

Water Clusters to Nanodrops: A Tight-Binding Density Functional Study

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Figure 1. Structures of small water clusters (1-10).

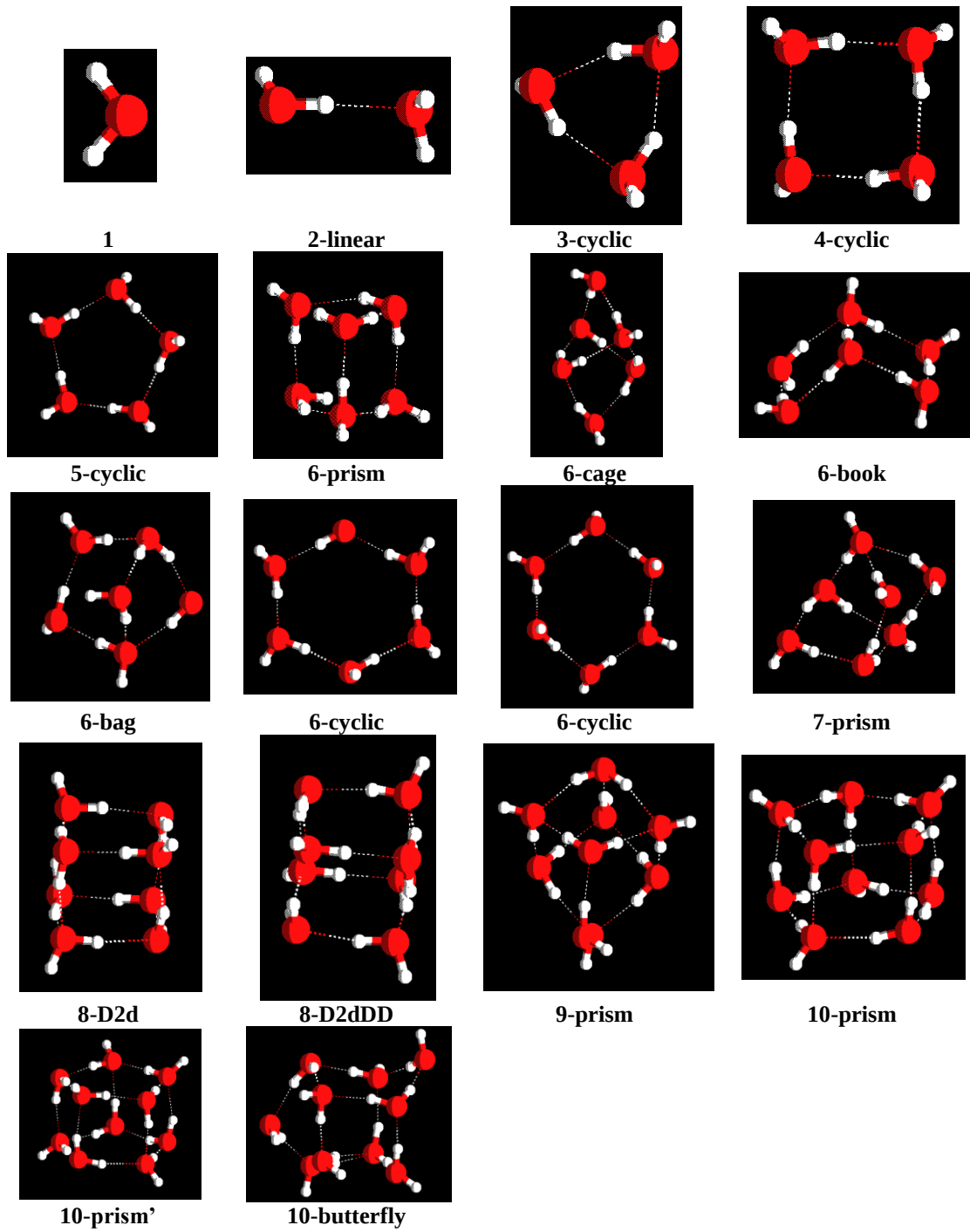


Figure 2. Structures of large water clusters (11-20).

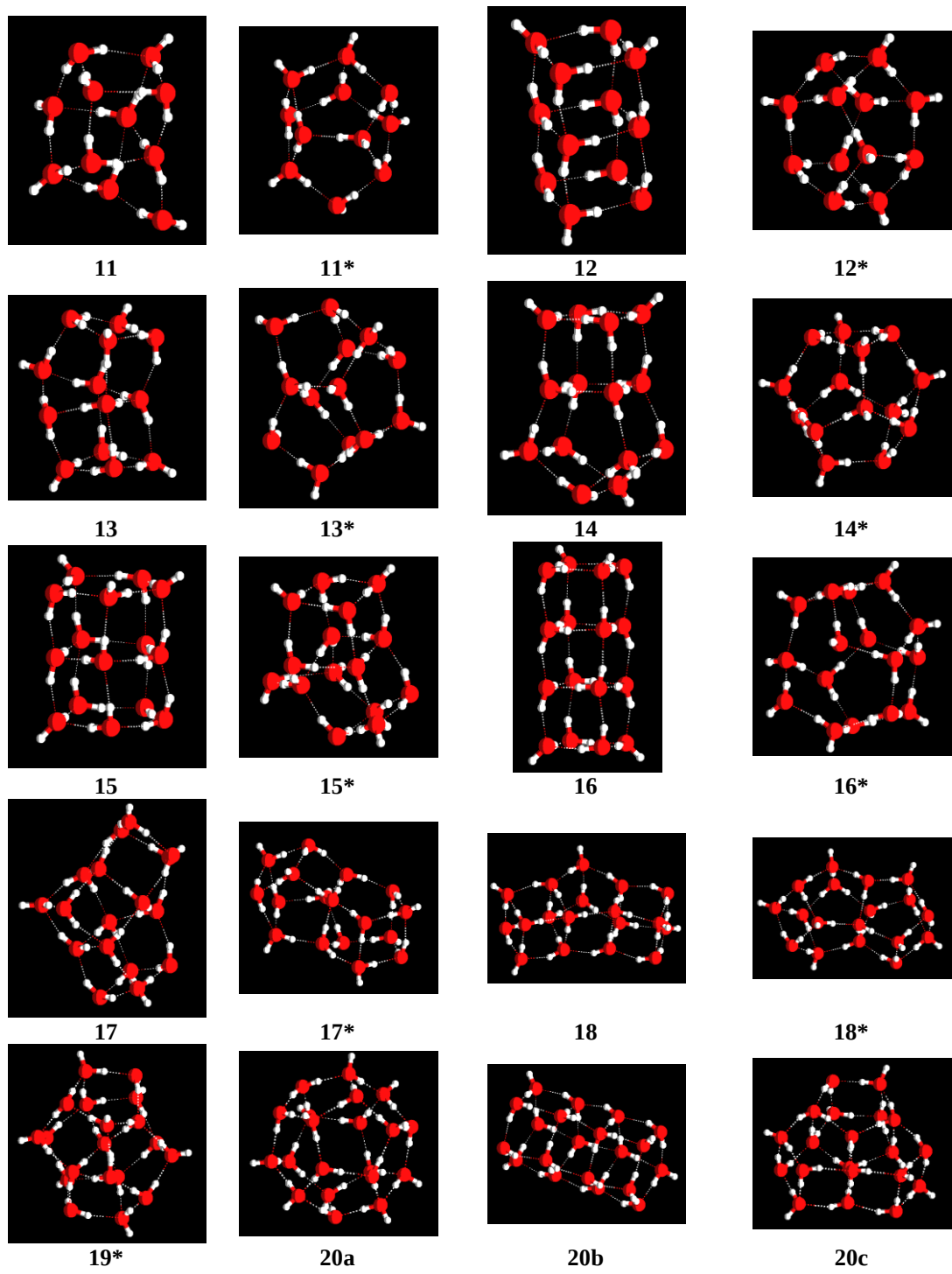


Figure 3. Structure of $(\text{H}_2\text{O})_{100}$ nanodrop.

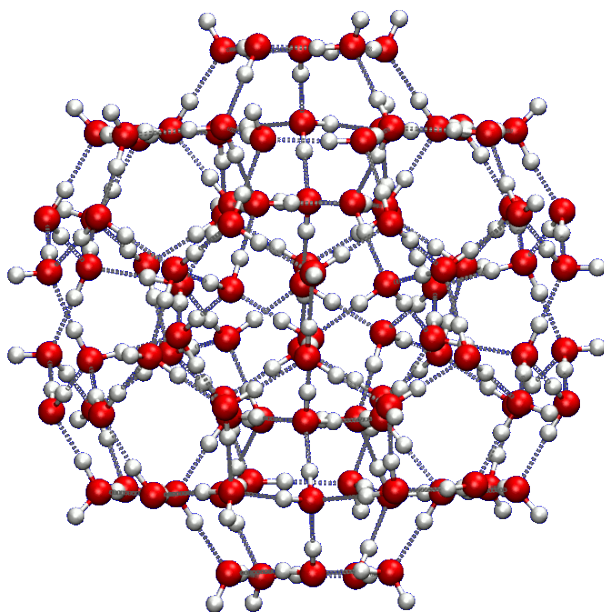


Table 1. Selected distances and angles for small water clusters (**1-10**) with the DFTB parameters implemented in Gaussian09 (DFTBA).

Label	Water Molecules	d(O-H)	d (O...H)	a (H-O-H)
1	1	0.966	-	107.24
2-cyclic	2	0.969	1.890	106.98
3-cyclic	3	0.974	1.883	106.79
4-cyclic	4	0.978	1.765	106.47
5-cyclic	5	0.979	1.756	106.37
6-prims	6	0.979	1.890	106.03
6-cage	6	0.979	1.830	106.52
6-book	6	0.979	1.788	106.50
6-bag	6	0.979	1.800	106.42
6-cyclic	6	0.979	1.756	106.19
6-cyclic	6	0.978	1.758	106.32
7-prism	7	0.980	1.844	106.33
8-D2d	8	0.982	1.818	106.37
8-D2dDD	8	0.982	1.812	106.37
9-Prism	9	0.982	1.800	106.35
10-Prism	10	0.982	1.799	106.37
10-Prism'	10	0.982	1.807	106.27
10-butterfly	10	0.981	1.844	106.16

Table 2. Total binding energies for small water clusters (1-10) optimized with the DFTB parameters implemented in Gaussian09 (DFTBA).

Label	Water Molecules	HB	DFTB	DFT (M06-L)	DFTB+E
1	1	-	0.0	0.0	0.0
2-cyclic	2	1	-3.3	-4.8	-5.5
3-cyclic	3	3	-9.5	-15.7	-16.2
4-cyclic	4	4	-17.6	-27.4	-26.6
5-cyclic	5	5	-23.0	-35.1	-34.1
6-prims	6	9	-29.4	-46.8	-48.0
6-cage	6	8	-29.2	-46.6	-46.8
6-book	6	7	-28.8	-44.3	-44.4
6-bag	6	7	-28.2	-43.6	-43.7
6-cyclic	6	6	-28.2	-43.4	-41.6
6-cyclic	6	6	-27.6	-42.2	-41.1
7-prism	7	10	-36.6	-57.7	-57.9
8-D2d	8	12	-46.1	-73.9	-72.7
8-D2dDD	8	12	-46.1	-73.6	-74.0
9-Prism	9	13	-51.9	-82.0	-80.7
10-Prism	10	15	-58.9	-92.5	-92.2
10-Prism'	10	15	-59.1	-92.3	-92.3
10-butterfly	10	15	-54.9	-86.1	-87.2

Table 3. Selected distances and angles for small water clusters (**1-10**) optimized at DFTB (mio-0-1 parameters).

Label	Water Molecules	d(O-H)	d (O...H)	a (H-O-H)
1	1	0.967	-	107.19
2-cyclic	2	0.971	1.889	106.93
3-cyclic	3	0.975	1.882	106.74
4-cyclic	4	0.979	1.785	106.42
5-cyclic	5	0.979	1.780	106.32
6-prims	6	0.980	1.898	106.00
6-cage	6	0.980	1.841	106.48
6-book	6	0.980	1.805	106.45
6-bag	6	0.979	1.816	106.38
6-cyclic	6	0.979	1.780	106.15
6-cyclic	6	0.979	1.781	106.27
7-prism	7	0.981	1.856	106.30
8-D2d	8	0.982	1.826	106.33
8-D2dDD	8	0.982	1.826	106.30
9-Prism	9	0.982	1.817	106.31
10-Prism	10	0.983	1.819	106.31
10-Prism'	10	0.983	1.819	106.27
10-butterfly	10	0.982	1.849	106.17

Table 4. Total binding energies for small water clusters (**1-10**) optimized at DFTB (mio-0-1 parameters).

Label	Water Molecules	HB	DFTB	DFT (M06-L)	DFTB+E
1	1	-	0.0	0.0	0.0
2-cyclic	2	1	-3.3	-4.8	-5.5
3-cyclic	3	3	-9.6	-15.7	-16.3
4-cyclic	4	4	-17.7	-27.5	-26.6
5-cyclic	5	5	-23.0	-35.1	-34.1
6-prims	6	9	-29.6	-46.8	-48.2
6-cage	6	8	-29.4	-46.6	-46.8
6-book	6	7	-28.9	-44.3	-44.4
6-bag	6	7	-28.3	-43.5	-43.7
6-cyclic	6	6	-28.2	-43.3	-41.5
6-cyclic	6	6	-27.7	-42.1	-41.0
7-prism	7	10	-36.7	-57.7	-58.0
8-D2d	8	12	-46.3	-73.9	-72.7
8-D2dDD	8	12	-46.2	-73.5	-72.6
9-Prism	9	13	-52.1	-81.9	-80.8
10-Prism	10	15	-59.3	-92.7	-92.2
10-Prism'	10	15	-59.3	-92.2	-92.2
10-butterfly	10	15	-55.3	-86.3	-87.3

Table 5. Selected distances and angles for small water clusters (**1-10**) with mio-1-1 parameters.

Label	Water Molecules	d(O-H)	d (O...H)	a (H-O-H)
1	1	0.967	-	107.19
2-cyclic	2	0.971	1.889	106.93
3-cyclic	3	0.975	1.882	106.74
4-cyclic	4	0.979	1.785	106.42
5-cyclic	5	0.979	1.779	106.32
6-prims	6	0.980	1.898	106.00
6-cage	6	0.980	1.841	106.47
6-book	6	0.980	1.805	106.45
6-bag	6	0.979	1.816	106.38
6-cyclic	6	0.979	1.779	106.14
6-cyclic	6	0.979	1.780	106.27
7-prism	7	0.981	1.855	106.30
8-D2d	8	0.982	1.826	106.33
8-D2dDD	8	0.982	1.826	106.30
9-Prism	9	0.982	1.816	106.31
10-Prism	10	0.983	1.818	106.31
10-Prism'	10	0.983	1.819	106.27
10-butterfly	10	0.982	1.848	106.17

Table 6. Total binding energies for small water clusters (**1-10**) optimized at DFTB (mio-1-1 parameters).

Label	Water Molecules	HB	DFTB	DFT (M06-L)	DFTB+E
1	1	-	0.0	0.0	0.0
2-cyclic	2	1	-3.3	-4.8	-5.5
3-cyclic	3	3	-9.6	-15.7	-16.3
4-cyclic	4	4	-17.7	-27.5	-26.6
5-cyclic	5	5	-23.0	-35.1	-34.1
6-prims	6	9	-29.6	-46.8	-48.2
6-cage	6	8	-29.4	-46.6	-46.8
6-book	6	7	-28.9	-44.3	-44.4
6-bag	6	7	-28.3	-43.5	-43.7
6-cyclic	6	6	-28.2	-43.3	-41.5
6-cyclic	6	6	-27.7	-42.1	-41.0
7-prism	7	10	-36.7	-57.7	-58.0
8-D2d	8	12	-46.3	-73.9	-72.7
8-D2dDD	8	12	-46.2	-73.5	-73.8
9-Prism	9	13	-52.1	-81.9	-80.8
10-Prism	10	15	-59.3	-92.7	-92.2
10-Prism'	10	15	-59.2	-92.2	-92.2
10-butterfly	10	15	-55.3	-86.3	-87.3

Table 7. Selected distances and angles for small water clusters (**1-10**) with pbc-0-1 parameters.

Label	Water Molecules	d(O-H)	d (O...H)	a (H-O-H)
1	1	0.957	-	103.04
2-cyclic	2	0.959	1.909	102.64
3-cyclic	3	0.963	1.914	102.24
4-cyclic	4	0.966	1.792	101.78
5-cyclic	5	0.967	1.782	101.67
6-prims	6	0.967	1.911	101.57
6-cage	6	0.967	1.859	101.87
6-book	6	0.967	1.818	101.81
6-bag	6	0.967	1.830	101.78
6-cyclic	6	0.967	1.780	101.52
6-cyclic	6	0.966	1.785	101.63
7-prism	7	0.967	1.870	101.72
8-D2d	8	0.969	1.842	101.62
8-D2dDD	8	0.969	1.842	101.67
9-Prism	9	0.969	1.829	101.59
10-Prism	10	0.969	1.835	101.59
10-Prism'	10	0.969	1.835	101.60
10-butterfly	10	0.968	1.866	101.55

Table 8. Total binding energies for small water clusters (**1-10**) optimized at DFTB (pbc-0-1 parameters).

Label	Water Molecules	HB	DFTB	DFT (M06-L)	DFTB+E
1	1	-	0.0	0.0	0.0
2-cyclic	2	1	-3.2	-4.6	-5.4
3-cyclic	3	3	-9.0	-15.0	-15.7
4-cyclic	4	4	-16.8	-26.4	-25.8
5-cyclic	5	5	-22.1	-34.0	-33.3
6-prims	6	9	-28.3	-45.9	-47.2
6-cage	6	8	-27.7	-45.2	-45.4
6-book	6	7	-27.5	-42.9	-43.1
6-bag	6	7	-27.0	-42.3	-42.5
6-cyclic	6	6	-27.2	-42.0	-40.6
6-cyclic	6	6	-26.6	-40.8	-40.1
7-prism	7	10	-34.9	-56.2	-56.4
8-D2d	8	12	-44.0	-71.3	-70.6
8-D2dDD	8	12	-43.9	-71.3	-71.5
9-Prism	9	13	-49.6	-79.2	-78.5
10-Prism	10	15	-56.4	-89.8	-89.7
10-Prism'	10	15	-56.5	-89.8	-89.7
10-butterfly	10	15	-52.5	-84.2	-85.1

Table 9. Selected distances and angles for small water clusters (**1-10**) with pbc-0-2 parameters.

Label	Water Molecules	d(O-H)	d (O...H)	a (H-O-H)
1	1	0.965	-	107.46
2-cyclic	2	0.968	1.894	107.21
3-cyclic	3	0.972	1.891	107.03
4-cyclic	4	0.976	1.772	106.73
5-cyclic	5	0.976	1.767	106.64
6-prims	6	0.976	1.901	106.29
6-cage	6	0.977	1.841	106.78
6-book	6	0.977	1.799	106.76
6-bag	6	0.976	1.813	106.68
6-cyclic	6	0.976	1.767	106.46
6-cyclic	6	0.976	1.768	106.59
7-prism	7	0.977	1.856	106.59
8-D2d	8	0.979	1.825	106.62
8-D2dDD	8	0.979	1.826	106.60
9-Prism	9	0.979	1.812	106.60
10-Prism	10	0.979	1.817	106.60
10-Prism'	10	0.979	1.818	106.56
10-butterfly	10	0.978	1.849	106.46

Table 10. Total binding energies for small water clusters (**1-10**) optimized at DFTB (pbc-1-1 parameters).

Label	Water Molecules	HB	DFTB	DFT (M06-L)	DFTB+E
1	1	-	0.0	0.0	0.0
2-cyclic	2	1	-3.3	-4.8	-5.5
3-cyclic	3	3	-9.5	-15.8	-16.3
4-cyclic	4	4	-17.5	-27.5	-26.6
5-cyclic	5	5	-22.8	-35.2	-34.2
6-prims	6	9	-29.3	-47.0	-48.3
6-cage	6	8	-29.0	-46.8	-47.0
6-book	6	7	-28.6	-44.5	-44.5
6-bag	6	7	-28.0	-43.7	-43.9
6-cyclic	6	6	-28.0	-43.5	-41.7
6-cyclic	6	6	-27.5	-42.3	-41.1
7-prism	7	10	-36.4	-57.9	-58.1
8-D2d	8	12	-45.9	-74.2	-73.0
8-D2dDD	8	12	-45.8	-73.8	-74.2
9-Prism	9	13	-51.7	-82.3	-81.1
10-Prism	10	15	-58.8	-93.1	-92.7
10-Prism'	10	15	-58.8	-92.7	-92.6
10-butterfly	10	15	-54.7	-86.6	-87.6

Table 11. Selected distances and angles for small water clusters (**1-10**) with pbc-0-3 parameters.

Label	Water Molecules	d(O-H)	d (O...H)	a (H-O-H)
1	1	0.965	-	107.47
2-cyclic	2	0.968	1.894	107.21
3-cyclic	3	0.972	1.891	107.03
4-cyclic	4	0.976	1.772	106.74
5-cyclic	5	0.976	1.767	106.64
6-prims	6	0.976	1.901	106.29
6-cage	6	0.977	1.841	106.77
6-book	6	0.977	1.799	106.75
6-bag	6	0.976	1.812	106.68
6-cyclic	6	0.976	1.767	106.45
6-cyclic	6	0.976	1.768	106.59
7-prism	7	0.977	1.855	106.59
8-D2d	8	0.979	1.825	106.62
8-D2dDD	8	0.979	1.826	106.60
9-Prism	9	0.979	1.813	106.61
10-Prism	10	0.979	1.818	106.60
10-Prism'	10	0.979	1.818	106.56
10-butterfly	10	0.978	1.850	106.46

Table 12. Total binding energies for small water clusters (**1-10**) optimized at DFTB (pbc-0-3 parameters).

Label	Water Molecules	HB	DFTB	DFT (M06-L)	DFTB+E
1	1	-	0.0	0.0	0.0
2-cyclic	2	1	-3.3	-4.8	-5.5
3-cyclic	3	3	-9.5	-15.8	-16.3
4-cyclic	4	4	-17.5	-27.5	-26.6
5-cyclic	5	5	-22.8	-35.2	-34.2
6-prims	6	9	-29.3	-47.0	-48.3
6-cage	6	8	-29.0	-46.8	-47.0
6-book	6	7	-28.6	-44.5	-44.5
6-bag	6	7	-28.0	-43.7	-43.9
6-cyclic	6	6	-28.0	-43.5	-41.7
6-cyclic	6	6	-27.5	-42.3	-41.1
7-prism	7	10	-36.4	-57.9	-58.1
8-D2d	8	12	-45.9	-74.2	-73.0
8-D2dDD	8	12	-45.8	-73.8	-74.2
9-Prism	9	13	-51.7	-82.3	-81.1
10-Prism	10	15	-58.8	-93.1	-92.7
10-Prism'	10	15	-58.8	-92.7	-92.7
10-butterfly	10	15	-54.7	-86.7	-87.6

Table 13. Hydrogen bond energy correction for different DFTB parameters.

$$E(r_{O-H}) = A \cdot \exp^{B \cdot (r_{O-H} - C)^2}$$

Parameters	A	B	C
DFTBA	-2.266	-5.500	1.8141176
mio-0-1	-2.237	-5.500	1.8275882
mio-1-1	-2.237	-5.500	1.8271176
pbc-0-1	-2.275	-5.500	1.8411176
pbc-0-2	-2.306	-5.500	1.8243529
pbc-0-3	-2.307	-5.500	1.8244706

Table 14. Cartesian coordinates of small water clusters (**1-10**) optimized with the DFTB parameters implemented in Gaussian09 (DFTBA).

