-0.861860	-1.965922
H	3.759816	-1.642729	-1.459725
H	3.418184	-0.707560	-2.677449
C	-0.067213	-0.045005	0.024511
C	0.931726	0.758677	0.860512
C	-1.312772	0.805291	-0.231523
C	-0.464581	-1.309492	0.788338
C	0.563776	-0.429979	-1.315388
H	1.827191	0.162903	1.085441
H	0.478634	1.062144	1.813782
H	1.248216	1.665054	0.328653
H	-2.042761	0.257699	-0.843205
H	-1.052506	1.732027	-0.761656
H	-1.797333	1.080094	0.713872
H	-1.229345	-1.874616	0.240583
H	-0.871049	-1.057776	1.777134
H	0.401974	-1.968675	0.935810
H	1.441689	-1.072539	-1.169471
H	0.882142	0.465254	-1.865600
H	-0.154046	-0.977372	-1.940645

Table S47. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the neo-C₅H₁₂@(H₂O)₃₀-C_{2v} A neopentane-clathrate.

O	-4.683649	-2.185584	-0.657147
H	-4.571790	-1.892789	0.271385
H	-3.874240	-2.710113	-0.868718
O	-2.465233	-3.651008	-1.279296
H	-1.942201	-3.859141	-0.475933
H	-1.884646	-3.163268	-1.898698
O	-4.699311	-0.020651	-2.286491
H	-4.669001	-0.817629	-1.697245
H	-3.906951	-0.066408	-2.862291
O	1.490854	-2.328719	-3.358899
H	1.877914	-2.762674	-2.567608
H	1.945987	-1.458932	-3.473471
O	-1.127205	-2.387528	-3.385726
H	-1.319331	-3.029748	-4.087006
H	-0.125183	-2.319615	-3.353475
O	-2.455014	-0.103854	-3.969617

H	-1.929251	-0.924995	-3.792112
H	-2.717572	-0.147115	-4.901774
O	2.610248	-3.691398	-1.211296
H	2.983970	-4.505235	-1.582848
H	3.392592	-3.147483	-0.910098
O	-4.593692	2.111658	-0.767308
H	-5.443326	2.570197	-0.853379
H	-4.644606	1.298982	-1.360255
O	1.445158	2.413561	-3.535536
H	0.448586	2.355898	-3.515672
H	1.662289	2.968626	-4.300119
O	-1.215367	2.341016	-3.540384
H	-1.610235	1.447397	-3.634173
H	-1.612672	2.739154	-2.736955
O	-2.432870	3.609277	-1.365577
H	-2.720579	4.454384	-1.745385
H	-3.264187	3.101715	-1.177861
O	2.819784	0.003092	-3.799740
H	2.307672	0.830763	-3.676803
H	3.576496	0.050697	-3.178882
O	-4.196431	1.377933	1.890037
H	-4.304576	1.615277	0.943895
H	-4.188254	0.396148	1.933469
O	-4.304338	-1.368379	1.999813
H	-3.491446	-1.811991	2.375296
H	-5.044380	-1.642186	2.562456
O	-2.182712	-2.606112	2.979639
H	-1.802550	-3.242826	2.334806
H	-1.445057	-2.068402	3.340848
O	-2.299685	2.736768	3.136023
H	-2.995792	2.177018	2.686962
H	-2.773293	3.281493	3.783051
O	-0.164555	1.467855	4.392518
H	-0.938920	1.865413	3.937344
H	0.624557	1.851025	3.953242
O	-0.117125	-1.193062	4.185760
H	-0.114892	-1.489798	5.108747
H	-0.139621	-0.195614	4.225335
O	1.303532	4.123924	1.040323
H	0.302377	4.187847	1.031654
H	1.620386	5.026706	1.201373
O	-1.318130	4.316334	1.080127
H	-1.687080	3.764182	1.805172
H	-1.722469	4.005511	0.240944
O	2.641697	3.602705	-1.335187
H	2.036299	3.708290	-0.570488
H	2.145404	3.155703	-2.055908
O	1.364541	-4.435152	1.173789
H	1.753128	-4.139761	0.322148
H	1.604202	-3.750338	1.845370
O	-1.265682	-4.425467	1.104713
H	-1.573199	-5.321186	1.310188
H	-0.262885	-4.462598	1.103373
O	2.021770	-2.627658	3.101763
H	2.776295	-2.075506	2.806385
H	1.309935	-2.021214	3.393746
O	2.072912	2.631771	3.177012
H	1.766354	3.174738	2.406603

H	2.416672	3.268372	3.823083
O	4.304492	1.324716	2.131322
H	3.501852	1.751143	2.500791
H	4.414640	1.668173	1.218474
O	4.303786	-1.325967	2.198477
H	4.292966	-0.327354	2.191247
H	5.046971	-1.583411	2.764591
O	4.729225	2.231932	-0.473266
H	3.949657	2.757775	-0.819618
H	5.492426	2.829216	-0.494060
O	4.987604	0.018970	-2.023110
H	5.836774	0.031727	-2.489860
H	4.959505	0.841368	-1.473021
O	4.673903	-2.227334	-0.400028
H	4.796598	-1.431468	-0.960818
H	4.552471	-1.903556	0.519792
C	-0.303777	0.628203	1.312557
C	-0.346210	-0.065986	-0.050624
C	0.182893	-1.495880	0.095057
C	-1.793336	-0.102895	-0.553159
C	0.518535	0.706964	-1.049953
H	-0.641712	1.670512	1.236768
H	-0.958642	0.114414	2.028216
H	0.714003	0.629949	1.725941
H	0.143417	-2.034973	-0.860876
H	1.226195	-1.498414	0.438386
H	-0.412021	-2.056095	0.827248
H	-1.862061	-0.629091	-1.513228
H	-2.186665	0.913897	-0.691893
H	-2.446770	-0.623593	0.159941
H	0.475629	0.245248	-2.045484
H	1.570628	0.731220	-0.733177
H	0.166537	1.742806	-1.144004

Table S48. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the neo-C₅H₁₂@(H₂O)₃₀-C_{2v} B neopentane-clathrate.

O	-1.447106	-2.692464	-3.540193
H	-1.756919	-3.242602	-4.275656
H	-0.878720	-1.976522	-3.948885
O	-3.370918	3.082361	1.779693
H	-3.785661	2.204930	1.634822
H	-2.528154	2.936176	2.260879
O	-1.741189	-1.600063	4.031249
H	-2.094846	-1.826997	4.904766
H	-2.527982	-1.558875	3.415503
O	5.048625	-0.571779	0.200877
H	4.774701	-0.241503	-0.685935
H	4.572776	-1.425215	0.327791
O	2.437890	-0.186541	3.748104
H	2.816164	-0.230720	4.640392
H	2.401260	-1.125288	3.434618
O	2.346802	-2.783979	2.936966
H	2.877313	-3.325616	3.541435

H	1.408815	-3.133365	3.000286
O	-4.595375	0.337628	-1.522975
H	-5.489522	0.366572	-1.897071
H	-4.082263	1.076186	-1.970505
O	-3.541464	-3.493132	0.367752
H	-4.278528	-4.122579	0.376212
H	-3.578915	-3.024898	-0.517658
O	-1.095740	-4.605416	0.682035
H	-1.181790	-5.566922	0.775518
H	-2.018582	-4.258971	0.582230
O	3.399541	2.920879	-1.575356
H	3.985192	3.578498	-1.980007
H	3.430228	3.093361	-0.588796
O	2.673807	-1.352136	-3.695942
H	2.628488	-2.129810	-3.084377
H	3.203805	-1.643488	-4.453935
O	2.551809	-3.442254	-1.953990
H	3.054417	-4.195996	-2.300018
H	1.602138	-3.754129	-1.885540
O	-0.969959	2.945685	3.184109
H	-0.677797	2.056495	3.540301
H	-1.153008	3.488270	3.967283
O	0.055667	-4.268445	-1.834864
H	-0.518772	-3.695458	-2.388913
H	-0.341076	-4.312868	-0.938843
O	0.944266	4.291602	1.770746
H	1.057707	5.122933	2.256459
H	0.290065	3.763614	2.291276
O	-3.816224	-1.610624	2.394286
H	-3.717156	-2.271574	1.675423
H	-4.082527	-0.770020	1.963900
O	4.328246	0.413064	-2.262209
H	3.915449	1.280093	-2.061802
H	3.668959	-0.123494	-2.747867
O	-3.655154	-2.230005	-1.943088
H	-3.911622	-1.287628	-1.844272
H	-2.852309	-2.269668	-2.506431
O	4.400440	1.138596	2.218873
H	4.630008	0.517187	1.483848
H	3.694012	0.695899	2.732397
O	0.868586	3.294009	-2.640857
H	0.451302	3.846379	-1.934318
H	1.757936	3.062439	-2.298166
O	-0.126932	-3.668564	3.120262
H	-0.708058	-2.935378	3.421165
H	-0.466421	-3.957070	2.245425
O	0.094280	-0.818362	-4.600349
H	1.007460	-0.955162	-4.265619
H	-0.198497	0.059412	-4.268824
O	-0.164334	0.663282	4.227598
H	-0.745609	-0.122553	4.129323
H	0.743679	0.374055	3.990234
O	3.729255	-2.951650	0.525733
H	3.119221	-2.920420	1.291127
H	3.199353	-3.121746	-0.280593
O	-3.279416	2.312989	-2.647202
H	-3.101859	2.970495	-1.938249
H	-2.408416	2.046084	-3.015136

O	-0.840437	1.676855	-3.836260
H	-0.944888	2.105099	-4.700643
H	-0.156451	2.227551	-3.356625
O	-4.685681	0.723157	1.166313
H	-4.659810	0.597789	0.183845
H	-5.620839	0.841235	1.393664
O	3.492115	3.398503	1.031387
H	2.590738	3.609443	1.351740
H	3.778529	2.570781	1.494223
O	-2.910849	4.141975	-0.606596
H	-3.496216	4.908226	-0.702694
H	-3.100144	3.752742	0.294627
O	-0.231613	4.841542	-0.706307
H	-1.183426	4.614158	-0.631100
H	0.171553	4.638822	0.164101
C	0.190319	0.090120	-0.032934
C	1.165357	1.062740	0.636742
C	0.819854	-0.421135	-1.331741
C	-1.120502	0.822888	-0.342157
C	-0.082199	-1.096277	0.897801
H	0.781321	1.408422	1.605781
H	1.327673	1.942968	0.000808
H	2.139946	0.587233	0.811096
H	0.152685	-1.126020	-1.845876
H	1.765559	-0.939746	-1.123204
H	1.034638	0.409894	-2.017498
H	-1.832945	0.164775	-0.857923
H	-0.934204	1.693775	-0.984652
H	-1.596221	1.180662	0.581054
H	-0.783524	-1.807013	0.438757
H	-0.514667	-0.759783	1.848508
H	0.846762	-1.637276	1.122187

Table S49. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the neo-C₅H₁₂@(H₂O)₃₀-4¹⁵1⁰6⁶-C_{2v} neopentane-clathrate.

O	-1.621765	4.406464	0.282017
H	-0.641013	4.417431	0.281171
H	-1.891825	3.896937	1.076780
O	-3.859303	-1.351805	2.163172
H	-3.891112	-1.820061	1.299810
H	-4.011239	-0.401383	1.972997
O	4.103658	-1.091208	2.383151
H	4.957777	-1.258449	2.810531
H	4.156489	-1.533546	1.483478
O	4.105716	1.650445	1.894783
H	3.280619	2.099553	2.174819
H	4.007167	0.695656	2.094243
O	2.130967	-1.965935	4.025011
H	2.841707	-1.659322	3.407453
H	2.586362	-2.335670	4.796512
O	1.634991	-2.818382	-3.448971
H	2.003169	-3.397129	-4.134037

H	2.047436	-1.931679	-3.594316
O	2.389802	-3.831884	-0.955418
H	2.065340	-3.463217	-1.803626
H	1.602546	-3.975118	-0.387996
O	-4.427572	1.322566	1.666581
H	-5.268450	1.528943	2.102876
H	-4.576961	1.464942	0.680579
O	-0.146795	2.215577	3.840942
H	-0.989070	2.344056	3.357224
H	-0.104695	1.273658	4.138158
O	0.180311	-4.461207	0.602609
H	0.204463	-5.428574	0.661661
H	0.161452	-4.134714	1.546697
O	4.773929	-0.256261	-1.939912
H	4.735930	0.643193	-1.491528
H	5.670640	-0.348474	-2.296296
O	-2.463905	2.980161	2.512182
H	-2.886477	3.609695	3.116852
H	-3.180880	2.357442	2.228278
O	-1.959046	-3.961870	-1.093667
H	-1.202052	-4.051141	-0.476348
H	-1.616972	-3.573079	-1.936268
O	1.931419	3.226870	2.602535
H	2.292561	3.860087	3.242255
H	1.143387	2.800931	3.056958
O	-4.089183	-2.677037	-0.243128
H	-4.804324	-3.329110	-0.193640
H	-3.271757	-3.177755	-0.535511
O	-1.982810	-2.054072	3.893773
H	-2.652746	-1.765053	3.212016
H	-2.492860	-2.436874	4.623430
O	1.160176	4.541893	0.371116
H	1.380774	5.474424	0.522468
H	1.452664	4.058969	1.188298
O	-0.001077	-0.319979	4.789859
H	-0.753420	-0.869516	4.482996
H	0.804824	-0.800691	4.509230
O	0.126762	-3.677972	3.134019
H	0.891639	-3.114697	3.378482
H	-0.671830	-3.148136	3.348985
O	4.328923	-2.200719	0.009839
H	4.467396	-1.522453	-0.685261
H	3.591878	-2.779967	-0.305011
O	-1.145151	-2.934655	-3.471175
H	-1.533552	-2.042405	-3.599007
H	-0.171580	-2.823770	-3.492866
O	4.628879	2.068557	-0.732938
H	4.420598	1.925677	0.223997
H	3.900914	2.615399	-1.097493
O	-4.632827	-0.724028	-2.160148
H	-4.438081	-1.417451	-1.493900
H	-3.851379	-0.685466	-2.753240
O	-4.770089	1.680757	-0.908346
H	-4.707599	0.803895	-1.364098
H	-4.031789	2.226970	-1.257004
O	-2.722811	3.307348	-1.863380
H	-3.130293	4.048727	-2.336750
H	-2.267764	3.708915	-1.069603

O	-2.470598	-0.542801	-3.903927
H	-2.002464	0.337797	-3.822549
H	-2.810300	-0.577702	-4.811047
O	2.849152	-0.407068	-3.828398
H	3.584915	-0.348605	-3.164944
H	3.273887	-0.382932	-4.700019
O	2.557476	3.622311	-1.777539
H	2.019159	3.959134	-1.019704
H	2.916788	4.406368	-2.220109
O	-1.328222	1.834431	-3.746592
H	-1.718509	2.377552	-3.028801
H	-0.345874	1.872535	-3.654911
O	1.380722	1.978089	-3.689787
H	1.765397	2.529713	-2.977128
H	1.864792	1.126867	-3.678125
C	-0.042723	-0.718870	1.203137
C	-0.220551	0.039859	-0.117015
C	0.354485	1.455053	0.017027
C	0.502035	-0.713101	-1.239822
C	-1.714875	0.129763	-0.448227
H	-0.461713	-1.731124	1.128220
H	1.019088	-0.810563	1.471077
H	-0.555726	-0.203174	2.025553
H	0.206643	2.028768	-0.908362
H	-0.140978	1.998133	0.833336
H	1.431958	1.429240	0.232969
H	0.342516	-0.222473	-2.209647
H	0.128241	-1.742644	-1.315505
H	1.584782	-0.759464	-1.055883
H	-1.877763	0.666613	-1.391239
H	-2.261150	0.661995	0.342270
H	-2.155773	-0.871535	-0.547589

Table S50. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the cyc-C₅H₁₀@(H₂O)₂₈ cyclopentane-clathrate.

O	3.947742	-2.555905	0.969449
H	4.272793	-1.651540	0.731963
H	4.725296	-3.063672	1.246465
O	-0.114596	3.696187	2.798609
H	-0.867727	3.744305	2.172968
H	0.706124	3.733750	2.262313
O	0.293119	1.561393	-4.327156
H	0.373535	1.835773	-5.253229
H	1.123728	1.855824	-3.876425
O	-3.998332	-2.572753	0.586461
H	-4.245356	-1.677711	0.269412
H	-3.388317	-2.959487	-0.076848
O	-3.759048	0.324213	-2.723321
H	-4.090510	0.278676	-1.800707
H	-3.247811	-0.501547	-2.856359
O	-2.275118	-2.005868	-3.194936
H	-2.682262	-2.492618	-3.928392
H	-2.219566	-2.650711	-2.445369

O	3.713894	1.612028	2.165031
H	3.131236	1.132442	2.794424
H	3.193185	2.374943	1.831201
O	3.972391	0.176291	-2.351942
H	3.447984	-0.628397	-2.562946
H	4.166879	0.136770	-1.390392
O	2.462316	-2.039248	-3.056757
H	1.584508	-1.731298	-3.422246
H	2.903602	-2.501053	-3.786261
O	-2.580431	0.173375	3.705240
H	-2.542532	-0.780774	3.400567
H	-3.105509	0.174100	4.519944
O	-0.183703	-3.712282	2.606348
H	0.647576	-3.181666	2.762267
H	-0.174023	-4.424704	3.263262
O	-0.063335	-4.700978	0.010398
H	-0.103654	-4.384143	0.938961
H	0.784579	-4.348082	-0.355165
O	-1.349281	4.144556	-1.360269
H	-1.682767	3.475887	-2.031361
H	-1.549755	5.018172	-1.730292
O	2.337734	-3.830168	-0.947629
H	2.896356	-3.405427	-0.264961
H	2.305984	-3.187658	-1.688875
O	-2.356192	3.869026	1.135393
H	-2.857295	4.669439	1.354248
H	-2.046876	3.982943	0.201691
O	2.552337	2.303129	-3.011221
H	3.094032	1.505073	-2.736100
H	3.133660	2.844769	-3.566763
O	-2.570060	-2.326102	2.887271
H	-1.704128	-2.770694	2.762492
H	-3.071577	-2.422613	2.040991
O	4.676402	-0.017326	0.326548
H	4.279115	0.615229	0.996030
H	5.635975	0.114896	0.373620
O	-4.738813	0.016392	-0.145332
H	-5.704993	0.092512	-0.139993
H	-4.407828	0.647480	0.555253
O	-0.172971	1.423757	4.268446
H	-0.176738	2.242292	3.712935
H	-0.986891	0.926035	4.037691
O	0.195428	-1.193498	-4.122271
H	0.184278	-0.214278	-4.182902
H	-0.662328	-1.467416	-3.731225
O	2.064611	-2.374059	3.005241
H	2.724892	-2.414607	2.281185
H	2.045948	-1.444683	3.323837
O	-2.104769	2.433277	-3.199201
H	-1.283306	2.072537	-3.593406
H	-2.690572	1.666275	-2.982710
O	-2.239952	-3.816001	-1.181828
H	-2.674068	-4.626863	-1.489157
H	-1.382868	-4.112888	-0.748715
O	2.262749	3.829636	1.351429
H	2.734137	4.648590	1.566611
H	1.983448	3.907991	0.395348
O	2.135329	0.207722	3.966182

H	2.553787	0.203112	4.840353
H	1.238559	0.642447	4.086593
O	1.432533	4.030219	-1.151007
H	0.455262	4.001390	-1.236814
H	1.803352	3.363996	-1.768136
O	-3.905675	1.650045	1.771034
H	-3.409876	1.150709	2.456951
H	-3.331229	2.395343	1.493778
C	-0.719788	0.825332	0.357920
C	-1.151839	-0.305050	-0.607092
C	-0.027577	-1.342448	-0.509686
C	1.221016	-0.459625	-0.437527
C	0.815863	0.662618	0.536063
H	-0.982924	1.811894	-0.040305
H	-1.229684	0.727610	1.323765
H	-1.193126	0.077671	-1.635986
H	-2.142646	-0.710779	-0.371135
H	-0.010052	-2.046258	-1.350291
H	-0.128090	-1.930565	0.414859
H	2.123303	-0.997802	-0.123783
H	1.415582	-0.038899	-1.434399
H	1.047600	0.363616	1.566189
H	1.360073	1.592912	0.343701

Table S51. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₄H₁₀_anti@(H₂O)₂₈ 5¹²6⁴-D₂ n-butane-clathrate.

O	2.846514	3.363663	1.540121
H	1.881113	3.534360	1.536231
H	2.995463	2.514198	2.007373
O	0.184562	4.158853	1.391764
H	-0.506307	3.673070	1.926587
H	0.178269	5.072408	1.715804
O	-1.710575	2.909680	2.750068
H	-1.481428	1.992797	3.019833
H	-2.504813	2.847999	2.176559
O	3.519228	0.990813	2.807477
H	4.031191	1.192595	3.605337
H	4.141804	0.500659	2.194735
O	1.333465	-0.546745	3.541320
H	1.462830	-1.433928	3.142786
H	2.075780	0.014747	3.226625
O	-1.143592	0.361776	3.635213
H	-1.266473	0.422589	4.595513
H	-0.208309	0.030791	3.514592
O	4.008348	-2.867879	0.963257
H	3.224419	-2.974526	1.558091
H	4.617874	-3.588065	1.185179
O	5.156249	-0.328884	1.180841
H	5.128714	0.070398	0.275287
H	4.775082	-1.227586	1.090752
O	-3.940928	2.818240	1.099986
H	-3.686625	2.963184	0.154067
H	-4.569555	3.522039	1.321725

O	-5.059812	0.278127	1.428194
H	-4.685383	1.177169	1.314962
H	-5.112844	-0.096437	0.523989
O	-3.299636	-1.218199	2.886415
H	-3.915170	-0.653404	2.356817
H	-2.505788	-0.672166	3.075304
O	-3.189688	3.164639	-1.491281
H	-3.694810	3.872985	-1.919203
H	-3.380020	2.330718	-2.013481
O	-0.581215	4.132636	-1.263059
H	-0.349665	4.124213	-0.307665
H	-1.460363	3.707748	-1.351163
O	1.462911	3.184930	-2.656281
H	0.669121	3.527539	-2.155981
H	1.586137	3.780548	-3.410549
O	-3.701452	0.941253	-2.823063
H	-2.862416	0.487064	-3.060902
H	-4.196996	0.321736	-2.244906
O	-1.351242	-0.329241	-3.584245
H	-1.456749	-0.404750	-4.545744
H	-1.407266	-1.266249	-3.240196
O	1.272642	0.586480	-3.535090
H	0.355747	0.251120	-3.440066
H	1.285421	1.505153	-3.187431
O	-5.132422	-0.789612	-1.161031
H	-4.684329	-1.669819	-1.133254
H	-6.031014	-0.951055	-1.486820
O	5.089831	0.792206	-1.306642
H	4.604755	1.648810	-1.221647
H	4.536342	0.235513	-1.892984
O	3.751102	3.162638	-1.032466
H	2.951292	3.168206	-1.598727
H	3.422690	3.239757	-0.105028
O	3.490853	-0.772465	-3.020932
H	2.636793	-0.292522	-3.209295
H	3.919233	-0.910468	-3.879064
O	-1.561103	-2.827873	-2.739945
H	-2.289304	-2.939611	-2.092801
H	-0.756068	-3.216281	-2.333339
O	-3.718519	-3.114222	-0.999401
H	-4.218879	-3.914339	-1.222175
H	-3.390083	-3.237945	-0.070408
O	1.792441	-3.079099	2.521455
H	1.048561	-3.482846	1.983122
H	1.934453	-3.673535	3.274210
O	-0.106212	-4.186872	1.073732
H	-1.003166	-3.809219	1.199321
H	0.110126	-4.116280	0.117822
O	-2.719816	-3.351883	1.489975
H	-3.129414	-4.086948	1.972167
H	-2.914155	-2.523932	2.030373
O	0.632235	-4.058698	-1.588813
H	0.696648	-4.958921	-1.942108
H	1.555813	-3.677217	-1.637130
O	3.113368	-3.137289	-1.657398
H	3.446425	-2.995980	-0.745134
H	3.240089	-2.290793	-2.140542
C	-1.900914	0.070823	0.125941

C	-0.488126	-0.504229	0.185449
C	0.585474	0.581484	0.263617
C	1.998033	0.019921	0.131805
H	-2.660316	-0.717370	0.057811
H	-2.016339	0.726181	-0.746208
H	-2.120902	0.666704	1.020566
H	-0.307457	-1.127300	-0.703802
H	-0.389374	-1.171639	1.055484
H	0.483279	1.122953	1.216594
H	0.411859	1.321837	-0.532304
H	2.754519	0.806611	0.217719
H	2.132615	-0.466165	-0.842542
H	2.200236	-0.730865	0.907032

Table S52. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₄H₁₀_anti@(H₂O)₃₀ 5¹²6⁵-D_{5h} n-butane-clathrate.

O	5.001488	-2.272776	-0.081439
H	5.813543	-2.797155	-0.158823
H	4.995155	-1.642050	-0.864797
O	2.760957	-3.840008	-0.132853
H	3.590159	-3.302166	-0.114130
H	3.044764	-4.765004	-0.193507
O	-1.308531	-3.532915	2.248980
H	-1.516599	-4.305838	2.795423
H	-0.313699	-3.481736	2.222634
O	1.352788	-3.466339	2.248759
H	1.769848	-2.698496	2.694007
H	1.821979	-3.581488	1.395428
O	4.922196	-0.806451	2.201100
H	5.725121	-0.982692	2.715080
H	4.988652	-1.360097	1.382187
O	2.607724	-1.341954	3.547258
H	3.470010	-1.172192	3.095501
H	2.830452	-1.629347	4.446103
O	4.837144	1.885623	1.462298
H	4.011186	2.289065	1.810536
H	4.836912	0.947290	1.747160
O	-1.393527	1.015738	3.803132
H	-0.395821	1.023334	3.753882
H	-1.607367	1.235051	4.723281
O	1.252945	1.079514	3.823820
H	1.716947	0.231300	3.662133
H	1.674560	1.755797	3.250268
O	2.496872	3.058116	2.352692
H	2.673853	3.814090	2.932770
H	1.994673	3.417959	1.564642
O	-2.676791	-1.417995	3.446730
H	-2.135818	-2.097223	2.991843
H	-2.131474	-0.605204	3.507499
O	4.849595	2.002663	-1.175003
H	4.853434	1.970658	-0.172540
H	5.642292	2.496718	-1.435188
O	-1.489140	3.907527	0.183273

H	-1.711218	4.850568	0.230923
H	-1.925086	3.492213	0.984257
O	1.251492	3.997100	0.231032
H	1.629365	3.642245	-0.602171
H	0.278038	3.864046	0.198628
O	2.546909	3.140328	-2.062278
H	3.405953	2.757915	-1.751054
H	2.777125	3.938272	-2.563270
O	-2.719785	2.914776	2.296311
H	-2.215551	2.227106	2.785108
H	-3.537024	2.479179	1.965337
O	4.956332	-0.606880	-2.114022
H	4.145204	-0.753764	-2.650292
H	4.919726	0.322457	-1.797624
O	-1.287612	1.288373	-3.776834
H	-0.288745	1.293705	-3.739942
H	-1.512916	1.571016	-4.676629
O	1.357424	1.346959	-3.821922
H	1.786433	0.472742	-3.695131
H	1.763018	1.959422	-3.171504
O	2.668142	-1.075933	-3.592246
H	2.911609	-1.360947	-4.486201
H	2.180061	-1.845980	-3.180703
O	-2.683623	3.080543	-2.176462
H	-2.193242	3.332173	-1.364661
H	-2.116396	2.452050	-2.672146
O	-1.284340	-3.260017	-2.480912
H	-1.491806	-3.985462	-3.089775
H	-1.720771	-2.448975	-2.870331
O	1.474198	-3.168539	-2.507869
H	1.845556	-3.400662	-1.630750
H	0.495202	-3.155519	-2.427018
O	-2.674952	-3.885703	-0.148396
H	-2.127373	-3.641408	-0.924289
H	-2.125139	-3.737729	0.649920
O	-2.526197	-1.170220	-3.526491
H	-3.367703	-1.006493	-3.045359
H	-2.045870	-0.313958	-3.559069
O	-4.977909	-2.410323	-0.113630
H	-4.140545	-2.933309	-0.097035
H	-4.993142	-1.871643	0.715696
O	-4.915700	-0.802299	-2.190410
H	-4.957380	-1.422282	-1.399928
H	-5.670264	-1.025712	-2.755481
O	-4.974962	1.839376	-1.354416
H	-4.945605	0.911005	-1.674015
H	-4.146303	2.272860	-1.673294
O	-5.020841	1.765133	1.292186
H	-5.817512	2.241041	1.571116
H	-5.005338	1.805157	0.291160
O	-5.034742	-0.896797	2.151623
H	-4.182260	-1.061083	2.620256
H	-5.021645	0.042718	1.871635
C	-2.023854	0.363555	0.275212
C	-0.538047	0.484005	0.611961
C	0.348260	0.581422	-0.631547
C	1.839455	0.507143	-0.303524
H	-2.636070	0.285196	1.180401

H	-2.374453	1.234895	-0.291812
H	-2.215021	-0.530165	-0.334332
H	-0.227358	-0.384217	1.212582
H	-0.366752	1.368771	1.243802
H	0.129000	1.522737	-1.158452
H	0.086057	-0.226547	-1.331079
H	2.456938	0.562085	-1.207340
H	2.081329	-0.435341	0.205278
H	2.139775	1.329327	0.358496

Table S53. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₄H₁₀_g⁻@(H₂O)₂₈ 5¹²6⁴-T_d n-butane-clathrate.

