SUPPORTING INFORMATION

# An Extensive Assessment of the Performance of Pairwise and Many-body Interaction Potentials in reproducing *ab initio* Benchmark Binding Energies for Water Clusters *n* = 2 – 25

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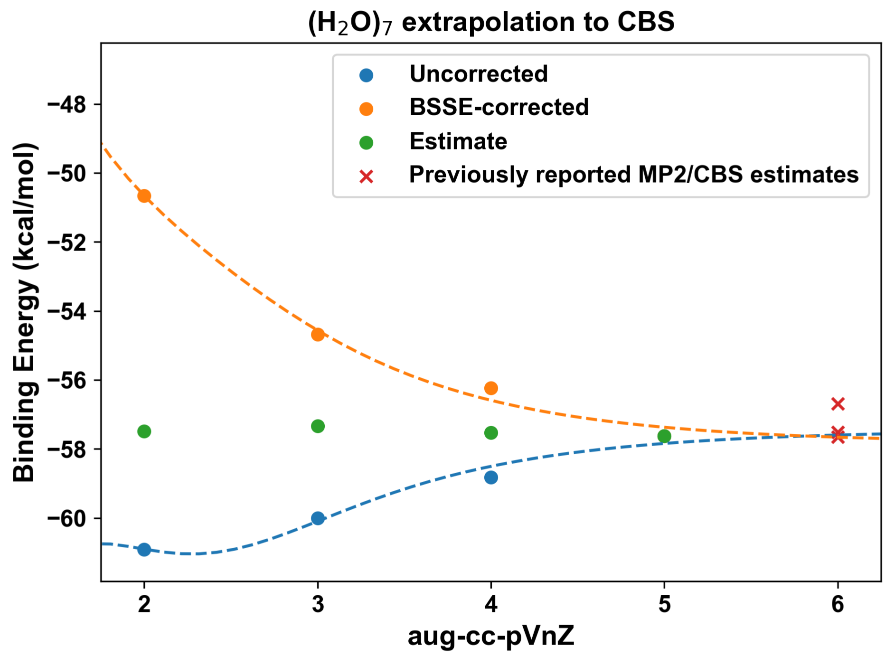
**Figure SF1**. Extrapolation to the complete basis set (CBS) limit for the water cluster isomers of *n* = 7, 10 structures used in MBE analysis.[1] The MP2/CBS values for this isomer and the minimum energy structure (slightly different that the one used in the MBE analysis) are indicated with red ×'s. The "estimate" is produced by averaging the BSSE-corrected and -uncorrected values for each basis set (for MP2/aVDZ: $\frac{2}{3}D_e + \frac{1}{3}D_e^{CP}$).[2]



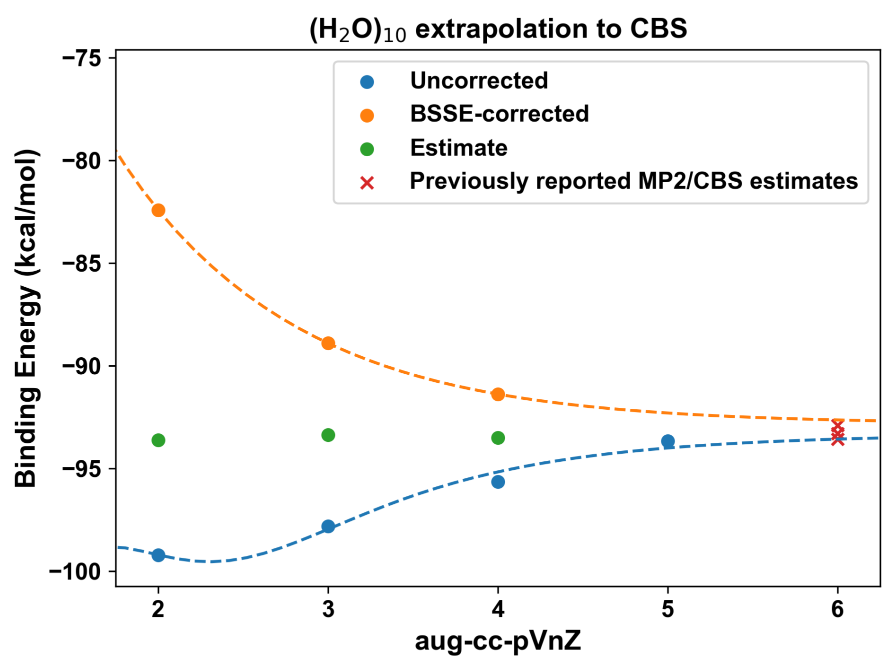



**Figure SF2.** A comparison of the pairwise additive potential performance relative to reference binding energies ($D_e$). The top panel shows the energetic difference (kcal/mol) with respect to the reference values and the bottom panel shows the percent deviation relative to the $D_e$ reference value for the lowest energy structures for water cluster sizes $n = 2 - 11, 16, 17, 20, 25$. The points for which the potential optimizes to a different structure (NSP in Table 2) have been excluded. The shaded gray regions represent the uncertainty in the CBS estimate of the $D_e$ calculation.

