

**Supplementary Information: The quantum chemical solvation of indole:  
Accounting for strong solute-solvent interactions using implicit/explicit models**

A. Manian,<sup>1, a)</sup> R. A. Shaw,<sup>2</sup> I. Lyskov,<sup>1</sup> and S. P. Russo<sup>1, b)</sup>

<sup>1)</sup>*ARC Centre of Excellence in Exciton Science, School of Science, RMIT University,  
Melbourne, 3000, Australia.*

<sup>2)</sup>*Department of Chemistry, University of Sheffield, Sheffield S3 7HF,  
UK*

(Dated: 2 December 2021)

SI begins with a number of snapshots of the explicit solvent molecules within a PCM described in the discussion, followed by the energetic differences calculated using two different basis sets for the smaller indole-water clusters. The optimised cartesian coordinates for all systems used in this study are then given; at the ground,  $L_a$ , and  $L_b$  excited states.

---

<sup>a)</sup>Electronic mail: [anjay.manian@rmit.edu.au](mailto:anjay.manian@rmit.edu.au)

<sup>b)</sup>Electronic mail: [salvy.russo@rmit.edu.au](mailto:salvy.russo@rmit.edu.au)

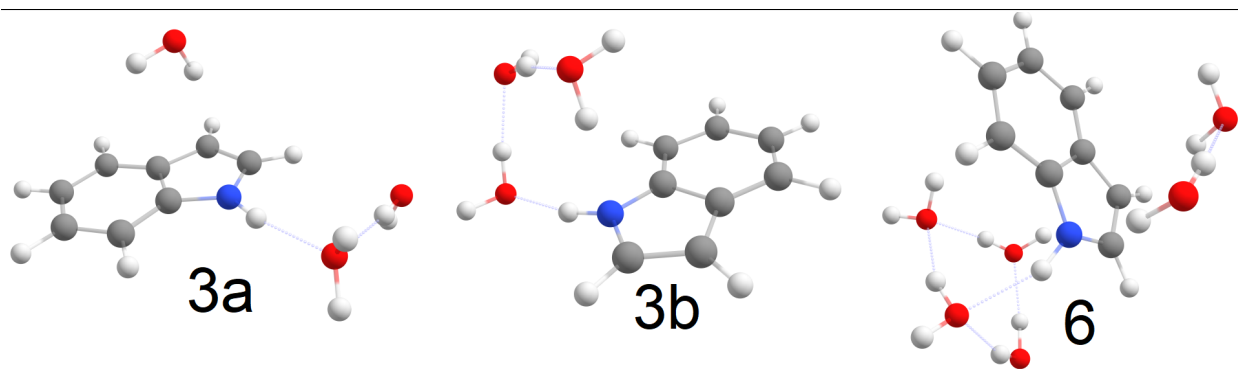


FIG. 1. Solute-solvent organisation upon equilibrium for smaller clusters. Labels indicate the number of solvent molecules.

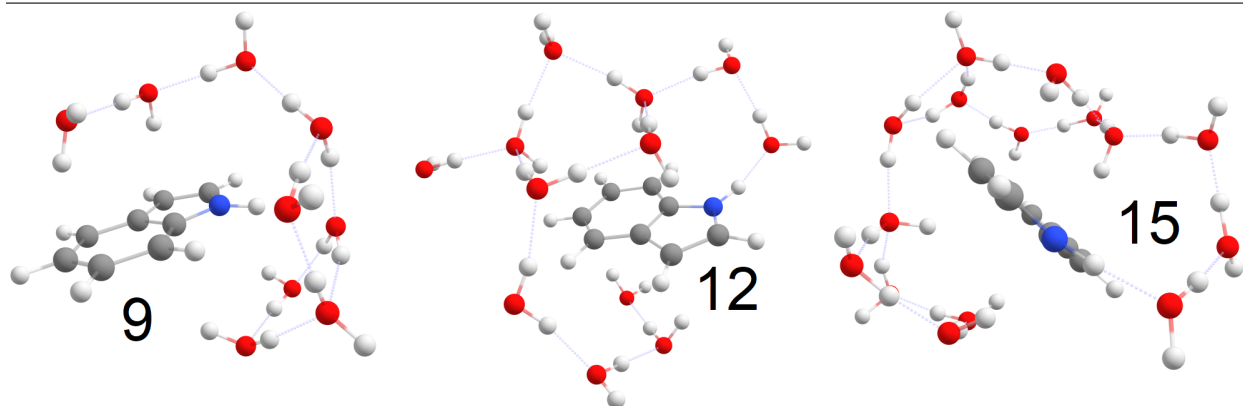


FIG. 2. Solute-solvent organisation upon equilibrium for larger clusters. Labels indicate the number of solvent molecules.

## I. CLUSTER SNAPSHOTS

Following are some snapshots of the studied QC clusters, to illustrate how the solvent couples to the indole chromophore.

## II. SHIFT OF BASIS SET

As per the explicit PCM indole-water clusters, the basis set for the larger clusters was required to be lowered in size, especially in the case of those basis sets with highly diffuse functions. As

TABLE I. Differences in computed absorption, emission, and adiabatic energies as a function of the aVDZ and aVTZ basis sets. Comparison given for explicit PCM indole-water clusters 3a, 3b, and 6 under the B3LYP/aug-cc-pVXZ and CAM-B3LYP/aug-cc-pVXZ method groups. Energies are given in units of eV.

B3LYP/aug-cc-pVXZ									
Cluster	Absorption			Emission			Adiabatic		
	aVTZ	aVDZ	$\Delta E$	aVTZ	aVDZ	$\Delta E$	aVTZ	aVDZ	$\Delta E$
3a	4.74	4.79	0.04	0.39	3.95	0.02	4.35	4.33	0.01
3b	4.79	4.81	0.02	3.92	3.92	0.01	4.39	4.35	0.05
6	4.76	4.75	0.00	3.74	3.73	0.00	4.32	4.28	0.04
CAM-B3LYP/aug-cc-pVXZ									
3a	4.74	4.80	0.05	3.97	3.99	0.01	4.33	4.33	0.00
3b	4.83	4.85	0.02	3.99	4.00	0.01	4.38	4.34	0.04
6	4.83	4.83	0.00	3.81	3.81	0.01	4.31	4.27	0.04

such, to ensure our drawn conclusions are related to cluster size, and not the changing of basis sets, the difference in energies computed using the aVTZ and aVDZ basis sets for the smaller clusters are given in Table I. Here, we see that the deviation between the two basis sets for computed energies for the smaller clusters are at most 0.05 eV, suggesting it's reasonable to use the smaller set for the larger systems.

### III. OPTIMISED GEOMETRIES - IMPLICIT PCM

Following are the optimised geometries using an implicit PCM.

#### A. Water

s0:

C	0.4230220	-1.6786269	0.0000000
C	-0.4943510	-0.6172290	0.0000000
C	0.0000000	0.7151769	0.0000000
C	1.3655999	1.0018279	0.0000000
C	2.2451968	-0.0687650	0.0000000
C	1.7785089	-1.3965369	0.0000000
C	-1.9254119	-0.5273180	0.0000000
C	-2.2419288	0.8036489	0.0000000
N	-1.0889899	1.5537319	0.0000000
H	0.0749700	-2.7046628	0.0000000
H	1.7254689	2.0231258	0.0000000
H	3.3114727	0.1194270	0.0000000
H	2.4953728	-2.2081948	0.0000000
H	-2.6285778	-1.3440459	0.0000000
H	-3.2052568	1.2862879	0.0000000
H	-1.0543339	2.5588638	0.0000000

-----  
La:

C	1.0012209	-1.4659989	0.0000040
C	-0.2391810	-0.7472719	0.0000130
C	-0.2394590	0.6568449	0.0000080
C	0.9149959	1.4399649	-0.0000010
C	2.1613938	0.6938089	-0.0000040

C	2.1908038	-0.6838759	-0.0000030
C	-1.5925299	-1.1594579	0.0000140
C	-2.4152328	0.0123900	0.0000080
N	-1.5874719	1.0628989	0.0000090
H	1.0269279	-2.5464758	0.0000050
H	0.8933989	2.5193488	-0.0000050
H	3.0931288	1.2461159	-0.0000090
H	3.1505428	-1.1872279	-0.0000070
H	-1.9699828	-2.1693058	0.0000160
H	-3.4856687	0.1164500	0.0000260
H	-1.8907939	2.0260208	0.0000100

-----

Lb:

C	0.4027610	-1.7223969	0.0000000
C	-0.5160050	-0.6378210	0.0000000
C	0.0000000	0.7319859	0.0000000
C	1.3879049	1.0459319	0.0000000
C	2.2595798	-0.0553830	0.0000000
C	1.7769159	-1.3995199	0.0000000
C	-1.9254769	-0.5364030	0.0000000
C	-2.2639328	0.8057729	0.0000000
N	-1.0706119	1.5537849	0.0000000
H	0.0656340	-2.7483918	0.0000000
H	1.7395199	2.0668968	0.0000000
H	3.3292857	0.1071570	0.0000000
H	2.5067168	-2.1995368	0.0000000
H	-2.6272398	-1.3545979	0.0000000
H	-3.2200758	1.2990269	0.0000000
H	-1.0300319	2.5599418	0.0000000

-----

**B. MCH**

s0:

C	0.4251930	-1.6762029	0.0000000
C	-0.4927850	-0.6166920	0.0000000
C	0.0000000	0.7144849	0.0000000
C	1.3643219	1.0027539	0.0000000
C	2.2447228	-0.0661040	0.0000000
C	1.7794579	-1.3931519	0.0000000
C	-1.9237639	-0.5292840	0.0000000
C	-2.2441818	0.7987269	0.0000000
N	-1.0911179	1.5522919	0.0000000
H	0.0780750	-2.7023868	0.0000000
H	1.7247149	2.0242358	0.0000000
H	3.3107277	0.1230700	0.0000000
H	2.4969588	-2.2040328	0.0000000
H	-2.6247918	-1.3475379	0.0000000
H	-3.2095038	1.2772689	0.0000000
H	-1.0561519	2.5561518	0.0000000

-----

La:

C	1.0147249	1.4478599	0.0000010
C	-0.2279700	0.7481569	-0.0000020
C	-0.2522110	-0.6491480	0.0000000
C	0.8904889	-1.4579579	0.0000050
C	2.1401598	-0.7315039	0.0000100
C	2.1922268	0.6452890	0.0000090
C	-1.5838569	1.1825799	-0.0000090

C	-2.4238708	0.0266790	-0.0000100
N	-1.6097319	-1.0346809	-0.0000040
H	1.0575289	2.5270738	-0.0000010
H	0.8519549	-2.5365148	0.0000060
H	3.0642608	-1.2962859	0.0000160
H	3.1596938	1.1323149	0.0000140
H	-1.9444039	2.1987578	-0.0000150
H	-3.4957517	-0.0608170	-0.0000140
H	-1.9233189	-1.9934898	-0.0000020

-----  
Lb:

C	0.4072390	-1.7166809	0.0000000
C	-0.5098370	-0.6388340	0.0000000
C	0.0000000	0.7299889	0.0000000
C	1.3805149	1.0452879	0.0000000
C	2.2607198	-0.0503170	0.0000000
C	1.7862209	-1.3977279	0.0000000
C	-1.9194659	-0.5416950	0.0000000
C	-2.2628578	0.8016699	0.0000000
N	-1.0866469	1.5543899	0.0000000
H	0.0699560	-2.7428028	0.0000000
H	1.7342539	2.0660938	0.0000000
H	3.3284047	0.1228730	0.0000000
H	2.5154278	-2.1971418	0.0000000
H	-2.6203738	-1.3604139	0.0000000
H	-3.2259248	1.2814799	0.0000000
H	-1.0504219	2.5590338	0.0000000

-----

#### IV. OPTIMISED GEOMETRIES - IMPLICIT PISALR

Following are the optimised geometries using an implicit PISALR method.

##### A. Water

s0:

C	0.4230220	-1.6786269	0.0000000
C	-0.4943510	-0.6172290	0.0000000
C	0.0000000	0.7151769	0.0000000
C	1.3655999	1.0018279	0.0000000
C	2.2451968	-0.0687650	0.0000000
C	1.7785089	-1.3965369	0.0000000
C	-1.9254119	-0.5273180	0.0000000
C	-2.2419288	0.8036489	0.0000000
N	-1.0889899	1.5537319	0.0000000
H	0.0749700	-2.7046628	0.0000000
H	1.7254689	2.0231258	0.0000000
H	3.3114727	0.1194270	0.0000000
H	2.4953728	-2.2081948	0.0000000
H	-2.6285778	-1.3440459	0.0000000
H	-3.2052568	1.2862879	0.0000000
H	-1.0543339	2.5588638	0.0000000

-----  
La:

C	1.0012209	-1.4659989	0.0000040
C	-0.2391810	-0.7472719	0.0000130
C	-0.2394590	0.6568449	0.0000080
C	0.9149959	1.4399649	-0.0000010
C	2.1613938	0.6938089	-0.0000040



C	2.1908038	-0.6838759	-0.0000030
C	-1.5925299	-1.1594579	0.0000140
C	-2.4152328	0.0123900	0.0000080
N	-1.5874719	1.0628989	0.0000090
H	1.0269279	-2.5464758	0.0000050
H	0.8933989	2.5193488	-0.0000050
H	3.0931288	1.2461159	-0.0000090
H	3.1505428	-1.1872279	-0.0000070
H	-1.9699828	-2.1693058	0.0000160
H	-3.4856687	0.1164500	0.0000260
H	-1.8907939	2.0260208	0.0000100

-----

Lb:

C	0.9834859	-1.4746889	-0.0000010
C	-0.2560620	-0.7790039	-0.0000010
C	-0.2504390	0.6846879	-0.0000010
C	0.9405069	1.4634619	0.0000000
C	2.1418018	0.7356839	0.0000000
C	2.1585018	-0.6924079	0.0000000
C	-1.6123439	-1.1756979	0.0000000
C	-2.3978338	-0.0359340	0.0000000
N	-1.5404489	1.0813949	0.0000000
H	1.0257329	-2.5538308	0.0000000
H	0.9130209	2.5430118	0.0000000
H	3.0877048	1.2610509	0.0000010
H	3.1216408	-1.1873539	0.0000010
H	-1.9845598	-2.1873118	0.0000000
H	-3.4660017	0.0926750	0.0000020
H	-1.8526359	2.0385648	0.0000000

-----

**B. MCH**

s0:

C	0.4251930	-1.6762029	0.0000000
C	-0.4927850	-0.6166920	0.0000000
C	0.0000000	0.7144849	0.0000000
C	1.3643219	1.0027539	0.0000000
C	2.2447228	-0.0661040	0.0000000
C	1.7794579	-1.3931519	0.0000000
C	-1.9237639	-0.5292840	0.0000000
C	-2.2441818	0.7987269	0.0000000
N	-1.0911179	1.5522919	0.0000000
H	0.0780750	-2.7023868	0.0000000
H	1.7247149	2.0242358	0.0000000
H	3.3107277	0.1230700	0.0000000
H	2.4969588	-2.2040328	0.0000000
H	-2.6247918	-1.3475379	0.0000000
H	-3.2095038	1.2772689	0.0000000
H	-1.0561519	2.5561518	0.0000000

-----

La:

C	1.0147249	1.4478599	0.0000010
C	-0.2279700	0.7481569	-0.0000020
C	-0.2522110	-0.6491480	0.0000000
C	0.8904889	-1.4579579	0.0000050
C	2.1401598	-0.7315039	0.0000100
C	2.1922268	0.6452890	0.0000090
C	-1.5838569	1.1825799	-0.0000090

C	-2.4238708	0.0266790	-0.0000100
N	-1.6097319	-1.0346809	-0.0000040
H	1.0575289	2.5270738	-0.0000020
H	0.8519549	-2.5365148	0.0000060
H	3.0642608	-1.2962859	0.0000160
H	3.1596938	1.1323149	0.0000130
H	-1.9444039	2.1987578	-0.0000130
H	-3.4957517	-0.0608170	-0.0000140
H	-1.9233199	-1.9934898	-0.0000030

-----  
Lb:

C	0.4072390	-1.7166809	0.0000000
C	-0.5098370	-0.6388340	0.0000000
C	0.0000000	0.7299889	0.0000000
C	1.3805149	1.0452879	0.0000000
C	2.2607198	-0.0503170	0.0000000
C	1.7862209	-1.3977279	0.0000000
C	-1.9194659	-0.5416950	0.0000000
C	-2.2628578	0.8016699	0.0000000
N	-1.0866469	1.5543899	0.0000000
H	0.0699560	-2.7428028	0.0000000
H	1.7342539	2.0660938	0.0000000
H	3.3284047	0.1228730	0.0000000
H	2.5154278	-2.1971418	0.0000000
H	-2.6203738	-1.3604139	0.0000000
H	-3.2259248	1.2814799	0.0000000
H	-1.0504219	2.5590338	0.0000000

-----

## V. OPTIMISED GEOMETRIES - EXPLICIT PCM

Following are the optimised geometries using an explicit PCM. Clusters are labelled according to the number of solvent molecules part of the complex.