O	4.542965	0.432724	1.560409
H	3.923353	0.776210	2.252306
H	5.434098	0.514027	1.933383
O	-2.412718	-2.616705	2.857911
H	-3.014752	-2.290546	2.156580
H	-2.076865	-1.820717	3.323100
O	-1.985950	4.412921	-0.094601
H	-2.363182	5.305608	-0.106681
H	-1.695761	4.247076	0.836993
O	-0.012275	-1.742425	-4.140687
H	-0.923776	-1.523451	-3.852012
H	0.510297	-0.913407	-4.135425
O	-2.831311	1.401094	-3.230067
H	-2.789719	0.421661	-3.199044
H	-1.911844	1.703636	-3.379891
O	-0.246451	2.400149	-3.734499
H	-0.306600	2.885105	-4.571978
H	0.473079	1.733949	-3.863771
O	1.274681	-0.728583	4.184383
H	1.453598	-1.552706	3.679290
H	0.305674	-0.573452	4.146786
O	1.489985	3.521283	2.297351
H	1.845334	3.624970	1.387105
H	1.885313	2.702993	2.667593
O	2.433832	3.908059	-0.282708
H	1.627724	4.026110	-0.860277
H	2.912550	4.749965	-0.318449
O	-0.855702	-4.410869	-0.824791
H	-0.110219	-4.053080	-1.389849
H	-0.919092	-5.354928	-1.035435
O	3.461606	-2.407314	-1.510168
H	3.599947	-2.349133	-0.522314
H	4.141644	-3.017827	-1.834061
O	3.811150	0.059004	-2.780776
H	3.688389	-0.794853	-2.310955
H	3.951070	0.739861	-2.077991
O	-4.439571	0.948157	1.077499
H	-4.211366	1.508457	0.276181
H	-5.350688	1.179306	1.315097
O	4.298649	1.899883	-0.824304
H	4.384038	1.413681	0.022133

H	3.595246	2.567863	-0.681145
O	-4.168514	-1.758443	0.855440
H	-5.048094	-2.109267	1.064488
H	-4.259288	-0.773163	0.882070
O	-1.131880	3.833272	2.418788
H	-0.142674	3.681492	2.391258
H	-1.276720	4.558459	3.045479
O	1.072691	-3.511395	-2.392517
H	1.867379	-3.095261	-1.994431
H	0.696470	-2.849684	-3.023128
O	2.751157	1.309763	3.405682
H	2.170882	0.542357	3.688592
H	3.193288	1.621380	4.210336
O	-2.660615	-1.367222	-3.369178
H	-3.206511	-1.647070	-4.119733
H	-2.883661	-1.991860	-2.622002
O	-0.365857	-4.127163	1.894950
H	-1.116053	-3.573044	2.222404
H	-0.486782	-4.204546	0.923583
O	0.251379	4.272309	-1.751487
H	-0.548734	4.305374	-1.184542
H	0.086541	3.583697	-2.431160
O	3.911617	-2.243064	1.100750
H	4.121375	-1.309189	1.316494
H	3.152069	-2.504222	1.666976
O	-3.848222	2.514802	-0.959273
H	-3.187120	3.173975	-0.659647
H	-3.462304	2.077865	-1.757770
O	1.645645	0.504461	-4.219205
H	1.960342	0.589062	-5.132170
H	2.465373	0.367650	-3.655145
O	-1.471025	-0.376789	4.214848
H	-1.773482	-0.420553	5.134584
H	-1.919885	0.421201	3.815337
O	1.872688	-3.049012	2.789693
H	2.225699	-3.709815	3.404720
H	1.042433	-3.452180	2.398654
O	-2.749350	1.699255	3.169758
H	-3.327443	1.454014	2.415027
H	-2.164954	2.425632	2.863938
O	-3.244841	-3.085197	-1.422117
H	-2.412158	-3.547147	-1.178390
H	-3.536842	-2.594776	-0.624274
C	-1.622043	0.020096	-0.266456
C	-0.818347	-1.278216	-0.264062
C	0.582378	-1.153102	0.337788
C	1.451722	-0.120781	-0.378203
H	-2.622855	-0.142760	-0.682799
H	-1.145655	0.797142	-0.875962
H	-1.741046	0.414086	0.752411
H	-0.726522	-1.649760	-1.295584
H	-1.375016	-2.041230	0.293981
H	1.072883	-2.135492	0.287124
H	0.504341	-0.902839	1.406960
H	2.489240	-0.160486	-0.029443
H	1.090166	0.901826	-0.218334
H	1.455471	-0.308852	-1.460243

Table S54. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₄H₁₀-g⁻@(H₂O)₃₀ 5¹²6⁵-C_{2v} B n-butane-clathrate.

O	-1.219450	-2.679906	-3.563152
H	-1.370906	-3.034746	-4.452188
H	-0.707619	-1.831576	-3.686796
O	-3.706182	2.738326	1.860057
H	-4.014039	1.838926	1.617041
H	-2.849262	2.633448	2.327836
O	-1.863761	-2.161220	3.637672
H	-2.156390	-2.409625	4.527436
H	-2.684014	-2.150431	3.066870
O	5.094296	-0.371678	0.341813
H	4.874030	0.035378	-0.527862
H	4.707204	-1.277208	0.344727
O	2.238878	-0.536277	3.726393
H	2.534489	-0.548846	4.649641
H	2.345877	-1.463262	3.394984
O	2.458643	-3.062464	2.746108
H	2.925709	-3.644703	3.364794
H	1.530124	-3.427481	2.673631
O	-4.536020	0.152558	-1.664031
H	-5.415443	0.186852	-2.071197
H	-4.047682	0.959107	-2.003368
O	-3.537786	-3.904917	-0.047466
H	-4.232417	-4.576732	-0.123168
H	-3.584612	-3.355397	-0.883861
O	-1.040883	-4.968378	0.250375
H	-1.125048	-5.932285	0.311142
H	-1.961132	-4.621797	0.137927
O	3.278752	3.260361	-1.325381
H	3.840410	3.991010	-1.626550
H	3.229655	3.348571	-0.329407
O	2.869413	-1.033083	-3.302026
H	2.892591	-1.904459	-2.833852
H	3.267608	-1.194354	-4.171581
O	2.874291	-3.435291	-2.000248
H	3.407516	-4.088862	-2.478176
H	1.940959	-3.794653	-1.990517
O	-1.261477	2.645008	3.189055
H	-0.945168	1.711045	3.346795
H	-1.450919	3.000794	4.071622
O	0.395801	-4.376057	-2.075411
H	-0.193427	-3.787437	-2.596685
H	-0.071355	-4.558646	-1.232696
O	0.582654	4.336968	2.076224
H	0.618774	5.086223	2.690410
H	-0.038362	3.683853	2.482951
O	-4.019026	-2.184375	2.092599
H	-3.872726	-2.784233	1.329190
H	-4.256370	-1.308704	1.718746
O	4.508133	0.857199	-2.054956
H	4.024179	1.678542	-1.823101

H	3.860947	0.258792	-2.482196
O	-3.630304	-2.422661	-2.234432
H	-3.853595	-1.483629	-2.059038
H	-2.772529	-2.438042	-2.713366
O	4.007593	1.133683	2.330616
H	4.383871	0.577063	1.604602
H	3.346570	0.573427	2.785690
O	0.765063	3.815079	-2.385520
H	0.274560	4.236977	-1.637764
H	1.632784	3.533977	-2.021873
O	-0.017026	-3.999589	2.657782
H	-0.676370	-3.352978	2.992420
H	-0.355879	-4.322364	1.795540
O	0.220964	-0.492691	-3.914436
H	1.150503	-0.580320	-3.614741
H	-0.095287	0.410624	-3.693878
O	-0.432305	0.204217	3.769121
H	-0.968099	-0.612481	3.673366
H	0.510064	-0.057866	3.696341
O	4.095493	-2.945805	0.472047
H	3.446097	-2.994954	1.203773
H	3.609477	-3.163172	-0.349999
O	-3.334909	2.347176	-2.520138
H	-3.267726	2.979992	-1.771235
H	-2.425380	2.228574	-2.872388
O	-0.779311	2.054251	-3.578645
H	-0.832942	2.370423	-4.493947
H	-0.162062	2.691460	-3.109669
O	-4.780228	0.294034	1.046033
H	-4.702356	0.251010	0.059685
H	-5.728503	0.381233	1.229491
O	3.167781	3.499415	1.321470
H	2.262033	3.716931	1.624050
H	3.405818	2.623448	1.717691
O	-3.239281	4.102773	-0.374703
H	-3.880413	4.825184	-0.452097
H	-3.457266	3.616673	0.470096
O	-0.603795	5.025554	-0.365697
H	-1.527509	4.696410	-0.337592
H	-0.204476	4.802945	0.501582
C	-0.871237	1.419729	-0.024170
C	0.595281	1.633459	0.347239
C	1.562434	0.712923	-0.397450
C	1.327066	-0.773671	-0.137371
H	-1.503062	2.208683	0.398465
H	-1.252705	0.459235	0.342857
H	-0.997562	1.437715	-1.114425
H	0.730691	1.497114	1.431649
H	0.865490	2.673168	0.129948
H	2.588259	0.964583	-0.100485
H	1.490806	0.917091	-1.477650
H	2.090788	-1.382734	-0.632593
H	0.347821	-1.103712	-0.504066
H	1.375545	-0.991085	0.938516

Table S55. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₅H₁₂_anti/anti@(H₂O)₃₀ 5¹²6⁵-D_{5h} n-pentane-clathrate.

O	5.046428	-1.095838	-1.993940
H	5.827307	-1.303549	-2.530332
H	4.949443	-0.096492	-2.010022
O	2.725388	-2.117078	-3.009061
H	3.593051	-1.772026	-2.682627
H	2.921351	-2.608199	-3.821951
O	-1.128304	-3.966767	-1.189739
H	-1.287160	-4.893633	-1.424987
H	-0.138023	-3.864627	-1.163080
O	1.534694	-3.825884	-1.158018
H	2.007410	-3.690478	-0.309673
H	1.945449	-3.213943	-1.804894
O	5.230537	-1.981114	0.592099
H	6.061941	-2.470173	0.692628
H	5.201210	-1.677418	-0.349262
O	3.013218	-3.497790	1.193739
H	3.824987	-2.976269	0.982271
H	3.324348	-4.365652	1.494017
O	5.113214	0.281203	2.264589
H	4.266122	0.223521	2.760405
H	5.161588	-0.526433	1.710483
O	-1.093865	-2.304938	3.287138
H	-0.099052	-2.268777	3.224862
H	-1.284041	-2.848428	4.067201
O	1.563765	-2.267988	3.247147
H	2.042210	-2.689527	2.502400
H	1.958231	-1.376735	3.369423
O	2.718710	0.208635	3.669205
H	2.915158	0.283165	4.615726
H	2.139505	0.992676	3.449832
O	-2.434458	-3.629181	1.242188
H	-1.918365	-3.683042	0.410442
H	-1.887506	-3.136509	1.889372
O	4.854046	2.375506	0.653757
H	4.974213	1.596917	1.272423
H	5.612385	2.961022	0.803069
O	-1.492920	2.369843	3.101634
H	-1.696965	2.918138	3.875154
H	-1.861317	1.463876	3.312512
O	1.273379	2.369327	3.146899
H	1.627284	2.868486	2.380508
H	0.297332	2.322464	3.045923
O	2.490681	3.697206	1.040781
H	3.350705	3.229082	0.900659
H	2.720366	4.603156	1.298739
O	-2.547471	0.021381	3.696990
H	-2.006601	-0.772619	3.494719
H	-3.399515	-0.072398	3.215983
O	4.763817	1.529798	-1.991327
H	3.903609	1.815955	-2.371999
H	4.788690	1.863120	-1.068171
O	-1.719058	3.805100	-1.311024
H	-0.724053	3.755331	-1.276038
H	-1.925932	4.693509	-1.639190

O	0.946129	3.827939	-1.292176
H	1.407170	3.264182	-1.950620
H	1.444756	3.728190	-0.454353
O	2.362366	2.315283	-3.137693
H	2.528781	2.820374	-3.948006
H	1.890695	1.479171	-3.416913
O	-3.087994	3.442745	1.081821
H	-2.495224	3.042157	1.753058
H	-2.559944	3.530521	0.259921
O	-1.565558	-0.075300	-3.777859
H	-1.736680	-0.066286	-4.732453
H	-2.086718	0.694680	-3.409347
O	1.186992	0.056743	-3.826867
H	1.630887	-0.732194	-3.451536
H	0.221329	-0.022806	-3.668613
O	-2.702879	-2.457548	-2.932268
H	-2.244169	-1.629800	-3.191326
H	-2.099662	-2.934800	-2.324490
O	-3.026349	1.954737	-2.908523
H	-3.820295	1.612325	-2.441168
H	-2.568567	2.574561	-2.300013
O	-5.066707	-1.735130	-1.731076
H	-4.217007	-2.002964	-2.155006
H	-4.993226	-2.003574	-0.781147
O	-5.310283	0.890061	-1.765365
H	-5.219331	-0.111201	-1.760633
H	-6.084173	1.091489	-2.312560
O	-5.361217	1.967882	0.796444
H	-5.387843	1.613359	-0.118879
H	-4.538948	2.513368	0.859942
O	-4.984537	-0.108290	2.399229
H	-5.718184	-0.124574	3.031950
H	-5.140831	0.683201	1.805669
O	-4.878127	-2.447895	0.884245
H	-3.984132	-2.842349	1.020145
H	-4.900482	-1.625905	1.417856
C	-2.413678	-0.045830	-0.054689
C	-1.081231	0.688920	-0.178147
C	0.121261	-0.237358	-0.014963
C	1.455939	0.493339	-0.144885
C	2.649965	-0.419242	0.105433
H	-3.265501	0.638352	-0.137411
H	-2.489776	-0.557694	0.913683
H	-2.518553	-0.806906	-0.838649
H	-1.021978	1.485359	0.578392
H	-1.019858	1.187632	-1.156047
H	0.071357	-1.041018	-0.767558
H	0.070525	-0.731680	0.968865
H	1.479498	1.332169	0.564731
H	1.530393	0.933745	-1.148463
H	3.596151	0.114560	-0.024664
H	2.643947	-1.269988	-0.587365
H	2.627597	-0.819304	1.126234

Table S56. M06-2X/6-31+G*/PCM optimized Cartesian

coordinates of the n-C₅H₁₂_anti/anti@ (H₂O)₃₂ 5¹²6⁶-D_{3d}
n-pentane-clathrate.

O	1.157095	4.158003	-0.213481
H	2.027471	3.888848	-0.595632
H	1.212875	5.120401	-0.106940
O	-1.278208	3.894969	-1.579348
H	-1.236923	3.257201	-2.336521
H	-0.410905	3.870423	-1.125916
O	-3.610872	2.812766	2.321204
H	-3.553995	3.136500	1.387512
H	-4.008042	3.536148	2.829876
O	1.146161	3.277510	2.426384
H	1.073155	3.506892	1.476438
H	0.300062	2.847753	2.703060
O	-1.118428	2.176932	3.399805
H	-1.104289	1.199963	3.490669
H	-1.977779	2.406079	2.987867
O	-3.541517	3.674675	-0.254823
H	-3.947843	4.551874	-0.328234
H	-2.648486	3.746844	-0.705755
O	3.502849	-2.694504	-2.397534
H	3.444486	-3.006081	-1.460483
H	4.073857	-1.897336	-2.396646
O	1.219532	-2.068629	-3.530662
H	1.336128	-2.231342	-4.479151
H	2.081679	-2.335955	-3.088768
O	-1.120497	-4.250820	-0.035589
H	-1.048735	-3.855937	-0.930721
H	-1.910830	-3.849515	0.387841
O	3.475503	-3.617564	0.154005
H	3.975152	-2.993956	0.721610
H	2.599303	-3.738087	0.577616
O	1.047356	-4.043335	1.466366
H	1.100503	-4.898222	1.920111
H	0.233822	-4.091305	0.886270
O	-1.009208	-3.316648	-2.648179
H	-0.177696	-2.868704	-2.946921
H	-1.092430	-4.110233	-3.199066
O	3.646954	3.503568	-1.161206
H	4.102836	4.322471	-1.410769
H	4.187167	3.098197	-0.412331
O	0.943750	0.653172	-3.014169
H	1.022024	-0.304711	-3.203379
H	1.845193	1.023536	-3.097352
O	-3.557034	0.670242	-3.631648
H	-3.991068	0.701056	-4.497350
H	-3.451130	-0.298835	-3.408405
O	-1.208640	2.175168	-3.669517
H	-2.009448	1.609608	-3.655604
H	-0.443652	1.579007	-3.493429
O	-3.394156	-1.899116	-3.027690
H	-2.526897	-2.327225	-2.871808
H	-3.963378	-2.103743	-2.244938
O	3.533751	1.710866	-3.176130
H	3.735357	2.135541	-4.023790
H	3.604265	2.414885	-2.481849
O	3.360119	-0.594045	3.470517

H	3.657790	-0.723148	4.384529
H	3.333975	0.387299	3.327301
O	3.396467	2.061742	2.994119
H	2.513285	2.495925	2.788170
H	3.768888	2.551001	3.743789
O	-3.457416	-3.362260	1.153757
H	-3.869639	-4.157606	1.524478
H	-3.474097	-2.678450	1.888196
O	-1.140027	-0.549480	3.856223
H	-0.349139	-1.100291	3.595136
H	-1.177743	-0.604807	4.823855
O	0.984105	-2.045481	3.378668
H	1.807988	-1.522864	3.290901
H	0.985107	-2.723708	2.668271
O	-3.582367	-1.593397	3.099216
H	-2.698501	-1.217020	3.303422
H	-4.158533	-0.828793	2.852438
O	-5.213231	0.506110	2.465015
H	-4.663511	1.315359	2.404608
H	-5.552081	0.347226	1.557529
O	-5.033096	-2.426036	-0.927110
H	-4.494811	-2.756696	-0.175233
H	-5.437217	-1.583973	-0.625468
O	-5.121086	1.886286	-1.698605
H	-4.550655	1.471338	-2.383318
H	-4.548655	2.504032	-1.194500
O	-6.120122	0.003606	-0.118274
H	-5.763853	0.718907	-0.719077
H	-7.085337	0.036008	-0.196176
O	6.154558	0.076029	0.023354
H	5.817991	-0.115429	-0.877323
H	5.780322	-0.621542	0.602038
O	5.050293	2.448931	0.781836
H	5.433840	1.576140	0.517043
H	4.475285	2.281336	1.559195
O	5.111337	-0.415187	-2.520819
H	5.797564	-0.516137	-3.198016
H	4.566570	0.362838	-2.794150
O	5.006281	-1.849347	1.690994
H	5.666207	-2.337869	2.206500
H	4.434256	-1.385053	2.349657
C	-2.440988	0.109053	0.447824
C	-1.206015	-0.774829	0.283814
C	0.102830	0.013691	0.353748
C	1.329470	-0.828217	0.007274
C	2.627341	-0.023971	0.014680
H	-3.368958	-0.471227	0.378752
H	-2.471021	0.885689	-0.328284
H	-2.437057	0.611177	1.423069
H	-1.258028	-1.300234	-0.681843
H	-1.200693	-1.556225	1.058813
H	0.219168	0.437264	1.364235
H	0.052026	0.864080	-0.342510
H	1.185933	-1.277871	-0.985536
H	1.409073	-1.663690	0.714970
H	3.488516	-0.650384	-0.244125
H	2.817311	0.413576	1.003518
H	2.579137	0.799587	-0.709446

Table S57. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₅H₁₂_g⁻/g⁻@(H₂O)₃₀ 5¹²6⁵-C_{2v} A n-pentane-clathrate.

O	5.045733	-1.676795	0.255897
H	4.803367	-1.322972	-0.625597
H	4.353103	-2.341460	0.485959
O	3.149665	-3.543413	0.926640
H	2.564088	-3.643142	0.145706
H	2.593464	-3.203614	1.658434
O	4.904238	0.350506	2.048626
H	4.948565	-0.398762	1.400844
H	4.142075	0.164917	2.636764
O	-0.848840	-2.965143	3.246246
H	-1.171420	-3.345005	2.400003
H	-1.344225	-2.119933	3.367211
O	1.763955	-2.633000	3.188038
H	2.081231	-3.222236	3.890261
H	0.763913	-2.731189	3.184673
O	2.706234	-0.151309	3.713537
H	2.317221	-1.045344	3.533989
H	2.971133	-0.158336	4.646111
O	-1.919124	-4.088150	0.931160
H	-2.213258	-4.972674	1.199062
H	-2.754915	-3.563636	0.772035
O	4.572453	2.616173	0.751980
H	5.387117	3.130336	0.857673
H	4.708840	1.758099	1.257342
O	-1.518336	1.949281	3.595828
H	-0.530005	2.008968	3.473835
H	-1.693574	2.296450	4.483866
O	1.112391	2.092788	3.375163
H	1.647205	1.272367	3.427366
H	1.537836	2.683652	2.718355
O	2.329889	3.862971	1.613767
H	2.573341	4.659009	2.110463
H	3.181224	3.454573	1.313119
O	-2.333641	-0.709844	3.641809
H	-1.988930	0.206915	3.587710
H	-3.178892	-0.703494	3.147064
O	4.071415	2.089012	-1.936929
H	4.249506	2.260068	-0.987189
H	4.167093	1.119564	-2.067902
O	4.429708	-0.623329	-2.273535
H	3.637269	-1.086760	-2.668928
H	5.168970	-0.791045	-2.877312
O	2.358592	-1.938852	-3.258248
H	2.094383	-2.627646	-2.607721
H	1.544271	-1.449412	-3.507210
O	1.851927	3.265369	-2.781888
H	2.672618	2.782158	-2.478494
H	2.155778	3.933239	-3.415128
O	-0.270746	1.896682	-3.931518
H	0.501613	2.331448	-3.508947

H	-1.058424	2.189092	-3.425794
O	0.033629	-0.734003	-4.157146
H	0.080874	-0.840213	-5.119958
H	-0.096543	0.244851	-4.007751
O	-1.882626	4.372059	-0.456427
H	-0.882381	4.423096	-0.456286
H	-2.193467	5.283470	-0.571603
O	0.749453	4.542622	-0.575488
H	1.134563	4.079692	-1.351883
H	1.286309	4.279836	0.202662
O	-3.112907	3.393906	1.850146
H	-2.597819	3.733311	1.087105
H	-2.487035	2.893403	2.419400
O	-0.814818	-4.424215	-1.604898
H	-1.206594	-4.267638	-0.718066
H	-1.210137	-3.753866	-2.214286
O	1.773102	-3.939982	-1.455158
H	2.199778	-4.732840	-1.815668
H	0.787876	-4.126831	-1.485251
O	-1.888541	-2.609799	-3.365543
H	-2.624651	-2.151743	-2.906334
H	-1.237097	-1.913251	-3.593036
O	-2.547924	2.859357	-2.626727
H	-2.312290	3.431229	-1.853480
H	-2.967342	3.450849	-3.271012
O	-4.508605	1.083485	-1.764654
H	-3.789347	1.669494	-2.084997
H	-4.640405	1.311019	-0.818637
O	-4.082439	-1.515523	-2.060239
H	-4.198413	-0.528242	-1.954379
H	-4.861471	-1.818659	-2.551569
O	-4.941815	1.720180	0.916852
H	-4.256867	2.359692	1.273170
H	-5.801916	2.153685	1.027175
O	-4.735527	-0.659348	2.210230
H	-5.523921	-0.810049	2.752945
H	-4.862415	0.215909	1.765559
O	-4.127955	-2.707075	0.428446
H	-4.348275	-1.992204	1.062947
H	-4.098208	-2.283236	-0.458345
C	1.685834	-0.584589	0.329555
C	0.377354	-1.352973	0.513965
C	-0.562350	-1.244934	-0.689493
C	-1.037531	0.171482	-1.022735
C	-1.779816	0.837305	0.134943
H	2.194998	-0.898601	-0.591934
H	1.514210	0.497429	0.266479
H	2.373597	-0.762488	1.163119
H	-0.130883	-1.010076	1.425968
H	0.594279	-2.417631	0.677432
H	-1.448590	-1.872286	-0.510983
H	-0.054469	-1.671012	-1.566107
H	-1.701424	0.122267	-1.898056
H	-0.187633	0.797524	-1.328251
H	-2.217333	1.792874	-0.170354
H	-1.114786	1.037502	0.984299
H	-2.595603	0.194896	0.497181

Table S58. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₅H₁₂_g⁻@(H₂O)₃₂ 5¹²6⁶-D₃ n-pentane-clathrate.

O	5.465156	-0.221329	-0.184172
H	5.096151	-0.492745	-1.062571
H	6.428666	-0.296132	-0.258635
O	4.416480	-1.760283	1.878392
H	4.791617	-1.180161	1.181370
H	3.887507	-1.188738	2.475542
O	3.402586	2.428827	2.793436
H	2.535597	2.885338	2.799157
H	3.230055	1.518864	3.114124
O	4.656302	2.389307	0.379038
H	4.940041	1.464858	0.216785
H	4.164441	2.390598	1.236292
O	-0.690926	-2.962000	3.461331
H	-0.230037	-3.482441	2.758611
H	-1.586395	-2.757403	3.115009
O	0.513551	-0.843810	4.446402
H	0.069336	-1.635378	4.015853
H	0.518727	-1.031480	5.397820
O	3.041071	-0.190022	3.701506
H	3.545682	-0.273730	4.525423
H	2.116157	-0.460848	3.928777
O	3.335673	3.256518	-1.738559
H	3.869929	3.982895	-2.094406
H	3.810856	2.944565	-0.913897
O	0.904797	3.643869	2.981842
H	0.451640	3.994881	2.174777
H	0.952210	4.385632	3.603999
O	-0.417983	4.630234	0.818064
H	-0.462117	5.595680	0.895442
H	0.030478	4.448559	-0.060964
O	0.751552	4.257997	-1.506329
H	1.652413	3.869575	-1.520248
H	0.224000	3.776887	-2.188309
O	-0.613277	1.685937	4.255483
H	-0.015045	2.288956	3.765551
H	-0.225691	0.784969	4.227387
O	3.269149	1.224324	-3.633125
H	3.251568	1.949994	-2.970807
H	2.339503	1.057373	-3.897789
O	4.383844	-0.928797	-2.575259
H	5.063759	-1.207999	-3.207648
H	3.942796	-0.125456	-2.979759
O	2.812567	-3.173567	-2.025268
H	3.290261	-2.340566	-2.221431
H	2.879597	-3.303969	-1.054818
O	0.676608	0.821155	-4.556031
H	0.189998	-0.028091	-4.406823
H	0.711473	0.937951	-5.517843
O	-0.791683	-1.445442	-4.248172
H	-0.408256	-2.163365	-3.659520
H	-0.882985	-1.850933	-5.124440

O	0.236700	-3.411816	-2.851493
H	1.164050	-3.272791	-2.538911
H	-0.268304	-3.765691	-2.087340
O	-0.668716	3.016324	-3.467878
H	-0.225365	2.222880	-3.834240
H	-1.598114	2.758199	-3.296696
O	0.519533	-4.510219	1.563273
H	1.388896	-4.151776	1.283848
H	-0.034432	-4.529297	0.753658
O	3.028419	-3.688461	0.700295
H	3.589400	-4.475517	0.776611
H	3.521595	-2.958357	1.170602
O	-3.453702	-3.572978	-0.027747
H	-3.817085	-2.885160	-0.626947
H	-3.391595	-3.167120	0.865006
O	-1.107315	-4.594646	-0.726277
H	-1.293831	-5.512319	-0.976771
H	-1.990365	-4.190677	-0.489887
O	-4.646359	-1.702501	-1.689821
H	-4.124564	-1.277222	-2.428053
H	-5.420900	-2.108056	-2.107955
O	-3.333268	-0.497225	-3.656197
H	-2.414795	-0.815337	-3.793927
H	-3.280554	0.462034	-3.458077
O	-5.485273	0.287164	0.081247
H	-5.154734	1.148925	-0.248505
H	-5.179446	-0.392647	-0.556700
O	-4.536480	2.784903	-0.760305
H	-5.267897	3.413556	-0.856291
H	-3.941759	3.155602	-0.046434
O	-3.333226	2.244703	-3.137918
H	-3.861473	2.687572	-3.819260
H	-3.759533	2.468892	-2.273559
O	-3.033813	3.744564	1.195121
H	-2.104649	4.002055	1.013002
H	-3.017974	3.144452	1.972693
O	-3.276284	-2.552841	2.543790
H	-3.835653	-3.116655	3.099751
H	-3.696080	-1.643422	2.572556
O	-4.496204	-0.213979	2.572034
H	-3.968339	0.563714	2.853654
H	-4.841717	-0.011283	1.668511
O	-3.093027	2.040447	3.388579
H	-2.167999	1.868112	3.722407
H	-3.568655	2.461917	4.120208
C	2.124249	-0.063286	-0.529258
C	1.078269	0.462360	0.454274
C	0.277803	-0.656850	1.129530
C	-0.399199	-1.631372	0.160837
C	-1.321125	-0.975051	-0.865401
H	2.761777	-0.819500	-0.051529
H	1.659211	-0.532802	-1.405321
H	2.772184	0.743246	-0.889066
H	0.396969	1.149442	-0.065883
H	1.577003	1.057630	1.231234
H	0.955378	-1.233036	1.778126
H	-0.481532	-0.214001	1.791414
H	-0.980344	-2.353719	0.746953

H	0.370371	-2.216363	-0.362642
H	-0.775375	-0.300659	-1.537123
H	-2.113713	-0.393613	-0.374205
H	-1.805588	-1.735022	-1.489069

Table S59. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₅H₁₂_anti/g⁻@(H₂O)₃₂ 5¹²6⁶-D₃ n-pentane-clathrate.