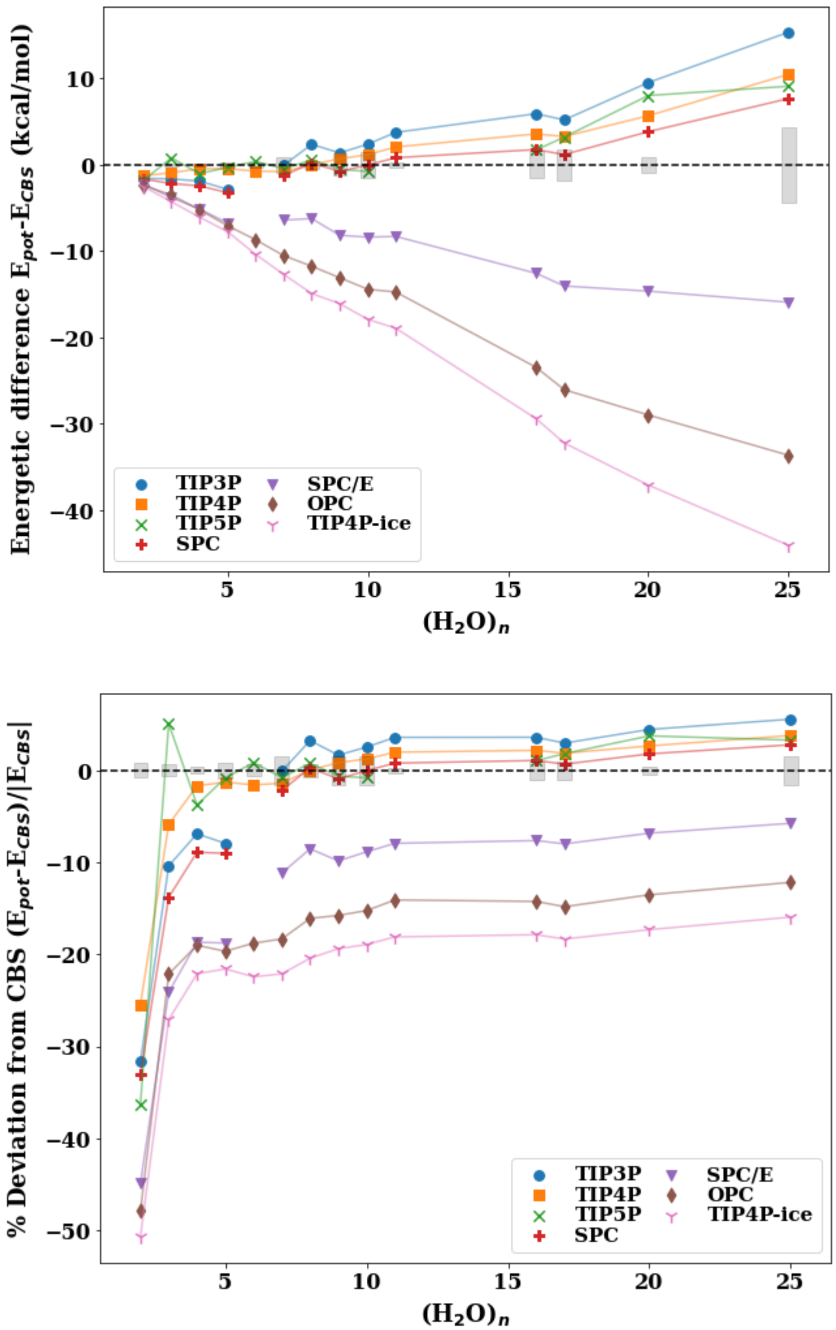


**Figure SF3.** Percent deviation with respect to the $D_e$ reference value for isomers of $n$ = 6, 8, 16, 20 with the pairwise additive potentials. The points for which the potential optimizes to a different structure (NSP in Table 2) have been excluded. The shaded gray regions represent the uncertainty in the CBS estimate of the $D_e$ calculation.

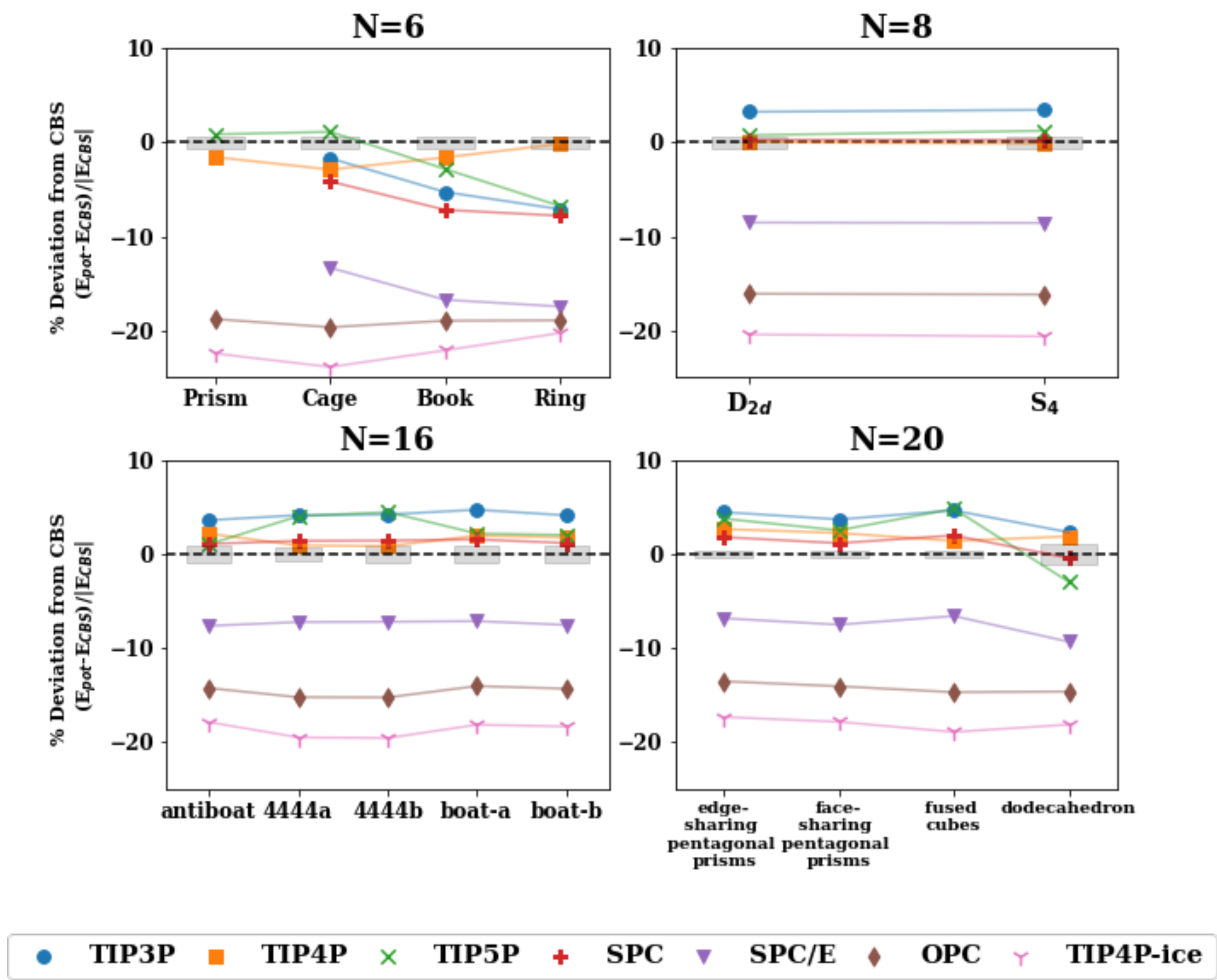
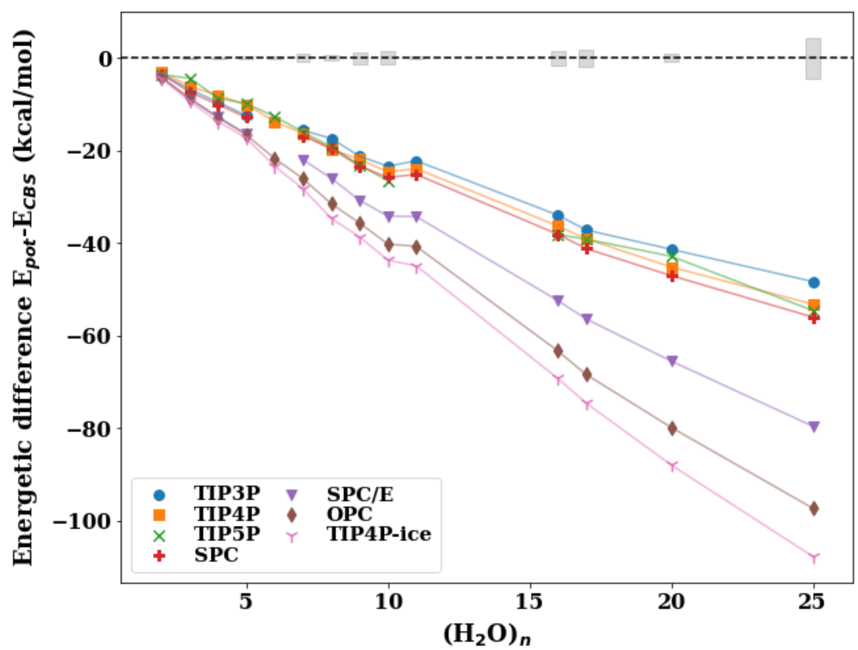


