

## Supporting information

The optimized geometry of the water cluster anions in Cartesian coordinates obtained by LC-BOP and MP2 using adz+diff basis set. Units in Å.

### Isomer 2L

<u>LC-BOP</u>			
	<u>x</u>	<u>y</u>	<u>z</u>
O	-0.0835	1.4980	0.0000
H	0.8593	1.7176	0.0000
H	-0.1040	0.5158	0.0000
O	-0.0791	-1.3267	0.0000
H	0.2830	-1.7961	0.7711
H	0.2830	-1.7961	-0.7711

  

<u>MP2</u>			
	<u>x</u>	<u>y</u>	<u>z</u>
O	-0.0838	1.5358	0.0000
H	0.8575	1.7495	0.0000
H	-0.0911	0.5606	0.0000
O	-0.0838	-1.3658	0.0000
H	0.2871	-1.8351	0.7612
H	0.2871	-1.8351	-0.7612

Isomer 3L

LC-BOP			
	x	y	z
O	-0.0822	0.8721	-0.0381
H	0.7786	0.3841	-0.0658
H	0.0226	1.5236	0.6707
H	-1.6574	0.0477	-0.0786
O	-2.5394	-0.3961	-0.0563
H	-2.3662	-1.2496	0.3651
O	2.3108	-0.4552	-0.0629
H	3.1003	0.0123	-0.3936
H	2.6087	-0.8846	0.7610

MP2			
	x	y	z
O	-0.0822	0.8721	-0.0381
H	0.7786	0.3841	-0.0658
H	0.0226	1.5236	0.6707
H	-1.6574	0.0477	-0.0786
O	-2.5394	-0.3961	-0.0563
H	-2.3662	-1.2496	0.3651
O	2.3108	-0.4552	-0.0629
H	3.1003	0.0123	-0.3936
H	2.6087	-0.8846	0.7610

Isomer 4L

LC-BOP			
	x	y	z
O	3.6335	0.1567	0.3619
H	3.4419	0.5830	1.2088
H	2.7480	-0.1255	0.0232
O	1.1665	-0.6903	-0.5100
H	0.3541	-0.1149	-0.4825
H	0.8927	-1.5340	-0.1231
H	-1.9032	0.4033	-0.1530
O	-1.0467	0.8361	-0.4138
H	-1.0151	1.6585	0.0976
O	-3.3562	-0.3554	0.3286
H	-3.5005	-0.4765	1.2882
H	-4.1950	0.0288	0.0069

MP2			
	x	y	z
O	3.6049	0.0983	0.5096
H	3.3245	0.3608	1.3946
H	2.7627	-0.1341	0.0665
O	1.1673	-0.6391	-0.7306
H	0.3804	-0.0582	-0.6249
H	0.8533	-1.5058	-0.4446
H	-1.8773	0.5028	-0.1292
O	-1.0674	0.9776	-0.4190
H	-1.0041	1.7207	0.1948
O	-3.3145	-0.4546	0.3915
H	-3.3751	-0.6655	1.3377
H	-4.1873	-0.0787	0.1931

Isomer 5L

LC-BOP			
	x	y	z
O	-4.7552	-0.5554	0.3436
H	-4.8786	-0.2997	1.2682
H	-3.9024	-0.1276	0.0820
O	-2.4379	0.7381	-0.3449
H	-1.5423	0.2983	-0.3568
H	-2.4928	1.2239	-1.1796
H	0.8011	-0.0175	-0.1373
O	-0.0459	-0.4174	-0.4896
H	0.0366	-1.3728	-0.3631
O	2.1903	0.6540	0.4365
H	3.0818	0.2667	0.2169
H	2.2391	0.8848	1.3766
O	4.6017	-0.4063	-0.1076
H	4.8670	-1.1621	0.4547
H	5.3665	0.2016	-0.0648

MP2			
	x	y	z
O	-4.8456	-0.5707	0.3798
H	-4.9325	-0.3225	1.3079
H	-4.0038	-0.1473	0.1121
O	-2.4685	0.7643	-0.3475
H	-1.5947	0.3108	-0.3755
H	-2.5170	1.2238	-1.1943
H	0.7912	-0.0492	-0.1987
O	-0.0282	-0.4740	-0.5473
H	0.0642	-1.4052	-0.3131
O	2.2233	0.7548	0.3921
H	3.0984	0.3359	0.2308
H	2.2492	0.9902	1.3287
O	4.6814	-0.4553	-0.0596
H	4.8845	-1.2051	0.5241
H	5.4612	0.1155	0.0376

