Evaluation of B3LYP, X3LYP, and M06-Class Density Functionals for Predicting the Binding Energies of Neutral, Protonated, and Deprotonated Water Clusters

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Supporting Information Available. Cartesian coordinates and energies for optimized clusters at the B3LYP/6-311++G(2d,2p) level of theory, and Table 1S comparing the performance of the various DFT methods employing the 6-311++G** basis set. This material is available free of charge via the Internet at http://pubs.acs.org.

Table 1S. Comparison of the benchmark water binding energies (MP2/CBS+ΔCCSD(T)) to those obtained with various DFT methods using the 6-311++G** basis set (kcal/mol). The lowest mean absolute errors (MAE) for BSSE uncorrected and corrected binding energies are in bold.

complex	$-\Delta E_e$, 6-311++G** (BSSE uncorrected)					$-\Delta E^b_e$, 6-311++G** (BSSE corrected)					$-\Delta E_e$, CBS	
	B3LYP	X3LYP	M06-L	M06-2X	M06	B3LYP	X3LYP	M06-L	M06-2X	M06	MP2	CCSD(T)
$(H_2O)_2$	5.83	6.23	5.81	6.45	6.20	5.02	5.41	5.08	5.63	5.35	4.98[a]	5.01
$(H_2O)_3$cyclic	17.32	18.47	18.41	20.04	19.48	15.44	16.55	16.75	18.12	17.50	15.8[a]	15.8
$(H_2O)_4$ cyclic	30.78	32.54	31.32	33.57	32.73	27.32	29.03	28.32	30.02	29.21	27.6[a]	27.4
$(H_2O)_5$ cyclic	40.85	43.13	40.62	43.88	42.46	36.04	38.26	36.45	39.01	37.66	36.3[a]	35.9
$(H_2O)_6$ prism	49.22	52.53	53.79	58.21	56.62	43.51	46.71	48.67	52.10	50.52	45.9[a]	46.0
$(H_2O)_6$ cage	49.22	52.43	53.13	57.20	55.71	43.66	46.77	48.22	51.34	49.89	45.8[a]	45.8
$(H_2O)_6$ book	50.29	53.30	51.43	55.41	53.71	44.55	47.47	46.44	49.47	47.82	45.6[a]	45.3
$(H_2O)_6$ cyclic	50.72	53.50	50.13	54.37	52.69	44.87	47.57	45.04	48.43	46.83	44.8[a]	44.3
$(H_2O_8$ cube (D_{2d})	77.88	82.76	83.11	89.02	87.29	69.24	73.98	75.61	79.85	78.27	72.7[b]	72.6[d]
$(H_2O)_8$ cube (S_4)	77.85	82.72	83.05	88.97	87.23	69.17	73.90	75.54	79.73	78.19	72.7[b]	
$(H_2O)_{20}$ dodecahedron	216.20	229.32	217.18	235.32	224.02	191.73	204.43	196.25	209.71	199.54	200.1[c]	
$(H_2O)_{20}$ fused cubes	216.14	230.53	235.91	253.48	248.64	192.52	206.47	215.12	227.91	223.42	212.6[c]	
$(H_2O)_{20}$ face sharing	218.52	232.83	233.03	250.89	242.89	193.33	207.19	210.86	223.95	216.32	215.0[c]	
$(H_2O)_{20}$-edge-sharing	221.45	235.60	234.65	251.78	244.55	196.57	210.28	212.96	225.36	218.54	217.9[c]	
$H_3O^+(H_2O)$	36.68	37.17	35.87	37.95	36.75	35.25	35.74	34.61	36.48	35.36	34.1	33.5
$H_3O^+(H_2O)_2$	61.44	62.43	60.34	63.19	61.07	59.18	60.16	58.28	60.76	58.76	57.5	56.9
$H_3O^+(H_2O)_3$	81.89	83.36	81.10	83.91	82.26	78.70	80.14	78.11	80.52	78.94	77.0	76.5
$H_3O^+(H_2O)_6$ $(3D_1)$	124.03	127.81	125.82	131.05	127.05	117.15	120.86	119.37	123.82	119.90	118.3[e]	117.8[e]
$H_3O^+(H_2O)_6$ $(2D_s)$	122.66	125.81	122.15	127.85	124.61	116.10	119.17	116.14	121.06	117.86	115.7[e]	114.9[e]
$OH^-(H_2O)$	29.39	29.94	28.39	31.59	29.17	27.79	28.32	27.50	30.30	27.92	26.4	26.6
$OH^-(H_2O)_2$	52.80	53.86	52.17	55.88	52.79	49.74	50.77	50.32	53.34	50.45	48.0	48.4
$OH^-(H_2O)_3$	72.35	73.91	74.78	78.66	76.23	68.24	69.74	71.39	74.55	72.20	66.8	67.6
$OH^-(H_2O)_4$ (C_4)	88.19	90.75	93.74	98.38	95.54	82.23	84.63	89.31	92.85	90.19	83.6	84.8
$OH^-(H_2O)_4$ (C_s)	88.81	91.39	93.00	97.89	94.71	82.92	85.40	88.78	92.53	89.62	83.9	84.8
$OH^-(H_2O)_5$	103.67	107.02	110.90	116.07	112.94	96.17	99.65	105.56	109.33	106.47	99.3	100.7
$OH^-(H_2O)_6$	119.16	123.28	126.91	133.09	129.58	110.38	114.33	120.45	124.67	121.62	114.3	115.7
$(H_2O)_8$ cube (S_4)– $H_3O^+(H_2O)_6OH^-$	24.02	24.32	30.57	24.63	31.05						25.3[f]	28.5[f]
MAE MP2, neutral	**4.61**	10.58	9.56	17.20	14.03	6.07	2.81	**2.10**	5.92	3.03		
MAE CCSD(T), neutral	**3.77**	6.31	5.51	8.89	7.64	**1.09**	1.51	1.38	3.98	2.77		
MAE CCSD(T), protonated	**5.43**	7.41	5.15	8.88	6.44	1.62	3.31	**1.40**	4.62	2.26		
MAE CCSD(T), deprotonated	**3.69**	5.95	7.34	11.86	8.92	2.50	**1.34**	3.54	7.01	4.28		
MAE CCSD(T), total	**4.16**	6.35	5.85	9.60	7.54	**1.69**	1.88	2.10	5.14	3.15		