### A. Water Cluster - Size 3a - B3LYP/def2TZVP Method Group

s0:

C	-2.6665508	0.6184150	-0.7238899
C	-1.2675889	0.6461000	-0.6399420
C	-0.5820700	-0.5147170	-0.1867510
C	-1.2579849	-1.6792969	0.1775500
C	-2.6397178	-1.6749859	0.0826100
C	-3.3373817	-0.5374490	-0.3643090
C	-0.2643970	1.6405979	-0.8960379
C	0.9488959	1.0658489	-0.6074810
N	0.7610519	-0.2265690	-0.1860130
H	-3.2129488	1.4899579	-1.0623369
H	-0.7213609	-2.5531508	0.5237130
H	-3.1941418	-2.5626708	0.3584220
H	-4.4176257	-0.5710310	-0.4245290
H	-0.4206670	2.6421508	-1.2612149
H	1.9454809	1.4717499	-0.6659569
H	1.5066309	-0.8466799	0.1119490
O	3.1729188	-1.7155909	0.5904600
H	3.3661037	-2.5634328	0.1709000
H	3.3216957	-1.8509229	1.5348569
O	-0.5939420	1.8946419	2.3548038
H	-1.2369489	1.1761369	2.3546498
H	-0.3411560	1.9762318	1.4221099
O	4.4376557	0.5864260	-0.5832400

H	4.0727137	-0.2207700	-0.1797880
H	4.2725727	0.4875290	-1.5273819

-----

La:

C	2.4431868	-1.1419099	-0.4474310
C	1.0241349	-1.0257739	-0.3287910
C	0.4106840	0.2291810	-0.3593630
C	1.1114929	1.4381859	-0.4822320
C	2.5168208	1.2839449	-0.7938189
C	3.1456918	0.0600760	-0.7665839
C	-0.0051590	-1.9793238	-0.0953550
C	-1.2420079	-1.2696689	0.0088150
N	-0.9688809	0.0225260	-0.1552350
H	2.9286838	-2.1068548	-0.4627720
H	0.6146790	2.3941738	-0.5459050
H	3.0923798	2.1707648	-1.0280659
H	4.2078967	0.0104270	-0.9716159
H	0.1015910	-3.0470658	0.0016870
H	-2.2491498	-1.6179549	0.1670370
H	-1.6785089	0.7582919	-0.1316490
O	-3.2417638	1.7831379	-0.0465730
H	-3.4488797	2.3069008	-0.8310049
H	-3.3162047	2.3890348	0.7018079
O	2.1427218	0.4047070	2.4427938
H	2.4519648	-0.3010840	1.8489419
H	1.7303709	1.0282449	1.8207609
O	-4.5372147	-0.7861919	0.1917470
H	-4.2139287	0.1272350	0.1052510
H	-4.7777436	-1.0512899	-0.7030119

-----  
**B. Water Cluster - Size 3b - B3LYP/def2TZVP Method Group**

s0:

C	-2.8934918	-0.1484600	0.2685780
C	-1.7778319	0.6782219	0.0756340
C	-0.5803390	0.1062720	-0.4316300
C	-0.4768840	-1.2486689	-0.7437969
C	-1.5976229	-2.0383188	-0.5452460
C	-2.7939898	-1.4934159	-0.0437440
C	-1.5119439	2.0729478	0.2826230
C	-0.2132180	2.2923658	-0.0885850
N	0.3633200	1.1086399	-0.5012020
H	-3.8187677	0.2597420	0.6559189
H	0.4468470	-1.6667659	-1.1218169
H	-1.5524809	-3.0941418	-0.7789819
H	-3.6491257	-2.1414298	0.0998210
H	-2.1959908	2.8137528	0.6621929
H	0.3621730	3.2031228	-0.0855470
H	1.2912879	1.0064739	-0.9194379
O	2.9478348	0.4405550	-1.5434439
H	3.6449907	1.1056539	-1.5544059
H	3.1991648	-0.2027730	-0.8418849
O	1.5362179	-0.0266190	2.1547398
H	1.0785359	0.4787390	1.4646909
H	0.8541629	-0.5816490	2.5520418
O	3.3929327	-1.3027139	0.5393910
H	3.1105138	-2.2028668	0.3410610
H	2.7414888	-0.9537859	1.1862609

-----  
La:

C	-2.9033388	-0.1548420	0.3724430
C	-1.7803369	0.7186099	0.2837440
C	-0.6193400	0.3233710	-0.3809980
C	-0.4330100	-0.9487159	-0.9558909
C	-1.6299759	-1.7745619	-0.9566239
C	-2.7845228	-1.3981439	-0.3078490
C	-1.5371639	2.0326798	0.7788459
C	-0.2076590	2.3983028	0.4018220
N	0.3085750	1.3827729	-0.2808680
H	-3.8115027	0.1391590	0.8775079
H	0.3904490	-1.1538659	-1.6266539
H	-1.5945289	-2.7300528	-1.4647539
H	-3.6313787	-2.0740028	-0.3168110
H	-2.2139828	2.6587858	1.3363979
H	0.3390560	3.3052137	0.5919600
H	1.2781589	1.3435579	-0.6437010
O	2.9286218	1.0791649	-1.1457919
H	3.5116987	1.8389079	-1.0379819
H	3.2741787	0.3781430	-0.5400830
O	1.2788439	-1.9951168	1.2691749
H	0.8898109	-1.6590999	2.0863828
H	0.6650049	-1.7007659	0.5466940
O	3.6756857	-0.8744809	0.5842140
H	4.2152737	-1.5797499	0.2095190
H	2.8346078	-1.3023719	0.8738609

-----

### C. Water Cluster - Size 6 - B3LYP/def2TZVP Method Group

s0:

C	1.7870229	-1.6373679	1.1804769
C	1.0508339	-0.4689880	0.9415029
C	0.4811620	-0.2631090	-0.3418780
C	0.6231410	-1.1892889	-1.3755019
C	1.3425209	-2.3450228	-1.1038269
C	1.9195799	-2.5649438	0.1603570
C	0.6916399	0.6763159	1.7389559
C	-0.0641510	1.4978189	0.9411799
N	-0.1710650	0.9561599	-0.3219540
H	2.2376228	-1.8137529	2.1491578
H	0.2004210	-1.0061209	-2.3551148
H	1.4701529	-3.0858228	-1.8824959
H	2.4789198	-3.4753367	0.3332840
H	0.9511989	0.8575159	2.7696398
H	-0.5494240	2.4305738	1.1738319
H	-0.9083429	1.1934829	-0.9827329
O	-2.6287098	0.6733359	-1.7826489
H	-2.6578018	-0.2765040	-1.5503369
H	-2.9330478	0.7461349	-2.6940728
O	3.5964827	1.6222259	0.5454380
H	4.0627277	0.7847319	0.4336750
H	2.8225568	1.3996389	1.0854649
O	-3.6753917	1.7421459	0.6843539
H	-3.4351677	1.5233739	-0.2312480
H	-3.3016627	1.0006909	1.1967949
O	2.2531038	2.4680648	-1.8046939
H	1.3758539	2.1336198	-1.5796309
H	2.7998088	2.2015398	-1.0411189



O	-2.4512088	-0.5512120	1.8823999
H	-1.5391439	-0.2725510	2.0491348
H	-2.4037248	-1.1043179	1.0799829
O	-2.3550138	-1.8743219	-0.6391070
H	-1.4513469	-2.1687478	-0.8335239
H	-2.9267428	-2.6356638	-0.8005459

-----

La:

C	-1.8780469	-0.3915360	1.6461019
C	-0.8722239	-0.7997729	0.7208299
C	-0.3114920	0.1038550	-0.1748130
C	-0.6485600	1.4726839	-0.2331880
C	-1.6520779	1.8743649	0.7272129
C	-2.2165898	0.9959099	1.6230689
C	-0.2898310	-2.0745168	0.4346140
C	0.6471680	-1.8908399	-0.6260990
N	0.6159670	-0.6107090	-0.9693479
H	-2.2293898	-1.0534769	2.4244548
H	-0.3355280	2.1181628	-1.0416289
H	-1.9626959	2.9112958	0.7388409
H	-2.9519018	1.3675839	2.3253228
H	-0.5087840	-3.0159588	0.9096919
H	1.3296969	-2.5909878	-1.0731099
H	1.2900929	-0.1613660	-1.5949129
O	2.8878788	0.8290939	-1.7966029
H	2.7957678	1.4617779	-1.0543589
H	3.1609298	1.3360039	-2.5692468
O	-4.0987697	-1.1170049	-0.3537020
H	-3.4661517	-0.9390899	0.3770160
H	-3.9789607	-2.0516528	-0.5615490

O	4.0039667	-1.4171359	-0.3054210
H	3.7879037	-0.7117989	-0.9358599
H	3.5186837	-1.1634459	0.5014720
O	-3.0049998	0.6074030	-2.3160628
H	-2.2728908	0.9996579	-1.8176619
H	-3.4161677	-0.0116410	-1.6812179
O	2.5803318	-0.3499930	1.9427259
H	1.6981589	-0.6776119	2.1534348
H	2.4425308	0.5490000	1.5838249
O	2.1872678	2.0847128	0.5806010
H	1.2112329	2.1296798	0.4500580
H	2.4602308	2.9413308	0.9321809

-----

#### D. Water Cluster - Size 9 - B3LYP/def2TZVP Method Group

s0:

C	-2.6751828	-2.0458288	-0.0876390
C	-1.7335569	-1.2864969	-0.7953579
C	-0.6363160	-0.7151699	-0.0887940
C	-0.4641200	-0.8907219	1.2856829
C	-1.4052629	-1.6597869	1.9542119
C	-2.5007548	-2.2316148	1.2760579
C	-1.5947629	-0.8847089	-2.1666308
C	-0.4523120	-0.1265570	-2.2440578
N	0.1160190	-0.0115850	-0.9981149
H	-3.5241327	-2.4828358	-0.5983200
H	0.3520270	-0.4168400	1.8145719
H	-1.3028809	-1.8154809	3.0203958
H	-3.2152738	-2.8251128	1.8319959

H	-2.2424568	-1.1432049	-2.9881358
H	0.0028750	0.3520310	-3.0954688
H	1.0203649	0.4153320	-0.8186819
O	3.0001108	0.7620509	-0.9372089
H	3.3093847	0.3528070	-0.1037400
H	3.0092018	0.0269870	-1.5866269
O	-2.7809838	1.9440679	-1.0128019
H	-3.0573008	1.5796949	-0.1437660
H	-2.5070268	1.1737079	-1.5339279
O	2.7895228	-1.6576599	-2.2905568
H	2.0276188	-1.7433999	-2.8751908
H	2.5270018	-2.1014168	-1.4512359
O	-0.6569759	3.6371897	-0.8332959
H	-1.0125559	4.4947677	-0.5760840
H	-1.4294389	3.0229308	-0.8736729
O	2.2039538	-2.6249968	0.2298140
H	1.2610859	-2.6006078	0.4387140
H	2.6037408	-1.9280359	0.7930079
O	3.3748207	-0.4729950	1.5405299
H	2.8275528	0.1824190	2.0480398
H	4.2097237	-0.5712930	2.0120668
O	-3.5337187	0.9207249	1.4531559
H	-3.0393478	1.3230919	2.1774958
H	-3.2978717	-0.0199020	1.4853269
O	1.6943699	2.9035558	0.3431610
H	0.8340679	3.1502228	-0.0676840
H	2.1500708	2.3254568	-0.2943900
O	1.7525409	1.3926909	2.5634578
H	1.6735959	2.0218468	1.7987559
H	2.0323118	1.9162189	3.3224807

-----  
La:

C	-2.6685978	-2.0380308	0.3183910
C	-1.5994789	-1.6716129	-0.5523560
C	-0.4490750	-1.0644819	-0.0578250
C	-0.1876130	-0.8570589	1.3119169
C	-1.2713219	-1.2634929	2.1843538
C	-2.4376378	-1.8274209	1.7092489
C	-1.4606989	-1.7226169	-1.9769358
C	-0.1996370	-1.1422999	-2.3050268
N	0.3751220	-0.7624199	-1.1696109
H	-3.5501847	-2.5453348	-0.0460430
H	0.5612580	-0.1588600	1.6524079
H	-1.1445389	-1.1415779	3.2542428
H	-3.2027618	-2.1202948	2.4183098
H	-2.1709088	-2.1060668	-2.6905928
H	0.2548330	-0.9775099	-3.2661128
H	1.2793909	-0.2660200	-1.1139719
O	2.7958258	0.6697449	-1.1464719
H	2.9527948	0.9438369	-0.2185110
H	3.3625977	-0.1247290	-1.2685509
O	-3.3579547	1.0416099	-0.2896850
H	-2.9102218	1.4074009	0.5077230
H	-3.3485487	0.0768940	-0.1464080
O	4.0596537	-1.7556679	-0.9203499
H	3.7151407	-2.4754528	-1.4611859
H	3.6431577	-1.8606709	-0.0331600
O	-1.7017599	1.6979839	-2.3379948
H	-2.1832168	2.3176878	-2.8971968
H	-2.3276638	1.4438259	-1.6137679
O	2.8662698	-1.6281269	1.5613159

H	1.9039699	-1.7953989	1.5478579
H	2.9188098	-0.6651679	1.7160719
O	2.8367198	1.2328349	1.5819069
H	2.0278028	1.7982229	1.6088839
H	3.5351587	1.7332949	2.0198408
O	-1.9875238	1.8386739	1.9677538
H	-1.0870469	2.1496358	1.7335289
H	-1.8562979	0.9267819	2.2719198
O	0.6850629	2.6138438	-1.4036639
H	-0.1530520	2.2548568	-1.7827209
H	1.3956899	1.9895338	-1.6225189
O	0.5706200	2.7443348	1.2448059
H	0.5869750	2.7496028	0.2443450
H	0.6800709	3.6626777	1.5213399

-----

### E. Water Cluster - Size 12 - B3LYP/def2TZVP Method Group

s0:

C	-1.2853389	-0.1466180	-0.6680039
C	-0.3985810	-0.9900399	0.0122850
C	0.8568839	-1.3006999	-0.5845020
C	1.2449439	-0.7696399	-1.8185279
C	0.3483480	0.0653650	-2.4681778
C	-0.9061999	0.3722710	-1.9003479
C	-0.4402660	-1.6919489	1.2638519
C	0.7493959	-2.3739388	1.3742469
N	1.5262999	-2.1453338	0.2651450
H	-2.2425728	0.1110650	-0.2345010
H	2.2019648	-1.0177589	-2.2589678

H	0.6133640	0.4884680	-3.4279817
H	-1.5871549	1.0167409	-2.4431978
H	-1.2495909	-1.6965319	1.9749178
H	1.1049309	-3.0132558	2.1655828
H	2.5015898	-2.4445438	0.1464930
O	4.9956026	0.0100930	0.4181640
H	4.1876467	0.5658800	0.3783550
H	5.6271426	0.4221200	-0.1820780
O	-2.4766938	-3.6440597	-0.2181060
H	-2.3423258	-3.3220977	-1.1358819
H	-1.6274189	-3.4832617	0.2167620
O	4.2840217	-2.5727688	-0.1326090
H	4.7852306	-3.1720398	0.4313610
H	4.6174206	-1.6668499	0.0677710
O	-2.0386948	-2.6257818	-2.7667808
H	-1.3489419	-3.0627058	-3.2806807
H	-1.7237429	-1.7179139	-2.6390628
O	-4.0338167	-1.9901148	1.3659279
H	-4.1182087	-2.4881158	2.1864508
H	-3.5164697	-2.5696628	0.7622129
O	-3.7802347	0.8082279	1.7002679
H	-3.7361527	-0.1610970	1.6108239
H	-2.8824758	1.1274999	1.9178949
O	-2.6656038	4.7453886	-1.5416389
H	-2.4084918	4.7871716	-2.4688038
H	-1.9551629	4.2329287	-1.1091389
O	1.1029569	0.7716559	2.6207488
H	0.8156839	-0.1397950	2.4590198
H	1.6508749	0.9925099	1.8401369
O	-0.6677009	3.1964888	-0.3069750
H	-0.6074340	2.3575468	-0.7888979

H	0.2397310	3.5617817	-0.2975590
O	2.5796908	1.3595289	0.2827290
H	2.1082428	0.9176099	-0.4401640
H	2.4969638	2.3196338	0.1036060
O	-1.3385679	2.1135528	2.2327728
H	-1.1550339	2.5688288	1.3894999
H	-0.5019150	1.6454989	2.4342118
O	2.0102068	4.0471587	-0.1701010
H	2.3860548	4.4794277	-0.9482789
H	2.1977198	4.6347876	0.5739400

-----  
La:

