Supporting Information for: "Achieving the CCSD(T) Basis-Set Limit in Sizable Molecular Clusters: Counterpoise Corrections for the Many-Body Expansion"

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Included in this document are figures analogous to Fig. 3 in the paper, but for each of the eight isomers of $(H_2O)_6$ that are considered in Ref. 1. These are Figs. S1–S8 below. In Table S1, we provide the numerical data used to produce Fig. 2 in the paper.

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[1] D. M. Bates and G. S. Tschumper, J. Phys. Chem. A **113**, 3555 (2009).

Method	mean unsigned error / kcal mol^{-1}	
	$Gly(H_2O)_{10}$	$F^-(H_2O)_{10}$
MBCP(2)	2.41	14.41
VMFC(3)	0.47	3.55
MBCP(3)	0.76	1.94
EE-MBCP(2)	0.64	2.00
EE-VMFC(3)	1.46	2.32
EE-MBCP(3)	0.23	0.73

TABLE S1: Numerical data for Fig. 2 in the paper.

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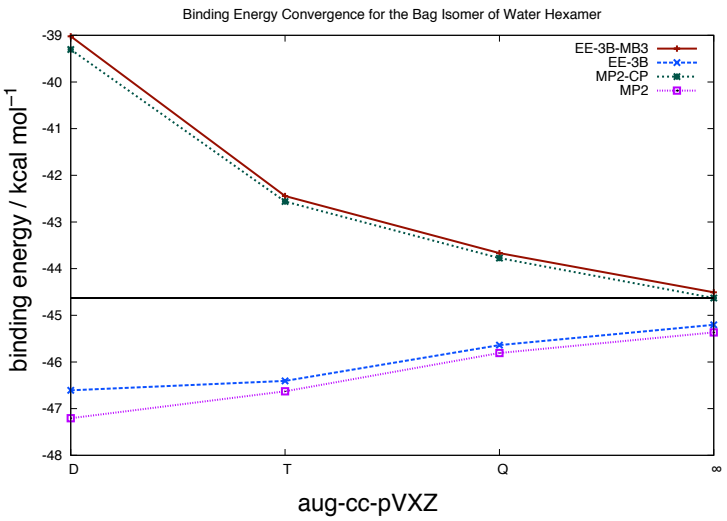

FIG. S1: Convergence to the CBS limit for the "bag" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.

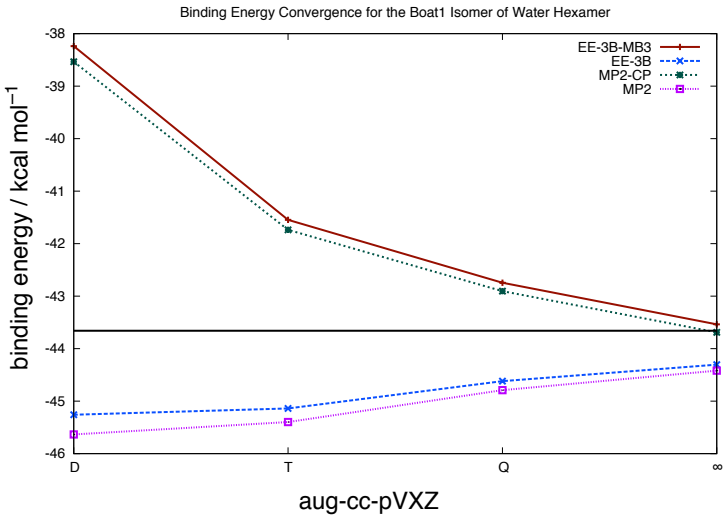

FIG. S2: Convergence to the CBS limit for the "boat1" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.