	Label	Name
	1	1
	2-cyclic	2
	3-cyclic	3
	4-cyclic	4
	5-cyclic	5
	6-prims	6a
	6-cage	6b
	6-book	6c
	6-bag	6d
	6-cyclic	6e
	6-cyclic	6f
	7-prism	7
	8-D2d	8a
	8-D2dDD	8b
	9-Prism	9
	10-Prism	10a
	10-Prism'	10b
	10-butterfly	10c

1	E= -4.077786 hartree		
	O	0.000000	-0.114557 -0.000002
	H	0.777546	0.458229 0.000019
	H	-0.777546	0.458229 -0.000002

2	E= -8.160809 hartree		
	O	0.003747	1.487634 0.000000
	H	0.910720	1.822487 0.000000
	H	0.063966	0.513143 0.000000
	O	0.003747	-1.375820 0.000000
	H	-0.517322	-1.615073 0.778157
	H	-0.517322	-1.615073 -0.778157

3	E= -12.248533 hartree		
	O	1.129783	-1.139034 -0.096630
	H	1.176320	-0.159432 -0.064717
	H	1.600152	-1.467064 0.682989
	O	0.431359	1.541415 0.117828
	H	0.478203	2.053842 -0.701980
	H	-0.448390	1.108413 0.127251
	O	-1.563321	-0.385340 -0.085746
	H	-0.763901	-0.935395 -0.215834
	H	-2.024949	-0.736687 0.688669

4	E= -16.339214 hartree		
	O	1.370984	-1.370984 0.005959
	H	0.389428	-1.479300 0.047188
	H	1.661504	-1.807765 -0.808141
	O	-1.370984	1.370984 0.005959
	H	-1.661504	1.807765 -0.808141
	H	-0.389428	1.479300 0.047188
	O	1.370984	1.370984 -0.005959
	H	1.479300	0.389428 -0.047188
	H	1.807765	1.661504 0.808141
	O	-1.370984	-1.370984 -0.005959
	H	-1.479300	-0.389428 -0.047188
	H	-1.807765	-1.661504 0.808141

5 E= -20.425531 hartree

O	1.011922	2.092227	0.085367
H	1.496540	1.238658	-0.036916
H	1.342523	2.476814	0.910275
O	0.419704	-2.280928	0.043762
H	-0.476952	-1.863882	0.013438
H	0.440225	-2.824784	0.844848
O	-1.678633	1.597447	-0.166185
H	-2.099333	2.204020	0.460255
H	-0.711231	1.797402	-0.148994
O	2.318177	-0.308272	-0.092045
H	1.645544	-1.027558	-0.000012
H	2.775290	-0.469315	-0.930570
O	-2.056395	-1.108783	0.071970
H	-1.929410	-0.129012	0.040486
H	-2.601400	-1.335867	-0.695762

6a E= -24.513616 hartree

O	1.214321	-1.142543	1.284952
H	1.209862	-1.498182	0.366370
H	1.650461	-0.273353	1.194472
O	-0.890733	1.918871	0.027214
H	-1.168030	1.313310	0.742573
H	-1.223835	1.512928	-0.791565
O	1.089992	-1.139296	-1.432830
H	1.524307	-0.280814	-1.266785
H	0.138027	-0.943134	-1.551090
O	-1.675409	-0.471533	-1.303947
H	-2.294472	-1.096865	-1.708426
H	-1.726036	-0.595092	-0.330808
O	-1.382274	-0.466408	1.461993
H	-0.423287	-0.745591	1.480708
H	-1.797997	-0.830944	2.258710
O	1.763445	1.274014	-0.064860
H	0.827661	1.596055	-0.028093
H	2.328609	2.056840	-0.146249

6b E= -24.513238 hartree

O	-2.865809	0.007590	0.178134
H	-3.402298	-0.794516	0.256056
H	-2.160420	-0.050972	0.866338
O	-0.809448	0.245463	-1.650188
H	-1.676214	0.209814	-1.184245
H	-0.345486	-0.585022	-1.420692
O	0.764714	-1.741614	-0.354860
H	1.575418	-1.181940	-0.260439
H	1.059105	-2.634540	-0.589245
O	0.626135	1.762475	0.046784
H	0.496879	2.713674	-0.090812
H	0.096892	1.293796	-0.658129
O	-0.577781	-0.250241	1.655438
H	-0.152757	0.584022	1.374892
H	-0.180799	-0.947540	1.096369
O	2.786726	0.045449	0.075947
H	3.130338	0.036394	0.981143
H	2.163046	0.803849	0.018728

6c E= -24.512577 hartree

O	-2.308540	-1.358648	-0.458423
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H	-3.127642	-1.626298	-0.017012
H	-2.355084	-0.380293	-0.571090
O	2.068355	-1.598902	-0.413058
H	1.738826	-2.111433	-1.166285
H	1.332964	-1.577389	0.253607
O	-0.090099	-1.240251	1.189770
H	-0.065338	-0.264732	1.265225
H	-0.874957	-1.446019	0.630556
O	2.372216	1.090946	-0.637232
H	3.250871	1.290530	-0.281261
H	2.303846	0.101930	-0.669780
O	-2.227795	1.396659	-0.546731
H	-2.016245	1.762805	-1.417541
H	-1.435150	1.534177	0.016614
O	0.169405	1.589804	0.874200
H	0.409572	2.194456	1.592195
H	0.970000	1.485400	0.296565

6d E= -24.511607 hartree

O	0.923634	1.817388	0.337714
H	1.427151	1.378197	-0.383155
H	0.993907	1.207592	1.105158
O	1.947753	0.018883	-1.525886
H	1.551078	0.105559	-2.403931
H	1.513293	-0.741246	-1.090312
O	-2.208992	-1.012083	-0.200244
H	-2.796022	-1.201280	-0.947512
H	-2.066352	-0.030053	-0.201233
O	-1.678917	1.648946	-0.359167
H	-2.145094	2.314555	0.168711
H	-0.709591	1.758837	-0.154669
O	0.344340	-1.939641	-0.233988
H	-0.604725	-1.650270	-0.259881
H	0.349470	-2.904790	-0.147575
O	0.874819	-0.381783	2.048076
H	0.023267	-0.459665	2.501058
H	0.842531	-0.991116	1.281300

6e E= -24.511609 hartree

O	-2.371957	1.369450	0.049936
H	-2.906692	1.547619	0.837441
H	-2.325399	0.385529	-0.034860
O	0.000000	-2.738900	0.049936
H	0.828822	-2.206619	-0.034860
H	0.113068	-3.291078	0.837441
O	0.000000	2.738900	-0.049936
H	-0.113068	3.291078	-0.837441
H	-0.828822	2.206619	0.034860
O	2.371957	-1.369450	-0.049936
H	2.325399	-0.385529	0.034860
H	2.906692	-1.547619	-0.837441
O	2.371957	1.369450	0.049936
H	2.793623	1.743459	0.837441
H	1.496577	1.821090	-0.034860
O	-2.371957	-1.369450	-0.049936
H	-2.793623	-1.743459	-0.837441
H	-1.496577	-1.821090	0.034860

6f E= -24.510774 hartree

O	1.306070	2.136082	-0.557562
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H	0.391091	2.125484	-0.184671
H	1.669434	3.013329	-0.368168
O	1.177839	-2.214944	0.610486
H	1.208721	-2.209544	1.578336
H	1.776715	-1.486747	0.310771
O	2.799057	-0.117473	-0.075140
H	2.252878	0.696573	-0.197754
H	3.269699	-0.256668	-0.910015
O	-1.305613	-2.135939	-0.558445
H	-1.669123	-3.013180	-0.369293
H	-0.391322	-2.124941	-0.183842
O	-1.179681	2.216303	0.606625
H	-1.213324	2.214453	1.574395
H	-1.777707	1.487010	0.307881
O	-2.799620	0.116970	-0.076441
H	-3.270692	0.255557	-0.911177
H	-2.253018	-0.696816	-0.198967

7 E= -28.602759 hartree

O	1.123983	1.698281	-1.027125
H	1.067768	0.780275	-1.375255
H	1.032146	2.297992	-1.782133
O	-1.015478	-1.858552	-0.184061
H	-1.745456	-1.250841	-0.453884
H	-0.736561	-1.562166	0.707374
O	1.107857	-1.024177	-1.599176
H	1.242730	-1.589039	-2.375909
H	0.306212	-1.381537	-1.118838
O	0.133409	-0.549332	2.053500
H	1.026934	-0.426619	1.638915
H	0.280657	-0.803013	2.977157
O	-1.043690	1.679220	0.782579
H	-0.294336	1.842598	0.170462
H	-0.737338	0.980244	1.396851
O	-2.783392	0.185577	-0.685997
H	-2.214959	0.834535	-0.199422
H	-3.643062	0.180641	-0.240105
O	2.454723	-0.136976	0.700277
H	2.366290	0.795034	0.436742
H	2.229684	-0.650432	-0.101938

8a E= -32.695809 hartree

O	-1.980628	-0.016281	1.391323
O	-0.024585	2.072140	-1.256681
O	-0.083603	-1.989034	-1.378257
O	2.089886	-0.072990	1.241804
H	-2.071651	0.018224	0.399633
H	0.016818	2.099514	-0.261809
H	-0.049456	-2.067753	-0.385807
H	2.110362	-0.038352	0.246686
H	-2.878271	-0.027361	1.757384
H	-0.026816	2.990994	-1.566290
H	-0.090423	-2.891712	-1.732396
H	3.010719	-0.087504	1.544835
O	-1.993740	0.073179	-1.313786
O	0.082970	1.887491	1.447184
O	0.025443	-1.979090	1.329073
O	1.883145	0.023230	-1.459427
H	-1.418575	0.852479	-1.470657
H	-0.702740	1.324747	1.615661

H	0.823281	-1.425888	1.469225
H	-1.445847	-0.711105	-1.529167
H	1.321546	0.821186	-1.560680
H	-0.739445	-1.400450	1.534960
H	0.859492	1.295940	1.545488
H	1.289901	-0.742111	-1.616920

8b	E= -32.695723 hartree		
O	1.432745	1.151535	1.566225
H	1.465671	0.156781	1.508261
H	2.079263	1.417608	2.237837
O	-1.454150	-1.541287	1.158442
H	-2.111974	-2.200464	1.427885
H	-1.490841	-1.482872	0.163842
O	-1.375570	-1.219117	-1.517629
H	-0.419499	-1.371923	-1.677594
H	-1.504619	-0.248588	-1.582010
O	1.347162	-1.524195	1.242568
H	0.387863	-1.679752	1.378787
H	1.492657	-1.589003	0.274384
O	1.396103	1.493885	-1.225593
H	1.531273	1.555772	-0.255738
H	0.442128	1.670282	-1.373413
O	-1.404909	1.572903	-1.176304
H	-1.455516	1.515316	-0.182267
H	-2.043588	2.247394	-1.453781
O	1.426654	-1.183113	-1.548378
H	1.480880	-0.189313	-1.490011
H	2.076507	-1.463775	-2.210770
O	-1.367368	1.249247	1.500496
H	-0.410214	1.380893	1.672401
H	-1.518525	0.281745	1.562583

9	E= -36.782847 hartree		
O	-2.524938	1.229697	-0.045306
H	-2.527983	0.234495	0.018363
H	-3.451159	1.514911	-0.069470
O	1.486962	-2.065850	0.082328
H	0.926446	-1.854424	0.858891
H	0.900151	-1.981981	-0.700038
O	-0.417028	1.540985	1.780294
H	-1.230450	1.612470	1.236315
H	0.323112	1.812579	1.195596
O	3.287027	-0.049986	-0.059837
H	3.875200	-0.174270	0.699902
H	2.679948	-0.837548	-0.075855
O	-0.296752	-1.143174	2.067321
H	-0.367584	-1.370250	3.006972
H	-0.295561	-0.148335	2.009290
O	-0.443032	1.259819	-1.929145
H	0.311984	1.582767	-1.389232
H	-1.246523	1.413173	-1.387612
O	-0.381108	-1.442524	-1.922997
H	-0.355191	-0.448154	-1.979869
H	-0.408349	-1.775724	-2.832839
O	1.576211	2.050678	-0.143080
H	2.084851	2.854317	-0.329495
H	2.225258	1.298310	-0.115243
O	-2.290474	-1.452315	0.123735
H	-1.735366	-1.634075	-0.665193

	H	-1.683739	-1.516903	0.893010
10a		E= -40.871787 hartree		
	O	1.593687	-1.210750	1.832737
	H	1.662934	-0.221041	1.730260
	H	2.236977	-1.471258	2.508444
	O	1.945676	-1.652392	-0.919054
	H	1.933570	-1.667119	0.063541
	H	1.054815	-1.957107	-1.199593
	O	1.799657	1.440007	1.370789
	H	2.077344	1.431951	0.429505
	H	0.903940	1.845656	1.380408
	O	-0.331002	2.099313	-1.689654
	H	0.576761	1.727486	-1.709069
	H	-0.480728	2.390889	-0.766607
	O	-2.496491	0.218768	1.167746
	H	-3.351957	0.062509	1.593780
	H	-1.952692	-0.608960	1.302049
	O	2.217313	1.003054	-1.334382
	H	2.133629	0.013275	-1.252307
	H	3.011648	1.183387	-1.860474
	O	-0.840332	2.420139	1.081153
	H	-1.453770	1.648420	1.146031
	H	-1.303132	3.188333	1.441220
	O	-1.051204	-2.033054	1.395286
	H	-0.140768	-1.793396	1.684107
	H	-0.966068	-2.317947	0.458917
	O	-2.092442	0.019577	-1.636387
	H	-1.468164	0.770748	-1.818592
	H	-2.426536	0.172072	-0.729814
	O	-0.731492	-2.291363	-1.365249
	H	-1.216663	-1.434454	-1.530220
	H	-1.104467	-2.946678	-1.968804
10b		E= -40.871985 hartree		
	O	1.547601	-1.651978	-1.571603
	H	1.881573	-0.725498	-1.417455
	H	2.169548	-2.077307	-2.181442
	O	-1.519852	-2.091799	1.058985
	H	-1.856288	-2.948408	1.364386
	H	-0.526170	-2.121459	1.154498
	O	1.169482	-2.161977	1.145397
	H	1.499766	-1.308399	1.501442
	H	1.395835	-2.155331	0.188994
	O	-1.268452	-1.557626	-1.735083
	H	-0.292738	-1.610913	-1.815822
	H	-1.479493	-1.832686	-0.819624
	O	-2.424871	0.502559	1.209129
	H	-3.245010	0.539413	1.722293
	H	-2.136212	-0.439130	1.187491
	O	0.217743	2.519990	-1.133913
	H	0.167540	3.334880	-1.656776
	H	-0.584473	1.974332	-1.373047
	O	-2.011241	1.067463	-1.548685
	H	-2.344894	1.005067	-0.630073
	H	-1.763823	0.141437	-1.796602
	O	-0.129228	2.121291	1.606999
	H	-0.965054	1.609112	1.575018
	H	0.021815	2.444867	0.691585
	O	1.990952	0.453164	1.797078

H	1.190523	1.046674	1.801702
H	2.558861	0.743297	2.527031
O	2.441278	0.821731	-0.944867
H	2.477557	0.728097	0.031893
H	1.723851	1.469430	-1.122995

10c		E= -40.865356 hartree	
O	3.442023	0.551887	-1.122664
H	4.026408	1.322998	-1.154432
H	2.545979	0.855939	-1.376089
O	0.572673	-2.390102	0.453786
H	1.456329	-1.996350	0.658451
H	-0.035239	-2.026207	1.130892
O	0.868735	1.291536	1.240951
H	1.052878	1.075753	0.297485
H	0.257975	2.052762	1.187325
O	0.735597	1.181052	-1.503289
H	0.302523	0.325837	-1.730576
H	0.017778	1.809783	-1.259946
O	-0.811538	-0.648353	2.173684
H	-0.756668	-0.706094	3.139710
H	-0.165653	0.045987	1.886802
O	-1.189673	2.614644	-0.099804
H	-1.859077	1.938078	0.198649
H	-1.690516	3.410286	-0.336586
O	-0.369149	-1.350159	-1.841872
H	-0.001303	-1.771951	-1.012511
H	-0.042740	-1.873939	-2.589787
O	2.773206	-0.901783	1.163274
H	3.167913	-0.521465	0.347813
H	2.352097	-0.157297	1.624331
O	-3.090674	-1.163824	-1.245133
H	-2.156692	-1.183903	-1.550786
H	-3.287075	-2.044387	-0.894328
O	-2.898480	0.708505	0.783530
H	-2.329937	0.183355	1.384751
H	-3.116747	0.113589	0.029134

Table 15. Cartesian coordinates of small water clusters (**1-10**) optimized at DFTB (mio-0-1 parameters).

		Label	Name
		1	1
		2-cyclic	2
		3-cyclic	3
		4-cyclic	4
		5-cyclic	5
		6-prims	6a
		6-cage	6b
		6-book	6c
		6-bag	6d
		6-cyclic	6e
		6-cyclic	6f
		7-prism	7
		8-D2d	8a
		8-D2dDD	8b
		9-Prism	9
		10-Prism	10a
		10-Prism'	10b
		10-butterfly	10c

1		E= -3019.614956 hartree		
O	0.00000000	-0.11469430	-0.00000200	
H	0.77848845	0.45931935	0.00001904	
H	-0.77848845	0.45931935	-0.00000199	

2		E= -6043.148439 hartree		
O	0.00335916	1.48763983	0.00000000	
H	0.91146772	1.82364502	0.00000000	
H	0.06506776	0.51185690	0.00000000	
O	0.00417635	-1.37590360	0.00000000	
H	-0.51857637	-1.61439136	0.77909673	
H	-0.51857637	-1.61439136	-0.77909673	

3		E= -9070.200434 hartree		
O	1.12975034	-1.13913876	-0.09701430	
H	1.17590015	-0.15822038	-0.06408931	
H	1.60262732	-1.46763158	0.68270428	
O	0.43146430	1.54148703	0.11832803	
H	0.47832448	2.05502470	-0.70249796	
H	-0.44921916	1.10731614	0.12651443	
O	-1.56347242	-0.38528487	-0.08592422	
H	-0.76256727	-0.93596329	-0.21455479	
H	-2.02637924	-0.73720448	0.68929388	

4		E= -12099.331426 hartree		
O	1.38100113	-1.38090019	0.00514617	
H	0.40033048	-1.49103244	0.04932445	
H	1.67030111	-1.82381427	-0.80762276	
O	-1.38100113	1.38090019	0.00514617	
H	-1.67030111	1.82381427	-0.80762276	
H	-0.40033048	1.49103244	0.04932445	
O	1.38090019	1.38100113	-0.00514617	
H	1.49103244	0.40033048	-0.04932445	
H	1.82381427	1.67030111	0.80762276	
O	-1.38090019	-1.38100113	-0.00514617	
H	-1.49103244	-0.40033048	-0.04932445	
H	-1.82381427	-1.67030111	0.80762276	

5	E= -15125.248681 hartree		
O	1.01926959	2.10941543	0.08880796
H	1.50405682	1.25786993	-0.03925457
H	1.35867346	2.49383092	0.91174263
O	0.42344449	-2.30036684	0.04587689
H	-0.47233025	-1.88395317	0.01190625
H	0.43835581	-2.84846902	0.84574460
O	-1.69181353	1.61082930	-0.16789195
H	-2.11325796	2.22807880	0.44959373
H	-0.72515336	1.81117527	-0.15228488
O	2.33772594	-0.31076124	-0.09533055
H	1.66676726	-1.02978607	0.00117840
H	2.79717547	-0.47894420	-0.93265829
O	-2.07394558	-1.11768454	0.07212274
H	-1.94688343	-0.13863962	0.04448677
H	-2.62411349	-1.34057484	-0.69478017

6a	E= -18152.619057 hartree		
O	1.22703976	-1.14909900	1.28678982
H	1.21763874	-1.50363654	0.36694317
H	1.66410025	-0.27933137	1.19537030
O	-0.90054374	1.92379097	0.02575472
H	-1.17739680	1.31890069	0.74317069
H	-1.23024143	1.51246341	-0.79335166
O	1.09106306	-1.13929047	-1.43477099
H	1.52608669	-0.28061459	-1.26382163
H	0.13781037	-0.94173999	-1.55046505
O	-1.67601927	-0.47073109	-1.30513834
H	-2.29463575	-1.09669365	-1.71268265
H	-1.73071046	-0.59509497	-0.33137626
O	-1.39615294	-0.46622663	1.46688109
H	-0.43979123	-0.74592330	1.49243576
H	-1.81748662	-0.83039145	2.26227144
O	1.77426724	1.27466560	-0.06715158
H	0.84123203	1.60221844	-0.02817784
H	2.34370709	2.05493161	-0.15800095

6b	E= -18152.330610 hartree		
O	-2.87483162	0.00873343	0.17752429
H	-3.41269589	-0.79386503	0.25768193
H	-2.17056954	-0.04873334	0.86714030
O	-0.81708043	0.23788798	-1.66088847
H	-1.68330834	0.20449549	-1.19237020
H	-0.35051204	-0.59025806	-1.42388815
O	0.76095201	-1.74909125	-0.35677924
H	1.57493064	-1.19470330	-0.26596604
H	1.05014972	-2.64488485	-0.59200420
O	0.62981032	1.77212674	0.05342811
H	0.49328665	2.72534663	-0.07088228
H	0.10387055	1.31128408	-0.65611358
O	-0.57306520	-0.25026256	1.65799237
H	-0.14759553	0.58426503	1.37467166
H	-0.17906487	-0.94889707	1.09641941
O	2.79886145	0.04923449	0.07919614
H	3.14942918	0.04335031	0.98321256
H	2.17404396	0.80745212	0.02447987

6c	E= -18151.780927 hartree		
O	-2.31567331	-1.36650558	-0.46159454

H	-3.13645429	-1.63408546	-0.02029802
H	-2.36384487	-0.38840722	-0.57701288
O	2.07808340	-1.61427559	-0.42016995
H	1.74306897	-2.13589230	-1.16631772
H	1.35005971	-1.59173031	0.25238296
O	-0.09558567	-1.23958487	1.20032293
H	-0.07049317	-0.26252233	1.26847626
H	-0.87894712	-1.44889083	0.63955669
O	2.38883819	1.10159071	-0.64398002
H	3.27518802	1.29687366	-0.30157157
H	2.31902211	0.11450743	-0.68374408
O	-2.23490684	1.40271386	-0.55026977
H	-2.01853235	1.77288292	-1.41974245
H	-1.44490206	1.53977387	0.01811235
O	0.16227226	1.59635064	0.88429484
H	0.40312382	2.18986744	1.61294561
H	0.96253757	1.49993812	0.30777504

6d	E= -18151.032597 hartree		
O	0.93905737	1.82277082	0.34164929
H	1.44135469	1.38124163	-0.37979253
H	1.00620023	1.21145346	1.10923078
O	1.95379974	0.01917376	-1.53041356
H	1.54410686	0.11281800	-2.40331585
H	1.52077209	-0.74174471	-1.09250677
O	-2.22887208	-1.02419526	-0.20125763
H	-2.83136356	-1.20999916	-0.93859509
H	-2.08985619	-0.04352180	-0.19838160
O	-1.69240061	1.66507534	-0.36159484
H	-2.15332696	2.34635953	0.15296494
H	-0.72432802	1.77298747	-0.16081950
O	0.35606806	-1.94896591	-0.23364671
H	-0.59404315	-1.66999555	-0.26504397
H	0.37000936	-2.91509529	-0.14549176
O	0.87654210	-0.38291793	2.05223782
H	0.01904074	-0.45379024	2.49810010
H	0.84560783	-0.99217646	1.28415526

