

ELECTRONIC SUPPLEMENTARY INFORMATION

Hybrid QTAIM and Electrostatic Potential-Based Quantum Topology Phase Diagrams for Water Clusters

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1. Complete tabulated list of topologies and topological features for W_n , $n = 7-10$

Table S1. The complete set of the critical point data for the four varying sets of critical points for the isomeric QTPDs of the heptamer molecular graphs W_n , $n = 7$. The numbers of QTAIM bond, ring and cage critical points are denoted by b , r and c respectively. The number of QTAIM hydrogen-bond BCPs are denoted by b_{HB} . The total number of BCPs is denoted b this includes the O-H sigma, H—O (b_{HB}) and O---O BCPs. The MESP critical points, the number of negative (3,+3) LCP critical points corresponding to the oxygen lone pairs are denoted by l . The bracketed values of b indicate the numbers of O---O BCPs. The topological complexity is denoted by the sum of the numbers of bond, ring and cage critical points; \sum_{brc} . The relative energy ΔE is listed in a.u., all the structures were optimized at the MP2/aug-cc-pvDZ level. of the critical point data for the four varying sets of critical points for the isomeric QTPD of the heptamer molecular graphs W_n , $n = 7$. The selection of critical point data can be found in the main Tables 1-4.

Molecular Graph	b	b_{HB}	r	c	l	\sum_{brc}	ΔE
H2O-7-1	24	10	5	1	4	30	0
H2O-7-2	24	10	4	0	4	28	0.0007
H2O-7-3	24	10	5	1	4	30	0.0010
H2O-7-t3	24	10	4	0	4	28	0.0018
H2O-7-t8	24	10	5	1	4	30	0.0024
H2O-7-t6	24	10	5	1	4	30	0.0025
H2O-7-4	23	9	3	0	5	26	0.0028
H2O-7-t29	24	10	4	0	4	28	0.0031
H2O-7-t18	23	9	3	0	5	26	0.0034
H2O-7-t21	23	9	3	0	5	26	0.0035
H2O-7-t5	24(1)	9	4	0	5	28	0.0039
H2O-7-t12	23	9	3	0	5	26	0.0040
H2O-7-5	23	9	3	0	5	26	0.0042
H2O-7-t28	24	10	4	0	4	28	0.0043
H2O-7-t7	24	10	5	1	5	30	0.0047
H2O-7-t11	22	8	2	0	6	24	0.0058
H2O-7-8	22	8	2	0	6	24	0.0058
H2O-7-t20	23	9	4	1	5	28	0.0060
H2O-7-t23	24	10	4	0	5	28	0.0060
H2O-7-t15	23(1)	8	3	0	6	26	0.0060
H2O-7-t16	25	11	6	1	5	32	0.0062
H2O-7-t1	25	11	6	1	5	32	0.0062
H2O-7-t2	23	9	3	0	5	26	0.0062
H2O-7-11	22	8	2	0	6	24	0.0064
H2O-7-6	22	8	2	0	6	24	0.0064
H2O-7-t13	23	9	3	0	5	26	0.0065
H2O-7-9	22	8	2	0	6	24	0.0068
H2O-7-10	22	8	2	0	6	24	0.0069
H2O-7-7	22	8	2	0	6	24	0.0069
H2O-7-t10	23	9	3	0	6	26	0.0074
H2O-7-13	22	8	2	0	6	24	0.0096
H2O-7-12	22	8	2	0	6	24	0.0096
H2O-7-t9	23	9	3	0	5	26	0.0103
H2O-7-t4	22	8	2	0	6	24	0.0105

Table S2. Critical point data for the isomeric QTPD of the octamer molecular graphs W_n , $n = 8$. See the caption of Table S1 for further details.

Molecular Graph	b	b_{HB}	r	c	l	\sum_{brc}	ΔE
H2O-8-1	28	12	6	1	4	35	0
H2O-8-2	28	12	6	1	4	35	3E-05
H2O-8-t23	27	11	5	1	5	33	0.0088
H2O-8-t2	27	11	5	1	5	33	0.0089
H2O-8-t15	27	11	5	1	5	33	0.0098
H2O-8-t22	28(1)	11	5	0	5	33	0.0106
H2O-8-t1	27	11	4	0	6	31	0.0131
H2O-8-t11	27	11	4	0	6	31	0.0134
H2O-8-t16	27	11	4	0	5	31	0.0147
H2O-8-t17	26	10	3	0	6	29	0.0147
H2O-8-t18	26	10	3	0	6	29	0.0159
H2O-8-t21	28(2)	10	6	1	6	35	0.0161
H2O-8-t14	26	10	3	0	6	29	0.0165
H2O-8-t8	28	12	6	1	7	35	0.0178
H2O-8-t10	26	10	3	0	6	29	0.0180
H2O-8-t7	28	12	5	0	8	33	0.0244

Table S3. Critical point data for the isomeric QTPD of the nonamer molecular graphs W_n , $n = 9$. See the caption of Table S1 for further details.

Molecular Graph	b	b_{HB}	r	c	l	\sum_{brc}	ΔE
H2O-9-1	31	13	6	1	5	38	0
H2O-9-2	31	13	6	1	5	38	0.0004
H2O-9-t12	31	13	6	1	5	38	0.0004
H2O-9-4	31	13	6	1	5	38	0.0006
H2O-9-5	31	13	6	1	5	38	0.0006
H2O-9-7	31	13	6	1	5	38	0.0009
H2O-9-6	31	13	6	1	5	38	0.0009
H2O-9-8	31	13	6	1	5	38	0.0012
H2O-9-t4	31	13	6	1	5	38	0.0042
H2O-9-t1	31	13	5	0	6	36	0.0082
H2O-9-t10	31	13	6	1	5	38	0.0107
H2O-9-t9	31	13	5	0	5	36	0.0110
H2O-9-t3	31	13	5	0	5	36	0.0113
H2O-9-t2	31	13	6	1	5	38	0.0112
H2O-9-t6	30	12	4	0	6	34	0.0133
H2O-9-t5	31	13	5	0	6	36	0.0163
H2O-9-t11	29	11	3	0	7	32	0.0177
H2O-9-t7	29	11	3	0	7	32	0.0194

Table S4. Critical point data for the isomeric QTPD of the decamer molecular graphs W_n , $n = 10$. See the caption of Table S1 for further details.