[a]Reference 31. [b]Reference 32. [c]Reference 33. [d]Reference 26. [e]Reference 37. [f]Reference 15.

Cartesian coordinates and absolute energies (in Hartrees) for optimized structures at the B3LYP/6-311++G(2d,2p) level of theory.

H_2O, E = -76.46204069

O	-0.11622642	0.00000000	0.00000000
H	0.46781527	0.76298442	0.00000000
H	0.46781527	-0.76298442	0.00000000

H_3O^+, E = -76.73396422

O	-0.05208978	-0.06463116	-0.02624429
H	-0.56801987	0.46326707	0.61776361
H	0.17856027	0.44866107	-0.82807856
H	0.73102210	-0.48812694	0.38240427

OH^-, E = -75.82936241

O	-0.06469672	-0.08439936	0.00000000
H	0.52204478	0.68102749	0.00000000

$(H_2O)_2$, E = -152.93199443

O	-0.19517759	-1.23632527	0.81892513
H	-0.15133027	-1.04007052	1.75750796
H	-0.05982301	-0.38771926	0.37174287
O	0.18781117	1.18784782	-0.76094679
H	-0.57698367	1.29743706	-1.33369137
H	0.93351552	1.04708639	-1.35176684

$(H_2O)_3$ cyclic, E = -229.41055335

O	1.20973995	1.08417068	-0.00835177
H	0.51894584	0.92546811	0.66012118
H	2.04930473	1.05021604	0.45625396
O	-1.12190738	0.03885630	1.17313197
H	-1.25479381	-0.55412549	1.91639572
H	-1.03910287	-0.52657796	0.38303733
O	-0.13831377	-1.05984324	-1.21406854
H	0.51651416	-0.35578191	-1.05237158
H	-0.51505372	-0.88055982	-2.07913773

$(H_2O)_4$ cyclic, E = -305.89185619

O	-1.44479529	1.26309054	-0.30928726
H	-0.48815144	1.46584980	-0.21358648
H	-1.89759930	1.79211824	0.35197611
O	-1.27860743	-1.46420408	-0.00652664
H	-1.46989581	-0.50719957	-0.12042474
H	-1.64425597	-1.90346534	-0.77822627
O	1.44669591	-1.26458475	0.29407104
H	0.49066557	-1.46778033	0.19332332
H	1.71417074	-1.64690626	1.13339179
O	1.27673598	1.46570143	0.02172280
H	1.46721628	0.50933144	0.14211008
H	1.82706905	1.75782123	-0.70900954

$(H_2O)_5$ cyclic, E = -382.3677864

O	-1.14734430	-1.54009464	1.29537659
H	-0.78673219	-2.01886875	2.04575194
H	-1.06308922	-0.58556099	1.52138946
O	0.05983627	-2.03880127	-1.10278820

H	-0.55032915	-2.56563161	-1.62382299
H	-0.38211631	-1.88817643	-0.23602884
O	0.84481463	2.15974715	-0.02128744
H	0.96914198	1.51385463	-0.75366115
H	1.72717564	2.40445965	0.26801259
O	-0.81856278	1.10756268	1.86723551
H	-0.21308019	1.51787293	1.20812153
H	-1.60058912	1.66408385	1.89211151
O	1.14699168	0.31237786	-2.00846950
H	0.74739666	0.53845503	-2.85159984
H	0.75835872	-0.55097738	-1.74275626