6e	E= -18151.013549 hartree		
O	-2.39148922	1.38074242	0.05265675
H	-2.93178968	1.55404711	0.83904220
H	-2.34437073	0.39813528	-0.03716915
O	0.00003851	-2.76169821	0.05266389
H	0.82731791	-2.22938079	-0.03718378
H	0.12027794	-3.31621325	0.83905955
O	-0.00003851	2.76169821	-0.05266389
H	-0.12027794	3.31621325	-0.83905955
H	-0.82731791	2.22938079	0.03718378
O	2.39148922	-1.38074242	-0.05265675
H	2.34437073	-0.39813528	0.03716915
H	2.93178968	-1.55404711	-0.83904220
O	2.39148127	1.38081166	0.05263223
H	2.81209073	1.76227398	0.83872250
H	1.51707154	1.83156544	-0.03711315
O	-2.39148127	-1.38081166	-0.05263223
H	-2.81209073	-1.76227398	-0.83872250
H	-1.51707154	-1.83156544	0.03711315

6f	E= -18150.406721 hartree		
O	1.31688503	2.15751823	-0.55548761

	H	0.40236020	2.14267933	-0.18348886
	H	1.67535115	3.03826115	-0.36628739
	O	1.18466468	-2.22559543	0.62914256
	H	1.22076557	-2.20583973	1.59791515
	H	1.78546748	-1.50574416	0.31639717
	O	2.81966840	-0.12053767	-0.09267915
	H	2.27609188	0.69590983	-0.20480391
	H	3.28182263	-0.25614690	-0.93435556
	O	-1.31265823	-2.15674544	-0.56180445
	H	-1.67097580	-3.03847206	-0.37692226
	H	-0.40054354	-2.14148359	-0.18387777
	O	-1.18798238	2.22860234	0.61988739
	H	-1.23040258	2.21979023	1.58856392
	H	-1.78620899	1.50477324	0.31143080
	O	-2.81958946	0.11610897	-0.08813080
	H	-3.28849798	0.25027115	-0.92629967
	H	-2.27405499	-0.69847638	-0.20451010
7			E= -21180.647963 hartree	
	O	1.12876304	1.70225286	-1.02700829
	H	1.07338851	0.78540127	-1.38013327
	H	1.03625395	2.30626678	-1.78026793
	O	-1.02443281	-1.86967821	-0.17547602
	H	-1.75562288	-1.26519142	-0.44877036
	H	-0.74422312	-1.56546710	0.71396320
	O	1.11781716	-1.02497044	-1.61096478
	H	1.25929859	-1.59271726	-2.38587624
	H	0.31913500	-1.38559134	-1.13362431
	O	0.12699545	-0.55260431	2.06352189
	H	1.02187828	-0.43166457	1.65445533
	H	0.26968098	-0.80784758	2.98876423
	O	-1.04025750	1.68594526	0.78748748
	H	-0.28911564	1.84583538	0.17501447
	H	-0.73749163	0.98390548	1.40154495
	O	-2.79872563	0.18560763	-0.69274535
	H	-2.23095121	0.83611487	-0.20921592
	H	-3.66066355	0.18645952	-0.24842051
	O	2.46761561	-0.13253258	0.69562351
	H	2.37209483	0.80012882	0.43181445
	H	2.24127609	-0.64763049	-0.10624250
8a			E= -24211.498753 hartree	
	O	-1.98417205	-0.01577641	1.39989886
	O	-0.02281112	2.07662444	-1.25959380
	O	-0.08090213	-1.99065339	-1.38529879
	O	2.08774088	-0.07043096	1.24519851
	H	-2.08026411	0.01693737	0.41026562
	H	0.01686073	2.10154533	-0.26588389
	H	-0.04328750	-2.07988829	-0.39520400
	H	2.10650125	-0.03885440	0.25105939
	H	-2.88106013	-0.01390993	1.77098299
	H	-0.02154965	2.99777816	-1.56551255
	H	-0.10604865	-2.89014275	-1.74916863
	H	3.01075726	-0.09266784	1.54462736
	O	-1.99425660	0.07080934	-1.32645009
	O	0.08287411	1.89133475	1.45979246
	O	0.02632366	-1.98250868	1.34033953
	O	1.88454602	0.01990643	-1.47342751
	H	-1.41737810	0.85072184	-1.47884431
	H	-0.70164846	1.32491310	1.62710023

H	0.82300599	-1.42647678	1.48315402
H	-1.43933531	-0.71400575	-1.52749102
H	1.31823156	0.81478235	-1.58187579
H	-0.74154294	-1.40495825	1.54308840
H	0.86289517	1.30449460	1.56690674
H	1.29553470	-0.74991194	-1.63076777

8b	E= -24211.449772 hartree		
O	-1.26359630	-1.34726558	0.19054168
H	-0.53959877	-1.42478432	-0.48741564
H	-1.61707979	-2.24043863	0.32995962
O	-0.29903287	1.00114904	-2.86606912
H	-0.29181889	1.32241717	-3.78197414
H	0.26032173	1.62911552	-2.33446395
O	1.17761365	2.57204786	-1.20080309
H	1.77065759	1.88789282	-0.82044700
H	0.51944202	2.77216804	-0.49999825
O	0.75154255	-1.29958255	-1.64207570
H	0.39124053	-0.62443777	-2.25753199
H	1.45664736	-0.84454924	-1.13200240
O	0.28614543	0.30440831	1.87202718
H	-0.31811470	-0.35691967	1.46967037
H	-0.11201536	1.18078598	1.67736403
O	-0.89632639	2.57350594	0.71134121
H	-1.50587563	2.04851384	0.12596959
H	-1.41845930	3.30385075	1.08030227
O	2.31310891	0.32799152	0.05198902
H	1.63941654	0.30243738	0.78362829
H	3.17942671	0.16920419	0.45994834
O	-2.36101873	0.97832327	-0.94134710
H	-2.19554135	0.11075757	-0.51192081
H	-1.80356899	0.98501548	-1.74980742

9	E= -27238.003787 hartree		
O	-2.53391659	1.24217198	-0.04576520
H	-2.54199446	0.24910638	0.01793802
H	-3.46006862	1.53155292	-0.07059227
O	1.48436514	-2.08452047	0.08364746
H	0.92411835	-1.87168910	0.86093183
H	0.89684330	-1.99977143	-0.69890021
O	-0.42027244	1.55613083	1.78415805
H	-1.23390860	1.62459144	1.23867434
H	0.31985422	1.82910869	1.19894802
O	3.31422252	-0.05194623	-0.05840505
H	3.91390091	-0.19132439	0.69119399
H	2.70908757	-0.83792475	-0.08061009
O	-0.29984315	-1.15615528	2.07709949
H	-0.37351343	-1.38520980	3.01727003
H	-0.29494955	-0.16330646	2.02198004
O	-0.44692474	1.27462499	-1.93468286
H	0.30794112	1.59913727	-1.39439436
H	-1.25069472	1.42467990	-1.39115310
O	-0.38455207	-1.45737248	-1.93176752
H	-0.35516446	-0.46554017	-1.99223586
H	-0.41430369	-1.79367084	-2.84164196
O	1.57757041	2.07191723	-0.14490035
H	2.08476312	2.87796137	-0.33094851
H	2.22779752	1.32399112	-0.11554610
O	-2.29437825	-1.46706785	0.12475048
H	-1.73851348	-1.64762064	-0.66488176

H -1.68666522 -1.52990411 0.89441310

10a		E= -30266.076232 hartree		
O	1.68447701	-1.08776795	1.84911628	
H	1.68172369	-0.09864844	1.74159309	
H	2.31473160	-1.29048235	2.55881602	
O	2.08321086	-1.56359757	-0.90124491	
H	2.05964069	-1.55408541	0.08067262	
H	1.20749210	-1.90858694	-1.18607652	
O	1.71558455	1.59495249	1.36215143	
H	1.98255916	1.58583251	0.41598265	
H	0.79956433	1.94710908	1.37969513	
O	-0.48187675	2.07857708	-1.69158501	
H	0.45303622	1.78146881	-1.72363672	
H	-0.64546444	2.35705822	-0.76660345	
O	-2.53107969	0.05474771	1.16813246	
H	-3.37444840	-0.15550424	1.60064141	
H	-1.93458324	-0.73159004	1.31049831	
O	2.15553508	1.12133782	-1.36715594	
H	2.13843944	0.13081468	-1.27626638	
H	2.93009373	1.33966484	-1.90968013	
O	-0.99629314	2.36745077	1.09373187	
H	-1.57074692	1.56956774	1.16848521	
H	-1.48634770	3.11241712	1.47515725	
O	-0.89691550	-2.10405474	1.40329295	
H	-0.00469283	-1.80782733	1.69160687	
H	-0.79668723	-2.37740955	0.46410417	
O	-2.12591522	-0.12604288	-1.65635659	
H	-1.56698129	0.66816186	-1.84773546	
H	-2.45346376	-0.00307016	-0.74063011	
O	-0.57227018	-2.33701662	-1.37295099	
H	-1.12015915	-1.52519881	-1.55674647	
H	-0.89548901	-3.03216601	-1.96839022	

10b		E= -30266.065348 hartree		
O	1.73446947	-1.47380795	-1.57768608	
H	1.96238236	-0.51601927	-1.43440478	
H	2.38435629	-1.82576287	-2.20678655	
O	-1.27534755	-2.26813260	1.05653970	
H	-1.51759503	-3.15470682	1.36920768	
H	-0.28732732	-2.18636590	1.16341267	
O	1.42428156	-2.02055472	1.15189647	
H	1.65819250	-1.13097909	1.49936325	
H	1.63167108	-1.99368571	0.19090575	
O	-1.08361209	-1.70234789	-1.73770639	
H	-0.10644882	-1.65455854	-1.81730972	
H	-1.26624665	-2.00122469	-0.82270022	
O	-2.47727175	0.23321957	1.20951146	
H	-3.30115789	0.17547606	1.71796860	
H	-2.08373679	-0.67026116	1.18799536	
O	-0.06640786	2.54268572	-1.14371855	
H	-0.21865439	3.35612701	-1.65112263	
H	-0.80443838	1.91567296	-1.38020407	
O	-2.13254883	0.83370102	-1.54877519	
H	-2.45181282	0.72837122	-0.62793844	
H	-1.79065464	-0.05774930	-1.80789539	
O	-0.37984040	2.10337306	1.60610385	
H	-1.15301484	1.49887666	1.56989657	
H	-0.26241071	2.44361012	0.69102014	
O	1.92888818	0.67327106	1.81058925	

H	1.07053829	1.17605144	1.81650568
H	2.46864852	1.03149377	2.53330812
O	2.34210993	1.10232225	-0.94350751
H	2.38420470	1.00205779	0.03279985
H	1.55932032	1.67090400	-1.12014251

10c	E= -30261.346787 hartree		
O	3.35708966	0.57053868	-1.25193706
H	3.88113601	1.38573507	-1.24713078
H	2.43949797	0.81974939	-1.49309256
O	0.67616309	-2.38528352	0.61214235
H	1.55212826	-1.95210968	0.76671112
H	0.07315612	-1.99189252	1.27822216
O	0.88487886	1.39089717	1.16542721
H	1.01047496	1.12342099	0.22445750
H	0.25547211	2.13726316	1.11112267
O	0.62092099	1.09848531	-1.56147067
H	0.20576603	0.21584571	-1.71063534
H	-0.10243808	1.72189647	-1.31976273
O	-0.73423828	-0.56553791	2.23251210
H	-0.67713251	-0.56047152	3.20117601
H	-0.11118550	0.12999943	1.90256957
O	-1.26734357	2.59974567	-0.16542144
H	-1.90285874	1.91836528	0.18585209
H	-1.80355203	3.36488396	-0.42949979
O	-0.34812364	-1.50728147	-1.73641765
H	0.03128804	-1.87047626	-0.88686940
H	0.03765563	-2.03113664	-2.45739141
O	2.83680553	-0.75551966	1.13955204
H	3.17906416	-0.41053944	0.28375054
H	2.40301713	-0.00031730	1.57376128
O	-3.08616316	-1.18985092	-1.25576402
H	-2.14376467	-1.29158814	-1.51609136
H	-3.40445721	-2.06917365	-1.00100215
O	-2.88411460	0.64174006	0.82533679
H	-2.28259580	0.14043594	1.41668666
H	-3.09740017	0.03677528	0.07607712

Table 16. Cartesian coordinates of small water clusters (**1-10**) optimized at DFTB (mio-1-1 parameters).

		Label	Name
		1	1
		2-cyclic	2
		3-cyclic	3
		4-cyclic	4
		5-cyclic	5
		6-prims	6a
		6-cage	6b
		6-book	6c
		6-bag	6d
		6-cyclic	6e
		6-cyclic	6f
		7-prism	7
		8-D2d	8a
		8-D2dDD	8b
		9-Prism	9
		10-Prism	10a
		10-Prism'	10b
		10-butterfly	10c

1

E= -3019.614956 hartree

O	0.00000000	-0.11469421	-0.00000200
H	0.77848874	0.45931861	0.00001904
H	-0.77848874	0.45931861	-0.00000199

2

E= -6043.148439 hartree

O	0.00353393	1.48770065	0.00000000
H	0.91176963	1.82335679	0.00000000
H	0.06487824	0.51189793	0.00000000
O	0.00400108	-1.37591384	0.00000000
H	-0.51862865	-1.61466939	0.77909856
H	-0.51862865	-1.61466939	-0.77909856

3

E= -9070.200434 hartree

O	1.12971344	-1.13914275	-0.09682509
H	1.17593166	-0.15822047	-0.06413935
H	1.60203610	-1.46745364	0.68330497
O	0.43147545	1.54150712	0.11806738
H	0.47831745	2.05493993	-0.70282529
H	-0.44921553	1.10735438	0.12633875
O	-1.56342449	-0.38531254	-0.08586910
H	-0.76247085	-0.93594074	-0.21446570
H	-2.02626479	-0.73717449	0.68941633

4

E= -12099.331426 hartree

O	1.38073880	-1.38077673	0.00523928
H	0.40004571	-1.49089206	0.04926979
H	1.66994035	-1.82238846	-0.80827493
O	-1.38073880	1.38077673	0.00523928
H	-1.66994035	1.82238846	-0.80827493
H	-0.40004571	1.49089206	0.04926979
O	1.38077673	1.38073880	-0.00523928
H	1.49089206	0.40004571	-0.04926979
H	1.82238846	1.66994035	0.80827493
O	-1.38077673	-1.38073880	-0.00523928
H	-1.49089206	-0.40004571	-0.04926979
H	-1.82238846	-1.66994035	0.80827493

5	E= -15125.248681 hartree		
O	1.01881885	2.10867614	0.08844243
H	1.50388562	1.25730287	-0.03988273
H	1.35418875	2.49016898	0.91438714
O	0.42317556	-2.29952117	0.04541374
H	-0.47259195	-1.88302503	0.01158316
H	0.43874108	-2.84619136	0.84625178
O	-1.69100602	1.61025210	-0.16823120
H	-2.11027752	2.22325344	0.45494629
H	-0.72424652	1.81045139	-0.15434539
O	2.33688753	-0.31062062	-0.09486539
H	1.66581836	-1.02961420	0.00134667
H	2.79555260	-0.47793348	-0.93280092
O	-2.07319410	-1.11706730	0.07251823
H	-1.94571304	-0.13804194	0.04426693
H	-2.62208146	-1.34034175	-0.69519792

6a	E= -18152.619057 hartree		
O	1.22757733	-1.14796774	1.28637129
H	1.21799404	-1.50361330	0.36696755
H	1.66371176	-0.27780521	1.19350969
O	-0.90075870	1.92346126	0.02629737
H	-1.17745245	1.31800252	0.74335013
H	-1.23041440	1.51262205	-0.79306214
O	1.09059304	-1.13987803	-1.43505491
H	1.52594990	-0.28124515	-1.26504251
H	0.13735408	-0.94213907	-1.55059342
O	-1.67608571	-0.47127931	-1.30555139
H	-2.29456939	-1.09752876	-1.71285140
H	-1.73066430	-0.59535527	-0.33176256
O	-1.39543420	-0.46560589	1.46630019
H	-0.43903496	-0.74530228	1.49179695
H	-1.81634231	-0.82832334	2.26257911
O	1.77373135	1.27431439	-0.06622439
H	0.84065588	1.60187628	-0.02786678
H	2.34361717	2.05492749	-0.15111100

6b	E= -18152.330610 hartree		
O	-2.87349836	0.00816972	0.17693577
H	-3.40951348	-0.79585410	0.25516150
H	-2.16978092	-0.04886934	0.86713728
O	-0.81618039	0.23816142	-1.66100867
H	-1.68244379	0.20490308	-1.19248238
H	-0.34981592	-0.59010186	-1.42396798
O	0.75984146	-1.74894572	-0.35650581
H	1.57393611	-1.19453915	-0.26650098
H	1.04878166	-2.64478145	-0.59189615
O	0.62981036	1.77252852	0.05376659
H	0.49749011	2.72588440	-0.07401077
H	0.10367473	1.31150355	-0.65553341
O	-0.57289816	-0.25043486	1.65908519
H	-0.14773706	0.58441836	1.37642227
H	-0.17880227	-0.94856467	1.09694638
O	2.79743338	0.04924093	0.07846210
H	3.14575330	0.04188442	0.98334337
H	2.17261747	0.80752071	0.02360097

6c	E= -18151.780927 hartree		
O	-2.31406969	-1.36576889	-0.46176538

H	-3.13418164	-1.63313592	-0.01909185
H	-2.36224364	-0.38764556	-0.57713064
O	2.07672587	-1.61398812	-0.42030034
H	1.74034085	-2.13471971	-1.16645349
H	1.34954542	-1.59150648	0.25318002
O	-0.09563236	-1.24002967	1.20158287
H	-0.07056539	-0.26309278	1.27104633
H	-0.87852195	-1.44860476	0.63986005
O	2.38718713	1.10134947	-0.64539687
H	3.27181109	1.29604306	-0.29820724
H	2.31713605	0.11426867	-0.68544428
O	-2.23324384	1.40303318	-0.55026807
H	-2.01530729	1.77176106	-1.41996746
H	-1.44360967	1.53956851	0.01882619
O	0.16215470	1.59548361	0.88460738
H	0.40237192	2.19405336	1.60932457
H	0.96156100	1.49865459	0.30690562

6d	E= -18151.032597 hartree		
O	0.93879260	1.82249319	0.34188575
H	1.44109516	1.38077548	-0.37945701
H	1.00532417	1.21106750	1.10943375
O	1.95232434	0.01901592	-1.52979068
H	1.54367979	0.11203042	-2.40325191
H	1.51937855	-0.74210005	-1.09210533
O	-2.22782359	-1.02341574	-0.20071716
H	-2.82680979	-1.20917000	-0.94092734
H	-2.08818921	-0.04277548	-0.19791999
O	-1.69167551	1.66529554	-0.36267202
H	-2.15277002	2.34248490	0.15712421
H	-0.72349363	1.77319354	-0.16227512
O	0.35641152	-1.94891563	-0.23376656
H	-0.59369967	-1.66976087	-0.26441184
H	0.37034317	-2.91508846	-0.14608644
O	0.87584037	-0.38314817	2.05192228
H	0.01879751	-0.45583467	2.49837016
H	0.84567768	-0.99238908	1.28380171

6e	E= -18151.013549 hartree		
O	-2.39065426	1.38021624	0.05231292
H	-2.92974368	1.55333059	0.83957403
H	-2.34334455	0.39759862	-0.03753517
O	0.00004860	-2.76061103	0.05231738
H	0.82728067	-2.22818381	-0.03754260
H	0.11979097	-3.31398434	0.83959552
O	-0.00004860	2.76061103	-0.05231738
H	-0.11979097	3.31398434	-0.83959552
H	-0.82728067	2.22818381	0.03754260
O	2.39065426	-1.38021624	-0.05231292
H	2.34334455	-0.39759862	0.03753517
H	2.92974368	-1.55333059	-0.83957403
O	2.39062184	1.38029132	0.05231002
H	2.81038771	1.76076170	0.83933422
H	1.51607840	1.83082406	-0.03746399
O	-2.39062184	-1.38029132	-0.05231002
H	-2.81038771	-1.76076170	-0.83933422
H	-1.51607840	-1.83082406	0.03746399

6f	E= -18150.406721 hartree		
O	1.31592463	2.15667839	-0.55583887

	H	0.40097460	2.14167275	-0.18484895
	H	1.67710134	3.03449780	-0.35836733
	O	1.18408921	-2.22488755	0.62990195
	H	1.21760039	-2.20219496	1.59870343
	H	1.78532431	-1.50561453	0.31660058
	O	2.81793933	-0.12058247	-0.09315564
	H	2.27365644	0.69543800	-0.20545041
	H	3.27895871	-0.25679752	-0.93536344
	O	-1.31129575	-2.15568267	-0.56274694
	H	-1.67216072	-3.03486074	-0.37079353
	H	-0.39896968	-2.14032975	-0.18527668
	O	-1.18762968	2.22803280	0.62000498
	H	-1.22820951	2.21758233	1.58874401
	H	-1.78610075	1.50441026	0.31147738
	O	-2.81799092	0.11575493	-0.08789521
	H	-3.28619468	0.25054225	-0.92636528
	H	-2.27158029	-0.69822702	-0.20485236
7	E= -21180.647963 hartree			
	O	1.12665214	1.70208805	-1.02749347
	H	1.07188805	0.78481696	-1.37969832
	H	1.03184743	2.30527220	-1.78113409
	O	-1.02382949	-1.87009150	-0.17557170
	H	-1.75431825	-1.26490017	-0.44931736
	H	-0.74389598	-1.56602032	0.71401552
	O	1.11792998	-1.02469247	-1.61045873
	H	1.25825625	-1.59077316	-2.38679903
	H	0.31949756	-1.38588592	-1.13306505
	O	0.12586996	-0.55240130	2.06275152
	H	1.02093023	-0.43194952	1.65390852
	H	0.26814335	-0.80698367	2.98823970
	O	-1.03968634	1.68689687	0.78824891
	H	-0.28869168	1.84652894	0.17547167
	H	-0.73706272	0.98450423	1.40199585
	O	-2.79616803	0.18590686	-0.69272407
	H	-2.22876129	0.83666731	-0.20903047
	H	-3.65714120	0.18407832	-0.24652616
	O	2.46707519	-0.13355315	0.69565436
	H	2.37203042	0.79912549	0.43181369
	H	2.24113477	-0.64859316	-0.10636660
8a	E= -24211.498753 hartree			
	O	-1.98373936	-0.01643104	1.40037377
	O	-0.02421483	2.07642726	-1.26237075
	O	-0.08179165	-1.98913387	-1.38617655
	O	2.08997870	-0.07160651	1.24830133
	H	-2.08060149	0.01690959	0.41080662
	H	0.01622040	2.10099860	-0.26866568
	H	-0.04407813	-2.07864596	-0.39609242
	H	2.10839540	-0.03950716	0.25416063
	H	-2.88036313	-0.01815260	1.77209932
	H	-0.02387229	2.99767205	-1.56802059
	H	-0.10246915	-2.88855982	-1.75048500
	H	3.01308657	-0.09177358	1.54759447
	O	-1.99581506	0.07165075	-1.32558668
	O	0.08405717	1.88940474	1.45647676
	O	0.02663277	-1.98166688	1.33914566
	O	1.88400167	0.02067250	-1.46975267
	H	-1.41890464	0.85139782	-1.47881934
	H	-0.70065128	1.32374303	1.62537359

H	0.82389601	-1.42685347	1.48332042
H	-1.44147975	-0.71327088	-1.52769165
H	1.31844715	0.81589070	-1.57965516
H	-0.74076076	-1.40350341	1.54215575
H	0.86393997	1.30258101	1.56484919
H	1.29457347	-0.74875066	-1.62772637