O	5.620009	-0.510621	0.240405
H	5.414371	0.448668	0.367910
H	6.586252	-0.583573	0.271662
O	4.638736	-1.522858	-2.169427
H	4.956636	-1.200064	-1.298607
H	3.892259	-2.132452	-1.986191
O	2.686435	-3.745412	1.063029
H	1.764704	-3.766907	1.393098
H	2.629626	-3.619901	0.092244
O	4.405397	-2.011679	2.271330
H	4.839586	-1.503516	1.553610
H	3.783168	-2.638565	1.829053
O	-0.629538	-1.560271	-4.197305
H	-0.002422	-0.797005	-4.199504
H	-1.514596	-1.204601	-3.963879
O	0.118159	-3.555047	-2.677713
H	-0.172780	-2.767635	-3.232495
H	0.070183	-4.323736	-3.267366
O	2.660232	-3.432363	-1.709232
H	3.047898	-4.245696	-2.068672
H	1.739812	-3.399265	-2.073403
O	2.982323	-0.306076	3.711010
H	3.363772	-0.362813	4.600672
H	3.499621	-0.959520	3.154970
O	0.041832	-4.105458	1.892369
H	-0.434846	-3.528334	2.540993
H	0.031768	-4.996094	2.275892
O	-1.310410	-2.538583	3.649700
H	-1.389652	-3.010340	4.493248
H	-0.736730	-1.738575	3.840802
O	0.253784	-0.514651	4.248453
H	1.189828	-0.507322	3.957181
H	-0.080697	0.411537	4.166050
O	-1.392816	-4.289223	-0.472284
H	-0.832921	-4.180534	0.326142
H	-0.882825	-3.940756	-1.235566
O	3.503239	2.257772	2.809970
H	3.276226	1.354670	3.125888
H	2.659722	2.752223	2.732583
O	4.989559	2.123765	0.623964
H	5.766180	2.689982	0.749322
H	4.434333	2.215187	1.451267
O	3.612258	2.833140	-1.704159
H	4.051819	2.582268	-0.864834
H	3.655558	2.043270	-2.283731
O	1.130433	3.719490	2.812838

H	0.744047	4.062435	1.968243
H	1.286747	4.498134	3.368633
O	-0.047532	4.656948	0.551317
H	0.419233	4.400907	-0.299154
H	-0.052136	5.626331	0.567495
O	1.184071	4.080284	-1.698379
H	2.041453	3.593085	-1.656471
H	0.636128	3.636480	-2.380797
O	-0.669824	2.032004	4.136147
H	-0.077093	2.631186	3.635902
H	-1.557555	2.107219	3.728838
O	1.077590	0.545876	-4.357332
H	1.976340	0.539447	-3.966333
H	0.655729	1.393009	-4.100205
O	3.699576	0.627115	-3.418670
H	4.273827	0.809033	-4.177751
H	4.062145	-0.195435	-2.983314
O	-2.815318	2.162572	-3.446042
H	-3.259498	2.449342	-2.618490
H	-2.944450	1.191057	-3.514420
O	-0.282054	2.892419	-3.733093
H	-0.278005	3.480328	-4.503363
H	-1.235839	2.630776	-3.591519
O	-4.151448	2.988776	-1.166300
H	-3.588591	3.374674	-0.438164
H	-4.805325	3.667513	-1.391380
O	-2.732577	3.961929	0.854700
H	-1.772490	4.121249	0.731502
H	-2.839142	3.370938	1.629876
O	-5.454807	0.693947	-0.247174
H	-5.207857	0.542924	0.689423
H	-4.980456	1.502396	-0.536366
O	-4.782940	0.169078	2.417511
H	-5.589875	0.197962	2.954232
H	-4.423468	-0.760849	2.511720
O	-3.227266	2.319588	3.055038
H	-3.768997	2.813340	3.689318
H	-3.745338	1.506550	2.834696
O	-3.904879	-2.324228	2.632208
H	-2.987550	-2.347606	2.980151
H	-3.862861	-2.700622	1.725092
O	-3.174170	-0.577203	-3.723003
H	-3.700690	-0.734547	-4.521448
H	-3.717024	-0.937147	-2.962393
O	-4.722431	-1.446764	-1.766186
H	-4.360183	-2.120754	-1.151228
H	-4.984916	-0.674930	-1.207436
O	-3.823681	-3.358747	0.038343
H	-2.903067	-3.678368	-0.181482
H	-4.397276	-4.136929	-0.035980
C	2.480309	-0.119160	0.045294
C	0.961616	0.008359	0.125923
C	0.260190	-1.027616	-0.754783
C	-1.251516	-0.822387	-0.880224
C	-1.959043	-0.798095	0.473718
H	2.790876	-1.148999	0.260508
H	2.840212	0.134447	-0.958807
H	2.981148	0.540242	0.762303

H	0.654721	1.020079	-0.179226
H	0.641549	-0.113530	1.169146
H	0.715185	-1.012601	-1.756348
H	0.456802	-2.029781	-0.339669
H	-1.676111	-1.628840	-1.494037
H	-1.450422	0.113695	-1.423721
H	-1.665808	0.071326	1.073969
H	-1.707930	-1.699218	1.049365
H	-3.046922	-0.767289	0.354916

Table S60. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₆H₁₄_g⁻/g⁻/g⁻@(H₂O)₃₂ 5¹²6⁶-D₃ n-hexane-clathrate.

O	4.666502	0.260180	-2.594633
H	4.998536	0.228996	-1.671290
H	4.085078	-0.521106	-2.712009
O	3.346923	-3.508113	-0.619071
H	2.464871	-3.860110	-0.376203
H	3.217380	-2.977010	-1.432542
O	4.682419	-2.071834	1.260067
H	5.003247	-1.264784	0.804795
H	4.155472	-2.575931	0.592538
O	-0.628020	0.153945	-4.568410
H	-0.123565	0.957156	-4.291291
H	-1.529951	0.258252	-4.194837
O	0.553130	-2.090320	-3.891108
H	0.091877	-1.218610	-4.089676
H	0.620551	-2.542267	-4.747140
O	3.111002	-2.018078	-2.972728
H	3.573627	-2.535325	-3.650582
H	2.173355	-1.955090	-3.285443
O	3.294841	-1.331354	3.380002
H	3.827863	-1.628098	4.133569
H	3.791809	-1.627252	2.561015
O	0.860296	-4.632098	-0.049276
H	0.420509	-4.317091	0.779968
H	0.970752	-5.589836	0.054477
O	-0.426876	-3.850862	2.219867
H	-0.515282	-4.650309	2.762488
H	0.018377	-3.174913	2.817041
O	0.704758	-2.189805	3.898847
H	1.601669	-1.888312	3.638220
H	0.168212	-1.375594	4.055561
O	-0.665934	-4.030266	-2.315759
H	-0.095537	-4.209684	-1.537533
H	-0.251042	-3.290800	-2.811103
O	3.250476	1.428489	3.474813
H	3.206648	0.446792	3.440374
H	2.331848	1.756962	3.575575
O	4.583656	2.375329	1.401767
H	5.263878	2.973639	1.746805
H	4.070898	2.043808	2.195523
O	3.010187	3.772223	-0.434869
H	3.514802	3.257802	0.229337

H	3.119183	3.301220	-1.288657
O	0.692711	2.386379	4.000973
H	0.217146	2.986275	3.372793
H	0.759672	2.874569	4.835701
O	-0.725536	3.984630	2.329230
H	-0.285138	4.148567	1.441963
H	-0.836074	4.858773	2.733828
O	0.432713	4.513314	0.036062
H	1.354144	4.190392	-0.111417
H	-0.078147	4.308726	-0.776476
O	-0.742101	0.037569	4.469397
H	-0.276218	0.876063	4.269070
H	-1.665183	0.147567	4.160642
O	0.685120	2.435209	-3.893162
H	1.585884	2.400870	-3.507870
H	0.144573	3.003740	-3.304501
O	3.283195	2.506650	-2.898363
H	3.803253	3.063919	-3.496724
H	3.793186	1.653623	-2.801398
O	-3.371704	3.000890	-2.341477
H	-3.767646	2.830762	-1.458817
H	-3.333512	2.133572	-2.802744
O	-0.945790	4.066020	-2.326322
H	-1.041966	4.919206	-2.775748
H	-1.862426	3.668614	-2.293026
O	-4.609983	2.531433	0.092591
H	-4.079856	2.689505	0.923553
H	-5.371219	3.129220	0.146779
O	-3.282305	2.886525	2.366104
H	-2.357569	3.209151	2.304737
H	-3.267672	2.043427	2.867164
O	-5.597173	-0.086192	0.006980
H	-5.248880	-0.560984	0.791258
H	-5.237565	0.825058	0.062821
O	-4.585705	-1.470962	2.227887
H	-5.301349	-1.908356	2.714243
H	-3.968675	-2.201060	1.929581
O	-3.399831	0.459005	3.730001
H	-3.930679	0.537160	4.537264
H	-3.820674	-0.258859	3.193208
O	-3.048232	-3.455015	1.387026
H	-2.117579	-3.485537	1.697260
H	-3.011941	-3.439168	0.404923
O	-3.220669	0.579038	-3.673932
H	-3.756444	0.646830	-4.479122
H	-3.665874	-0.119641	-3.110024
O	-4.479458	-1.216978	-2.214494
H	-3.932839	-1.978190	-1.922870
H	-4.873830	-0.818900	-1.400031
O	-3.074758	-3.453492	-1.379992
H	-2.164200	-3.632328	-1.753036
H	-3.618562	-4.211947	-1.643333
C	2.317268	-0.044075	0.142309
C	1.242236	-0.983154	0.686735
C	0.310801	-1.523740	-0.402156
C	-0.448113	-0.460271	-1.203002
C	-1.259311	0.517377	-0.346434
C	-2.247224	-0.187678	0.582483

O	5.619091	0.263359	0.024053
H	2.902889	-0.545882	-0.638420
H	1.885036	0.864705	-0.295014
H	3.008533	0.265014	0.933682
H	0.660939	-0.472778	1.468307
H	1.728251	-1.836408	1.180228
H	-0.411173	-2.219327	0.050084
H	0.911937	-2.120698	-1.103006
H	0.251886	0.101462	-1.836778
H	-1.134926	-0.973803	-1.893739
H	-1.807783	1.195926	-1.014144
H	-0.583792	1.150987	0.245921
H	-1.735306	-0.748638	1.375185
H	-2.863313	-0.901537	0.021422
H	-2.919116	0.530664	1.064049
H	5.280894	1.048915	0.522225
H	6.586345	0.318992	0.055204

Table S61. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the n-C₆H₁₄_g⁻/g⁻/g⁻@(H₂O)₃₂ 5¹²6⁶-C₂ A n-hexane-clathrate.

O	-5.256511	-2.266401	0.164843
H	-4.928233	-2.037065	1.079789
H	-6.078539	-2.764703	0.286591
O	-3.254010	-3.722980	-1.093956
H	-3.990166	-3.215615	-0.689160
H	-2.961630	-3.207813	-1.875974
O	-4.365056	-1.610786	2.579215
H	-4.216259	-0.643711	2.659837
H	-3.512620	-2.043309	2.801053
O	1.136716	-4.556695	0.251063
H	0.166225	-4.408991	0.456353
H	1.294201	-5.504817	0.377384
O	-1.406246	-4.243032	0.833222
H	-2.045844	-3.994711	0.122061
H	-1.579018	-3.664595	1.604605
O	-1.940559	-2.829452	3.174284
H	-2.036291	-3.494376	3.873144
H	-1.312531	-2.149757	3.527960
O	1.847730	-3.789332	-2.241469
H	1.874961	-4.584947	-2.794412
H	1.556642	-4.089253	-1.343166
O	-4.017672	1.134954	2.823385
H	-4.664125	1.442804	3.477538
H	-4.282114	1.558221	1.966768
O	-4.854367	2.204281	0.484413
H	-5.609799	2.792188	0.638033
H	-4.160785	2.755395	0.009003
O	-3.080088	3.601320	-0.832756
H	-2.802321	3.115037	-1.639570
H	-2.263629	3.897734	-0.361444
O	-1.535001	1.580553	4.008879
H	-2.378431	1.435216	3.529619
H	-1.073420	0.714241	4.012623

O	-0.079981	3.485331	2.839445
H	-0.619668	2.753486	3.252460
H	-0.114158	4.222910	3.468048
O	-0.870521	4.594878	0.393087
H	-0.148779	4.472919	-0.258567
H	-0.595574	4.132624	1.213150
O	2.624165	3.077500	2.423408
H	1.651694	3.134072	2.552270
H	2.799425	3.230969	1.470995
O	2.204412	-1.280320	3.615338
H	2.436812	-1.993559	2.972119
H	2.770631	-0.506452	3.406206
O	-0.322186	-0.916286	4.215466
H	-0.322269	-1.062752	5.174499
H	0.634943	-1.022223	3.932065
O	3.892195	0.873343	3.171407
H	3.390316	1.701573	2.928873
H	4.366588	1.073234	3.992615
O	2.959279	-3.294079	1.958594
H	3.714844	-2.988975	1.412279
H	2.296329	-3.670822	1.343448
O	0.198042	2.525988	-3.582955
H	-0.756826	2.369450	-3.413620
H	0.522237	3.103168	-2.858955
O	-2.525893	2.292350	-3.208129
H	-3.034410	1.428903	-3.254083
H	-2.910729	2.857563	-3.895548
O	1.545882	0.319747	-4.145930
H	1.641607	0.349795	-5.110035
H	1.049944	1.149671	-3.893874
O	1.084592	4.284459	-1.613271
H	1.283532	5.133143	-2.038198
H	1.921404	3.998639	-1.172365
O	-5.654253	0.121076	-1.213297
H	-5.373703	0.838738	-0.607114
H	-5.530219	-0.716146	-0.716454
O	-3.969857	0.088129	-3.357571
H	-4.565355	0.074749	-2.568343
H	-3.427287	-0.728513	-3.314882
O	0.154656	-1.980350	-3.498351
H	0.642192	-1.148714	-3.683746
H	0.755665	-2.574096	-3.001221
O	-2.482043	-2.264361	-3.336513
H	-2.699164	-2.766342	-4.136712
H	-1.497351	-2.121810	-3.366649
O	3.316746	3.542180	-0.237097
H	3.914181	4.305853	-0.192754
H	3.862993	2.799590	-0.606488
O	4.918820	1.583690	-1.165265
H	4.555723	0.981418	-1.885634
H	5.707730	2.001932	-1.544007
O	4.080650	-0.014829	-3.063575
H	4.138510	-0.948245	-2.740530
H	3.163846	0.120625	-3.387848
O	5.645198	0.163798	1.123097
H	5.378457	0.677398	0.329688
H	5.033843	0.432658	1.843500
O	5.159150	-2.379610	0.519989

H	5.957378	-2.893143	0.714385
H	5.364781	-1.432673	0.764407
O	4.346879	-2.550864	-2.132923
H	3.479839	-3.008452	-2.136089
H	4.639061	-2.516365	-1.196688
C	-2.147384	-0.160181	-0.624967
C	-1.178097	-0.389398	0.534907
C	-0.443334	0.886543	0.955018
C	0.375267	1.558550	-0.151646
C	1.409467	0.662691	-0.839680
C	2.396184	0.022695	0.136414
H	-2.753612	-1.051376	-0.822016
H	-1.616591	0.091091	-1.552108
H	-2.833566	0.668643	-0.403667
H	-0.456525	-1.173964	0.264587
H	-1.734409	-0.772194	1.402061
H	0.207849	0.669632	1.814519
H	-1.189564	1.610546	1.312554
H	0.899721	2.417962	0.289609
H	-0.304985	1.974960	-0.907829
H	1.964010	1.269355	-1.570322
H	0.902733	-0.119701	-1.422474
H	3.176795	-0.535786	-0.393804
H	1.897313	-0.672331	0.822235
H	2.885991	0.791201	0.748537

Table S62. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_2@(\text{H}_2\text{O})_{26}$ $5^{12}6^3$ - D_{3h} clathrate.

O	4.182091	2.376274	0.515454
H	4.865309	3.023660	0.746399
H	3.552845	2.348952	1.290360
O	2.272624	-0.232654	3.656996
H	2.630970	-0.214697	4.557474
H	1.363200	-0.614251	3.734100
O	2.500255	2.312940	2.577457
H	2.357381	1.411928	2.938073
H	1.614655	2.690213	2.392017
O	3.929490	-1.744404	1.963176
H	3.338724	-2.394517	1.525300
H	3.351463	-1.214890	2.550796
O	2.253851	-3.596781	0.727752
H	2.273685	-3.434671	-0.258480
H	2.605746	-4.490057	0.860225
O	2.541358	0.968673	-3.323527
H	2.952523	1.210174	-4.167857
H	3.117666	0.263405	-2.936791
O	2.630884	3.203348	-1.656824
H	2.570155	2.415655	-2.237681
H	3.191784	2.927301	-0.900224
O	4.103877	-0.986663	-2.236952
H	4.524816	-0.697472	-1.373249
H	4.831696	-1.245597	-2.822632
O	5.151422	-0.207411	0.067422
H	4.878766	0.720105	0.238295

H	4.719058	-0.749857	0.772841
O	-0.198033	-3.477875	2.018810
H	0.638931	-3.481628	1.505282
H	-0.140218	-2.733327	2.655817
O	2.366221	-3.136595	-1.876413
H	1.483350	-2.935238	-2.255566
H	2.938967	-2.354435	-2.030789
O	-2.356686	2.513500	2.580926
H	-2.804929	3.042243	3.259030
H	-2.939210	2.556296	1.766021
O	-2.176523	3.282872	-1.687659
H	-2.507971	4.086873	-2.115438
H	-1.259202	3.506052	-1.358705
O	0.004140	-0.045961	-3.927054
H	0.867077	0.335102	-3.662097
H	-0.002435	-0.972207	-3.603511
O	-2.383929	1.161505	-3.453512
H	-2.263675	1.906315	-2.825061
H	-1.489941	0.766326	-3.596797
O	-4.021503	-0.649659	-2.461461
H	-3.405440	0.050080	-2.837087
H	-4.649054	-0.866055	-3.167984
O	-5.116933	0.162728	-0.113063
H	-4.809571	-0.136477	-1.005514
H	-6.080152	0.254700	-0.168957
O	-2.554259	-3.485686	0.795212
H	-2.916786	-4.374405	0.929185
H	-1.652840	-3.486500	1.224555
O	-2.445948	-0.116517	3.494153
H	-2.378584	0.796128	3.141405
H	-3.074579	-0.603667	2.907243
O	-0.179691	-1.404111	3.862785
H	-1.021799	-0.881064	3.705509
H	-0.272769	-1.797726	4.743937
O	-4.188334	-1.537980	1.940589
H	-4.549703	-0.976854	1.223863
H	-3.640196	-2.224704	1.502979
O	-2.492540	-2.912546	-1.906545
H	-3.026231	-2.102420	-2.056536
H	-2.494143	-3.080264	-0.938546
O	-0.109356	-2.673275	-3.042811
H	-0.163344	-3.253731	-3.817249
H	-0.983280	-2.772938	-2.567351
O	-3.857881	2.611391	0.408672
H	-3.273654	2.809232	-0.357068
H	-4.290999	1.751168	0.221173
O	0.083733	3.590960	2.036568
H	0.097367	4.453392	2.478872
H	-0.792399	3.186459	2.256977
O	0.189218	3.978977	-0.721657
H	1.055394	3.659311	-1.074291
H	0.201888	3.830196	0.247069
C	1.633155	0.174340	-0.244010
H	2.700155	0.392839	-0.321964
H	1.415356	-0.216211	0.754402
H	1.354726	-0.572015	-0.994164
H	1.061074	1.090746	-0.412266
C	-1.649042	-0.129358	-0.071190

H	-2.730024	-0.278826	-0.039941
H	-1.326642	-0.006639	-1.109366
H	-1.390406	0.766739	0.500618
H	-1.149632	-0.998543	0.366594

Table S63. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_2@(\text{H}_2\text{O})_{28}$ $5^{12}6^4$ - D_2 clathrate.

O	-2.840048	3.500836	-1.453057
H	-1.880251	3.694919	-1.491463
H	-2.987368	2.656352	-1.929417
O	-0.161659	4.296542	-1.403069
H	0.514791	3.799707	-1.943597
H	-0.134865	5.212668	-1.718012
O	1.713488	3.005614	-2.776869
H	1.482407	2.101163	-3.081887
H	2.507075	2.918544	-2.206630
O	-3.480933	1.131649	-2.765758
H	-3.995917	1.377289	-3.549413
H	-4.106285	0.613283	-2.180586
O	-1.350264	-0.421125	-3.632945
H	-1.501681	-1.315981	-3.259879
H	-2.076253	0.146969	-3.293611
O	1.151024	0.468098	-3.751217
H	1.290485	0.525665	-4.708967
H	0.215182	0.141301	-3.640505
O	-4.064924	-2.811355	-1.026551
H	-3.284628	-2.879908	-1.631883
H	-4.670949	-3.521759	-1.286566
O	-5.150995	-0.237081	-1.216313
H	-5.104156	0.129568	-0.296936
H	-4.829434	-1.161258	-1.157552
O	3.943231	2.868853	-1.109572
H	3.673243	3.014194	-0.168409
H	4.579687	3.568577	-1.320734
O	5.037400	0.314807	-1.398859
H	4.682154	1.219942	-1.272348
H	5.112316	-0.074190	-0.502986
O	3.273119	-1.129265	-2.900287
H	3.880026	-0.575948	-2.350214
H	2.493815	-0.575079	-3.119592
O	3.138871	3.163504	1.472439
H	3.661762	3.832507	1.940379
H	3.292941	2.302532	1.959980
O	0.549357	4.188431	1.281838
H	0.321644	4.215242	0.326515
H	1.431403	3.765754	1.352416
O	-1.427371	3.189073	2.752423
H	-0.664023	3.547930	2.219245
H	-1.538244	3.792107	3.502778
O	3.615411	0.902646	2.759702
H	2.805394	0.426280	3.047711
H	4.129056	0.274727	2.208292
O	1.364908	-0.446466	3.680608
H	1.525370	-0.563643	4.629907

H	1.384000	-1.366582	3.290108
O	-1.214614	0.592400	3.681478
H	-0.303425	0.240486	3.589184
H	-1.216319	1.504922	3.318767
O	5.110904	-0.843203	1.158104
H	4.665108	-1.723616	1.105627
H	6.000190	-1.004551	1.508269
O	-4.977549	0.797919	1.290951
H	-4.523297	1.673907	1.235672
H	-4.398880	0.234901	1.846933
O	-3.718838	3.219023	1.125783
H	-2.924165	3.212849	1.699121
H	-3.386359	3.333946	0.203994
O	-3.348477	-0.803097	2.926114
H	-2.511505	-0.314210	3.162812
H	-3.813653	-0.946102	3.764367
O	1.498752	-2.890565	2.673896
H	2.229412	-2.969614	2.024632
H	0.694425	-3.246749	2.238046
O	3.663887	-3.141608	0.926346
H	4.140983	-3.960255	1.132766
H	3.344399	-3.234360	-0.008899
O	-1.875188	-2.956849	-2.639586
H	-1.116824	-3.358688	-2.123663
H	-2.033962	-3.550687	-3.389383
O	0.056943	-4.080930	-1.239217
H	0.975541	-3.756241	-1.356095
H	-0.144446	-4.064768	-0.277646
O	2.709098	-3.328322	-1.594416
H	3.135140	-4.038822	-2.098338
H	2.894825	-2.477417	-2.099558
O	-0.667484	-4.095109	1.431376
H	-0.695087	-5.011195	1.746811
H	-1.603275	-3.748471	1.508653
O	-3.158681	-3.205982	1.586584
H	-3.492548	-3.047985	0.677441
H	-3.196034	-2.339023	2.049274
C	1.733430	-0.453703	0.040918
H	1.531054	0.336793	-0.687553
H	1.305875	-1.394555	-0.317437
H	1.282772	-0.191374	1.001926
H	2.814095	-0.564217	0.160510
C	-1.737688	-0.410466	0.104643
H	-2.794858	-0.637519	-0.052500
H	-1.270417	-1.219645	0.673461
H	-1.649615	0.524598	0.665894
H	-1.237255	-0.307683	-0.862002

Table S64. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_3@(\text{H}_2\text{O})_{30}$ $5^{12}6^5-C_{2v}$ B clathrate.

O	-2.368505	-1.014439	-3.484382
H	-2.484431	-1.107474	-4.441857
H	-1.473293	-0.593250	-3.346482
O	-1.222551	4.131670	2.069080

H	-2.008618	3.599597	1.823485
H	-0.588053	3.534319	2.521834
O	-2.587935	-0.878342	3.442224
H	-2.879620	-0.952297	4.363258
H	-3.314221	-0.392661	2.955471
O	4.164117	-3.417790	0.117978
H	4.131463	-2.855401	-0.690363
H	3.363888	-3.990642	0.096736
O	1.645914	-2.087077	3.505541
H	1.802977	-2.297165	4.438523
H	1.220643	-2.888690	3.109051
O	0.397717	-4.218775	2.371303
H	0.352358	-4.967711	2.985460
H	-0.542161	-3.902599	2.259056
O	-3.618112	2.859130	-1.430033
H	-4.244680	3.511541	-1.779702
H	-2.714190	3.169100	-1.724896
O	-5.202367	-1.041560	-0.148252
H	-6.159645	-1.179348	-0.215917
H	-4.934933	-0.523096	-0.963128
O	-3.754458	-3.347275	0.004941
H	-4.354816	-4.108386	0.005405
H	-4.327612	-2.542008	-0.052651
O	4.526260	0.936262	-1.386992
H	5.437572	1.099184	-1.675364
H	4.553865	0.948555	-0.386322
O	1.752267	-2.208967	-3.440664
H	1.306575	-2.985055	-3.016951
H	1.863587	-2.437527	-4.375718
O	0.473101	-4.279992	-2.225413
H	0.449649	-5.056842	-2.805319
H	-0.474186	-3.975278	-2.143734
O	0.680510	2.592964	3.376324
H	0.425551	1.628256	3.322725
H	0.696464	2.820057	4.318496
O	-2.053622	-3.453659	-2.203998
H	-2.182914	-2.592966	-2.659827
H	-2.610649	-3.425021	-1.397873
O	3.086763	3.110950	2.187507
H	3.605841	3.575487	2.861824
H	2.218336	2.903206	2.612917
O	-4.530320	0.393272	2.156186
H	-4.768347	-0.102694	1.342861
H	-4.200354	1.267122	1.855123
O	4.137602	-1.754469	-2.078407
H	4.200143	-0.805917	-1.838111
H	3.303782	-1.863531	-2.580891
O	-4.471169	0.336778	-2.297309
H	-4.139593	1.218989	-2.024643
H	-3.710134	-0.120128	-2.719962
O	4.035496	-1.571855	2.137285
H	4.069815	-2.250925	1.420354
H	3.193732	-1.724683	2.613112
O	3.108365	3.183799	-2.255011
H	2.948248	3.741087	-1.454809
H	3.579401	2.380998	-1.942304
O	-2.115048	-3.349647	2.262877
H	-2.269397	-2.474938	2.682049

H	-2.658386	-3.360694	1.447068
O	0.037921	-0.084051	-2.947349
H	0.724255	-0.744153	-3.179789
H	0.377071	0.809134	-3.175820
O	-0.024590	0.076556	3.070320
H	-0.942825	-0.226886	3.238589
H	0.569446	-0.679133	3.267817
O	1.876284	-5.003925	0.105286
H	1.337833	-4.721790	0.873777
H	1.359611	-4.739707	-0.684412
O	-1.267688	3.848704	-2.159814
H	-0.841243	4.357077	-1.435469
H	-0.553500	3.328848	-2.589486
O	0.823253	2.507015	-3.397736
H	0.903103	2.782378	-4.323293
H	1.687996	2.756293	-2.955064
O	-3.621586	2.899361	1.300114
H	-3.640308	2.907665	0.310563
H	-4.285323	3.548997	1.579704
O	4.589776	0.942162	1.259291
H	3.997595	1.622991	1.641447
H	4.310741	0.059362	1.606630
O	-0.099874	5.244607	-0.064453
H	-0.321617	6.187888	-0.074211
H	-0.527449	4.861661	0.753379
O	2.664460	4.760457	-0.053256
H	1.705812	4.967551	-0.046957
H	2.814262	4.194481	0.733489
C	1.062350	1.739651	0.037082
H	2.155804	1.745263	0.039667
H	0.699038	2.771444	0.007782
H	0.694692	1.243792	0.940158
H	0.701125	1.198915	-0.842101
C	-2.059568	-0.067886	-0.012399
H	-2.499853	-1.066451	0.075158
H	-2.857447	0.668894	-0.129140
H	-1.481431	0.150911	0.889806
H	-1.396771	-0.037574	-0.882074
C	0.713043	-1.879864	0.106859
H	-0.051483	-2.662926	0.076689
H	1.700183	-2.336278	0.219506
H	0.513624	-1.214321	0.951285
H	0.672596	-1.301213	-0.820387

Table S65. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_3@(\text{H}_2\text{O})_{32}$ $5^{12}6^6$ - D_{3h} clathrate.