$(H_2O)_6$ prism, E = -458.8424124

O	1.48177134	-0.38076297	1.41635148
H	0.54980015	-0.71156814	1.53229732
H	1.98817476	-0.68311212	2.17396904
O	0.79080509	2.00892143	-0.06382021
H	1.11722198	1.46540185	0.67093808
H	1.15245966	1.55820226	-0.83911778
O	1.67906423	-0.50648504	-1.35763923
H	2.40812997	-0.93324027	-1.81457409
H	1.81915992	-0.64714738	-0.40117327
O	-1.86394951	1.26508891	-0.07019175
H	-0.96601505	1.66494403	-0.08043747
H	-2.49003750	1.98807965	-0.15585021
O	-1.15027391	-1.29159516	-1.37171807
H	-0.21826757	-1.10964569	-1.56988648
H	-1.55550097	-0.41679332	-1.27664261
O	-1.07806450	-1.13929446	1.43000657
H	-1.13819160	-1.47458503	0.51189678
H	-1.56304826	-0.30353340	1.36806551

$(H_2O)_6$ cage, E = -458.84248274

O	-2.09310434	0.94069596	1.80770489
H	-2.15498359	1.48296081	2.59705672
H	-1.56549711	1.44746440	1.15498067
O	-0.59106170	-1.33237051	1.15691929
H	-1.16566678	-0.65848264	1.56898494
H	0.30612199	-0.97536138	1.24573215
O	1.86190124	0.19642784	0.62347286
H	2.07238872	-0.18199939	-0.25894749
H	2.69639006	0.31888026	1.08258395
O	-0.80916079	-0.82290783	-1.46783498
H	-1.51233760	-1.29523596	-1.92044258
H	-0.82820366	-1.11569032	-0.51742769
O	-0.42057643	1.85377260	-0.21033026
H	-0.69502704	1.18475664	-0.85524568
H	0.43450758	1.52637657	0.11155128
O	1.92534308	-0.88903936	-1.88948836
H	2.18689389	-0.35106806	-2.64104038
H	0.94856946	-0.95214941	-1.92646790

$(H_2O)_6$ book, E = -458.84370096

O	0.11686174	1.56289206	0.84007195
H	0.96118359	1.52321678	0.32605918
H	0.26366886	2.17576794	1.56506016

O	-0.02579259	-1.38542362	0.98167723
H	-0.03593492	-0.43457327	1.16845279
H	-0.86187213	-1.54673512	0.50214739
O	-2.35142036	1.37967689	-0.46526184
H	-1.48476456	1.55359917	-0.04875198
H	-2.34487572	1.84582381	-1.30469781
O	-2.46529336	-1.40594408	-0.42198718
H	-2.53737649	-0.43337846	-0.49985796
H	-3.25791235	-1.69398336	0.03736509
O	2.42882747	1.19981882	-0.49930477
H	2.48621287	0.21350430	-0.51259049
H	2.52857012	1.48550763	-1.41062743
O	2.27866928	-1.49734629	-0.42970831
H	1.42494162	-1.58329527	0.06153585
H	2.91910755	-2.02927089	0.04847900

$(H_2O)_6$ cyclic, E = -458.84337175

O	1.86301361	1.96991034	0.11917558
H	0.90570062	2.17870841	0.02391191
H	2.15225320	2.42042653	0.91617407
O	0.77446713	-2.59832716	0.11913996
H	1.02003452	-3.07410012	0.91611433
H	1.43395833	-1.87368000	0.02386486
O	2.63746956	-0.62845078	-0.11922513
H	2.33967123	0.30500927	-0.02393778
H	3.17224773	-0.65367330	-0.91622263
O	-1.86300447	-1.96988666	-0.11909327
H	-2.15227890	-2.42043559	-0.91605989
H	-0.90569072	-2.17868952	-0.02386488
O	-0.77445715	2.59831663	-0.11919499
H	-1.02000133	3.07406568	-0.91618927
H	-1.43394791	1.87367194	-0.02392443
O	-2.63745971	0.62844613	0.11918951
H	-3.17224656	0.65370271	0.91618191
H	-2.33964636	-0.30502022	0.02394759

$(H_2O)_8$ cube (D_{2d}), E = -611.80846999

O	1.46447377	-1.46434860	1.35004576
O	-1.46415790	-1.46461808	-1.34974237
O	1.46446652	1.46450702	-1.34988383
O	-1.46454587	1.46435360	1.34959413
H	1.53493918	-1.53434199	0.36261049
H	-1.53482995	-1.53451804	-0.36231394
H	1.53458362	1.53469535	-0.36243956
H	-1.53509775	1.53422720	0.36215733
H	2.08957826	-2.08937022	1.72559373
H	-2.08916810	-2.08965237	-1.72542272
H	2.08952723	2.08963433	-1.72532983
H	-2.08962259	2.08937932	1.72517757
O	1.40552959	-1.40540868	-1.33868287
O	-1.40536187	-1.40545571	1.33896308
O	1.40515451	1.40556244	1.33886063
O	-1.40540078	1.40517218	-1.33912450
H	0.46244433	-1.55274529	-1.52669224
H	-0.46232062	-1.55289525	1.52709162
H	0.46202781	1.55269038	1.52682658

H	1.55277922	-0.46243081	-1.52724198
H	-1.55224942	0.46207479	-1.52743813
H	1.55258708	0.46260534	1.52737747
H	-1.55247443	-0.46239995	1.52726749
H	-0.46238588	1.55285371	-1.52718488