8b	E= -24211.449772 hartree		
O	-1.26359630	-1.34726558	0.19054168
H	-0.53959877	-1.42478432	-0.48741564
H	-1.61707979	-2.24043863	0.32995962
O	-0.29903287	1.00114904	-2.86606912
H	-0.29181889	1.32241717	-3.78197414
H	0.26032173	1.62911552	-2.33446395
O	1.17761365	2.57204786	-1.20080309
H	1.77065759	1.88789282	-0.82044700
H	0.51944202	2.77216804	-0.49999825
O	0.75154255	-1.29958255	-1.64207570
H	0.39124053	-0.62443777	-2.25753199
H	1.45664736	-0.84454924	-1.13200240
O	0.28614543	0.30440831	1.87202718
H	-0.31811470	-0.35691967	1.46967037
H	-0.11201536	1.18078598	1.67736403
O	-0.89632639	2.57350594	0.71134121
H	-1.50587563	2.04851384	0.12596959
H	-1.41845930	3.30385075	1.08030227
O	2.31310891	0.32799152	0.05198902
H	1.63941654	0.30243738	0.78362829
H	3.17942671	0.16920419	0.45994834
O	-2.36101873	0.97832327	-0.94134710
H	-2.19554135	0.11075757	-0.51192081
H	-1.80356899	0.98501548	-1.74980742

9	E= -27238.003787 hartree		
O	-2.53221246	1.24220160	-0.04601064
H	-2.54047551	0.24912776	0.01783664
H	-3.45831523	1.53174223	-0.07084861
O	1.48345381	-2.08417462	0.08327808
H	0.92356391	-1.87096863	0.86075473
H	0.89570268	-1.99904718	-0.69912142
O	-0.42029737	1.55621056	1.78510300
H	-1.23390504	1.62449597	1.23952930
H	0.31979608	1.82890983	1.19969166
O	3.31296196	-0.05199236	-0.05847594
H	3.90756035	-0.18866165	0.69566149
H	2.70821231	-0.83826287	-0.08188069
O	-0.29876150	-1.15563507	2.07651195
H	-0.37082194	-1.38514630	3.01669634
H	-0.29446547	-0.16272663	2.02178667
O	-0.44659115	1.27425582	-1.93543097
H	0.30809065	1.59843615	-1.39462239
H	-1.25053042	1.42431258	-1.39211887
O	-0.38383061	-1.45646484	-1.93111388
H	-0.35476599	-0.46453905	-1.99176191
H	-0.41098054	-1.79302680	-2.84097793
O	1.57533968	2.07022928	-0.14473094
H	2.08224015	2.87634997	-0.33125776
H	2.22572543	1.32233746	-0.11601075
O	-2.29368160	-1.46695086	0.12484919
H	-1.73798041	-1.64761640	-0.66486582

H -1.68586710 -1.52990984 0.89441078

10a	E= -30266.076232 hartree		
O	1.68303368	-1.08743307	1.84833454
H	1.68091394	-0.09830442	1.74066484
H	2.30953405	-1.29009990	2.56136464
O	2.08436066	-1.56408211	-0.90210222
H	2.06133048	-1.55481220	0.07978744
H	1.20785671	-1.90767033	-1.18642037
O	1.71562690	1.59506645	1.36225242
H	1.98275406	1.58603932	0.41615003
H	0.79941374	1.94680629	1.37962913
O	-0.48138601	2.07662476	-1.69139277
H	0.45338826	1.77891586	-1.72335729
H	-0.64475841	2.35543704	-0.76647947
O	-2.53159996	0.05476926	1.16793770
H	-3.37447614	-0.15499173	1.60164725
H	-1.93495665	-0.73148486	1.31038911
O	2.15483293	1.12061523	-1.36721130
H	2.13869138	0.13005365	-1.27624170
H	2.92746000	1.33947268	-1.91227176
O	-0.99534869	2.36588098	1.09395060
H	-1.57030041	1.56831986	1.16852202
H	-1.48478643	3.11100487	1.47585906
O	-0.89690434	-2.10297383	1.40399815
H	-0.00471528	-1.80594899	1.69183777
H	-0.79667927	-2.37662510	0.46492638
O	-2.12746466	-0.12592709	-1.65624305
H	-1.56815109	0.66804708	-1.84752037
H	-2.45498374	-0.00295237	-0.74050346
O	-0.57061044	-2.33409026	-1.37242015
H	-1.11972484	-1.52296706	-1.55582700
H	-0.89091220	-3.02855731	-1.97023004

10b	E= -30266.062626 hartree		
O	1.73553870	-1.47446364	-1.57549031
H	1.96310260	-0.51638487	-1.43345141
H	2.38698885	-1.82760303	-2.20230708
O	-1.27699314	-2.26865302	1.05379421
H	-1.51991896	-3.15312707	1.37183964
H	-0.28910762	-2.18639007	1.16169283
O	1.42208872	-2.01932612	1.15334460
H	1.65600334	-1.12957134	1.50039849
H	1.63051735	-1.99311321	0.19252826
O	-1.08203817	-1.70152853	-1.74081859
H	-0.10476131	-1.65359908	-1.81888346
H	-1.26598847	-2.00249772	-0.82680924
O	-2.47439067	0.23375712	1.21100852
H	-3.29879763	0.17606027	1.71863100
H	-2.08187368	-0.67019246	1.18819256
O	-0.06740026	2.54004413	-1.14278860
H	-0.21855443	3.35297220	-1.65134274
H	-0.80593869	1.91346962	-1.37894099
O	-2.13454816	0.83268099	-1.54810900
H	-2.45198685	0.72661277	-0.62671064
H	-1.79180607	-0.05813684	-1.80828320
O	-0.37901637	2.10476164	1.60789022
H	-1.15173831	1.49962447	1.57247290
H	-0.26232048	2.44421298	0.69242761
O	1.92939408	0.67411023	1.80897869

H	1.07126843	1.17730007	1.81593383
H	2.47015160	1.03202546	2.53110540
O	2.34195095	1.10254350	-0.94486685
H	2.38456042	1.00266261	0.03146753
H	1.55815940	1.66987736	-1.12125134

10c		E= -30261.346787 hartree	
O	3.35706651	0.56982049	-1.25374952
H	3.88137174	1.38484666	-1.24788191
H	2.43926450	0.81978801	-1.49344492
O	0.67483681	-2.38425666	0.61260000
H	1.55123713	-1.95166887	0.76640979
H	0.07231962	-1.98989080	1.27859248
O	0.88436013	1.39157072	1.16753696
H	1.01042480	1.12404178	0.22660941
H	0.25504084	2.13795835	1.11285457
O	0.62208430	1.09870718	-1.55882848
H	0.20696818	0.21615870	-1.70874185
H	-0.10152430	1.72216094	-1.31771465
O	-0.73571643	-0.56503273	2.23131472
H	-0.67998725	-0.56030236	3.20006333
H	-0.11241024	0.13086526	1.90248502
O	-1.26730040	2.59838096	-0.16599063
H	-1.90291224	1.91710553	0.18539434
H	-1.80363891	3.36273593	-0.43207240
O	-0.34764200	-1.50560855	-1.73564321
H	0.03116761	-1.86927208	-0.88596824
H	0.03779681	-2.02974920	-2.45659252
O	2.83699926	-0.75625378	1.13672162
H	3.17871650	-0.41111734	0.28071911
H	2.40476791	-0.00086258	1.57211355
O	-3.08451528	-1.19081770	-1.25483151
H	-2.14213649	-1.29031748	-1.51616748
H	-3.39825993	-2.06971566	-0.99303437
O	-2.88458877	0.64126206	0.82448747
H	-2.28306342	0.13997504	1.41588573
H	-3.09725345	0.03648956	0.07483772

Table 17. Cartesian coordinates of small water clusters (**1-10**) optimized at DFTB (pbc-0-1 parameters).

		Label	Name	
		1	1	
		2-cyclic	2	
		3-cyclic	3	
		4-cyclic	4	
		5-cyclic	5	
		6-prims	6a	
		6-cage	6b	
		6-book	6c	
		6-bag	6d	
		6-cyclic	6e	
		6-cyclic	6f	
		7-prism	7	
		8-D2d	8a	
		8-D2dDD	8b	
		9-Prism	9	
		10-Prism	10a	
		10-Prism'	10b	
		10-butterfly	10c	

1		E= -3021.925254 hartree		
O	0.00000000	-0.11708346	-0.00000205	
H	0.74901384	0.47829281	0.00001899	
H	-0.74901384	0.47829281	-0.00000125	

2		E= -6047.616650 hartree		
O	0.00198013	1.49508937	0.00000000	
H	0.92582339	1.74769839	0.00000000	
H	0.05168956	0.53130128	0.00000000	
O	0.00698556	-1.37711574	0.00000000	
H	-0.53042280	-1.63567434	0.74906779	
H	-0.53042280	-1.63567434	-0.74906779	

3		E= -9076.415655 hartree		
O	1.13315455	-1.14557400	-0.09683386	
H	1.19298165	-0.17926691	-0.08257917	
H	1.59092656	-1.38932747	0.70925718	
O	0.43662540	1.54536893	0.12133946	
H	0.40975326	2.00669148	-0.71857958	
H	-0.43581188	1.12736560	0.15044885	
O	-1.57129166	-0.38217520	-0.08905405	
H	-0.79391962	-0.93672144	-0.23782539	
H	-1.95709359	-0.77425619	0.69566329	

4		E= -12107.565778 hartree		
O	1.37924713	-1.37317105	0.01005584	
H	0.41428009	-1.48808749	0.06851448	
H	1.57974131	-1.81787434	-0.81567917	
O	-1.37924713	1.37317105	0.01005584	
H	-1.57974131	1.81787434	-0.81567917	
H	-0.41428009	1.48808749	0.06851448	
O	1.37317105	1.37924713	-0.01005584	
H	1.48808749	0.41428009	-0.06851448	
H	1.81787434	1.57974131	0.81567917	
O	-1.37317105	-1.37924713	-0.01005584	
H	-1.48808749	-0.41428009	-0.06851448	
H	-1.81787434	-1.57974131	0.81567917	

5	E= -15135.670877 hartree		
O	1.01351254	2.10117004	0.08485435
H	1.49698033	1.26738659	-0.05773248
H	1.37746543	2.39426063	0.92234566
O	0.42473011	-2.28666873	0.03869442
H	-0.46009735	-1.88072792	-0.00650154
H	0.36422865	-2.79251196	0.85130610
O	-1.68867666	1.59932326	-0.17058689
H	-2.02762473	2.22559421	0.47142997
H	-0.73656692	1.80056655	-0.16516123
O	2.32647192	-0.30489676	-0.08766761
H	1.66878943	-1.01565265	0.01964332
H	2.72115167	-0.53288357	-0.93158129
O	-2.06069874	-1.11682457	0.07749182
H	-1.94116909	-0.15056707	0.06467294
H	-2.59032211	-1.25553642	-0.71005672

6a	E= -18164.918881 hartree		
O	1.22396173	-1.15466767	1.29554900
H	1.23439410	-1.49385219	0.38483376
H	1.65582742	-0.30182946	1.15751031
O	-0.90463017	1.94700139	0.03539644
H	-1.19153651	1.33872378	0.72858900
H	-1.24970878	1.50853325	-0.74913833
O	1.10770035	-1.16770387	-1.43738698
H	1.51267751	-0.30216163	-1.30731432
H	0.17649752	-0.93551384	-1.55421041
O	-1.66711261	-0.45528601	-1.31298579
H	-2.29573692	-1.07469116	-1.68785468
H	-1.74540700	-0.61998739	-0.36217235
O	-1.38591627	-0.46753268	1.46677675
H	-0.44425747	-0.74077598	1.48576372
H	-1.71449532	-0.83539188	2.29034768
O	1.74690128	1.27049499	-0.07671344
H	0.82968952	1.59942056	-0.03326073
H	2.25251202	2.08537225	-0.10332102

6b	E= -18164.284841 hartree		
O	-2.86250378	-0.00730847	0.17518944
H	-3.32388036	-0.83742052	0.30615720
H	-2.18075251	-0.04028527	0.86825535
O	-0.82520181	0.26659139	-1.69006241
H	-1.66973974	0.20405576	-1.21485592
H	-0.40821002	-0.57271135	-1.45656195
O	0.75075578	-1.72113427	-0.34763341
H	1.55876404	-1.18227095	-0.27034292
H	1.10441938	-2.59427612	-0.52898089
O	0.62963009	1.74331232	0.04744992
H	0.39573007	2.66439486	-0.08829862
H	0.11660921	1.29940773	-0.65992815
O	-0.58681542	-0.24697425	1.68814929
H	-0.14203728	0.55318127	1.37833852
H	-0.18304191	-0.91923655	1.12309351
O	2.82046139	0.03431459	0.07463131
H	3.07267379	0.07594811	0.99874975
H	2.23475083	0.80132548	-0.00958146

6c	E= -18163.952855 hartree		
O	-2.29851599	-1.35285069	-0.45987945

H	-3.12750955	-1.54225503	-0.01691292
H	-2.35502931	-0.39176853	-0.59240039
O	2.07799852	-1.60366071	-0.41759601
H	1.66430103	-2.11356825	-1.11700720
H	1.37326130	-1.58912090	0.25819301
O	-0.07911711	-1.25974060	1.20982258
H	-0.09884166	-0.29454000	1.25915689
H	-0.85570439	-1.44057468	0.65435484
O	2.38188943	1.09725633	-0.64148130
H	3.25100495	1.19811420	-0.24797433
H	2.30680626	0.12612885	-0.70070191
O	-2.25598960	1.41215262	-0.55565013
H	-1.95568995	1.78440207	-1.38654444
H	-1.49248319	1.56179659	0.02114103
O	0.15705085	1.58749925	0.86881835
H	0.48014570	2.15495517	1.57148125
H	0.94498986	1.49291602	0.30035269

6d	E= -18163.386845 hartree		
O	0.92245608	1.84692928	0.33844535
H	1.43661688	1.39220432	-0.34705977
H	1.01253162	1.22435213	1.07682229
O	1.96709313	0.01966308	-1.50747643
H	1.51024084	0.06286383	-2.34854334
H	1.56257469	-0.75112473	-1.09029809
O	-2.22425121	-1.02062725	-0.18945099
H	-2.79060980	-1.12262156	-0.95718062
H	-2.08971724	-0.05400622	-0.17452065
O	-1.68947570	1.65271772	-0.36436907
H	-2.07459380	2.33216105	0.19304428
H	-0.73485679	1.76661974	-0.17774690
O	0.33976847	-1.96313537	-0.24220549
H	-0.59181213	-1.67331563	-0.26891728
H	0.25511926	-2.91313711	-0.13915067
O	0.88711013	-0.38286136	2.03206741
H	0.01057886	-0.49107691	2.40428853
H	0.87182578	-1.00210208	1.28918772

6e	E= -18163.683456 hartree		
O	-2.37699981	1.37745768	0.04434029
H	-2.90731465	1.46357656	0.83884739
H	-2.33429176	0.40967644	-0.05712393
O	-0.00440903	-2.74724886	0.04433479
H	0.81230484	-2.22626404	-0.05708931
H	0.18634551	-3.24979391	0.83866118
O	0.00440903	2.74724886	-0.04433479
H	-0.18634551	3.24979391	-0.83866118
H	-0.81230484	2.22626404	0.05708931
O	2.37699981	-1.37745768	-0.04434029
H	2.33429176	-0.40967644	0.05712393
H	2.90731465	-1.46357656	-0.83884739
O	2.38144567	1.36980708	0.04433630
H	2.72152339	1.78627218	0.83856308
H	1.52200546	1.81681655	-0.05702460
O	-2.38144567	-1.36980708	-0.04433630
H	-2.72152339	-1.78627218	-0.83856308
H	-1.52200546	-1.81681655	0.05702460

6f	E= -18162.981386 hartree		
O	1.31616697	2.14461286	-0.55271871

	H	0.41009887	2.12849107	-0.19740492
	H	1.61031263	3.02097143	-0.29775689
	O	1.18271850	-2.22273792	0.61420163
	H	1.25132281	-2.11736005	1.56496742
	H	1.78446824	-1.52502656	0.29689523
	O	2.81135652	-0.12428487	-0.08153784
	H	2.27882312	0.68420180	-0.18172508
	H	3.22583530	-0.19051652	-0.94390127
	O	-1.31188931	-2.14365635	-0.55905059
	H	-1.60642299	-3.02095007	-0.30775250
	H	-0.40812109	-2.12709270	-0.19785118
	O	-1.18612531	2.22564404	0.60493643
	H	-1.26099290	2.13133810	1.55639186
	H	-1.78523064	1.52377370	0.29183454
	O	-2.81123589	0.11975362	-0.07693735
	H	-3.23238161	0.18484005	-0.93615580
	H	-2.27659128	-0.68683654	-0.18146784
7	E= -21194.656700 hartree			
	O	1.12868429	1.69705456	-0.99989510
	H	1.05029199	0.81074960	-1.38385474
	H	1.08510623	2.26428162	-1.77186183
	O	-1.02346822	-1.90607792	-0.20217247
	H	-1.73892005	-1.29247011	-0.44359760
	H	-0.78197143	-1.58118537	0.67619781
	O	1.11362085	-1.03252190	-1.60792530
	H	1.19733156	-1.64429413	-2.34305429
	H	0.33081372	-1.39273606	-1.13832770
	O	0.12385633	-0.52325499	2.01895794
	H	1.01046916	-0.42126271	1.62256768
	H	0.33423645	-0.76011182	2.92459091
	O	-1.07752150	1.73082098	0.79512213
	H	-0.31765929	1.87451793	0.21242394
	H	-0.73990392	1.04090205	1.38363178
	O	-2.78069115	0.17617056	-0.66771640
	H	-2.22885924	0.83459916	-0.20634835
	H	-3.59713666	0.21657189	-0.16630256
	O	2.48799187	-0.14899462	0.70465239
	H	2.38119645	0.75620316	0.39469347
	H	2.27416846	-0.64468294	-0.09704034
8a	E= -24227.265386 hartree			
	O	-1.93364839	-0.01639208	1.39683145
	O	-0.02328982	2.02624901	-1.25959092
	O	-0.08005718	-1.94051650	-1.38252018
	O	2.03687000	-0.06956214	1.24549806
	H	-2.05328853	0.01602749	0.42544988
	H	0.01589267	2.07626211	-0.28240284
	H	-0.04354400	-2.05358121	-0.41050060
	H	2.08072636	-0.03898690	0.26770442
	H	-2.84129355	-0.01238817	1.70852457
	H	-0.01944399	2.95379727	-1.50581295
	H	-0.10310495	-2.85029147	-1.68709686
	H	2.96594841	-0.08997038	1.48504219
	O	-2.05470940	0.07124784	-1.31341096
	O	0.08325316	1.95329340	1.45167324
	O	0.02499797	-2.04372831	1.32784849
	O	1.94594046	0.01871947	-1.46585464
	H	-1.46232448	0.81767874	-1.48583632
	H	-0.66693369	1.36911453	1.63546708

H	0.78871557	-1.47100918	1.49072592
H	-1.48340044	-0.67935648	-1.53254218
H	1.36166874	0.78053793	-1.59275370
H	-0.70807914	-1.45061060	1.54834365
H	0.82985701	1.34952215	1.57762652
H	1.34005314	-0.71647100	-1.63974624

8b	E= -24227.216404 hartree		
O	-1.24236563	-1.31929252	0.17532550
H	-0.53008405	-1.40830004	-0.49071020
H	-1.53825111	-2.22703137	0.27243936
O	-0.29019935	0.99913106	-2.82834350
H	-0.24874220	1.37530207	-3.71024748
H	0.26048065	1.62516432	-2.31481425
O	1.19490953	2.60202975	-1.22474163
H	1.76316523	1.93135803	-0.81834114
H	0.56296382	2.77480283	-0.51159763
O	0.75560507	-1.33924374	-1.65603358
H	0.42606045	-0.65107306	-2.25243061
H	1.44416700	-0.85965812	-1.17262158
O	0.30411093	0.29897946	1.90917924
H	-0.31371839	-0.32533563	1.50137126
H	-0.11713493	1.14649786	1.70385190
O	-0.88866169	2.54176428	0.69153712
H	-1.49714141	2.03416061	0.11624012
H	-1.45816374	3.24456544	1.01203833
O	2.27537354	0.33373918	0.04928694
H	1.62089282	0.30405970	0.77705684
H	3.09726265	0.16212071	0.51407364
O	-2.40033544	0.99348328	-0.94062364
H	-2.21768543	0.12838184	-0.54548834
H	-1.83900287	0.96580790	-1.72925957

9	E= -27255.895677 hartree		
O	-2.48492278	1.25267510	-0.04741937
H	-2.51891301	0.27591877	0.01624666
H	-3.41640059	1.48244194	-0.07063222
O	1.54923744	-2.10519248	0.08024580
H	0.96641143	-1.89120847	0.82313044
H	0.93997189	-2.02292602	-0.66843252
O	-0.41738839	1.55390216	1.84695820
H	-1.20001280	1.64819129	1.28463363
H	0.28692472	1.83686255	1.24522398
O	3.29469419	-0.02854545	-0.06058782
H	3.81583297	-0.20359768	0.72559317
H	2.72405214	-0.82172233	-0.09726219
O	-0.29671687	-1.15389668	2.01905278
H	-0.37615103	-1.32542094	2.95984480
H	-0.29301203	-0.17521581	1.99277748
O	-0.44150835	1.26112260	-1.99352674
H	0.27800197	1.59467640	-1.43553247
H	-1.21386066	1.43960978	-1.43758981
O	-0.38284678	-1.45197113	-1.87525062
H	-0.35265633	-0.47720720	-1.96087822
H	-0.42149670	-1.72915543	-2.79316059
O	1.53613223	2.05133645	-0.14164541
H	2.10270052	2.80196261	-0.33229540
H	2.17993433	1.31652664	-0.11089661
O	-2.35735885	-1.45143989	0.12564620
H	-1.78381047	-1.64566759	-0.63070454

H -1.73144580 -1.53320406 0.86088589

10a	E= -30285.829423 hartree		
O	1.65337946	-1.10393196	1.80307423
H	1.66631618	-0.12796817	1.72314376
H	2.29019178	-1.25105675	2.50578898
O	2.13441245	-1.54683512	-0.94635589
H	2.07913486	-1.56946899	0.02043319
H	1.26445816	-1.89610622	-1.19389286
O	1.75986609	1.58087384	1.42199210
H	1.98973689	1.60293310	0.48069109
H	0.86340405	1.94575367	1.40916596
O	-0.53310909	2.07579161	-1.72763068
H	0.39361216	1.79576078	-1.73461244
H	-0.64377221	2.35785052	-0.80965512
O	-2.51121982	0.07355134	1.15039094
H	-3.32168926	-0.18213211	1.59672687
H	-1.94455665	-0.71214249	1.30483100
O	2.10972769	1.13783772	-1.33265383
H	2.11611447	0.16104166	-1.26200277
H	2.88579336	1.30017745	-1.87333083
O	-0.94924982	2.36789455	1.07866395
H	-1.52294906	1.58833699	1.16089074
H	-1.48922790	3.06324540	1.45883550
O	-0.95340154	-2.11811546	1.45074172
H	-0.06057042	-1.83552371	1.70149667
H	-0.81429922	-2.38822646	0.53015059
O	-2.13079370	-0.15511321	-1.68806646
H	-1.59828524	0.64356745	-1.86101333
H	-2.44529950	0.01974000	-0.79059690
O	-0.54441237	-2.31488152	-1.32327340
H	-1.08950481	-1.52398699	-1.52045112
H	-0.91218089	-2.96021789	-1.93115873

10b	E= -30285.867520 hartree		
O	1.70972330	-1.45872693	-1.53278688
H	1.94527059	-0.51562771	-1.41375143
H	2.37402479	-1.74938369	-2.16141593
O	-1.24726380	-2.27064519	1.05733928
H	-1.41650573	-3.15875418	1.37968190
H	-0.27645484	-2.19687584	1.17564554
O	1.44100353	-2.05982146	1.19649455
H	1.67182407	-1.16788148	1.49797589
H	1.65589397	-2.00221309	0.25275696
O	-1.11726008	-1.69029202	-1.74628086
H	-0.15125387	-1.65410137	-1.79781677
H	-1.25357242	-1.99875566	-0.84030210
O	-2.45959616	0.23262496	1.17247574
H	-3.26169289	0.10489099	1.68235890
H	-2.07008557	-0.65665366	1.16976321
O	-0.07249532	2.51403386	-1.10555142
H	-0.27908862	3.28792281	-1.63441512
H	-0.79613279	1.90226756	-1.35871588
O	-2.14392102	0.85423856	-1.59467945
H	-2.46546588	0.70692836	-0.69452971
H	-1.81745794	-0.03595120	-1.82132497
O	-0.37890760	2.12073674	1.65742269
H	-1.14260978	1.53051294	1.57811431
H	-0.29530085	2.44928774	0.74920582

O	1.90970109	0.67408068	1.76502918
H	1.06418845	1.16707328	1.79426559
H	2.39292735	1.06973093	2.49366210
O	2.37438251	1.10866120	-0.98651066
H	2.39441505	1.04053143	-0.02040866
H	1.59263557	1.66594128	-1.12218743

10c	E= -30281.260528 hartree		
O	3.39969685	0.57124259	-1.21482631
H	3.84511958	1.41937020	-1.18942324
H	2.51028600	0.81105189	-1.50616662
O	0.68294142	-2.42530192	0.58393978
H	1.53214518	-1.98276684	0.76554506
H	0.11929921	-2.02213281	1.25946376
O	0.89166768	1.40756670	1.13606311
H	0.99626825	1.18012020	0.19609672
H	0.25665796	2.13148380	1.05555268
O	0.65260427	1.12724644	-1.59687719
H	0.21776382	0.26770063	-1.72499581
H	-0.09760179	1.70933629	-1.40420555
O	-0.71667361	-0.55935797	2.17019488
H	-0.60204502	-0.48967440	3.12021491
H	-0.11173888	0.13128558	1.84009410
O	-1.29308036	2.56453977	-0.17334565
H	-1.92352618	1.90359114	0.18202961
H	-1.87158636	3.31244915	-0.33957783
O	-0.35450849	-1.47283228	-1.71787548
H	0.02221750	-1.84504807	-0.89081796
H	0.05301802	-2.03254366	-2.38302818
O	2.81894314	-0.78082300	1.16688934
H	3.18111204	-0.43449951	0.33662513
H	2.40634196	0.00457306	1.53798012
O	-3.09841548	-1.20160120	-1.20459156
H	-2.17584296	-1.27342629	-1.49140257
H	-3.30024409	-2.10033329	-0.93958659
O	-2.93056162	0.66378897	0.85445647
H	-2.32970448	0.13681129	1.39999406
H	-3.13287265	0.04435637	0.13344356

Table 18. Cartesian coordinates of small water clusters (**1-10**) optimized at DFTB (pbc-0-2 parameters).