C	1.1206149	0.1713300	1.3686919
C	0.5164950	-0.6699779	0.3867010
C	-0.7234329	-1.2497669	0.6104450
C	-1.5279299	-0.9905179	1.7442189
C	-0.8811409	-0.1891920	2.7522138
C	0.3625110	0.3751140	2.5693098
C	0.9545429	-1.1193729	-0.9048939
C	-0.0676780	-1.9677548	-1.4282929
N	-1.0416819	-2.0339258	-0.5276270
H	2.0577288	0.6772529	1.1853249
H	-2.4232408	-1.5567819	1.9566879
H	-1.4064209	-0.0119180	3.6826967
H	0.7836259	0.9873079	3.3571627
H	1.8793369	-0.8822999	-1.4023089
H	-0.1114390	-2.4907758	-2.3681528
H	-1.9563019	-2.5115878	-0.6599819
O	-5.0552236	-0.7268269	-0.6484090
H	-4.4203907	-0.0203880	-0.3949230

H	-5.7556416	-0.7030119	0.0133000
O	3.5219847	-3.0803128	-0.0314120
H	3.1826218	-2.8532118	0.8658089
H	2.8257468	-3.5982867	-0.4513190
O	-3.5945807	-3.0199388	-0.7669469
H	-3.8561207	-3.5288517	-1.5423769
H	-4.1842377	-2.2270728	-0.7427569
O	2.6293268	-2.2668908	2.4208718
H	1.9654318	-2.8123718	2.8597648
H	2.1680798	-1.4285919	2.2036458
O	4.2919437	-0.8958949	-1.4904549
H	4.5881016	-1.2336969	-2.3427108
H	4.0343857	-1.6860579	-0.9609739
O	3.3221197	1.7266829	-1.5732239
H	3.6175677	0.7982159	-1.5076999
H	2.3913208	1.7148649	-1.8823979
O	3.0269258	3.4316787	0.6290740
H	3.2089718	2.8102638	-0.1063800
H	2.0581628	3.4688187	0.6666809
O	-1.7345049	0.7607649	-2.4757088
H	-1.7847389	-0.1634070	-2.7439248
H	-2.1796638	0.8090929	-1.6011089
O	0.1678120	2.9645278	0.4609060
H	0.2628180	2.0828598	0.8676309
H	-0.7379889	3.2629258	0.6692579
O	-2.9921338	0.9589649	-0.0029890
H	-2.5286878	0.4168410	0.6800679
H	-2.9642858	1.8823209	0.3190130
O	0.6617869	2.1481828	-2.1655138
H	0.4450780	2.5232358	-1.2877139
H	-0.0995120	1.5667089	-2.3655238



O	-2.5628618	3.5856407	0.8944059
H	-2.8445478	3.7977447	1.7938359
H	-2.9086318	4.2955507	0.3376090

-----

### F. Water Cluster - Size 15 - B3LYP/def2TZVP Method Group

s0:

C	0.6545170	0.6109900	0.4931890
C	0.1169290	-0.3663460	-0.3708190
C	-0.9308309	-1.2163709	0.1099800
C	-1.4349029	-1.1192569	1.4131169
C	-0.8638199	-0.1601290	2.2576838
C	0.1723700	0.6940229	1.8002359
C	0.3432930	-0.7345829	-1.7492919
C	-0.5424940	-1.7534359	-2.0465248
N	-1.3030849	-2.0633648	-0.9247389
H	1.4031099	1.3119319	0.1463990
H	-2.2551368	-1.7469889	1.7374169
H	-1.2356319	-0.0512910	3.2702868
H	0.5573440	1.4665159	2.4542508
H	1.0688539	-0.3015850	-2.4190758
H	-0.6843859	-2.2901478	-2.9710458
H	-2.1523468	-2.6751108	-0.8654919
O	-4.6249126	0.9924359	-0.4510530
H	-3.7816617	1.4948159	-0.2091740
H	-4.8324106	1.0922469	-1.3954329
O	1.0798829	-3.7628727	0.0863520
H	1.2641619	-3.2748137	0.9642689
H	0.1817580	-3.5523417	-0.2336520

O	-4.8575146	-1.3508459	0.5689490
H	-5.0324706	-1.3078829	1.5230059
H	-4.7718296	-0.4192110	0.1608870
O	1.6331069	-2.4277608	2.2113338
H	1.0238279	-1.7183239	2.4850288
H	2.6045928	-2.1666348	2.3262498
O	3.2994947	-0.9282039	-0.2297610
H	3.2517358	-1.7586629	-0.8502419
H	2.4060678	-0.8140219	0.1598160
O	3.4592467	1.5167959	-1.3582029
H	3.4838767	0.5898120	-0.9914659
H	2.6647018	1.6737539	-1.9281369
O	0.9454669	4.0383217	1.7716089
H	1.3777929	3.9787587	2.6372318
H	1.5813059	3.8656547	0.9807319
O	-1.2240599	1.8700359	-2.2065178
H	-1.1963969	0.9210399	-2.4389668
H	-1.6521229	1.9694208	-1.2957699
O	2.3691308	3.6503217	-0.2872550
H	3.0187988	2.8976408	-0.3922670
H	1.7879129	3.5460817	-1.0943449
O	-2.3217048	2.0039618	0.1846650
H	-1.9553579	1.2605059	0.7044639
H	-2.0574908	2.9067408	0.6608619
O	1.1980929	2.6769808	-2.4576348
H	1.3427649	3.0899888	-3.3276447
H	0.2188880	2.3817338	-2.3531408
O	-1.5310759	4.0498697	1.3519219
H	-0.5206460	4.0627957	1.5647279
H	-1.8908779	4.9366986	1.1929809
O	-3.5787517	-3.3257587	-0.4320250

H	-4.1388037	-2.5747828	-0.0214510
H	-3.5965917	-4.1229127	0.1246370
O	2.8970758	-3.0483928	-1.5513449
H	2.1562978	-3.4402827	-0.9510749
H	2.5920868	-2.9620788	-2.4709878
O	4.1201297	-1.6881679	2.1387678
H	4.0588707	-1.3432899	1.1954039
H	4.8318136	-2.3453228	2.2300238

-----  
La:

C	0.8561939	-0.1459860	-0.4010580
C	-0.1224520	0.3041200	0.5441020
C	-1.3204579	0.8763799	0.1338100
C	-1.6756619	1.1068969	-1.2264479
C	-0.7550779	0.5314870	-2.1722528
C	0.4446240	-0.0655010	-1.7867599
C	-0.1311970	0.3231610	2.0016038
C	-1.3706849	0.9104829	2.4115558
N	-2.0621828	1.2314429	1.3069669
H	1.6317309	-0.8452399	-0.1092250
H	-2.6764498	1.4015939	-1.5108929
H	-1.0153989	0.5577840	-3.2263328
H	1.0775279	-0.5317390	-2.5353088
H	0.6401460	-0.0419350	2.6584708
H	-1.7534699	1.0702079	3.4054277
H	-3.0604298	1.6183629	1.2525349
O	-3.9401507	-2.0634888	-0.4257090
H	-2.9623308	-2.2593118	-0.5902280
H	-4.3018557	-2.6302538	0.2749680
O	-0.0684840	3.6742517	-0.8193839

H	0.6691319	3.4703027	-1.4908459
H	-0.7997849	3.0295138	-0.9842049
O	-5.0658576	0.1858160	-0.8202059
H	-5.1878526	0.3848210	-1.7625329
H	-4.6002396	-0.7150059	-0.6783819
O	1.7566269	2.8647368	-2.4872528
H	1.4628329	1.9399009	-2.6138928
H	2.6957758	2.8876408	-2.1018878
O	2.7301238	1.7265139	0.7069939
H	2.1111828	2.4145288	1.1578519
H	2.1355728	1.1585749	0.1179550
O	3.5920957	-0.5116820	1.9090659
H	3.3338437	0.3931370	1.5727689
H	2.8298508	-0.9701109	2.3413508
O	2.3361748	-3.1026438	-1.8874819
H	3.0060978	-3.3331597	-2.5515138
H	2.7509408	-2.8976018	-0.9689299
O	-0.8109959	-2.5402648	1.7993689
H	-1.5408659	-2.2192138	2.3543508
H	-1.0381879	-2.4798178	0.8116379
O	3.2565858	-2.6685798	0.4414140
H	3.6421427	-1.7932629	0.7387429
H	2.5897788	-2.8630698	1.1572279
O	-1.3854389	-2.4235978	-0.7405539
H	-1.0437979	-1.5785709	-1.1066739
H	-0.8821259	-3.2103468	-1.2198799
O	1.6272729	-2.3858398	2.5395768
H	1.7863279	-2.8834298	3.3616327
H	0.6382750	-2.4354448	2.2705828
O	0.0347900	-4.1442717	-1.8524189
H	0.9948209	-3.7651867	-1.9068819

H	-0.2285380	-4.6013766	-2.6677068
O	-4.4861457	1.9898118	0.8511089
H	-4.8096026	1.2960329	0.1640440
H	-5.1739256	2.2328968	1.4920599
O	0.9801319	3.4032707	1.4914769
H	0.4842240	3.5728307	0.6025010
H	0.3688200	3.2402078	2.2297208
O	4.0226997	2.8586868	-1.2277829
H	3.6718537	2.4332068	-0.3748330
H	4.8021276	2.3844278	-1.5654899

-----

### G. Water Cluster - Size 3a - B3LYP/aug-cc-pVXZ Method Group

s0:

C	2.7763978	-1.0503709	-0.1739720
C	1.3753269	-1.0257589	-0.1860550
C	0.7126509	0.2216340	-0.3363020
C	1.4084029	1.4210049	-0.4763190
C	2.7927408	1.3630869	-0.4650300
C	3.4697507	0.1395930	-0.3139970
C	0.3526890	-2.0259778	-0.0715410
C	-0.8510899	-1.3819989	-0.1487320
N	-0.6434980	-0.0231180	-0.2855960
H	3.3074027	-1.9857538	-0.0574880
H	0.8869529	2.3616278	-0.5876000
H	3.3633477	2.2751668	-0.5727410
H	4.5511357	0.1331240	-0.3072700
H	0.4955750	-3.0850418	0.0582420
H	-1.8558629	-1.7663459	-0.1096640

H	-1.3775279	0.6516940	-0.4702110
O	-3.0320238	1.6432009	-0.7036429
H	-3.1751288	2.0626268	-1.5598469
H	-3.2107138	2.3264268	-0.0472390
O	-0.4264690	0.6236800	2.8179268
H	-0.5813960	0.3909460	1.8925429
H	0.4950450	0.9017929	2.8417278
O	-4.2275197	-0.9165639	-0.2878460
H	-3.9406037	0.0009510	-0.4345050
H	-5.1868536	-0.8751929	-0.2266050

-----  
La:

C	2.4668708	-1.1176879	-0.4387390
C	1.0436959	-1.0190369	-0.3668380
C	0.4190300	0.2321130	-0.3882500
C	1.1122349	1.4458929	-0.4563460
C	2.5258358	1.3125219	-0.7316659
C	3.1662178	0.0938470	-0.7111179
C	0.0216110	-1.9850538	-0.1792470
C	-1.2234439	-1.2892459	-0.0913630
N	-0.9628909	0.0091320	-0.2257500
H	2.9621448	-2.0766108	-0.4542580
H	0.6108430	2.3992238	-0.5064090
H	3.0985388	2.2086918	-0.9289639
H	4.2334607	0.0585480	-0.8842679
H	0.1356150	-3.0523858	-0.0993170
H	-2.2291648	-1.6531009	0.0288390
H	-1.6786539	0.7372239	-0.2023030
O	-3.2334918	1.7741149	-0.1037530
H	-3.4552327	2.2843878	-0.8913729

H	-3.2883087	2.3944348	0.6326140
O	2.0316348	0.3559230	2.5079958
H	2.3745418	-0.3363520	1.9179259
H	1.6339829	0.9870639	1.8849189
O	-4.4759417	-0.7870259	0.2772420
H	-4.2005677	0.1313740	0.1195200
H	-5.2268806	-0.9306089	-0.3071410

-----

#### H. Water Cluster - Size 3b - B3LYP/aug-cc-pVXZ Method Group

s0:

C	-2.9889748	0.0519340	0.3623280
C	-1.7964519	0.7444239	0.1119700
C	-0.6889299	0.0331740	-0.4218840
C	-0.7491569	-1.3295529	-0.7088489
C	-1.9429969	-1.9849858	-0.4548750
C	-3.0513678	-1.3011009	0.0766710
C	-1.3725099	2.1055238	0.2740470
C	-0.0729460	2.1731908	-0.1468160
N	0.3574870	0.9236599	-0.5468660
H	-3.8474337	0.5677970	0.7714769
H	0.1048900	-1.8547049	-1.1133129
H	-2.0244008	-3.0419498	-0.6677939
H	-3.9664287	-1.8461429	0.2639990
H	-1.9559969	2.9240828	0.6591979
H	0.5974690	3.0142788	-0.1873890
H	1.2473029	0.7255509	-1.0089409
O	2.8713378	0.1576620	-1.6967309
H	3.4727517	0.8379559	-2.0153548

H	3.3156637	-0.2560990	-0.9235509
O	1.6749159	-0.1088470	2.0701038
H	1.1389819	0.2696970	1.3566159
H	1.1131239	-0.7735109	2.4834198
O	3.8584007	-0.9620059	0.6082660
H	3.9372837	-1.9212919	0.5946070
H	3.1071558	-0.7614049	1.2064169

-----  
La:

C	-2.9219348	-0.2035370	0.3527010
C	-1.8157259	0.6933889	0.2792720
C	-0.6342770	0.3174740	-0.3636070
C	-0.4170910	-0.9492639	-0.9310879
C	-1.5962169	-1.7981079	-0.9521639
C	-2.7695688	-1.4431919	-0.3249810
C	-1.6094439	2.0104928	0.7724049
C	-0.2813660	2.4023008	0.4179460
N	0.2691930	1.3960459	-0.2530030
H	-3.8432097	0.0736390	0.8415939
H	0.4295480	-1.1498929	-1.5710329
H	-1.5336409	-2.7519198	-1.4584369
H	-3.6024007	-2.1340448	-0.3484950
H	-2.3070708	2.6236988	1.3165769
H	0.2416400	3.3212877	0.6119660
H	1.2425659	1.3791909	-0.6005840
O	2.9072478	1.1728119	-1.1078409
H	3.4769977	1.9374589	-0.9771419
H	3.2779167	0.4544550	-0.5420970
O	1.3420549	-1.8685709	1.3543459
H	0.7117639	-1.6578969	0.6218180



H	1.2872599	-2.8234328	1.4758679
O	3.7330967	-0.8532939	0.5052080
H	4.2415597	-1.5412189	0.0636730
H	2.9072618	-1.2885639	0.8207109

-----

**I. Water Cluster - Size 6 - B3LYP/aug-cc-pVXZ Method Group**

s0:

C	1.7284619	1.7644749	-1.1739169
C	1.0502249	0.5538220	-0.9349129
C	0.4802180	0.3202890	0.3490320
C	0.5687840	1.2563199	1.3889699
C	1.2319169	2.4533718	1.1184409
C	1.8070059	2.7029948	-0.1490250
C	0.7502999	-0.6109650	-1.7378719
C	0.0277710	-1.4729519	-0.9352679
N	-0.1144730	-0.9302489	0.3253840
H	2.1779898	1.9642229	-2.1460908
H	0.1483730	1.0516039	2.3725648
H	1.3178029	3.2053988	1.9020229
H	2.3218398	3.6478597	-0.3210410
H	1.0204539	-0.7797559	-2.7750028
H	-0.4066480	-2.4380848	-1.1681809
H	-0.8222929	-1.2198409	0.9989419
O	-2.5815218	-0.7797949	1.7989569
H	-2.6455998	0.1668300	1.5578669
H	-2.9360828	-0.8545579	2.6930148
O	3.5394637	-1.7792269	-0.6278310
H	4.1137327	-1.0024309	-0.5997110

H	2.7372578	-1.4707539	-1.0829229
O	-3.6339617	-1.8263939	-0.6925069
H	-3.3779227	-1.6150089	0.2223050
H	-3.2575548	-1.0833439	-1.2044449
O	2.3823568	-2.4022238	1.8792089
H	1.4913989	-2.0643158	1.7175489
H	2.8549838	-2.1989728	1.0468819
O	-2.4351738	0.4654770	-1.9177579
H	-1.5132179	0.1912670	-2.0438348
H	-2.4208148	1.0078029	-1.1053129
O	-2.4302108	1.7692149	0.6233370
H	-1.5493369	2.1279238	0.8185719
H	-3.0487528	2.4953428	0.7791859

-----

La:

C	1.9049549	-0.4168610	-1.6389079
C	0.8851669	-0.8191669	-0.7143789
C	0.3058760	0.0974160	0.1674510
C	0.6426400	1.4729659	0.2180720
C	1.6430589	1.8738459	-0.7547059
C	2.2249968	0.9821049	-1.6401059
C	0.3100950	-2.0998038	-0.4138920
C	-0.6428330	-1.9064359	0.6412080
N	-0.6257020	-0.6147960	0.9668029
H	2.2608438	-1.0895529	-2.4162938
H	0.3154060	2.1329498	1.0186729
H	1.9426649	2.9213638	-0.7848719
H	2.9612918	1.3554989	-2.3520208
H	0.5431380	-3.0533678	-0.8751939
H	-1.3229089	-2.6118368	1.1016349