O	4.047393	-1.636690	-2.235084
H	4.118550	-2.279236	-1.496751
H	3.151002	-1.747515	-2.619560
O	4.863832	0.786607	-1.528890
H	4.522526	-0.107788	-1.814750
H	5.764667	0.851925	-1.880808
O	3.441853	3.042262	-2.291101
H	3.917469	2.214371	-2.060029

H	3.362521	3.542724	-1.452019
O	1.542919	-2.046245	-3.373447
H	1.642486	-2.203894	-4.324900
H	1.198904	-2.895169	-2.993310
O	-2.702097	-0.257807	-3.436807
H	-1.730546	-0.100736	-3.284569
H	-2.827538	-0.289965	-4.396760
O	-0.131081	0.116945	-2.875223
H	0.481586	-0.621994	-3.074740
H	0.330132	0.954212	-3.097499
O	1.044210	2.577552	-3.350363
H	1.948556	2.721181	-2.950626
H	1.127051	2.803699	-4.289159
O	-3.655501	-2.621436	-2.271532
H	-4.195626	-2.406421	-1.473039
H	-3.308019	-1.774802	-2.620274
O	0.738472	5.437877	0.136519
H	1.691634	5.171657	0.138741
H	0.723593	6.407313	0.137861
O	3.272648	4.471144	0.127653
H	3.382352	3.871498	0.910931
H	3.982897	5.128754	0.185450
O	-3.125502	3.924940	-1.439124
H	-3.636964	4.685922	-1.752738
H	-2.185189	4.088077	-1.727258
O	-0.604854	4.455883	-2.125914
H	-0.052945	3.761854	-2.548221
H	-0.102222	4.780045	-1.349934
O	-4.422002	1.574864	-2.229533
H	-3.782995	0.952097	-2.636569
H	-3.912885	2.375704	-1.984838
O	3.504149	2.770695	2.226004
H	4.012857	1.978979	1.881794
H	4.050838	3.152467	2.930290
O	4.916636	0.766156	1.247130
H	4.913442	0.771409	0.264555
H	4.636910	-0.133766	1.521600
O	4.216871	-1.800978	2.066312
H	4.271716	-2.422969	1.298325
H	4.891167	-2.098185	2.696609
O	-0.595819	4.324975	2.252885
H	-0.106895	4.762702	1.514803
H	-0.684655	4.998011	2.945364
O	0.998995	2.318560	3.379181
H	1.871840	2.401096	2.938999
H	0.417078	2.980631	2.949808
O	4.303793	-3.428286	-0.112272
H	3.553583	-4.095297	-0.116618
H	5.126926	-3.934626	-0.187851
O	2.245153	-5.075637	-0.105964
H	1.686403	-4.842820	-0.880150
H	1.724318	-4.835864	0.693169
O	-0.034519	-0.127009	3.694148
H	-0.079952	-0.174268	4.662457
H	0.344853	0.774996	3.506239
O	1.796161	-2.208138	3.373401
H	2.608796	-1.947748	2.890189
H	1.189771	-1.436605	3.376243

O	0.842960	-4.391096	2.187768
H	0.936517	-5.086131	2.856851
H	1.174005	-3.552480	2.616938
O	-1.767645	-4.402639	-1.470729
H	-1.783578	-4.393845	-0.482934
H	-2.407636	-3.712389	-1.774850
O	0.698254	-4.399593	-2.329765
H	-0.265924	-4.374501	-2.036821
H	0.761762	-5.106508	-2.990281
O	-3.652983	-2.692361	2.234940
H	-4.193432	-3.121037	2.915500
H	-3.305661	-1.852301	2.647727
O	-1.770977	-4.473637	1.247939
H	-0.876359	-4.339112	1.625499
H	-2.367453	-3.806500	1.649838
O	-3.179866	3.763238	1.333961
H	-3.154016	3.822383	0.353654
H	-2.264395	3.920965	1.647482
O	-4.352546	1.534736	2.187519
H	-4.986561	1.819018	2.863264
H	-3.887726	2.364051	1.883950
O	-2.804390	-0.437125	3.361140
H	-1.838294	-0.277092	3.325463
H	-3.249213	0.312284	2.907951
O	-5.721916	0.528698	-0.049265
H	-5.255047	0.909836	-0.830329
H	-5.268120	0.895568	0.738362
O	-5.203212	-2.165035	-0.056010
H	-4.652510	-2.330092	0.737781
H	-5.414813	-1.200909	-0.039056
C	1.444585	1.638262	0.021108
H	2.516521	1.455989	-0.097259
H	1.268844	2.711200	0.145489
H	1.082881	1.107794	0.905767
H	0.913681	1.279027	-0.864032
C	-2.130323	-0.535523	0.062971
H	-3.161598	-0.172802	0.039713
H	-1.536971	0.089884	0.736643
H	-2.118548	-1.568860	0.422918
H	-1.697450	-0.494330	-0.939893
C	0.912033	-1.954733	-0.011377
H	0.299212	-2.840888	-0.200020
H	1.967833	-2.239829	0.027016
H	0.619038	-1.515222	0.945719
H	0.752110	-1.224236	-0.808540

Table S66. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_4@(\text{H}_2\text{O})_{34}$ $5^{12}6^7\text{-C}_{3v}$ clathrate.

O	5.466167	1.364218	1.130611
H	5.226154	0.516094	1.607672
H	6.385665	1.559050	1.368496
O	3.748966	3.376473	1.795583
H	4.227447	4.026813	2.332203
H	4.403812	2.667209	1.576244

O	5.197592	0.999256	-1.619860
H	5.292031	1.134680	-0.651900
H	4.509088	1.633687	-1.918333
O	4.582826	-1.536058	-2.040717
H	5.225323	-1.854764	-2.693132
H	4.779845	-0.561601	-1.910180
O	2.083921	-2.322751	-3.025193
H	1.791189	-3.161776	-2.610597
H	2.915210	-2.040517	-2.589649
O	3.348728	2.869338	-2.504495
H	3.803939	3.389167	-3.184851
H	3.141216	3.510646	-1.766485
O	0.940280	2.162858	-3.648399
H	0.712030	1.218102	-3.512645
H	1.803352	2.323598	-3.207536
O	0.227100	-0.515829	-3.625443
H	0.905669	-1.168404	-3.298426
H	0.215824	-0.640365	-4.587760
O	0.147459	5.343500	-0.693432
H	0.127929	6.291055	-0.898002
H	-0.202605	4.883689	-1.497434
O	2.816271	4.563781	-0.532974
H	3.062047	4.158350	0.325854
H	1.869447	4.817536	-0.489293
O	-1.602247	4.886407	1.451217
H	-1.242462	4.200218	2.052795
H	-0.949004	5.005791	0.730768
O	-1.263223	-5.294435	-1.315152
H	-1.888176	-4.605288	-1.623941
H	-1.322112	-5.265020	-0.327311
O	1.265371	-4.807537	-2.023860
H	1.507144	-5.527113	-2.625953
H	0.308636	-4.961220	-1.773976
O	-1.445256	-5.181578	1.402503
H	-0.585259	-4.830600	1.716826
H	-2.116252	-4.506958	1.660763
O	-4.870524	-2.637025	-0.040031
H	-4.289245	-2.916646	-0.791068
H	-5.629462	-3.240279	-0.055413
O	-3.324651	-3.327585	2.175681
H	-2.951808	-2.545321	2.634021
H	-3.862204	-2.996789	1.426284
O	-2.432311	-1.161631	-3.222269
H	-1.489894	-0.889234	-3.209001
H	-2.981479	-0.394990	-2.946688
O	-3.211301	-3.405651	-2.074463
H	-3.745689	-3.831167	-2.763095
H	-2.864812	-2.562839	-2.487972
O	2.750256	-4.750093	0.320022
H	2.281977	-4.776790	-0.543345
H	3.440954	-4.055954	0.260032
O	4.765334	-2.817449	0.340119
H	4.763883	-2.357788	-0.537459
H	5.613665	-3.283986	0.395340
O	4.807803	-0.884861	2.367760
H	3.921942	-0.768473	2.778559
H	4.724396	-1.595039	1.696566
O	0.993012	-4.114442	2.201136

H	1.330963	-4.429713	3.052484
H	1.680022	-4.352112	1.516247
O	0.319251	-1.428721	2.392582
H	-0.546721	-1.376833	2.853456
H	0.500274	-2.381448	2.239993
O	2.392987	-0.386646	3.618453
H	2.411354	-0.677677	4.542458
H	1.591036	-0.818608	3.199549
O	-2.152496	-1.253782	3.624441
H	-2.147550	-1.465041	4.569989
H	-2.509900	-0.323904	3.547862
O	1.718085	2.277965	3.369621
H	2.382766	2.684979	2.775828
H	1.976547	1.335215	3.467793
O	-0.857069	2.973509	3.319743
H	0.089430	2.667727	3.277832
H	-0.936528	3.434156	4.169270
O	-3.044878	1.241183	3.466027
H	-2.283848	1.832039	3.283468
H	-3.717077	1.392024	2.767346
O	-5.070403	1.730400	1.611737
H	-5.899247	1.985862	2.043541
H	-5.313171	1.063670	0.910606
O	-5.723825	0.026798	-0.356816
H	-5.432328	-0.895727	-0.196765
H	-5.212465	0.321782	-1.143193
O	-0.791627	4.003247	-2.875300
H	-0.162111	3.270277	-3.139619
H	-0.862616	4.581814	-3.650176
O	-3.402352	3.273233	-2.226934
H	-2.462085	3.463685	-2.429559
H	-3.557561	3.535805	-1.284844
O	-4.253717	0.807681	-2.579257
H	-3.892677	1.734631	-2.454276
H	-4.840181	0.855479	-3.349720
O	-3.923336	3.958272	0.336747
H	-3.098687	4.253029	0.791385
H	-4.276189	3.187125	0.827253
C	-2.675429	-0.125856	0.505653
H	-2.875228	0.939964	0.356170
H	-2.688333	-0.636771	-0.462428
H	-3.449202	-0.549526	1.151095
H	-1.695575	-0.257263	0.971725
C	2.476053	0.223125	0.061037
H	1.679748	-0.138771	0.717110
H	2.806326	1.213190	0.391025
H	2.104385	0.292569	-0.966133
H	3.320379	-0.470018	0.093801
C	-0.251153	-2.333465	-0.646852
H	-1.093087	-2.602623	-0.002049
H	-0.080320	-1.256075	-0.587173
H	-0.472310	-2.617180	-1.679012
H	0.646450	-2.861402	-0.309799
C	-0.276728	2.123980	-0.359734
H	-1.141587	2.793778	-0.362041
H	0.615113	2.665789	-0.688342
H	-0.463564	1.287275	-1.040147
H	-0.117998	1.738989	0.651281

Table S67. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_4@(\text{H}_2\text{O})_{36}$ $5^{12}6^8$ clathrate.

O	-2.753603	-4.236670	-1.195370
H	-3.496872	-3.629439	-0.984907
H	-2.175653	-4.272722	-0.403323
O	2.628495	-3.328185	3.054781
H	3.388877	-2.851872	2.617639
H	3.026324	-3.868181	3.754934
O	2.520454	-1.134394	-4.221530
H	2.827043	-1.386495	-5.105569
H	1.993030	-1.909930	-3.881990
O	2.714390	4.450169	1.048906
H	3.038364	5.317345	1.336551
H	2.229247	4.609706	0.191373
O	4.891376	2.001464	-1.992851
H	5.705089	2.310639	-2.420072
H	4.150675	2.480231	-2.441385
O	2.774649	3.288966	-3.168420
H	3.072797	3.855430	-3.896803
H	2.208466	2.580405	-3.589200
O	-1.244325	-4.604737	1.128037
H	-1.588980	-5.465042	1.413923
H	-0.252622	-4.712098	1.127168
O	-1.545575	-3.391562	-3.401864
H	-1.742256	-4.075487	-4.060378
H	-1.979784	-3.699279	-2.555409
O	-1.392281	1.267648	-4.502853
H	-1.569336	1.535558	-5.417755
H	-1.843933	1.951853	-3.933588
O	2.547948	1.069373	3.967663
H	2.892048	1.297388	4.845549
H	3.346261	0.924632	3.398799
O	-1.409881	3.490369	3.482227
H	-1.525869	4.205979	4.125729
H	-0.428058	3.423061	3.329632
O	-1.307708	4.662283	-1.188437
H	-1.727252	4.502208	-0.298242
H	-1.574593	5.560717	-1.437494
O	4.731725	-2.767350	-0.805347
H	4.702344	-1.974664	-1.413402
H	5.581020	-3.201808	-0.979402
O	-2.673950	3.083973	-3.047968
H	-3.456893	2.687700	-2.608328
H	-2.174753	3.581629	-2.364969
O	4.685920	-2.075023	1.888262
H	4.649613	-1.098725	1.969133
H	4.701160	-2.274522	0.927437
O	1.219936	-3.271645	-3.336684
H	0.241299	-3.303755	-3.263540
H	1.605206	-3.693925	-2.540970
O	1.233622	3.382459	3.149501
H	1.683606	2.544402	3.387533
H	1.695191	3.740916	2.360923

O	-2.621865	-3.029404	2.972803
H	-2.124110	-2.404880	3.542226
H	-1.990385	-3.455855	2.357733
O	4.882274	2.715674	0.706017
H	4.112896	3.316325	0.818065
H	4.883787	2.448076	-0.238394
O	1.209498	-1.330943	4.398278
H	1.635842	-2.036941	3.866269
H	1.666369	-0.492215	4.175960
O	1.372064	1.383071	-4.355848
H	1.713794	0.466990	-4.274025
H	0.391762	1.333072	-4.331178
O	-2.780521	1.246964	4.485259
H	-2.213731	1.965134	4.133589
H	-2.226619	0.438942	4.526222
O	4.671770	-0.747560	-2.525083
H	3.906722	-0.838887	-3.134831
H	4.728647	0.199688	-2.279113
O	1.469825	4.879084	-1.271528
H	1.842580	4.309073	-1.977223
H	0.503571	4.708848	-1.237112
O	1.393951	-5.018120	1.207891
H	1.820160	-4.416727	1.857753
H	1.822130	-4.828828	0.346106
O	-1.430394	-1.209964	4.711386
H	-1.574206	-1.540831	5.611034
H	-0.444630	-1.235451	4.568752
O	2.638258	-4.472784	-1.247558
H	3.420801	-3.882858	-1.113221
H	2.989127	-5.298278	-1.615948
O	4.719357	0.677605	2.387775
H	5.519714	0.773904	2.927191
H	4.763304	1.415093	1.710917
O	-2.870692	-1.103300	-4.304170
H	-2.282861	-0.318722	-4.306745
H	-2.346150	-1.857518	-3.960192
O	-2.611142	4.294837	1.108460
H	-2.176579	3.985672	1.933193
H	-3.390643	3.717656	0.962172
O	-4.755894	-1.825442	1.778685
H	-3.967231	-2.246388	2.196452
H	-4.741042	-0.875177	2.046777
O	-5.042139	-0.615811	-2.721516
H	-5.027885	-1.277901	-1.996274
H	-4.256582	-0.808984	-3.290207
O	-4.936691	-2.563721	-0.739137
H	-5.736812	-3.109479	-0.778257
H	-4.879805	-2.228162	0.204944
O	-4.955896	1.911253	-1.961345
H	-5.721904	2.317572	-2.394869
H	-4.985843	0.938652	-2.206329
O	-4.858456	2.711973	0.644035
H	-5.666353	3.229810	0.780016
H	-4.907588	2.371286	-0.282785
O	-4.774082	0.754743	2.652126
H	-4.042603	0.954586	3.282547
H	-4.742518	1.432758	1.947477
C	-1.797100	-1.081130	-0.940001

H	-2.798486	-1.214812	-1.354303
H	-1.062254	-1.507186	-1.628362
H	-1.729985	-1.590806	0.025479
H	-1.596950	-0.014947	-0.802687
C	2.090412	1.491735	-0.374091
H	1.112952	1.220771	-0.783131
H	2.408338	2.443650	-0.802022
H	2.819816	0.715650	-0.621229
H	2.017992	1.589310	0.713166
C	1.495926	-1.716254	0.680300
H	0.698586	-2.233247	1.221403
H	1.078029	-1.218582	-0.197832
H	2.253882	-2.436844	0.364642
H	1.958489	-0.972308	1.335434
C	-0.809694	0.583274	2.048421
H	-1.399193	-0.318087	2.238057
H	-1.475805	1.400984	1.759114
H	-0.098576	0.388034	1.244385
H	-0.263366	0.859407	2.955159

Table S68. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_5@(\text{H}_2\text{O})_{36}$ 5¹²6⁸ clathrate.

O	2.875238	-3.444004	-3.221904
H	3.634577	-3.049832	-2.740246
H	2.423940	-2.688447	-3.659247
O	-2.009561	1.391425	-3.937203
H	-2.920760	1.258805	-3.550396
H	-2.098460	1.255836	-4.892826
O	-3.222073	-4.231292	0.691194
H	-3.539356	-5.140550	0.805599
H	-2.600596	-4.263053	-0.087933
O	-2.503794	3.089804	2.847508
H	-2.666920	3.422807	3.742802
H	-1.965779	2.249291	2.948499
O	-5.169921	-0.522923	2.172666
H	-5.912248	-0.545989	2.796408
H	-4.369817	-0.759511	2.705119
O	-2.948742	-1.124260	3.653461
H	-3.169097	-1.108769	4.597539
H	-2.606390	-2.047909	3.461875
O	1.549193	-1.274172	-4.357294
H	1.237253	-1.427067	-5.261913
H	0.732044	-1.106935	-3.807429
O	1.128303	-4.544523	-1.496069
H	1.196806	-5.491172	-1.696547
H	1.760346	-4.101880	-2.128244
O	0.702177	-3.630242	3.273882
H	0.915415	-4.266212	3.974022
H	1.092602	-2.766906	3.575133
O	-2.265117	4.822082	-1.159233
H	-2.632842	5.703213	-1.327730
H	-3.042517	4.221889	-1.052382
O	1.663176	4.578859	1.618852
H	1.949658	5.492906	1.769277
H	0.673641	4.629393	1.511204

O	1.084105	1.199165	4.594688
H	1.718943	1.891446	4.258468
H	0.905487	1.417328	5.521496
O	-5.082293	-1.534496	-2.152769
H	-5.239417	-1.904950	-1.237387
H	-5.849924	-1.795271	-2.684401
O	1.960129	-1.428484	4.151277
H	2.805108	-1.315944	3.664292
H	1.614214	-0.525409	4.311655
O	-4.413425	1.106751	-2.839725
H	-4.436690	1.741622	-2.090623
H	-4.627108	0.219685	-2.482773
O	-1.671422	-4.378531	-1.474977
H	-0.695387	-4.287817	-1.465230
H	-2.015057	-3.736595	-2.131901
O	-0.985901	4.863319	1.353763
H	-1.355020	4.825991	0.446472
H	-1.521400	4.234432	1.885840
O	3.134588	1.032921	-4.118145
H	2.579834	1.743932	-3.735527
H	2.552775	0.250277	-4.221152
O	-4.775285	2.206780	1.551074
H	-3.989569	2.492082	2.069056
H	-4.882382	1.243571	1.700783
O	-0.840527	3.841385	-3.392258
H	-1.295225	2.989891	-3.576074
H	-1.275732	4.207390	-2.593713
O	-2.072618	-3.552207	3.122070
H	-2.392066	-3.789748	2.224080
H	-1.090352	-3.569518	3.099084
O	3.044290	3.926388	-0.728910
H	2.468968	4.077695	0.050279
H	2.471340	3.681075	-1.485222
O	-5.466275	-2.580048	0.276549
H	-4.698267	-3.171813	0.431673
H	-5.384917	-1.860392	0.939665
O	-1.146551	0.852316	2.960168
H	-1.712336	0.116857	3.280397
H	-0.365568	0.913915	3.550580
O	-0.603360	-0.746444	-2.876231
H	-1.004678	0.086561	-3.207675
H	-1.323010	-1.405097	-2.970085
O	1.777261	3.318544	-3.135235
H	2.180579	3.991943	-3.704671
H	0.796588	3.484958	-3.193880
O	-2.754344	-2.496737	-3.185284
H	-3.612464	-2.162521	-2.822526
H	-2.929441	-2.772668	-4.097398
O	-4.417847	3.101165	-0.915557
H	-5.223308	3.609318	-1.100232
H	-4.541585	2.730360	0.006047
O	2.240982	-4.442568	1.056231
H	1.638805	-4.129905	1.763781
H	1.743440	-4.411823	0.211676
O	2.820803	3.029986	3.659908
H	2.381263	3.551734	2.953911
H	3.528888	2.520076	3.210112
O	5.259330	0.350438	-2.465463

H	4.511883	0.610840	-3.052747
H	5.168272	0.912808	-1.660558
O	4.450700	-2.853664	0.821646
H	4.585802	-2.578745	-0.110719
H	3.632893	-3.406586	0.856392
O	5.031977	-2.247705	-1.846530
H	5.889593	-2.648155	-2.054440
H	5.119594	-1.276002	-2.065002
O	4.382978	-1.137331	2.816916
H	5.066268	-1.479513	3.414023
H	4.408943	-1.731961	2.009492
O	4.837792	1.519982	2.420489
H	5.700351	1.697598	2.826023
H	4.674390	0.552801	2.548198
O	5.029705	2.078930	-0.336275
H	4.306065	2.733423	-0.480380
H	4.967354	1.820235	0.605389
C	2.364590	-0.870001	-1.282507
H	1.467948	-0.250283	-1.355565
H	2.918703	-0.809125	-2.218384
H	2.065532	-1.905991	-1.100261
H	2.997354	-0.522822	-0.460538
C	-0.098848	-1.948647	0.834792
H	-0.631059	-1.465858	1.659103
H	-0.279259	-1.390470	-0.088527
H	-0.458559	-2.975400	0.713911
H	0.973327	-1.958404	1.049939
C	1.687352	1.178054	1.417291
H	2.486110	1.652472	0.838464
H	1.091794	0.535570	0.769506
H	1.041376	1.942999	1.853238
H	2.130756	0.572987	2.214041
C	-2.959822	-0.490090	-0.010642
H	-3.970077	-0.105182	-0.170197
H	-2.358615	-0.351053	-0.913526
H	-3.006876	-1.556277	0.231129
H	-2.490835	0.045713	0.819772
C	-0.896683	2.035618	-0.611670
H	-0.223803	2.885110	-0.759261
H	-0.440242	1.125242	-1.010871
H	-1.840796	2.214650	-1.135459
H	-1.089906	1.902328	0.456521

Table S69. M06-2X/6-31+G*/PCM optimized Cartesian coordinates of the $(\text{CH}_4)_6@(\text{H}_2\text{O})_{36}$ $5^{12}6^8$ clathrate.

O	2.564605	4.874804	-0.804437
H	3.327419	4.268471	-0.681402
H	2.040378	4.801383	0.022538
O	-2.439355	2.599383	3.585459
H	-3.158769	2.133679	3.075416
H	-2.905699	3.166263	4.219838
O	-2.632223	1.667456	-3.852899
H	-3.048443	1.935433	-4.686951
H	-2.226571	2.500984	-3.483547

O	-2.527020	-4.605419	0.582412
H	-2.660747	-5.538415	0.807898
H	-2.049735	-4.596623	-0.293907
O	-4.920539	-1.961420	-2.024537
H	-5.724309	-2.193774	-2.514599
H	-4.166634	-2.312143	-2.559266
O	-2.740694	-2.861235	-3.466714
H	-3.006855	-3.407580	-4.222410
H	-2.255044	-2.081386	-3.857506
O	1.206848	4.646247	1.653027
H	1.402470	5.465685	2.133388
H	0.213337	4.580596	1.647455
O	1.116051	3.958893	-2.880605
H	1.296437	4.603635	-3.582585
H	1.636036	4.281584	-2.093152
O	1.269431	-0.734729	-4.868022
H	1.502469	-0.856663	-5.800840
H	1.761997	-1.441641	-4.368810
O	-2.399062	-1.848191	4.179451
H	-2.702543	-2.429329	4.893761
H	-3.194014	-1.675343	3.618218
O	1.738788	-4.008890	2.883915
H	1.731983	-4.725999	3.535691
H	0.785390	-3.807005	2.692490
O	1.519449	-4.408449	-1.721890
H	2.042367	-4.462637	-0.876245
H	1.687206	-5.252787	-2.169199
O	-4.910467	2.576778	-0.226796
H	-4.851538	1.898680	-0.957816
H	-5.822760	2.904923	-0.238383
O	2.682907	-2.617477	-3.552577
H	3.408095	-2.184605	-3.052132
H	2.211901	-3.177440	-2.899280
O	-4.415345	1.414698	2.246830
H	-4.428048	0.435417	2.208004
H	-4.579267	1.756692	1.341554
O	-1.667840	3.985262	-2.919709
H	-0.697182	3.965028	-2.773733
H	-2.086288	4.214477	-2.062975
O	-0.813285	-3.358291	2.395600
H	-1.333906	-2.805484	3.013791
H	-1.443733	-3.783239	1.776092
O	2.464512	2.753724	3.332152
H	1.929321	2.023983	3.707032
H	1.890071	3.295458	2.753248
O	-4.886746	-3.106120	0.569620
H	-4.083252	-3.671390	0.554246
H	-4.930501	-2.684027	-0.314585
O	-1.327549	0.573018	5.196480
H	-1.698011	1.280018	4.624382
H	-1.701448	-0.266601	4.854335
O	-1.508999	-0.781356	-4.598525
H	-1.782464	0.097605	-4.262387
H	-0.527660	-0.781703	-4.638082
O	2.860568	-1.659039	4.033453
H	2.387855	-2.427257	3.651722
H	2.201836	-0.952447	4.195298
O	-4.734063	0.839347	-2.229150

H	-3.962255	1.047583	-2.799243
H	-4.740500	-0.130139	-2.082498
O	-1.272150	-4.543649	-1.773676
H	-1.673172	-3.880763	-2.375054
H	-0.311912	-4.354590	-1.711825
O	-1.463114	4.551040	1.811475
H	-1.774396	3.816770	2.383396
H	-1.997439	4.519628	0.989971
O	1.339852	0.606082	4.763897
H	1.726939	0.787285	5.634301
H	0.356204	0.578844	4.913023
O	-3.044031	4.578358	-0.528296
H	-3.741603	3.884786	-0.432031
H	-3.514538	5.423606	-0.591335
O	-4.553323	-1.347032	2.549250
H	-5.366968	-1.434212	3.070172
H	-4.658481	-1.982032	1.784010
O	2.375307	1.746774	-4.085088
H	1.865667	0.934357	-4.285125
H	1.785302	2.380806	-3.628708
O	3.063791	-4.704319	0.478847
H	2.590120	-4.493804	1.312297
H	3.782392	-4.040115	0.408655
O	4.724528	1.949115	1.979809
H	3.903613	2.203875	2.462507
H	4.762612	0.964964	2.010254
O	4.503794	1.186199	-2.461060
H	4.527818	1.828884	-1.719242
H	3.711582	1.401231	-3.009405
O	4.720117	3.088470	-0.433775
H	5.583448	3.520881	-0.516510
H	4.719237	2.643074	0.462039
O	4.778758	-1.420621	-2.151980
H	5.571584	-1.601074	-2.680812
H	4.661270	-0.426215	-2.182473
O	5.074587	-2.723247	0.247941
H	5.975373	-3.081321	0.240777
H	4.971295	-2.236823	-0.605809
O	4.867516	-0.786356	2.323230
H	4.133488	-1.089520	2.905735
H	4.913180	-1.429806	1.587444
C	1.970956	1.808183	-0.021097
H	1.103205	1.370971	0.476868
H	2.357283	2.620919	0.592685
H	1.669495	2.189022	-1.001436
H	2.743932	1.046336	-0.150878
C	0.672358	-0.415212	-1.996079
H	0.347766	-1.390976	-2.368913
H	0.513563	-0.370509	-0.919073
H	0.091866	0.376729	-2.480439
H	1.736041	-0.271762	-2.204645
C	2.089815	-1.746426	0.698360
H	2.731681	-2.273367	1.401519
H	1.892933	-0.743976	1.082964
H	1.145837	-2.290720	0.591825
H	2.587356	-1.674386	-0.273788
C	-1.721926	1.903730	-0.336146
H	-2.277748	1.913558	0.606628

H	-1.011026	2.734364	-0.353746
H	-2.418561	1.994923	-1.172744
H	-1.182001	0.962549	-0.424984
C	-2.256954	-1.502598	-0.611355
H	-2.727958	-2.458470	-0.834012
H	-2.888081	-0.927244	0.073138
H	-2.116080	-0.941921	-1.540787
H	-1.286136	-1.688905	-0.146210
C	-0.664279	0.073750	2.230931
H	-0.185107	-0.583506	2.959523
H	-0.379815	1.113720	2.417613
H	-1.752072	-0.023540	2.305669
H	-0.352003	-0.221461	1.229516

Table S70. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₆ hollow clathrate in the decahedron 4²⁵₈ configuration.