Molecular Graph	b	b_{HB}	r	c	l	\sum_{brc}	ΔE
H2O-10-1	35	15	7	1	5	43	0
H2O-10-2	35	15	7	1	5	43	0.0002
H2O-10-3	35	15	7	1	5	43	0.0011
H2O-10-4	35	15	7	1	5	43	0.0011
H2O-10-5	35	15	7	1	5	43	0.0012
H2O-10-6	35	15	7	1	5	43	0.0025
H2O-10-8	35	15	7	1	5	43	0.0026
H2O-10-7	35	15	7	1	5	43	0.0026
H2O-10-t8	35	15	7	1	5	43	0.0033
H2O-10-12	35	15	7	1	5	43	0.0034
H2O-10-9	35	15	7	1	5	43	0.0034
H2O-10-10	35	15	7	1	5	43	0.0034
H2O-10-14	35	15	7	1	5	43	0.0038
H2O-10-15	35	15	7	1	5	43	0.0038
H2O-10-20	35	15	7	1	5	43	0.0041
H2O-10-16	34	14	6	1	6	41	0.0042
H2O-10-25	35	15	7	1	5	43	0.0043
H2O-10-17	34	14	6	1	6	41	0.0044
H2O-10-19	34	14	6	1	6	41	0.0044
H2O-10-18	34	14	6	1	6	41	0.0045
H2O-10-21	34	14	6	1	6	41	0.0049
H2O-10-22	34	14	6	1	6	41	0.0049
H2O-10-t24	35	15	7	1	6	43	0.0053
H2O-10-27	34	14	6	1	6	41	0.0054
H2O-10-E18	35	15	8	2	6	45	0.0058
H2O-10-t26	34	14	5	0	6	39	0.0059
H2O-10-t5	35	15	7	1	5	43	0.0061
H2O-10-E15	35	15	7	1	6	43	0.0062
H2O-10-E8	35	15	7	1	7	43	0.0065
H2O-10-E11	35	15	7	1	7	43	0.0070
H2O-10-E1	35	15	7	1	6	43	0.0070
H2O-10-29	34	14	5	0	6	39	0.0072
H2O-10-28	34	14	6	1	6	41	0.0072
H2O-10-E2	35	15	7	1	7	43	0.0073
H2O-10-30	34	14	6	1	6	41	0.0075
H2O-10-E16	35	15	7	1	6	43	0.0082
H2O-10-t9	36	16	8	1	6	45	0.0088
H2O-10-E7	35	15	7	1	7	43	0.0089
H2O-10-t14	34	14	6	1	6	41	0.0089
H2O-10-t11	34	14	6	1	6	41	0.0090

H2O-10-t12	35	15	7	1	5	43	0.0096
H2O-10-E17	34	14	6	1	6	41	0.0099
Molecular Graphs	b	b_{HB}	r	c	l	\sum_{brc}	ΔE
H2O-10-t25	34	14	5	0	6	39	0.0118
H2O-10-t10	36(1)	15	8	1	5	45	0.0122
H2O-10-t15	34	14	6	1	6	41	0.0137
H2O-10-t7	35	15	7	1	6	43	0.0148
H2O-10-t17	34	14	5	0	6	39	0.0165
H2O-10-t27	36	16	7	0	6	43	0.0169
H2O-10-t23	37(2)	15	9	1	5	47	0.0170
H2O-10-t22	35	15	7	1	5	43	0.0181
H2O-10-t16	35	15	6	0	8	41	0.0182
H2O-10-t13	36(1)	15	8	1	7	45	0.0193
H2O-10-t28	33	13	4	0	8	37	0.0205
H2O-10-t18	33	13	4	0	7	37	0.0208

2. Ratio of hydrogen-bond $BCPs$ and lone pair CPs (b_{HB}/l)

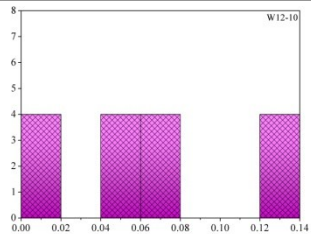
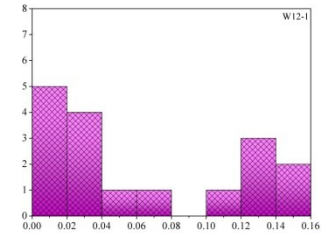
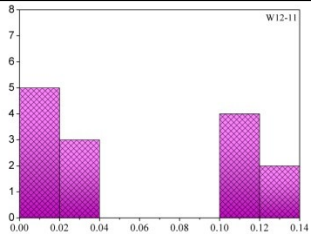
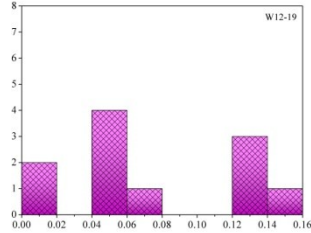
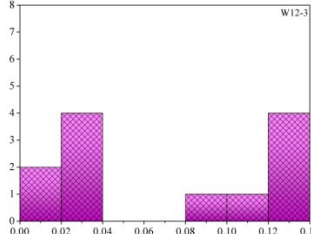
The use of ratio of hydrogen bonds to lone pairs in water clusters have been briefly mentioned in main article. Here we express this result, with the help of Table S5 where the value of (b_{HB}/l) may be seen to be maximum for each of the structures that correspond to global energy minimum. The results from Table S5 of the W_n , $n = 7-10$ hybrid topologies also reflect the pattern of higher b_{HB}/l values, including that of GM for even number water cluster $n = 8, 10$ in contrast with the odd numbered ones, $n = 7, 9$. This implies even-numbered water clusters could allow better utilization of the $LCPs$ in hydrogen-bonding, thus increasing the value of b_{HB}/l and increasing the overall relative energetic stability ΔE , see Tables S1-S4. This is in agreement with the literature where extra energetic stability has been reported amongst water clusters containing an even number of water monomers compared with those containing an odd number.