$(H_2O)_8$ cube (S_4), E = -611.80842354

O	1.99059117	-0.10840032	-1.46522917
H	1.33029282	-0.84678682	-1.53045193
H	2.70353962	-0.31034519	-2.07624010
O	-0.10840032	-1.99059117	1.46522917
H	-0.31034519	-2.70353962	2.07624010
H	-0.84678682	-1.33029282	1.53045193
O	-1.93875330	-0.02557563	1.40160929
H	-2.17246674	0.02636080	0.45836949
H	-1.39882408	0.76704418	1.56446481
O	0.02557563	-1.93875330	-1.40160929
H	-0.02636080	-2.17246674	-0.45836949
H	-0.76704418	-1.39882408	-1.56446481
O	-0.02557563	1.93875330	-1.40160929
H	0.76704418	1.39882408	-1.56446481
H	0.02636080	2.17246674	-0.45836949
O	0.10840032	1.99059117	1.46522917
H	0.84678682	1.33029282	1.53045193
H	0.31034519	2.70353962	2.07624010
O	-1.99059117	0.10840032	-1.46522917
H	-1.33029282	0.84678682	-1.53045193
H	-2.70353962	0.31034519	-2.07624010
O	1.93875330	0.02557563	1.40160929
H	2.17246674	-0.02636080	0.45836949
H	1.39882408	-0.76704418	1.56446481

$(H_2O)_{20}$ dodecahedron, E = -1529.55176042

O	1.58696351	3.63236080	0.11775373
O	3.44667146	1.54384844	0.87269541
O	-0.58457184	3.48702391	1.79682854
O	0.61922836	2.90116692	-2.47913802
O	2.55255532	0.23610998	2.97699260
O	-0.01645720	1.30115820	3.62625980
O	3.65914411	-0.19395474	-1.24960742
O	-2.66914954	2.72251843	0.37232549
O	1.92618620	0.58912792	-3.38761791
O	-1.99228450	2.48799424	-2.33780690
O	2.02533254	-2.40374883	2.17991844
O	-1.89491114	-0.67065363	3.30094865
O	2.78288317	-2.80035115	-0.30085484
O	-3.72383572	0.20710044	1.22747618
O	0.09594073	-1.29521336	-3.64738294
O	-2.39162771	-0.26092588	-3.05188194
O	-0.73830031	-2.90438756	2.55278347
O	0.58381962	-3.46308545	-1.78293818
O	-3.49375682	-1.66708622	-0.75901908
O	-1.67512828	-3.42849123	-0.03770833
H	0.82632541	3.64786792	0.74188588
H	1.97664289	4.51071857	0.13755118
H	2.84282655	2.25331551	0.60029213

H	3.54611109	0.95093408	0.09368798
H	-0.87067787	4.25554121	2.29830610
H	-1.37794736	3.19612910	1.26090514
H	0.99548546	3.13349696	-1.61284399
H	1.10728711	2.11599868	-2.79659646
H	3.21155354	0.33203219	3.66995064
H	2.90697930	0.73430476	2.18377930
H	0.87654840	0.96845879	3.42392930
H	-0.16870930	2.04606718	3.02243849
H	3.36275140	-1.07550705	-0.97033816
H	3.09475805	0.05206367	-2.00394412
H	-2.47598812	2.65912293	-0.58363388
H	-3.04055790	1.86229151	0.63614090
H	1.23456199	-0.12459722	-3.50203879
H	2.35826299	0.68250777	-4.24099768
H	-2.40913755	3.10168649	-2.94874365
H	-1.00941722	2.64902868	-2.40796539
H	1.07908127	-2.56928574	2.34971812
H	2.20962366	-1.49570883	2.49129634
H	-2.51704612	-0.34565846	2.63038648
H	-1.23891402	0.05040098	3.44185359
H	3.54183445	-3.38854400	-0.25510451
H	2.49163143	-2.64984679	0.64762531
H	-4.63262053	0.26195153	1.53576340
H	-3.70995762	-0.47451037	0.51659023
H	0.24085616	-2.03523624	-3.03612622
H	-0.80662830	-0.95424348	-3.45813434
H	-2.29647053	0.67694456	-2.81037087
H	-2.78572968	-0.70032949	-2.28107226
H	-0.92935575	-3.56142845	3.22768557
H	-1.18208145	-2.05619259	2.85407562
H	0.71243262	-4.31104216	-2.21678937
H	1.41067440	-3.27799629	-1.27917578
H	-4.25899924	-2.17609580	-1.04085577
H	-2.80105392	-2.33781051	-0.48730356
H	-0.89475237	-3.45479494	-0.61978622
H	-1.33879424	-3.28848392	0.86938827

