Supporting Information for:

CCSD(T) Complete Basis Set Limit Relative Energies for Low-Lying Water Hexamer Structures

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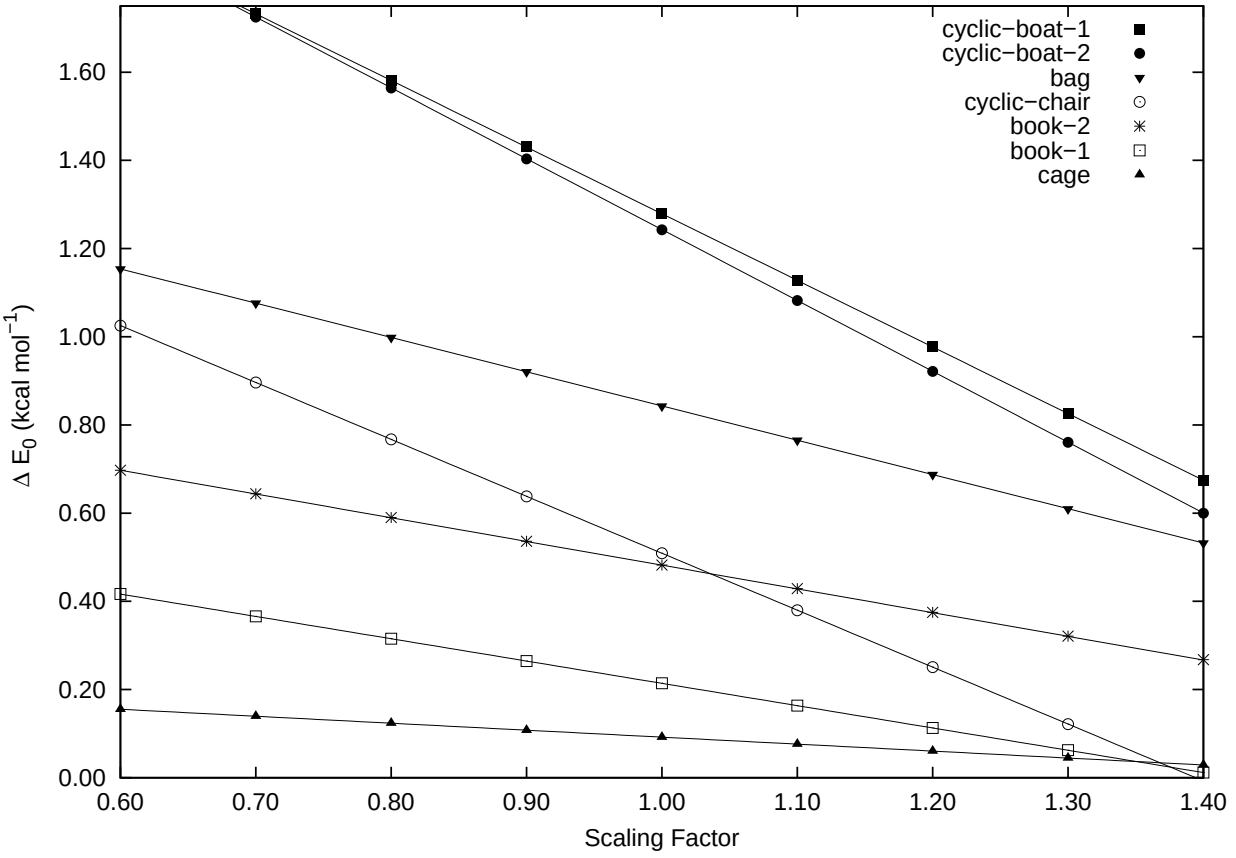

Figure S1: Effect of scaling factors for MP2/haTZ harmonic vibrational frequencies on the relative energies of the water hexamer isomers. All relative energies increase with respect to the prism for scaling factors less than 1. Only with a scaling factor larger than 1.39 does another structure (cyclic-chair) become more stable than the prism. The relative stability cyclic-chair and book-2 structures inverts at a value of 1.04.

Table S1: Cartesian coordinates (in Å) of the MP2/haTZ optimized book-2 water hexamer

O	2.4032053362	1.3270659373	−0.4231241288
O	2.0682038153	−1.4035016261	−0.6521599818
O	−0.1643579518	−1.5595899492	1.0026524632
O	−2.3181617136	−1.1551868762	−0.5453543706
O	−2.0641196909	1.5200844007	−0.4985515003
O	0.0821770896	1.3511908817	1.1316718732
H	3.2824705291	1.5275529981	−0.0914460180
H	2.4010102640	0.3610726372	−0.5799178960
H	−1.8529134608	2.0431806726	−1.2764401766
H	−1.2682598521	1.5827252635	0.0837206366
H	0.0581169390	0.4025609972	1.3290652908
H	0.9279954625	1.4655873732	0.6566010635
H	−3.2290937865	−1.3858096501	−0.3443798320
H	−2.3092654357	−0.1705337451	−0.6170936879
H	1.8644694205	−1.8074627322	−1.5001929598
H	1.2809613207	−1.5678898278	−0.0972909741
H	−1.0129241853	−1.5230335341	0.4985855505
H	−0.2826661794	−2.2325735230	1.6787417375

Table S2: Cartesian coordinates (in Å) of the MP2/haTZ optimized cyclic-boat-2 water hexamer.