Table S5. The hybrid topologies expressed as the number of hydrogen-bond $BCPs$ (b_{HB}) from the QTAIM analysis and the numbers (l) of negative MESP (3,+3) $LCPs$ for the W_n , $n = 7-10$. The value of the ratio (b_{HB}/l) corresponding to the global minimum of each hybrid-QTPD are indicated in a bold font, see Figure 5.

Hybrid QTPD	b_{HB} W_n , $n = 7-10$	b_{HB}/l
W_7	$n + 1, n + 2, \mathbf{n + 3}, n + 4$	1.33, 1.78, 2.50 , 2.38
W_8	$n + 2, n + 3, \mathbf{n + 4}$	1.66, 2.22, 3.00
W_9	$n + 2, n + 3, \mathbf{n + 4}$	1.56, 2.00, 2.63
W_{10}	$n + 3, n + 4, \mathbf{n + 5}, n + 6$	1.85, 2.32, 3.00 , 2.63

3. Table of topological features including histogram for W_n , $n = 12$

Table S6: W_n , $n = 12$ clusters are arranged in order of decreasing energetic stability using MP2/3-21G (opt) energies. The number of hydrogen-bond BCPs (b_{HB}), lone pairs LCPs (l) and histograms of negative (3,+3) MESP critical points are provided. The x-axis of the histogram represents the negative valued (3,+3) critical points and the y-axis represents their count. The left hand side of x-axis starts with a value of 0 a.u. and stretches up to -0.14 a.u. (-0.16 a.u. in few cases), partitioned into the smaller segments of size 0.02 a.u. All the accounted critical points are negative valued although negative sign is not carried off in the histogram. The MP2/aug-cc-pvDZ energies belong to the structures which are successfully optimized starting with MP2/3-21G geometries.

Rank	Molecule	b_{HB}	l	Histogram	MP2/3-21G (opt)	MP2/aug-cc-pvDZ (opt)
1	W12-10	20	4		-908.9903133	-915.3306569
2	W12-1	18	6		-908.9621305	-915.3196938
3	W12-11	20	6		-908.9582291	-915.3163258
4	W12-19	18	4		-908.9560104	-915.3173443
5	W12-3	19	5		-908.9535198	-NC-

6	W12-7	18	5	<p>W12-7</p>	-908.95285	-915.3155026
7	W12-9	19	5	<p>W12-9</p>	-908.9487784	-915.3120727
8	W12-15	20	5	<p>W12-15</p>	-908.9485384	-915.3126055
9	W12-14	19	3	<p>W12-14</p>	-908.9478547	-915.3149325
10	W12-20	20	3	<p>W12-20</p>	-908.9405999	-NC-
11	W12-6	18	4	<p>W12-6</p>	-908.937249	-NC-
12	W12-17	19	6	<p>W12-17</p>	-908.9278839	-915.3041912

13	W12-5	18	5		-908.9259688	-NC-
14	W12-12	20	2		-908.9202275	-NC-

4. Coordinates of some of the most stable W_n , $n = 7-10$ cluster (H_2O)₇

H2O-7-1

O 1.0958991846 -1.2898738996 -1.3823317062
H 0.2880513219 -1.5745548180 -0.8627933679
H 1.2721231991 -2.0016908551 -2.0091729557
O 2.4704778884 0.0051103004 0.7217089558
H 2.2177830677 -0.6108896459 0.0056257004
H 2.4381927845 0.8626282645 0.2691618203
O 0.2004444154 -0.1647001125 2.2040900666
H 1.1018322829 -0.1042056082 1.8006749394
H 0.3421194263 -0.2160001167 3.1571320425
O -0.9658824724 -1.8490803435 0.1755725132
H -0.6926158543 -1.4332105111 1.0143158752
H -1.7365529340 -1.3113341008 -0.1112346088
O -1.0521594782 1.7740615360 0.4578616351
H -0.3338352257 1.7926632382 -0.2037735155
H -0.6757424503 1.2521424981 1.1902630930
O -2.8183564137 0.0259461020 -0.6705454535
H -3.7319958833 0.1735627133 -0.3987181303
H -2.2991826732 0.7602356578 -0.2619745201
O 1.0728196798 1.4751293134 -1.4605595132
H 1.0079975782 1.9416319467 -2.3031393738
H 1.0110519787 0.5214994396 -1.6835145303

H2O-7-2

O -0.9401233410 -1.3217030221 -1.5488870226
H -1.6889620132 -1.2534927150 -0.9305999180
H -0.2260184326 -1.6911048582 -0.9977835948
O -1.0704304975 1.4677971128 -1.3163989462
H -0.8760463369 0.5542947000 -1.6227040897

H -1.8542257667 1.3026731838 -0.7622030965
O -0.3658045649 -0.1556426767 1.9509623682
H 0.1658553197 -0.8757787214 1.5613020448
H 0.1046138669 0.6466398924 1.6585798941
O 2.8190917266 0.1155268141 -0.3518217562
H 2.2263899451 0.8677140178 -0.1275866176
H 3.0585559044 0.2557968536 -1.2766522525
O 0.8976189301 1.9445452051 0.4025828240
H 1.0401255324 2.8895678966 0.5370287894
H 0.1593920610 1.8691648426 -0.2674853863
O 1.1793405412 -1.9437252714 0.3155088191
H 1.8799456278 -1.3017272054 0.0459979024
H 1.6438489330 -2.7585968662 0.5421247399
O -2.6551504188 -0.1222889961 0.4865417730
H -1.9042002977 -0.1477228692 1.1310445551
H -3.4548167033 -0.2421973205 1.0125189904