$(H_2O)_{20}$ fused cubes, E = -1529.55263508

O	-0.00406748	1.93708469	-5.68374907
O	-2.00810203	-0.13854281	-5.73517779
O	-0.13854281	2.00810203	5.73517779
O	-1.93708469	-0.00406748	5.68374907
O	-1.97376851	0.02275421	2.80812961
O	1.97376851	-0.02275421	2.80812961
O	-1.96877420	0.02156078	-2.89395442
O	1.96877420	-0.02156078	-2.89395442
O	0.00406748	-1.93708469	-5.68374907
O	2.00810203	0.13854281	-5.73517779
O	0.13854281	-2.00810203	5.73517779
O	1.93708469	0.00406748	5.68374907
O	1.98093142	0.08917777	-0.04438928
O	0.02275421	1.97376851	-2.80812961
O	0.02156078	1.96877420	2.89395442
O	-0.02156078	-1.96877420	2.89395442
O	-0.08917777	1.98093142	0.04438928

O	0.08917777	-1.98093142	0.04438928
O	-0.02275421	-1.97376851	-2.80812961
O	-1.98093142	-0.08917777	-0.04438928
H	-0.79532299	1.38382435	-5.80381124
H	-0.05298783	2.25334714	-4.76722491
H	-1.33022757	-0.86056736	-5.78903184
H	-2.66722955	-0.32022695	-6.40994976
H	-0.32022695	2.66722955	6.40994976
H	-0.86056736	1.33022757	5.78903184
H	-1.38382435	-0.79532299	5.80381124
H	-2.25334714	-0.05298783	4.76722491
H	-2.36753392	-0.00490556	1.92171758
H	-1.35126214	0.78149133	2.79459793
H	2.36753392	0.00490556	1.92171758
H	1.35126214	-0.78149133	2.79459793
H	-2.29317207	-0.03161487	-3.80936866
H	-1.34965060	0.78293607	-2.88702651
H	1.34965060	-0.78293607	-2.88702651
H	2.29317207	0.03161487	-3.80936866
H	0.05298783	-2.25334714	-4.76722491
H	0.79532299	-1.38382435	-5.80381124
H	1.33022757	0.86056736	-5.78903184
H	2.66722955	0.32022695	-6.40994976
H	0.86056736	-1.33022757	5.78903184
H	0.32022695	-2.66722955	6.40994976
H	1.38382435	0.79532299	5.80381124
H	2.25334714	0.05298783	4.76722491
H	1.33572253	0.82795822	-0.04228444
H	2.35281077	0.07832224	-0.94113578
H	-0.00490556	2.36753392	-1.92171758
H	0.78149133	1.35126214	-2.79459793
H	0.78293607	1.34965060	2.88702651
H	-0.03161487	2.29317207	3.80936866
H	0.03161487	-2.29317207	3.80936866
H	-0.78293607	-1.34965060	2.88702651
H	-0.82795822	1.33572253	0.04228444
H	-0.07832224	2.35281077	0.94113578
H	0.07832224	-2.35281077	0.94113578
H	0.82795822	-1.33572253	0.04228444
H	0.00490556	-2.36753392	-1.92171758
H	-0.78149133	-1.35126214	-2.79459793
H	-2.35281077	-0.07832224	-0.94113578
H	-1.33572253	-0.82795822	-0.04228444

$(H_2O)_{20}$ face sharing, E = -1529.55505856

O	-0.46747713	-1.37922145	2.34108811
H	-0.51043158	-0.49635672	2.73695585
H	-1.15441451	-1.37712012	1.63766515
O	-1.18053876	-4.37506733	-2.02318313
H	-1.60063866	-5.04407786	-2.56980138
H	-1.62970246	-4.40792750	-1.13208742
O	-0.38912566	-4.30519700	2.36352663
H	-0.41227530	-3.38901572	2.67663470
H	0.49540362	-4.41525952	1.97524604
O	-2.37087055	-1.36465301	0.33034360
H	-2.76874891	-0.48263858	0.37504413

H	-1.90085679	-1.39485585	-0.53285126
O	-1.04126497	-1.54092109	-2.09126006
H	-0.07413861	-1.51143591	-1.91969289
H	-1.22112626	-2.46646758	-2.33482219
O	1.64025978	-4.31556314	-1.60449206
H	0.69072031	-4.44269614	-1.78785526
H	1.82339940	-3.39682709	-1.85625437
O	-2.33250751	-4.28268920	0.36967113
H	-1.67496004	-4.37972822	1.09317217
H	-2.66338762	-3.37663777	0.45731838
O	1.67869673	-1.43123617	-1.59094507
H	1.80420572	-1.43195906	-0.61491737
H	1.96908504	-0.55576433	-1.88849975
O	2.01773546	-1.53360265	1.14433851
H	1.13428286	-1.50035651	1.57503644
H	2.31867326	-2.45348059	1.25279900
O	2.18241888	-4.35665248	1.02977847
H	2.85539154	-5.00992522	1.23705429
H	2.00306928	-4.42630916	0.05597571
O	-0.41528352	4.42067255	2.28621876
H	-0.56802690	5.10179210	2.94653533
H	-1.11281359	4.52407611	1.60243134
O	-1.10470486	1.31242606	-2.08007605
H	-1.27383696	0.42248033	-2.42928799
H	-1.54218331	1.33381605	-1.19986087
O	-0.33438519	1.51858292	2.31438861
H	0.53476010	1.44656203	1.85926847
H	-0.37975966	2.43502288	2.62809624
O	-2.27503489	4.41331661	0.23260087
H	-1.79889520	4.38271145	-0.64415032
H	-2.98130003	5.05777033	0.13575270
O	-0.99342577	4.17958644	-2.08575796
H	-0.02992861	4.30652852	-2.00367001
H	-1.10883182	3.25804126	-2.37019922
O	1.63439522	1.43185076	-1.69322409
H	0.66376266	1.39726802	-1.84269469
H	1.89363780	2.34410252	-1.90542503
O	-2.32155197	1.51493819	0.39153141
H	-2.62505267	2.43653071	0.38643610
H	-1.61930474	1.48895374	1.07981050
O	1.81449810	4.28553183	-1.65133122
H	2.40204754	4.92645154	-2.05990913
H	1.98089406	4.32073207	-0.67351068
O	2.16925159	4.16843895	1.01108429
H	2.38097649	3.23753339	1.19195985
H	1.33724344	4.33725595	1.48523272
O	2.09576742	1.30602142	1.02133154
H	2.41828310	0.41327445	1.22708069
H	1.93531899	1.30668468	0.05064121