Isomer 6L

LC-BOP			
	x	y	z
O	-5.8388	-0.0863	-0.6881
H	-5.9244	-0.9219	-1.1678
H	-4.9998	-0.1822	-0.1730
O	-3.5419	-0.4427	0.7688
H	-2.6862	-0.0084	0.4958
H	-3.6372	-0.2484	1.7117
H	-0.3797	0.3505	0.0829
O	-1.2790	0.7912	0.1003
H	-1.3046	1.3804	-0.6662
O	1.0813	-0.3806	0.0564
H	1.9671	0.0888	0.0765
H	1.2152	-1.1792	-0.4731
O	3.4238	0.8421	0.0854
H	3.5717	1.5312	-0.5811
H	4.2393	0.2694	0.0398
H	6.4647	-0.2625	0.1039
O	5.6183	-0.6969	-0.1247
H	5.7638	-1.0323	-1.0336

MP2			
	x	y	z
O	-5.9154	-0.3846	-0.7291
H	-5.9529	-1.3379	-0.8710
H	-5.0975	-0.2671	-0.2028
O	-3.5931	-0.1295	0.8539
H	-2.7467	0.1803	0.4571
H	-3.7028	0.4304	1.6318
H	-0.3796	0.4108	0.0214
O	-1.2464	0.8269	-0.2039
H	-1.2010	0.9861	-1.1541
O	1.1226	-0.3226	0.4797
H	1.9766	0.1355	0.2884
H	1.2792	-1.2360	0.2094
O	3.4892	0.9360	-0.0540
H	3.5489	1.3993	-0.9004
H	4.2658	0.3311	-0.0699
H	6.5101	-0.4210	-0.1772
O	5.6289	-0.8283	-0.1350
H	5.6132	-1.3942	-0.9260

Isomer 3AA

LC-BOP			
	x	y	z
O	0.0000	0.0000	0.8969
H	-0.7690	0.0000	1.5026
H	0.7690	0.0000	1.5026
H	0.0000	1.5896	-0.1627
O	0.0000	2.4537	-0.6274
H	0.0000	3.1032	0.0916
H	0.0000	-1.5896	-0.1627
O	0.0000	-2.4537	-0.6274
H	0.0000	-3.1032	0.0916

MP2			
	x	y	z
O	0.0000	0.0000	0.9786
H	-0.7597	0.0000	1.5845
H	0.7597	0.0000	1.5845
H	0.0000	1.6216	-0.1698
O	0.0000	2.4580	-0.6697
H	0.0000	3.1257	0.0283
H	0.0000	-1.6216	-0.1698
O	0.0000	-2.4580	-0.6697
H	0.0000	-3.1257	0.0283

Isomer 4AA

LC-BOP			
	x	y	z
O	0.0422	2.2155	0.0000
H	0.0541	1.6056	0.7656
H	0.0541	1.6056	-0.7656
O	0.0422	0.0777	1.9754
H	-0.8029	-0.0485	2.4327
H	0.0927	-0.6783	1.3463
O	0.0422	0.0777	-1.9754
H	0.0927	-0.6783	-1.3463
H	-0.8029	-0.0485	-2.4327
O	0.0441	-1.9517	0.0000
H	0.7397	-2.6418	0.0000
H	-0.7925	-2.4697	0.0000

MP2			
	x	y	z
O	-0.0220	-2.2730	0.0000
H	-0.0299	-1.6609	0.7564
H	-0.0299	-1.6609	-0.7564
O	-0.0481	-0.0804	2.0136
H	0.7644	0.0808	2.5106
H	-0.0864	0.6764	1.3969
O	-0.0481	-0.0804	-2.0136
H	-0.0864	0.6764	-1.3969
H	0.7644	0.0808	-2.5106
O	-0.0481	2.0068	0.0000
H	-0.7388	2.6916	0.0000
H	0.7732	2.5326	0.0000

Isomer 5AA-1

LC-BOP			
	x	y	z
O	-0.1831	2.4312	-0.4399
H	-0.9151	1.7795	-0.4010
H	0.5991	1.9436	-0.1240
O	-2.3304	0.5828	0.0498
H	-1.9695	-0.3415	0.0848
H	-2.3966	0.8612	0.9751
H	2.1847	0.5501	1.4872
O	2.1370	0.7162	0.5219
H	3.0549	0.9523	0.2803
O	-1.2460	-1.9268	0.1719
H	-0.3042	-1.8566	-0.1537
H	-1.1646	-2.2587	1.0786
H	1.6178	-0.7648	-0.2661
O	1.2909	-1.6267	-0.6316
H	1.9471	-2.2794	-0.3374