H2O-7-3

O -0.9430556709 -1.8448817718 0.0178870617
H -0.7217480144 -1.4596170009 0.8864748065
H -1.7281669722 -1.3293017110 -0.2652278759
O 1.2158637887 1.5030226113 -1.3883203099
H 1.1754610792 0.5584729301 -1.6511563258
H 1.2915548205 2.0000115005 -2.2121000797
O 2.4491096953 -0.0315075267 0.8403363448
H 2.2402658404 -0.6313455745 0.0974746906
H 2.4378803847 0.8352720445 0.4043199277
O 0.0766366573 -0.2159174629 2.1587911817
H 0.1404914901 -0.2988071712 3.1180133975
H 1.0068812894 -0.1544021576 1.8296922733
O -1.0509064923 1.7847572772 0.3851179506
H -0.2956895086 1.7913658226 -0.2326719988
H -0.7280123829 1.2518471166 1.1351294542
O 1.2028624752 -1.2560687710 -1.3989163910
H 0.3608303776 -1.5404600654 -0.9348114122
H 1.4227766439 -1.9697621626 -2.0096092147
O -2.9333571976 0.0125371143 -0.5005854143
H -3.4972451085 0.3208425796 -1.2188393365
H -2.3506531353 0.7728823802 -0.2648488141

H2O-7-t3

O -1.6261227758 3.1166306362 -2.1961096821
H -2.0841074123 3.2169164243 -1.3414982359
H -2.3557200287 3.0015956675 -2.8297863089
O -3.6736277280 1.7017373733 -3.7422691135
H -4.3420119317 1.7910921797 -4.4319941254
H -4.1692808204 1.4780710044 -2.9157285836
O -3.1777051045 3.0007325106 0.2533182540
H -2.7329812371 2.3495168489 0.8463094701
H -3.3918444255 3.7592382192 0.8099531039
O -1.9578753811 0.9154581460 1.5031182707
H -2.1023178514 0.2212976768 0.8215143991
H -2.2408073846 0.5155556937 2.3344944170
O -4.6803351086 1.0918237578 -1.2888977157

H	-4.1312524658	0.3333052627	-1.0165898186
H	-4.3597560809	1.8154363705	-0.7181128948
O	-1.3149415603	0.3872855342	-2.7327310632
H	-1.1461020556	1.3122132653	-2.4466522120
H	-2.0328863143	0.5308566300	-3.3752551685
O	-2.5198078075	-0.7251879205	-0.6496740307
H	-2.3956868760	-1.6821942066	-0.6673467040
H	-2.0098321042	-0.3763789472	-1.4380641989

H2O-7-t8

O	1.3351384567	-1.7168646934	-0.4366468530
H	0.9238980257	-0.8369410378	-0.5124433594
H	0.6362010457	-2.2554957416	-0.0253718013
O	-1.2997540886	-0.4241912657	4.3482942446
H	-0.4680278233	-0.9306437603	4.2481547740
H	-1.0883720404	0.2937362281	4.9574366266
O	2.3368356030	-0.5550810257	1.8963055552
H	2.2419272030	-1.0898001787	1.0767747982
H	1.8351883135	0.2411935851	1.6416666960
O	0.3718774575	0.9149815584	0.4081460427
H	0.1565121413	1.7613542070	-0.0016703029
H	-0.4712686159	0.5984608546	0.8247886198
O	0.8828064439	-1.9961105064	3.5651715332
H	1.4892453282	-1.4330058889	2.9977146921
H	1.4675542469	-2.4945461821	4.1498974123
O	-0.6256248933	-2.8955918229	1.3988042002
H	-0.1169585614	-2.7816593632	2.2309258673
H	-1.0525863760	-3.7582109750	1.4709942377
O	-1.7683229369	-0.2384121988	1.5684565370
H	-1.6048583490	-1.1857692033	1.4105286460
H	-1.7334073140	-0.1714031918	2.5440738705

(H₂O)₈

H2O-8-1

H	2.1562222484	0.1988412771	0.3524763209
O	1.9275988805	0.1855327133	-1.3298385561
H	1.2890949454	0.9002393629	-1.5196099421
H	1.4316179099	-0.6327872862	-1.5269499850
O	-0.1991614913	2.0747136906	-1.3446437131
O	0.1856081597	-2.0632274116	-1.3641096252
O	2.0758651644	0.1868529523	1.3448037416
H	-1.4468347350	0.6456680002	-1.5069972563
H	-0.2022330689	2.1558128081	-0.3523084251
H	-0.2842906052	2.9727124747	-1.6871791568
H	0.2672405238	-2.9582910453	-1.7150751800
H	-1.3042741513	-0.8873711216	-1.5140664135
H	0.1986613791	-2.1527237994	-0.3725783766
H	2.9741279974	0.2688121368	1.6874206945
H	0.9013704898	-1.3029036828	1.5070433265
H	0.6469297704	1.4328092043	1.5197991705
O	0.1865704690	-1.9396399595	1.3117852456
H	-2.1525731480	-0.2018715540	0.3725142048
H	-0.8860986091	1.2901043933	1.5270237100

O -0.1732827500 1.9285153096 1.3299847095
H -0.6316620649 -1.4455822307 1.5140341231
O -2.0622496137 -0.1982588197 1.3640510029
O -1.9408092825 -0.1743294541 -1.3118275004
H -2.9570284230 -0.2831369523 1.7149718846