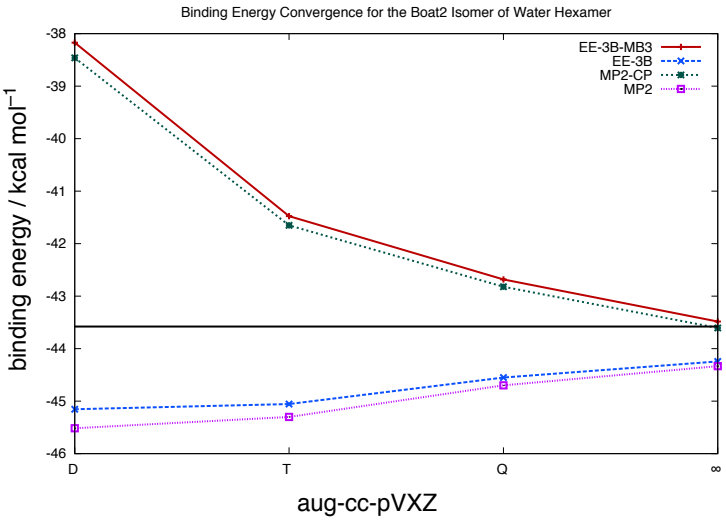

FIG. S3: Convergence to the CBS limit for the "boat2" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.

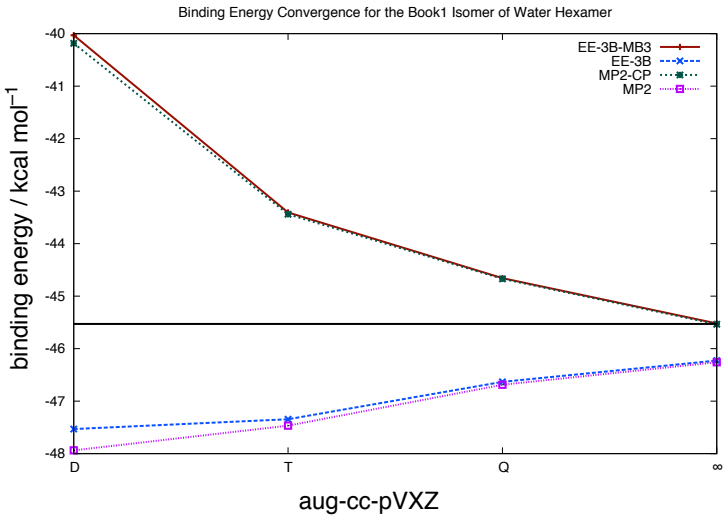

FIG. S4: Convergence to the CBS limit for the "book1" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.

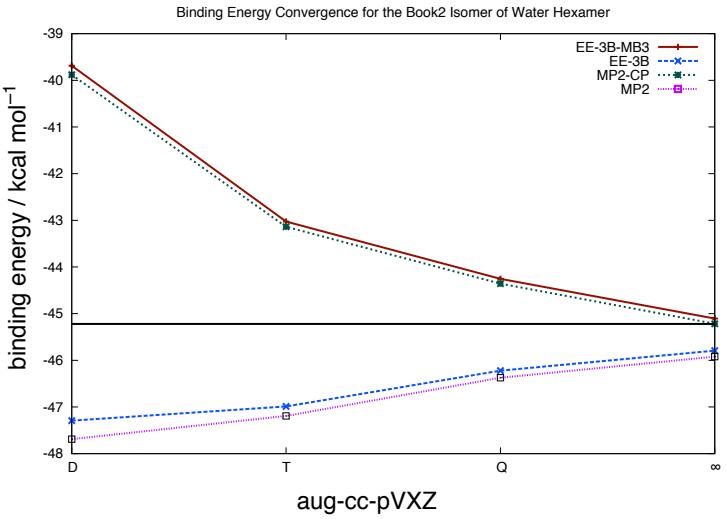

FIG. S5: Convergence to the CBS limit for the "book2" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.