$(H_2O)_{20}$ edge-sharing, E = -1529.55949201

O	1.44499155	-2.31823325	1.38587940
H	0.95238179	-1.48325716	1.52953184
H	2.36949785	-2.11294656	1.61232771
O	1.41990983	-2.46160643	-1.40004921
H	1.44127578	-2.49356944	-0.41874697

H	0.77720259	-3.14584346	-1.65690975
O	0.00687792	0.01822269	1.40337794
H	0.38937322	0.90756653	1.56320255
H	-0.96090951	0.05133024	1.56164437
O	-2.73668764	-0.07070426	1.35950427
H	-2.78815399	-0.09360762	0.37856555
H	-2.97855778	-0.97075328	1.64205712
O	4.04550515	1.46379507	-1.46060607
H	4.78814812	1.76498858	-1.99063136
H	4.03336485	0.47419132	-1.53068744
O	-1.00076295	4.22596381	1.49894861
H	-1.15214824	5.00926484	2.03422392
H	-1.83279877	3.68661619	1.54229494
O	-3.22719970	2.75022575	-1.54466338
H	-3.84121665	3.21273809	-2.12112599
H	-2.37029657	3.24959637	-1.58820863
O	0.06158681	-0.05986372	-1.34981672
H	0.54045034	-0.88821053	-1.56823748
H	0.05254324	-0.05072815	-0.36544420
O	1.35061742	2.36344066	-1.42488798
H	2.29438361	2.21904174	-1.61586638
H	0.92560265	1.48879746	-1.55887205
O	4.07975243	-1.26958675	1.51083644
H	4.81847125	-1.52971676	2.06741761
H	4.00886149	-0.28230534	1.57994294
O	-0.91180083	4.11568732	-1.39616566
H	-0.86991638	4.32997169	-0.44869382
H	-0.08970644	3.63155343	-1.58531208
O	-2.68497880	-0.04147855	-1.42677802
H	-2.98310293	0.85700376	-1.65555563
H	-1.71319303	-0.04280549	-1.56287159
O	-3.12950848	-2.86554855	-1.32927553
H	-3.11404942	-1.91813988	-1.54743550
H	-3.30320066	-2.90158324	-0.37303026
O	1.22447490	2.47901375	1.36019988
H	0.58128415	3.16680100	1.60827679
H	1.27288390	2.51710355	0.37996280
O	-0.81277222	-4.23212894	-1.52327044
H	-0.94661993	-5.02036497	-2.05599138
H	-1.66332823	-3.72223960	-1.55370713
O	-3.24984545	2.75546188	1.34864533
H	-3.19242208	1.81302377	1.57970229
H	-3.43471886	2.76769634	0.39351954
O	4.03742468	-1.23035330	-1.38058044
H	3.23356683	-1.71850679	-1.62341979
H	4.16044458	-1.40022237	-0.43063219
O	-3.09397429	-2.88411501	1.56681667
H	-2.21797775	-3.35005851	1.59505978
H	-3.68978353	-3.38577968	2.12925734
O	-0.73321285	-4.16493199	1.37043860
H	0.07096396	-3.65283678	1.56257730
H	-0.68794871	-4.35877693	0.41835805
O	3.90984823	1.41747180	1.42638398
H	3.06608912	1.85057710	1.63743322
H	4.05546347	1.59384347	0.48081512

$H_3O^+(H_2O)$, E = -153.25223859

O	-1.19970341	0.02896035	0.05616498
H	-1.63130086	-0.73358971	0.46853942
H	-1.69416532	0.29596499	-0.73175069
O	1.19975299	-0.02907987	0.05618059
H	0.00015426	-0.00017724	-0.00334555
H	1.69414757	-0.29563008	-0.73193877
H	1.63109466	0.73354588	0.46869206

$H_3O^+(H_2O)_2$, E = -229.75148804

O	1.21794628	1.42235117	1.06614926
H	1.84588013	1.17199915	1.75269642
H	1.24261957	2.38177884	0.97538881
O	-0.35779393	-1.50099719	-1.50363771
H	-0.08516774	-2.42003034	-1.40688288
H	-0.80291090	-1.41014320	-2.35390072
O	-0.79381380	0.15172990	0.31437223
H	0.04813046	0.65227631	0.66791581
H	-0.61261875	-0.57405290	-0.41003241
H	-1.36300907	-0.16788569	1.02682223