H2O-8-2

H -1.3490865106 -0.8137355835 1.5326065141
O -0.0627102875 -1.8997315757 1.3653619390
H 0.7509425539 -1.3817324235 1.5204375435
H 0.2745467058 -2.7061660372 -2.1007312563
O 2.0019963333 0.0637472373 1.4756559612
O -2.0020047048 -0.0637678604 1.4756549716
H -2.7061742818 -0.2745526363 2.1007385007
H -2.1384609909 0.0081017853 -0.4193274669
H -0.7509518251 1.3817049698 1.5203952199
O 0.0627014407 1.8997083502 1.3653255528
H 0.0080794291 2.1384782156 0.4193107693
H 1.3490868811 0.8137154801 1.5325904642
O 1.8996961897 -0.0627007406 -1.3653355172
O -1.8996987350 0.0627243223 -1.3653424759
H -1.3817003554 -0.7509337060 -1.5204103279
H -0.2745313173 2.7061917235 -2.1007526350
O 0.0637539515 -2.0020085625 -1.4756351274
H -0.0080893849 -2.1384908576 0.4193465062
H 0.8137151573 -1.3490815681 -1.5325924115
H 2.1384500051 -0.0080846191 -0.4193185529
H 2.7062036141 0.2745262504 2.1006935418
O -0.0637513670 2.0020271102 -1.4756632585
H -0.8137134110 1.3491023807 -1.5326072126
H 1.3817009004 0.7509583498 -1.5204082377

H2O-8-t23

H -3.3636854964 -1.3745548644 -1.0240110321
O -2.4760429175 -0.1431918387 -3.6696753455
H -2.7570528275 0.4499452884 -4.3773055829
H -1.9456469309 0.4150287940 -3.0644480020
O -3.0579946854 2.8175767557 -0.6947372571
O -1.2051738738 1.1456794864 -1.5369598225
O -4.1100771948 -1.1424818852 -1.6060651218
H -1.4043108768 -0.2807075646 -0.4419278938
H -3.8869307425 2.3052369530 -0.6170682295
H -2.8247976597 3.0269437128 0.2362457582
H -1.8797734706 1.8208174099 -1.2182637715
H -1.0530764524 -1.6304322260 0.2434917569
H -0.3649115523 1.6212407717 -1.5581711993
H -3.6647591248 -0.8624948537 -2.4324336956
H -2.5017930370 3.4326610785 2.7001131332
H -4.8641630880 0.1515312351 -0.8306314881
O -2.2505501569 2.8853601490 1.9466338730
H -2.8257046377 -0.1617777333 1.5045854463
H -6.1063123277 0.9688399858 -0.3468441308
O -5.1444679963 0.9324230553 -0.2798773559
H -2.6635345708 2.0030429506 2.1121704544
O -3.4353236285 0.4297411069 1.9829186097
O -1.7814807598 -1.0151140385 0.0939634196

H -4.1634413124 0.5566886715 1.3452956012

H2O-8-t2

H 2.1407756174 1.1970607769 -1.3177389818
O 1.3110125992 -1.0121069147 0.4007413819
H 1.9652180911 -0.5908430041 -0.2133304259
H 1.7252497662 -1.8301377453 0.7009618262
O 0.8554960506 2.3004429988 -1.0803701872
O -1.4991803453 1.2899951870 -2.4042134296
O 2.7665210573 0.4258642797 -1.3469692989
H -1.3208113796 -0.3414541102 -1.4066089613
H 0.5541564895 2.1112371498 -0.1644640402
H 0.1062355194 2.0272609591 -1.6410011498
H -1.7756864859 1.3751140936 -3.3247722569
H -0.3962246186 -1.0571784862 -0.3872431212
H -2.1493376312 1.8139191135 -1.8753829240
H 3.6393858165 0.8029954021 -1.1826632186
H -2.6803080503 3.3842456201 -0.2556802118
H 0.6175871460 0.5487516795 1.3795718299
O -3.0739088233 2.5730798112 -0.6031108038
H -2.1678418484 -0.1244837005 0.5447658000
H -0.7474789142 1.1895563079 1.6239455712
O 0.1911542764 1.4166406432 1.5007666916
H -3.0006345863 1.9246647620 0.1315184368
O -2.5494612601 0.5338501487 1.1902706020
O -1.3333822762 -0.9575685528 -0.6492861809
H -3.1865379671 0.0460960214 1.7262933884

H2O-8-t15

H -5.4825172870 2.6824888956 1.3719557468
O -3.5696507117 -0.2485459542 2.1710582247
H -4.1957018784 0.4759594314 1.9884411934
H -4.0868835411 -1.0664434115 2.0107990698
O -4.9494099497 -2.4866714849 1.2317408736
O -4.0298204692 -1.6028952178 -1.1982117057
O -5.1018596073 1.8882210075 0.9766861445
H -6.9755245362 0.0934583146 -1.0451270036
H -4.6066478117 -2.3491517378 0.3170754705
H -4.7968307600 -3.4185274686 1.4287335605
H -3.2181772208 -1.1305411329 -0.9320526207
H -5.9048105214 0.9476583647 -0.3090147966
H -4.7056921764 -0.9016269080 -1.2568688394
H -4.3373461071 2.2044326348 0.4115660417
H -2.5095196281 1.6259531692 -0.4986327133
H -2.4336576137 -0.1585187809 0.9250486158
O -3.0819324416 2.4042453919 -0.6506507385
H -5.1999959832 1.3274660745 -2.5468618938
H -1.0184443097 -0.2885176466 0.2654883232
O -1.9365883584 -0.0692539198 0.0650727549
H -3.4353859868 2.2797681019 -1.5554960125
O -4.5257033515 1.8613681884 -3.0094538226
O -6.0768836167 0.4348086310 -1.1328881875
H -4.1970247686 1.2878669102 -3.7134060506