	Label	Name
	1	1
	2-cyclic	2
	3-cyclic	3
	4-cyclic	4
	5-cyclic	5
	6-prims	6a
	6-cage	6b
	6-book	6c
	6-bag	6d
	6-cyclic	6e
	6-cyclic	6f
	7-prism	7
	8-D2d	8a
	8-D2dDD	8b
	9-Prism	9
	10-Prism	10a
	10-Prism'	10b
	10-butterfly	10c

1	E= -3019.076158 hartree			
O	0.00000000	-0.11436352	-0.00000200	
H	0.77827958	0.45669249	0.00001899	
H	-0.77827958	0.45669249	-0.00000204	

2	E= -6042.032747 hartree			
O	0.00398606	1.48904631	0.00000000	
H	0.90946949	1.82617527	0.00000000	
H	0.06259424	0.51613633	0.00000000	
O	0.00328936	-1.37708711	0.00000000	
H	-0.51427500	-1.61956692	0.77884779	
H	-0.51427500	-1.61956692	-0.77884779	

3	E= -9068.409885 hartree			
O	1.13177343	-1.14074653	-0.09663798	
H	1.17990722	-0.16373951	-0.06475812	
H	1.60178780	-1.47337575	0.68032111	
O	0.43173953	1.54431819	0.11777697	
H	0.48158063	2.05950622	-0.69923637	
H	-0.44627917	1.11322240	0.12758774	
O	-1.56569205	-0.38649910	-0.08554052	
H	-0.76869522	-0.93606917	-0.21640534	
H	-2.03086472	-0.73636827	0.68654268	

4	E= -12096.944934 hartree			
O	1.37285571	-1.37327628	0.00523544	
H	0.39496576	-1.48179202	0.04694428	
H	1.66749795	-1.81167849	-0.80548736	
O	-1.37285571	1.37327628	0.00523544	
H	-1.66749795	1.81167849	-0.80548736	
H	-0.39496576	1.48179202	0.04694428	
O	1.37327628	1.37285571	-0.00523544	
H	1.48179202	0.39496576	-0.04694428	
H	1.81167849	1.66749795	0.80548736	
O	-1.37327628	-1.37285571	-0.00523544	
H	-1.48179202	-0.39496576	-0.04694428	
H	-1.81167849	-1.66749795	0.80548736	

5	E= -15122.326112 hartree		
O	1.01339184	2.09774468	0.08666973
H	1.49626777	1.24809592	-0.03711708
H	1.34577403	2.48702184	0.90764113
O	0.42088807	-2.28827128	0.04542632
H	-0.47204939	-1.87312628	0.01322432
H	0.44205505	-2.83684038	0.84220225
O	-1.68198642	1.60245869	-0.16606321
H	-2.10697351	2.21187356	0.45342526
H	-0.71809419	1.80167414	-0.14921831
O	2.32520754	-0.30948730	-0.09400496
H	1.65588180	-1.02614294	-0.00041180
H	2.78767361	-0.47129446	-0.92841885
O	-2.06277296	-1.11076028	0.07123044
H	-1.93536774	-0.13485156	0.04087556
H	-2.61262606	-1.33983080	-0.69133807

6a	E= -18149.013467 hartree		
O	1.22244055	-1.14624327	1.28780678
H	1.21601988	-1.50846378	0.37560754
H	1.65636537	-0.27839766	1.19413822
O	-0.89483039	1.92175142	0.02563640
H	-1.17159825	1.31945591	0.74123030
H	-1.22485701	1.51656640	-0.79327718
O	1.09202062	-1.14005766	-1.43694487
H	1.52745243	-0.28509838	-1.26613050
H	0.14196182	-0.94553808	-1.55458106
O	-1.67878405	-0.47136288	-1.30669336
H	-2.29811520	-1.09091897	-1.71759372
H	-1.73218156	-0.59660600	-0.33679187
O	-1.38998094	-0.46736836	1.46802363
H	-0.43792919	-0.74591044	1.49000641
H	-1.81078031	-0.82346298	2.26448577
O	1.76861994	1.27638292	-0.06531164
H	0.83777025	1.59947020	-0.02860394
H	2.33887871	2.05410681	-0.14859264

6b	E= -18148.714135 hartree		
O	-2.87284900	0.00810392	0.18029842
H	-3.41570097	-0.78846865	0.26063633
H	-2.16896921	-0.05027082	0.86496900
O	-0.81320469	0.24184941	-1.65654535
H	-1.67829814	0.20919528	-1.19430682
H	-0.34814797	-0.58479939	-1.42472193
O	0.76691416	-1.74654079	-0.35546284
H	1.57523759	-1.19045307	-0.26212003
H	1.05510378	-2.63991988	-0.59189472
O	0.62732508	1.77033154	0.04832081
H	0.49192016	2.72148878	-0.07485209
H	0.10324656	1.30766913	-0.65532182
O	-0.57691108	-0.25072698	1.65612526
H	-0.15244219	0.58214390	1.37735426
H	-0.18303156	-0.94886407	1.09936172
O	2.79355574	0.04550029	0.07788747
H	3.14641306	0.03580623	0.97861951
H	2.17371582	0.80309430	0.02226640

6c	E= -18148.224319 hartree		
O	-2.31567983	-1.36285498	-0.45938249

H	-3.13430089	-1.63322373	-0.02054095
H	-2.36121742	-0.38793023	-0.57348914
O	2.07315075	-1.60413436	-0.41485029
H	1.74814088	-2.12103377	-1.16583318
H	1.34296799	-1.58266939	0.25046299
O	-0.09201055	-1.24054616	1.19125215
H	-0.06681240	-0.26721540	1.26651779
H	-0.87400169	-1.44976301	0.63506519
O	2.37909532	1.09453831	-0.63870423
H	3.26036999	1.29805313	-0.29418852
H	2.31111589	0.11022264	-0.67282283
O	-2.23074559	1.39787492	-0.54878207
H	-2.02247788	1.76688301	-1.41831256
H	-1.44211018	1.53572297	0.01548036
O	0.16951180	1.59525783	0.87920077
H	0.40777160	2.19240571	1.60280708
H	0.96571293	1.49330277	0.30334582

6d	E= -18147.546740 hartree		
O	0.92990887	1.82161148	0.33841859
H	1.43164119	1.38506657	-0.38136708
H	1.00019456	1.21645821	1.10584835
O	1.95099175	0.01622305	-1.52934549
H	1.55552666	0.10442941	-2.40703695
H	1.51740836	-0.74095767	-1.09212309
O	-2.21702025	-1.01565163	-0.20679055
H	-2.81070021	-1.20653252	-0.94708777
H	-2.07703008	-0.03817925	-0.20399358
O	-1.68783074	1.65682229	-0.35726347
H	-2.15451587	2.32634632	0.16327657
H	-0.72360149	1.76593405	-0.15782631
O	0.34633259	-1.94582055	-0.23187848
H	-0.59853604	-1.65976246	-0.26152807
H	0.35741421	-2.91017245	-0.14819013
O	0.88037297	-0.38198026	2.05324265
H	0.03232453	-0.45831882	2.51145196
H	0.84691003	-0.98996068	1.28846881

6e	E= -18147.508643 hartree		
O	-2.37832247	1.37286919	0.05205827
H	-2.91724860	1.55323011	0.83513399
H	-2.33140313	0.39302566	-0.03469288
O	0.00033979	-2.74691084	0.05205039
H	0.82544460	-2.21634268	-0.03474074
H	0.11346449	-3.30343831	0.83541497
O	-0.00033979	2.74691084	-0.05205039
H	-0.11346449	3.30343831	-0.83541497
H	-0.82544460	2.21634268	0.03474074
O	2.37832247	-1.37286919	-0.05205827
H	2.33140313	-0.39302566	0.03469288
H	2.91724860	-1.55323011	-0.83513399
O	2.37798902	1.37345897	0.05203862
H	2.80397871	1.74997500	0.83494985
H	1.50613097	1.82311396	-0.03461804
O	-2.37798902	-1.37345897	-0.05203862
H	-2.80397871	-1.74997500	-0.83494985
H	-1.50613097	-1.82311396	0.03461804

6f	E= -18146.901816 hartree		
O	1.31217005	2.14802171	-0.54737835

	H	0.39967166	2.13437154	-0.17815935
	H	1.67657360	3.02378887	-0.35739880
	O	1.17948346	-2.21577580	0.62091839
	H	1.21374166	-2.20569430	1.58774517
	H	1.77617796	-1.49501290	0.31236469
	O	2.80455330	-0.11933490	-0.09296451
	H	2.26258412	0.69465746	-0.20499891
	H	3.26977013	-0.25786230	-0.92998872
	O	-1.30814627	-2.14734236	-0.55338593
	H	-1.67237012	-3.02411464	-0.36772090
	H	-0.39796824	-2.13327774	-0.17844229
	O	-1.18260719	2.21863342	0.61193678
	H	-1.22293263	2.21905291	1.57858048
	H	-1.77688167	1.49412116	0.30753663
	O	-2.80448705	0.11516778	-0.08873888
	H	-3.27613547	0.25228009	-0.92239234
	H	-2.26071063	-0.69708709	-0.20478029
7			E= -21176.457315 hartree	
	O	1.12899477	1.70240132	-1.02907675
	H	1.07239445	0.78912571	-1.38082346
	H	1.04571640	2.30880832	-1.77860046
	O	-1.02225765	-1.86351188	-0.17980408
	H	-1.75076931	-1.26136224	-0.45190743
	H	-0.74220179	-1.56625845	0.70829278
	O	1.11472414	-1.02800423	-1.60871545
	H	1.26058011	-1.59558864	-2.37998346
	H	0.31848213	-1.38343404	-1.13320168
	O	0.13448237	-0.55129730	2.06155814
	H	1.02388975	-0.42905142	1.64933004
	H	0.27685845	-0.80611888	2.98462276
	O	-1.04354186	1.68083707	0.78521997
	H	-0.29668937	1.84583190	0.17469791
	H	-0.74074463	0.98298232	1.39885290
	O	-2.79489902	0.18664234	-0.68859321
	H	-2.22792116	0.83291239	-0.20590703
	H	-3.65588910	0.18316604	-0.24723309
	O	2.45939939	-0.13321600	0.69961096
	H	2.36801915	0.79786040	0.43832298
	H	2.23708218	-0.64818878	-0.09966336
8a			E= -24206.744817 hartree	
	O	-1.98387734	-0.01633492	1.39346695
	O	-0.02421314	2.07603784	-1.25601575
	O	-0.08218965	-1.98982319	-1.37935215
	O	2.09084210	-0.07195023	1.24192832
	H	-2.07674164	0.01710851	0.40753809
	H	0.01591519	2.09725544	-0.26622261
	H	-0.04479487	-2.07505566	-0.39290862
	H	2.10587750	-0.03959925	0.25175510
	H	-2.87779473	-0.02159572	1.76573668
	H	-0.02500510	2.99446029	-1.56292894
	H	-0.09831847	-2.88667263	-1.74418108
	H	3.01115887	-0.09027809	1.54255034
	O	-1.99508809	0.07202025	-1.31816430
	O	0.08373689	1.88856682	1.44844669
	O	0.02613010	-1.98037790	1.33175697
	O	1.88360547	0.02121794	-1.46166688
	H	-1.42213512	0.85010040	-1.47275301
	H	-0.69991594	1.32810252	1.61948534

H	0.82250627	-1.43077765	1.47728596
H	-1.44629169	-0.71195200	-1.52221342
H	1.32298255	0.81547086	-1.57309389
H	-0.73957938	-1.40618705	1.53586006
H	0.86204593	1.30569877	1.55831460
H	1.29805913	-0.74653300	-1.62084574

8b	E= -24206.712162 hartree		
O	-1.25623035	-1.34963910	0.18730395
H	-0.53612011	-1.42185541	-0.48936548
H	-1.60916840	-2.24051526	0.32690634
O	-0.29678011	1.00833429	-2.86237357
H	-0.28993201	1.32853275	-3.77623410
H	0.26139551	1.62972976	-2.32948748
O	1.17694245	2.56641878	-1.20368645
H	1.76904394	1.88587634	-0.82435202
H	0.52085407	2.77090352	-0.50708656
O	0.74552699	-1.29798843	-1.64051661
H	0.38740056	-0.62588255	-2.25502732
H	1.45086764	-0.84917664	-1.13197479
O	0.28971557	0.30782914	1.86777636
H	-0.31119633	-0.35460691	1.47077148
H	-0.10767954	1.18116069	1.67540728
O	-0.90135048	2.57199172	0.70478056
H	-1.50540457	2.04472441	0.12274107
H	-1.42184510	3.30084027	1.07300658
O	2.30851233	0.32467009	0.05809466
H	1.63435818	0.30256061	0.78382468
H	3.17295101	0.16613689	0.46470469
O	-2.35789459	0.97896627	-0.93578512
H	-2.19442575	0.11388630	-0.50852815
H	-1.80610735	0.98863552	-1.74386175

9	E= -27232.702890 hartree		
O	-2.53142883	1.23535637	-0.04567787
H	-2.53683272	0.24636738	0.01783917
H	-3.45457137	1.52669581	-0.07036737
O	1.48615360	-2.07281006	0.08270494
H	0.92893848	-1.86269470	0.85885596
H	0.90214588	-1.99053852	-0.69862312
O	-0.41775496	1.54832867	1.78277024
H	-1.23013254	1.61929205	1.24192219
H	0.32166269	1.81925766	1.20125375
O	3.29631630	-0.05137854	-0.05890490
H	3.88984799	-0.17752423	0.69510166
H	2.69299583	-0.83498248	-0.07805582
O	-0.29674605	-1.14845099	2.07395727
H	-0.36690247	-1.38000987	3.01146061
H	-0.29413962	-0.15952291	2.01679904
O	-0.44408091	1.26644816	-1.93246106
H	0.30986989	1.58861106	-1.39579735
H	-1.24667066	1.41882482	-1.39403911
O	-0.38158876	-1.44848118	-1.92914273
H	-0.35447166	-0.46005142	-1.98647676
H	-0.40879016	-1.78623055	-2.83616848
O	1.57867398	2.05880134	-0.14384195
H	2.08338056	2.86404170	-0.32873073
H	2.22408325	1.31035600	-0.11609053
O	-2.29295079	-1.46013264	0.12426332

H	-1.74129910	-1.64156179	-0.66377761
H	-1.68971064	-1.52454895	0.89276077

10a	E= -30260.154901 hartree		
O	1.68070067	-1.08062347	1.84732324
H	1.67843391	-0.09583423	1.73742664
H	2.30177387	-1.28554543	2.56136384
O	2.08124878	-1.55757637	-0.90424399
H	2.06243841	-1.55089090	0.07420048
H	1.20809745	-1.89910004	-1.18925690
O	1.71260650	1.58831405	1.36299164
H	1.98197474	1.58157185	0.42128975
H	0.79946466	1.93861210	1.38284539
O	-0.48309088	2.06785202	-1.69080150
H	0.44850002	1.77120586	-1.72432020
H	-0.64807596	2.34932550	-0.77037699
O	-2.52371659	0.05471961	1.16923067
H	-3.36329664	-0.14623209	1.60825581
H	-1.93011006	-0.72865966	1.30887841
O	2.15251731	1.11357471	-1.36679415
H	2.13557728	0.12728523	-1.27361367
H	2.92071331	1.33465246	-1.91318624
O	-0.99794301	2.35801389	1.09453423
H	-1.56790769	1.56047559	1.16675623
H	-1.48515243	3.10142446	1.47712200
O	-0.89803287	-2.09501593	1.40364138
H	-0.00953287	-1.79899723	1.69190964
H	-0.80055451	-2.37186255	0.46907699
O	-2.11744686	-0.12482701	-1.65550953
H	-1.55837113	0.66588794	-1.84313803
H	-2.45246989	-0.00494674	-0.74576757
O	-0.57231479	-2.32619242	-1.37334147
H	-1.11789832	-1.51708015	-1.55292390
H	-0.88651857	-3.01825469	-1.97344963

10b	E= -30260.152180 hartree		
O	1.73578835	-1.46827110	-1.57368795
H	1.96140361	-0.51439258	-1.42883080
H	2.38627812	-1.82336562	-2.19686695
O	-1.27412174	-2.26255042	1.05418316
H	-1.52324468	-3.13840054	1.38398154
H	-0.29045670	-2.18103864	1.15919205
O	1.41436850	-2.01654788	1.15285225
H	1.64795267	-1.13120417	1.50129003
H	1.62454210	-1.99349799	0.19606761
O	-1.08111004	-1.69406531	-1.74236956
H	-0.10727233	-1.64613699	-1.82119243
H	-1.26816422	-1.99781364	-0.83352557
O	-2.46892808	0.22869040	1.21268898
H	-3.29188091	0.17168532	1.71857594
H	-2.07476763	-0.67101534	1.18683415
O	-0.07106568	2.53412287	-1.14446468
H	-0.21933726	3.34505432	-1.65265217
H	-0.80580049	1.90854213	-1.37627887
O	-2.12688520	0.82990537	-1.54670043
H	-2.44838239	0.72800763	-0.62979977
H	-1.78416587	-0.05738355	-1.80509481
O	-0.37430800	2.09923273	1.60779569
H	-1.14422501	1.49583552	1.57635777
H	-0.25968459	2.44079757	0.69680335

O	1.92347683	0.67659554	1.80808081
H	1.06883614	1.17774338	1.81182763
H	2.46536463	1.03263992	2.52722648
O	2.33740795	1.09662705	-0.94590170
H	2.38329591	0.99938220	0.02701677
H	1.55707753	1.66173413	-1.12481580

10c	E= -30255.286674 hartree		
O	3.35743852	0.57059181	-1.25337615
H	3.88547742	1.38066697	-1.25248130
H	2.44297688	0.81888777	-1.49389610
O	0.67654161	-2.37862945	0.60933388
H	1.54935241	-1.94742304	0.76237121
H	0.07341364	-1.99128172	1.27385889
O	0.87888406	1.38734210	1.16953658
H	1.00839334	1.11942589	0.23355881
H	0.25203467	2.13200039	1.11609108
O	0.62020540	1.09589485	-1.55842884
H	0.20860082	0.21581193	-1.70686599
H	-0.09891649	1.71943500	-1.32060434
O	-0.73209559	-0.55938423	2.22927514
H	-0.67704365	-0.55550852	3.19581312
H	-0.11217989	0.13309051	1.89778084
O	-1.27180983	2.59386657	-0.16300455
H	-1.90280144	1.91306837	0.18563456
H	-1.80438645	3.35911276	-0.42557142
O	-0.34599319	-1.50570958	-1.73112495
H	0.03126528	-1.86590585	-0.88515320
H	0.03522470	-2.02737908	-2.45291378
O	2.83453286	-0.76042629	1.13485374
H	3.17685995	-0.41585999	0.28324442
H	2.40706141	-0.00910472	1.57607618
O	-3.08216916	-1.18916674	-1.25305566
H	-2.14292839	-1.28717462	-1.51312496
H	-3.39807315	-2.06424588	-0.98905543
O	-2.88055632	0.64362738	0.81929840
H	-2.28311629	0.14592809	1.41223230
H	-3.09370354	0.04196163	0.07227300

Table 19. Cartesian coordinates of small water clusters (**1-10**) optimized at DFTB (pbc-0-3 parameters).