**Figure SF4.** A comparison of the pairwise additive potential performance relative to reference binding energies ($D_0$). The top panel shows the energetic difference (kcal/mol) with respect to the reference values and the bottom panel shows the percent deviation relative to the $D_0$ reference value for the lowest energy structures for water cluster sizes $n = 2 – 11, 16, 17, 20, 25$. The points for which the potential optimizes to a different structure (NSP in Table 2) have been excluded. The shaded gray regions represent the uncertainty in the CBS estimate of the $D_e$ calculation.



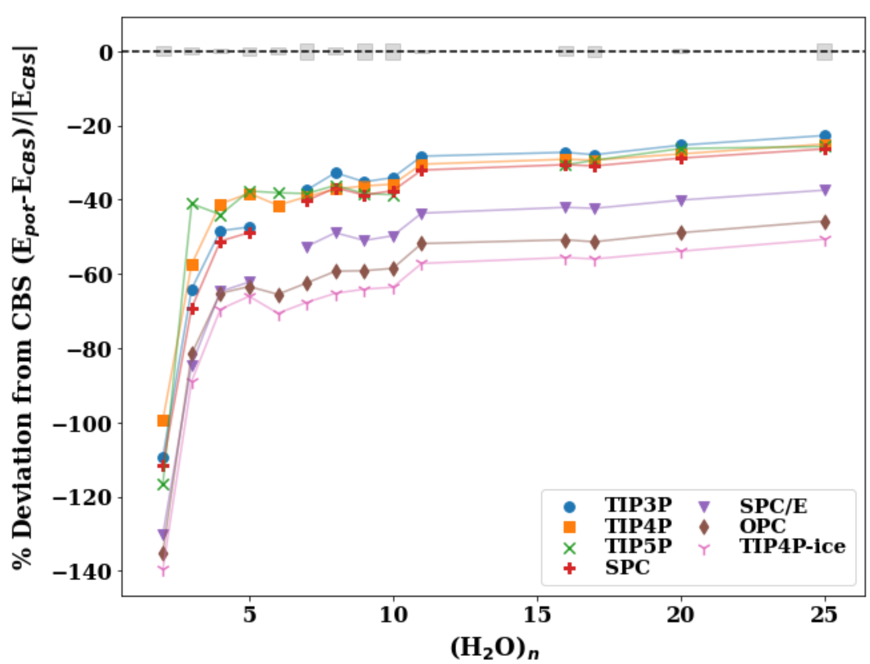



**Figure SF5.** Percent deviation with respect to the $D_0$ reference value for isomers of *n* = 6, 8, 16, 20 with the pairwise additive potentials. The points for which the potential optimizes to a different structure (NSP in Table 2) have been excluded. The shaded gray regions represent the uncertainty in the CBS estimate of the $D_e$ calculation.