MP2			
	x	y	z
O	-0.7107	2.3378	-0.6248
H	-1.2897	1.5677	-0.4781
H	0.1246	2.0674	-0.2127
O	-2.4056	0.0637	0.1556
H	-1.8562	-0.7510	0.1517
H	-2.4397	0.3120	1.0885
H	1.7501	0.9420	1.6326
O	1.8296	1.1754	0.6907
H	2.6976	1.6100	0.6494
O	-0.7544	-2.2111	0.1421
H	0.1243	-1.9177	-0.1947
H	-0.5557	-2.5332	1.0314
H	1.7801	-0.3897	-0.2906
O	1.6909	-1.2608	-0.7330
H	2.4666	-1.7482	-0.4216



Isomer 5AA-2

LC-BOP			
	x	y	z
O	-0.0688	-1.8156	-0.1201
H	-0.5138	-1.2682	-0.8056
H	0.8522	-1.4859	-0.1008
O	-1.6076	0.2292	-1.3837
H	-0.9045	0.8939	-1.2323
H	-0.9408	0.7189	1.3067
O	-1.5667	-0.0187	1.4478
H	-1.0417	-0.7996	1.1534
H	-1.9910	0.1572	-0.4820
H	0.8016	2.5378	0.1017
O	0.4104	1.6517	0.0577
H	1.1854	1.0314	0.0453
O	2.4004	-0.2273	-0.0039
H	3.0262	-0.1240	-0.7537
H	2.9848	-0.2159	0.7850

MP2			
	x	y	z
O	-0.0414	-1.8652	-0.1221
H	-0.4764	-1.3232	-0.8075
H	0.8712	-1.5282	-0.1126
O	-1.6456	0.2220	-1.4322
H	-0.9564	0.8915	-1.2744
H	-0.9749	0.7075	1.3584
O	-1.5951	-0.0279	1.5009
H	-1.0619	-0.7936	1.2086
H	-2.0305	0.1515	-0.5392
H	0.7845	2.5811	0.0969
O	0.3970	1.6964	0.0586
H	1.1787	1.1017	0.0429
O	2.4539	-0.2136	-0.0057
H	3.0805	-0.0979	-0.7428
H	3.0360	-0.1843	0.7747

Isomer 6AA-1

LC-BOP			
	x	y	z
O	-1.3883	-0.9432	1.3744
H	-0.4055	-0.9496	1.5122
H	-1.6097	-0.0031	1.2212
O	1.3718	-0.9357	1.3807
H	1.4359	-1.1762	0.4206
H	1.6378	0.0034	1.3523
O	1.3871	-0.9484	-1.3724
H	0.4044	-0.9536	-1.5102
H	1.6104	-0.0082	-1.2234
H	-1.4364	-1.1775	-0.4177
O	-1.3729	-0.9388	-1.3783
H	-1.6389	0.0004	-1.3511
O	1.9498	1.5977	-0.0013
H	2.7365	2.1692	-0.0565
H	1.2018	2.2393	0.0018
H	-1.2000	2.2409	-0.0084
O	-1.9477	1.5990	-0.0023
H	-2.7346	2.1703	0.0527

MP2			
	x	y	z
O	1.4033	-0.9545	-1.4249
H	0.4295	-0.9539	-1.5541
H	1.6135	-0.0158	-1.2797
O	-1.4299	-0.9593	-1.4103
H	-1.4773	-1.1860	-0.4561
H	-1.6980	-0.0256	-1.3822
O	-1.4034	-0.9533	1.4255
H	-0.4296	-0.9528	1.5547
H	-1.6135	-0.0148	1.2796
H	1.4772	-1.1859	0.4569
O	1.4298	-0.9583	1.4109
H	1.6980	-0.0247	1.3819
O	-2.0171	1.6268	0.0120
H	-2.8245	2.1595	0.0814
H	-1.3193	2.3088	-0.0079
H	1.3196	2.3088	0.0064
O	2.0173	1.6266	-0.0130
H	2.8248	2.1591	-0.0825