H	-1.3092859	-0.1606660	1.5855179
O	-2.8777218	0.8346049	1.7985939
H	-2.7893008	1.4692409	1.0560449
H	-3.1582898	1.3466449	2.5666648
O	4.1204377	-1.0658029	0.3750250
H	3.4787897	-0.9244829	-0.3587490
H	4.0556007	-2.0096158	0.5730470
O	-4.0325617	-1.3858819	0.2940000
H	-3.7970337	-0.6889019	0.9295139
H	-3.5289097	-1.1404339	-0.5068130
O	2.9746798	0.6242070	2.3274888
H	2.2419908	1.0048529	1.8171589
H	3.4010917	0.0106810	1.6940679
O	-2.5846218	-0.3606760	-1.9434699
H	-1.6999389	-0.6927669	-2.1431898
H	-2.4389218	0.5370800	-1.5802879
O	-2.1926378	2.0713738	-0.5856520
H	-1.2161779	2.1251728	-0.4599570
H	-2.4644588	2.9247278	-0.9488869

-----

## J. Water Cluster - Size 9 - B3LYP/aug-cc-pVXZ Method Group

s0:

C	-2.6668258	-2.0662838	-0.0543320
C	-1.7360419	-1.2999479	-0.7818709
C	-0.6258490	-0.7197379	-0.0939440
C	-0.4295440	-0.8864849	1.2846099
C	-1.3612649	-1.6598419	1.9756918
C	-2.4699118	-2.2431558	1.3146469

C	-1.6183419	-0.9066329	-2.1633648
C	-0.4727610	-0.1404150	-2.2603438
N	0.1139560	-0.0191660	-1.0205789
H	-3.5265097	-2.5129218	-0.5528750
H	0.3984660	-0.4056940	1.8013959
H	-1.2411899	-1.8092239	3.0481198
H	-3.1771288	-2.8405598	1.8890659
H	-2.2807658	-1.1728359	-2.9796998
H	-0.0278290	0.3378860	-3.1259548
H	1.0208639	0.4135690	-0.8535099
O	2.9869558	0.7865269	-0.9635989
H	3.2879717	0.3922200	-0.1189360
H	3.0001588	0.0315150	-1.5919929
O	-2.8298748	1.8974239	-1.0208389
H	-3.0735328	1.5397369	-0.1380920
H	-2.5332258	1.1233149	-1.5269989
O	2.8312368	-1.6558909	-2.2864318
H	2.0664528	-1.7509609	-2.8683558
H	2.5628538	-2.0826358	-1.4384679
O	-0.7151979	3.5932957	-0.8715319
H	-1.0739649	4.4532457	-0.6221620
H	-1.4898459	2.9781638	-0.8966939
O	2.2503168	-2.6045118	0.2407980
H	1.3024899	-2.5777958	0.4330270
H	2.6305768	-1.8866029	0.7921629
O	3.3752357	-0.4136460	1.5348029
H	2.8317908	0.2438080	2.0436628
H	4.2190267	-0.4891800	1.9964458
O	-3.5123337	0.9027109	1.4766009
H	-3.0285028	1.3606669	2.1765148
H	-3.1990858	-0.0158800	1.5274569

O	1.6374589	2.9024338	0.3242860
H	0.7716639	3.1273678	-0.0889940
H	2.0932048	2.3156428	-0.3066870
O	1.7506289	1.4478139	2.5821898
H	1.6502529	2.0496718	1.7974719
H	2.1059388	1.9973938	3.2913737

-----

La:

C	2.6294918	-2.0256648	-0.5684460
C	1.5766969	-1.7469689	0.3635880
C	0.4319830	-1.0471029	-0.0322310
C	0.1676110	-0.6394290	-1.3598299
C	1.2392249	-0.9434629	-2.2956358
C	2.3989018	-1.6043809	-1.9161539
C	1.4393589	-2.0052528	1.7680299
C	0.1875830	-1.4430309	2.1857128
N	-0.3798490	-0.8854189	1.1168729
H	3.5075357	-2.6006038	-0.2840990
H	-0.5756750	0.1153400	-1.5931909
H	1.1096259	-0.6649319	-3.3426397
H	3.1557248	-1.8143089	-2.6727488
H	2.1436848	-2.5115588	2.4193248
H	-0.2650800	-1.4090159	3.1689188
H	-1.2796479	-0.3728120	1.1323219
O	-2.8019618	0.5350050	1.2317619
H	-2.9398528	0.9148059	0.3375630
H	-3.3402197	-0.2895840	1.2254139
O	3.3574637	0.9726779	0.3885670
H	2.9098798	1.4366689	-0.3571780
H	3.3281847	0.0320410	0.1309490

O	-3.9952007	-1.8850229	0.6963899
H	-3.5871897	-2.6369578	1.1446339
H	-3.5796267	-1.8561369	-0.1990590
O	1.7112669	1.3906159	2.5034938
H	2.1880198	1.9965588	3.0838728
H	2.3249668	1.2214659	1.7432379
O	-2.8537628	-1.4171239	-1.7659729
H	-1.8821929	-1.5369859	-1.7355119
H	-2.9439848	-0.4445100	-1.7931209
O	-2.8564598	1.4379989	-1.4127529
H	-2.0450358	1.9998288	-1.3804959
H	-3.5658097	2.0110628	-1.7291549
O	2.0261478	2.0876598	-1.7614629
H	1.1199259	2.3505788	-1.4903049
H	1.9045379	1.2158889	-2.1732038
O	-0.6617399	2.4387088	1.6786749
H	0.1737590	2.0241098	2.0057248
H	-1.3725209	1.7917519	1.8201509
O	-0.5542310	2.8636858	-0.9456129
H	-0.5646120	2.7523858	0.0478760
H	-0.6627309	3.8109637	-1.1022829

-----

**K. Water Cluster - Size 12 - B3LYP/aug-cc-pVXZ Method Group**

s0:

C	1.2265789	-0.4117690	0.6928099
C	0.2273510	-1.0295869	-0.0812910
C	-1.0874799	-1.1633519	0.4609930
C	-1.4263529	-0.6744869	1.7331779

C	-0.4201740	-0.0539040	2.4728568
C	0.8972019	0.0666720	1.9623319
C	0.1956720	-1.6359829	-1.3883159
C	-1.0957349	-2.0960168	-1.5778349
N	-1.8620819	-1.8156069	-0.4696480
H	2.2429518	-0.3231090	0.3163620
H	-2.4331738	-0.7882879	2.1315068
H	-0.6457020	0.3323050	3.4654317
H	1.6653119	0.5282240	2.5826018
H	1.0132639	-1.7006749	-2.0975108
H	-1.5302089	-2.6062978	-2.4303508
H	-2.8775608	-1.9539079	-0.3853280
O	-4.8461746	0.9553039	-0.2802870
H	-3.9523567	1.3552769	-0.1980860
H	-5.3820696	1.3874189	0.3963740
O	1.8681979	-3.9315587	0.1099290
H	1.5865049	-3.7110667	1.0256589
H	1.1484449	-3.5930387	-0.4443440
O	-4.6498126	-1.7692829	-0.0396010
H	-5.2578496	-2.1746248	-0.6697819
H	-4.7851886	-0.7960939	-0.1306890
O	1.1441579	-3.1727878	2.6798228
H	0.3194830	-3.5463157	3.0171518
H	0.9781569	-2.2181328	2.6240858
O	3.8545387	-2.1174428	-0.5311810
H	4.6342776	-2.6185408	-0.7994269
H	3.1788888	-2.7966468	-0.2977410
O	3.2817507	-0.3061840	-2.6603898
H	3.4110097	-0.8864879	-1.8864119
H	2.7100148	0.4360330	-2.3726458
O	3.6914287	4.1083587	1.4925539

H	3.5656747	4.2601467	2.4370578
H	2.8483938	3.7131527	1.1891569
O	-1.0072789	1.1277979	-2.5446238
H	-0.8574469	0.1737620	-2.4443898
H	-1.4616619	1.3843879	-1.7145739
O	1.3539169	2.9434708	0.4814580
H	1.1227179	2.1178418	0.9354479
H	0.5370580	3.4821717	0.4982390
O	-2.2315248	1.8410499	-0.1094010
H	-1.8359369	1.2732569	0.5710610
H	-1.9434989	2.7510718	0.1120650
O	1.6535139	1.9247419	-2.1602878
H	1.6301959	2.3040908	-1.2608539
H	0.7199569	1.6748459	-2.3316938
O	-1.0981299	4.3288937	0.4225230
H	-1.3606189	4.8132796	1.2173829
H	-1.1734869	4.9668796	-0.3007020

-----  
La:

C	1.3082339	-0.1904240	0.9837709
C	0.4205100	-0.8444139	0.0719350
C	-0.8781679	-1.1819799	0.4510590
C	-1.4441619	-0.8712349	1.7144599
C	-0.4827330	-0.3811950	2.6770828
C	0.8222929	-0.0559650	2.3291198
C	0.5683960	-1.2597619	-1.2993669
C	-0.6780419	-1.8448239	-1.7026749
N	-1.5106739	-1.7876079	-0.6643669
H	2.3592908	-0.0597000	0.7406399
H	-2.4084008	-1.2656019	2.0253578



H	-0.8044399	-0.2450040	3.7095317
H	1.4872899	0.3418650	3.0953228
H	1.4352529	-1.1428059	-1.9396219
H	-0.9649729	-2.2741948	-2.6551268
H	-2.5140988	-2.0671608	-0.6778929
O	-5.0321436	0.3655570	-0.2725250
H	-4.2191227	0.8754859	-0.0523870
H	-5.6431586	0.5283230	0.4569840
O	2.6793498	-3.4524237	0.0421190
H	2.1542438	-3.3552037	0.8699029
H	2.0462788	-3.7417077	-0.6266250
O	-4.2203707	-2.2214028	-0.5456680
H	-4.6739896	-2.6114778	-1.3030059
H	-4.5821337	-1.3047739	-0.4586510
O	1.3382849	-3.2071788	2.4426438
H	0.5521080	-3.7622417	2.5248268
H	1.0099809	-2.2954158	2.5560338
O	4.1123167	-1.2093839	-0.6731119
H	4.9956616	-1.5396309	-0.8775839
H	3.5933617	-2.0078118	-0.4188960
O	3.1465118	0.2260680	-2.9336268
H	3.4632847	-0.1984300	-2.1130978
H	2.4411498	0.8555199	-2.6708108
O	3.3488337	3.9874557	1.4206269
H	3.4019397	3.7176657	2.3454868
H	2.5440608	3.5423997	1.0775749
O	-1.6046089	1.3246789	-2.3895148
H	-1.8908509	0.4830420	-2.7660928
H	-1.9433439	1.3266029	-1.4660139
O	1.1041819	2.7442378	0.3419410
H	1.0844649	1.7958939	0.6162330

H	0.2496080	3.1239098	0.6269340
O	-2.5761528	1.4726179	0.2105860
H	-2.1878978	0.8057359	0.8273029
H	-2.2935328	2.3443328	0.5538900
O	1.1005409	2.0437358	-2.3764208
H	1.1495579	2.3794598	-1.4582469
H	0.1798300	1.7148539	-2.4469388
O	-1.4119499	3.8680427	1.0660929
H	-1.5175019	4.1353247	1.9895438
H	-1.6255259	4.6567626	0.5485510

-----

#### L. Water Cluster - Size 15 - B3LYP/aug-cc-pVXZ Method Group

s0:

C	-0.4721280	-0.5896040	-0.5414720
C	0.4578000	-0.0050480	0.3462460
C	1.2920219	1.0593899	-0.1274960
C	1.2147739	1.5447829	-1.4404689
C	0.2898570	0.9434599	-2.2994358
C	-0.5443010	-0.1147910	-1.8533849
C	0.7952889	-0.2039950	1.7396689
C	1.7850839	0.7110019	2.0509698
N	2.1032958	1.4618159	0.9255789
H	-1.1386769	-1.3769909	-0.2095900
H	1.8403449	2.3656758	-1.7712369
H	0.1955190	1.3008399	-3.3193037
H	-1.2593149	-0.5534730	-2.5410268
H	0.3762210	-0.9362439	2.4131578
H	2.2923588	0.8836439	2.9874148

H	2.6632688	2.3323458	0.9095239
O	-1.3254649	4.3415087	0.4206400
H	-1.7787179	3.4605697	0.2375270
H	-1.8656049	4.9197296	0.9848489
O	4.0389117	-0.9183339	-0.0683250
H	3.6155177	-1.0165779	-0.9856039
H	3.7261627	-0.1019250	0.3673760
O	1.0261719	5.0861516	-0.3719760
H	1.0184679	5.4515656	-1.2725859
H	0.1024060	4.7919446	-0.0781010
O	2.8604528	-1.2649319	-2.3801098
H	2.2433998	-0.5442450	-2.6106018
H	2.3967998	-2.1610748	-2.4123038
O	1.2646339	-3.1951778	0.4269990
H	2.1754228	-3.3523427	0.8524829
H	1.1384349	-2.2242338	0.3742940
O	-1.3128769	-3.6778757	1.1995179
H	-0.3440130	-3.6291187	0.9870149
H	-1.5821509	-2.9910218	1.8573209
O	-4.3738457	-1.1095099	-1.8077629
H	-4.1936117	-1.3920819	-2.7194538
H	-4.0189547	-1.7639209	-1.1104929
O	-2.0963298	0.8539339	2.3363088
H	-1.1503699	0.9424639	2.5663748
H	-2.2627448	1.3031809	1.4529219
O	-3.5478867	-2.6311078	0.0917080
H	-2.7570288	-3.2267538	0.0914620
H	-3.5097747	-2.1630008	0.9717169
O	-2.3771768	1.9787248	-0.0724540
H	-1.7320229	1.4752129	-0.6113650
H	-3.3171267	1.8255959	-0.4594000

O	-2.7968388	-1.6467139	2.4700388
H	-3.2643008	-1.8730639	3.2934097
H	-2.5437418	-0.6602539	2.4485548
O	-4.5992256	1.3407789	-1.1130589
H	-4.5865746	0.3691940	-1.4253679
H	-5.4835406	1.7396279	-1.0985779
O	3.1451138	3.9269457	0.5719080
H	2.3571248	4.4518817	0.2098140
H	3.8571197	4.4998727	0.9015959
O	3.7039647	-3.1443088	1.2096209
H	3.9631127	-2.2567088	0.7870879
H	4.2106087	-3.3628787	2.0084718
O	1.6173189	-3.5424587	-2.1667718
H	1.4199099	-3.6052817	-1.1845139
H	1.7472309	-4.4070257	-2.5899228

-----  
La:

C	0.6213890	0.3904380	-0.7843059
C	-0.3670100	0.1720900	0.2382130
C	-1.6818709	-0.1704340	-0.0955830
C	-2.1556658	-0.3067820	-1.4219879
C	-1.1688829	-0.0661450	-2.4426578
C	0.1530680	0.2659810	-2.1476098
C	-0.3022780	0.2352270	1.6810399
C	-1.6051879	-0.1012090	2.1838098
N	-2.4026318	-0.3366390	1.1274719
H	1.6807879	0.4412930	-0.5529900
H	-3.1736138	-0.5859050	-1.6554599
H	-1.4656669	-0.1683790	-3.4829997
H	0.8594729	0.4080480	-2.9596928

H	0.5524360	0.4917410	2.2854128
H	-1.9449029	-0.1902530	3.2026068
H	-3.3835727	-0.7071549	1.1603629
O	-1.3185479	-4.1045347	-0.0926110
H	-0.4883430	-3.5444967	-0.2135520
H	-1.1047779	-4.9769356	0.2799370
O	-2.9529788	2.9496268	0.1741940
H	-2.5316998	2.9817418	-0.7530399
H	-3.5638957	2.1983888	0.2652350
O	-3.8197337	-3.5632797	-0.4849140
H	-4.1101977	-3.7248267	-1.3983519
H	-2.8327148	-3.7602947	-0.3625280
O	-1.7312779	3.1018928	-2.1113108
H	-1.3720119	2.2297798	-2.3810078
H	-0.9998719	3.7933007	-2.0713038
O	1.0029359	3.1814458	0.2612260
H	0.2625960	3.2946407	0.9524109
H	0.8468909	2.3264028	-0.2336200
O	3.2685348	2.2069658	1.3824109
H	2.4592908	2.6729508	1.0326499
H	3.0245018	1.4513229	1.9709058
O	4.4283807	-1.3804079	-1.9176619
H	5.2266186	-1.3199309	-2.4677978
H	4.4539687	-0.7496639	-1.1150269
O	1.4822939	-2.2980028	2.1962268
H	0.7666739	-2.5167538	2.8173438
H	1.2315479	-2.5045358	1.2406489
O	4.4296107	0.0957370	0.1785610
H	4.1507687	1.0449969	0.2579610
H	4.1008577	-0.3284450	1.0156869
O	0.8754599	-2.6615508	-0.3397730