(H₂O)₉

H2O-9-1

O -0.4054400308 1.0767620821 -1.9864131534
H 0.3331510255 1.4601291122 -1.4735391146
H -1.1995790891 1.3072111009 -1.4667251108
O -0.3709060283 -1.1006420839 2.1761891644
H -0.3412930260 -0.1075660081 2.1107941596
H -0.3714660285 -1.3049720991 3.1191832391
O -2.3690201791 -1.3724131042 0.1697110131
H -1.8033441359 -1.6407951252 -0.5805560418
H -1.7817691350 -1.4565341095 0.9461130718
O -0.4079120310 -1.5987761232 -1.8754211412
H -0.3988060304 -1.9987071527 -2.7534942110
H -0.3631670280 -0.6153050479 -2.0220641527
O 1.6086221221 2.0522251551 -0.2167140165
H 2.0631201579 2.8868642189 -0.3845160295
H 2.3251561795 1.3677031038 -0.1518680114
O -2.5423801964 1.2802741004 -0.1224100094
H -3.4484792660 1.6090531211 -0.1624740126
H -2.6109271978 0.2923650224 -0.0142400011
O 3.3175982539 -0.0026830002 -0.1160450088
H 4.0308013098 -0.1349870100 0.5197860398
H 2.6987222067 -0.7681560601 0.0213060016
O -0.4015440305 1.5377481167 1.7273301313
H -1.1979590923 1.6347171223 1.1699680871
H 0.3329260257 1.8072631380 1.1414810893
O 1.4948821136 -1.9453511473 0.2042910154
H 0.9010860677 -1.9451111496 -0.5718510443
H 0.9029800671 -1.7402171319 0.9538660742

H2O-9-2

O -0.4700290949 1.4727375698 1.7857040070
H -1.2693902738 1.5678192542 1.2319680600
H 0.2481791418 1.8013673308 1.2110835136
O 3.3535904667 0.0942277320 0.0086929332
H 2.7792256611 0.8873195374 -0.0513563946
H 3.9582538872 0.2731814883 0.7390504329
O 1.4770258741 -1.9667873821 0.0956084396
H 0.9565603378 -1.7680844578 0.8978287277
H 2.2005185594 -1.3048337192 0.1016172869
O 1.4513148449 2.1175326921 -0.2395805502
H 0.8069708832 1.7893069580 -0.9305373904
H 1.7018880353 3.0034383261 -0.5307005386
O -0.3855552924 1.1889738584 -1.9143739790
H -0.3094773451 0.2223114909 -2.0502703479
H -1.2342919154 1.2930687278 -1.4420984187
O -0.2547996217 -1.6282753894 -1.8782687868
H -0.1091585242 -2.2569295209 -2.5956961960
H 0.4638347085 -1.8079321133 -1.2071321418
O -2.3112958050 -1.4214760215 0.0708450139
H -1.7370541443 -1.5243991179 0.8546032228
H -1.7216708399 -1.6466118733 -0.6760561519
O -0.3484061329 -1.1850337422 2.1277691921
H -0.3516190739 -0.1905138947 2.0968298229
H -0.3579161673 -1.4193019497 3.0637887794
O -2.5816012001 1.2248915049 -0.1058888739
H -3.4976188717 1.5214067158 -0.1677595900

H -2.6170581025 0.2311360306 -0.0377090414

H2O-9-4

O 3.3360485161 0.1268603265 -0.2545654020
H 2.7449843529 -0.6637597078 -0.1424068540
H 4.0773587528 -0.0225933732 0.3442384689
O -2.5204759149 1.3260386718 -0.0320248816
H -3.2431284255 1.9241713624 -0.2576259690
H -1.8755022535 1.3713533526 -0.7904699671
O 1.5333594804 2.0982272689 -0.1448568881
H 2.2859856646 1.4506953847 -0.1537392107
H 1.9364059404 2.9623569628 -0.2943031426
O -0.5258932988 -1.6114658783 -1.8787243926
H -1.2476578743 -1.6648045373 -1.1950800559
H -0.7739513765 -2.2319907412 -2.5749920991
O -0.5809597776 1.2350297419 -1.8592506433
H -0.4525486595 0.2819783282 -2.0328677984
H 0.2268343239 1.5207709622 -1.3890885588
O -0.2358671949 -1.2520119924 2.1202554361
H -0.2471776511 -0.2561136238 2.1197271002
H -0.1991884777 -1.5159687104 3.0476488310
O -2.2733942307 -1.5026435775 0.1470106421
H -2.5683311334 -0.5712521585 0.1440993380
H -1.6969185053 -1.5566399403 0.9341432148
O 1.5822183576 -1.8828173140 0.0239149957
H 1.0134073043 -1.7506393731 0.8072605284
H 0.9516133190 -1.9015975553 -0.7215778098
O -0.3816454229 1.4016543700 1.8442701487
H -1.1984203126 1.5247164602 1.3226302782
H 0.3229744988 1.7291453257 1.2511647055

H2O-9-7

O 3.3336794319 0.2620525727 -0.2321379807
H 2.7299252279 1.0311105270 -0.1523847869
H 4.0491017726 0.4347676785 0.3918476813
O 1.6026406676 -1.9007484533 0.0219208137
H 2.2763483891 -1.1890403125 -0.0184731375
H 1.1230357696 -1.7508729414 0.8585199017
O -2.1807519952 -1.5499544525 0.2698421465
H -2.5203295921 -0.6419309240 0.1479835239
H -1.6761630518 -1.7173555635 -0.5507742373
O 1.3346322246 2.1847847809 -0.1128641090
H 1.5045036514 3.1330946898 -0.0503207142
H 0.7166609330 1.9739958081 0.6419584518
O -0.2597068739 -1.3185698535 2.1130213926
H -1.0302948850 -1.4883753872 1.5039543390
H -0.4374313885 -1.8335136792 2.9098365759
O -2.5679618735 1.2371503086 -0.0957974897
H -1.9289936382 1.2768848154 -0.8599641693
H -3.3316708655 1.7664338217 -0.3554375365
O -0.2772513910 -1.6567700973 -1.8331635914
H 0.4881485880 -1.7982879743 -1.2068456346
H -0.1341758094 -2.2691831969 -2.5650536529
O -0.4287437300 1.4949213521 1.7629726691
H -1.2805393558 1.4972223577 1.2845615685
H -0.3204914499 0.5630559702 2.0401363019