Isomer 6AA-2

LC-BOP			
	x	y	z
O	0.0475	1.3882	1.2535
H	-0.1551	0.4572	1.5317
H	0.9253	1.3316	0.8224
O	-0.5785	-1.2785	1.6321
H	-1.2313	-1.2592	0.8868
H	0.2021	-1.6506	1.1779
O	-1.7470	-1.0825	-0.8556
H	-1.8272	-0.0992	-0.9277
H	-0.8139	-1.2691	-1.0876
H	-1.0695	1.6723	0.0309
O	-1.7259	1.6840	-0.7277
H	-1.2696	2.1380	-1.4514
H	1.6825	-2.1739	-1.1964
O	1.1037	-1.5780	-0.6965
H	1.6123	-0.7282	-0.6317
H	2.5596	1.3083	-1.1895
O	2.4090	0.8125	-0.3531
H	3.3154	0.7076	0.0127

MP2			
	x	y	z
O	0.1043	1.4090	1.3174
H	-0.1139	0.4863	1.5734
H	0.9718	1.3254	0.8829
O	-0.6212	-1.3183	1.6741
H	-1.2660	-1.2676	0.9365
H	0.1396	-1.7092	1.2123
O	-1.8206	-1.0497	-0.8888
H	-1.8544	-0.0729	-0.9592
H	-0.8987	-1.2577	-1.1245
H	-1.0412	1.7505	0.0086
O	-1.6814	1.7897	-0.7444
H	-1.1840	2.2230	-1.4502
H	1.6294	-2.2343	-1.2502
O	1.0690	-1.6468	-0.7257
H	1.5957	-0.8192	-0.6691
H	2.6039	1.2639	-1.2033
O	2.4564	0.7744	-0.3720
H	3.3651	0.6448	-0.0424

Isomer 3I-1

LC-BOP			
	x	y	z
O	0.2794	-3.1331	0.0000
H	0.9799	-2.4569	0.0000
H	-0.5369	-2.6026	0.0000
O	-2.9154	1.3402	0.0000
H	-2.0527	1.7914	0.0000
H	-2.6697	0.3980	0.0000
H	1.6249	2.1268	0.0000
O	2.5626	1.8644	0.0000
H	2.5178	0.8919	0.0000

MP2			
	x	y	z
O	0.3208	-3.5527	0.0000
H	1.0139	-2.8759	0.0000
H	-0.4887	-3.0204	0.0000
O	-3.3003	1.5166	0.0000
H	-2.4391	1.9602	0.0000
H	-3.0513	0.5804	0.0000
H	1.9722	2.3640	0.0000
O	2.9065	2.1077	0.0000
H	2.8560	1.1402	0.0000

Isomer 3I-2

LC-BOP			
	x	y	z
O	0.0000	0.0000	1.5395
H	0.0000	0.7653	0.9312
H	0.0000	-0.7653	0.9312
O	0.0000	2.0072	-0.5972
H	-0.7667	1.7872	-1.1560
H	0.7667	1.7872	-1.1560
O	0.0000	-2.0072	-0.5972
H	0.7667	-1.7872	-1.1560
H	-0.7667	-1.7872	-1.1560

MP2			
	x	y	z
O	0.0000	0.0000	1.5314
H	0.0000	0.7576	0.9223
H	0.0000	-0.7576	0.9223
O	0.0000	2.1170	-0.5887
H	-0.7584	1.9541	-1.1692
H	0.7584	1.9541	-1.1692
O	0.0000	-2.1170	-0.5887
H	0.7584	-1.9541	-1.1692
H	-0.7584	-1.9541	-1.1692

Isomer 4I

LC-BOP			
	x	y	z
O	-1.8638	4.3591	0.0000
H	-0.9143	4.5479	0.0000
H	-1.9043	3.3730	0.0000
O	-1.8638	1.5680	0.0000
H	-1.4208	1.1477	0.7638
H	-1.4208	1.1477	-0.7638
O	1.8638	-1.5680	0.0000
H	1.4208	-1.1477	-0.7638
H	1.4208	-1.1477	0.7638
O	1.8638	-4.3591	0.0000
H	1.9043	-3.3730	0.0000
H	0.9143	-4.5479	0.0000

MP2			
	x	y	z
O	-2.1825	4.3008	0.0000
H	-1.2324	4.4724	0.0000
H	-2.2208	3.3228	0.0000
O	-2.1825	1.4321	0.0000
H	-1.7056	1.0469	0.7549
H	-1.7056	1.0469	-0.7549
O	2.1825	-1.4321	0.0000
H	1.7056	-1.0469	-0.7549
H	1.7056	-1.0469	0.7549
O	2.1825	-4.3008	0.0000
H	2.2208	-3.3228	0.0000
H	1.2324	-4.4724	0.0000