$H_3O^+(H_2O)_3$, E = -306.24434718

O	0.26921644	1.30291506	-2.11024129
H	0.76644777	2.10955919	-2.28439924
H	0.21118957	0.82101119	-2.94200762
O	-1.94075973	0.46073695	1.49923095
H	-2.82059816	0.43908161	1.10827226
H	-1.99782366	1.00035579	2.29534610
O	1.41459001	-2.01820390	0.39568177
H	2.25774298	-2.10718183	0.85330636
H	0.96914481	-2.86997483	0.45482577
O	0.28851919	0.28157953	0.24281549
H	0.69204871	-0.64507504	0.31535426
H	0.28847985	0.64236428	-0.70408903
H	-0.61337883	0.35939372	0.69813168

$H_3O^+(H_2O)_6$ (3D), E = -535.69357394

O	-0.80118137	1.05999292	2.17965287
H	-0.95013195	0.10138390	2.07909355
H	-1.48521330	1.41876151	2.75268789
O	1.65121824	-1.66013591	-0.04930397
H	2.33014344	-2.34317521	-0.02169340
H	1.08546669	-1.79304956	0.73146386
O	-0.78541855	-1.66014393	1.45299253
H	-1.14958875	-2.34336534	2.02643091
H	-1.17873463	-1.79180047	0.57247691
O	2.28801453	1.06074047	-0.39395678
H	2.27549536	0.10179984	-0.21645913
H	3.12624009	1.41902274	-0.08737438
O	-1.48536047	1.06356313	-1.78260477
H	-1.63895747	1.42341124	-2.66118142
H	-1.32529748	0.10478291	-1.86224137
O	-0.86816615	-1.65792403	-1.40835468
H	-1.18386316	-2.34001429	-2.01112825
H	0.09089439	-1.79098215	-1.30919034
O	0.00089676	2.12091950	0.00192714

H	-0.36095656	1.76527163	0.88658552
H	0.94797818	1.76554975	-0.12756574
H	-0.58475959	1.76665971	-0.75407322

$H_3O^+(H_2O)_6$ (2D), E = -535.69079083

O	1.84293295	-1.54018495	0.95993339
H	1.26501702	-2.28824813	0.73963702
O	1.07944259	0.97486317	0.52691058
H	1.40182348	0.05362784	0.70173094
O	-0.00068094	-3.56511078	-0.00029857
O	-1.84389363	-1.53946520	-0.95926744
H	-1.26604837	-2.28761124	-0.73895382
O	-1.07991771	0.97487012	-0.52771082
H	-1.40213940	0.05336882	-0.70223517
H	-0.00120935	0.98023631	-0.00092013
H	-2.36721653	-1.79489071	-1.72407811
H	2.36590939	-1.79552669	1.72500114
H	-1.76978553	1.47872904	-0.03394626
H	1.76954694	1.47871056	0.03371012
O	-2.99096672	2.39015074	0.72349115
O	2.99128214	2.39124536	-0.72356575
H	0.43232731	-4.14750591	-0.63559166
H	-0.43339606	-4.14818079	0.63457644
H	-3.17933273	2.44908156	1.66468262
H	-3.43464842	3.13409395	0.30510948
H	3.43621708	3.13401374	-0.30444609
H	3.18187433	2.44935560	-1.66435011

$OH^-(H_2O)$, E = -152.33763572

H	-0.09745925	-0.08920841	0.02051282
H	1.52120235	0.49391655	0.65998459
O	-1.22690889	-0.08001380	0.06874490
O	1.24014230	-0.06500659	-0.06970788
H	-1.46733144	0.51833439	-0.64238336

$OH^-(H_2O)_2$, E = -228.83488584

H	-1.45861503	0.03175994	0.00399257
O	-2.42513990	-0.30263609	-0.15411643
H	-0.01886411	1.45888413	0.37966318
H	-2.44767086	-0.44264423	-1.10296193
O	-0.00681470	0.52994938	0.13695644
H	1.45747805	0.06516752	0.02095134
O	2.43272218	-0.28060707	0.00303681
H	2.46333355	-0.86586133	0.76261458

$OH^-(H_2O)_3$, E = -305.32686092

H	1.83974625	-1.89097449	-0.68847645
O	2.20526675	-1.15039340	-0.19973206
H	1.37883398	-0.68647662	0.16059481
H	-0.01858462	-0.01517331	1.61882376
H	-0.09831507	1.53565056	0.16267264
H	0.73651358	2.53864525	-0.66255118
O	-0.09986133	2.48428414	-0.19515244
O	-0.00736471	-0.00655837	0.65854277
H	-1.28515537	-0.85405435	0.12786929
O	-2.09720816	-1.32791425	-0.25157258