O -0.6417386475 1.1399517353 -1.9368941329
H 0.1388001533 1.5161230873 -1.4878846335
H -0.4379622744 0.1878533756 -2.0396195286

H2O-9-8

O 2.5544237361 1.2787515781 0.0326439537
H 1.9004447162 1.4104685156 0.7724281715
H 3.3048646670 1.8514784636 0.2315289786
O 0.4375491336 1.2540801282 -1.8721309287
H 1.2828177866 1.3269996418 -1.3883218180
H 0.3552268324 0.2976414339 -2.0592081357
O 2.2181020293 -1.5403740635 -0.0210033777
H 1.6763868091 -1.6061082127 0.7902645458
H 2.5428960543 -0.6192120165 -0.0017631497
O 0.5812999168 1.3985137665 1.8306111684
H 0.3782382051 0.4598788260 2.0204350277
H -0.1823554828 1.7189762112 1.3139530255
O -1.3694820231 2.1639284874 -0.1421878006
H -1.5816231073 3.0732811609 -0.3882132629
H -0.7377395233 1.8458680629 -0.8476295345
O 0.3563195993 -1.5838764922 -1.9428557855
H 1.1117678239 -1.6628576307 -1.2986670686
H 0.5711024966 -2.1736160294 -2.6760244292
O 0.2237935603 -1.3985450515 1.9984190951
H 0.0727697210 -1.9477369429 2.7773869660
H -0.5113711855 -1.6244719174 1.3597024889
O -1.5796598332 -1.9040303154 0.1248322955
H -1.0763897212 -1.8735223950 -0.7109257628
H -2.2671482934 -1.2102287124 0.0375182827
O -3.3700375337 0.2281979481 -0.0612763230
H -3.9987545420 0.3932849903 0.6519033169
H -2.7607118236 0.9971306112 -0.0520298934

(H₂O)₁₀

H2O-10-1

O -0.8375009073 2.3789661555 -1.2203051098
H -1.1576957629 3.1170848925 -1.7532273250
H -1.4922626122 1.6533357423 -1.3496053901
O 1.8109064916 1.3493089185 -1.3585473426
H 0.9240965783 1.7568440134 -1.3998428852
H 2.0630263560 1.4176092969 -0.4161786131
O -2.4820840102 0.1900809510 -1.2921342643
H -3.2536356578 0.0518085104 -1.8553876547
H -1.9186561871 -0.6294757426 -1.4055311437
O 1.7442480708 -1.2856212936 -1.7565605966
H 1.7970028356 -0.2915971333 -1.7068309265
H 2.3331885928 -1.5472567545 -2.4746365178
O 2.1956962888 1.0869874534 1.4302194743
H 2.1300979530 0.0931787318 1.4012827712
H 2.9410683102 1.2857484972 2.0097827426
O 1.9179967635 -1.5442088153 1.0892563697
H 1.0170638662 -1.8596716197 1.3064663369
H 1.9758151883 -1.6397505663 0.1197491644
O -2.1671829804 -0.0353979536 1.5997349818
H -2.5035732739 0.0941139377 0.6951985674

H -1.5713245613 0.7395121771 1.7323280887
O -0.7780076682 -2.2815422427 1.4147803312
H -1.1192751662 -2.9459060910 2.0256659712
H -1.3171314969 -1.4549550340 1.5792982835
O -0.9548023687 -1.9687958585 -1.3905340065
H -0.0228763463 -1.7891992916 -1.6301821103
H -0.9098554025 -2.2738415283 -0.4625545906
O -0.4473844479 2.1201515639 1.6569853402
H 0.4815535588 1.8201253731 1.6939842439
H -0.5574520096 2.4225237086 0.7383057377

H2O-10-2

O -1.6693940175 -1.3859804045 1.5911674275
H -2.0192761877 -1.4780996276 0.6871922744
H -1.6826253326 -0.4096380749 1.7323168014
O -2.1794357674 -1.2397721279 -1.2707743527
H -2.2104032358 -0.2588147483 -1.3682677571
H -2.8952119212 -1.5781875616 -1.8226020655
O 0.5171168534 -2.1587258548 -1.3923999595
H -0.4230842449 -1.8974273845 -1.4393742672
H 0.6511003381 -2.3911522820 -0.4519438496
O 0.5335932226 2.1533162239 -1.3451947665
H 1.1314292828 1.4225288779 -1.6032030137
H 0.7806132047 2.3434658076 -0.4181313189
O 2.1660541500 -0.1034468151 -1.7623198284
H 1.5627334428 -0.8961575701 -1.7297287066
H 2.7910881640 -0.2756792181 -2.4769424659
O 0.8070335589 -2.2949286543 1.4233164047
H 0.9450745456 -3.0322664316 2.0302526256
H -0.1276932896 -1.9775033907 1.5867990006
O -2.0224972631 1.4914707672 -1.2495421316
H -1.0637067290 1.7553485267 -1.3645161656
H -2.5273644427 2.1194427310 -1.7810063683
O 2.4555418077 -0.0325354240 1.0883015064
H 1.9495948102 -0.8413416282 1.3081492052
H 2.5622389697 -0.0800010853 0.1192753634
O 1.0511030287 2.2029975325 1.4347898353
H 1.5229390226 2.8260837403 2.0006227955
H 1.6125046004 1.3799281725 1.4095082388
O -1.6673919706 1.3695641197 1.6561164629
H -1.9419493102 1.5585508893 0.7413894281
H -0.7541052928 1.7140608901 1.6963695633