## Isomer 5I

LC-BOP			
	x	y	z
O	0.7444	-1.3007	-0.9144
H	0.6240	-0.3519	-1.1585
H	-0.1312	-1.5842	-0.5625
O	0.8218	1.4857	-0.8594
H	-0.0340	1.7276	-0.4362
H	1.7748	-0.2464	1.8469
O	2.2635	-0.1780	1.0129
H	1.7669	-0.7691	0.3799
H	1.4073	1.2207	-0.1189
O	-1.6935	1.9884	0.3271
H	-1.7758	1.6235	1.2308
H	-2.3914	1.5102	-0.1626
H	-2.5190	-1.6901	-0.3047
O	-1.7436	-1.9847	0.2111
H	-1.8632	-1.5254	1.0679

MP2			
	x	y	z
O	0.6067	-1.3952	-0.9666
H	0.5762	-0.4447	-1.1960
H	-0.2884	-1.5814	-0.6198
O	1.0098	1.4503	-0.8762
H	0.1913	1.7788	-0.4547
H	1.7341	-0.4640	1.8828
O	2.2474	-0.4337	1.0645
H	1.7031	-0.9574	0.4310
H	1.5379	1.1188	-0.1279
O	-1.4934	2.2495	0.3334
H	-1.6162	1.9469	1.2490
H	-2.2446	1.8320	-0.1201
H	-2.7421	-1.5337	-0.2552
O	-1.9713	-1.8978	0.2106
H	-2.0451	-1.4803	1.0864

Isomer 6I

LC-BOP			
	x	y	z
O	-6.6375	-0.5069	0.2722
H	-6.3306	-1.4173	0.3863
H	-5.8075	0.0120	0.1282
O	-4.3123	0.9321	-0.0466
H	-3.4873	0.5155	-0.4142
H	-4.0190	1.3751	0.7631
H	-1.3325	0.4566	-1.2410
O	-2.0232	-0.1873	-0.9786
H	-1.5518	-0.7383	-0.3174
O	2.0300	0.1823	0.9992
H	1.3429	-0.4642	1.2646
H	1.5512	0.7362	0.3457
H	4.0080	-1.3620	-0.7791
O	4.3089	-0.9295	0.0336
H	3.4879	-0.5161	0.4133
O	6.6349	0.5085	-0.2831
H	5.8052	-0.0113	-0.1403
H	6.3283	1.4205	-0.3833

MP2			
	x	y	z
O	-6.4111	-0.5980	0.4168
H	-6.0091	-1.4697	0.5136
H	-5.6424	-0.0218	0.2207
O	-4.1633	1.0474	-0.0798
H	-3.3990	0.6356	-0.5426
H	-3.7656	1.3862	0.7332
H	-1.2323	0.5223	-1.4481
O	-1.9449	-0.1286	-1.3117
H	-1.5173	-0.7542	-0.6971
O	1.9447	0.1254	1.3154
H	1.2334	-0.5269	1.4521
H	1.5153	0.7506	0.7018
H	3.7661	-1.3836	-0.7333
O	4.1637	-1.0458	0.0802
H	3.3992	-0.6357	0.5441
O	6.4096	0.6029	-0.4143
H	5.6416	0.0255	-0.2189
H	6.0066	1.4743	-0.5093



Isomer 3D

LC-BOP			
	x	y	z
O	-0.2948	1.5522	-0.0832
H	0.5503	1.0396	-0.0424
H	-0.3073	2.1106	0.7093
O	1.4916	-0.5208	-0.0833
H	1.9816	-0.7894	0.7092
H	-1.6744	-1.3214	0.7089
O	-1.1969	-1.0314	-0.0835
H	-1.1756	-0.0432	-0.0427
H	0.6251	-0.9963	-0.0425

MP2			
	x	y	z
O	-1.5736	-0.4270	-0.0835
H	-1.1415	0.4497	-0.0246
H	-2.1477	-0.4682	0.6926
O	0.4170	1.5760	-0.0835
H	0.6678	2.0938	0.6927
H	1.4797	-1.6259	0.6923
O	1.1566	-1.1489	-0.0835
H	0.1814	-1.2135	-0.0245
H	0.9605	0.7636	-0.0244