O	-0.659167	1.838198	2.556905
H	-0.200714	0.985139	2.769836
H	-1.571514	1.587448	2.280682
O	-0.666768	2.670409	-1.796043
H	-0.192004	2.904101	-0.956169
H	-0.713522	3.497992	-2.309102
O	3.198710	-1.912018	-0.363229
H	2.325869	-2.366665	-0.423927
H	3.220136	-1.484581	0.523880
O	0.668655	-0.537705	3.129306
H	0.237942	-1.300015	2.679114
H	1.579543	-0.488013	2.756666
O	3.235664	0.297294	-1.969554
H	3.269709	-0.567724	-1.473155
H	4.004610	0.299308	-2.568063
O	-3.205247	-1.591175	1.128581
H	-3.237596	-1.570130	0.144227
H	-2.336934	-1.996419	1.359118
O	3.234677	-0.296204	1.970844
H	4.003462	-0.297701	2.569547
H	3.268289	0.568797	1.474350
O	-3.205715	1.590734	-1.128501
H	-2.337120	1.995369	-1.359324
H	-3.237734	1.569406	-0.144111
O	-0.658144	-1.838003	-2.557150
H	-1.570613	-1.587387	-2.281300
H	-0.199770	-0.984948	-2.770269
O	3.197355	1.912989	0.364613
H	2.324389	2.367498	0.424607
H	3.219655	1.485813	-0.522587
O	-3.235276	1.088293	1.661748
H	-3.265738	0.094674	1.573471
H	-3.992993	1.335225	2.222490
O	-3.234821	-1.089268	-1.661990
H	-3.992400	-1.335992	-2.223008
H	-3.265527	-0.095732	-1.573250

O	0.661078	3.148222	0.594689
H	0.717077	4.085627	0.856459
H	0.162896	2.688707	1.333620
O	0.662916	-3.148125	-0.595432
H	0.719572	-4.085249	-0.858073
H	0.164369	-2.688395	-1.333978
O	-0.666410	-2.671378	1.794774
H	-0.190968	-2.904847	0.955237
H	-0.711628	-3.498661	2.308438
O	0.669999	0.537624	-3.129501
H	0.238622	1.299852	-2.679847
H	1.580577	0.488413	-2.756063

Table S71. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₆ hollow clathrate in the decahedron 4³5⁶6¹ configuration.

O	2.383151	1.257924	2.149119
H	2.965543	1.603199	2.850449
H	2.162028	2.038319	1.577259
O	-3.658424	-0.205942	0.556898
H	-3.285805	-1.129749	0.658903
H	-4.615586	-0.278415	0.726197
O	1.578596	2.166801	-2.199536
H	1.755589	2.540182	-1.306151
H	1.971115	1.262055	-2.198242
O	1.228671	-2.629454	-1.961570
H	0.249999	-2.520843	-2.015061
H	1.422205	-2.909684	-1.037369
O	2.767390	-0.385466	-2.149410
H	2.174221	-1.187629	-2.184232
H	3.437235	-0.517649	-2.844815
O	-2.226108	1.589672	2.098089
H	-2.801421	0.956596	1.594266
H	-2.800208	1.978158	2.783452
O	-1.138952	2.383807	-2.314100
H	-0.150548	2.260836	-2.375925
H	-1.382528	2.973205	-3.050952
O	3.544064	-0.783088	0.559493
H	3.167593	-0.056642	1.109144
H	3.369620	-0.530615	-0.376439
O	-2.473787	-2.645940	0.615753
H	-1.677791	-2.621235	1.208810
H	-2.121573	-2.696851	-0.301976
O	-1.073119	3.464388	0.315158
H	-1.505361	2.827956	0.931670
H	-1.242394	3.118009	-0.591425
O	-0.273913	-2.520117	2.290389
H	-0.164974	-1.587219	2.602995
H	0.546385	-2.726193	1.786111
O	-2.749285	0.080239	-2.125609
H	-3.132263	0.118833	-1.219501
H	-2.165252	0.870612	-2.207172
O	1.641899	3.286261	0.420036
H	2.044644	4.164284	0.550389
H	0.653004	3.424068	0.463107

O	-1.575537	-2.384277	-2.082313
H	-1.966116	-1.474150	-2.202912
H	-1.985239	-2.944126	-2.766634
O	-0.029288	0.122705	3.160396
H	0.793512	0.544554	2.822319
H	-0.773172	0.661778	2.806356
O	2.034302	-3.055771	0.726852
H	2.574794	-3.827724	0.974614
H	2.645471	-2.267846	0.755607

Table S72. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₇ hollow clathrate in the undecahedron 4⁴5⁶6¹ configuration.

O	1.879351	1.578956	1.784797
H	1.826694	0.666184	2.161285
H	2.730436	1.577883	1.289070
O	-0.546325	-3.422637	0.073678
H	-1.309414	-3.061258	-0.433626
H	0.259200	-3.178212	-0.438090
O	-2.772094	-2.287600	-1.251016
H	-3.245940	-1.702377	-0.592111
H	-3.436818	-2.920869	-1.578288
O	1.810579	-2.683894	-1.334237
H	2.256870	-3.434922	-1.766250
H	2.472517	-2.310982	-0.686064
O	-3.311694	1.581111	-1.393503
H	-2.712893	1.075169	-1.987170
H	-2.752783	2.265292	-0.957315
O	2.432644	1.610979	-2.410774
H	1.936013	0.794428	-2.706877
H	2.801710	2.014520	-3.217305
O	-1.779637	-0.303109	-2.939133
H	-2.144663	-1.085508	-2.451563
H	-2.132701	-0.374502	-3.845307
O	-2.287432	-0.078700	2.711296
H	-2.786384	-0.038967	3.547582
H	-1.781579	0.777710	2.660482
O	3.526563	-1.597815	0.486449
H	3.766532	-0.677627	0.231012
H	3.021606	-1.497193	1.327191
O	-0.901321	2.290454	2.479137
H	-1.255591	2.757792	1.686945
H	0.053043	2.160424	2.297688
O	-3.908983	-0.460871	0.406054
H	-3.370790	-0.317852	1.219004
H	-3.755586	0.338938	-0.157859
O	1.944263	-1.058656	2.758868
H	2.297850	-1.181364	3.658645
H	1.057192	-1.524823	2.740953
O	0.891481	3.005976	-0.521537
H	1.340145	2.596757	-1.297378
H	1.151705	2.445781	0.241494
O	1.048173	-0.615030	-3.095843
H	0.071434	-0.508240	-3.017897
H	1.290728	-1.361753	-2.498502

O	-0.470581	-2.249336	2.590749
H	-0.533206	-2.662101	1.691501
H	-1.140124	-1.526782	2.611887
O	3.962512	1.149740	-0.120791
H	4.866989	1.509977	-0.165982
H	3.546579	1.338314	-0.999678
O	-1.720550	3.448993	0.004286
H	-1.971964	4.389096	-0.046114
H	-0.792393	3.388574	-0.349197

Table S73. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₈ hollow clathrate in the undecahedron 4²5⁸6¹ configuration.

O	2.293037	-2.386130	1.642592
H	1.486115	-2.817253	1.252819
H	2.756137	-3.092087	2.130520
O	-2.427218	-1.258536	-2.597573
H	-3.006501	-1.424689	-1.819243
H	-2.357701	-0.277031	-2.643087
O	2.292099	1.599906	-2.520042
H	2.906162	1.665557	-1.753567
H	2.216883	0.632330	-2.688683
O	-2.234296	2.162164	2.023730
H	-1.450555	2.653131	1.662425
H	-2.661509	2.775920	2.649054
O	-2.150544	-2.420369	1.715110
H	-1.885360	-1.636910	2.261596
H	-2.811650	-2.082041	1.066677
O	2.262600	-1.233226	-2.782843
H	2.633270	-1.617208	-3.598040
H	1.407719	-1.724395	-2.614293
O	-2.404412	1.584677	-2.493622
H	-2.809688	2.070765	-3.234513
H	-1.541434	2.052004	-2.301295
O	2.216507	2.175744	1.910423
H	2.851140	1.928277	1.196702
H	2.000021	1.335316	2.377363
O	0.022243	-3.453266	0.484597
H	-0.039934	-4.423648	0.555753
H	-0.794872	-3.095352	0.942880
O	-0.015518	-2.592193	-2.230285
H	-0.020104	-2.898227	-1.293966
H	-0.864402	-2.097000	-2.357112
O	-0.097743	2.868497	-1.876971
H	-0.048220	3.056666	-0.911397
H	0.743098	2.395767	-2.103431
O	-3.969046	-1.411288	-0.199769
H	-4.882169	-1.751077	-0.182932
H	-4.038422	-0.421515	-0.090043
O	3.940299	1.439636	-0.192945
H	4.009790	0.444007	-0.218540
H	4.854828	1.775685	-0.175090
O	-0.002604	3.382873	0.922456
H	0.079471	4.334490	1.117784

H	0.823665	2.958747	1.295299
O	3.866212	-1.271052	-0.448311
H	3.327862	-1.366534	-1.268966
H	3.332800	-1.685666	0.268616
O	-3.905483	1.311024	-0.103529
H	-3.404124	1.511977	-0.928334
H	-3.340275	1.635614	0.635825
O	1.504742	-0.233522	3.227682
H	1.811733	-1.022369	2.711330
H	1.898895	-0.331280	4.113908
O	-1.340089	-0.246777	3.248554
H	-0.356207	-0.211275	3.261755
H	-1.632730	0.604011	2.848203

Table S74. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₁₉ hollow clathrate in the undecahedron 4²5¹⁰ configuration.

O	1.969578	-2.058135	-2.370883
H	2.721562	-1.537163	-1.990333
H	1.659411	-2.648270	-1.643785
O	2.349258	2.040960	2.147684
H	1.491437	1.811266	2.609483
H	2.838292	2.612763	2.767654
O	-1.015058	3.677045	-0.351654
H	-0.017403	3.636594	-0.280762
H	-1.234771	4.613454	-0.510444
O	3.914498	-0.316107	-1.399245
H	3.474499	0.499492	-1.726559
H	3.859191	-0.273220	-0.416694
O	1.671006	3.394086	-0.239556
H	1.943208	2.913057	0.577117
H	1.901390	2.806637	-0.995562
O	-1.704006	1.997642	-2.527358
H	-0.994115	1.331743	-2.629873
H	-1.423634	2.585024	-1.787271
O	2.251204	1.748378	-2.473767
H	1.504849	1.185458	-2.790749
H	2.549615	2.253051	-3.252655
O	-3.821611	0.332772	-1.722283
H	-3.175284	1.026720	-1.998923
H	-3.379588	-0.498916	-2.024633
O	-2.219614	-1.785465	-2.604814
H	-1.400050	-1.275950	-2.775934
H	-2.011909	-2.374238	-1.834860
O	1.089547	-3.684581	-0.234548
H	1.420233	-3.268800	0.611646
H	1.433516	-4.596347	-0.235198
O	-2.159102	2.495288	1.877883
H	-1.783116	2.980211	1.097601
H	-2.658118	3.161745	2.384994
O	-3.755993	0.284287	1.052347
H	-3.222681	1.066619	1.323353
H	-3.796619	0.315973	0.060721
O	0.000456	1.387620	3.332310

H	-0.768816	1.765436	2.844777
H	-0.146506	0.413149	3.355328
O	-0.351589	-1.424331	3.372786
H	-1.183259	-1.665288	2.886104
H	-0.468525	-1.770481	4.276653
O	0.224136	-0.163343	-3.178912
H	0.838769	-0.905285	-2.890537
H	0.208820	-0.209729	-4.154174
O	3.657256	-0.296125	1.430749
H	3.241393	0.554116	1.729801
H	4.504876	-0.354228	1.908784
O	1.925242	-2.461619	2.045606
H	2.521499	-1.699625	1.858032
H	1.150856	-2.089196	2.528383
O	-1.717777	-3.416806	-0.416933
H	-2.020506	-2.959678	0.401288
H	-0.747151	-3.547769	-0.308334
O	-2.616663	-2.022616	1.891698
H	-3.298933	-2.516265	2.382858
H	-3.058570	-1.173661	1.593826

Table S75. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₀ hollow clathrate in the regular dodecahedron 5¹² configuration.

O	-1.638592	-3.482380	-0.409326
H	-0.900218	-3.537482	0.239947
H	-1.224521	-3.191859	-1.262696
O	2.647635	0.525845	-2.785015
H	2.956419	0.957050	-1.954738
H	1.796216	0.975792	-3.026816
O	-3.562384	0.366375	-1.554931
H	-3.568700	-0.342344	-0.869767
H	-3.321703	1.198598	-1.082844
O	0.434951	2.673478	2.809885
H	0.883650	2.987145	1.991416
H	0.904855	1.848266	3.073499
O	0.482166	-3.594691	1.487829
H	1.332492	-3.338660	1.046735
H	0.628446	-4.493854	1.834909
O	-2.256409	2.176150	2.335359
H	-1.294356	2.332816	2.516809
H	-2.413211	1.219581	2.509602
O	2.244553	-2.117403	-2.407738
H	2.415479	-1.141378	-2.563478
H	2.799258	-2.588495	-3.056503
O	-0.211561	-1.696405	3.470499
H	0.009513	-2.371307	2.787186
H	-1.094928	-1.337295	3.220973
O	-1.792575	-0.224268	-3.534700
H	-2.466139	-0.003629	-2.830541
H	-2.289274	-0.263580	-4.372140
O	-0.424119	3.598047	-1.530720

H	0.280007	3.617028	-0.842858
H	-1.250030	3.334152	-1.062338
O	-2.728913	-0.591846	2.772258
H	-3.066026	-1.012402	1.938428
H	-3.408733	-0.769679	3.447931
O	3.539569	1.698284	-0.356633
H	3.567790	0.973070	0.332184
H	4.451630	2.036550	-0.420706
O	-0.523094	-2.644615	-2.807243
H	0.435214	-2.443664	-2.700681
H	-0.945099	-1.800533	-3.092302
O	3.549839	-0.291874	1.485421
H	3.287134	-1.148269	1.075479
H	2.905290	-0.130075	2.214798
O	0.263236	1.740480	-3.495246
H	-0.005170	2.398977	-2.806073
H	-0.464006	1.077001	-3.524405
O	-3.529700	-1.714409	0.367405
H	-4.376771	-2.195372	0.406109
H	-2.846251	-2.390555	0.083478
O	1.657267	3.590852	0.407288
H	2.099418	4.452634	0.516479
H	2.371117	2.958520	0.132724
O	2.809967	-2.730237	0.226549
H	3.541511	-3.374738	0.245714
H	2.642501	-2.545678	-0.736099
O	-2.815384	2.759991	-0.252815
H	-3.515735	3.437743	-0.258028
H	-2.633007	2.567162	0.712186
O	1.690960	0.243668	3.541154
H	2.083099	0.240469	4.433352
H	0.993536	-0.472045	3.548835

Table S76. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₀ hollow clathrate in the irregular dodecahedron 4³5⁶6³ configuration.

O	1.063194	-1.865457	-3.087217
H	0.302049	-2.378964	-2.730578
H	1.807181	-1.994950	-2.454928
O	2.192177	2.377446	-2.175915
H	1.565101	1.808269	-2.712908
H	2.709169	2.882488	-2.830470
O	-2.886825	0.137030	2.505835
H	-2.046379	-0.213613	2.883065
H	-3.164244	-0.501251	1.807385
O	-1.684476	-3.701570	0.448926
H	-0.962539	-3.476757	1.081255
H	-2.408749	-3.057641	0.625319
O	-2.592615	2.715596	1.713783
H	-2.735659	1.767228	1.994286
H	-3.281658	3.235271	2.166041
O	2.977081	-2.480657	1.305672
H	3.192214	-1.580737	1.643935

H	2.070692	-2.683867	1.635113
O	-3.245522	-1.200846	-2.084406
H	-2.537354	-1.859075	-2.272441
H	-2.876522	-0.320164	-2.331026
O	3.953209	0.626845	-0.808896
H	3.331575	1.233404	-1.275708
H	3.758282	-0.276861	-1.149060
O	1.371682	1.191270	3.274122
H	2.152064	0.915532	2.739454
H	0.980520	1.980519	2.820853
O	-2.203105	1.307177	-2.862018
H	-2.715349	1.667790	-3.608729
H	-2.196503	2.027762	-2.170575
O	3.300315	-2.079191	-1.375197
H	3.155670	-2.332149	-0.421028
H	3.996424	-2.674723	-1.707343
O	3.622697	0.227213	1.870006
H	4.463420	0.422057	2.322655
H	3.761676	0.481169	0.914990
O	0.497509	0.804934	-3.577945
H	-0.445536	0.961714	-3.337921
H	0.673022	-0.152926	-3.390874
O	-0.446649	-0.777827	3.622852
H	-0.536680	-0.901844	4.585705
H	0.235085	-0.051952	3.507955
O	0.378532	-3.068086	2.292975
H	0.085728	-2.272936	2.811155
H	0.451995	-3.787520	2.947019
O	0.625643	4.047869	-0.610776
H	1.222599	3.483829	-1.168811
H	0.871670	4.969849	-0.809038
O	-1.249385	-3.222595	-2.204278
H	-1.327761	-3.475527	-1.242445
H	-1.446299	-4.031872	-2.710067
O	0.135756	3.399091	2.123517
H	0.408821	3.629696	1.207021
H	-0.825442	3.195456	2.052737
O	-2.086559	3.295487	-1.006951
H	-2.354371	3.055664	-0.089284
H	-1.154367	3.603617	-0.925274
O	-3.712745	-1.714791	0.552588
H	-4.637660	-2.000891	0.663614
H	-3.621205	-1.446607	-0.404461

Table S77. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₂ hollow clathrate in the tridecahedron 4¹⁵8⁶2 configuration.

O	1.947493	-3.764351	0.354454
H	2.221841	-3.188929	1.106399
H	2.282894	-3.318025	-0.456588
O	-1.722034	-3.022190	-2.094723
H	-1.391574	-3.409986	-1.231037
H	-1.939399	-3.788535	-2.657153
O	-1.786392	2.995290	1.989588

H	-1.359852	3.379751	1.188505
H	-1.082746	2.497499	2.468702
O	2.666234	2.365625	2.169878
H	2.436562	2.872833	1.357670
H	1.808305	2.144305	2.601331
O	-4.002699	1.606508	1.263986
H	-3.194084	2.107492	1.569726
H	-4.765923	2.066512	1.658090
O	2.791877	1.964896	-2.310025
H	1.956265	1.675009	-2.747301
H	2.524703	2.601243	-1.606198
O	0.202534	-1.070895	3.545471
H	1.034561	-1.457314	3.183095
H	-0.539984	-1.569080	3.130090
O	0.438359	-1.645754	-3.310260
H	-0.313408	-2.106936	-2.869635
H	1.255547	-1.960062	-2.857685
O	-1.623400	2.660741	-2.448100
H	-0.955418	2.038442	-2.819011
H	-2.400354	2.113522	-2.168357
O	-1.921239	-2.564571	2.423114
H	-2.299541	-3.153519	3.101397
H	-2.694103	-2.046206	2.060486
O	2.823752	-2.457348	-2.016558
H	3.352369	-1.647766	-1.791328
H	3.404068	-2.999879	-2.581444
O	0.427858	1.061483	-3.570486
H	0.459109	1.219693	-4.531785
H	0.390255	0.068770	-3.468297
O	-0.813524	-4.014974	0.250887
H	-1.183009	-3.522420	1.020757
H	0.171464	-3.916040	0.310534
O	-0.673773	4.102732	-0.368135
H	-0.963807	5.023712	-0.502515
H	-1.030319	3.588741	-1.151270
O	2.067559	3.756079	-0.236735
H	1.094948	3.947772	-0.292926
H	2.509921	4.621454	-0.311961
O	-3.983109	-1.539974	-1.481770
H	-3.194878	-2.082473	-1.746839
H	-4.751571	-1.968693	-1.900762
O	2.634698	-2.079408	2.523229
H	3.173798	-1.309312	2.179505
H	3.189839	-2.508769	3.199453
O	-3.880716	1.307037	-1.562982
H	-3.893345	0.326750	-1.645027
H	-3.968909	1.476418	-0.596688
O	-4.024683	-1.218753	1.342467
H	-4.001233	-0.236273	1.417513
H	-4.053970	-1.396138	0.373883
O	0.229030	1.645792	3.435315
H	0.213409	1.939372	4.364551
H	0.183135	0.648647	3.471635
O	4.028513	0.028945	1.542162
H	3.550297	0.873280	1.746201
H	4.087889	-0.014623	0.559810
O	4.163479	-0.141587	-1.294289
H	3.679652	0.644236	-1.681766

H 5.078051 -0.077069 -1.625667

Table S78. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₄ hollow clathrate in the tetradecahedron 5¹²6² configuration.

O	1.988800	-1.951760	-3.045629
H	2.394140	-2.292692	-3.863871
H	2.209194	-0.977628	-3.027759
O	4.355608	1.241679	-0.755565
H	5.248212	1.526165	-1.024782
H	3.984711	1.993346	-0.223059
O	2.669220	0.677588	-2.965582
H	3.247614	0.902106	-2.200036
H	1.958631	1.361345	-2.981901
O	4.311179	-1.157983	0.765716
H	3.762282	-0.980608	1.564747
H	4.342777	-0.308936	0.267826
O	2.685027	-0.726508	3.051648
H	1.957068	-1.410224	3.033336
H	3.175563	-0.893098	3.877223
O	-1.102173	-4.391711	-0.759630
H	-1.300107	-5.307436	-1.028849
H	-0.266410	-4.445039	-0.225962
O	-0.745620	-2.647875	-2.968122
H	-0.840780	-3.261982	-2.203383
H	0.201863	-2.374510	-2.983851
O	1.219424	-4.346486	0.741121
H	1.947535	-3.933764	0.188447
H	1.555822	-5.220103	1.013140
O	3.136929	-3.165971	-0.747077
H	2.752396	-2.739184	-1.548186
H	3.561238	-2.434920	-0.228299
O	1.908263	1.987905	2.963807
H	2.152882	1.032672	2.969563
H	2.368875	2.389419	2.190416
O	0.766344	-2.649342	2.963431
H	-0.183230	-2.383497	2.968416
H	0.884542	-3.248114	2.189460
O	0.699509	2.697708	-3.044807
H	0.791961	3.218550	-3.863464
H	-0.254223	2.401530	-3.026386
O	-2.682283	-0.743477	-3.045580
H	-3.178952	-0.923424	-3.864692
H	-1.948570	-1.421071	-3.027582
O	-3.159249	-3.155043	0.761237
H	-2.440506	-3.607037	0.262390
H	-2.730093	-2.769231	1.560093
O	-4.310715	-1.132582	-0.749642
H	-3.748132	-1.012466	-1.550179
H	-3.889940	-1.865775	-0.230947
O	-4.376734	1.117340	0.740090
H	-4.382900	0.280828	0.186818
H	-5.301693	1.262029	1.011930
O	-3.253265	3.152146	-0.758004

H	-3.719221	2.455009	-0.226127
H	-3.945661	3.782740	-1.028341
O	-0.716570	2.687089	3.049783
H	-0.818229	3.195703	3.874974
H	0.239553	2.398630	3.032341
O	1.175152	4.299930	-0.746620
H	0.999141	3.753789	-1.548182
H	0.329016	4.301363	-0.229250
O	3.154745	3.229878	0.744014
H	2.433800	3.654036	0.190656
H	3.742382	3.958106	1.017364
O	-1.152567	4.311675	0.763605
H	-1.903959	3.915943	0.265011
H	-1.032912	3.746697	1.562157
O	-2.679833	0.658227	2.961453
H	-3.257695	0.856053	2.187853
H	-1.974737	1.347570	2.966925
O	-1.973076	-1.964696	3.048762
H	-2.363962	-2.306641	3.873538
H	-2.201227	-0.992434	3.030753
O	-1.918082	1.972239	-2.964528
H	-2.155325	1.015054	-2.981310
H	-2.403002	2.361358	-2.200029

Table S79. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₄ hollow clathrate in the tetradecahedron 4¹⁵10⁶3 configuration.

O	0.791964	-2.084995	-3.397397
H	0.942054	-2.476272	-4.277351
H	1.283642	-1.215696	-3.407164
O	4.407626	0.101911	-1.626399
H	5.260671	0.170525	-2.093135
H	4.386929	0.868785	-0.996106
O	2.202619	0.238476	-3.408845
H	2.966731	0.221666	-2.786843
H	1.723893	1.082544	-3.232463
O	4.070246	-2.358119	-0.238429
H	3.854544	-2.136645	0.696300
H	4.213561	-1.495877	-0.691752
O	3.373432	-1.760267	2.451469
H	2.464454	-2.100292	2.661261
H	3.964176	-2.173092	3.107800
O	-2.434314	-3.563375	-0.512987
H	-2.782489	-4.441639	-0.753890
H	-1.560017	-3.739830	-0.055272
O	-1.971544	-2.007296	-2.840682
H	-2.103419	-2.555846	-2.032415
H	-1.001132	-2.005403	-3.017504
O	-0.039384	-4.050975	0.631406
H	0.674490	-3.910818	-0.044086
H	0.218433	-3.519558	1.419615
O	1.886274	-3.708211	-1.324905
H	1.529873	-3.145794	-2.050437
H	2.671356	-3.220691	-0.969195

O	3.371035	1.066548	2.651023
H	3.396429	0.085598	2.559362
H	3.672795	1.432391	1.786584
O	0.782152	-2.628402	2.952992
H	0.239874	-1.831190	3.224173
H	0.740278	-3.239246	3.711790
O	0.895918	2.695936	-2.941997
H	1.000922	3.284593	-3.711704
H	-0.086799	2.663289	-2.766084
O	-3.310091	0.352948	-2.788409
H	-3.808221	0.393088	-3.625222
H	-2.793016	-0.501241	-2.826762
O	-4.258471	-2.086646	0.955087
H	-3.609945	-2.657562	0.466140
H	-4.960779	-2.688910	1.261497
O	-5.002354	0.222804	-0.524735
H	-4.434039	0.259995	-1.330508
H	-4.797443	-0.640040	-0.095809
O	-4.164007	1.998943	1.353833
H	-4.535171	1.418684	0.628973
H	-4.928770	2.460121	1.744948
O	-2.321780	3.698073	0.181811
H	-2.998026	3.126892	0.631722
H	-2.727814	4.582649	0.126290
O	0.876055	1.931015	3.318079
H	0.959735	2.380389	4.179109
H	1.799413	1.625860	3.088875
O	2.159301	3.774780	-0.636813
H	1.715064	3.410059	-1.437634
H	1.459415	3.817356	0.064414
O	4.181187	2.186056	0.181484
H	3.450178	2.799013	-0.128087
H	4.975004	2.744581	0.272436
O	0.248947	3.896512	1.371172
H	-0.664551	3.773419	1.025376
H	0.393940	3.191263	2.044038
O	-3.252869	-0.243904	2.885455
H	-3.524633	0.595990	2.450840
H	-3.556674	-0.948468	2.268881
O	-0.613957	-0.446259	3.724641
H	-1.537553	-0.340230	3.383861
H	-0.145958	0.403910	3.551954
O	-1.769311	2.688930	-2.414378
H	-2.285428	1.857361	-2.535481
H	-1.985385	3.018460	-1.511143

Table S80. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₆ hollow clathrate in the pentadecahedron 5¹²6³ configuration.

O	4.104752	2.308441	-1.139942
H	4.823665	2.927490	-1.362640
H	3.530253	2.788532	-0.478793
O	2.371907	2.106559	3.087952
H	2.771243	2.655901	3.787424

H	1.487087	1.833734	3.445938
O	2.502515	3.563747	0.663182
H	2.366293	3.056435	1.496779
H	1.608313	3.773245	0.306376
O	3.969441	-0.202917	2.595654
H	3.389973	-0.993420	2.698365
H	3.398904	0.576674	2.786423
O	2.345813	-2.517918	2.814879
H	2.318840	-2.956301	1.917525
H	2.738691	-3.178104	3.414616
O	2.475033	-1.273083	-3.490907
H	2.905464	-1.529127	-4.327381
H	3.065503	-1.625276	-2.774738
O	2.469322	1.570430	-3.327751
H	2.461635	0.586478	-3.365888
H	3.069789	1.806782	-2.582827
O	4.028292	-2.212714	-1.393233
H	4.408607	-1.440182	-0.879206
H	4.795277	-2.745305	-1.673417
O	4.991910	-0.118755	0.014102
H	4.703258	0.738459	-0.378173
H	4.627451	-0.128262	0.936192
O	-0.104080	-1.606505	3.873515
H	0.741001	-1.913340	3.468295
H	-0.042860	-0.625053	3.940627
O	2.352454	-3.676015	0.358424
H	1.488366	-3.826396	-0.092413
H	2.914047	-3.175982	-0.279050
O	-2.348420	3.683001	0.669033
H	-2.827332	4.505066	0.883078
H	-2.919729	3.212224	-0.004799
O	-2.309672	1.630004	-3.398565
H	-2.681978	1.981913	-4.227727
H	-1.418348	2.073104	-3.300138
O	-0.049221	-2.574978	-3.313569
H	0.821054	-2.116146	-3.356976
H	-0.021665	-3.135391	-2.503566
O	-2.448186	-1.197688	-3.474311
H	-2.314837	-0.221836	-3.440327
H	-1.550639	-1.613550	-3.419377
O	-4.053556	-2.111641	-1.502860
H	-3.473080	-1.776973	-2.248606
H	-4.731285	-2.669627	-1.926777
O	-5.046326	0.047393	-0.085670
H	-4.753428	-0.742842	-0.610790
H	-6.019575	0.052277	-0.139597
O	-2.461038	-2.437015	2.810776
H	-2.837930	-3.053867	3.464468
H	-1.577673	-2.159274	3.185547
O	-2.360162	2.094066	3.030184
H	-2.327089	2.630249	2.204404
H	-2.960732	1.329319	2.835565
O	-0.047026	1.218959	4.116257
H	-0.884280	1.571233	3.693443
H	-0.117398	1.454882	5.059709
O	-4.019490	-0.080705	2.559669
H	-4.391919	-0.070998	1.648132
H	-3.505359	-0.918398	2.631064

O	-2.436513	-3.635182	0.254622
H	-3.015582	-3.084282	-0.322184
H	-2.421853	-3.195696	1.137322
O	-0.079622	-4.187675	-0.978452
H	-0.128902	-5.135087	-1.201889
H	-0.929191	-3.985979	-0.493122
O	-3.864804	2.383424	-1.166012
H	-3.341090	2.102536	-1.953976
H	-4.281656	1.564001	-0.810366
O	0.060664	4.275039	-0.576152
H	0.061362	5.238785	-0.723391
H	-0.794674	4.083786	-0.109461
O	0.054471	2.913722	-3.075743
H	0.899867	2.401634	-3.147568
H	0.086495	3.375999	-2.206783

Table S81. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₆ hollow clathrate in the pentadecahedron 4¹⁵10⁶4 configuration.