O	−1.3867441060	−2.1368119633	−0.3756225893
H	−0.4863499895	−2.1789552080	0.0153601788
H	−1.7732871574	−3.0024272951	−0.2236401630
O	−1.1321912700	2.2124077551	0.6482442718
H	−1.2992914850	2.2386321163	1.5937908372
H	−1.7207166238	1.5020492418	0.3064145725
O	−2.7262340741	0.2257234831	−0.2955282394
H	−2.2736190362	−0.6453266868	−0.3243346978
H	−3.0650993684	0.3594784483	−1.1846860058
O	1.3867422071	2.1368108756	−0.3756286314
H	1.7732934243	3.0024220545	−0.2236436139
H	0.4863369901	2.1789706344	0.0153257188
O	1.1321572604	−2.2123721845	0.6483234883
H	1.2992212246	−2.2385310875	1.5938783399
H	1.7206916453	−1.5020336282	0.3064678630
O	2.7262138391	−0.2257363978	−0.2955339749
H	3.0650364573	−0.3595167569	−1.1847041922
H	2.2736040400	0.6453160882	−0.3243422191

Table S3: Cartesian coordinates (in Å) of the MP2/haTZ optimized water monomer.

O	−1.3867441060	−2.1368119633	−0.3756225893
H	−0.4863499895	−2.1789552080	0.0153601788
H	−1.7732871574	−3.0024272951	−0.2236401630

Table S4: Cartesian coordinates (in Å) of the MP2/haTZ optimized cyclic-boat-1 water hexamer.[a]

O	−1.726744	−1.949373	−0.286967
O	−2.590266	0.622599	−0.361636
O	−0.794610	2.415041	0.610617
O	2.590163	−0.622736	−0.361901
O	0.794557	−2.414847	0.610989
O	1.726922	1.949301	−0.286706
H	−1.948340	1.276484	−0.005295
H	0.134410	2.266967	0.327985
H	2.049592	1.021469	−0.329144
H	−0.134451	−2.266742	0.328301
H	−2.049611	−1.021593	−0.329106
H	0.754378	−2.535812	1.562971
H	−0.754427	2.536367	1.562552
H	2.876251	−0.991167	−1.201866
H	−2.876587	0.990982	−1.201544
H	1.948264	−1.276555	−0.005381
H	2.495054	2.475673	−0.052229
H	−2.494719	−2.475947	−0.052417

[a] Private communication from the authors of Reference 19 (the MP2/haTZ boat structure in the Supporting Information for that reference is actually the book structure)

Table S5: Harmonic ZPVE corrections (δ_{ZPVE} in kcal mol^{-1}) computed with various methods and basis sets.

Method	MP2	BLYP	B3LYP	BLYP	B3LYP	PBE
Basis	haTZ	6-31+G(d,p)	6-31+G$(d,2p)$	MG3S	MG3S	MG3S
prism	+0.00	+0.00	+0.00	+0.00	+0.00	+0.00
cage	−0.16	−0.13	−0.14	−0.02	−0.16	−0.08
bag	−0.78	−0.67	−0.62	−0.60	−0.69	−0.60
cyclic-ring	−1.29	−1.11	−1.04	−0.92	−1.14	−0.93
book-1	−0.51	−0.40	−0.38	−0.32	−0.45	−0.34
book-2	−0.54	−0.37	−0.30	−0.33	−0.47	−0.32
cyclic-boat-1	−1.51	−1.27	−1.29	−1.10	−1.28	−1.10
cyclic-boat-2	−1.61	−1.36	−1.41	−1.18	−1.46	−1.11
6 monomers	−13.71	−14.21	−14.07	−13.35	−13.82	−13.42

Table S6: Total electronic energies and sum of electronic and zero-point vibrational energies (E_e and $E_{+\mathrm{ZPVE}}$, respectively, in E_h) from the MP2/haTZ computations as well as the corresponding relative energies (ΔE_e and $\Delta E_{+\mathrm{ZPVE}}$ in kcal mol^{-1}).

Structure	$E_e^{\mathrm{MP2/haTZ}}$	$\Delta E_e^{\mathrm{MP2/haTZ}}$	$E_{+\mathrm{ZPVE}}^{\mathrm{MP2/haTZ}}$	$\Delta E_{+\mathrm{ZPVE}}^{\mathrm{MP2/haTZ}}$	δ_{ZPVE}
prism	−458.042669	+0.00	−457.892242	+0.00	+0.00
cage	−458.042650	−0.15	−457.892475	+0.01	−0.16
bag	−458.040790	+0.40	−457.891601	+1.18	−0.78
cyclic-ring	−458.040683	−0.05	−457.892314	+1.25	−1.29
book-1	−458.042171	−0.19	−457.892550	+0.31	−0.51
book-2	−458.041693	+0.07	−457.892123	+0.61	−0.54
cyclic-boat-1	−458.039088	+0.74	−457.891068	+2.25	−1.51
6yclic-boat-2	−458.038958	+0.72	−457.891092	+2.33	−1.61
6 monomers	−457.968327	+32.94	−457.839750	+46.65	−13.71