Isomer 4D

LC-BOP			
	x	y	z
O	-1.8660	-0.3597	-0.0799
H	-1.1179	-1.0209	-0.0610
H	-2.4083	-0.5511	0.7004
O	0.3597	-1.8659	-0.0800
H	1.0209	-1.1179	-0.0610
H	0.5512	-2.4085	0.7002
O	1.8660	0.3597	-0.0799
H	1.1179	1.0209	-0.0610
H	2.4083	0.5511	0.7004
H	-1.0209	1.1179	-0.0610
O	-0.3597	1.8659	-0.0800
H	-0.5512	2.4085	0.7002

MP2			
	x	y	z
O	1.3849	1.3849	-0.0815
H	0.4084	1.5135	-0.0506
H	1.7136	1.8440	0.7027
O	-1.3849	1.3849	-0.0815
H	-1.5135	0.4084	-0.0506
H	-1.8440	1.7136	0.7027
O	-1.3849	-1.3849	-0.0815
H	-0.4084	-1.5135	-0.0506
H	-1.7136	-1.8440	0.7027
H	1.5135	-0.4084	-0.0506
O	1.3849	-1.3849	-0.0815
H	1.8440	-1.7136	0.7027

Isomer 5D

LC-BOP			
	x	y	z
O	-1.8916	-1.0929	-0.3684
H	-2.6216	-1.6150	-0.0066
H	-1.0465	-1.5420	-0.0732
H	0.5365	-2.2071	1.3544
O	0.4304	-2.1510	0.3922
H	1.1320	-1.5080	0.0848
H	1.7577	0.5926	-0.2436
O	2.1479	-0.3055	-0.4550
H	3.0776	-0.2740	-0.1885
H	-0.0185	1.8763	0.0629
O	0.9717	2.0104	0.1221
H	1.1344	2.3274	1.0238
H	-1.8064	0.5588	-0.1429
O	-1.6571	1.5398	-0.0213
H	-2.1563	1.7848	0.7724

MP2			
	x	y	z
O	-1.9896	-1.0523	-0.4128
H	-2.7250	-1.5296	-0.0094
H	-1.1810	-1.5117	-0.0816
H	0.4518	-2.1815	1.4241
O	0.3479	-2.1951	0.4632
H	1.0640	-1.6020	0.1349
H	1.8511	0.4838	-0.2844
O	2.1894	-0.4121	-0.5248
H	3.1095	-0.4152	-0.2340
H	0.1112	1.9187	0.0937
O	1.0919	2.0097	0.1564
H	1.2448	2.2595	1.0775
H	-1.8245	0.6895	-0.1464
O	-1.6379	1.6501	-0.0261
H	-2.1156	1.8864	0.7798

Isomer 6D

LC-BOP			
	x	y	z
O	-0.0047	-1.3124	1.0908
H	-0.8390	-1.4799	0.5825
H	-0.0150	-0.3445	1.2477
H	-2.3982	-0.4291	-0.4769
O	-2.3184	-1.4169	-0.3814
H	-2.2455	-1.7576	-1.2857
H	0.9324	1.4953	0.3069
O	0.1018	1.5313	0.8830
H	0.2465	2.2274	1.5400
O	-2.2672	1.2819	-0.4255
H	-1.4023	1.4828	0.0154
H	-2.2625	1.7715	-1.2629
H	1.3717	-1.5084	0.2003
O	2.2310	-1.4371	-0.3193
H	2.1168	-1.9831	-1.1112
O	2.2483	1.2064	-0.5601
H	2.3392	0.2074	-0.5681
H	2.2293	1.4924	-1.4872

MP2			
	x	y	z
O	-0.0318	-1.3384	1.1559
H	-0.8568	-1.4862	0.6465
H	-0.0300	-0.3744	1.2974
H	-2.4457	-0.4505	-0.5137
O	-2.3899	-1.4263	-0.4010
H	-2.3003	-1.7618	-1.3025
H	0.9475	1.5256	0.3607
O	0.1327	1.5586	0.9283
H	0.2883	2.2766	1.5541
O	-2.2881	1.3502	-0.4571
H	-1.4292	1.5398	-0.0233
H	-2.2505	1.8311	-1.2950
H	1.3976	-1.5658	0.1696
O	2.2359	-1.5137	-0.3556
H	2.0607	-2.0320	-1.1515
O	2.3328	1.2160	-0.5750
H	2.3885	0.2301	-0.6070
H	2.2977	1.4965	-1.4997