		Label	Name	
		1	1	
		2-cyclic	2	
		3-cyclic	3	
		4-cyclic	4	
		5-cyclic	5	
		6-prims	6a	
		6-cage	6b	
		6-book	6c	
		6-bag	6d	
		6-cyclic	6e	
		6-cyclic	6f	
		7-prism	7	
		8-D2d	8a	
		8-D2dDD	8b	
		9-Prism	9	
		10-Prism	10a	
		10-Prism'	10b	
		10-butterfly	10c	

1		E= -3019.076158 hartree		
O	0.00000000	-0.11436026	-0.00000200	
H	0.77829937	0.45666656	0.00001899	
H	-0.77829937	0.45666656	-0.00000204	

2		E= -6042.032747 hartree		
O	0.00399367	1.48891538	0.00000000	
H	0.90940297	1.82624443	0.00000000	
H	0.06281033	0.51601515	0.00000000	
O	0.00329439	-1.37701046	0.00000000	
H	-0.51445012	-1.61910983	0.77884685	
H	-0.51445012	-1.61910983	-0.77884685	

3		E= -9068.409885 hartree		
O	1.13173516	-1.14069724	-0.09663727	
H	1.17988258	-0.16368758	-0.06476235	
H	1.60149825	-1.47331711	0.68047799	
O	0.43171754	1.54425740	0.11776725	
H	0.48160672	2.05929496	-0.69933850	
H	-0.44630524	1.11316265	0.12759860	
O	-1.56562926	-0.38648583	-0.08554038	
H	-0.76862862	-0.93604468	-0.21645633	
H	-2.03065727	-0.73626068	0.68667306	

4		E= -12096.944934 hartree		
O	1.37293527	-1.37331045	0.00516669	
H	0.39505132	-1.48184229	0.04690208	
H	1.66762044	-1.81202331	-0.80537189	
O	-1.37293527	1.37331045	0.00516669	
H	-1.66762044	1.81202331	-0.80537189	
H	-0.39505132	1.48184229	0.04690208	
O	1.37331045	1.37293527	-0.00516669	
H	1.48184229	0.39505132	-0.04690208	
H	1.81202331	1.66762044	0.80537189	
O	-1.37331045	-1.37293527	-0.00516669	
H	-1.48184229	-0.39505132	-0.04690208	
H	-1.81202331	-1.66762044	0.80537189	

5	E= -15122.326112 hartree		
O	1.01333235	2.09763060	0.08660375
H	1.49623481	1.24799440	-0.03717980
H	1.34484131	2.48631556	0.90820811
O	0.42078881	-2.28802559	0.04524293
H	-0.47213780	-1.87283976	0.01314418
H	0.44214963	-2.83625412	0.84224912
O	-1.68174093	1.60224490	-0.16619382
H	-2.10635739	2.21098803	0.45421036
H	-0.71783464	1.80145380	-0.14966569
O	2.32504341	-0.30943089	-0.09384062
H	1.65567879	-1.02606070	-0.00031180
H	2.78715547	-0.47092510	-0.92851172
O	-2.06269980	-1.11070363	0.07140145
H	-1.93524623	-0.13479355	0.04108289
H	-2.61187548	-1.33979001	-0.69165227

6a	E= -18149.013467 hartree		
O	1.22250710	-1.14601578	1.28762618
H	1.21598514	-1.50821552	0.37540440
H	1.65643106	-0.27816614	1.19389952
O	-0.89491436	1.92181928	0.02591709
H	-1.17178982	1.31965585	0.74157523
H	-1.22496309	1.51660118	-0.79296608
O	1.09173525	-1.14006115	-1.43680129
H	1.52730319	-0.28511403	-1.26628070
H	0.14166704	-0.94543732	-1.55432287
O	-1.67841813	-0.47157663	-1.30658112
H	-2.29707104	-1.09195386	-1.71726780
H	-1.73170493	-0.59650518	-0.33661105
O	-1.38980079	-0.46713892	1.46764026
H	-0.43769447	-0.74553341	1.48973287
H	-1.81100217	-0.82459671	2.26327954
O	1.76835495	1.27615696	-0.06528851
H	0.83751227	1.59926255	-0.02848883
H	2.33865890	2.05390970	-0.14798809

6b	E= -18148.714135 hartree		
O	-2.87085563	0.00742379	0.17949347
H	-3.41084012	-0.79136469	0.25710675
H	-2.16758883	-0.05021119	0.86486774
O	-0.81264501	0.24237402	-1.65720283
H	-1.67759029	0.20984396	-1.19457366
H	-0.34781343	-0.58450223	-1.42572602
O	0.76532552	-1.74601895	-0.35538896
H	1.57388123	-1.19013502	-0.26265373
H	1.05314877	-2.63976605	-0.59088050
O	0.62717388	1.77001732	0.04889147
H	0.49588810	2.72133533	-0.07747092
H	0.10299488	1.30735376	-0.65470718
O	-0.57659897	-0.25068565	1.65759454
H	-0.15241349	0.58253614	1.37954727
H	-0.18266464	-0.94823333	1.10011511
O	2.79218584	0.04552615	0.07746795
H	3.14382651	0.03486015	0.97867072
H	2.17210277	0.80301072	0.02201144

6c	E= -18148.224319 hartree		
O	-2.31212396	-1.36139831	-0.45982742

H	-3.13070431	-1.63257286	-0.02139908
H	-2.35843057	-0.38643580	-0.57358082
O	2.07087922	-1.60410411	-0.41546914
H	1.74393343	-2.12027615	-1.16611537
H	1.34206407	-1.58262763	0.25136962
O	-0.09154974	-1.24118006	1.19388149
H	-0.06608426	-0.26791891	1.26976395
H	-0.87291568	-1.44962167	0.63648679
O	2.37768927	1.09403837	-0.63976288
H	3.25797430	1.29687587	-0.29231930
H	2.30927162	0.10974442	-0.67428025
O	-2.23030815	1.39883779	-0.54892874
H	-2.02112626	1.76670867	-1.41872546
H	-1.44168688	1.53609989	0.01556710
O	0.16885063	1.59384849	0.87881844
H	0.40640999	2.19452320	1.59973289
H	0.96462093	1.49173922	0.30234281

6d	E= -18147.546740 hartree		
O	0.93079157	1.82161172	0.33970676
H	1.43307831	1.38520639	-0.37981189
H	0.99951502	1.21579945	1.10677485
O	1.95053696	0.01816404	-1.52940678
H	1.55312469	0.10875398	-2.40597811
H	1.51738549	-0.73975936	-1.09303732
O	-2.21582239	-1.01586533	-0.20152969
H	-2.81045605	-1.20837793	-0.94064521
H	-2.07517891	-0.03844885	-0.20166081
O	-1.68546453	1.65552020	-0.36007248
H	-2.15300356	2.32493845	0.15984555
H	-0.72151618	1.76507791	-0.15941246
O	0.34732971	-1.94536980	-0.23426847
H	-0.59777309	-1.65981668	-0.26154148
H	0.35921046	-2.90960828	-0.14938866
O	0.87553575	-0.38290462	2.05212358
H	0.02469525	-0.45832613	2.50529248
H	0.84554230	-0.99032294	1.28676098

6e	E= -18147.505922 hartree		
O	-2.37801066	1.37259839	0.05165067
H	-2.91633373	1.55290684	0.83515465
H	-2.33094210	0.39274851	-0.03499925
O	0.00034989	-2.74631999	0.05163750
H	0.82548009	-2.21576361	-0.03502029
H	0.11307822	-3.30231262	0.83543995
O	-0.00034989	2.74631999	-0.05163750
H	-0.11307822	3.30231262	-0.83543995
H	-0.82548009	2.21576361	0.03502029
O	2.37801066	-1.37259839	-0.05165067
H	2.33094210	-0.39274851	0.03499925
H	2.91633373	-1.55290684	-0.83515465
O	2.37764543	1.37320754	0.05163220
H	2.80317265	1.74920106	0.83504690
H	1.50562936	1.82258231	-0.03491127
O	-2.37764543	-1.37320754	-0.05163220
H	-2.80317265	-1.74920106	-0.83504690
H	-1.50562936	-1.82258231	0.03491127

6f	E= -18146.899094 hartree		
O	1.31078839	2.14680253	-0.54825534

	H	0.39816007	2.13313448	-0.17935298
	H	1.67652664	3.02116363	-0.35439489
	O	1.17956206	-2.21524304	0.62169798
	H	1.21153977	-2.20314244	1.58857920
	H	1.77663614	-1.49482517	0.31305960
	O	2.80396675	-0.11913987	-0.09261683
	H	2.26125479	0.69431786	-0.20512564
	H	3.26834584	-0.25836642	-0.92999390
	O	-1.30620935	-2.14583081	-0.55515893
	H	-1.67154149	-3.02161665	-0.36701811
	H	-0.39618646	-2.13182583	-0.17981496
	O	-1.18303006	2.21832742	0.61180939
	H	-1.22221483	2.21859841	1.57849944
	H	-1.77737921	1.49361954	0.30800514
	O	-2.80403871	0.11439210	-0.08737683
	H	-3.27549161	0.25222318	-0.92102721
	H	-2.25928538	-0.69708059	-0.20449507
7			E= -21176.457315 hartree	
	O	1.12651322	1.70218428	-1.02880008
	H	1.07029447	0.78811993	-1.37875577
	H	1.03863992	2.30706478	-1.77903869
	O	-1.02213598	-1.86542098	-0.17958217
	H	-1.74956800	-1.26212025	-0.45220730
	H	-0.74204019	-1.56810702	0.70849933
	O	1.11373767	-1.02709079	-1.60786735
	H	1.25622444	-1.59019517	-2.38304015
	H	0.31825165	-1.38397954	-1.13211982
	O	0.13309931	-0.55067511	2.05967850
	H	1.02280317	-0.42911586	1.64787929
	H	0.27485500	-0.80546975	2.98284619
	O	-1.04315198	1.68299964	0.78601403
	H	-0.29618320	1.84754360	0.17543111
	H	-0.74075475	0.98476680	1.39943077
	O	-2.79054571	0.18663659	-0.68903474
	H	-2.22437032	0.83336336	-0.20592514
	H	-3.65135555	0.18154298	-0.24732855
	O	2.45968468	-0.13476348	0.69991843
	H	2.36940939	0.79641959	0.43875272
	H	2.23785087	-0.64944777	-0.09964224
8a			E= -24206.744817 hartree	
	O	-1.98519047	-0.01619622	1.39334230
	O	-0.02391639	2.07737103	-1.25522291
	O	-0.08153899	-1.99052684	-1.37911941
	O	2.09087466	-0.07139359	1.24112570
	H	-2.07794133	0.01693574	0.40742463
	H	0.01627585	2.09816993	-0.26545143
	H	-0.04393981	-2.07595726	-0.39271507
	H	2.10552039	-0.03938668	0.25094434
	H	-2.87911835	-0.01784581	1.76561867
	H	-0.02360467	2.99594711	-1.56167781
	H	-0.10232194	-2.88726141	-1.74399407
	H	3.01132529	-0.09161303	1.54122052
	O	-1.99516194	0.07142279	-1.31870768
	O	0.08377066	1.88923393	1.44957908
	O	0.02638840	-1.98105743	1.33225345
	O	1.88388832	0.02046042	-1.46283819
	H	-1.42282557	0.84998259	-1.47297215
	H	-0.69951577	1.32799067	1.61973720

H	0.82233301	-1.43074651	1.47746574
H	-1.44534203	-0.71210093	-1.52180014
H	1.32276103	0.81436399	-1.57405289
H	-0.73973082	-1.40747509	1.53632457
H	0.86248648	1.30690470	1.55924763
H	1.29893971	-0.74768710	-1.62213925

8b	E= -24206.712162 hartree		
O	-1.25623035	-1.34963910	0.18730395
H	-0.53612011	-1.42185541	-0.48936548
H	-1.60916840	-2.24051526	0.32690634
O	-0.29678011	1.00833429	-2.86237357
H	-0.28993201	1.32853275	-3.77623410
H	0.26139551	1.62972976	-2.32948748
O	1.17694245	2.56641878	-1.20368645
H	1.76904394	1.88587634	-0.82435202
H	0.52085407	2.77090352	-0.50708656
O	0.74552699	-1.29798843	-1.64051661
H	0.38740056	-0.62588255	-2.25502732
H	1.45086764	-0.84917664	-1.13197479
O	0.28971557	0.30782914	1.86777636
H	-0.31119633	-0.35460691	1.47077148
H	-0.10767954	1.18116069	1.67540728
O	-0.90135048	2.57199172	0.70478056
H	-1.50540457	2.04472441	0.12274107
H	-1.42184510	3.30084027	1.07300658
O	2.30851233	0.32467009	0.05809466
H	1.63435818	0.30256061	0.78382468
H	3.17295101	0.16613689	0.46470469
O	-2.35789459	0.97896627	-0.93578512
H	-2.19442575	0.11388630	-0.50852815
H	-1.80610735	0.98863552	-1.74386175

9	E= -27232.702890 hartree		
O	-2.53246649	1.23535397	-0.04566067
H	-2.53767906	0.24638277	0.01785693
H	-3.45567377	1.52648204	-0.07042797
O	1.48643178	-2.07336028	0.08274913
H	0.92914662	-1.86334069	0.85885525
H	0.90253966	-1.99097080	-0.69862925
O	-0.41783709	1.54850569	1.78303869
H	-1.23021912	1.61942089	1.24222012
H	0.32155217	1.81953284	1.20156018
O	3.29693480	-0.05149228	-0.05871022
H	3.89264820	-0.17885618	0.69336572
H	2.69349821	-0.83498845	-0.07744294
O	-0.29692181	-1.14858232	2.07500772
H	-0.36684584	-1.37996698	3.01257191
H	-0.29427813	-0.15968348	2.01769941
O	-0.44429120	1.26658232	-1.93280778
H	0.30969970	1.58892931	-1.39635229
H	-1.24680999	1.41889040	-1.39428468
O	-0.38179160	-1.44874339	-1.93018791
H	-0.35471938	-0.46032607	-1.98740006
H	-0.40893885	-1.78636373	-2.83726376
O	1.57967906	2.05978244	-0.14398381
H	2.08459882	2.86496736	-0.32853157
H	2.22497714	1.31130268	-0.11590626
O	-2.29329110	-1.46031394	0.12427925
H	-1.74163502	-1.64172479	-0.66374453

H -1.69011950 -1.52471751 0.89281253

10a		E= -30260.157622 hartree	
O	1.68189221	-1.08062317	1.84799111
H	1.67932024	-0.09585841	1.73803257
H	2.30458282	-1.28542966	2.56065608
O	2.08156445	-1.55756346	-0.90363660
H	2.06237656	-1.55062057	0.07481336
H	1.20878095	-1.89962562	-1.18897491
O	1.71281434	1.58853807	1.36289996
H	1.98214641	1.58168483	0.42118982
H	0.79969085	1.93884265	1.38276465
O	-0.48322116	2.06861642	-1.69091936
H	0.44840942	1.77217753	-1.72448884
H	-0.64823643	2.35017929	-0.77053596
O	-2.52455804	0.05440213	1.17005634
H	-3.36361842	-0.14621087	1.61022839
H	-1.93096038	-0.72901411	1.30931686
O	2.15341839	1.11374808	-1.36721383
H	2.13627175	0.12749774	-1.27383843
H	2.92230072	1.33461426	-1.91272565
O	-0.99840765	2.35877618	1.09452609
H	-1.56828390	1.56121621	1.16689667
H	-1.48538405	3.10202929	1.47771323
O	-0.89835358	-2.09565161	1.40347623
H	-0.00989148	-1.79995472	1.69203624
H	-0.80084826	-2.37191091	0.46872858
O	-2.11740146	-0.12474538	-1.65619032
H	-1.55833616	0.66604813	-1.84345336
H	-2.45285005	-0.00505384	-0.74661054
O	-0.57325256	-2.32723769	-1.37410995
H	-1.11837154	-1.51789388	-1.55392421
H	-0.88948417	-3.02000518	-1.97233644

10b		E= -30260.154901 hartree	
O	1.73593515	-1.46833623	-1.57407516
H	1.96160695	-0.51450473	-1.42905723
H	2.38575116	-1.82308340	-2.19815463
O	-1.27408878	-2.26276270	1.05431840
H	-1.52303946	-3.13895668	1.38333402
H	-0.29043238	-2.18120705	1.15931015
O	1.41451614	-2.01667501	1.15290957
H	1.64808933	-1.13133269	1.50134832
H	1.62481882	-1.99369337	0.19616812
O	-1.08120461	-1.69436385	-1.74227931
H	-0.10737040	-1.64638528	-1.82113010
H	-1.26820721	-1.99798172	-0.83337648
O	-2.46938997	0.22873620	1.21275002
H	-3.29218432	0.17179590	1.71890030
H	-2.07521825	-0.67094863	1.18694872
O	-0.07109243	2.53453099	-1.14468357
H	-0.21948734	3.34547767	-1.65281096
H	-0.80581882	1.90892189	-1.37641875
O	-2.12689576	0.83005757	-1.54669610
H	-2.44855470	0.72820078	-0.62985240
H	-1.78424469	-0.05725720	-1.80503807
O	-0.37426518	2.09930684	1.60767810
H	-1.14423676	1.49599230	1.57620424
H	-0.25959035	2.44091666	0.69671195
O	1.92356398	0.67662581	1.80850954

H	1.06894416	1.17779709	1.81207285
H	2.46522631	1.03252001	2.52789957
O	2.33757721	1.09660206	-0.94589960
H	2.38346424	0.99937900	0.02701154
H	1.55733047	1.66180148	-1.12483354

10c	E= -30255.289396 hartree		
O	3.35793964	0.57097141	-1.25335047
H	3.88612588	1.38094974	-1.25343125
H	2.44352551	0.81915629	-1.49411363
O	0.67660117	-2.37932624	0.60932118
H	1.54933225	-1.94811391	0.76259643
H	0.07332246	-1.99208897	1.27374057
O	0.87930697	1.38775950	1.16933870
H	1.00915040	1.11959204	0.23352965
H	0.25214221	2.13213110	1.11549559
O	0.62006964	1.09625044	-1.55944479
H	0.20851263	0.21615924	-1.70774688
H	-0.09897497	1.71963125	-1.32110505
O	-0.73225255	-0.55957913	2.23037376
H	-0.67746805	-0.55576857	3.19692226
H	-0.11226371	0.13283812	1.89911447
O	-1.27214387	2.59471745	-0.16263762
H	-1.90322128	1.91392272	0.18579394
H	-1.80447918	3.36054619	-0.42398609
O	-0.34573322	-1.50680326	-1.73189897
H	0.03145402	-1.86677739	-0.88584119
H	0.03594815	-2.02833366	-2.45354262
O	2.83514557	-0.76056562	1.13551474
H	3.17754136	-0.41596491	0.28397784
H	2.40776094	-0.00921651	1.57676493
O	-3.08295253	-1.18943582	-1.25338543
H	-2.14378212	-1.28815169	-1.51335819
H	-3.40036354	-2.06474804	-0.99198971
O	-2.88093660	0.64408343	0.81954989
H	-2.28353940	0.14643133	1.41254072
H	-3.09425827	0.04226752	0.07274040

Table 20. Cartesian coordinates of large water clusters (**11-20**) optimized with the DFTB parameters implemented in Gaussian09 (DFTBA).

Label	Name
1	1
2-cyclic	2
3-cyclic	3
4-cyclic	4
5-cyclic	5
6-prims	6a
6-cage	6b
6-book	6c
6-bag	6d
6-cyclic	6e
6-cyclic	6f
7-prism	7
8-D2d	8a
8-D2dDD	8b
9-Prism	9
10-Prism	10a
10-Prism'	10b
10-butterfly	10c

11a

E= hartree

O	-0.857429	-1.723812	0.171658
H	-1.819723	-1.954455	0.174286
H	-0.742776	-1.038566	-0.527973
O	2.834784	1.305732	-0.347429
H	2.750291	0.610649	-1.034924
H	2.063087	1.898196	-0.456885
O	-3.577317	-1.767021	-0.032279
H	-3.524229	-0.820612	-0.310656
H	-4.038291	-2.244294	-0.737382
O	-0.316266	0.191465	-1.805278
H	-0.034599	1.063887	-1.449920
H	0.509912	-0.258489	-2.093736
O	-2.970396	0.743221	-0.928399
H	-2.200809	0.505172	-1.479994
H	-2.609303	1.243188	-0.166248
O	-1.558466	2.034850	1.181090
H	-1.994117	2.567731	1.865069
H	-1.138251	1.255062	1.650167
O	-0.399316	-0.090597	2.327487
H	0.581860	-0.054895	2.333380
H	-0.632004	-0.797212	1.677399
O	0.353474	2.665813	-0.660540
H	-0.316428	2.561717	0.059544
H	0.102780	3.447181	-1.175833
O	2.379129	-0.172742	1.873483
H	3.125033	-0.099185	2.487864
H	2.581374	0.419226	1.099580
O	1.835980	-2.409228	0.256307
H	2.097543	-1.765261	0.949230
H	0.855690	-2.445107	0.285732
O	2.217678	-0.922315	-1.954931
H	2.727642	-1.402061	-2.626643
H	2.120494	-1.534792	-1.171411

11b

E= hartree

O	0.06980300	-2.34679600	-1.50545600
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H	0.52443400	-1.51952500	-1.82944100
H	0.20065000	-3.02176200	-2.18881600
O	1.46946000	-2.30964000	0.91079600
H	0.98144400	-2.50862200	0.08061800
H	0.80044900	-1.93803000	1.52835600
O	-2.02295800	2.20914700	-0.25167500
H	-2.60108500	1.42348200	-0.44430500
H	-2.60933300	2.97915000	-0.20137000
O	2.08191400	2.11436800	0.77385000
H	2.49981700	1.24602900	0.56324100
H	2.79068000	2.72039700	1.03538000
O	-3.61821600	0.07424200	-0.73669600
H	-3.15771800	-0.71200000	-0.33947100
H	-3.80957800	-0.15885200	-1.65734800
O	1.50316900	-0.19422300	-2.24549500
H	2.21057100	-0.19648200	-1.56838300
H	1.05414200	0.68343000	-2.15784100
O	0.47659300	2.25111800	-1.56657100
H	-0.44420800	2.24766000	-1.23007500
H	1.05040500	2.38462800	-0.78519900
O	-2.16366200	-2.01592500	0.18693100
H	-1.70126700	-1.74414500	1.00933800
H	-1.45853800	-2.20017600	-0.46958300
O	-0.59738100	-1.07099900	2.32690300
H	-0.53591000	-0.08404100	2.20131700
H	-0.86162800	-1.21855200	3.24775400
O	3.11915700	-0.34981200	0.10413600
H	4.02562100	-0.69337300	0.12703300
H	2.52827600	-1.07620400	0.45570700
O	-0.43148000	1.60106000	1.96882300
H	-1.04618200	1.84963500	1.24191600
H	0.46777700	1.83702700	1.65681300

12a

E= hartree

O	0.943085	1.731648	2.817169
H	1.121768	2.389634	3.506604
H	-0.031300	1.522857	2.860409
O	-0.943085	-1.731648	2.817169
H	-1.121768	-2.389634	3.506604
H	0.031300	-1.522857	2.860409
O	1.731648	-0.943085	-2.817169
H	2.389634	-1.121768	-3.506604
H	1.522857	0.031300	-2.860409
O	-0.996862	-1.655452	-2.763764
H	-1.146300	-1.903490	-1.828737
H	-0.024145	-1.595410	-2.873138
O	-1.731648	0.869101	-0.044858
H	-1.947156	1.090670	-0.978279
H	-1.526371	-0.100111	-0.040303
O	1.731648	-0.869101	-0.044858
H	1.526371	0.100111	-0.040303
H	1.947156	-1.090670	-0.978279
O	0.869101	1.731648	0.044858
H	1.090670	1.947156	0.978279
H	-0.100111	1.526371	0.040303
O	-0.869101	-1.731648	0.044858
H	-1.090670	-1.947156	0.978279
H	0.100111	-1.526371	0.040303
O	0.996862	1.655452	-2.763764
H	1.146300	1.903490	-1.828737

H	0.024145	1.595410	-2.873138
O	1.655452	-0.996862	2.763764
H	1.903490	-1.146300	1.828737
H	1.595410	-0.024145	2.873138
O	-1.731648	0.943085	-2.817169
H	-2.389634	1.121768	-3.506604
H	-1.522857	-0.031300	-2.860409
O	-1.655452	0.996862	2.763764
H	-1.903490	1.146300	1.828737
H	-1.595410	0.024145	2.873138

12b

E= hartree

O	-1.522827	0.441991	-2.486175
H	-0.599485	0.054366	-2.505380
H	-1.729734	0.703179	-3.396931
O	-3.023141	-1.038238	-0.722815
H	-3.860272	-1.303421	-1.131575
H	-2.518324	-0.518955	-1.394455
O	1.143029	-2.611920	-0.538411
H	1.236274	-3.543122	-0.792126
H	0.292240	-2.543032	-0.017564
O	1.614049	0.763826	2.289319
H	2.200731	0.139227	1.812937
H	1.466041	1.518293	1.674707
O	0.939713	-0.611721	-2.551111
H	1.010253	-1.369100	-1.931467
H	1.611826	0.049886	-2.244126
O	-0.763150	-0.424097	2.743192
H	0.112305	0.024253	2.575411
H	-0.843886	-0.521920	3.704258
O	2.730782	1.036321	-1.320627
H	2.212071	1.710832	-0.830394
H	3.042593	0.396800	-0.648825
O	-2.779255	0.924267	1.312164
H	-3.038291	0.215795	0.688709
H	-2.105010	0.529321	1.905652
O	-1.404934	2.460589	-0.489938
H	-1.459245	1.844509	-1.251474
H	-1.944698	2.046757	0.229462
O	1.150825	2.679100	0.315589
H	1.321349	3.626139	0.433901
H	0.201169	2.597758	0.015456
O	3.064674	-1.006999	0.620861
H	2.403578	-1.618485	0.218000
H	3.868386	-1.519955	0.790747
O	-1.149297	-2.443553	0.853393
H	-1.862804	-2.065380	0.295875
H	-1.020810	-1.810271	1.595675