H	0.7114349	-1.7333549	-0.6308640
H	1.6550299	-3.0519878	-0.8810699
O	3.1668468	-0.3646430	2.5320068
H	3.6924257	-0.4474020	3.3476057
H	2.4881688	-1.1197149	2.4585668
O	2.9061868	-3.4307677	-1.6689089
H	3.5601847	-2.6650318	-1.8318859
H	2.9521998	-4.1279127	-2.3431638
O	-4.7274096	-1.5693689	0.8700099
H	-4.4668287	-2.3980168	0.3406250
H	-5.5274276	-1.6934659	1.4063299
O	-1.0335189	3.4169517	1.8319249
H	-1.8635779	3.2097428	1.2803259
H	-1.1108399	3.1392218	2.7599928
O	0.2252400	4.7740526	-1.6613269
H	0.6955929	4.2986557	-0.9071119
H	0.8093639	5.3407866	-2.1913838

-----

### M. Water Cluster - Size 3a - CAM-B3LYP/def2TZVP Method Group

s0:

C	2.6852898	-0.5927790	-0.0105780
C	1.4060519	-0.6241650	-0.5751720
C	0.5702140	0.5049470	-0.4411140
C	0.9748809	1.6483569	0.2433320
C	2.2384748	1.6485229	0.7906869
C	3.0882088	0.5378170	0.6635939
C	0.6545580	-1.6052109	-1.3027679
C	-0.5596690	-1.0438329	-1.5776889

N	-0.6132160	0.2240410	-1.0711069
H	3.3456677	-1.4458349	-0.0999630
H	0.3192000	2.5033888	0.3410680
H	2.5846658	2.5206268	1.3293819
H	4.0748167	0.5755350	1.1061039
H	0.9821499	-2.5867728	-1.6021209
H	-1.4046469	-1.4580039	-2.1023888
H	-1.4399199	0.8114569	-1.0562609
O	-3.0989908	1.6647229	-0.5764050
H	-3.8076807	1.6735819	-1.2300179
H	-3.0462308	2.5627648	-0.2294530
O	-0.8061629	-1.8672649	1.6118129
H	-0.1512040	-1.3896339	2.1324608
H	-0.4124880	-1.9518669	0.7292369
O	-3.2817107	-0.4913250	1.3730759
H	-3.1982908	0.2386330	0.7423249
H	-2.4066688	-0.9131709	1.4277489

-----  
La:

C	2.4458908	-1.1006529	-0.4895610
C	1.0218369	-1.0116459	-0.3611330
C	0.3965640	0.2500210	-0.3600240
C	1.0790089	1.4464919	-0.4719430
C	2.5006528	1.3228549	-0.7535729
C	3.1375668	0.1110500	-0.7508969
C	0.0204890	-1.9634099	-0.1579570
C	-1.2246399	-1.2718249	-0.0362840
N	-0.9691549	0.0259080	-0.1666910
H	2.9457968	-2.0580558	-0.5170220
H	0.5816150	2.4042468	-0.4766740

H	3.0655038	2.2237718	-0.9534699
H	4.2030867	0.0777680	-0.9390679
H	0.1365040	-3.0323898	-0.0879620
H	-2.2280528	-1.6344499	0.1152020
H	-1.6858679	0.7524779	-0.1250100
O	-3.2513308	1.7696399	-0.0182080
H	-3.4672027	2.2978328	-0.7959939
H	-3.3289257	2.3633538	0.7382109
O	2.1435108	0.2876560	2.4720088
H	2.4633198	-0.3563760	1.8202449
H	1.6948949	0.9438279	1.9194949
O	-4.4953727	-0.7998149	0.2079240
H	-4.1922037	0.1191040	0.1199290
H	-4.8430666	-1.0396279	-0.6566109

-----

**N. Water Cluster - Size 3b - CAM-B3LYP/def2TZVP Method Group**

s0:

C	-2.9041478	-0.1134700	0.3053350
C	-1.7770719	0.6837099	0.0825660
C	-0.6085130	0.0848830	-0.4326080
C	-0.5388260	-1.2738349	-0.7280139
C	-1.6660509	-2.0327008	-0.5009520
C	-2.8392658	-1.4575929	0.0120130
C	-1.4803529	2.0741728	0.2636360
C	-0.1912650	2.2574038	-0.1321280
N	0.3524940	1.0614659	-0.5353940
H	-3.8134957	0.3199450	0.7018649
H	0.3687680	-1.7155519	-1.1176609



H	-1.6477509	-3.0919098	-0.7208999
H	-3.7047517	-2.0852508	0.1786420
H	-2.1418138	2.8352188	0.6425780
H	0.4011190	3.1571058	-0.1536390
H	1.2709069	0.9335449	-0.9661889
O	2.8954368	0.3305870	-1.5963009
H	3.5958407	0.9710899	-1.7538689
H	3.2046858	-0.2469090	-0.8626609
O	1.5970589	0.0309860	2.1279798
H	1.0866299	0.4771680	1.4361249
H	0.9603299	-0.4975320	2.6215648
O	3.4889277	-1.2115479	0.5737210
H	3.3072557	-2.1507618	0.4668640
H	2.8263848	-0.8720419	1.2127619

-----  
La:

C	-2.8955188	-0.1967430	0.3363510
C	-1.7886929	0.7041049	0.2808810
C	-0.6053350	0.3257480	-0.3803260
C	-0.4162780	-0.9102369	-0.9771959
C	-1.5863299	-1.7830909	-0.9747219
C	-2.7459988	-1.4339019	-0.3379460
C	-1.5787509	1.9940998	0.7774429
C	-0.2525360	2.3901058	0.4188640
N	0.2917560	1.3910379	-0.2653220
H	-3.8121577	0.0701390	0.8417289
H	0.4570250	-1.1387749	-1.5708129
H	-1.5177439	-2.7365898	-1.4812299
H	-3.5777077	-2.1272778	-0.3500220
H	-2.2720658	2.6045668	1.3322749

H	0.2775710	3.3032157	0.6261520
H	1.2639349	1.3719289	-0.6173060
O	2.9176588	1.1179279	-1.1108589
H	3.5196267	1.8619189	-1.0105479
H	3.2688108	0.3901310	-0.5440970
O	1.2625409	-1.7806189	1.4287409
H	0.6441280	-1.5869039	0.6920619
H	1.1477429	-2.7148578	1.6340339
O	3.6707767	-0.9170269	0.4971630
H	4.1285067	-1.6427159	0.0610530
H	2.8388678	-1.2948189	0.8635169

-----

**O. Water Cluster - Size 6 - CAM-B3LYP/def2TZVP Method Group**

s0:

C	1.7834599	1.6919739	-1.1725539
C	1.0722509	0.5124050	-0.9324249
C	0.4780530	0.3142600	0.3300030
C	0.5695920	1.2592639	1.3494249
C	1.2642029	2.4209458	1.0788419
C	1.8669949	2.6345938	-0.1707770
C	0.7610239	-0.6513660	-1.7195139
C	0.0091410	-1.4719429	-0.9302239
N	-0.1442350	-0.9156259	0.3153600
H	2.2537898	1.8636309	-2.1323678
H	0.1257760	1.0817499	2.3206238
H	1.3543619	3.1772348	1.8474399
H	2.4081238	3.5553797	-0.3442040
H	1.0466279	-0.8411499	-2.7417688

H	-0.4472890	-2.4200808	-1.1606749
H	-0.8828969	-1.1682219	0.9681939
O	-2.6126978	-0.7164819	1.7564339
H	-2.6803888	0.2292410	1.5194569
H	-2.9174528	-0.8042919	2.6651518
O	3.5878167	-1.7384369	-0.5165240
H	4.1898527	-0.9865479	-0.4927480
H	2.8396038	-1.4496259	-1.0589909
O	-3.5809927	-1.8507489	-0.6888939
H	-3.3634487	-1.6145179	0.2266920
H	-3.2377078	-1.0996179	-1.2060179
O	2.2660088	-2.3800568	1.8746759
H	1.3913189	-2.0493898	1.6414239
H	2.8087278	-2.1768918	1.0903739
O	-2.4601408	0.4698310	-1.8791849
H	-1.5369609	0.2551710	-2.0668958
H	-2.4405988	1.0370159	-1.0868139
O	-2.4559888	1.8204379	0.6094460
H	-1.5857879	2.1948628	0.8094979
H	-3.0963588	2.5282588	0.7498239

-----  
La:

C	1.9438949	-0.4065760	-1.6595789
C	0.9061399	-0.8018959	-0.7600759
C	0.3405260	0.1291760	0.1237420
C	0.7160389	1.4652699	0.1872570
C	1.7517299	1.8538419	-0.7556229
C	2.3175108	0.9646059	-1.6276999
C	0.3006180	-2.0367308	-0.4918260
C	-0.6579999	-1.8342179	0.5465190

N	-0.6116420	-0.5567640	0.8894049
H	2.3130838	-1.0805739	-2.4193308
H	0.3500800	2.1449588	0.9434449
H	2.0754748	2.8859738	-0.7625329
H	3.0782508	1.3165819	-2.3121738
H	0.5077400	-2.9848498	-0.9593009
H	-1.3672279	-2.5182818	0.9777959
H	-1.2782729	-0.0981180	1.5151399
O	-2.8406808	0.9148839	1.7819989
H	-2.7714048	1.5138389	1.0125119
H	-3.0620778	1.4529969	2.5486908
O	4.0955147	-1.1233239	0.4399440
H	3.4988447	-0.9498979	-0.3170930
H	4.0114007	-2.0663128	0.6188960
O	-4.0616417	-1.3725129	0.5022650
H	-3.8049377	-0.6372990	1.0791169
H	-3.6422887	-1.1604739	-0.3510200
O	2.9651238	0.5555940	2.3850338
H	2.2449468	0.9544859	1.8785989
H	3.3930927	-0.0545220	1.7545249
O	-2.8027848	-0.4351090	-1.8640859
H	-1.9827278	-0.8362199	-2.1703488
H	-2.5685558	0.4649080	-1.5683209
O	-2.1937058	2.0338938	-0.6725629
H	-1.2220989	2.1007178	-0.5872560
H	-2.4971828	2.8611808	-1.0642139

-----

**P. Water Cluster - Size 9 - CAM-B3LYP/def2TZVP Method Group**

s0:

C	-2.6695188	-2.0748188	-0.0239450
C	-1.7223579	-1.3519279	-0.7560219
C	-0.6352040	-0.7575649	-0.0738440
C	-0.4757030	-0.8670639	1.3069809
C	-1.4207069	-1.5945729	1.9996618
C	-2.5087278	-2.1954668	1.3416519
C	-1.5721029	-1.0153099	-2.1415958
C	-0.4306950	-0.2723600	-2.2419898
N	0.1291330	-0.1047440	-1.0045169
H	-3.5136617	-2.5352308	-0.5213860
H	0.3398710	-0.3734350	1.8190709
H	-1.3286339	-1.7001009	3.0726448
H	-3.2281488	-2.7616078	1.9188329
H	-2.2133108	-1.3099019	-2.9558758
H	0.0355790	0.1590110	-3.1127208
H	1.0264409	0.3417500	-0.8349519
O	2.9501538	0.7911379	-0.9006029
H	3.2775937	0.4158700	-0.0594220
H	3.0473738	0.0646860	-1.5515079
O	-2.7458988	1.8849489	-1.1209819
H	-3.0960118	1.5393069	-0.2718850
H	-2.4435548	1.1078809	-1.6124789
O	3.0021828	-1.6159609	-2.2215778
H	2.3436308	-1.8124229	-2.8954138
H	2.6989578	-2.0651728	-1.4006479
O	-0.7609879	3.6712307	-0.7409389
H	-0.7482819	4.2441777	-1.5135049
H	-1.4817679	3.0137998	-0.8920279

O	2.3209598	-2.5520048	0.2618590
H	1.3788269	-2.6110478	0.4574420
H	2.6656478	-1.8398579	0.8406159
O	3.3671907	-0.3710070	1.5888489
H	2.8038908	0.2837490	2.0786758
H	4.2034057	-0.4438860	2.0603928
O	-3.6806347	0.9017859	1.2704879
H	-3.3394287	1.3554729	2.0490428
H	-3.4091017	-0.0227500	1.3708949
O	1.6212009	2.9238388	0.3054590
H	0.7602859	3.1725688	-0.1010030
H	2.0760758	2.3356458	-0.3220050
O	1.7134889	1.4723079	2.5407158
H	1.6211029	2.0889938	1.7681179
H	1.9281409	2.0099928	3.3091747

-----  
La:

C	-2.7031708	-2.1484148	0.0109230
C	-1.6938009	-1.5288899	-0.7899269
C	-0.5954390	-0.8972619	-0.1727620
C	-0.4035900	-0.8466999	1.1939479
C	-1.4662429	-1.4477939	1.9932558
C	-2.5463628	-2.0648118	1.4128529
C	-1.5246349	-1.3836139	-2.1724768
C	-0.3114030	-0.6619609	-2.3896238
N	0.2065580	-0.3870730	-1.1963609
H	-3.5526357	-2.6411738	-0.4384670
H	0.3640290	-0.2418530	1.6515659
H	-1.3723469	-1.4337279	3.0711398
H	-3.2972797	-2.5129488	2.0512088

H	-2.1759438	-1.7392059	-2.9537988
H	0.1604940	-0.3574470	-3.3070607
H	1.1080819	0.0869110	-1.0532399
O	2.8404228	0.6632719	-0.9674079
H	3.1277878	0.6000090	-0.0333960
H	3.1736148	-0.1609960	-1.3829879
O	-3.0435788	1.5094709	-0.8597799
H	-3.0789208	1.4550309	0.1209500
H	-2.8992818	0.6016980	-1.1535799
O	3.3541917	-1.9335379	-1.6046419
H	4.2301357	-2.3133668	-1.7243829
H	3.0637028	-2.1763158	-0.6963199
O	-1.0240119	3.0792888	-1.7430429
H	-1.3867899	3.9552707	-1.9060159
H	-1.7687309	2.5232258	-1.4136229
O	2.4804258	-2.2284448	0.9788939
H	1.5134039	-2.1632468	1.0463859
H	2.8017348	-1.3940489	1.3744599
O	3.2704208	0.3400990	1.7515799
H	2.6011728	1.0109979	2.0458628
H	4.0986287	0.5412520	2.1989618
O	-3.0955828	1.2391769	1.8673639
H	-2.4430928	1.7969389	2.3056908
H	-2.7843878	0.3254250	2.0029778
O	1.3102229	2.9704078	-0.3751290
H	0.4561170	3.0130098	-0.8626419
H	1.8612439	2.3130938	-0.8288559
O	1.3406169	2.1260878	2.1673838
H	1.2622929	2.5067218	1.2553479
H	1.4939179	2.8643588	2.7654578

-----  
**Q. Water Cluster - Size 12 - CAM-B3LYP/def2TZVP Method Group**

s0:

C	1.2518009	-0.1828560	0.6946149
C	0.3787180	-1.0254669	0.0013720
C	-0.8706119	-1.3488109	0.5794530
C	-1.2703239	-0.8385539	1.8161089
C	-0.3897950	-0.0090980	2.4785138
C	0.8629019	0.3151420	1.9243149
C	0.4339930	-1.7084719	-1.2580269
C	-0.7452509	-2.3895668	-1.3841909
N	-1.5296859	-2.1813558	-0.2830490
H	2.2086828	0.0892650	0.2683210
H	-2.2287358	-1.0997009	2.2456428
H	-0.6635869	0.3991480	3.4420787
H	1.5335639	0.9595189	2.4797478
H	1.2488609	-1.6996499	-1.9630779
H	-1.0910099	-3.0194918	-2.1875968
H	-2.5036568	-2.4852038	-0.1750080
O	-4.9694396	-0.0194350	-0.4581740
H	-4.1732997	0.5486610	-0.3936630
H	-5.6461516	0.4023110	0.0806970
O	2.5945518	-3.5988287	0.1584070
H	2.4734028	-3.3045087	1.0863589
H	1.7226799	-3.5014007	-0.2452290
O	-4.2801517	-2.5854088	0.0984080
H	-4.8187756	-3.1998468	-0.4093000
H	-4.6142056	-1.6820409	-0.1064120
O	2.2003148	-2.6415408	2.7077048



H	1.6276969	-3.1275068	3.3110307
H	1.8089039	-1.7606799	2.6232148
O	4.0360407	-1.8879329	-1.4269799
H	4.1746997	-2.3749968	-2.2449238
H	3.5563947	-2.5006368	-0.8259719
O	3.7443467	0.8923309	-1.6299469
H	3.7259517	-0.0802060	-1.5909429
H	2.8479978	1.2045679	-1.8581889
O	2.6350738	4.8414596	1.3858289
H	2.4588268	4.9209696	2.3276798
H	1.9144829	4.2845657	1.0363169
O	-1.1028879	0.7935029	-2.5644358
H	-0.8212619	-0.1222230	-2.4289778
H	-1.6610939	0.9984589	-1.7883059
O	0.6195570	3.1970698	0.3685050
H	0.5825560	2.3650698	0.8611349
H	-0.2914970	3.5513057	0.3650440
O	-2.5891588	1.3499069	-0.2441810
H	-2.1305808	0.9047659	0.4831880
H	-2.5159608	2.3092088	-0.0604200
O	1.3028929	2.1488728	-2.1622748
H	1.1111429	2.5979768	-1.3189859
H	0.4731770	1.6766609	-2.3771468
O	-2.0471528	4.0209477	0.2328030
H	-2.4304198	4.4399307	1.0134469
H	-2.2314738	4.6137426	-0.5066920