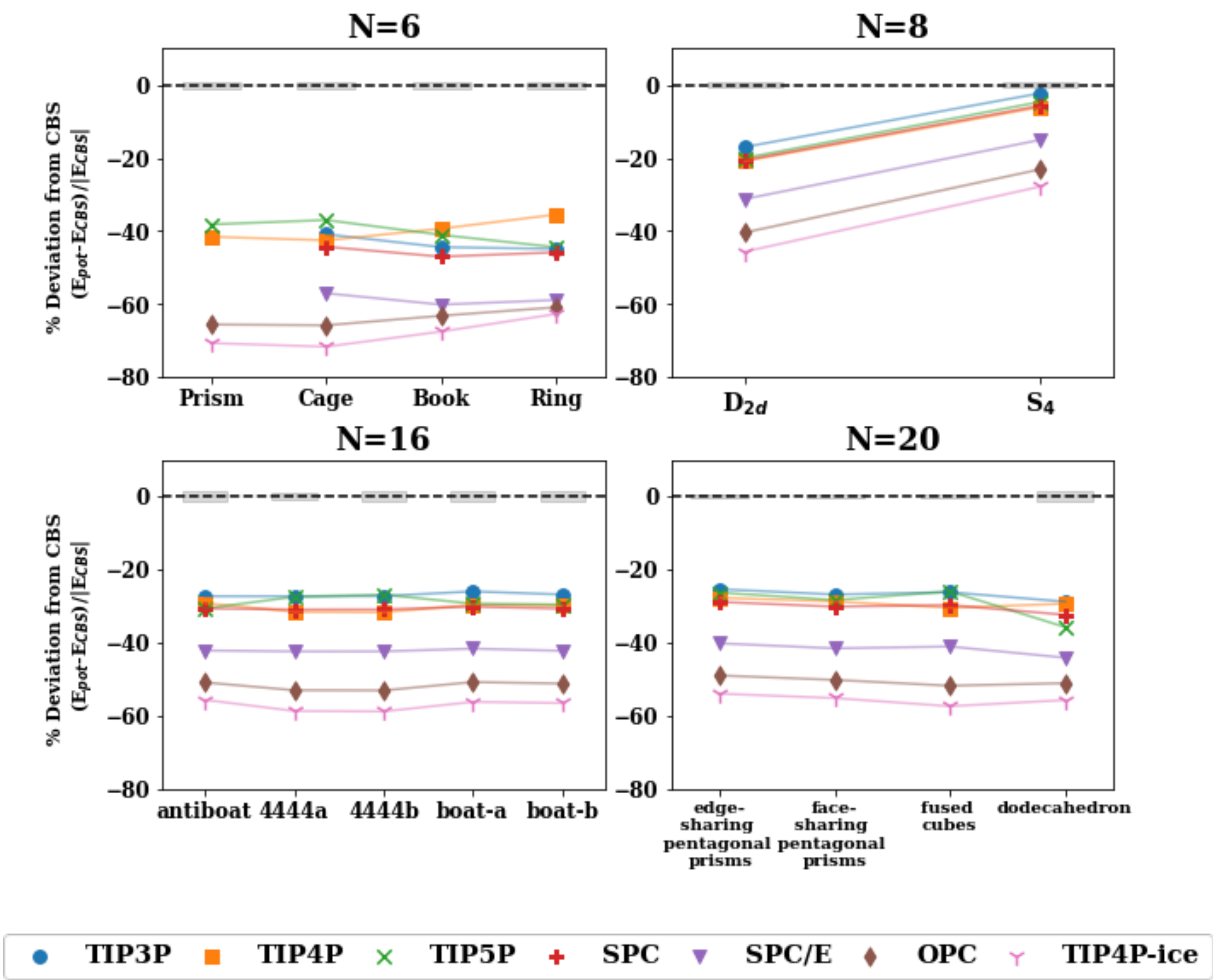


**Figure SF6.** A comparison of the different versions of the AMOEBA potential (AMOEBA03, AMOEBA14, iAMOEBA, AMOEBA+, AMOEBA+CF) through the percent error on the total binding energy of water clusters, *n* = 2-11, 16-17, 20, 25. The shaded gray regions represent the uncertainty in the CBS estimate of the $D_e$ calculation.

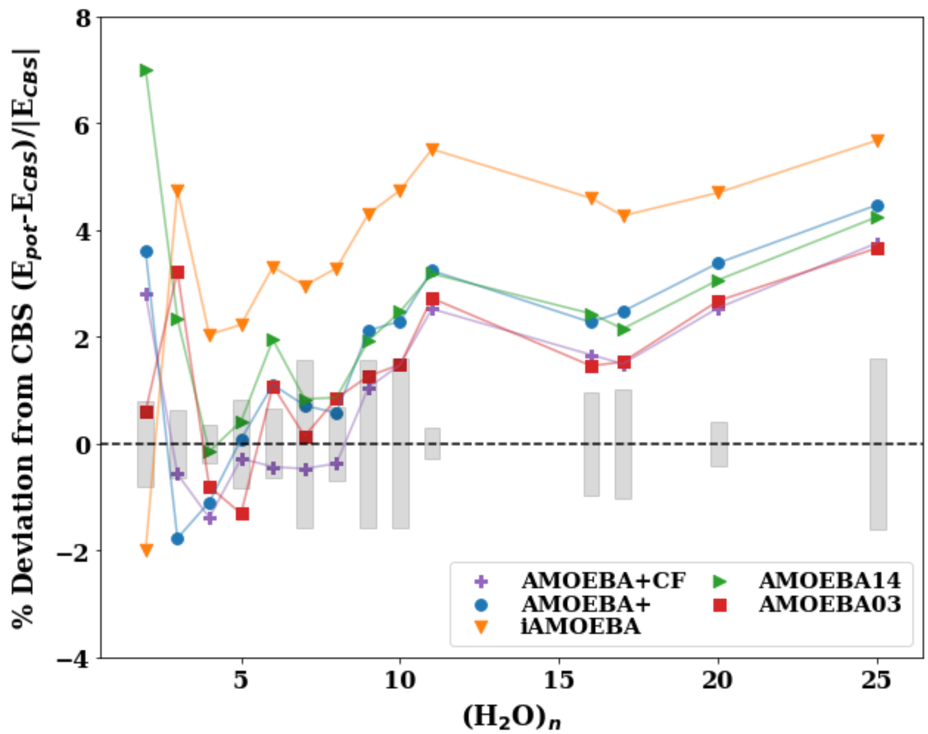


**Figure SF7.** A comparison of the different versions of the EFP potential (EFP1(RHF), EFP1(DFT), EFP1(RHF)-D3, EFP2(E6), EFP2(E6+E7), EFP2(E6+E7+E8)) through the percent error on the total binding energy of water clusters, *n* = 2-11, 16-17, 20, 25. The shaded gray regions represent the uncertainty in the CBS estimate of the $D_e$ calculation.