13a

E= hartree

O	-2.392629	-0.042602	-2.237697
H	-1.426426	-0.001666	-2.385461
H	-2.583102	-0.909918	-1.826273
O	2.487360	-2.318832	0.356352
H	2.613029	-1.712526	1.117461
H	1.517236	-2.363366	0.217611
O	1.092341	2.532848	-0.801613
H	1.921966	2.162909	-0.387854
H	1.337956	3.372364	-1.219863
O	-3.106638	-0.531990	1.664659

H	-3.230072	0.311470	1.178861
H	-2.222519	-0.477475	2.087157
O	-2.831036	-2.188644	-0.443741
H	-3.306126	-3.026129	-0.329545
H	-3.020418	-1.631989	0.362168
O	-0.341319	-0.202173	2.152423
H	-0.295714	-0.725354	1.313577
H	-0.491823	0.746557	1.891413
O	0.459190	0.190027	-2.148897
H	1.369972	-0.161471	-2.266365
H	0.571948	1.078699	-1.737670
O	3.292875	1.329287	0.160982
H	3.045283	0.835655	0.973608
H	3.400010	0.657278	-0.545921
O	-3.142837	1.579957	-0.200495
H	-3.925992	2.084569	-0.467686
H	-2.863720	1.040171	-0.988111
O	-0.150310	-1.638814	-0.191941
H	-1.047290	-2.017717	-0.344576
H	0.012618	-0.982160	-0.914397
O	2.367948	-0.277046	2.289534
H	2.699907	-0.259005	3.200062
H	1.376151	-0.223149	2.342376
O	-0.835062	2.303011	1.228917
H	-1.694919	2.201463	0.768788
H	-0.167307	2.495247	0.536098
O	3.068607	-0.734090	-1.738409
H	3.769385	-1.113692	-2.290761
H	2.892047	-1.388276	-1.005284

13b

E= hartree

O	0.151965	1.991848	0.691688
H	0.152855	1.285007	1.376519
H	1.073563	2.359652	0.672591
O	0.131760	-0.093302	2.574260
H	-0.719047	-0.550007	2.311792
H	0.016253	0.203185	3.490365
O	-1.350566	-2.848280	-0.331993
H	-1.610871	-3.759091	-0.538045
H	-0.364029	-2.795044	-0.471426
O	1.312229	-2.686280	-0.724224
H	1.735890	-2.375473	0.104224
H	1.508129	-1.998650	-1.399578
O	3.618810	0.246273	-0.307203
H	3.317935	-0.376009	0.386823
H	3.095485	0.027873	-1.108477
O	1.826511	-0.472503	-2.354133
H	2.019525	-0.497463	-3.303793
H	1.040741	0.131077	-2.235372
O	-3.666933	0.685657	0.418522
H	-4.608133	0.912937	0.462215
H	-3.179321	1.516362	0.168966
O	-2.168276	-1.252961	1.826051
H	-2.755409	-0.581442	1.415801
H	-1.944529	-1.897353	1.118292
O	-2.228235	2.813932	-0.432517
H	-1.417701	2.745425	0.118503
H	-1.944378	2.572240	-1.330432
O	2.786718	2.676438	0.596410
H	3.167572	1.809649	0.301194

H	3.079399	3.339814	-0.045750
O	-2.406078	-0.650408	-1.706400
H	-2.995839	-0.262219	-1.026416
H	-2.057996	-1.485653	-1.324612
O	-0.313405	1.104114	-1.909076
H	-0.149352	1.380552	-0.975765
H	-1.080487	0.474485	-1.896930
O	2.337613	-1.437505	1.588535
H	2.788565	-1.862655	2.332756
H	1.574263	-0.933392	1.957193

14a

E= hartree

O	-3.571932	-0.240088	-1.493396
H	-4.312187	-0.473945	-2.073998
H	-2.998282	-1.052118	-1.418345
O	3.337608	1.540500	1.130921
H	3.355051	1.486239	0.133429
H	4.019342	2.179734	1.389648
O	0.594325	1.387682	1.440427
H	0.541749	0.400899	1.536884
H	1.552462	1.612326	1.491282
O	-2.074685	2.144000	-1.613321
H	-2.165170	2.424439	-0.680268
H	-2.628370	1.339869	-1.710461
O	-2.141630	-2.012886	1.716415
H	-2.680246	-1.179256	1.617726
H	-2.614737	-2.578950	2.345423
O	3.325930	-1.261449	1.434440
H	2.387874	-1.438694	1.653565
H	3.441371	-0.290150	1.505746
O	3.324747	-1.557925	-1.251600
H	3.378827	-1.512737	-0.257282
H	3.984671	-2.206289	-1.541542
O	0.521420	-1.335482	1.381179
H	0.516459	-1.452175	0.396161
H	-0.357220	-1.655665	1.691130
O	0.471968	1.292042	-1.342093
H	-0.407820	1.649123	-1.639699
H	0.489259	1.416496	-0.363284
O	-1.931975	2.461969	1.209340
H	-2.035096	3.249057	1.764526
H	-1.008340	2.139058	1.330897
O	-2.050485	-2.430273	-1.077992
H	-1.124115	-2.219186	-1.322301
H	-2.071082	-2.473972	-0.098385
O	-3.614354	0.202851	1.265760
H	-3.083888	1.023725	1.359490
H	-3.786733	0.103441	0.303489
O	3.248919	1.244618	-1.543232
H	2.296471	1.404845	-1.716178
H	3.380630	0.277263	-1.635972
O	0.552933	-1.429725	-1.353719
H	1.499373	-1.649420	-1.507429
H	0.476898	-0.449820	-1.488535

14b

E= hartree

O	2.478475	-0.300093	2.128847
H	3.030449	-0.348032	2.923428
H	1.559482	-0.081503	2.422490
O	-0.837709	2.195424	-2.082904

H	-1.614454	2.100069	-1.490962
H	-0.125389	2.587262	-1.534539
O	-1.723328	-2.111756	-1.717888
H	-2.082868	-2.811143	-2.283153
H	-1.170098	-2.549081	-1.028633
O	-2.862465	1.902711	-0.140331
H	-3.074100	0.930074	-0.055371
H	-3.711445	2.365478	-0.209685
O	-0.830365	2.562744	1.642723
H	-1.617652	2.378447	1.080123
H	-0.122919	2.857245	1.025675
O	0.025958	-0.247950	-2.971825
H	-0.292703	0.662877	-2.744127
H	-0.628052	-0.872030	-2.590895
O	-0.063382	0.343821	2.930823
H	-0.352711	1.158430	2.423565
H	-0.272896	0.519223	3.861554
O	-1.764342	-1.739322	2.017661
H	-1.179279	-1.026380	2.350992
H	-1.207518	-2.323846	1.462345
O	2.496808	-0.643410	-2.013415
H	3.058970	-0.776990	-2.792150
H	1.569252	-0.488157	-2.357899
O	-0.164966	-3.286271	0.240914
H	-0.092078	-4.237539	0.413712
H	0.767991	-2.928259	0.219888
O	-3.408424	-0.720538	0.071571
H	-2.960795	-1.163362	-0.680117
H	-2.957664	-1.065502	0.881134
O	1.117742	3.153598	-0.274934
H	1.539551	4.015350	-0.412015
H	1.850759	2.480965	-0.222084
O	3.090224	1.314682	-0.117489
H	2.957621	0.674296	-0.852893
H	2.969109	0.802548	0.710032
O	2.349343	-2.340757	0.186932
H	2.462984	-1.696411	0.918849
H	2.467911	-1.827086	-0.644735

15a		E= hartree	
O	3.050621	-0.186005	2.173800
H	3.748457	-0.360307	2.822774
H	3.046889	-0.938732	1.535413
O	0.258311	0.035985	2.338273
H	1.213878	-0.011542	2.554316
H	0.145314	0.842251	1.772856
O	2.884004	-2.245151	0.344329
H	2.796592	-1.859061	-0.574308
H	3.446544	-3.031128	0.260135
O	-2.748572	-2.327115	0.680175
H	-2.842312	-1.614954	1.361581
H	-1.813216	-2.605323	0.724928
O	-0.068100	1.354086	-1.861434
H	0.861405	1.578910	-2.090374
H	-0.115113	0.363701	-1.866031
O	0.093165	-2.186389	0.755006
H	0.058084	-1.396510	1.352753
H	1.039088	-2.443228	0.709132
O	-3.004603	-1.304095	-1.787899
H	-3.682080	-1.806101	-2.267280

H	-2.982744	-1.668650	-0.856617
O	2.727372	2.233584	0.726580
H	1.788085	2.456110	0.887349
H	2.922520	1.444873	1.275817
O	-0.084792	2.224460	0.739509
H	-0.111181	1.927846	-0.206170
H	-1.017434	2.433925	0.976248
O	-0.246699	-1.373181	-1.842060
H	-1.201688	-1.446678	-2.071796
H	-0.170847	-1.687282	-0.904749
O	-2.592458	-0.242502	2.449130
H	-2.765195	0.607675	1.992211
H	-1.646013	-0.238355	2.684152
O	-2.887840	1.502649	-1.643350
H	-3.034514	0.535969	-1.742239
H	-1.961229	1.662290	-1.911992
O	2.702866	1.573828	-1.894452
H	2.768794	1.820422	-0.930785
H	3.288192	2.176327	-2.378570
O	2.545662	-1.224876	-2.120018
H	2.690504	-0.253239	-2.117377
H	1.589994	-1.359211	-2.287894
O	-2.833620	2.171237	0.970624
H	-3.519376	2.831674	1.155494
H	-2.928757	1.917013	0.011381

15b

E= hartree

O	-1.697449	-2.649570	-1.417614
H	-0.856897	-2.215131	-1.682311
H	-1.545032	-2.985184	-0.507606
O	-1.045304	1.127196	1.456839
H	-1.406968	2.033020	1.577923
H	-0.218170	1.023980	2.002683
O	3.436746	1.580586	1.106839
H	4.079879	2.263857	1.349601
H	3.093961	1.813679	0.201034
O	3.890174	-1.121033	0.495823
H	3.874727	-0.208901	0.858448
H	3.070504	-1.552148	0.815937
O	1.306913	0.485429	2.582890
H	2.059577	0.985451	2.201368
H	1.311504	-0.388870	2.130378
O	2.526304	2.020685	-1.399052
H	1.546566	1.972663	-1.361132
H	2.825411	1.192384	-1.829150
O	1.204706	-1.789571	0.956451
H	0.466833	-2.365378	1.256655
H	0.973420	-1.534173	0.030223
O	-2.937106	1.916255	-1.524996
H	-3.365946	2.161587	-2.358271
H	-3.176911	0.976411	-1.341226
O	0.600792	-1.104980	-1.662150
H	0.281705	-0.174400	-1.555109
H	1.521744	-1.043457	-2.004935
O	-3.564314	-0.746641	-1.109143
H	-4.401576	-1.163025	-1.366410
H	-2.848331	-1.424893	-1.283631
O	-1.258380	-3.054861	1.329961
H	-1.530381	-3.777727	1.915858
H	-1.853148	-2.280117	1.531274

O	-2.470520	3.412665	0.876629
H	-3.339237	3.537251	1.284028
H	-2.623042	2.998767	0.003395
O	-0.212020	1.450727	-1.111218
H	-1.056702	1.754149	-1.507795
H	-0.423037	1.317222	-0.150166
O	3.289836	-0.613870	-2.081832
H	3.953990	-0.990672	-2.679298
H	3.573147	-0.841969	-1.151984
O	-2.879396	-0.922260	1.644168
H	-2.237094	-0.176811	1.718053
H	-3.278349	-0.833631	0.753392

16a	E= hartree		
	O	-1.426036	1.486053 1.241462
	H	-2.362113	1.643540 1.500070
	H	-1.413992	1.508567 0.250984
	O	1.417287	-1.438350 1.300401
	H	1.407695	-1.506750 0.311835
	H	2.354063	-1.577869 1.566842
	O	4.140820	1.416949 1.333774
	H	3.205164	1.622654 1.534173
	H	4.252839	0.461903 1.529421
	O	1.336829	1.299827 1.435074
	H	1.325589	0.311626 1.493813
	H	0.419143	1.593357 1.619324
	O	1.349452	-1.308961 -1.440858
	H	1.338594	-0.320651 -1.501278
	H	0.434036	-1.603165 -1.633989
	O	-4.146365	1.364939 -1.382406
	H	-3.210915	1.560068 -1.593961
	H	-4.261360	0.403331 -1.539609
	O	-4.184063	-1.457651 -1.314994
	H	-4.868810	-2.057081 -1.649752
	H	-4.235711	-1.483325 -0.319364
	O	4.191440	1.412788 -1.362901
	H	4.234627	1.474132 -0.368365
	H	4.876636	2.003124 -1.712316
	O	4.184561	-1.401080 1.375110
	H	4.879068	-1.973789 1.735641
	H	4.239796	-1.465714 0.381292
	O	-4.152634	-1.358500 1.381400
	H	-3.218199	-1.556056 1.595278
	H	-4.267084	-0.397183 1.540666
	O	1.425747	1.429179 -1.307790
	H	2.362943	1.575812 -1.569102
	H	1.410217	1.495563 -0.319097
	O	-1.418828	-1.494091 -1.247029
	H	-1.406967	-1.518114 -0.256745
	H	-2.356920	-1.643241 -1.504213
	O	-4.191129	1.464994 1.314481
	H	-4.879642	2.059381 1.650153
	H	-4.240868	1.492755 0.318907
	O	4.158820	-1.409078 -1.323298
	H	3.226273	-1.622005 -1.530300
	H	4.265816	-0.454065 -1.518554
	O	-1.339312	1.236894 -1.492699
	H	-1.330921	0.247097 -1.514017
	H	-0.421550	1.520779 -1.691010
	O	-1.345467	-1.245587 1.490156

H	-0.425314	-1.525363	1.683967
H	-1.341091	-0.255907	1.510237

16b

		E= hartree	
O	0.002089	-2.980052	-1.644724
H	0.296577	-2.176783	-2.129721
H	0.525612	-3.008124	-0.813174
O	-2.594112	-2.551472	-1.027525
H	-3.087952	-3.318635	-1.353801
H	-1.636858	-2.712083	-1.251878
O	-3.263603	0.137441	-1.515736
H	-3.078267	-0.824080	-1.444755
H	-3.431176	0.448098	-0.600806
O	3.142451	0.296284	-1.788296
H	2.977258	1.174156	-1.382837
H	3.378177	-0.305022	-1.047151
O	-0.138233	3.288260	-0.806793
H	-0.229022	4.083409	-1.355341
H	-0.464093	2.527378	-1.379569
O	2.510741	2.683716	-0.410499
H	1.542294	2.870857	-0.478899
H	2.970202	3.534770	-0.462790
O	-1.031645	1.401387	-2.452303
H	-0.395926	0.669664	-2.621932
H	-1.879408	0.973836	-2.160268
O	0.652166	0.734592	2.973806
H	0.711114	1.049302	3.887310
H	1.545856	0.867970	2.571483
O	-2.689029	-1.715548	1.669516
H	-2.924764	-0.768498	1.587518
H	-2.699868	-2.080660	0.759185
O	3.124902	1.094670	1.851494
H	2.947167	1.699813	1.101298
H	3.375604	0.234939	1.454736
O	-3.507636	0.969282	1.175472
H	-4.333943	1.182600	1.633408
H	-2.926915	1.766428	1.241979
O	0.862737	-0.624460	-2.910292
H	1.057346	-0.716965	-3.855521
H	1.698490	-0.293080	-2.480758
O	-0.115263	-1.903500	2.602626
H	-1.067786	-1.887827	2.329749
H	0.134677	-0.964192	2.778597
O	-2.115582	3.332271	1.157750
H	-2.662130	4.037617	0.783226
H	-1.322678	3.254134	0.581632
O	1.459353	-2.975637	0.755517
H	1.594644	-3.881697	1.075131
H	0.851014	-2.535954	1.429244
O	3.613455	-1.324579	0.441342
H	2.828687	-1.919214	0.554567
H	4.403738	-1.883406	0.479285

17a

		E= hartree	
O	4.625569	0.128218	0.567621
H	4.218632	-0.648564	1.043178
H	5.470384	0.318699	1.004350
O	-0.016034	-2.013417	-0.055962
H	-0.340893	-1.395452	-0.758901
H	0.817560	-2.417949	-0.390346

O	-0.114486	3.543441	-1.252392
H	-0.218644	4.462381	-1.545193
H	0.111228	3.571591	-0.280949
O	2.211511	1.447421	0.564175
H	3.156443	1.170993	0.600097
H	1.915286	1.334009	-0.371715
O	1.274922	1.219311	-2.023995
H	0.861479	2.109935	-1.996721
H	0.538193	0.582726	-2.141589
O	-3.457350	-0.660144	2.038350
H	-3.111642	-1.468539	1.567589
H	-3.990718	-0.980201	2.782425
O	3.272210	-1.900084	1.715731
H	2.998717	-2.389461	0.911895
H	2.456761	-1.484453	2.073275
O	3.574660	-0.476325	-1.978448
H	4.104625	-0.148688	-1.222041
H	2.871171	0.183881	-2.140703
O	-1.079131	-0.317113	-1.922075
H	-1.496727	0.427357	-1.415345
H	-1.828869	-0.892819	-2.193208
O	-4.511408	0.358355	-0.362349
H	-4.325020	0.055589	0.552715
H	-3.852579	1.060745	-0.541001
O	2.527838	-2.719921	-0.891123
H	2.902864	-1.918150	-1.349085
H	2.844379	-3.496157	-1.378388
O	0.367611	3.369713	1.390794
H	-0.337997	2.810508	1.771872
H	1.162948	2.800041	1.337199
O	-2.608059	-2.783448	0.600757
H	-2.964074	-2.577272	-0.289867
H	-1.632820	-2.711459	0.517683
O	-1.337450	1.171864	2.047217
H	-0.562205	0.566119	2.157835
H	-2.135388	0.624920	2.230188
O	-3.500134	-1.662313	-1.835474
H	-4.172639	-2.045018	-2.419783
H	-3.939570	-0.916486	-1.339132
O	-2.113798	1.775784	-0.516624
H	-1.569967	2.511665	-0.879031
H	-1.803903	1.623246	0.412261
O	0.880036	-0.468609	2.017316
H	0.505342	-1.067209	1.323041
H	1.375578	0.241633	1.539243

17b

E= hartree

O	-2.360330	-2.788228	0.402599
H	-2.570969	-2.297083	1.225166
H	-1.460399	-2.486913	0.140868
O	4.009221	-1.283886	1.328371
H	4.383820	-0.703399	0.630669
H	3.426457	-0.714779	1.875378
O	-3.916469	-1.512744	-1.392312
H	-4.479414	-2.145405	-1.863853
H	-3.335175	-2.042851	-0.780159
O	2.748380	-1.024958	-2.438952
H	2.609553	-1.810517	-1.871457
H	1.879855	-0.571626	-2.505002
O	-2.910223	-0.915381	2.449045

H	-3.416436	-1.117664	3.250868
H	-3.532552	-0.432594	1.834806
O	2.272915	0.527858	2.648879
H	1.311732	0.366946	2.484943
H	2.360060	0.803136	3.573732
O	-0.351825	0.066135	1.993567
H	-1.208748	-0.239453	2.372613
H	-0.192082	-0.518538	1.207689
O	-3.223824	2.373123	-0.454086
H	-2.407062	2.467477	0.110690
H	-3.604220	3.259833	-0.546616
O	-4.594428	0.236009	0.688050
H	-4.204386	1.075271	0.353876
H	-4.555103	-0.387410	-0.069945
O	2.500741	-2.840012	-0.277635
H	2.660463	-3.780899	-0.107552
H	3.071779	-2.325986	0.357229
O	0.058402	-1.560173	-0.159749
H	0.118573	-0.925555	-0.922601
H	0.888577	-2.093786	-0.170413
O	0.280704	0.288441	-2.140821
H	0.534566	1.155510	-1.748995
H	-0.671616	0.377120	-2.416199
O	4.546673	0.294607	-0.920238
H	5.374354	0.367550	-1.419691
H	3.882941	-0.140312	-1.524795
O	-0.967070	2.599269	0.995311
H	-0.258481	2.740836	0.328441
H	-0.767606	1.733099	1.421037
O	3.231457	2.228130	0.606392
H	2.929257	1.703288	1.379435
H	3.799650	1.631003	0.071428
O	1.062532	2.695342	-0.917622
H	1.228627	3.503559	-1.426549
H	1.870965	2.540890	-0.353407
O	-2.395456	0.603479	-2.504122
H	-2.905737	-0.196011	-2.253853
H	-2.692448	1.309172	-1.891185

18a		E= hartree	
O	2.162808	1.286936	-1.459057
H	3.142168	1.218728	-1.551606
H	1.819341	0.357704	-1.523248
O	-1.326411	-1.473709	1.140267
H	-0.392635	-1.583676	1.429129
H	-1.304633	-1.413189	0.153295
O	4.748150	0.497398	1.432802
H	3.885960	0.926234	1.623867
H	4.609184	-0.462562	1.573821
O	4.027347	-2.225826	1.276153
H	4.062198	-2.234134	0.278902
H	4.465656	-3.035533	1.581003
O	-0.040780	2.966338	1.589100
H	-0.815079	2.391716	1.765701
H	-0.093210	3.221206	0.651239
O	0.128052	3.132582	-1.291398
H	0.270131	3.881523	-1.888829
H	0.894730	2.520354	-1.400448
O	1.310802	-1.298329	-1.312811
H	1.288755	-1.378845	-0.325379

H	0.375972	-1.366311	-1.613021
O	-2.111066	1.513763	-1.118824
H	-1.394496	2.153184	-1.339234
H	-2.121536	1.449847	-0.128896
O	-4.018614	-2.219702	1.185695
H	-3.063661	-2.150088	1.393097
H	-4.413684	-1.359613	1.442647
O	2.094193	1.327326	1.322952
H	1.386592	1.957309	1.624899
H	2.119088	1.411238	0.339722
O	4.014190	-2.037376	-1.417998
H	4.408255	-1.148137	-1.542274
H	3.058335	-1.937929	-1.608410
O	4.842600	0.651062	-1.252796
H	5.668588	1.059525	-1.554014
H	4.873670	0.634568	-0.254929
O	-2.149186	1.097712	1.583543
H	-1.803272	0.169685	1.562453
H	-3.119747	1.016554	1.725570
O	-4.786707	0.708662	-1.289544
H	-4.634379	-0.224332	-1.551972
H	-3.932526	1.169155	-1.424218
O	-4.050707	-1.995287	-1.507355
H	-4.036888	-2.137000	-0.519637
H	-4.487102	-2.770622	-1.893285
O	-1.431634	-1.090316	-1.586956
H	-1.643812	-0.122954	-1.547486
H	-2.286519	-1.545273	-1.764480
O	1.416044	-1.308974	1.430145
H	2.272087	-1.777537	1.559524
H	1.617699	-0.342561	1.532217
O	-4.844896	0.467416	1.400513
H	-5.647395	0.855141	1.785312
H	-4.901308	0.599219	0.413512