-----

La:

C	1.0910279	0.1101680	1.4007489
C	0.5034470	-0.7114809	0.3898970

C	-0.7436519	-1.3108439	0.6057830
C	-1.5222269	-1.1029899	1.7391709
C	-0.8959599	-0.2990670	2.7688578
C	0.3331000	0.2813860	2.5986988
C	0.9384029	-1.1195199	-0.8829789
C	-0.0758560	-1.9638309	-1.4334339
N	-1.0499199	-2.0623288	-0.5406680
H	2.0182908	0.6397010	1.2291919
H	-2.4445858	-1.6356769	1.9177049
H	-1.4299539	-0.1486210	3.6981197
H	0.7450639	0.8844269	3.3979487
H	1.8628199	-0.8659799	-1.3750669
H	-0.1141470	-2.4612458	-2.3876528
H	-1.9603189	-2.5418648	-0.6857259
O	-5.0287076	-0.7334329	-0.6892809
H	-4.4050047	-0.0260140	-0.4192970
H	-5.7740176	-0.6862699	-0.0821830
O	3.7176837	-2.9846778	-0.1093490
H	3.3728467	-2.7839288	0.7907369
H	3.0662728	-3.5627067	-0.5199110
O	-3.6000997	-3.0251208	-0.7827609
H	-3.8963357	-3.5835597	-1.5081429
H	-4.1891457	-2.2333118	-0.7705259
O	2.7890638	-2.2557508	2.3349778
H	2.2201968	-2.8566728	2.8285368
H	2.2478328	-1.4584519	2.1620148
O	4.2349437	-0.7747719	-1.5956189
H	4.6170276	-1.0746239	-2.4258448
H	4.0747937	-1.5808819	-1.0525399
O	3.2489858	1.8149089	-1.5518529
H	3.5599417	0.8901549	-1.5389039

H	2.3208318	1.8155409	-1.8665819
O	2.9650468	3.4314097	0.6857889
H	3.1487798	2.8375248	-0.0705390
H	1.9978968	3.4593547	0.7361539
O	-1.7347219	0.8212419	-2.4744558
H	-1.7686639	-0.0911070	-2.7790418
H	-2.1888378	0.8371629	-1.6057149
O	0.1322940	2.9332218	0.5430950
H	0.2357340	2.0462138	0.9310399
H	-0.7732159	3.2250168	0.7573869
O	-2.9837088	0.9423729	-0.0015310
H	-2.5142878	0.3902650	0.6577919
H	-2.9629418	1.8581409	0.3416210
O	0.6064740	2.2580108	-2.1148988
H	0.3954120	2.5854548	-1.2185689
H	-0.1424920	1.6709299	-2.3384558
O	-2.5882798	3.5256877	0.9560139
H	-2.8874428	3.7155267	1.8537469
H	-2.9244218	4.2440747	0.4058940

-----

### **R. Water Cluster - Size 15 - CAM-B3LYP/def2TZVP Method Group**

s0:

C	-0.6117980	0.6206560	-0.5071840
C	-0.1226770	-0.3822240	0.3498860
C	0.8915609	-1.2601559	-0.1221070
C	1.4174249	-1.1665399	-1.4142819
C	0.8989079	-0.1816520	-2.2498568
C	-0.1090960	0.7026779	-1.7989339

C	-0.3812170	-0.7550749	1.7191039
C	0.4572010	-1.8039089	2.0124818
N	1.2175269	-2.1296798	0.9026339
H	-1.3442929	1.3395359	-0.1628870
H	2.2198458	-1.8195189	-1.7320109
H	1.2895099	-0.0738190	-3.2547948
H	-0.4556510	1.4964679	-2.4482798
H	-1.1011169	-0.3048440	2.3834068
H	0.5656380	-2.3540458	2.9333088
H	2.0466428	-2.7670618	0.8474539
O	4.6656776	0.8377719	0.4133370
H	3.8283527	1.3683909	0.2259470
H	5.0460986	1.0420009	1.2808279
O	-1.2499739	-3.6929527	-0.1065710
H	-1.4127389	-3.1914208	-0.9792349
H	-0.3447000	-3.5391577	0.2185040
O	4.8198936	-1.5153839	-0.5332910
H	5.1083456	-1.5168209	-1.4578999
H	4.7681536	-0.5730240	-0.1465210
O	-1.7418739	-2.3091638	-2.1940418
H	-1.0845619	-1.6651509	-2.5063168
H	-2.6956598	-1.9995868	-2.3288078
O	-3.3154997	-0.8398709	0.2436190
H	-3.3417297	-1.6792399	0.8507559
H	-2.4170268	-0.7937459	-0.1425650
O	-3.3695017	1.6138459	1.3081069
H	-3.4347117	0.6805529	0.9686509
H	-2.5936468	1.7605819	1.9034259
O	-0.7629709	4.0623867	-1.7430969
H	-1.1778399	4.1115617	-2.6154808
H	-1.4220569	3.9080847	-0.9675069

O	1.2267059	1.8126629	2.2278548
H	1.1821449	0.8704969	2.4731618
H	1.6948029	1.9067199	1.3386319
O	-2.2260078	3.6977767	0.2687540
H	-2.8964228	2.9637348	0.3620540
H	-1.6714879	3.5915117	1.0914419
O	2.3860488	1.9233639	-0.1176700
H	1.9905768	1.2000219	-0.6411000
H	2.1611338	2.8422468	-0.5873740
O	-1.1408799	2.7170448	2.4604488
H	-1.2872099	3.1331588	3.3262947
H	-0.1745280	2.3806358	2.3657378
O	1.6816139	3.9921227	-1.2580479
H	0.6795659	4.0486487	-1.5017709
H	2.1174938	4.8533666	-1.1937329
O	3.4572117	-3.4307947	0.4250440
H	4.0538207	-2.7000338	0.0330820
H	3.5172937	-4.2598137	-0.0742740
O	-3.0738218	-2.9976598	1.5027969
H	-2.3266538	-3.3939067	0.9169819
H	-2.8498778	-3.0131208	2.4463528
O	-4.1519177	-1.4326189	-2.1432238
H	-4.0946137	-1.1360149	-1.1863889
H	-4.9450416	-1.9605449	-2.3243098

-----

La:

C	-0.8119069	0.2200740	-0.3921170
C	0.0975580	-0.3083720	0.5754950
C	1.2665529	-0.9708579	0.1769620
C	1.6251329	-1.2096449	-1.1575359

C	0.7494059	-0.5914300	-2.1324738
C	-0.3994990	0.0863560	-1.7684969
C	0.0801130	-0.3329700	2.0035708
C	1.2675699	-1.0084899	2.4384868
N	1.9536049	-1.3709789	1.3498049
H	-1.5562639	0.9593039	-0.1194130
H	2.5906808	-1.6117169	-1.4285239
H	1.0229209	-0.6524080	-3.1804288
H	-0.9951419	0.5770160	-2.5312278
H	-0.6664199	0.0951360	2.6514478
H	1.6184049	-1.1955389	3.4388947
H	2.9258058	-1.8187429	1.2963999
O	4.1197917	1.8492479	-0.4453250
H	3.1507298	2.0995648	-0.5775420
H	4.6031006	2.5024818	0.0814920
O	-0.2138750	-3.6680877	-0.7583059
H	-0.9055259	-3.4183437	-1.4626979
H	0.5794640	-3.1044398	-0.8925939
O	5.0697936	-0.4723220	-0.7460409
H	5.2426756	-0.6905309	-1.6738359
H	4.6816556	0.4680490	-0.6338150
O	-1.9109679	-2.7839418	-2.4788248
H	-1.5535779	-1.9054439	-2.7035888
H	-2.8570018	-2.7185598	-2.1166478
O	-2.8537358	-1.5192379	0.6735549
H	-2.3181188	-2.2664578	1.1381439
H	-2.2016368	-1.0032229	0.1088650
O	-3.5424177	0.7809419	1.8296579
H	-3.3637797	-0.1475940	1.5153519
H	-2.7560408	1.1922799	2.2630198
O	-2.0985898	3.2507388	-1.9153109

H	-2.5468148	2.8269638	-2.6608398
H	-2.5498208	3.0776208	-1.0082949
O	0.9340749	2.5983058	1.7858379
H	1.6174519	2.2639438	2.3868778
H	1.1961159	2.4792268	0.8157999
O	-3.0853448	2.8889638	0.3781070
H	-3.5309317	2.0439858	0.6739439
H	-2.4203348	3.0469108	1.1023909
O	1.5946279	2.3196858	-0.7139099
H	1.2285599	1.4747199	-1.0469019
H	1.1287909	3.1056678	-1.2370439
O	-1.5031129	2.5224448	2.4738198
H	-1.6525509	3.0165638	3.2975177
H	-0.5087590	2.5322158	2.2114338
O	0.2783230	4.0118457	-1.9380509
H	-0.7154449	3.7334947	-1.9765308
H	0.4186220	4.9690736	-1.9557789
O	4.3322477	-2.2266728	0.9012379
H	4.7063546	-1.5542219	0.2190980
H	4.5920956	-3.1419338	0.7184469
O	-1.3232719	-3.3509337	1.4966179
H	-0.8047099	-3.5560017	0.6310280
H	-0.7511959	-3.2839027	2.2767708
O	-4.1690617	-2.5368988	-1.2887149
H	-3.8188117	-2.1453348	-0.4229380
H	-4.7831796	-3.2735928	-1.1450509

-----

**S. Water Cluster - Size 3a - CAM-B3LYP/aug-cc-pVXZ Method Group**

s0:

C	2.7867428	-1.0226889	-0.1787650
C	1.3895019	-1.0040839	-0.2078750
C	0.7254479	0.2346930	-0.3208750
C	1.4142839	1.4402229	-0.4102600
C	2.7911028	1.3898629	-0.3836470
C	3.4719997	0.1687890	-0.2673730
C	0.3731160	-2.0132558	-0.1449920
C	-0.8252929	-1.3752239	-0.2166800
N	-0.6262540	-0.0159230	-0.2995600
H	3.3210307	-1.9587379	-0.0892190
H	0.8885359	2.3807978	-0.4960320
H	3.3578757	2.3076508	-0.4522950
H	4.5527727	0.1681690	-0.2473170
H	0.5199060	-3.0755048	-0.0528860
H	-1.8284009	-1.7666689	-0.2071220
H	-1.3603239	0.6605979	-0.4747860
O	-3.0035458	1.6594539	-0.7041609
H	-3.1393458	2.0856478	-1.5570279
H	-3.1857548	2.3335448	-0.0408380
O	-0.6081760	0.4744180	2.8264928
H	-0.6498270	0.3026260	1.8773889
H	0.2990760	0.7482039	2.9886778
O	-4.1570017	-0.8993379	-0.3259800
H	-3.8868837	0.0238430	-0.4610920
H	-5.1164996	-0.8848659	-0.2785380

-----

La:



C	2.4682378	-1.0774029	-0.4814080
C	1.0396089	-1.0041339	-0.3933230
C	0.4026170	0.2516850	-0.3814560
C	1.0765499	1.4544169	-0.4450870
C	2.5034798	1.3491469	-0.6979359
C	3.1528908	0.1430260	-0.7024489
C	0.0459420	-1.9682778	-0.2313230
C	-1.2072049	-1.2910779	-0.1240450
N	-0.9655809	0.0114390	-0.2266130
H	2.9767078	-2.0289748	-0.5161290
H	0.5712180	2.4069848	-0.4447080
H	3.0640168	2.2577498	-0.8668199
H	4.2218537	0.1242970	-0.8646739
H	0.1699270	-3.0362648	-0.1780420
H	-2.2077908	-1.6707789	-0.0081790
H	-1.6884559	0.7301169	-0.1846900
O	-3.2444728	1.7604989	-0.0649100
H	-3.4710437	2.2768698	-0.8459189
H	-3.3033677	2.3681098	0.6803499
O	2.0523768	0.2427140	2.5237908
H	2.4010058	-0.3848820	1.8722819
H	1.6089599	0.9033239	1.9738438
O	-4.4308677	-0.8040199	0.2538570
H	-4.1814297	0.1257270	0.1298200
H	-5.3115466	-0.8901909	-0.1205820

-----

**T. Water Cluster - Size 3b - CAM-B3LYP/aug-cc-pVXZ Method Group**

s0:

C	-2.9834248	0.0727160	0.3776710
C	-1.7900679	0.7447989	0.0975060
C	-0.7006289	0.0151990	-0.4213360
C	-0.7745299	-1.3523649	-0.6688939
C	-1.9647038	-1.9866118	-0.3872410
C	-3.0599728	-1.2804179	0.1331420
C	-1.3552169	2.1054098	0.2149760
C	-0.0668170	2.1470988	-0.2186600
N	0.3491050	0.8883349	-0.5845300
H	-3.8333757	0.6077910	0.7788579
H	0.0711580	-1.8953079	-1.0666929
H	-2.0573948	-3.0480608	-0.5690650
H	-3.9773237	-1.8119849	0.3438390
H	-1.9279769	2.9404498	0.5796530
H	0.6083320	2.9823768	-0.2914530
H	1.2336969	0.6669959	-1.0444329
O	2.8364968	0.0465130	-1.7049859
H	3.4459347	0.6562829	-2.1292688
H	3.3052247	-0.3183760	-0.9231059
O	1.7200179	-0.0022210	2.0577618
H	1.1558939	0.3302910	1.3452359
H	1.1702149	-0.6060550	2.5665218
O	3.8695517	-0.9145459	0.6249080
H	3.9954727	-1.8653079	0.6897779
H	3.1300438	-0.6903819	1.2273809

-----  
La:

C	-2.9066588	-0.1826760	0.3521460
C	-1.7920919	0.7108989	0.2864930
C	-0.6160170	0.3205570	-0.3817380

C	-0.4443330	-0.9150639	-0.9790549
C	-1.6226239	-1.7742149	-0.9741099
C	-2.7753978	-1.4158629	-0.3283450
C	-1.5669859	1.9930698	0.7873609
C	-0.2382190	2.3760588	0.4247850
N	0.2932340	1.3762479	-0.2684040
H	-3.8171847	0.0934990	0.8616959
H	0.4267640	-1.1571079	-1.5686659
H	-1.5680299	-2.7249538	-1.4851579
H	-3.6127557	-2.1006068	-0.3375400
H	-2.2484598	2.6073218	1.3506859
H	0.2997460	3.2842267	0.6297040
H	1.2608249	1.3521529	-0.6260230
O	2.9179378	1.1027989	-1.1354439
H	3.5211627	1.8481449	-1.0705809
H	3.2834637	0.3926680	-0.5590530
O	1.2926189	-1.7936109	1.4093589
H	0.6590489	-1.6046359	0.6876809
H	1.1750309	-2.7228698	1.6298299
O	3.6978227	-0.8933329	0.5102980
H	4.2053007	-1.6080729	0.1158780
H	2.8693888	-1.2969369	0.8514409

-----

**U. Water Cluster - Size 6 - CAM-B3LYP/aug-cc-pVXZ Method Group**

s0:

C	1.7327079	1.8216589	-1.1461129
C	1.0577089	0.6057210	-0.9470969
C	0.4917480	0.3298320	0.3195230

C	0.5812150	1.2284659	1.3891499
C	1.2404909	2.4271828	1.1604649
C	1.8121789	2.7203848	-0.0955640
C	0.7620349	-0.5307670	-1.7872029
C	0.0461270	-1.4142869	-1.0153349
N	-0.1008270	-0.9147239	0.2560210
H	2.1806258	2.0544308	-2.1112008
H	0.1625330	0.9902739	2.3657148
H	1.3285969	3.1516218	1.9688288
H	2.3263838	3.6702877	-0.2352100
H	1.0326759	-0.6657389	-2.8289338
H	-0.3838210	-2.3733878	-1.2804179
H	-0.7960799	-1.2374869	0.9264849
O	-2.5414448	-0.8678599	1.7696489
H	-2.6252718	0.0870460	1.5769719
H	-2.8799258	-0.9990149	2.6622008
O	3.4802747	-1.8216739	-0.6291890
H	4.1180757	-1.0974999	-0.6295380
H	2.7071368	-1.4750329	-1.1028529
O	-3.6217107	-1.8067029	-0.7262999
H	-3.3498907	-1.6348479	0.1908510
H	-3.2601718	-1.0434599	-1.2158879
O	2.3829348	-2.4547898	1.8676509
H	1.4842989	-2.1244538	1.7519879
H	2.8236518	-2.2378258	1.0225179
O	-2.4648638	0.5248510	-1.8581989
H	-1.5420009	0.2852760	-2.0265178
H	-2.4468298	1.0362459	-1.0275219
O	-2.4614018	1.7216189	0.7163639
H	-1.5972999	2.1132608	0.9139349
H	-3.1124648	2.4106608	0.8996809