O	-2.669976	-3.886660	-0.371957
H	-3.072410	-4.769790	-0.460619
H	-1.754904	-4.041916	-0.002035
O	0.095806	-2.818678	3.081614
H	0.142257	-3.502834	3.774882
H	0.925323	-2.270989	3.202152
O	-0.173925	-4.238277	0.642543
H	-0.003439	-3.699059	1.449750
H	0.539428	-4.025878	-0.002914
O	-2.273213	-1.394444	3.406009
H	-2.614443	-1.660522	4.279596
H	-1.410474	-1.875493	3.307961
O	-2.262837	1.462175	3.329839
H	-2.920645	1.716550	2.634886
H	-2.228644	0.479060	3.324781
O	-3.809762	0.002778	-2.545855
H	-4.519013	0.007287	-3.214780
H	-4.277119	-0.002233	-1.670208
O	-2.391215	-2.456434	-2.799939
H	-2.866496	-1.600602	-2.693909
H	-2.531536	-2.950064	-1.958735
O	-4.989435	-0.005276	-0.032732
H	-4.673100	-0.804428	0.480302
H	-5.962280	-0.066479	-0.042321
O	-4.075919	-2.149475	1.348138
H	-3.587704	-2.778225	0.765190
H	-3.443589	-1.901548	2.062751
O	2.384798	1.458325	3.586483
H	1.551201	1.956924	3.351176
H	2.665172	1.815744	4.448583
O	-4.066181	2.282932	1.368516
H	-3.585057	2.854166	0.727286
H	-4.400352	1.515511	0.849425
O	4.043368	-2.363477	-0.944973
H	4.827392	-2.859325	-1.245199

H	4.015715	-1.540443	-1.513529
O	1.570285	-0.083707	-4.010842
H	1.765110	-0.117285	-4.965236
H	1.069550	-0.926640	-3.812253
O	-2.317155	2.412322	-2.806316
H	-2.822198	1.574085	-2.695323
H	-2.458360	2.925938	-1.978344
O	0.392741	2.408255	-3.385801
H	0.730149	1.503014	-3.581444
H	-0.574367	2.321904	-3.188237
O	1.748221	3.744812	-1.481005
H	1.245202	3.245064	-2.192170
H	2.018307	4.583472	-1.899879
O	4.039293	2.261568	-0.917594
H	3.232073	2.810277	-1.095271
H	4.790404	2.811366	-1.207659
O	0.122607	2.820314	2.985505
H	0.078379	3.295216	2.125311
H	-0.727192	2.316668	3.074556
O	4.516085	-1.465132	1.719672
H	4.340148	-1.788693	0.806846
H	4.608208	-0.483006	1.639586
O	2.351095	-1.380528	3.467621
H	3.093343	-1.514372	2.824473
H	2.270956	-0.402146	3.553525
O	4.529260	1.328401	1.724478
H	4.292989	1.702942	0.845644
H	3.758502	1.493826	2.314465
O	-0.031605	4.336781	0.571224
H	0.625556	4.128657	-0.143752
H	0.135199	5.267480	0.810088
O	-2.606523	3.936134	-0.424160
H	-3.015413	4.807688	-0.576829
H	-1.701360	4.126517	-0.067649
O	3.931637	-0.119123	-2.465038
H	3.109528	-0.078225	-3.009438
H	3.951057	0.713063	-1.937280
O	1.721872	-3.807365	-1.415762
H	2.003742	-4.681680	-1.742315
H	2.564084	-3.314459	-1.231405
O	0.306197	-2.413381	-3.453111
H	-0.651877	-2.393650	-3.200822
H	0.768854	-2.905148	-2.736112

Table S82. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₈ hollow clathrate in the hexadecahedron 5¹²6⁴-T_d configuration.

O	-0.477096	-4.775944	0.790598
H	-1.296415	-4.478647	0.315552
H	-0.589211	-5.734537	0.927882
O	-0.162467	0.824832	-4.731513
H	-0.103129	1.686837	-4.259196
H	-1.016989	0.423717	-4.448855
O	-3.667082	2.333596	2.175785

H	-4.418565	2.774601	2.612845
H	-4.071733	1.687036	1.540736
O	4.253879	1.559858	1.733829
H	3.754438	2.322164	1.359094
H	3.708555	1.212420	2.476788
O	0.501843	4.017224	2.064183
H	1.313640	3.902152	1.517569
H	0.546763	3.329304	2.767015
O	0.508121	2.062294	4.137176
H	0.609564	2.499291	5.002727
H	1.285141	1.448911	4.063408
O	-1.837980	-2.938608	-2.952676
H	-0.860559	-3.003078	-3.068624
H	-2.095517	-2.036820	-3.258010
O	-3.922437	-1.963884	1.225490
H	-3.363196	-1.924133	2.037058
H	-3.467474	-2.573972	0.599301
O	-2.397034	-1.751002	3.594897
H	-2.247725	-0.779454	3.772056
H	-2.901282	-2.079094	4.361766
O	3.821630	0.608103	-2.621703
H	4.125794	0.221525	-1.750334
H	4.633410	0.729421	-3.147319
O	3.650599	-2.810122	0.740134
H	2.992630	-3.299276	0.169782
H	4.387925	-3.433334	0.874179
O	2.429541	-2.163415	3.220738
H	2.839503	-2.396719	2.355176
H	1.518371	-2.552666	3.205597
O	-2.190266	3.693104	-1.840963
H	-2.068459	3.873015	-0.862704
H	-2.690770	4.457261	-2.182016
O	-0.084664	-3.339922	3.214411
H	-0.254547	-3.839967	2.383434
H	-0.872281	-2.762385	3.344601
O	0.102846	3.304104	-3.356432
H	0.133525	4.052885	-3.979911
H	-0.692191	3.472538	-2.786461
O	-4.676764	0.487740	0.360372
H	-4.394715	-0.427921	0.648518
H	-5.651371	0.466042	0.345857
O	4.669291	-0.356327	-0.236830
H	4.285156	-1.207351	0.078471
H	4.508772	0.302947	0.485642
O	-2.710768	-3.810286	-0.545346
H	-2.408652	-3.461694	-1.433410
H	-3.362839	-4.505972	-0.748713
O	2.871965	3.734313	0.547251
H	3.399974	4.552909	0.576864
H	2.758789	3.525094	-0.422660
O	1.957919	-0.871079	-4.152263
H	1.217528	-0.239633	-4.340874
H	2.597318	-0.381155	-3.584321
O	-2.077332	0.910287	4.039687
H	-2.597755	1.438693	3.390883
H	-1.167038	1.287697	4.040508
O	1.838337	-4.191004	-0.741245
H	1.016508	-4.394204	-0.237057

H	1.544024	-3.820186	-1.606600
O	-1.968291	4.149837	0.811092
H	-2.550486	3.525411	1.302346
H	-1.074282	4.077707	1.232625
O	2.742253	0.439876	3.865677
H	3.273388	0.429864	4.683133
H	2.592338	-0.523417	3.635390
O	-2.592560	-0.392968	-3.904547
H	-3.221707	-0.479577	-4.643915
H	-3.034538	0.218475	-3.250204
O	0.964392	-3.216075	-3.239032
H	1.173102	-3.866982	-3.933917
H	1.362649	-2.353975	-3.555609
O	-3.752860	1.348269	-2.173862
H	-3.212872	2.158493	-2.019704
H	-4.039480	1.031859	-1.285624
O	2.630406	3.115935	-2.087557
H	3.008373	2.230434	-2.302109
H	1.735215	3.147543	-2.497470

Table S83. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₂₈ hollow clathrate in the hexadecahedron 5¹²6⁴-D₂ configuration.

O	2.928245	3.501383	1.536117
H	1.972222	3.732521	1.586277
H	3.041624	2.663248	2.041674
O	0.226885	4.362144	1.513852
H	-0.460981	3.848125	2.023745
H	0.193175	5.266165	1.876727
O	-1.729655	3.012409	2.834350
H	-1.559650	2.096685	3.158412
H	-2.527554	2.961865	2.258476
O	3.433712	1.081631	2.923417
H	3.946596	1.279737	3.728344
H	4.051921	0.556336	2.336850
O	1.243352	-0.554709	3.634932
H	1.420681	-1.460043	3.289277
H	2.004978	0.008211	3.358997
O	-1.282584	0.417138	3.872754
H	-1.408202	0.469557	4.837980
H	-0.357270	0.065034	3.751806
O	4.008207	-2.985946	1.091021
H	3.236265	-3.097599	1.704778
H	4.640826	-3.685935	1.335864
O	5.058598	-0.357730	1.296747
H	5.065939	0.015311	0.376781
H	4.716615	-1.277366	1.212492
O	-3.982533	2.994033	1.119464
H	-3.700075	3.174434	0.185293
H	-4.625038	3.693454	1.338966
O	-5.046635	0.369337	1.314804
H	-4.705500	1.288811	1.225022
H	-5.080747	0.007831	0.399554
O	-3.368377	-1.217082	2.856178

H	-3.945688	-0.618659	2.316263
H	-2.617231	-0.663588	3.173661
O	-3.096836	3.369332	-1.486854
H	-3.619462	4.024198	-1.985398
H	-3.205139	2.508656	-1.984835
O	-0.445533	4.332703	-1.234200
H	-0.236145	4.338856	-0.270276
H	-1.355427	3.963454	-1.316391
O	1.528153	3.267226	-2.769602
H	0.778353	3.642771	-2.227553
H	1.644957	3.885728	-3.513703
O	-3.463894	1.033107	-2.809257
H	-2.681587	0.530188	-3.138312
H	-4.009814	0.387101	-2.303535
O	-1.264608	-0.436361	-3.827714
H	-1.433375	-0.547770	-4.781538
H	-1.325976	-1.356863	-3.445276
O	1.359190	0.613186	-3.703563
H	0.435364	0.269748	-3.685769
H	1.333999	1.535012	-3.354701
O	-5.063734	-0.752928	-1.295674
H	-4.654130	-1.653930	-1.237181
H	-5.952252	-0.892699	-1.671520
O	5.083494	0.739907	-1.247334
H	4.633301	1.622553	-1.216195
H	4.549870	0.193834	-1.869017
O	3.833484	3.219370	-1.086314
H	3.039147	3.250611	-1.667245
H	3.491957	3.331266	-0.163758
O	3.517430	-0.878485	-2.997126
H	2.704120	-0.360188	-3.253131
H	3.982442	-1.059802	-3.834177
O	-1.523075	-2.946813	-2.810641
H	-2.286408	-3.049567	-2.196914
H	-0.760163	-3.386804	-2.366493
O	-3.762381	-3.201846	-1.078651
H	-4.309188	-3.977541	-1.302476
H	-3.468643	-3.344154	-0.139752
O	1.773557	-3.185762	2.726024
H	1.034940	-3.601151	2.194093
H	1.905729	-3.773810	3.492372
O	-0.159441	-4.340785	1.222731
H	-1.081144	-4.003051	1.311282
H	0.055553	-4.322653	0.260227
O	-2.845615	-3.500569	1.516123
H	-3.320335	-4.193528	2.011308
H	-3.005686	-2.652744	2.026532
O	0.578395	-4.301669	-1.505804
H	0.662352	-5.203563	-1.865902
H	1.495849	-3.908308	-1.559381
O	3.087501	-3.272597	-1.574280
H	3.433866	-3.137147	-0.661871
H	3.217767	-2.419833	-2.052760

Table S84. MP2/6-31+G*/PCM optimized Cartesian coordinates of the (H₂O)₃₀ hollow clathrate in the heptadecahedron 5¹²6⁵-C_{2v} A configuration.

O	-4.974235	2.131637	0.526761
O	-2.852139	3.773267	1.270082
O	-4.968208	-0.076381	2.190844
O	1.283233	2.467742	3.283654
O	-1.415266	2.550339	3.405652
O	-2.658421	0.105200	3.849108
O	2.654180	3.888889	1.250959
O	-4.869052	-2.297891	0.663646
O	1.479093	-2.398144	3.446527
O	-1.231756	-2.282980	3.320777
O	-2.665418	-3.800954	1.401858
O	2.727716	0.136219	3.729282
O	-4.421364	-1.520392	-2.024754
O	-4.508526	1.293059	-2.158605
O	-2.312768	2.647829	-3.009234
O	-2.293699	-2.856595	-3.045905
O	-0.052253	-1.387353	-3.932737
O	-0.073961	1.324670	-4.128992
O	1.432761	-4.471454	-0.949073
O	-1.273433	-4.484201	-0.970759
O	2.877835	-3.674891	1.351909
O	1.261890	4.561485	-1.125332
O	-1.442357	4.514002	-1.069525
O	2.115183	2.809255	-3.097128
O	2.238898	-2.787993	-3.006390
O	4.471480	-1.301872	-2.081319
O	4.414864	1.413328	-2.212215
O	4.992303	-2.181400	0.560883
O	5.072695	0.110756	2.114734
O	4.756829	2.368715	0.432195
H	-1.647863	-3.916017	-1.685069
H	-1.749510	-4.232462	-0.145050
H	-2.977903	-4.613587	1.840923
H	-3.488922	-3.303155	1.155136
H	-3.069539	-2.336337	-2.690244
H	-2.654415	-3.391329	-3.776671
H	-1.710780	-1.433969	3.463126
H	-1.733058	-2.779396	2.633020
H	-0.842147	-1.876620	-3.602827
H	0.735301	-1.861996	-3.579276
H	0.485898	-2.343371	3.372630
H	1.644176	-2.910700	4.258984
H	1.963238	-3.419893	-2.291628
H	2.538303	-3.351434	-3.743757
H	2.286863	-3.915501	0.600916
H	2.315319	-3.236870	2.033467
H	0.432389	-4.474676	-0.923161
H	1.688068	-5.397839	-1.114508
H	4.224865	-2.748836	0.862593
H	5.781084	-2.751345	0.619275
H	3.682961	-1.803143	-2.395137
H	4.651861	-1.628188	-1.168740
H	2.280092	-0.733548	3.610300
H	3.542897	0.096375	3.178528

H	5.895801	0.122077	2.636808
H	5.105491	-0.726846	1.583100
H	4.411922	0.414964	-2.187573
H	5.170663	1.654482	-2.778440
H	4.888632	1.573620	0.999558
H	4.649234	2.028542	-0.487555
H	2.868858	2.237233	-2.823301
H	1.406190	2.210701	-3.427354
H	3.033777	4.700091	1.635766
H	3.438333	3.342020	0.960168
H	1.748852	2.948544	2.560057
H	1.774791	1.617590	3.413222
H	1.726279	4.320115	-0.290023
H	1.584442	3.921542	-1.810163
H	-0.095129	1.477093	-5.091456
H	-0.066375	0.332809	-4.024427
H	-1.580614	3.130745	4.171494
H	-0.418801	2.499164	3.331609
H	-1.971408	3.289050	-2.341868
H	-1.528338	2.164919	-3.360890
H	-2.276367	4.012763	0.507272
H	-2.271476	3.351601	1.943855
H	-1.723582	5.413059	-1.319798
H	-0.442043	4.544434	-1.054699
H	-4.812661	1.857406	-0.405141
H	-4.215359	2.720982	0.766719
H	-3.689926	1.759822	-2.489207
H	-5.226720	1.581071	-2.751103
H	-2.184917	0.965861	3.703337
H	-2.907701	0.107476	4.791593
H	-4.964202	0.725059	1.604346
H	-4.171523	0.007133	2.764027
H	-4.591540	-1.756526	-1.082994
H	-4.422203	-0.534850	-2.067114
H	-5.723168	-2.756847	0.764753
H	-4.927216	-1.484191	1.247365

Table S85. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $\text{CH}_4@(\text{H}_2\text{O})_{16}$ 4²5⁸ methane-clathrate.

O	0.736488	3.324263	0.693378
H	0.294334	3.195668	-0.183069
H	1.623484	2.907036	0.591278
O	0.517595	-0.663264	3.194268
H	0.127026	0.233933	3.042333
H	0.594232	-0.749124	4.162553
O	-3.133352	-1.012100	-1.627524
H	-2.274439	-1.293452	-2.021416
H	-3.103632	-0.028386	-1.591675
O	-0.522820	2.922099	-1.810069
H	-0.102431	2.176788	-2.293992
H	-1.427396	2.595743	-1.596136
O	-3.164060	-1.632816	1.039698
H	-3.184680	-1.502985	0.050157
H	-3.999899	-2.079647	1.267694
O	3.153986	0.389936	-1.866900

H	3.144569	-0.518898	-1.487265
H	2.301069	0.481588	-2.351834
O	-3.032791	1.793550	-1.101899
H	-3.823920	2.310804	-1.340294
H	-3.076327	1.665451	-0.112774
O	3.053643	-0.552280	1.900193
H	2.186820	-0.599751	2.366228
H	3.101532	0.355250	1.520086
O	0.533471	-3.338540	-0.656444
H	1.438790	-2.965795	-0.544499
H	0.087184	-3.190058	0.214234
O	-3.064652	1.169011	1.560376
H	-2.199937	1.404858	1.970554
H	-3.089434	0.185123	1.524629
O	3.166536	1.885688	0.428627
H	3.188199	1.426225	-0.457110
H	3.992799	2.400251	0.481726
O	3.050825	-2.050292	-0.388641
H	3.833418	-2.631032	-0.413754
H	3.079135	-1.591315	0.497396
O	-0.559344	1.906356	2.660611
H	-0.643135	2.488964	3.438025
H	-0.088825	2.450136	1.966107
O	-0.632304	-1.855913	-2.656048
H	-0.715618	-2.446588	-3.427447
H	-0.212884	-2.411372	-1.938091
O	0.638980	0.626150	-3.181575
H	0.185053	-0.241685	-3.034920
H	0.709173	0.719927	-4.149576
O	-0.755372	-2.903561	1.834018
H	-0.310911	-2.186282	2.338231
H	-1.636458	-2.530457	1.599053
C	0.010794	-0.009652	-0.026220
H	0.719967	-0.643192	-0.554640
H	0.552330	0.770755	0.502908
H	-0.551953	-0.614629	0.680431
H	-0.676637	0.447772	-0.734354

Table S86. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $\text{CH}_4@(\text{H}_2\text{O})_{16}$ 4³5⁶6¹ methane-clathrate.

O	2.383679	1.110353	2.248134
H	2.996113	1.400602	2.949096
H	2.210092	1.915439	1.695505
O	-3.653186	-0.085784	0.514441
H	-3.304636	-1.020231	0.602825
H	-4.612434	-0.137447	0.681293
O	1.717729	2.242902	-2.191729
H	1.879009	2.570277	-1.277889
H	2.046132	1.313755	-2.199136
O	1.187843	-2.670390	-2.080218
H	0.220184	-2.490466	-2.129803
H	1.354145	-2.957399	-1.152988
O	2.742395	-0.406837	-2.149210
H	2.146510	-1.203931	-2.221049

H	3.449096	-0.545718	-2.806242
O	-2.179167	1.585595	2.171839
H	-2.783605	1.004381	1.641417
H	-2.744256	2.006939	2.845498
O	-1.023694	2.465031	-2.270608
H	-0.036422	2.342088	-2.339575
H	-1.257195	3.116791	-2.956974
O	3.468517	-0.908926	0.562738
H	3.106785	-0.198143	1.141660
H	3.297277	-0.615434	-0.361849
O	-2.508236	-2.546945	0.541822
H	-1.737812	-2.565617	1.166900
H	-2.124178	-2.568447	-0.364295
O	-0.957345	3.450097	0.402463
H	-1.396741	2.808763	1.008385
H	-1.125313	3.118064	-0.509835
O	-0.378180	-2.598192	2.333666
H	-0.242427	-1.679486	2.675509
H	0.429167	-2.806802	1.810810
O	-2.800653	0.247652	-2.204121
H	-3.166838	0.263932	-1.290689
H	-2.163336	0.997989	-2.246269
O	1.754250	3.198845	0.518908
H	2.185756	4.056491	0.689218
H	0.770571	3.371261	0.557378
O	-1.614505	-2.235106	-2.158577
H	-2.002399	-1.323444	-2.270687
H	-2.066933	-2.796441	-2.814709
O	-0.058555	0.022918	3.294854
H	0.772904	0.411692	2.940134
H	-0.783056	0.572817	2.918877
O	1.876227	-3.130239	0.657312
H	2.384707	-3.931027	0.881552
H	2.520807	-2.370518	0.711525
C	0.012299	0.001174	-0.150843
H	-1.012929	0.080077	0.207484
H	0.590761	0.849802	0.211076
H	0.017006	-0.001840	-1.240053
H	0.452743	-0.923604	0.217239

Table S87. MP2/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₁₇ 4⁴5⁶6¹ methane-clathrate.

O	2.360992	1.952660	1.253761
H	2.090674	1.212154	1.848944
H	3.113048	1.566876	0.748762
O	-1.059317	-3.212663	1.258892
H	-1.795798	-2.935985	0.666867
H	-0.261374	-3.243512	0.681565
O	-3.108292	-2.195798	-0.425854
H	-3.427007	-1.345968	-0.004706
H	-3.896714	-2.762122	-0.517284
O	1.261067	-3.237397	-0.402829
H	1.598402	-4.139719	-0.553191
H	1.985492	-2.761115	0.092379
O	-2.990530	1.455663	-1.874498

H	-2.540730	0.682214	-2.281853
H	-2.286612	2.110161	-1.658349
O	2.342737	0.401347	-2.738455
H	1.755648	-0.407761	-2.782419
H	2.748494	0.482138	-3.621266
O	-1.998489	-1.105540	-2.764645
H	-2.422320	-1.595974	-2.015304
H	-2.455410	-1.415802	-3.568489
O	-2.129449	1.186848	2.620904
H	-2.619701	1.533164	3.388960
H	-1.505746	1.912755	2.351217
O	3.180037	-1.864330	0.978186
H	3.563702	-1.143553	0.427701
H	2.741618	-1.391348	1.724326
O	-0.412260	3.161533	1.699211
H	-0.722801	3.337755	0.779760
H	0.524072	2.893956	1.601934
O	-3.813304	0.261053	0.504215
H	-3.235259	0.590376	1.230198
H	-3.556135	0.782358	-0.297862
O	1.843662	-0.291280	2.898015
H	2.223877	-0.227495	3.793329
H	0.909358	-0.630484	3.022200
O	1.503287	2.757340	-1.405130
H	1.706770	1.972020	-1.963277
H	1.724378	2.472983	-0.491075
O	0.768396	-1.826520	-2.818334
H	-0.185324	-1.579492	-2.801215
H	0.921924	-2.337253	-1.988510
O	-0.689739	-1.202252	3.166912
H	-0.856169	-1.889687	2.473074
H	-1.255169	-0.428385	2.942545
O	4.020968	0.405855	-0.505147
H	4.959935	0.525029	-0.738144
H	3.528831	0.373371	-1.364301
O	-1.106779	3.406151	-1.049995
H	-1.305672	4.294157	-1.400060
H	-0.172767	3.202626	-1.333551
C	-0.138101	-0.013001	-0.155282
H	-0.818337	-0.862813	-0.138721
H	0.881871	-0.358200	0.016831
H	-0.418961	0.691765	0.625486
H	-0.195385	0.477463	-1.126487

Table S88. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $\text{CH}_4@(\text{H}_2\text{O})_{18}$ $4^25^86^1$ methane-clathrate.

O	2.080889	-2.584371	1.609757
H	1.251945	-2.964298	1.212000
H	2.503393	-3.321595	2.088503
O	-2.451363	-1.057541	-2.695538
H	-3.026865	-1.195234	-1.908840
H	-2.245814	-0.095150	-2.680747
O	2.398491	1.543531	-2.486493
H	2.992979	1.528841	-1.701961

H	2.200593	0.594285	-2.655960
O	-2.055992	2.263445	2.080953
H	-1.253701	2.745285	1.750486
H	-2.490547	2.874551	2.703987
O	-2.345726	-2.367717	1.713670
H	-2.030879	-1.608738	2.268320
H	-2.956475	-1.972075	1.048490
O	2.085560	-1.286716	-2.773297
H	2.463521	-1.664042	-3.588710
H	1.226967	-1.778690	-2.624139
O	-2.119051	1.777491	-2.463299
H	-2.527050	2.295295	-3.181364
H	-1.263442	2.248881	-2.247764
O	2.324733	2.016310	2.011798
H	2.923433	1.734200	1.280003
H	2.020765	1.179712	2.434485
O	-0.241175	-3.490051	0.425970
H	-0.363423	-4.455733	0.486971
H	-1.027089	-3.090722	0.903632
O	-0.210309	-2.665641	-2.314642
H	-0.237321	-2.940082	-1.369272
H	-0.999055	-2.080249	-2.443660
O	0.177883	3.088810	-1.822388
H	0.213577	3.212200	-0.846306
H	0.963677	2.529987	-2.049542
O	-3.962447	-1.177732	-0.273749
H	-4.901904	-1.436235	-0.295033
H	-3.950376	-0.187837	-0.140055
O	3.954412	1.182554	-0.126209
H	3.953429	0.185221	-0.176435
H	4.890522	1.451422	-0.093524
O	0.232454	3.437069	1.027002
H	0.361143	4.372786	1.269443
H	1.021980	2.949104	1.401963
O	3.702306	-1.506040	-0.463341
H	3.143234	-1.533074	-1.275766
H	3.157631	-1.914840	0.248087
O	-3.678662	1.520411	-0.117382
H	-3.138619	1.706651	-0.921298
H	-3.120087	1.794757	0.646905
O	1.433839	-0.400214	3.221930
H	1.692020	-1.196915	2.691687
H	1.819746	-0.540469	4.106321
O	-1.402834	-0.253538	3.264917
H	-0.419037	-0.293281	3.266927
H	-1.624080	0.616502	2.861372
C	-0.061204	-0.007231	-0.102469
H	-0.985931	-0.556641	0.074361
H	0.053613	0.176664	-1.170323
H	0.786796	-0.591926	0.257623
H	-0.096102	0.944397	0.426663

Table S89. MP2/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₁₉ 4²5¹⁰ methane-clathrate.

O	2.119176	-2.037399	-2.297912
H	2.828058	-1.445707	-1.939070
H	1.819354	-2.578511	-1.529456
O	3.917382	-0.125923	-1.363571
H	3.434694	0.647607	-1.730046
H	3.827495	-0.058928	-0.384703
O	2.134291	1.766257	-2.549635
H	1.444133	1.141604	-2.878456
H	2.417001	2.279656	-3.328961
O	1.467952	3.452037	-0.365474
H	1.720498	3.003134	0.475468
H	1.722694	2.839251	-1.092560
O	1.303157	-3.556568	-0.062169
H	1.587386	-3.114965	0.788291
H	1.693448	-4.449310	-0.038441
O	2.116915	2.220768	2.092202
H	1.280744	1.972771	2.583958
H	2.591198	2.839175	2.678306
O	-0.165621	1.534982	3.389337
H	-0.931365	1.837630	2.847413
H	-0.243073	0.554014	3.440349
O	-0.300026	-1.306089	3.491467
H	-1.099305	-1.611124	2.985855
H	-0.425129	-1.634309	4.401132
O	3.577652	-0.042973	1.455708
H	3.087250	0.780316	1.715950
H	4.425875	-0.001383	1.934915
O	2.048172	-2.298192	2.233568
H	2.578038	-1.501951	1.994650
H	1.252618	-1.959038	2.705490
O	0.278287	-0.308312	-3.256880
H	0.930544	-0.992954	-2.914136
H	0.300945	-0.397115	-4.229257
O	-1.749709	1.783592	-2.676622
H	-1.008815	1.148369	-2.751378
H	-1.514353	2.394730	-1.940513
O	-3.754646	0.035123	-1.773565
H	-3.151543	0.751146	-2.088856
H	-3.274458	-0.783384	-2.052677
O	-3.724219	0.122215	0.999269
H	-3.243651	0.944938	1.247732
H	-3.740679	0.106086	0.006683
O	-2.304958	2.463463	1.779020
H	-1.953652	2.931848	0.977568
H	-2.869972	3.113010	2.236656
O	-2.076019	-2.041882	-2.617576
H	-1.282742	-1.508397	-2.833429
H	-1.835528	-2.570720	-1.814238
O	-1.501566	-3.496845	-0.326213
H	-1.837416	-3.012860	0.463344
H	-0.525074	-3.548678	-0.203358
O	-2.460440	-2.071711	1.937920
H	-3.130958	-2.589095	2.421159
H	-2.940204	-1.257561	1.601921
O	-1.224925	3.566333	-0.524848
H	-0.227342	3.602707	-0.445483
H	-1.510399	4.473466	-0.740293
C	0.019585	0.038417	0.091179

H	-0.397698	1.039958	0.200846
H	0.993526	0.099721	-0.396821
H	-0.654241	-0.572517	-0.510135
H	0.137740	-0.414132	1.075291

Table S90. MP2/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₂₀ 5¹² methane-clathrate.