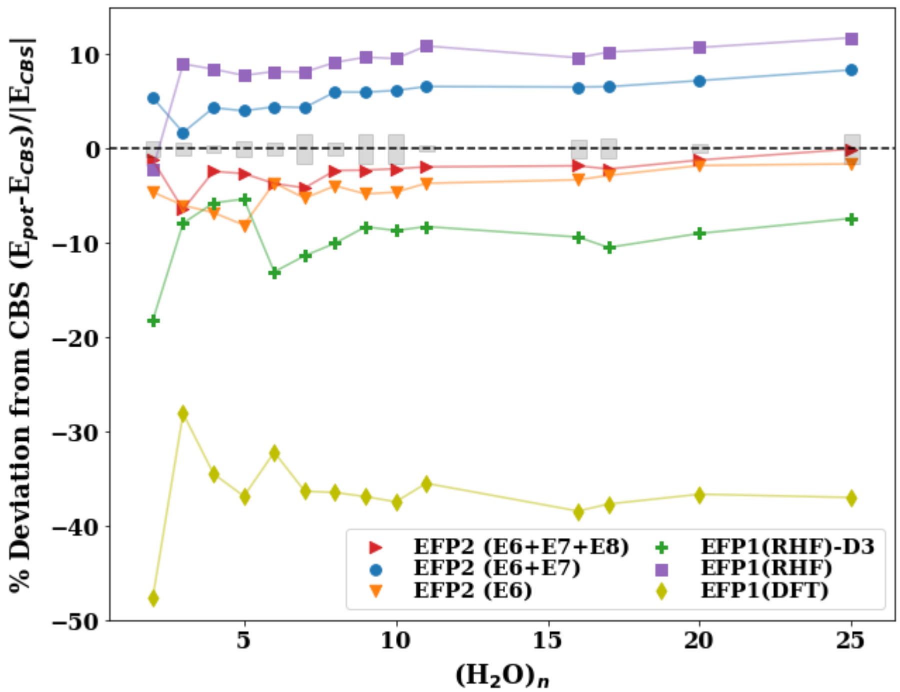


**Table ST1.** Classification and properties of pairwise and many-body potentials used in this study.

**Pairwise additive potentials (2-body potentials)**

| | Rigid/flexible | Number of sites | Dissociable | Polarizable | Permanent molecular dipole | Reference |
|---|---|---|---|---|---|---|
| **TIP3P** | Rigid | 3 | No | No | 2.35 | Jorgensen, W. L. Quantum and Statistical Mechanical Studies of Liquids. 10. Transferable Intermolecular Potential Functions for Water, Alcohols, and Ethers. Application to Liquid Water. J. Am. Chem. Soc. 1981, 103 (2), 335–340. |
| **TIP4P** | Rigid | 4 | No | No | 2.18 | Jorgensen, W. L. Quantum and Statistical Mechanical Studies of Liquids. 10. Transferable Intermolecular Potential Functions for Water, Alcohols, and Ethers. Application to Liquid Water. J. Am. Chem. Soc. 1981, 103 (2), 335–340.; Abascal, J. L. F.; Vega, C. A General Purpose Model for the Condensed Phases of Water: TIP4P/2005. J. Chem. Phys. 2005, 123 (23), 234505. |
| **TIP5P** | Rigid | 5 | No | No | 2.29 | Mahoney, M. W.; Jorgensen, W. L. A Five-Site Model for Liquid Water and the Reproduction of the Density Anomaly by Rigid, Nonpolarizable Potential Functions. *J. Chem. Phys.* **2000**, *112* (20), 8910–8922. |
| **SPC** | Rigid | 3 | No | No | 2.27 | Berendsen, H. J. C.; Postma, J. P. M.; Gunsteren, W. F. V.; Hermans, J. *Company. INTERACTION MODELS FOR WATER IN RELATION TO PROTEIN HYDRATION*. |
| **SPC/E** | Rigid | 3 | No | No | 2.35 | Berendsen, H. J. C.; Grigera, J. R.; Straatsma, T. P. The Missing Term in Effective Pair Potentials. *J. Phys. Chem.* **1987**, *91* (24), 6269–6271. |
| **OPC** | Rigid | 4 | No | No | 2.48 | Izadi, S.; Anandakrishnan, R.; Onufriev, A. V. Building Water Models: A Different Approach. J. Phys. Chem. Lett. 2014, 5 (21), 3863–3871. |
| **TIP4P-ice** | Rigid | 4 | No | No | 2.43 | Abascal, J. L. F.; Sanz, E.; García Fernández, R.; Vega, C. A Potential Model for the Study of Ices and Amorphous Water: TIP4P/Ice. J. Chem. Phys. 2005, 122 (23), 234511 |