-----  
La:

C	2.0357938	-0.4091570	-1.6609099
C	0.9640529	-0.8109199	-0.7922119
C	0.3664050	0.1180540	0.0827500
C	0.7399169	1.4605689	0.1682370
C	1.7970239	1.8609649	-0.7544919
C	2.3967948	0.9719309	-1.6185099
C	0.3444920	-2.0519448	-0.5569840
C	-0.6535400	-1.8540659	0.4549860
N	-0.6158150	-0.5741610	0.8128039
H	2.4251408	-1.0816089	-2.4224488
H	0.3483060	2.1414088	0.9207729
H	2.1142318	2.9028528	-0.7543739
H	3.1757398	1.3358089	-2.2879158
H	0.5648110	-3.0027368	-1.0302089
H	-1.3744339	-2.5477538	0.8702129
H	-1.2914059	-0.1203090	1.4396739
O	-2.7822298	0.9182389	1.8015159
H	-2.7285408	1.5214069	1.0328999
H	-2.9530468	1.4642809	2.5769978
O	4.1243797	-1.1041039	0.4890850
H	3.5382857	-0.9471029	-0.2821740
H	4.0809357	-2.0556298	0.6437170
O	-4.1228537	-1.3364909	0.6059700
H	-3.8138247	-0.6080120	1.1682799
H	-3.7693537	-1.1093469	-0.2753030
O	2.9197648	0.5236910	2.4212338
H	2.2120238	0.9231009	1.8946159
H	3.3698447	-0.0756360	1.7927409

O	-3.0589238	-0.3855200	-1.8304019
H	-2.3185538	-0.8426599	-2.2457498
H	-2.7053818	0.4770290	-1.5367029
O	-2.1836728	2.0119258	-0.6701519
H	-1.2085869	2.0622908	-0.6116830
H	-2.4728318	2.8472278	-1.0581619

-----

### V. Water Cluster - Size 9 - CAM-B3LYP/aug-cc-pVXZ Method Group

s0:

C	-2.6465258	-2.1337008	-0.0187380
C	-1.7215729	-1.3917389	-0.7719089
C	-0.6134560	-0.7966229	-0.1145370
C	-0.4119050	-0.9186849	1.2653719
C	-1.3359049	-1.6637579	1.9821768
C	-2.4446038	-2.2670588	1.3474389
C	-1.6126129	-1.0416879	-2.1638048
C	-0.4716250	-0.2862630	-2.2875788
N	0.1235050	-0.1297790	-1.0626219
H	-3.5075997	-2.5962998	-0.4991900
H	0.4201400	-0.4253270	1.7629819
H	-1.2106509	-1.7789939	3.0578668
H	-3.1481188	-2.8462178	1.9438269
H	-2.2781388	-1.3335159	-2.9685598
H	-0.0291230	0.1584320	-3.1721768
H	1.0223029	0.3268770	-0.9080299
O	2.8960608	0.8680309	-0.8708319
H	3.1926858	0.5099410	-0.0101920
H	3.0839838	0.1454160	-1.5080209

O	-2.8456838	1.7874119	-1.1079669
H	-3.0985078	1.4538839	-0.2195260
H	-2.5264048	1.0088459	-1.5899979
O	3.0977248	-1.5051069	-2.2117028
H	3.9356577	-1.8847789	-2.4986418
H	2.8596348	-1.9719208	-1.3777079
O	-0.8413099	3.5761127	-0.9720889
H	-1.2346789	4.4392307	-0.8050229
H	-1.5909019	2.9322038	-1.0034929
O	2.4277358	-2.4911948	0.2529720
H	1.4792969	-2.6054818	0.3919990
H	2.6888818	-1.7577289	0.8484939
O	3.2807977	-0.2578600	1.6477159
H	2.7046698	0.3970140	2.1220408
H	4.1205657	-0.2857290	2.1196668
O	-3.5386727	0.8595979	1.3867809
H	-3.1375448	1.3663259	2.1033278
H	-3.1924698	-0.0405950	1.4921079
O	1.4623129	2.9498658	0.3033390
H	0.6100520	3.1661728	-0.1389380
H	1.9484069	2.3656518	-0.3053750
O	1.5884039	1.5709699	2.5828978
H	1.4763939	2.1504468	1.7837629
H	1.8772169	2.1490608	3.2977227

-----

La:

C	-2.6602288	-2.1485808	0.1494340
C	-1.6591549	-1.5600879	-0.6977249
C	-0.5791350	-0.8452959	-0.1249910
C	-0.4019800	-0.6704729	1.2394969

C	-1.4685509	-1.2170479	2.0803808
C	-2.5274198	-1.9256629	1.5450319
C	-1.4680729	-1.5471989	-2.0909398
C	-0.2569700	-0.8231609	-2.3568058
N	0.2333810	-0.4169150	-1.1831769
H	-3.4943647	-2.7091428	-0.2656880
H	0.3571020	-0.0116180	1.6514749
H	-1.3925669	-1.0970869	3.1605838
H	-3.2783967	-2.3379228	2.2189328
H	-2.0990858	-1.9976338	-2.8497848
H	0.2259600	-0.5916970	-3.2984267
H	1.1351299	0.0727140	-1.0690519
O	2.8733938	0.5964910	-1.0175519
H	3.1697378	0.5679590	-0.0833870
H	3.1535958	-0.2722080	-1.3808189
O	-3.0375708	1.4356869	-1.0112279
H	-3.1589118	1.4399849	-0.0348640
H	-2.8407168	0.5134040	-1.2232529
O	3.3592057	-2.0594998	-1.4627999
H	2.8126238	-2.5400008	-2.0954048
H	2.9700928	-2.2383838	-0.5747590
O	-0.9930659	2.9856418	-1.8369519
H	-1.3570919	3.8577057	-2.0238948
H	-1.7500169	2.4349628	-1.5209489
O	2.4190568	-2.1702538	1.1032869
H	1.4586219	-2.0301078	1.1754819
H	2.7961588	-1.3309689	1.4378189
O	3.3457487	0.3906900	1.7040959
H	2.7009268	1.0897359	1.9885148
H	4.1873147	0.5957540	2.1263328
O	-3.3512457	1.2824749	1.6999209



H	-2.8836928	1.9454829	2.2223928
H	-2.9219408	0.4341100	1.9223599
O	1.3410569	2.9147268	-0.4794310
H	0.4825750	2.9387808	-0.9625509
H	1.8848919	2.2391918	-0.9168219
O	1.4594579	2.2260688	2.1014548
H	1.3478729	2.5529818	1.1711589
H	1.6612819	3.0012528	2.6371908

-----

#### W. Water Cluster - Size 12 - CAM-B3LYP/aug-cc-pVXZ Method Group

s0:

C	1.1996449	-0.4171640	0.7273629
C	0.2171740	-1.0341879	-0.0632250
C	-1.0934589	-1.1856549	0.4573080
C	-1.4496339	-0.7221579	1.7317369
C	-0.4630730	-0.1059360	2.4872218
C	0.8548539	0.0376700	1.9935428
C	0.2060580	-1.6189849	-1.3781439
C	-1.0727019	-2.0821358	-1.5867679
N	-1.8522039	-1.8259389	-0.4883880
H	2.2172588	-0.3111630	0.3582280
H	-2.4592968	-0.8521429	2.1171428
H	-0.7023059	0.2620420	3.4831647
H	1.6101059	0.5013090	2.6274038
H	1.0323939	-1.6704119	-2.0782858
H	-1.4927149	-2.5819688	-2.4527458
H	-2.8665968	-1.9712938	-0.4188770
O	-4.8187976	0.9346619	-0.3447360

H	-3.9376047	1.3510379	-0.2316200
H	-5.4052986	1.3902239	0.2696950
O	1.9008739	-3.9371007	0.0794110
H	1.6248239	-3.7303077	0.9987099
H	1.1657409	-3.6253607	-0.4670010
O	-4.6354026	-1.7704769	-0.0965370
H	-5.2707186	-2.1896448	-0.6872179
H	-4.7736346	-0.7996009	-0.1924510
O	1.1885889	-3.2179338	2.6394298
H	0.4183350	-3.6414317	3.0371238
H	0.9760109	-2.2731428	2.6141578
O	3.8598437	-2.1817028	-0.7117589
H	4.4179987	-1.9686788	0.0440340
H	3.1860908	-2.8171048	-0.3782260
O	3.3331227	-0.2019890	-2.6368968
H	3.4440047	-0.8278649	-1.8982269
H	2.7332758	0.5109300	-2.3380838
O	3.6819687	4.0983917	1.4483739
H	3.5699747	4.3343827	2.3756308
H	2.8251198	3.7140607	1.1764369
O	-0.9934779	1.1633069	-2.4971188
H	-0.8509499	0.2080030	-2.4172308
H	-1.4606069	1.4094499	-1.6727479
O	1.3211029	2.9522578	0.5282760
H	1.0978789	2.1262998	0.9817019
H	0.5039760	3.4888997	0.5447360
O	-2.2377298	1.8470709	-0.0794030
H	-1.8557299	1.2769969	0.6045920
H	-1.9553329	2.7568878	0.1464120
O	1.6478729	1.9536919	-2.1027238
H	1.6198499	2.3348148	-1.2059189

H	0.7169139	1.7073029	-2.2852468
O	-1.1201149	4.3202167	0.4662750
H	-1.3865959	4.7973956	1.2629949
H	-1.1929279	4.9597996	-0.2545130

-----  
La:

C	-1.1725299	-0.0777580	-1.4715499
C	-0.5167100	-0.8134029	-0.4273530
C	0.7813229	-1.3175339	-0.6226720
C	1.5341619	-1.1130049	-1.7813239
C	0.8381229	-0.4073470	-2.8447568
C	-0.4394600	0.0852260	-2.6916558
C	-0.9105749	-1.1902309	0.8731709
C	0.1749320	-1.9299209	1.4535869
N	1.1525189	-1.9891008	0.5559150
H	-2.1833078	0.3063530	-1.3485229
H	2.4966858	-1.5901479	-1.9458639
H	1.3544189	-0.2622350	-3.7928507
H	-0.9035419	0.6163850	-3.5215857
H	-1.8476839	-0.9713729	1.3700619
H	0.2598520	-2.3801688	2.4354788
H	2.0941558	-2.4036068	0.7132369
O	5.0828716	-0.4821650	0.5302630
H	4.4149477	0.1762340	0.2400630
H	5.7865306	-0.4559750	-0.1279720
O	-3.8424807	-2.9337248	0.1087810
H	-3.3540397	-2.9308678	-0.7456959
H	-3.3060467	-3.4577097	0.7148569
O	3.7509537	-2.8215538	0.8232259
H	4.0554137	-3.2696508	1.6202549

H	4.2994937	-2.0049198	0.7376789
O	-2.5722208	-2.6975698	-2.2901058
H	-1.9004709	-3.3441167	-2.5392458
H	-2.0901318	-1.8550929	-2.1757918
O	-4.3653877	-0.4168420	1.0205939
H	-4.5965826	0.1267100	0.2595730
H	-4.1824327	-1.3167849	0.6654909
O	-2.9310258	0.7736859	3.1204338
H	-3.4026077	0.3991950	2.3542688
H	-2.1205728	1.1975779	2.7689958
O	-2.6086178	4.4669087	-0.9943269
H	-2.6679158	4.5745357	-1.9497739
H	-1.8536069	3.8602787	-0.8510359
O	1.8966399	0.9197229	2.4362818
H	2.0139808	0.0239420	2.7721348
H	2.2635008	0.9154869	1.5258589
O	-0.5224390	2.7321828	-0.4417940
H	-0.6630249	1.8553959	-0.8524449
H	0.3768090	3.0147838	-0.6973569
O	2.9180628	1.0364409	-0.1284260
H	2.4536268	0.4390260	-0.7516349
H	2.7633658	1.9418979	-0.4640350
O	-0.6278230	2.0499228	2.2715078
H	-0.6252660	2.3365948	1.3377109
H	0.2287920	1.5893239	2.3844968
O	2.1132978	3.5361157	-1.0218069
H	2.3103998	3.7748737	-1.9369179
H	2.3873728	4.2965847	-0.4925270

-----

**X. Water Cluster - Size 15 - CAM-B3LYP/aug-cc-pVXZ Method Group**

s0:

C	0.4193110	0.5736260	-0.5895560
C	-0.4936920	-0.0239300	0.3015800
C	-1.3287199	-1.0749129	-0.1698300
C	-1.2716759	-1.5404689	-1.4884819
C	-0.3647830	-0.9314039	-2.3479728
C	0.4727670	0.1187120	-1.9019979
C	-0.8124059	0.1589230	1.6987479
C	-1.7910209	-0.7565509	2.0086748
N	-2.1222918	-1.4916959	0.8840779
H	1.0843689	1.3623969	-0.2570930
H	-1.9037069	-2.3554498	-1.8203209
H	-0.2861800	-1.2731399	-3.3738537
H	1.1730419	0.5693020	-2.5962768
H	-0.3822910	0.8806079	2.3763798
H	-2.2834628	-0.9411229	2.9504638
H	-2.6782408	-2.3631218	0.8654819
O	1.3390109	-4.2553187	0.4807400
H	1.7838779	-3.3798537	0.2630060
H	1.8482469	-4.7819576	1.1165659
O	-4.0499247	0.9310359	-0.0178520
H	-3.6543697	1.0407659	-0.9443289
H	-3.7699357	0.0912580	0.3895400
O	-0.9638199	-5.0790826	-0.3282020
H	-0.9262879	-5.5579616	-1.1706939
H	-0.0537590	-4.7542346	-0.0278120
O	-2.9369538	1.3113489	-2.3359918
H	-2.3479908	0.5913190	-2.6232888
H	-2.4761468	2.2069568	-2.3738698

O	-1.2850199	3.1737888	0.4584230
H	-2.1828388	3.3400117	0.9026729
H	-1.1687989	2.2044658	0.3937570
O	1.3168969	3.6026507	1.1085749
H	0.3400700	3.5871007	0.9449489
H	1.6012899	2.9583198	1.8000849
O	4.5605507	1.1026889	-1.7346509
H	4.9908186	1.5329329	-2.4886808
H	4.1556427	1.7562949	-1.0648339
O	2.1297238	-0.7973109	2.3060248
H	1.2111969	-0.9426699	2.5962478
H	2.2836728	-1.2474829	1.4228459
O	3.5661937	2.5962758	0.0744820
H	2.7603208	3.1669548	0.0370880
H	3.5361667	2.1681308	0.9722669
O	2.3813488	-1.9193839	-0.0876990
H	1.7367409	-1.4182399	-0.6254400
H	3.3243597	-1.7884959	-0.4774670
O	2.8125308	1.6856419	2.4640858
H	3.2569168	1.9262379	3.2937137
H	2.5611978	0.6998869	2.4399878
O	4.6188856	-1.3558299	-1.0940269
H	4.6822846	-0.3825620	-1.3913349
H	5.4335186	-1.8662859	-1.2088979
O	-3.1210628	-3.9664037	0.5421300
H	-2.3172458	-4.4779607	0.2007200
H	-3.8721747	-4.5367827	0.7666219
O	-3.6703317	3.0810758	1.3323469
H	-3.9664607	2.2331958	0.8600119
H	-4.3807437	3.5888537	1.7505869
O	-1.7210319	3.5700637	-2.0972618

H	-1.4653679	3.6186477	-1.1308189
H	-1.5863419	4.3916607	-2.5924868

-----

La:

C	0.5040790	0.4703970	-0.8206169
C	-0.4528180	0.0971550	0.1876260
C	-1.7086649	-0.4264290	-0.1884730
C	-2.1290908	-0.5769390	-1.5072639
C	-1.1739039	-0.1533070	-2.5151958
C	0.0762590	0.3413720	-2.1851308
C	-0.4172050	0.1228840	1.6030269
C	-1.6623329	-0.4185990	2.0786768
N	-2.4025848	-0.7358659	1.0067869
H	1.5316579	0.7146029	-0.5701500
H	-3.0972578	-0.9779319	-1.7732469
H	-1.4468799	-0.2571600	-3.5605607
H	0.7644229	0.6172470	-2.9774098
H	0.3849630	0.4744480	2.2317448
H	-1.9942918	-0.5912660	3.0891198
H	-3.3084397	-1.2614969	1.0168039
O	-0.5556390	-4.2414677	0.0929370
H	0.1549920	-3.5561217	-0.1063370
H	-0.2099690	-4.9742486	0.6271680
O	-3.3925067	2.5154378	0.3378120
H	-3.0285418	2.6007578	-0.6080140
H	-3.9577347	1.7359609	0.4558570
O	-3.0787988	-4.2337737	-0.4058900
H	-3.3236817	-4.6781766	-1.2321329
H	-2.0790058	-4.2321457	-0.2432290
O	-2.3127598	2.8427268	-1.9790058