C	-0.053484	-0.015243	0.003432
H	-0.534922	0.921052	-0.283385
H	-0.089090	-0.714293	-0.833656
H	-0.575014	-0.444034	0.860434
H	0.986565	0.178736	0.272396
O	1.641416	-3.204630	1.357573
H	0.841292	-3.419238	0.825066
H	1.322107	-2.641497	2.109315
O	-2.326027	1.501750	2.721054
H	-2.704776	1.634526	1.821189
H	-1.445633	1.961168	2.714742
O	3.757877	0.712505	0.994242
H	3.673494	-0.178345	0.580405
H	3.457513	1.357346	0.310317
O	-0.732741	1.649365	-3.470550
H	-1.084825	2.220715	-2.750220
H	-1.211442	0.791622	-3.391042
O	-0.647188	-3.821643	-0.209803
H	-1.438724	-3.395635	0.209172
H	-0.832361	-4.778879	-0.200504
O	1.982316	1.218689	-3.100768
H	1.009048	1.354898	-3.232128
H	2.104368	0.250357	-2.968358
O	-1.980375	-1.130020	3.181206
H	-2.129703	-0.148104	3.033699
H	-2.468616	-1.351837	3.995653
O	-0.165477	-2.781959	-2.791589
H	-0.324186	-3.172886	-1.900721
H	0.737051	-2.387258	-2.752864
O	2.166445	0.844510	3.192809
H	2.774795	0.803716	2.400623
H	2.737295	1.061308	3.952400
O	0.598455	3.890407	0.237338
H	-0.176158	3.708422	-0.342201
H	1.363573	3.439805	-0.190362
O	2.381388	-1.556462	-2.676388
H	2.793908	-1.687688	-1.782428
H	3.013239	-1.938743	-3.312935
O	-3.446954	1.836609	0.136587
H	-3.548065	0.932459	-0.281999
H	-4.348236	2.204928	0.188755
O	0.807829	-1.615240	3.468559
H	-0.154760	-1.421625	3.393818
H	1.263043	-0.744002	3.392749
O	-3.668560	-0.622515	-0.968036
H	-3.364649	-1.300389	-0.321304
H	-3.091788	-0.726976	-1.761615

O	0.129285	2.772215	2.747399
H	0.314363	3.168315	1.858877
H	0.849266	2.117787	2.899692
O	3.437949	-1.857305	-0.134322
H	4.263480	-2.375880	-0.116667
H	2.783177	-2.371231	0.425899
O	-1.672733	3.327128	-1.375056
H	-2.117915	4.126126	-1.712519
H	-2.357702	2.844249	-0.842785
O	-2.816714	-2.525466	0.951683
H	-3.543393	-3.123221	1.207895
H	-2.552707	-2.052233	1.785564
O	2.825750	2.567717	-0.911056
H	3.513667	3.191751	-1.206717
H	2.530769	2.081299	-1.735257
O	-2.027574	-0.855744	-3.248201
H	-2.524254	-1.108897	-4.047776
H	-1.347136	-1.575511	-3.113275

Table S91. MP2/6-31+G*/PCM optimized Cartesian coordinates of the CH₄@(H₂O)₂₂ 4¹⁵1⁰6² methane-clathrate.

O	2.003441	-3.698649	0.397880
H	2.266520	-3.092292	1.129453
H	2.312100	-3.266649	-0.431233
O	-1.691359	-3.039037	-2.013658
H	-1.341900	-3.389134	-1.140481
H	-1.915273	-3.830435	-2.537729
O	-1.771620	2.965808	1.938885
H	-1.364336	3.322485	1.115503
H	-1.059517	2.484213	2.421906
O	2.650020	2.472785	2.141717
H	2.388951	2.937790	1.313810
H	1.807828	2.232224	2.593348
O	-4.005427	1.593408	1.268913
H	-3.186499	2.088648	1.557593
H	-4.758416	2.063569	1.670679
O	2.687172	1.939612	-2.389439
H	1.850950	1.618553	-2.803375
H	2.419623	2.572156	-1.682263
O	0.264066	-1.008486	3.668337
H	1.088250	-1.366824	3.261478
H	-0.481374	-1.490435	3.239628
O	0.423235	-1.749626	-3.380320
H	-0.314786	-2.174778	-2.883623
H	1.249006	-2.019108	-2.914874
O	-1.708608	2.559771	-2.530732
H	-1.040638	1.932953	-2.893917
H	-2.473282	2.013760	-2.216327
O	-1.842134	-2.486721	2.504157
H	-2.208084	-3.088176	3.178518
H	-2.628374	-1.990442	2.138045
O	2.806368	-2.449679	-2.025455
H	3.320318	-1.626778	-1.812822
H	3.404686	-3.000503	-2.563155

O	0.347230	0.955192	-3.617750
H	0.384357	1.108578	-4.579823
H	0.337043	-0.038919	-3.511765
O	-0.750223	-3.954010	0.342204
H	-1.110568	-3.444369	1.105286
H	0.235301	-3.848247	0.383090
O	-0.749178	4.017336	-0.473681
H	-1.056988	4.931607	-0.614659
H	-1.104975	3.488483	-1.248229
O	1.986870	3.725363	-0.314822
H	1.010311	3.895393	-0.378721
H	2.411850	4.595475	-0.427805
O	-3.981590	-1.619185	-1.388415
H	-3.178349	-2.138376	-1.656368
H	-4.740794	-2.079414	-1.790541
O	2.656947	-1.958750	2.524646
H	3.176034	-1.182889	2.161573
H	3.238705	-2.377887	3.184833
O	-3.924852	1.219068	-1.548973
H	-3.928195	0.236582	-1.601260
H	-3.996496	1.416909	-0.586863
O	-3.985584	-1.219866	1.422830
H	-3.981117	-0.235060	1.468239
H	-4.024932	-1.426859	0.460614
O	0.251998	1.694782	3.430887
H	0.211486	2.022399	4.348144
H	0.223761	0.697748	3.505220
O	4.010619	0.144387	1.498495
H	3.529311	0.986454	1.705041
H	4.038055	0.081708	0.515664
O	4.093761	-0.107349	-1.328430
H	3.593162	0.658776	-1.735929
H	5.007125	-0.031934	-1.661193
C	0.221882	-0.021442	0.019664
H	-0.486481	-0.611093	0.605312
H	0.905885	-0.691634	-0.504301
H	0.789830	0.629455	0.686717
H	-0.319590	0.585708	-0.708622

Table S92. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $C_2H_6@(H_2O)_{22}$ $4^15^{10}6^2$ ethane-clathrate.

O	1.457692	-3.891674	0.348231
H	1.795975	-3.353087	1.101347
H	1.850819	-3.491499	-0.460777
O	-2.032566	-2.820882	-2.092358
H	-1.774917	-3.264613	-1.230793
H	-2.346717	-3.540777	-2.670585
O	-1.393192	3.148143	1.985446
H	-0.921629	3.466270	1.180354
H	-0.763548	2.554382	2.458635
O	2.930955	2.073331	2.231986
H	2.767352	2.576063	1.401417
H	2.042871	1.909355	2.625858
O	-3.755940	2.033545	1.268843

H	-2.890831	2.435302	1.569055
H	-4.455890	2.582991	1.666443
O	3.046370	1.666955	-2.340694
H	2.169548	1.446549	-2.736010
H	2.860794	2.311844	-1.618799
O	0.017292	-1.136231	3.545621
H	0.810853	-1.589867	3.175609
H	-0.765239	-1.528978	3.092295
O	0.258461	-1.703171	-3.323368
H	-0.533017	-2.061938	-2.857599
H	1.040459	-2.090900	-2.866129
O	-1.284926	2.825475	-2.435291
H	-0.695614	2.117157	-2.785341
H	-2.126744	2.385567	-2.152841
O	-2.251053	-2.359614	2.379107
H	-2.705776	-2.875323	3.070309
H	-2.945991	-1.744513	2.008552
O	2.538627	-2.724652	-2.005721
H	3.154194	-1.980317	-1.774525
H	3.064166	-3.341849	-2.547301
O	0.564015	0.987820	-3.514105
H	0.603264	1.150027	-4.474834
H	0.410402	0.004354	-3.422507
O	-1.306746	-3.969764	0.247502
H	-1.639659	-3.439862	1.009270
H	-0.317375	-3.934720	0.307911
O	-0.146315	4.108029	-0.358829
H	-0.335474	5.057259	-0.477323
H	-0.571958	3.647264	-1.142224
O	2.537662	3.472734	-0.216074
H	1.593878	3.775282	-0.280155
H	3.077103	4.282793	-0.275823
O	-4.076778	-1.044322	-1.516306
H	-3.351093	-1.677975	-1.757858
H	-4.879085	-1.387702	-1.950916
O	2.356280	-2.322556	2.516415
H	2.984308	-1.617648	2.182252
H	2.858357	-2.828105	3.181511
O	-3.701726	1.776808	-1.561534
H	-3.804845	0.802998	-1.654478
H	-3.747745	1.936655	-0.590659
O	-4.174448	-0.761935	1.304665
H	-4.011142	0.205137	1.397582
H	-4.185436	-0.919767	0.332348
O	0.408239	1.545717	3.427609
H	0.407374	1.836944	4.357963
H	0.225138	0.563478	3.458189
O	4.011792	-0.397343	1.568795
H	3.637544	0.494338	1.787905
H	4.041530	-0.438441	0.584930
O	4.116921	-0.576468	-1.266736
H	3.743191	0.259175	-1.673712
H	5.040952	-0.627076	-1.574120
C	-0.817631	-0.150889	-0.056581
C	0.664723	0.205947	-0.001504
H	-1.239164	0.058673	-1.043958
H	-1.388347	0.423899	0.679049
H	-0.973924	-1.211901	0.153675

H	1.086464	-0.018025	0.981765
H	0.822659	1.270733	-0.197276
H	1.234503	-0.359522	-0.744798

Table S93. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $C_2H_6@(H_2O)_{24} 5^{12}6^2$ ethane-clathrate.

C	-0.778784	-0.041462	-0.034440
C	0.742096	-0.182615	-0.017680
H	-1.079547	1.010602	0.007880
H	-1.230100	-0.552808	0.820581
H	-1.205385	-0.472845	-0.943972
H	1.040717	-1.234979	-0.056046
H	1.168775	0.250929	0.891263
H	1.196482	0.323487	-0.874335
O	-1.012156	-2.544403	3.037551
H	-1.215842	-3.093204	3.817241
H	-1.666245	-1.788743	3.071196
O	-4.425337	-0.772614	0.740865
H	-5.368864	-0.909468	0.944864
H	-4.388204	0.064425	0.206767
O	-2.849323	-0.544342	3.084696
H	-3.412046	-0.599667	2.277321
H	-2.460170	0.362172	3.075184
O	-3.368771	-2.851762	-0.863658
H	-2.946647	-2.445288	-1.655620
H	-3.750235	-2.105959	-0.345499
O	-2.088204	-1.759790	-3.150561
H	-1.128329	-2.036353	-3.114466
H	-2.440781	-2.155087	-3.968991
O	2.873246	-3.412018	0.789129
H	3.444217	-4.157913	1.050322
H	2.152142	-3.809137	0.233031
O	1.775142	-2.099469	3.046964
H	2.123668	-2.572561	2.255962
H	0.794972	-2.200797	3.016197
O	0.794041	-4.310220	-0.776536
H	-0.043513	-4.250202	-0.226344
H	0.859979	-5.241663	-1.057482
O	-1.443806	-4.081558	0.693862
H	-1.308879	-3.527666	1.498081
H	-2.141091	-3.623660	0.156903
O	-2.620305	1.008413	-3.087213
H	-2.412553	0.044845	-3.106325
H	-3.158412	1.153880	-2.274007
O	0.484612	-2.602723	-3.006633
H	1.224116	-1.950236	-2.997638
H	0.622646	-3.184992	-2.223442
O	-1.825318	2.075654	3.066965
H	-2.127646	2.541597	3.868219
H	-0.832902	2.192658	3.056017
O	2.739635	0.431199	3.104871
H	3.274067	0.486195	3.918430
H	2.361105	-0.494540	3.098082
O	4.227339	-1.462957	-0.760795

H	3.753288	-2.163845	-0.257259
H	3.670846	-1.273803	-1.551691
O	4.370768	0.811501	0.808658
H	3.802410	0.662732	1.600036
H	4.311405	-0.019614	0.270428
O	3.452220	2.852796	-0.688155
H	3.813191	2.098847	-0.132422
H	4.223182	3.404157	-0.916805
O	1.549874	4.146786	0.829878
H	2.274390	3.731613	0.291586
H	1.893889	5.015974	1.106466
O	-0.478750	2.676777	-3.035985
H	-0.595321	3.227874	-3.831792
H	-1.238402	2.026720	-3.056631
O	-2.904448	3.327973	0.763335
H	-2.519990	2.897679	1.562713
H	-2.133637	3.682814	0.249368
O	-4.171009	1.517527	-0.774107
H	-3.713787	2.205566	-0.203916
H	-5.025911	1.912682	-1.026887
O	-0.799879	4.303212	-0.738682
H	0.038555	4.259945	-0.223770
H	-0.660161	3.734280	-1.531346
O	2.209552	1.825496	-3.010140
H	2.617074	2.210572	-2.199364
H	1.258430	2.084707	-2.991269
O	2.686334	-0.845621	-3.063287
H	3.198394	-1.009984	-3.876336
H	2.490123	0.134344	-3.065963
O	0.850699	2.517762	3.033103
H	1.485736	1.763561	3.059332
H	1.121684	3.073660	2.265864

Table S94. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $C_2H_6@(H_2O)_{26}$ $5^{12}6^3$ ethane-clathrate.

O	4.034918	2.271601	-1.333040
H	4.752039	2.880119	-1.588470
H	3.441942	2.794327	-0.720974
O	2.321999	2.410618	2.869496
H	2.700430	3.031380	3.519363
H	1.430781	2.165011	3.232533
O	2.408021	3.647403	0.339640
H	2.292542	3.208763	1.214433
H	1.506352	3.793982	-0.029194
O	3.964396	0.103634	2.622977
H	3.394059	-0.687487	2.765597
H	3.374845	0.884647	2.732219
O	2.382021	-2.209977	2.976354
H	2.386226	-2.749563	2.134095
H	2.761088	-2.793321	3.659128
O	2.484685	-1.507284	-3.331980
H	2.911107	-1.853548	-4.137630
H	3.075465	-1.786268	-2.583794
O	2.477576	1.321634	-3.482223
H	2.473693	0.339171	-3.413865

H	3.054004	1.638483	-2.748180
O	4.047986	-2.246515	-1.173541
H	4.399440	-1.420410	-0.724655
H	4.835354	-2.762430	-1.427469
O	4.949463	-0.018847	0.037495
H	4.641125	0.792890	-0.429508
H	4.595989	0.048773	0.961644
O	-0.065146	-1.221696	3.934242
H	0.777952	-1.551054	3.542812
H	-0.030353	-0.237411	3.896404
O	2.470342	-3.659029	0.690514
H	1.596562	-3.837989	0.269528
H	3.006073	-3.180702	0.015000
O	-2.450591	3.674841	0.315115
H	-2.940871	4.507309	0.448674
H	-3.009587	3.135360	-0.317754
O	-2.327253	1.232124	-3.510341
H	-2.685599	1.517446	-4.370812
H	-1.436359	1.681765	-3.433720
O	0.008139	-2.847637	-3.025270
H	0.860527	-2.361396	-3.108225
H	0.048140	-3.322096	-2.162583
O	-2.417808	-1.579811	-3.372127
H	-2.310201	-0.600999	-3.418408
H	-1.511011	-1.962033	-3.253758
O	-3.977998	-2.307773	-1.302667
H	-3.409568	-2.039861	-2.085378
H	-4.647700	-2.919349	-1.660522
O	-5.016344	-0.058668	-0.086897
H	-4.698703	-0.884474	-0.538601
H	-5.989102	-0.086725	-0.142970
O	-2.414441	-2.189450	3.016594
H	-2.760968	-2.754692	3.731145
H	-1.528521	-1.859986	3.342659
O	-2.438362	2.333092	2.810562
H	-2.414759	2.779880	1.932855
H	-3.015705	1.534926	2.694995
O	-0.098775	1.599313	3.918625
H	-0.948126	1.894960	3.474067
H	-0.176159	1.900789	4.842877
O	-4.034371	0.083194	2.566175
H	-4.387885	0.001323	1.650725
H	-3.492109	-0.725958	2.716115
O	-2.342190	-3.609127	0.595261
H	-2.925127	-3.127966	-0.037230
H	-2.347236	-3.088677	1.433014
O	0.020852	-4.237185	-0.561831
H	-0.034631	-5.198305	-0.715202
H	-0.831145	-3.994942	-0.097952
O	-3.921072	2.188367	-1.396922
H	-3.374081	1.839036	-2.140643
H	-4.310017	1.397704	-0.954841
O	-0.041571	4.170869	-0.947112
H	-0.056177	5.111535	-1.203423
H	-0.900995	4.015983	-0.473741
O	0.012037	2.554774	-3.275302
H	0.880971	2.079309	-3.318552
H	0.032063	3.099571	-2.455402

C	-0.721283	0.129098	-0.001719
C	0.793692	-0.070978	0.038380
H	-1.158834	-0.338508	-0.890002
H	-0.978301	1.193142	-0.023754
H	-1.200979	-0.310921	0.878896
H	1.229081	0.393837	0.929074
H	1.274763	0.374051	-0.838969
H	1.051654	-1.134841	0.057963

Table S95. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $C_3H_8@(H_2O)_{24}$ $5^{12}6^2$ propane-clathrate.

C	-1.299130	-0.210109	-0.031428
C	-0.019279	0.460198	-0.512119
C	1.206412	-0.203615	0.101158
H	-2.186462	0.251957	-0.465419
H	-1.380566	-0.140665	1.056820
H	-1.300576	-1.272395	-0.299867
H	-0.037323	1.524629	-0.245709
H	0.036589	0.412058	-1.605672
H	2.134906	0.278805	-0.212604
H	1.255262	-1.259754	-0.183644
H	1.153686	-0.154826	1.193124
O	1.435813	-2.731781	2.781548
H	1.626753	-3.353339	3.508196
H	0.442538	-2.631163	2.782947
O	-2.462512	-3.747239	0.452311
H	-2.973355	-4.556119	0.640315
H	-3.098732	-3.128243	0.006743
O	-1.295313	-2.628598	2.787022
H	-1.700482	-3.008996	1.973609
H	-1.788403	-1.790647	2.951613
O	-0.174520	-4.183972	-1.165957
H	-0.214549	-3.506545	-1.881243
H	-0.983723	-4.044380	-0.622533
O	-0.223896	-2.251332	-3.229013
H	0.658133	-1.780958	-3.202807
H	-0.234785	-2.716104	-4.086392
O	4.652462	-0.254129	0.564514
H	5.606342	-0.368199	0.732509
H	4.398334	-1.003113	-0.036349
O	3.159925	-0.494787	2.987347
H	3.667468	-0.444802	2.143998
H	2.558497	-1.270466	2.894684
O	3.780634	-2.270411	-1.118568
H	3.198238	-2.895367	-0.593173
H	4.491855	-2.824407	-1.490473
O	2.160662	-3.905211	0.297511
H	1.913543	-3.497421	1.160225
H	1.310104	-4.006127	-0.202573
O	-2.703983	-0.903283	-3.080259
H	-1.819052	-1.338086	-3.087113
H	-3.175429	-1.265826	-2.294654
O	2.232703	-1.094300	-3.189561
H	2.247270	-0.114636	-3.077418

H	2.773068	-1.463716	-2.452631
O	-2.793630	-0.262841	3.195358
H	-3.272831	-0.274113	4.044434
H	-2.177813	0.521758	3.246613
O	1.686323	1.788046	3.219165
H	1.989789	2.211821	4.043381
H	2.214850	0.942442	3.150251
O	4.015360	2.205394	-0.732867
H	4.271361	1.339533	-0.340064
H	3.457916	1.998586	-1.518675
O	2.345787	3.505438	1.056287
H	2.122021	2.877460	1.782530
H	2.953272	3.016316	0.443865
O	0.189032	4.423006	-0.270143
H	1.001160	4.095951	0.220144
H	0.310317	5.385665	-0.368183
O	-1.989392	3.720580	1.270113
H	-1.221084	4.029683	0.721252
H	-2.350045	4.524501	1.687868
O	-2.518058	1.804034	-2.802843
H	-3.008518	2.172532	-3.560978
H	-2.558960	0.812810	-2.922546
O	-4.591368	0.070236	0.982800
H	-3.969047	-0.023005	1.741007
H	-4.339819	0.914851	0.530089
O	-4.119427	-1.916508	-0.811189
H	-4.315442	-1.188310	-0.151641
H	-4.988398	-2.280030	-1.064154
O	-3.890260	2.411391	-0.373434
H	-3.231651	2.894066	0.177446
H	-3.425063	2.215256	-1.219588
O	0.006585	3.123667	-2.774051
H	0.038500	3.587323	-1.904825
H	-0.832592	2.606682	-2.766893
O	2.336111	1.713430	-2.974569
H	2.751838	2.063216	-3.784358
H	1.462923	2.194211	-2.901994
O	-1.143760	1.894805	3.254715
H	-0.165467	1.786710	3.205358
H	-1.386626	2.539008	2.549595

Table S96. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $C_3H_8@(H_2O)_{26}$ $5^{12}6^3$ propane-clathrate.

O	4.067118	-1.447639	2.128397
H	4.784744	-1.864808	2.639288
H	3.517491	-2.202703	1.771027
O	2.477317	-3.335943	-1.675472
H	2.876042	-4.149767	-2.035559
H	1.573277	-3.287705	-2.082154
O	2.555259	-3.472445	1.141463
H	2.460420	-3.414413	0.162321
H	1.642798	-3.452228	1.512457
O	4.064513	-1.057433	-2.345007
H	3.459188	-0.399589	-2.760074

H	3.500542	-1.834235	-2.127253
O	2.371871	0.874454	-3.526553
H	2.321246	1.700476	-2.964663
H	2.729006	1.167943	-4.384878
O	2.332634	2.769582	2.437845
H	2.766383	3.377194	3.065640
H	2.945213	2.726545	1.657326
O	2.419862	0.227471	3.690670
H	2.368808	1.095531	3.228394
H	3.016945	-0.333333	3.142227
O	3.990922	2.596226	0.224699
H	4.395874	1.682197	0.136196
H	4.743637	3.215215	0.257942
O	5.026202	0.114718	-0.017211
H	4.703922	-0.445621	0.727596
H	4.686864	-0.321050	-0.840915
O	-0.014732	-0.506097	-4.027563
H	0.812952	-0.026055	-3.788235
H	0.037896	-1.393672	-3.602489
O	2.332864	3.107297	-1.999329
H	1.455411	3.422192	-1.677074
H	2.885269	2.955341	-1.197409
O	-2.367545	-3.552537	1.136923
H	-2.825036	-4.379644	1.377789
H	-2.940257	-2.818182	1.506560
O	-2.318996	0.190951	3.683880
H	-2.693021	0.299565	4.577639
H	-1.430705	-0.250147	3.821128
O	-0.118979	3.991583	1.695490
H	0.727960	3.552685	1.940653
H	-0.101275	4.067781	0.712840
O	-2.463551	2.706272	2.416564
H	-2.300565	1.829557	2.836233
H	-1.580384	3.094407	2.189248
O	-4.065780	2.518352	0.262547
H	-3.480207	2.598137	1.073826
H	-4.754715	3.200511	0.366897
O	-5.040685	-0.062149	0.044473
H	-4.754035	0.884812	0.128724
H	-6.014908	-0.044734	0.077568
O	-2.369228	0.729515	-3.556929
H	-2.713062	0.942908	-4.443924
H	-1.478702	0.302500	-3.715468
O	-2.383958	-3.387952	-1.687493
H	-2.360864	-3.434671	-0.703313
H	-2.969620	-2.616909	-1.902991
O	0.005276	-3.098805	-2.909236
H	-0.860146	-3.213924	-2.415251
H	-0.041316	-3.729034	-3.652223
O	-4.002231	-1.227214	-2.332932
H	-4.368607	-0.814199	-1.517711
H	-3.445523	-0.529406	-2.751178
O	-2.445178	3.056481	-1.985705
H	-3.024547	2.844180	-1.217111
H	-2.380428	2.227201	-2.515726
O	-0.126188	4.165534	-1.125303
H	-0.179936	5.089127	-1.432908
H	-0.961005	3.728408	-1.459721

O	-3.905337	-1.566753	2.150193
H	-3.361839	-0.937861	2.682217
H	-4.303513	-1.028261	1.426933
O	0.060828	-3.443752	2.459706
H	0.053776	-4.216833	3.054128
H	-0.796720	-3.495320	1.960722
O	0.023938	-1.097609	4.047002
H	0.868044	-0.602705	3.885879
H	0.065652	-1.901775	3.479800
C	-1.261338	-0.141609	0.048595
C	-0.015398	0.676646	-0.278553
C	1.260570	-0.144892	-0.119762
H	-2.175409	0.449429	-0.065565
H	-1.222780	-0.506343	1.081258
H	-1.337261	-1.012050	-0.612150
H	0.029265	1.555910	0.374506
H	-0.082830	1.054051	-1.306078
H	2.151813	0.443344	-0.356349
H	1.245329	-1.015352	-0.785377
H	1.360701	-0.512348	0.908146

Table S97. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $C_3H_8@(H_2O)_{28}$ $5^{12}6^4-T_d$ propane-clathrate.

O	-2.451143	-1.147584	3.981240
H	-1.708458	-1.800344	3.890792
H	-2.901058	-1.380128	4.814380
O	4.668071	1.022908	1.179715
H	4.535486	1.082866	0.205807
H	4.454797	0.091060	1.417736
O	-0.081136	-3.737953	-2.981699
H	-0.096491	-4.529771	-3.550458
H	0.324913	-4.034482	-2.124944
O	-2.022840	3.856765	-2.069479
H	-1.256988	3.530918	-2.596789
H	-2.673867	3.118568	-2.033210
O	-0.391025	0.459317	-4.382675
H	-0.146276	1.352799	-4.046737
H	-1.294142	0.273627	-4.037545
O	-2.998937	-0.194362	-3.482391
H	-3.608603	-0.211035	-4.243354
H	-3.370492	0.491680	-2.867658
O	1.920824	-1.414785	3.751583
H	1.759564	-0.448958	3.870905
H	2.632819	-1.497400	3.073667
O	-0.928998	-4.290040	1.271329
H	-1.750964	-3.895823	0.894011
H	-0.712425	-3.767362	2.078474
O	-3.279174	-3.261498	0.108968
H	-3.082970	-3.065417	-0.851721
H	-3.955322	-3.963760	0.094218
O	1.601519	4.310912	0.570710
H	0.600396	4.331445	0.567482
H	1.876093	5.237615	0.697581
O	-2.718810	3.022460	2.282497

H	-2.210958	2.463578	2.937320
H	-3.222313	3.658647	2.822794
O	-4.471890	1.402298	0.758939
H	-3.858466	1.953390	1.298926
H	-4.350331	0.473455	1.082490
O	3.608617	-1.255038	-2.578929
H	2.778109	-1.342492	-3.135393
H	4.332935	-1.565233	-3.153937
O	-4.222599	-1.174131	1.758469
H	-3.606632	-1.187711	2.526227
H	-3.887435	-1.866969	1.143518
O	4.261343	1.261154	-1.623329
H	5.091921	1.487503	-2.081538
H	3.992266	0.380372	-1.994801
O	1.038537	-4.466722	-0.560956
H	0.328181	-4.378462	0.140450
H	1.291911	-5.408462	-0.551880
O	-1.092377	4.436478	0.473696
H	-1.630677	3.914988	1.114243
H	-1.443862	4.212111	-0.425684
O	-0.328379	-2.891533	3.632288
H	0.519952	-2.359493	3.641556
H	-0.240207	-3.531429	4.362806
O	0.268278	3.049078	-3.517178
H	0.415960	3.629687	-4.286084
H	1.082911	3.151979	-2.946840
O	2.938688	2.748803	2.495819
H	3.539086	2.139815	1.994418
H	2.440442	3.262850	1.818287
O	-2.704913	-2.812511	-2.495951
H	-1.779718	-3.091471	-2.688989
H	-2.788263	-1.882755	-2.812004
O	-1.412600	1.476055	4.075575
H	-1.733565	0.544696	4.052122
H	-0.427375	1.431467	4.060969
O	1.406709	-1.607317	-4.081914
H	0.883305	-2.355832	-3.712814
H	0.772611	-0.848585	-4.156104
O	-3.982755	1.814165	-1.861462
H	-4.831848	2.150277	-2.203549
H	-4.147978	1.622071	-0.890894
O	4.023795	-1.648514	1.904650
H	4.780706	-2.109724	2.310330
H	3.799908	-2.173269	1.083889
O	1.392095	1.317679	4.175125
H	1.682019	1.578146	5.068771
H	1.943430	1.870495	3.546355
O	3.440976	-3.001062	-0.366969
H	3.465526	-2.404443	-1.151662
H	2.571441	-3.463609	-0.401889
O	2.451207	3.402829	-1.950900
H	2.184072	3.695278	-1.047189
H	3.049689	2.629945	-1.826209
C	1.249758	0.137091	0.070240
C	0.015632	-0.681638	-0.302131
C	-1.249666	0.173160	-0.305686
H	2.154037	-0.477562	0.075574
H	1.135565	0.578939	1.067440

H	1.399667	0.956081	-0.643027
H	-0.103298	-1.512145	0.406098
H	0.158865	-1.132577	-1.292632
H	-2.136275	-0.414134	-0.563262
H	-1.161500	0.990754	-1.031130
H	-1.418843	0.619243	0.681597

Table S98. MP2/6-31+G*/PCM optimized Cartesian coordinates of the $i\text{-C}_4\text{H}_{10} @ (\text{H}_2\text{O})_{28}$ $5^{12}6^4\text{-}T_d$ isobutane-clathrate.