H	-2.55034426	-0.62890013	-0.72800614

$OH^-(H_2O)_4$ (C_4), E = -381.81239950

H	-0.02662582	1.58204086	0.31510162
H	1.58174647	0.02700289	0.31517494
H	0.02695733	-1.58197798	0.31516060
H	-1.58173802	-0.02714841	0.31501718
O	-0.00020517	0.00004775	0.99077486
H	-0.00036946	0.00028624	1.95057893
O	0.03124140	2.41837000	-0.22199349
O	2.41802173	-0.03067005	-0.22203363
O	-0.03062031	-2.41813440	-0.22222726
O	-2.41821737	0.03021965	-0.22197359
H	0.84255058	2.27794451	-0.71875169
H	2.27728738	-0.84149400	-0.71949611
H	-0.84206619	-2.27787670	-0.71881140
H	-2.27820217	0.84135065	-0.71912779

$OH^-(H_2O)_4$ (C_s), E = -381.81370415

O	2.06634339	-0.01342915	-0.80001802
O	-0.00046967	-1.50145009	-0.38233810
H	0.76361835	1.41965001	-0.44311651
H	2.47352865	-0.04549555	0.06968647
O	0.00006586	1.94313869	-0.13662768
H	-0.76326695	1.41985366	-0.44402152
O	-2.06600911	-0.01255917	-0.80298766
H	-2.47455023	-0.04459268	0.06607793
H	-1.28977059	-0.67247945	-0.71558848
O	-0.00100694	-0.28263837	2.07037986
H	-0.00106082	0.58952941	1.65213634
H	-0.00091823	-0.88502749	1.28625055
H	1.28958358	-0.67288266	-0.71361000
H	-0.00014896	-2.42587851	-0.63556515

$OH^-(H_2O)_5$, E = -458.29826071

H	1.48556600	-0.41508216	0.00040350
H	0.05383348	-2.03002855	-0.02454962
H	-1.31319848	-0.40273695	0.38988380
O	0.07828075	1.94808296	-1.10108314
O	1.92130900	-0.27034141	-0.88442481
O	-0.17123471	-2.54032960	-0.84159252
O	-1.97740395	-0.08690311	-0.25978413
H	0.76000710	1.25553516	-1.19590054
H	1.54577601	-0.99913254	-1.39362189
H	-0.96441287	-2.07559788	-1.13449086
H	-1.48753474	0.60681031	-0.73064846
O	0.31729375	-0.74531936	1.20923392
H	0.53921189	-1.21590220	2.01570729
O	-0.12812280	1.79220440	1.80336271
H	0.06880605	2.10721499	-0.14001378
H	-1.08931237	1.79570664	1.81746330
H	0.09404032	0.81880058	1.64556779

$OH^-(H_2O)_6$, E = -534.78377972

O	0.16980212	-1.79664123	-1.68297955
H	0.29357596	-1.47334608	-2.57876751

H	-0.54755437	-1.19766777	-1.29401562
O	-0.87992216	-1.85610659	1.45648583
H	-0.38596820	-2.50881022	0.95203817
H	-1.23068340	-1.23735429	0.74837480
O	-0.99682541	2.01664108	0.98666927
H	-1.34381128	1.20774825	0.52810911
H	-0.50148980	2.43226864	0.26805164
O	0.97344426	0.25975532	2.11961883
H	0.41116716	-0.53460951	2.05277015
H	0.36209232	0.97620727	1.85911652
O	0.20445981	1.69095637	-1.75162938
H	1.01036323	1.27070483	-1.40505195
H	-0.49849616	1.07031868	-1.46530789
O	2.20917947	-0.06680663	-0.46942710
H	1.89624990	0.06058189	0.44807405
H	1.63078566	-0.76505610	-0.82322796
O	-1.54662312	-0.19107239	-0.51706788
H	-2.45363503	-0.28732852	-0.81678624

$H_3O^+(H_2O)_6OH^-$, E = -611.76950580

O	-1.73898816	1.35311679	-1.42334173
O	-1.19645743	1.47504815	1.04143185
O	1.27996855	1.95175620	1.19700734
O	-1.52571786	-0.85810836	1.95365696
O	0.56828278	-2.23924474	1.31613048
O	1.18924456	-1.46633615	-1.03507935
O	2.42341931	0.75378752	-0.79198236
O	-0.99326476	-0.97847211	-2.26385676
H	-1.49047217	0.43987578	-1.78364913
H	-2.61871350	1.56376573	-1.74427174
H	-1.58888543	-1.70229050	-2.05493128
H	-1.75644644	-0.99781285	2.87481689
H	-0.70963529	-1.42278684	1.75178665
H	-0.10088604	-1.20919629	-1.80187077
H	-1.46343616	1.43566522	0.04570105
H	-1.33707171	0.54143345	1.45728181
H	2.34899460	1.19875799	-1.63979671
H	0.84504439	-1.96850293	0.36055437
H	-0.19541233	1.71640627	1.10470699
H	1.34328331	-2.08999908	1.86333002
H	1.71980369	-2.12043671	-1.49679578
H	1.96336661	-0.16061423	-0.91541360
H	1.60305122	2.85158145	1.28197965
H	1.76041040	1.52491354	0.41432719