18b

E= hartree

O	1.646425	2.720331	-1.071090
H	1.831046	3.661929	-1.211043
H	1.614220	2.586242	-0.079907
O	3.732941	-2.358383	-0.224529
H	4.352220	-1.605749	-0.097057
H	3.203792	-2.136405	-1.021461
O	-0.348232	-1.032871	-1.448037
H	-0.321363	-1.079857	-0.457092
H	-1.186028	-1.479450	-1.715456
O	1.574952	2.424986	1.592485
H	2.277133	1.801829	1.907700
H	0.721969	2.056673	1.909604
O	-0.781318	1.160227	2.516020
H	-1.662467	1.466709	2.160575
H	-0.845922	1.201347	3.482524
O	-0.351015	-1.272562	1.278113
H	-0.480174	-0.406775	1.737281
H	0.528900	-1.616975	1.565931
O	2.206290	-2.058713	1.970606
H	2.411528	-2.783480	2.580917
H	2.737454	-2.223335	1.141598
O	-2.872687	-2.105369	-1.826807
H	-3.236316	-2.662199	-2.532350
H	-3.503161	-1.339084	-1.712337

O	-4.584507	-0.083214	-1.348621
H	-4.109691	0.778292	-1.385705
H	-4.781392	-0.237301	-0.398860
O	-2.780842	-2.591087	0.952219
H	-1.896783	-2.225494	1.182509
H	-2.805731	-2.630862	-0.027345
O	-0.689342	1.642908	-2.155554
H	0.109541	2.102511	-1.809162
H	-0.552844	0.684870	-1.971416
O	-3.106008	2.275411	-1.151979
H	-3.402014	3.077504	-1.608918
H	-2.199360	2.060944	-1.509800
O	-4.583485	-0.635233	1.396644
H	-5.314975	-0.983429	1.928940
H	-3.917081	-1.371500	1.303487
O	2.184518	-1.418456	-2.391668
H	1.256455	-1.286972	-2.072137
H	2.128584	-1.857876	-3.253328
O	3.387676	0.498320	2.331095
H	4.056830	0.430723	1.617716
H	2.922277	-0.363394	2.347424
O	3.616983	0.997540	-2.039783
H	2.941625	1.650192	-1.743002
H	3.125038	0.184127	-2.283822
O	5.031670	0.090394	0.064106
H	4.543381	0.496354	-0.704824
H	5.967947	0.315717	-0.046489
O	-3.228452	1.824415	1.615163
H	-3.767744	1.004193	1.635401
H	-3.191418	2.100858	0.672843

19

E= hartree			
O	3.622198	-1.836807	-0.553621
H	3.213208	-1.815123	-1.446178
H	2.887797	-2.061272	0.063924
O	-0.735968	-3.658489	0.099419
H	0.040639	-3.186595	0.491767
H	-0.607237	-4.606213	0.255080
O	1.952982	1.110090	-1.905638
H	2.725434	1.152932	-1.295585
H	2.043959	0.268849	-2.411135
O	-1.333981	-0.676214	3.241591
H	-0.365394	-0.791786	3.327900
H	-1.455024	0.214397	2.846880
O	-2.077443	-0.358469	-2.029373
H	-2.143407	0.592307	-2.279513
H	-2.850580	-0.545181	-1.443994
O	1.293717	-2.050969	0.918558
H	0.850248	-1.297676	0.450250
H	1.405416	-1.740737	1.849815
O	0.274014	3.341064	-1.595879
H	0.439399	3.495326	-0.639518
H	0.911501	2.648412	-1.869614
O	0.006115	0.035445	-0.304901
H	-0.728769	-0.204754	-0.926787
H	0.680073	0.525761	-0.841683
O	2.614876	1.595187	2.227864
H	1.990309	2.278947	1.900085
H	3.165926	1.335486	1.457955
O	-3.475926	2.002340	0.232089

H	-3.129629	2.233163	-0.655995
H	-3.825384	1.087739	0.162836
O	-2.178273	2.407803	-2.242130
H	-2.514672	2.971447	-2.955692
H	-1.287977	2.775520	-1.983514
O	4.017950	0.776356	-0.088290
H	4.945357	1.015772	-0.238997
H	3.953246	-0.215459	-0.186103
O	-1.195941	1.594482	1.634301
H	-2.077457	1.835561	1.240437
H	-0.771069	0.984518	0.982660
O	0.723386	3.429396	1.188020
H	-0.035552	2.834820	1.435298
H	0.618544	4.248298	1.695919
O	-0.373262	-2.540899	-2.478119
H	-1.025996	-1.808921	-2.492724
H	-0.519731	-3.016406	-1.630741
O	2.080294	-1.487576	-2.880088
H	1.187290	-1.898378	-2.705296
H	2.331707	-1.751064	-3.778653
O	-2.778627	-2.311459	1.563388
H	-2.280910	-1.784355	2.238019
H	-2.114632	-2.829814	1.061029
O	-4.068620	-0.712881	-0.156951
H	-4.961040	-1.076119	-0.265635
H	-3.608981	-1.287385	0.522378
O	1.513241	-0.653125	3.264980
H	2.002522	-0.828557	4.083018
H	1.865004	0.204343	2.900358

20a

E= hartree

O	3.876031	-0.401977	0.187957
O	3.203470	2.118727	-0.914538
O	2.778926	-2.271314	-1.501696
O	2.672028	-0.814224	2.705471
O	1.597666	1.741113	-3.043670
O	1.233103	-1.002797	-3.529705
O	1.755669	3.315508	1.078772
O	1.014425	-3.768632	-0.107036
O	1.362000	1.578098	3.244750
O	0.837720	-2.787400	2.490762
O	-0.881740	2.855565	-2.429349
O	-1.433437	-1.567141	-3.234571
O	-0.875988	3.795326	0.089160
O	-1.597796	-3.381170	-1.062110
O	-1.261747	1.021444	3.515223
O	-1.668952	-1.664435	3.079559
O	-2.699370	0.728856	-2.637955
O	-2.737636	2.328756	1.475030
O	-3.225406	-2.105642	0.752695
O	-3.895478	0.338798	-0.149575
H	3.473041	-1.060547	-0.428279
H	4.834145	-0.542426	0.167931
H	3.467976	1.270562	-0.497446
H	2.734371	2.635837	-0.211002
H	3.337746	-2.918168	-1.959603
H	2.113300	-2.798929	-0.975560
H	3.121090	-0.661995	1.844817
H	2.219556	0.032441	2.931118
H	2.030657	2.221262	-3.766140

H	2.178929	1.863316	-2.239734
H	1.350821	-0.033978	-3.414867
H	1.762300	-1.434136	-2.826817
H	0.846864	3.487964	0.754803
H	1.669933	2.703465	1.842704
H	0.960610	-3.452880	0.825179
H	0.109631	-3.672459	-0.479832
H	0.390073	1.358324	3.315206
H	1.616386	1.960454	4.098397
H	1.105268	-3.444290	3.151639
H	1.498936	-2.042602	2.556840
H	-1.539350	2.127862	-2.517544
H	-0.007591	2.470944	-2.674370
H	-1.452397	-2.210747	-2.493682
H	-0.476916	-1.390060	-3.425194
H	-0.966256	4.756180	-0.006162
H	-0.848457	3.423621	-0.839465
H	-2.078210	-4.172166	-1.348052
H	-2.163629	-2.924380	-0.393141
H	-1.811925	1.447257	2.823144
H	-1.433206	0.048400	3.447187
H	-0.795669	-2.081735	2.911006
H	-2.206143	-1.808629	2.271933
H	-3.329245	0.850644	-3.365561
H	-2.201155	-0.114464	-2.839473
H	-3.345798	2.973281	1.866613
H	-2.056575	2.841788	0.974281
H	-4.066364	-2.500646	1.030650
H	-3.444988	-1.191894	0.411613
H	-3.521651	1.027566	0.443906
H	-3.504010	0.496277	-1.040411

20b	E= hartree		
O	1.310871	-0.621898	2.281928
H	0.389017	-0.643995	2.608675
H	1.351824	-1.273941	1.537375
O	4.256214	-1.114108	-1.999028
H	4.924403	-1.563086	-2.539786
H	4.262717	-1.562489	-1.104707
O	4.151094	-0.467686	2.354028
H	3.213696	-0.510107	2.623866
H	4.285720	0.415056	1.951256
O	1.275731	-2.360307	0.165094
H	0.357439	-2.693934	0.214215
H	1.337591	-1.833623	-0.670677
O	1.511912	-0.871296	-2.130453
H	1.481482	0.092579	-1.901728
H	2.458961	-1.065874	-2.321747
O	4.210315	1.663464	-1.604883
H	4.330497	0.705894	-1.790245
H	3.271593	1.859988	-1.795776
O	4.122251	-2.368910	0.381427
H	4.267203	-1.727263	1.121396
H	3.187402	-2.646095	0.444480
O	1.385749	1.782729	-1.455988
H	1.400242	1.852111	-0.467847
H	0.472126	2.003495	-1.732528
O	1.514985	1.922228	1.283076
H	1.456841	1.007611	1.663325
H	2.463236	2.181740	1.352518

O	4.263411	2.070961	1.072722
H	4.924608	2.749356	1.279526
H	4.307706	1.918361	0.089024
O	-4.293470	-0.488727	2.243247
H	-4.962914	-0.734401	2.899184
H	-4.358338	-1.134970	1.499609
O	-1.243871	-1.098337	-2.088430
H	-0.313753	-1.186030	-2.391129
H	-1.289503	-1.546776	-1.207261
O	-1.496166	-0.309733	2.287259
H	-1.394200	0.570344	1.840801
H	-2.440181	-0.372978	2.546128
O	-4.297440	-2.244045	0.117022
H	-4.248898	-1.726081	-0.737678
H	-4.878918	-3.002271	-0.049215
O	-4.046918	-0.882607	-2.194827
H	-4.174613	0.079493	-2.041691
H	-3.104142	-0.998217	-2.433743
O	-1.391662	1.609148	-1.686490
H	-1.339315	0.634834	-1.860539
H	-2.334153	1.856225	-1.824942
O	-1.512920	-2.278666	0.379885
H	-2.465584	-2.515229	0.339257
H	-1.438890	-1.582195	1.081343
O	-4.149215	1.848231	-1.546783
H	-4.743551	2.521608	-1.912155
H	-4.167074	1.955051	-0.556492
O	-4.043510	2.121469	1.145488
H	-3.094093	2.318778	1.280930
H	-4.211138	1.259637	1.582025
O	-1.232353	2.097117	1.009667
H	-0.307339	2.331459	1.240990
H	-1.237762	1.933709	0.032289

20c

E= hartree

O	2.572871	1.091311	1.395421
H	1.669823	0.718065	1.530397
H	2.486536	2.058413	1.556086
O	2.663891	1.026412	-1.341348
H	2.721989	1.058380	-0.352145
H	3.197923	0.246352	-1.613893
O	0.003263	0.097910	1.453879
H	-0.850203	0.592815	1.557796
H	-0.186465	-0.870556	1.551856
O	-0.323296	-2.601534	1.286786
H	-0.306533	-2.653830	0.296610
H	0.550905	-2.944020	1.582851
O	-0.866372	4.069673	-1.430551
H	-1.035188	4.899069	-1.903276
H	0.115769	3.907456	-1.480240
O	-4.283889	-0.458889	1.510898
H	-5.081965	-0.550311	2.053668
H	-3.837290	-1.350658	1.503336
O	-3.086343	-2.668887	-1.536643
H	-3.642143	-3.220393	-2.108413
H	-3.503976	-1.763072	-1.520924
O	0.103801	0.152474	-1.278351
H	1.003684	0.495414	-1.518870
H	0.088414	0.149735	-0.286018
O	-2.195292	1.634563	-1.454091

H	-1.898697	2.565008	-1.577018
H	-1.383984	1.081552	-1.564239
O	1.805389	3.756794	1.480476
H	2.122074	4.504025	2.010672
H	0.809999	3.780197	1.519861
O	-4.268653	-0.255282	-1.299196
H	-4.422335	-0.222167	-0.330407
H	-3.651607	0.478795	-1.504750
O	-0.304080	-2.550471	-1.453406
H	-1.262599	-2.698975	-1.624253
H	-0.149577	-1.579217	-1.556435
O	2.307243	-3.540195	-1.227257
H	1.380892	-3.332991	-1.473667
H	2.311828	-3.636189	-0.250407
O	-2.326447	1.494350	1.282889
H	-3.079081	0.914280	1.539866
H	-2.359346	1.562581	0.294580
O	3.962778	-1.432746	-1.555242
H	4.723270	-1.733677	-2.075856
H	3.325181	-2.198517	-1.514079
O	-3.107820	-2.876249	1.277845
H	-2.158115	-2.868301	1.522070
H	-3.131687	-2.986267	0.302703
O	1.810026	3.714807	-1.340678
H	2.152012	2.832540	-1.592635
H	1.965766	3.799978	-0.375303
O	2.353965	-3.313418	1.581926
H	2.971413	-2.531294	1.537155
H	2.783654	-3.972320	2.148687
O	4.083899	-1.266015	1.252415
H	3.686391	-0.397226	1.472955
H	4.198987	-1.270820	0.277299
O	-0.891491	3.919004	1.385871
H	-1.405397	3.114461	1.605176
H	-1.027879	4.072770	0.426051

Table 21. Cartesian coordinates of (H₂O)₁₀₀ nanodrop optimized with the DFTB parameters implemented in Gaussian09 (DFTBA).

O	0.189174	-0.102064	7.832840
O	5.215305	-0.020676	4.020654
O	-5.674452	3.745398	3.763608
O	-0.822401	2.177370	3.100788
O	-2.397669	-3.713960	6.456280
O	-1.176587	-0.499552	3.542718
O	6.412374	-2.561399	3.823432
O	-4.011550	2.910400	5.926431
O	3.096298	-0.050370	2.280172
O	1.182385	-1.811757	3.155156
O	0.027945	-5.106250	5.928259
O	-6.333567	-0.548304	4.699209
O	7.110509	-3.127829	1.305246
O	2.001631	-3.235278	5.353349
O	2.494186	-1.340477	7.282116
O	3.035991	3.103220	6.426817
O	3.052136	4.195272	3.889286
O	-5.199962	-2.588454	3.195341
O	0.388610	2.580393	7.339772
O	-4.231604	-4.741013	4.696922
O	-6.475264	1.051671	0.408885
O	-7.102291	1.482440	3.123116
O	3.786405	-0.541491	-0.319172
O	4.492351	-4.315561	4.683701
O	-4.327702	0.305894	6.472361
O	4.278051	0.715817	6.528273
O	-3.046284	-1.581152	1.871470
O	-1.892365	-0.971796	6.141356
O	-1.716777	-7.479282	-1.157428
O	4.018912	-4.781033	-1.753584
O	-6.960814	-2.008125	-3.196693
O	-1.789884	-2.348828	-2.325871
O	-3.005729	-6.515205	3.135331
O	-1.750602	-3.349594	0.222614
O	5.674875	-5.368089	0.387886
O	-5.693658	-4.357426	-3.095307
O	2.349312	-2.779046	-0.934034
O	0.801507	-3.618385	1.154417
O	-0.304395	-6.790902	3.846765
O	-6.827465	-3.344918	1.127508
O	1.486175	-6.200870	1.780088
O	1.044604	-7.747499	-0.530757
O	0.855055	-6.187876	-4.676084
O	1.388881	-3.559856	-5.408525
O	-1.739132	-6.646459	-3.717077
O	-7.670044	-1.268602	-0.641657
O	4.150370	-6.086540	2.476899
O	-5.558886	-5.319187	-0.458217
O	2.507747	-6.961087	-2.712340
O	-3.052311	-5.723138	0.506311
O	1.716777	7.479282	1.157428
O	-4.018912	4.781033	1.753584
O	6.960814	2.008125	3.196693
O	1.789884	2.348828	2.325871
O	3.005729	6.515205	-3.135331
O	1.750602	3.349594	-0.222614
O	-5.674875	5.368089	-0.387886

O	5.693658	4.357426	3.095307
O	-2.349312	2.779046	0.934034
O	-0.801507	3.618385	-1.154417
O	0.304395	6.790902	-3.846765
O	6.827465	3.344918	-1.127508
O	-7.110509	3.127829	-1.305246
O	-1.486175	6.200870	-1.780088
O	-1.044604	7.747499	0.530757
O	-0.855055	6.187876	4.676084
O	-1.388881	3.559856	5.408525
O	5.199962	2.588454	-3.195341
O	1.739132	6.646459	3.717077
O	4.231604	4.741013	-4.696922
O	6.475264	-1.051671	-0.408885
O	7.670044	1.268602	0.641657
O	-3.786405	0.541491	0.319172
O	-4.150370	6.086540	-2.476899
O	5.558886	5.319187	0.458217
O	-2.507747	6.961087	2.712340
O	3.046284	1.581152	-1.871470
O	3.052311	5.723138	-0.506311
O	-0.189174	0.102064	-7.832840
O	-5.215305	0.020676	-4.020654
O	5.674452	-3.745398	-3.763608
O	0.822401	-2.177370	-3.100788
O	2.397669	3.713960	-6.456280
O	1.176587	0.499552	-3.542718
O	-6.412374	2.561399	-3.823432
O	4.011550	-2.910400	-5.926431
O	-3.096298	0.050370	-2.280172
O	-1.182385	1.811757	-3.155156
O	-0.027945	5.106250	-5.928259
O	6.333567	0.548304	-4.699209
O	-2.001631	3.235278	-5.353349
O	-2.494186	1.340477	-7.282116
O	-3.035991	-3.103220	-6.426817
O	-3.052136	-4.195272	-3.889286
O	-0.388610	-2.580393	-7.339772
O	7.102291	-1.482440	-3.123116
O	-4.492351	4.315561	-4.683701
O	4.327702	-0.305894	-6.472361
O	-4.278051	-0.715817	-6.528273
O	1.892365	0.971796	-6.141356
H	2.422924	-0.706691	2.595587
H	2.648091	0.835589	2.306370
H	2.227240	2.716996	-0.819777
H	2.216671	4.224169	-0.310868
H	1.773721	-2.573742	-1.718686
H	2.944041	-3.522214	-1.215054
H	0.303629	0.951256	-3.399163
H	1.420127	0.650428	-4.492461
H	-0.303629	-0.951256	3.399163
H	-1.420127	-0.650428	4.492461
H	-1.773721	2.573742	1.718686
H	-2.944041	3.522214	1.215054
H	-2.227240	-2.716996	0.819777
H	-2.216671	-4.224169	0.310868
H	-2.422924	0.706691	-2.595587
H	-2.648091	-0.835589	-2.306370
H	-1.038581	2.481682	-2.434436

H	-1.463542	2.318461	-3.959371
H	-1.772777	-2.721258	-1.406080
H	-2.248647	-3.021683	-2.895518
H	-3.270038	1.354604	0.562866
H	-3.561665	0.346041	-0.628462
H	1.381126	-3.317707	0.406048
H	-0.132890	-3.547090	0.824740
H	-0.976065	1.212432	3.271582
H	0.133885	2.264713	2.847546
H	2.368360	1.203808	-2.491832
H	3.346789	0.825109	-1.300283
H	0.132890	3.547090	-0.824740
H	-1.381126	3.317707	-0.406048
H	0.976065	-1.212432	-3.271582
H	-0.133885	-2.264713	-2.847546
H	-2.368360	-1.203808	2.491832
H	-3.346789	-0.825109	1.300283
H	1.038581	-2.481682	2.434436
H	1.463542	-2.318461	3.959371
H	1.772777	2.721258	1.406080
H	2.248647	3.021683	2.895518
H	3.561665	-0.346041	0.628462
H	3.270038	-1.354604	-0.562866
H	-1.247996	7.238889	-0.285914
H	-0.085888	7.635058	0.705364
H	-1.175291	3.056305	4.583371
H	-1.204225	4.508288	5.205143
H	4.962391	5.258172	-5.070884
H	3.742738	5.366907	-4.079018
H	-3.199590	6.195442	-2.225757
H	-4.177871	5.460380	-3.230930
H	-4.502186	3.233378	5.141413
H	-3.064964	3.174890	5.803873
H	2.050194	6.628432	-3.344093
H	3.054563	6.266254	-2.177751
H	-6.231278	6.149291	-0.243068
H	-5.078235	5.598405	-1.156645
H	0.780202	4.581939	-6.113797
H	-0.748804	4.457258	-5.749528
H	-4.624842	0.320951	7.395785
H	-4.183985	1.263854	6.220443
H	-4.591936	4.431578	2.472772
H	-4.609485	5.013373	0.997193
H	-3.046526	6.214065	2.368916
H	-2.002532	7.317355	1.937333
H	0.831844	6.481774	4.062580
H	2.225168	5.792244	3.793775
H	3.048714	3.831480	4.808548
H	3.997427	4.268776	3.608514
H	-2.869890	3.637837	-5.120412
H	-2.175010	2.566313	-6.062256
H	2.081986	8.376207	1.203943
H	1.705966	7.136554	2.095769
H	-4.934745	4.849902	-5.360045
H	-5.153543	3.651280	-4.365549
H	2.055109	1.933768	-6.267645
H	2.752986	0.508677	-6.284811
H	3.052359	4.058880	-5.799534
H	2.700022	3.993793	-7.333118
H	-6.165830	2.928023	3.504811

H	-6.318816	4.351967	4.158068
H	0.139237	7.671794	-4.216427
H	0.169920	6.143724	-4.592451
H	-1.459018	6.441234	3.917859
H	-1.033865	6.827027	5.383296
H	-0.864222	6.461938	-2.498293
H	-1.243944	5.274070	-1.530251
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H	-6.376998	-1.287665	-3.528312
H	-4.865974	-3.350620	3.725069
H	-4.411150	-2.206380	2.724950
H	-1.274970	-2.794236	-6.978692
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H	-7.263343	2.488548	-4.283778
H	-6.634155	2.750534	-2.864030
H	-5.962468	-1.298762	4.175624
H	-5.633256	-0.273784	5.333973
H	-3.471266	-2.204874	-6.436205
H	-3.450601	-3.610884	-7.141394
H	-6.940032	2.371286	-0.693027
H	-6.623829	3.901908	-0.943755
H	-2.773715	1.664703	-8.152706
H	-1.630132	0.853738	-7.439441
H	-6.695674	1.197258	1.356196
H	-5.502833	0.864606	0.368281
H	-7.288575	-0.423644	-0.315069
H	-7.348768	-1.976017	-0.044473
H	-5.574505	-5.004880	-1.389876
H	-6.014208	-4.632352	0.075776
H	-2.594183	-6.374745	-0.080613
H	-3.978069	-5.615221	0.154302
H	-6.140266	-3.458737	-3.104346
H	-6.262518	-4.943309	-3.618508
H	-0.257502	-0.881921	-7.721833
H	0.549364	0.393051	-7.252593
H	-6.777414	0.721019	3.685995
H	-8.068952	1.483611	3.203929
H	-3.664276	0.010385	-6.776544
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H	-7.628109	-3.696272	1.544754
H	-6.226219	-3.057285	1.859723
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H	4.865974	3.350620	-3.725069
H	4.411150	2.206380	-2.724950
H	1.274970	2.794236	6.978692
H	-0.273959	2.934362	6.703679
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H	6.634155	-2.750534	2.864030
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H	6.777414	-0.721019	-3.685995
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H	1.175291	-3.056305	-4.583371
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H	6.231278	-6.149291	0.243068
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H	0.748804	-4.457258	5.749528
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H	4.591936	-4.431578	-2.472772
H	3.046526	-6.214065	-2.368916
H	2.002532	-7.317355	-1.937333
H	-0.831844	-6.481774	-4.062580
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H	-3.997427	-4.268776	-3.608514
H	-3.048714	-3.831480	-4.808548
H	-2.081986	-8.376207	-1.203943
H	-1.705966	-7.136554	-2.095769
H	-3.052359	-4.058880	5.799534
H	-2.700022	-3.993793	7.333118
H	6.318816	-4.351967	-4.158068
H	6.165830	-2.928023	-3.504811
H	-0.139237	-7.671794	4.216427
H	-0.169920	-6.143724	4.592451
H	1.033865	-6.827027	-5.383296

H	1.459018	-6.441234	-3.917859
H	0.864222	-6.461938	2.498293
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