H	-1.8761179	2.0416378	-2.3301858
H	-1.6859739	3.6291037	-1.9676548
O	0.4497330	3.2873907	0.2998720
H	-0.2781800	3.3029607	1.0138159
H	0.4008570	2.4330058	-0.2027080
O	2.8646428	2.6157918	1.2930029
H	1.9859618	2.9759318	1.0000469
H	2.7776648	1.8462399	1.9058489
O	4.6672796	-0.6974539	-1.9063249
H	5.3490416	-0.4506020	-2.5490458
H	4.5906916	-0.0512720	-1.1204809
O	1.9485119	-2.0109128	2.1760958
H	1.3248339	-2.3741128	2.8248328
H	1.7016239	-2.2463448	1.2294059
O	4.4158687	0.7930439	0.1430090
H	3.9424957	1.6622449	0.2064680
H	4.2025317	0.3317640	0.9946209
O	1.3228339	-2.4639678	-0.3344180
H	0.9936409	-1.5831019	-0.6279320
H	2.1442288	-2.7292068	-0.8886179
O	3.2828837	0.1585280	2.5067098
H	3.7919077	0.1897060	3.3338487
H	2.7372728	-0.6970079	2.4350488
O	3.4066247	-2.8966468	-1.6954869
H	3.9755447	-2.0639848	-1.8411179
H	3.7551997	-3.6992177	-2.1102668
O	-4.4374847	-2.3855298	0.7327699
H	-3.9978807	-3.1799618	0.2793210
H	-5.3014936	-2.5829768	1.1244019
O	-1.5308289	3.2701908	1.9234389
H	-2.3382378	2.9383848	1.4022969



H	-1.5294669	3.0030798	2.8554558
O	-0.5702300	4.7186946	-1.6176719
H	-0.0327720	4.3545437	-0.8517049
H	-0.2644730	5.5701686	-1.9635139

-----

## Y. MCH

s0:

C	3.6312937	-1.8798639	0.4555890
C	2.8224868	-1.5268729	-0.6416350
C	1.5045919	-2.0751818	-0.7338189
C	0.9898449	-2.9512108	0.2308750
C	1.8140599	-3.2796447	1.3084869
C	3.1219528	-2.7490668	1.4202269
C	2.9944018	-0.6483520	-1.7742869
C	1.8227429	-0.6786959	-2.4991138
N	0.9214389	-1.5434189	-1.8781859
H	4.6336376	-1.4737459	0.5523010
H	-0.0150190	-3.3527387	0.1520740
H	1.4447929	-3.9520077	2.0764238
H	3.7341557	-3.0247538	2.2731698
H	3.8713557	-0.0645640	-2.0096018
H	1.5508499	-0.1585890	-3.4041267
H	-0.0191880	-1.7194379	-2.1905828
C	-2.8295078	-1.4509919	1.2411049
C	-4.3394407	-1.6696549	1.0322789
C	-4.9956256	-0.4310130	0.3926510
C	-4.2943727	-0.0419730	-0.9224739
C	-2.7813068	0.1865680	-0.7243819

C	-2.1341158	-1.0529359	-0.0727400
H	-2.3638238	-2.3554058	1.6546749
H	-2.6788948	-0.6520010	1.9827888
H	-4.8253756	-1.9064919	1.9879788
H	-4.4912937	-2.5388128	0.3733310
H	-6.0625875	-0.6166790	0.2115690
H	-4.9348726	0.4128890	1.0970299
H	-4.7533966	0.8622739	-1.3457759
H	-4.4362137	-0.8465379	-1.6623059
H	-2.6591948	1.0305049	-0.0265590
H	-1.0700959	-0.8650279	0.1068130
H	-2.1990278	-1.8958199	-0.7824239
C	-2.0866948	0.5534890	-2.0447218
H	-2.5232208	1.4584869	-2.4846768
H	-1.0161059	0.7324299	-1.8919789
H	-2.1990958	-0.2594840	-2.7766348
C	2.3618268	1.7087719	1.0858999
C	1.0988279	0.8506089	1.2727519
C	-0.0903780	1.7108949	1.7355789
C	-0.3467760	2.8725018	0.7578429
C	0.9096619	3.7442117	0.5450400
C	2.1001888	2.8651298	0.1043090
H	3.1861678	1.0839049	0.7235669
H	2.6713288	2.1199098	2.0596388
H	1.2895839	0.0347610	1.9809268
H	0.8510989	0.3780910	0.3133230
H	-0.9923779	1.0931459	1.8325739
H	0.1224720	2.1192818	2.7357238
H	-1.1765019	3.4985987	1.1157129
H	-0.6554449	2.4638148	-0.2165270
H	1.1708219	4.1985177	1.5160999

H	2.9992848	3.4884227	-0.0036690
H	1.8812569	2.4453318	-0.8904139
C	0.6422510	4.8743636	-0.4608920
H	-0.1876660	5.5120376	-0.1310170
H	1.5285039	5.5082506	-0.5904590
H	0.3785440	4.4588827	-1.4430859

-----

La:

C	-4.1854457	-0.9363409	-0.3526120
C	-3.1539368	-1.1386269	0.6222450
C	-1.8907219	-1.6268009	0.2306720
C	-1.5410119	-1.9466639	-1.0922609
C	-2.5919158	-1.7170829	-2.0701478
C	-3.8469007	-1.2402209	-1.7112459
C	-3.1042928	-0.9261099	2.0386688
C	-1.7960229	-1.3042799	2.5041918
N	-1.1014569	-1.7139619	1.4156479
H	-5.1619576	-0.5568750	-0.0765790
H	-0.5584000	-2.2953248	-1.3796959
H	-2.3781588	-1.9272769	-3.1138128
H	-4.5938146	-1.0862259	-2.4844938
H	-3.8957237	-0.5470520	2.6679808
H	-1.3760889	-1.2900139	3.4960527
H	-0.1437470	-2.0371268	1.4326369
C	2.4196038	-0.6882779	-1.5904789
C	3.7861307	-1.3663129	-1.7989059
C	4.7857136	-0.9483579	-0.7033769
C	4.2260397	-1.2293299	0.7040069
C	2.8607368	-0.5459020	0.9271889
C	1.8708849	-0.9626229	-0.1796910

H	1.6994219	-1.0297079	-2.3451228
H	2.5279638	0.3975570	-1.7277769
H	4.1848277	-1.1187429	-2.7913408
H	3.6561717	-2.4592878	-1.7711509
H	5.7409536	-1.4718049	-0.8406719
H	4.9961256	0.1279240	-0.7990699
H	4.9378696	-0.8942259	1.4709729
H	4.1033267	-2.3165068	0.8369089
H	3.0140428	0.5425080	0.8455309
H	0.9165409	-0.4397090	-0.0467100
H	1.6700559	-2.0437258	-0.0806660
C	2.2980958	-0.8438319	2.3256388
H	2.9991358	-0.5364380	3.1108598
H	1.3537779	-0.3108330	2.4937668
H	2.1198508	-1.9225409	2.4484978
C	-1.8902729	1.9807138	-0.8299459
C	-0.8067899	1.7364709	-1.8950419
C	0.3199280	2.7822278	-1.7923179
C	0.9143219	2.8368158	-0.3723410
C	-0.1617500	3.0648578	0.7112739
C	-1.2786349	2.0079148	0.5811920
H	-2.6631288	1.2070259	-0.8912649
H	-2.3826468	2.9462038	-1.0278129
H	-1.2517929	1.7546209	-2.8986038
H	-0.3924680	0.7279739	-1.7538179
H	1.1118539	2.5622798	-2.5214228
H	-0.0836600	3.7733167	-2.0519878
H	1.6761179	3.6269917	-0.3086310
H	1.4261289	1.8879189	-0.1574640
H	-0.6147950	4.0547637	0.5328760
H	-2.0584938	2.1949538	1.3332449

H	-0.8551769	1.0185169	0.8083649
C	0.4561440	3.0608508	2.1181738
H	1.2319589	3.8309267	2.2152418
H	-0.3054080	3.2451058	2.8865718
H	0.9201169	2.0880218	2.3297218

-----

## VI. OPTIMISED GEOMETRIES - EXPLICIT PISALR

Following are the optimised geometries used in the study.

### A. Water

s0:

C	2.3120798	0.5128560	0.0006860
C	0.9614539	0.8892729	0.0000900
C	-0.0346070	-0.1270030	-0.0001020
C	0.2908330	-1.4836239	0.0003780
C	1.6342439	-1.8223139	0.0009370
C	2.6354818	-0.8333859	0.0010810
C	0.2664120	2.1430138	-0.0006060
C	-1.0736639	1.8545629	-0.0012600
N	-1.2594289	0.4931670	-0.0009620
H	3.0912988	1.2652739	0.0008000
H	-0.4802520	-2.2434008	0.0003190
H	1.9196299	-2.8664938	0.0012510
H	3.6752127	-1.1350559	0.0014860
H	0.7031419	3.1280188	-0.0006520
H	-1.9219069	2.5190088	-0.0019260
H	-2.1576138	0.0157630	-0.0012780

O	-3.7790777	-0.9778359	-0.0079490
H	-3.9098247	-1.4978409	0.7942999
H	-3.8244667	-1.6150299	-0.7311999

-----

La:

C	2.3259688	0.5924160	0.0005380
C	0.9287889	0.8987349	0.0000510
C	-0.0225130	-0.1323980	0.0001290
C	0.2984740	-1.4920989	0.0008410
C	1.7192439	-1.7841339	0.0009630
C	2.6728278	-0.7901379	0.0008330
C	0.2071090	2.1193318	-0.0006670
C	-1.1904169	1.8053569	-0.0012140
N	-1.2922579	0.4741020	-0.0007780
H	3.0753678	1.3707319	0.0004210
H	-0.4488380	-2.2705128	0.0015200
H	2.0332488	-2.8206288	0.0011570
H	3.7197547	-1.0691629	0.0009320
H	0.6116510	3.1183288	-0.0008000
H	-2.0496168	2.4521368	-0.0019430
H	-2.1759378	-0.0480210	-0.0010620
O	-3.7171377	-1.0200039	-0.0082440
H	-3.8539227	-1.5377079	0.7947619
H	-3.7656957	-1.6562669	-0.7324289

-----

Lb:

C	2.3434898	0.5298950	0.0001200
C	0.9732669	0.9100319	0.0000810
C	-0.0568460	-0.1300300	0.0006000

C	0.2392700	-1.5230969	0.0014590
C	1.6036269	-1.8524749	0.0010550
C	2.6229258	-0.8522059	0.0003380
C	0.2898160	2.1462988	-0.0007540
C	-1.0717729	1.8860099	-0.0009220
N	-1.2520529	0.4905110	-0.0001230
H	3.1339008	1.2653169	-0.0003540
H	-0.5424020	-2.2674338	0.0024550
H	1.9049789	-2.8915018	0.0013700
H	3.6541507	-1.1818959	0.0000230
H	0.7379829	3.1263318	-0.0012130
H	-1.9199559	2.5479158	-0.0014280
H	-2.1542928	0.0145090	-0.0005240
O	-3.7534687	-0.9576809	-0.0088730
H	-3.8854537	-1.4782389	0.7929349
H	-3.7994457	-1.5936899	-0.7332779

-----

## B. MCH

s0:

C	-1.6755199	0.8092829	-1.5902709
C	-1.8076969	-0.3231730	-0.7768759
C	-1.9502199	-0.1459670	0.6248500
C	-1.9626839	1.1150759	1.2168649
C	-1.8315859	2.2139298	0.3850750
C	-1.6892309	2.0624118	-1.0049019
C	-1.8224419	-1.7359819	-1.0204249
C	-1.9697358	-2.3515398	0.1906830
N	-2.0496778	-1.3991669	1.1840809

H	-1.5569129	0.7031939	-2.6611888
H	-2.0634128	1.2328119	2.2883488
H	-1.8291649	3.2075138	0.8134179
H	-1.5810799	2.9440848	-1.6229609
H	-1.7328139	-2.2303138	-1.9730118
H	-2.0210788	-3.3995137	0.4331600
H	-2.1443408	-1.5935219	2.1645978
C	1.7346109	-1.4172219	1.0620219
C	2.4233878	-1.8764419	-0.2239150
C	2.0734808	-0.9584869	-1.3959729
C	2.3924428	0.5023710	-1.0752049
C	1.7008089	0.9723749	0.2078330
C	2.0524718	0.0455630	1.3749909
H	2.0318188	-2.0556008	1.8989409
H	0.6534150	-1.5313349	0.9449159
H	2.1424708	-2.9074678	-0.4546830
H	3.5093587	-1.8718239	-0.0734860
H	2.6084958	-1.2733409	-2.2960958
H	1.0048959	-1.0510189	-1.6121849
H	2.0929118	1.1448429	-1.9083129
H	3.4773437	0.6223080	-0.9608379
H	0.6235910	0.8982889	0.0432620
H	1.5126919	0.3653910	2.2714778
H	3.1216018	0.1460120	1.6012329
C	2.0263228	2.4273238	0.5246140
H	1.7337629	3.0834258	-0.2982970
H	1.4991499	2.7618648	1.4210589
H	3.0985798	2.5612518	0.6958819

-----  
La:



C	-4.3663127	-0.2249270	0.1632390
C	-3.2236548	0.5832450	-0.1009860
C	-1.9611419	-0.0003980	-0.2433000
C	-1.7111339	-1.3730829	-0.1384910
C	-2.8838318	-2.1771618	0.1187580
C	-4.1386147	-1.6275059	0.2613360
C	-3.0492678	1.9873828	-0.2627680
C	-1.6635619	2.2391908	-0.5059300
N	-1.0528169	1.0494989	-0.4909510
H	-5.3500276	0.2052610	0.2764830
H	-0.7311049	-1.8062899	-0.2564780
H	-2.7631838	-3.2497068	0.2035290
H	-4.9778686	-2.2832218	0.4563210
H	-3.8100957	2.7491398	-0.2130420
H	-1.1366169	3.1601938	-0.6786369
H	-0.0616970	0.9186769	-0.6287680
C	2.2176698	-1.6555899	0.1768790
C	3.6960767	-1.7877249	-0.1901980
C	4.1887237	-0.5574520	-0.9535389
C	3.9092947	0.7314159	-0.1795670
C	2.4285228	0.8755299	0.1894660
C	1.9497219	-0.3652590	0.9512769
H	1.8892359	-2.5177478	0.7616309
H	1.6200199	-1.6581979	-0.7421769
H	3.8602837	-2.6913678	-0.7819649
H	4.2844197	-1.9013979	0.7271729
H	5.2573946	-0.6437340	-1.1641839
H	3.6822817	-0.5106730	-1.9243339
H	4.2327617	1.6006709	-0.7587399
H	4.4975717	0.7354219	0.7456299
H	1.8797549	0.9256659	-0.7653279

H	0.8867139	-0.2834960	1.1948989
H	2.4769168	-0.4025850	1.9115569
C	2.1631978	2.1592798	0.9703379
H	2.4736648	3.0401908	0.4041860
H	1.1050829	2.2705508	1.2193139
H	2.7200888	2.1544878	1.9105019

-----

Lb:

C	2.2806628	0.4753900	1.4143989
C	2.0954998	-0.4490340	0.3600910
C	1.7567609	0.0462310	-0.9712259
C	1.6127559	1.4193839	-1.2762809
C	1.7980969	2.3061098	-0.2029450
C	2.1236868	1.8460849	1.1087509
C	2.1293168	-1.8571589	0.2680420
C	1.8212429	-2.2158388	-1.0356519
N	1.6001279	-1.0487199	-1.7695089
H	2.5289168	0.1469950	2.4122788
H	1.3651319	1.7598959	-2.2697888
H	1.6868909	3.3692607	-0.3651840
H	2.2513928	2.5823028	1.8907619
H	2.3395078	-2.5475258	1.0676269
H	1.7434739	-3.1832208	-1.4993189
H	1.3507529	-1.0220359	-2.7426208
C	-1.9580579	1.6167839	-0.1865100
C	-3.1974818	1.0296999	-0.8626759
C	-3.0145928	-0.4607890	-1.1537379
C	-2.6465548	-1.2331399	0.1134710
C	-1.3972159	-0.6597299	0.7903329
C	-1.5769919	0.8348089	1.0705269

H	-2.1219788	2.6690028	0.0607580
H	-1.1149399	1.5881989	-0.8840069
H	-3.4195537	1.5719619	-1.7858399
H	-4.0652547	1.1608269	-0.2058160
H	-3.9216537	-0.8755919	-1.6015039
H	-2.2141608	-0.5857230	-1.8925159
H	-2.4879818	-2.2904008	-0.1190210
H	-3.4850027	-1.1906369	0.8198029
H	-0.5683260	-0.7672669	0.0823450
H	-0.6547240	1.2384809	1.4958019
H	-2.3592908	0.9593169	1.8301319
C	-1.0326819	-1.4276999	2.0553688
H	-0.8571059	-2.4841088	1.8394419
H	-0.1262060	-1.0208169	2.5078358
H	-1.8374589	-1.3644909	2.7936648

-----