H2O-10-3

O -1.1318909688 -1.9813995641 1.3219540108
H -1.3013269780 -2.1470558719 0.3733919929
H -0.1585026326 -2.0009877532 1.4008595193
O 2.3918557756 0.7741160670 1.1815322610
H 2.3596845241 0.8661096317 0.1787649564
H 3.2369977642 1.1557813584 1.4508441206
O 1.7068724458 -1.8784572586 1.2915439512
H 2.0498006078 -0.9583230749 1.3791631357
H 2.2892812377 -2.4283103729 1.8297633736
O -0.2765467561 2.4985048883 -1.3191979605
H -0.1948756091 2.5433178667 -0.3277147204
H -0.3700801292 3.4114215600 -1.6183742344
O -2.1619769663 0.4500048516 1.6909930642

H -1.7959445393 -0.4759386384 1.6502603493
H -2.8128873033 0.4440010875 2.4033144104
O -0.0460837214 2.2760789268 1.3363474256
H 0.7809728918 1.7762555790 1.4748162468
H -0.7611135840 1.6656460085 1.6075053041
O 1.3260309776 -1.7515545481 -1.6068641265
H 0.3587683003 -1.8631968927 -1.6865561776
H 1.5137947762 -2.0050253332 -0.6861660938
O -1.5105449717 -1.8988009752 -1.4826975746
H -1.8671938743 -0.9690388612 -1.4621800868
H -2.0907003523 -2.3903768680 -2.0766623541
O -2.3828087708 0.6022333539 -1.1577310643
H -2.4902731711 0.6644610264 -0.1892677839
H -1.7206330757 1.2922512919 -1.3617994860
O 2.0860010413 0.8914753039 -1.4209909829
H 1.7980756578 -0.0265007839 -1.6364740014
H 1.3048174153 1.4517880034 -1.5897774006

H2O-10-6

O 0.9105877098 -1.2116790126 2.1298482872
H 0.8779085857 -1.4931066552 3.0523122373
H 0.8858488321 -0.2123839009 2.1430425122
O 1.0034838074 -1.4539598315 -1.9583065335
H 1.0292519189 -1.8458361800 -2.8397580667
H 0.9891605086 -0.4632138878 -2.0954521205
O -3.6952204776 -1.3009963692 0.1167354973
H -4.1290399810 -1.9565504377 -0.4424354192
H -2.7396215384 -1.5149508539 0.0694363420
O -0.9280908452 -1.4741330314 0.0518072298
H -0.3272139229 -1.6431306701 -0.7039197154
H -0.3629343673 -1.5575843629 0.8483379811
O 2.9437023058 -1.2483705544 0.1269905475
H 2.3626757884 -1.4117598880 0.8946208817
H 2.3944927240 -1.5020325683 -0.6395662267
O 0.9593347136 1.2005365348 -2.0063675755
H 1.7123879174 1.4698445154 -1.4462859994
H 0.1705430454 1.4318865996 -1.4722613103
O -3.8899052426 1.4592047348 -0.1816463980
H -4.3950662743 1.8227071283 0.5561585258
H -3.9640799964 0.4853507575 -0.0798130617
O 3.0093720859 1.4364392067 -0.0331570576
H 3.1255117015 0.4514378091 0.0290035027
H 3.8985162794 1.8110823583 -0.0355473893
O 0.8584401970 1.4311789679 1.8417828886
H 0.1045592378 1.5873845458 1.2346244504
H 1.6444309539 1.6333021870 1.2989085745
O -1.1147649197 1.3281990909 -0.1361476228
H -1.1367947274 0.3492205542 -0.0721258473
H -2.0640160180 1.5771231586 -0.1592191094

H2O-10-t8

O 0.0762972594 -1.6611270306 -0.2294472969
H -0.4493688853 -2.4513284402 -0.4048363549
H -0.0332393294 -1.4906783984 0.7311142083
O -2.7547248021 1.9450841298 3.4830752764
H -2.3755641120 1.8780937720 2.5833723034

H	-2.6466490170	1.0482089319	3.8505374398
O	-0.7505132535	0.7713699493	-1.3109275604
H	-0.1166806253	1.0896321649	-1.9652391735
H	-0.4267335655	-0.1196081847	-1.0525030888
O	-1.7829273664	-0.5343257362	4.6186862501
H	-1.0994190917	-0.0467631638	5.1556948038
H	-2.1895908904	-1.1709905105	5.2190114544
O	0.1206401660	0.9516586219	5.7653619445
H	0.8953895539	0.8409329710	5.1820386073
H	-0.1674990681	1.8726384309	5.6057845762
O	1.9277822510	0.5930723802	3.5829502642
H	2.7842028960	0.1606732361	3.4784469281
H	1.2797257193	0.0381159855	3.0826696808
O	-0.9225123433	3.3924199216	4.7936857749
H	-1.6891037850	2.9472623193	4.3395383614
H	-1.2880645632	4.1700642726	5.2326542365
O	0.8692819064	3.1025639301	2.5782396440
H	1.4216592121	2.3752681485	2.9185227823
H	0.3593571238	3.3922601577	3.3589004905
O	-0.1712736984	-0.6196385334	2.3315522444
H	-0.5518396827	0.2123239652	1.9418273560
H	-0.7764580573	-0.8276400650	3.0727648744
O	-1.0640460163	1.6926692543	1.2687500222
H	-0.9704555216	1.5732773100	0.2988023827
H	-0.3396724006	2.2925092983	1.5699787683