**Many-body potentials**

| | Rigid/flexible | Implicit/Explicit many-body potentials | Dissociable | Polarizable | Reference |
|---|---|---|---|---|---|
| **TTM2.1-F** | Flexible | Implicit | No | Yes | Fanourgakis, G. S.; Xantheas, S. S. The Flexible, Polarizable, Thole-Type Interaction Potential for Water (TTM2-F) Revisited. *J. Phys. Chem. A* **2006**, *110* (11), 4100–4106. |
| **TTM3-F** | Flexible | Implicit | No | Yes | Fanourgakis, G. S.; Xantheas, S. S. Development of Transferable Interaction Potentials for Water. V. Extension of the Flexible, Polarizable, Thole-Type Model Potential (TTM3-F, v. 3.0) to Describe the Vibrational Spectra of Water Clusters and Liquid Water. *J. Chem. Phys.* **2008**, *128* (7), 074506 |
| **EFP2** | Rigid | Implicit | No | Yes | Guidez, E. B.; Gordon, M. S. Dispersion Interactions in Water Clusters. *J. Phys. Chem. A* **2017**, *121* (19), 3736–3745. |
| **AMOEBA+CF** | Flexible | Implicit | No | Yes | Liu, C.; Piquemal, J.-P.; Ren, P. Implementation of Geometry-Dependent Charge Flux into the Polarizable AMOEBA+ Potential. *J. Phys. Chem. Lett.* **2020**, *11* (2), 419–426. |
| **MB-UCB** | Flexible | Implicit | No | Yes | Das, A. K.; Urban, L.; Leven, I.; Loipersberger, M.; Aldossary, A.; Head-Gordon, M.; Head-Gordon, T. Development of an Advanced Force Field for Water Using Variational Energy Decomposition Analysis. J. Chem. Theory Comput. 2019, 15 (9), 5001–5013 |
| **HIPPO** | Flexible | Implicit | No | Yes | Rackers, J. A.; Silva, R. R.; Wang, Z.; Ponder, J. W. Polarizable Water Potential Derived from a Model Electron Density. *J. Chem. Theory Comput.* **2021**, *17* (11), 7056–7084 |
| **CC-pol** | Rigid | Explicit | No | No | Góra, U.; Cencek, W.; Podeszwa, R.; van der Avoird, A.; Szalewicz, K. Predictions for Water Clusters from a First-Principles Two- and Three-Body Force Field. *J. Chem. Phys.* **2014**, *140* (19), 194101.; Bukowski, R.; Szalewicz, K.; Groenenboom, G. C. Predictions of the Properties of Water from First Principles. 2007, 315, 5.; |
| **WHBB5** | Flexible | Explicit | No | Yes (base model is TTM3-F) | Wang, Y.; Huang, X.; Shepler, B. C.; Braams, B. J.; Bowman, J. M. Flexible, *Ab Initio* Potential, and Dipole Moment Surfaces for Water. I. Tests and Applications for Clusters up to the 22-Mer. *J. Chem. Phys.* **2011**, *134* (9), 094509.; óra, U.; Podeszwa, R.; Cencek, W.; Szalewicz, K. Interaction Energies of Large Clusters from Many-Body Expansion. J. Chem. Phys. 2011, 135 (22), 224102. |
| **WHBB6** | Flexible | Explicit | No | Yes (base model is TTM3-F) | Wang, Y.; Huang, X.; Shepler, B. C.; Braams, B. J.; Bowman, J. M. Flexible, *Ab Initio* Potential, and Dipole Moment Surfaces for Water. I. Tests and Applications for Clusters up to the 22-Mer. *J. Chem. Phys.* **2011**, *134* (9), 094509. |
| **MB-pol** | Flexible | Explicit | No | Yes (base model is TTM4-F) | Babin, V.; Leforestier, C.; Paesani, F. Development of a "First Principles" Water Potential with Flexible Monomers: Dimer Potential Energy Surface, VRT Spectrum, and Second Virial Coefficient. *J. Chem. Theory Comput.* **2013**, *9* (12), 5395–5403; Babin, V.; Medders, G. R.; Paesani, F. Development of a "First Principles" Water Potential with Flexible Monomers. II: Trimer Potential Energy Surface, Third Virial Coefficient, and Small Clusters. J. Chem. Theory Comput. 2014, 10 (4), 1599–1607. |
| **q-AQUA** | Flexible | Explicit | No | No | Yu, Q.; Qu, C.; Houston, P. L.; Conte, R.; Nandi, A.; Bowman, J. M. Q-AQUA: A Many-Body CCSD(T) Water Potential, Including Four-Body Interactions, Demonstrates the Quantum Nature of Water from Clusters to the Liquid Phase. *J. Phys. Chem. Lett.* **2022**, 5068–5074. |

**Table ST2.** Binding energies (kcal/mol) of water clusters with the pairwise additive potentials, obtained using Gromacs compiled in mixed precision (default). NSP (Not a Stationary Point) means that the water cluster optimized to a different structure.

| *n* | Isomer | TIP3P | TIP4P | TIP5P | SPC | SPC/E | OPC | TIP4P/ice |
|---|---|---|---|---|---|---|---|---|
| **2** | | -6.57 | -6.26 | -6.80 | -6.64 | -7.23 | -7.37 | -7.52 |
| **3** | | -17.44 | -16.73 | -15 | -17.98 | -19.61 | -19.30 | -20.07 |
| **4** | | -29.28 | -27.86 | -28.43 | -29.83 | -32.51 | -32.60 | -33.46 |
| **5** | | -38.74 | -36.35 | -36.08 | -39.12 | -42.62 | -42.94 | -43.64 |
| **6** | prism | *NSP* | -46.93 | -45.81 | *NSP* | *NSP* | -54.87 | -56.56 |
| | cage | -46.67 | -47.22 | -45.38 | -47.80 | -52.02 | -54.88 | -56.85 |
| | book | -47.79 | -46.12 | -46.68 | -48.65 | -52.99 | -53.98 | -55.43 |
| | ring | -47.45 | -44.38 | -47.30 | -47.76 | -52.03 | -52.68 | -53.27 |
| **7** | | -57.45 | -58.20 | -57.84 | -58.64 | -63.80 | -67.91 | -70.09 |
| **8** | $D_{2d}$ | -70.64 | -72.97 | -72.45 | -72.81 | -79.23 | -84.74 | -87.91 |
| | $S_4$ | -70.38 | -73.00 | -72.01 | -72.72 | -79.14 | -84.69 | -87.94 |
| **9** | $D_{2d}$DD | -81.62 | -82.28 | -83.53 | -83.75 | -91.16 | -96.08 | -99.07 |
| **10** | | -92.20 | -93.43 | -95.37 | -94.62 | -102.98 | -109.01 | -112.51 |
| **11** | 43'4 | -100.84 | -102.54 | *NSP* | -103.77 | -112.89 | -119.33 | -123.54 |
| **16** | antiboat | -158.68 | -161.02 | -162.89 | -162.83 | -177.16 | -188.04 | -194.00 |
| | 4444-a | -157.43 | -162.71 | -157.62 | -161.91 | -176.08 | -189.18 | -196.19 |
| | 4444-b | -157.20 | -162.72 | -156.76 | -161.76 | -175.92 | -189.09 | -196.20 |
| | boat a | -156.66 | -161.19 | -160.82 | -161.85 | -176.13 | -187.47 | -194.22 |
| | boat b | -157.45 | -161.26 | -160.87 | -162.27 | -176.57 | -187.67 | -194.29 |
| **17** | sphere | -170.49 | -172.42 | -172.49 | -174.52 | -189.73 | -201.73 | -207.91 |
| **20** | edge-sharing pentagonal prisms | -204.67 | -208.51 | -206.17 | -210.36 | -228.83 | -243.16 | -251.29 |
| | face-sharing pentagonal prisms | -204.11 | -207.16 | -206.56 | -209.46 | -227.81 | -241.68 | -249.69 |
| | fused cubes | -200.85 | -207.65 | -200.48 | -206.44 | -224.48 | -241.53 | -250.44 |
| | pentagonal dodecahedron (A3) | -196.16 | -197.05 | -206.75 | -201.65 | -219.51 | -230.13 | -237.20 |
| **25** | isomer 2 | -260.92 | -265.81 | -267.20 | -268.61 | -292.21 | -309.91 | -320.33 |