O	0.548501	-0.202393	4.586254
H	1.339287	0.285117	4.234964
H	0.671646	-0.236142	5.552876
O	-0.108026	4.797577	-1.334268
H	-0.162941	4.165995	-2.088034
H	0.753069	4.597791	-0.900199
O	3.853225	-2.284780	-1.997203
H	4.620262	-2.668295	-2.461342
H	4.220849	-1.548042	-1.442409
O	-4.315640	-2.192330	-1.290520
H	-3.783412	-1.842479	-2.042770
H	-3.724542	-2.833926	-0.833390
O	-0.385769	-2.568979	-3.520680
H	-1.215081	-2.043071	-3.436102
H	-0.372821	-3.188728	-2.756156
O	-0.244187	-4.425990	-1.373984
H	-0.325059	-5.319785	-1.756184
H	-1.056262	-4.314088	-0.812601
O	1.686881	3.456143	2.520198
H	0.702318	3.496653	2.566552
H	1.925675	3.693424	1.592679
O	4.129039	-0.831149	2.094329
H	3.588885	-1.656556	2.094375
H	3.582310	-0.140649	2.535353
O	2.680003	-3.258168	2.074762
H	2.576697	-3.616684	1.147705
H	3.179361	-3.940331	2.560504
O	-3.956661	2.316892	-0.727084
H	-4.252611	1.466422	-0.289094
H	-4.782239	2.792949	-0.934136
O	-3.650275	-0.659145	2.854111
H	-2.995729	0.012349	3.198559
H	-4.342519	-0.716316	3.538144
O	-2.344994	-3.156931	2.562771
H	-2.789540	-2.282849	2.664045
H	-1.402157	-3.010808	2.828872
O	2.035214	1.492547	-3.639692
H	1.968825	0.492293	-3.691360
H	2.488664	1.757432	-4.461977
O	0.253919	-2.768784	3.431066
H	0.386414	-1.877495	3.827592
H	1.069663	-2.949684	2.908716
O	-0.310884	2.946320	-3.482807
H	-0.360184	3.409678	-4.339575

H	0.507938	2.386610	-3.538753
O	4.775903	-0.168141	-0.441696
H	4.544886	-0.387659	0.508311
H	5.748506	-0.097311	-0.462510
O	-4.826014	-0.009104	0.379118
H	-4.393114	-0.216914	1.240287
H	-4.641573	-0.789750	-0.202596
O	2.702642	1.158720	3.508849
H	2.340778	1.997238	3.096603
H	3.314419	1.462304	4.205186
O	-2.805236	-1.132241	-3.435425
H	-3.259675	-1.273872	-4.286230
H	-2.743913	-0.140003	-3.331744
O	-2.232488	4.287987	0.399662
H	-1.493479	4.442360	-0.242401
H	-2.787350	3.568259	0.020914
O	2.442351	-4.202517	-0.462330
H	2.898100	-3.551536	-1.044813
H	1.505546	-4.241037	-0.763182
O	-1.853974	1.093800	3.870103
H	-0.998563	0.669176	4.112421
H	-1.621300	1.945457	3.429939
O	1.980637	-1.187208	-3.811301
H	2.611781	-1.584568	-3.167957
H	1.116397	-1.652540	-3.669825
O	-2.608302	-4.059598	0.039842
H	-3.079198	-4.909546	0.124474
H	-2.492065	-3.727976	0.979618
O	2.399569	4.193771	-0.092107
H	3.002161	4.960165	-0.088884
H	2.893124	3.470081	-0.571055
O	-1.125110	3.565545	2.755181
H	-1.373273	4.272503	3.379152
H	-1.552487	3.819113	1.885157
O	3.688134	2.243151	-1.486759
H	3.121195	1.939503	-2.234601
H	4.041443	1.424541	-1.067458
O	-2.735191	1.558760	-3.148723
H	-3.130367	1.852719	-2.294162
H	-1.864459	2.014206	-3.224925
C	-0.017650	-0.011125	-0.631468
C	-1.289897	-0.707072	-0.159473
C	1.215909	-0.707390	-0.065925
C	-0.034488	1.459920	-0.230283
H	0.022315	-0.071277	-1.729130
H	-2.181248	-0.225132	-0.571587
H	-1.360975	-0.666378	0.935478
H	-1.302093	-1.760290	-0.458436
H	2.137581	-0.235752	-0.421516
H	1.239936	-1.764302	-0.349842
H	1.209724	-0.652514	1.030805
H	0.867287	1.975211	-0.575795
H	-0.081744	1.555608	0.862553
H	-0.904478	1.973095	-0.649571

Table S99. MP2/6-31+G*/PCM optimized Cartesian coordinates of the neo-C₅H₁₂@(H₂O)₂₈ 5¹²6⁴-T_d neopentane-clathrate.

O	3.494352	-1.492159	-2.924384
H	3.852424	-1.345774	-2.009813
H	4.268787	-1.730860	-3.467127
O	-0.579239	-3.247068	3.650577
H	-1.210461	-2.500739	3.769997
H	0.315755	-2.835888	3.670787
O	1.196917	4.252257	1.857085
H	1.422832	5.121271	2.237470
H	1.943957	3.649220	2.110355
O	-4.201064	0.345071	-2.485177
H	-4.325635	0.627131	-1.549202
H	-3.546825	0.972558	-2.870933
O	-3.149348	3.449768	0.637543
H	-3.636056	2.603008	0.504639
H	-2.686891	3.625534	-0.213822
O	-1.715927	3.995413	-1.767490
H	-2.011753	4.832389	-2.171475
H	-1.879306	3.303022	-2.459649
O	3.249635	-2.902428	1.202817
H	2.602605	-3.459396	0.708905
H	2.787343	-2.597037	2.019219
O	4.481734	1.749150	0.196896
H	4.002652	2.169351	-0.555579
H	4.421618	0.778962	0.035541
O	3.064749	2.960572	-1.948870
H	2.277930	3.476300	-1.612249
H	3.618902	3.612462	-2.416694
O	-3.245448	-3.209700	0.039678
H	-3.180651	-2.853080	-0.893620
H	-3.910987	-3.921149	-0.005659
O	-0.730913	-2.347404	-3.935857
H	0.075256	-2.795455	-3.552008
H	-0.907197	-2.815469	-4.772879
O	-0.293202	0.404127	-4.509862
H	-0.428254	-0.543757	-4.275930
H	0.626640	0.624052	-4.214914
O	-0.934506	1.218375	4.346586
H	-1.136689	1.986169	3.735908
H	-1.062341	1.569310	5.247770
O	2.332754	0.945842	-3.802440
H	2.763034	0.118557	-3.485720
H	2.556780	1.637468	-3.137210
O	-2.440352	-1.098310	3.988140
H	-2.962223	-1.210701	4.804321
H	-1.936577	-0.253133	4.115350
O	3.220835	2.463060	2.507102
H	3.682087	2.173591	1.667591
H	3.920175	2.854721	3.062907
O	-3.157089	-2.234544	-2.478023
H	-2.288333	-2.246214	-2.942368
H	-3.485632	-1.300072	-2.508214
O	4.455916	-1.043643	-0.351932
H	3.986241	-1.690750	0.250375

H	5.394505	-1.308106	-0.318537
O	-4.613627	1.064441	0.233650
H	-5.560125	1.252606	0.373111
H	-4.418929	0.273141	0.811609
O	-0.906777	-4.375468	1.118563
H	-0.800513	-3.946085	2.005229
H	-1.687345	-3.939509	0.703905
O	0.975987	4.388480	-0.959594
H	0.997196	4.329722	0.023482
H	0.052683	4.178508	-1.232249
O	1.529004	-3.554623	-2.965140
H	2.225882	-2.858813	-2.933823
H	1.439965	-3.870135	-2.035202
O	-1.342369	3.348884	2.743173
H	-0.476409	3.667071	2.399570
H	-1.969245	3.350162	1.975178
O	-2.273314	2.050346	-3.678359
H	-2.622064	2.445148	-4.499082
H	-1.523187	1.453535	-3.969306
O	2.023861	-2.100422	3.604910
H	2.563316	-2.443170	4.341493
H	1.972172	-1.113510	3.754867
O	1.417141	-4.480327	-0.279231
H	1.666639	-5.422304	-0.242829
H	0.541474	-4.423488	0.201486
O	1.815514	0.559695	4.092069
H	0.867366	0.827732	4.122072
H	2.266773	1.187443	3.481920
O	-4.182346	-1.161293	1.744161
H	-3.843684	-1.888104	1.169575
H	-3.553413	-1.102025	2.500421
C	0.045839	-0.043991	-0.010744
C	-0.974225	0.800579	-0.769276
C	1.229553	0.829099	0.394828
C	0.534430	-1.175325	-0.910753
C	-0.599953	-0.632211	1.240416
H	-1.826726	0.189284	-1.086928
H	-0.518294	1.240102	-1.664120
H	-1.350264	1.614405	-0.139988
H	1.972572	0.241079	0.946411
H	0.901751	1.654425	1.037795
H	1.717448	1.255522	-0.488065
H	1.297686	-1.773803	-0.402563
H	0.970229	-0.776623	-1.833682
H	-0.294874	-1.839048	-1.183151
H	-1.440554	-1.282527	0.975981
H	-0.973909	0.164673	1.893406
H	0.125772	-1.226554	1.806388

Table S100. MP2/6-31+G*/PCM optimized Cartesian coordinates of the cyc-C₅H₁₀@(H₂O)₂₈ 5¹²6⁴-T_d cyclopentane-clathrate.

O	0.446032	4.445988	-1.639309
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H	1.291874	4.226103	-1.167846
H	0.584300	5.333983	-2.017965
O	3.623900	-2.736292	-1.754994
H	3.084956	-3.273488	-1.129710
H	3.992347	-1.993440	-1.221949
O	0.318734	0.125604	4.682389
H	0.406802	0.168275	5.652557
H	1.154564	0.523923	4.322593
O	-4.268713	-1.898429	-1.277746
H	-3.765099	-2.532246	-0.716089
H	-4.396023	-1.084763	-0.737643
O	-2.632277	-2.732823	2.771103
H	-2.686833	-3.135721	1.873020
H	-3.044076	-1.842471	2.686757
O	-3.777931	-0.127964	2.649434
H	-4.559562	-0.107286	3.232773
H	-4.118905	0.133283	1.754246
O	4.065546	1.793918	-1.701775
H	3.485821	1.495016	-2.441981
H	4.268942	0.980830	-1.182247
O	1.908079	3.518548	2.361246
H	0.926088	3.614564	2.362011
H	2.185697	3.540336	1.415959
O	-0.909829	3.795871	2.494454
H	-1.295424	2.991867	2.945566
H	-1.135208	4.547123	3.074011
O	-0.521477	-2.770197	-3.511504
H	-1.326422	-2.173888	-3.513246
H	-0.638438	-3.354694	-4.283418
O	-2.506521	1.553226	-3.576544
H	-1.563815	1.882299	-3.615096
H	-2.926492	1.880920	-4.393213
O	-3.806365	2.607912	-1.285693
H	-3.350341	2.253700	-2.084601
H	-3.130017	3.166978	-0.825232
O	2.213946	-3.247214	2.506919
H	1.344054	-3.007748	2.943237
H	2.649869	-3.865206	3.122958
O	-1.939878	4.288995	-0.086641
H	-1.118764	4.351121	-0.625300
H	-1.625729	4.075191	0.822788
O	2.008603	-4.323836	-0.031374
H	2.344658	-5.237562	0.027101
H	2.055807	-3.967571	0.894246
O	2.612815	1.222457	3.593127
H	2.367997	2.066574	3.111320
H	3.239206	1.496843	4.288690
O	-2.754966	-1.251984	-3.506173
H	-2.635599	-0.273252	-3.507176
H	-3.301409	-1.459903	-2.705445
O	2.781391	3.741166	-0.316416
H	3.243527	2.990384	-0.792624
H	3.422787	4.476315	-0.323953
O	-2.829350	-3.851637	0.197390
H	-3.318576	-4.694963	0.195276
H	-1.972514	-4.042379	-0.280081
O	2.058190	-1.663204	-3.769822
H	2.593537	-2.065860	-3.038756

H	1.139052	-1.999785	-3.653076
O	-1.890071	1.629608	3.794437
H	-1.139924	1.067303	4.097641
H	-2.523438	1.024571	3.343036
O	0.014281	2.533569	-3.663230
H	0.189740	3.192152	-2.951417
H	0.815479	1.959308	-3.705648
O	-0.052085	-2.516276	3.762434
H	0.042907	-1.588644	4.079228
H	-0.958196	-2.584185	3.365719
O	-4.749478	0.512308	0.138082
H	-5.713528	0.657946	0.163331
H	-4.376997	1.299272	-0.360280
O	4.715875	-0.569143	-0.290000
H	5.684535	-0.668458	-0.238681
H	4.390282	-0.672042	0.649230
O	2.371560	1.012853	-3.827457
H	2.798116	1.197341	-4.684722
H	2.231904	0.020649	-3.810094
O	3.839667	-0.934208	2.250488
H	3.241587	-1.711903	2.344180
H	3.374040	-0.174366	2.670916
O	-0.564826	-4.397042	-1.204551
H	-0.517126	-3.807030	-1.993637
H	0.310651	-4.323052	-0.758446
C	0.680033	-1.075802	-0.108625
C	-0.866124	-0.940849	-0.080371
C	-1.155248	0.574825	-0.090218
C	0.137037	1.208456	0.428567
C	1.217006	0.359351	-0.241578
H	1.039758	-1.519049	0.826994
H	1.025508	-1.720929	-0.921469
H	-1.273155	-1.402358	0.825108
H	-1.334537	-1.442078	-0.932077
H	-2.033462	0.844564	0.504781
H	-1.338943	0.919003	-1.115800
H	0.214594	2.273814	0.192366
H	0.199999	1.099866	1.520638
H	1.295626	0.640673	-1.300034
H	2.206900	0.484166	0.207830

Table S101. MP2/6-31+G*/PCM optimized Cartesian coordinates of the neo-C₅H₁₂@(H₂O)₃₀-4¹⁵10⁶-C_{2v} neopentane-clathrate.

O	-1.239482	4.510826	-0.952799
H	-0.258638	4.486022	-0.866374
H	-1.594963	4.261973	-0.067473
O	-4.196360	-0.520874	2.218183
H	-4.211033	-1.183684	1.487550
H	-4.225676	0.363523	1.784300
O	3.784735	-0.662233	2.883886
H	4.597899	-0.784201	3.408834
H	3.854095	-1.331327	2.140317
O	4.173184	1.871341	1.693433

H	3.402898	2.472108	1.819416
H	3.941451	1.014761	2.121049
O	1.662647	-1.042851	4.618530
H	2.409394	-0.921888	3.975151
H	2.090251	-1.232935	5.474031
O	1.585316	-3.854967	-2.589947
H	1.956455	-4.600943	-3.096568
H	2.043915	-3.048715	-2.941318
O	2.097233	-4.232456	0.189190
H	1.851839	-4.083950	-0.752286
H	1.259857	-4.202342	0.707187
O	-4.388448	2.041211	1.039531
H	-5.238276	2.419457	1.333143
H	-4.470484	1.943212	0.043475
O	-0.141553	3.237190	3.234865
H	-0.945357	3.327026	2.673835
H	-0.235332	2.392846	3.744719
O	-0.261779	-4.340795	1.745236
H	-0.314509	-5.259452	2.067802
H	-0.317971	-3.775176	2.567178
O	4.756597	-1.101003	-1.542783
H	4.793247	-0.118018	-1.341849
H	5.665324	-1.350622	-1.793960
O	-2.337720	3.817912	1.554618
H	-2.766556	4.608341	1.932435
H	-3.077970	3.173624	1.397231
O	-2.296699	-4.106058	-0.198441
H	-1.575702	-4.120508	0.472810
H	-1.865987	-3.972140	-1.081321
O	2.136363	3.810595	1.912296
H	2.513121	4.555390	2.417032
H	1.299411	3.559915	2.402908
O	-4.358587	-2.409063	0.148829
H	-5.142181	-2.974135	0.279718
H	-3.586765	-3.040756	0.058658
O	-2.443093	-0.896554	4.245537
H	-3.062072	-0.750845	3.474614
H	-3.023457	-1.050411	5.013514
O	1.582276	4.554801	-0.697433
H	1.870696	5.483223	-0.779317
H	1.796368	4.297804	0.238935
O	-0.360365	0.954912	4.791039
H	-1.142865	0.391115	4.591738
H	0.405653	0.340972	4.722377
O	-0.425209	-2.867032	4.022880
H	0.363880	-2.300641	4.185606
H	-1.186432	-2.241363	4.051293
O	4.065978	-2.418314	0.864277
H	4.289881	-1.966650	0.017519
H	3.327268	-3.044006	0.649540
O	-1.236430	-3.770415	-2.733237
H	-1.523172	-2.911896	-3.122673
H	-0.252014	-3.754046	-2.733110
O	4.818092	1.522803	-0.967150
H	4.563517	1.664425	-0.018563
H	4.164422	2.030274	-1.501811
O	-4.575384	-0.933483	-2.261762
H	-4.483034	-1.462286	-1.435539

H	-3.771996	-1.129215	-2.798263
O	-4.581447	1.763651	-1.633674
H	-4.560669	0.799501	-1.866693
H	-3.798465	2.163837	-2.079695
O	-2.350238	2.975627	-2.889140
H	-2.663275	3.616844	-3.553670
H	-1.896614	3.526018	-2.188894
O	-2.305653	-1.427848	-3.879430
H	-1.793295	-0.576769	-3.999510
H	-2.611065	-1.666571	-4.774061
O	2.922918	-1.596377	-3.538796
H	3.620154	-1.419013	-2.852164
H	3.415527	-1.828734	-4.348400
O	2.944788	2.961776	-2.527628
H	2.431874	3.529483	-1.896395
H	3.403596	3.587199	-3.118705
O	-1.016713	0.916697	-4.278948
H	-1.391453	1.655757	-3.746077
H	-0.033596	0.946340	-4.162428
O	1.745415	0.943249	-4.123583
H	2.133608	1.616791	-3.520310
H	2.140592	0.080060	-3.864558
C	0.164877	-0.483746	1.347831
C	-0.015606	0.005072	-0.089486
C	0.666305	1.363420	-0.257735
C	0.612580	-1.007223	-1.047108
C	-1.507215	0.144795	-0.399325
H	-0.312303	-1.460995	1.487399
H	1.229896	-0.587868	1.592387
H	-0.280373	0.218944	2.061988
H	0.538194	1.738998	-1.280227
H	0.234319	2.097816	0.432153
H	1.741519	1.290987	-0.050028
H	0.472487	-0.699548	-2.089598
H	0.154975	-1.994477	-0.917650
H	1.689816	-1.103509	-0.860391
H	-1.659224	0.494054	-1.427029
H	-1.980145	0.865645	0.279212
H	-2.023195	-0.816712	-0.285853

Table S102. MP2/6-31+G*/PCM optimized Cartesian coordinates of the n-C₄H₁₀ gauche@(H₂O)₂₈ 5¹²6⁴-T_d n-butane-clathrate.

O	-4.957791	0.120379	-0.883681
H	-4.597288	0.979744	-1.225674
H	-5.910688	0.134727	-1.090026
O	2.425540	0.405842	-4.091909
H	3.108554	0.396708	-3.382815
H	1.871978	1.204073	-3.923680
O	1.164180	3.689442	2.753312
H	1.332989	4.465897	3.318464
H	0.710707	4.045670	1.945061
O	1.235438	-4.111581	2.099953
H	2.024821	-3.535331	1.975609

H	0.598607	-3.592675	2.643069
O	3.202721	-0.245625	3.268051
H	3.319287	-1.017410	2.666440
H	2.303454	-0.347805	3.655152
O	0.625315	-0.467696	4.459774
H	0.734342	-0.569567	5.423572
H	0.117251	-1.270385	4.169722
O	-1.927528	1.734698	-3.633129
H	-1.875669	0.756958	-3.753702
H	-0.995600	2.051501	-3.573496
O	-2.701242	3.757250	0.513758
H	-2.865322	3.159794	1.281453
H	-3.026042	3.273362	-0.281488
O	-3.115875	2.121688	2.775631
H	-2.230748	2.026084	3.229428
H	-3.691031	2.568199	3.423950
O	1.768204	-3.595621	-2.210478
H	1.112673	-3.948945	-1.540735
H	2.091396	-4.380633	-2.690072
O	-2.654864	-3.832195	-0.276956
H	-2.997744	-3.194120	-0.965837
H	-3.198809	-4.635224	-0.376232
O	-3.016498	-2.630252	2.259463
H	-2.917243	-3.041020	1.368971
H	-3.471619	-1.761919	2.113411
O	4.037624	2.548201	-0.438271
H	3.890665	2.410066	0.543524
H	4.798497	3.155176	-0.501299
O	-4.389138	-0.246631	1.889764
H	-4.592350	-0.093213	0.939096
H	-3.911395	0.561117	2.190180
O	4.404424	0.299647	-2.041909
H	5.309297	0.367781	-2.398653
H	4.301937	1.077883	-1.434983
O	-0.126227	4.583683	0.474758
H	-1.071449	4.252584	0.453660
H	-0.196450	5.556153	0.452745
O	0.073098	-4.606389	-0.368489
H	-0.856023	-4.278580	-0.354249
H	0.450474	-4.416392	0.528325
O	-3.742953	2.455600	-1.768268
H	-3.042773	2.205389	-2.439111
H	-4.338526	3.071263	-2.234550
O	3.575939	-2.550011	1.678748
H	4.356638	-3.031358	2.009702
H	3.735776	-2.429401	0.699703
O	0.735878	-1.788743	-4.088802
H	1.354526	-1.014795	-4.057439
H	1.058798	-2.419407	-3.402948
O	-0.697162	1.965209	3.987733
H	-0.025052	2.547872	3.563464
H	-0.256600	1.093249	4.119850
O	-3.647197	-2.091405	-2.105834
H	-4.086687	-1.310696	-1.697096
H	-2.987653	-1.729496	-2.743653
O	3.578165	2.295229	2.216179
H	2.736900	2.772292	2.402158
H	3.438748	1.373240	2.551934

O	-0.704701	-2.740905	3.639586
H	-0.932377	-3.298417	4.406684
H	-1.558182	-2.648541	3.121557
O	0.742930	2.628945	-3.647910
H	0.832641	3.266344	-4.380243
H	1.098357	3.101794	-2.841504
O	-1.855968	-1.054241	-4.004107
H	-2.193472	-1.270530	-4.892974
H	-0.898982	-1.351211	-4.007241
O	1.768920	3.889048	-1.492451
H	2.520186	3.405904	-1.075293
H	1.108889	4.064892	-0.782862
O	3.968685	-2.310584	-0.999198
H	3.188541	-2.706312	-1.454717
H	4.061361	-1.392750	-1.343675
C	1.646600	0.270615	-0.097990
C	0.731865	-0.840506	0.408975
C	-0.647203	-0.824192	-0.249164
C	-1.387820	0.496281	-0.052897
H	2.663051	0.145229	0.283291
H	1.296958	1.258525	0.218970
H	1.690120	0.263458	-1.194033
H	0.612615	-0.752129	1.498597
H	1.202582	-1.812819	0.224551
H	-1.249051	-1.641642	0.162974
H	-0.534977	-1.027698	-1.323895
H	-2.412420	0.432225	-0.426980
H	-0.896511	1.319694	-0.581123
H	-1.434878	0.758510	1.010915

Table S103. MP2/6-31+G*/PCM optimized Cartesian coordinates of the n-C₄H₁₀ anti@ (H₂O)₂₈ 5¹²6⁴-D₂ n-butane-clathrate.

O	-2.988487	3.414168	-1.567964
H	-2.018525	3.584081	-1.587262
H	-3.136387	2.568471	-2.051427
O	-0.268363	4.178312	-1.464261
H	0.421806	3.694806	-2.002454
H	-0.250985	5.095675	-1.794386
O	1.684133	2.930680	-2.864957
H	1.493752	2.008041	-3.157960
H	2.483486	2.880488	-2.290767
O	-3.603512	0.996793	-2.891167
H	-4.140841	1.186061	-3.682478
H	-4.209556	0.491778	-2.275315
O	-1.380714	-0.567786	-3.692796
H	-1.513113	-1.457515	-3.290634
H	-2.127718	-0.011560	-3.368484
O	1.178029	0.329633	-3.806698
H	1.303056	0.381150	-4.772777
H	0.238053	0.010520	-3.693189
O	-4.050496	-2.958673	-0.962548
H	-3.277211	-3.057248	-1.577198
H	-4.656019	-3.689364	-1.186234

O	-5.235820	-0.390280	-1.200872
H	-5.209614	0.002537	-0.290326
H	-4.845730	-1.289515	-1.108028
O	3.954010	2.900267	-1.180746
H	3.701894	3.048968	-0.231998
H	4.567912	3.624802	-1.402065
O	5.142522	0.340158	-1.467306
H	4.755601	1.239882	-1.364195
H	5.196723	-0.017953	-0.551880
O	3.396123	-1.229699	-2.971083
H	3.987025	-0.641434	-2.434756
H	2.600081	-0.693400	-3.193730
O	3.193321	3.267892	1.465546
H	3.688187	3.994349	1.888281
H	3.401330	2.453547	2.009754
O	0.510741	4.160053	1.238736
H	0.280422	4.143730	0.279406
H	1.415223	3.778103	1.316220
O	-1.535511	3.176259	2.714137
H	-0.754251	3.519151	2.193572
H	-1.651371	3.805352	3.449828
O	3.772068	1.039959	2.897171
H	2.949026	0.567311	3.167381
H	4.265371	0.411382	2.320052
O	1.413542	-0.289044	3.747048
H	1.549814	-0.387375	4.708209
H	1.474888	-1.219388	3.385680
O	-1.288317	0.570420	3.709853
H	-0.354804	0.261410	3.642415
H	-1.308322	1.483431	3.336984
O	5.229409	-0.702196	1.186542
H	4.795741	-1.593213	1.158245
H	6.136356	-0.862790	1.506991
O	-5.178231	0.742500	1.345512
H	-4.707090	1.610381	1.262028
H	-4.615930	0.203945	1.947307
O	-3.861113	3.181033	1.066913
H	-3.049344	3.186057	1.624193
H	-3.539988	3.269100	0.134431
O	-3.544170	-0.823983	3.109988
H	-2.695750	-0.346690	3.330046
H	-3.983202	-0.980881	3.966079
O	1.641750	-2.821964	2.815471
H	2.375594	-2.924002	2.166463
H	0.844716	-3.214073	2.387277
O	3.828415	-3.098030	1.035099
H	4.346805	-3.892556	1.261837
H	3.503752	-3.247504	0.106779
O	-1.827083	-3.136839	-2.614991
H	-1.068039	-3.518930	-2.084656
H	-1.966872	-3.759711	-3.352433
O	0.147417	-4.221532	-1.129985
H	1.060575	-3.871338	-1.250388
H	-0.056347	-4.147591	-0.167656
O	2.826614	-3.417207	-1.513582
H	3.253751	-4.152693	-1.991206
H	3.012631	-2.599628	-2.066201
O	-0.555661	-4.084084	1.592772

H	-0.605501	-4.988310	1.954234
H	-1.488625	-3.727514	1.653650
O	-3.118224	-3.212379	1.695700
H	-3.463363	-3.075417	0.782813
H	-3.268598	-2.365397	2.178598
C	1.912895	0.070835	-0.036774
C	0.506278	-0.513176	-0.083050
C	-0.564893	0.567833	-0.195654
C	-1.971669	-0.004653	-0.077138
H	2.675017	-0.709005	0.047267
H	2.019865	0.742589	0.820567
H	2.123142	0.648430	-0.942007
H	0.322285	-1.105858	0.823793
H	0.412721	-1.204871	-0.931812
H	-0.452120	1.093314	-1.154025
H	-0.403714	1.317475	0.591703
H	-2.733892	0.769582	-0.185981
H	-2.111154	-0.477983	0.899720
H	-2.147430	-0.765671	-0.844479