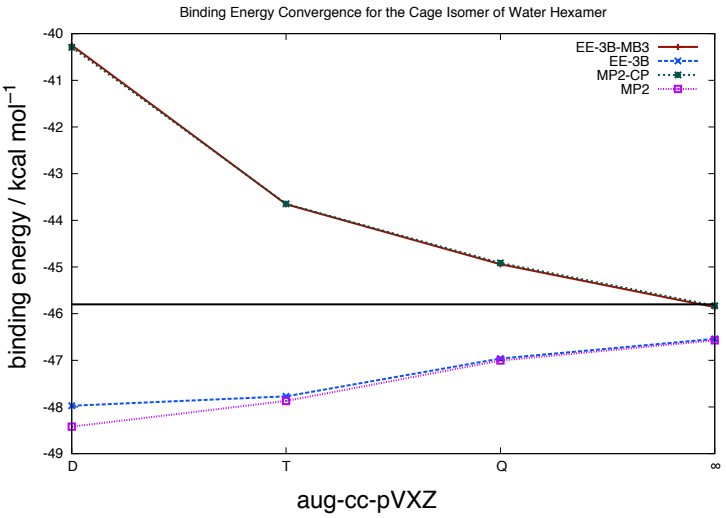

FIG. S6: Convergence to the CBS limit for the "cage" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.

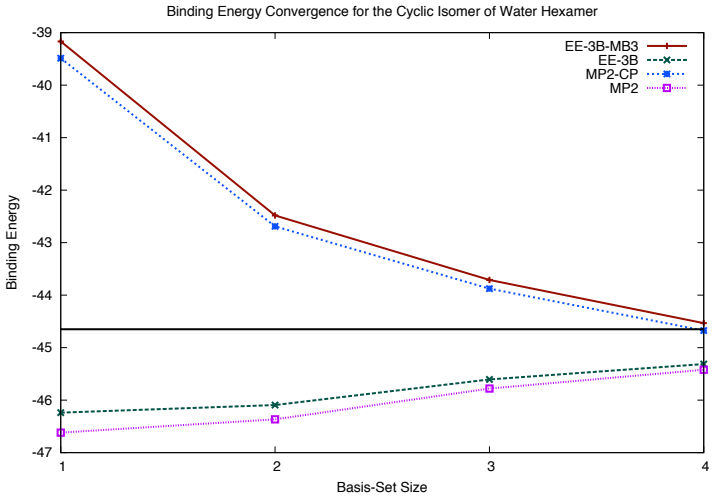

FIG. S7: Convergence to the CBS limit for the "cyclic" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.

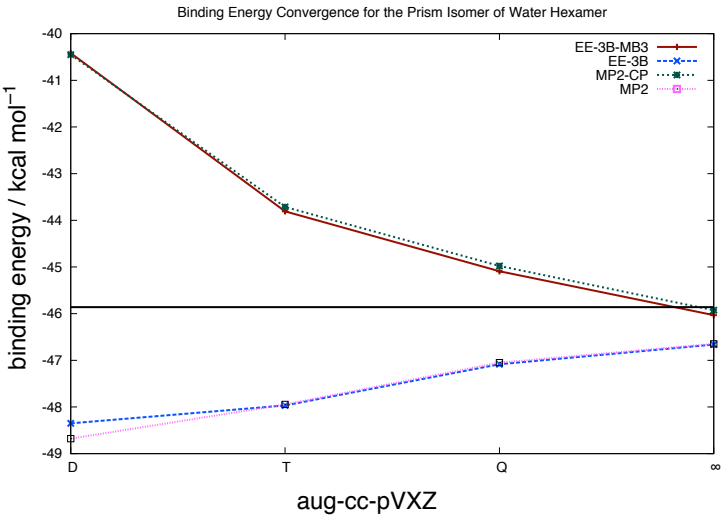

FIG. S8: Convergence to the CBS limit for the "prism" isomer[1] of $(H_2O)_6$. CP-MP2 denotes traditional counterpoise-corrected MP2, EE-MBCP(3) is a three-body approximation to the binding energy defined by Eq. (3) from the main text and EE-MB(3) represents a three-body approximation to the cluster energy, following which the binding energy is computed with no attempt at counterpoise correction. The horizontal line is the benchmark MP2/CBS value from Ref. 1.