**Table ST3.** Binding energies (kcal/mol) of water clusters with additional (often older variants) many-body potentials.

| ***n*** | Isomer | **AMOEBA-03** | **iAMOEBA** | **AMOEBA-14** | **AMOEBA+** | **EFP1(RHF)** | **EFP1(DFT)** | **EFP1(RHF)-D3** | **EFP2(E6)** | **EFP2(E6+E7)** |
|---|---|---|---|---|---|---|---|---|---|---|
| **2** | | -4.96 | -5.09 | -4.64 | -4.81 | -5.10 | -7.37 | -5.90 | -5.22 | -4.72 |
| **3** | | -15.29 | -15.05 | -15.43 | -16.08 | -14.38 | -20.24 | -17.05 | -16.75 | -15.53 |
| **4** | | -27.62 | -26.84 | -27.44 | -27.70 | -25.09 | -36.85 | -28.98 | -29.26 | -26.21 |
| **5** | | -36.37 | -35.10 | -35.75 | -35.87 | -33.11 | -49.14 | -37.82 | -38.81 | -34.46 |
| **6** | prism | -45.70 | -44.67 | -45.30 | -45.69 | -42.42 | -61.08 | -52.24 | -47.88 | -44.15 |
| | cage | -45.73 | -44.41 | -45.84 | -45.79 | -41.90 | -61.52 | -50.95 | -47.62 | -43.48 |
| | book | -45.60 | -44.18 | -45.10 | -45.43 | -41.76 | -62.05 | -48.97 | -48.53 | -43.59 |
| | ring | -44.63 | -43.39 | -43.50 | -44.00 | -41.15 | -60.66 | -46.66 | -48.33 | -43.00 |
| **7** | | -57.32 | -55.70 | -56.92 | -56.99 | -52.73 | -78.26 | -63.925 | -60.42 | -54.90 |
| **8** | $D_{2d}$ | -72.38 | -70.60 | -72.37 | -72.58 | -66.32 | -99.63 | -80.33 | -75.88 | -68.61 |
| | $S_4$ | -72.37 | -70.63 | -72.36 | -72.56 | -66.25 | -99.24 | -80.25 | -75.77 | -68.51 |
| **9** | $D_{2d}$DD | -81.95 | -79.43 | -81.40 | -81.24 | -74.95 | -113.64 | -89.88 | -86.99 | -78.03 |
| **10** | | -93.20 | -90.11 | -92.26 | -92.43 | -85.56 | -130.05 | -102.82 | -98.97 | -88.76 |
| **11** | 43'4 | -101.75 | -98.83 | -101.27 | -101.21 | -93.21 | -141.74 | -113.25 | -108.45 | -97.71 |
| **16** | antiboat | -162.20 | -157.03 | -160.59 | -160.86 | -148.73 | -227.89 | -180.04 | -170.04 | -153.84 |
| | 4444-a | -161.18 | -157.75 | -161.83 | -161.12 | -147.83 | -223.41 | -183.18 | -168.26 | -154.28 |
| | 4444-b | -160.98 | -157.72 | -161.50 | -160.57 | -147.45 | -222.12 | -182.84 | -167.68 | -153.75 |
| | boat a | -161.35 | -157.89 | -160.75 | -161.43 | -147.98 | -226.25 | -179.16 | -170.36 | -153.97 |
| | boat b | -161.52 | -157.93 | -160.68 | -161.16 | -148.08 | -226.08 | -179.37 | -170.69 | -154.26 |
| **17** | sphere | -173.01 | -168.20 | -171.92 | -171.35 | -157.70 | -241.94 | -194.13 | -180.70 | -164.15 |
| **20** | edge-sharing pentagonal prisms | -208.47 | -204.13 | -207.63 | -206.95 | -191.20 | -292.73 | -233.46 | -218.03 | -198.74 |
| | face-sharing pentagonal prisms | -206.13 | -199.63 | -204.85 | -203.68 | -189.14 | -289.23 | -232.84 | -218.40 | -198.19 |
| | fused cubes | -205.79 | -201.51 | -206.63 | -205.67 | -188.83 | -285.71 | -234.86 | -214.36 | -197.00 |
| | pentagonal dodecahedron (A3) | -197.24 | -191.78 | -193.75 | -194.72 | -181.62 | -280.59 | -214.91 | -212.29 | -187.66 |
| **25** | isomer 2 | -266.17 | -260.60 | -264.56 | -263.94 | -243.79 | -378.56 | -296.73 | -280.77 | -253.22 |

**Table ST4.** The differences between BSSE-corrected MP2/aVTZ many-body terms and average (BSSE-corrected and -uncorrected) MP2/aVTZ many-body terms against MP2/aV5Z results. The italicized values indicate the smallest errors, and the bold values indicate the most comparable MP2/aVTZ value to the MP2/aV5Z reference. This justifies our use of averaged MP2/aVTZ 2- and 3-body terms and BSSE-corrected MP2/aVTZ values for the 4-body as an estimate of those respective values with a larger (aV5Z) basis set for $(H_2O)_{16}$. All $(H_2O)_7$ and $(H_2O)_{10}$ results are taken from the SI of Heindel et. al 2020.[1]

| | *n*-body | MP2/AVTZ | BSSE MP2/aVTZ | Average MP2/aVTZ | MP2/aV5Z | BSSE MP2/aV5Z | BSSE MP2/aVTZ vs. MP2/aV5Z | Average MP2/aVTZ vs. MP2/aV5Z |
|---|---|---|---|---|---|---|---|---|
| | 2B | -49.459 | -43.958 | **-46.709** | -47.160 | -47.165 | 3.202 | *0.456* |
| **$(H_2O)_7$** | 3B | -12.030 | -12.313 | **-12.172** | -12.191 | -12.181 | -0.122 | *0.009* |
| | 4B | -1.106 | **-0.874** | -0.990 | -0.841 | -0.854 | *-0.033* | -0.136 |
| | 2B | -78.707 | -69.504 | **-74.106** | -74.796 | n/a | 5.292 | *0.691* |
| **$(H_2O)_{10}$** | 3B | -21.285 | -21.989 | **-21.637** | -21.625 | n/a | -0.364 | *-0.012* |
| | 4B | -3.028 | **-1.978** | -2.503 | -1.878 | n/a | *-0.100* | -0.625 |
| | 2B | -138.62 | -122.523 | **-130.572** | n/a | n/a | n/a | n/a |
| **$(H_2O)_{16}$** | 3B | -36.417 | -37.657 | **-37.037** | n/a | n/a | n/a | n/a |
| | 4B | -4.997 | **-2.142** | -3.570 | n/a | n/a | n/a | n/a |

**Table ST5.** The ratio of SPC and SPC/E energies (obtained with Gromacs in DP).

| ***n*** | **Isomer** | **SPC** | **SPC/E** | **Ratio SPC: SPC/E** |
|---|---|---|---|---|
| **2** | | -6.64 | -7.23 | 0.918 |
| **3** | | -17.98 | -19.61 | 0.917 |
| **4** | | -29.84 | -32.52 | 0.918 |
| **5** | | -39.14 | -42.64 | 0.918 |
| **6** | **prism** | -47.35 | -51.52 | 0.919 |
| | **cage** | -47.81 | -52.02 | 0.919 |
| | **book** | -48.66 | -53.00 | 0.918 |
| | **ring** | -47.76 | -52.03 | 0.918 |
| **7** | | -58.65 | -63.81 | 0.919 |
| **8** | **D2d** | -72.81 | -79.23 | 0.919 |
| | **S4** | -72.81 | -79.23 | 0.919 |
| **9** | **D2dDD** | -83.77 | -91.17 | 0.919 |
| **10** | | -94.63 | -102.98 | 0.919 |
| **11** | **43'4** | -103.78 | -112.9 | 0.919 |
| **16** | **antiboat** | -162.84 | -177.17 | 0.919 |
| | **4444-a** | -161.91 | -176.08 | 0.920 |
| | **4444-b** | -161.76 | -175.92 | 0.920 |
| | **boat a** | -161.86 | -176.13 | 0.919 |
| | **boat b** | -162.29 | -176.58 | 0.919 |
| **17** | **sphere** | -174.52 | -189.74 | 0.920 |
| **20** | **edge-sharing pentagonal prisms** | -210.37 | -228.84 | 0.919 |
| | **face-sharing pentagonal prisms** | -209.47 | -227.82 | 0.919 |
| | **fused cubes** | -206.44 | -224.48 | 0.920 |
| | **pentagonal dodecahedron (A3)** | -201.66 | -219.52 | 0.919 |
| **25** | **isomer 2** | -268.63 | -292.22 | 0.919 |

**Table ST6.** Cartesian coordinates for water clusters used in molecular dipole analysis.

**Singly solvated monomer (*N* = 5)**

15
-381.680759840801 a.u. (MP2/aVTZ)
O -0.00354472 -0.08149026 0.01491547
H -0.39032271 0.74241384 -0.32014335
H 0.92751433 -0.05263168 -0.25792714
O -0.08995661 -0.11714257 2.87959018
H -0.07602037 -0.13535657 1.90811717
H -0.42363594 -0.98426489 3.12351228
O 2.70157691 -0.05359097 -0.85190341
H 3.43241397 0.55483635 -0.71236704
H 3.05524812 -0.75650624 -1.40467879
O -1.30672697 -2.41143972 -1.00824991
H -2.03478178 -2.10209935 -1.55236159
H -0.89189792 -1.59812893 -0.67322552
O -1.33926007 2.26076533 -0.95303245
H -2.26755199 2.39679908 -0.7418469
H -1.08742531 3.02190474 -1.48316964

**Singly solvated dimer (*N* = 8)**

24
-610.699899359085 a.u. (MP2/aVTZ)
O 0.02277885 -0.00642763 -1.36056841
H -0.35350277 0.81470964 -1.71809042
H 0.94041503 -0.02947048 -1.68218566
O 0.03595643 0.03255532 1.39201696
H 0.01870483 0.00391823 0.41419927
H -0.43363577 -0.76623765 1.68057286
O 2.663003 -0.05776818 -2.30923264
H 3.35691317 0.59089219 -2.16129158
H 3.06006981 -0.74071521 -2.85701841
O -1.36962325 -2.34584098 -2.28008022
H -2.10685088 -2.02443086 -2.80480773
H -0.92024782 -1.53860689 -1.9775137
O -1.28291767 2.31025356 -2.33233582
H -2.20040577 2.45386539 -2.08176456
H -1.05242828 3.0590831 -2.88888718
O -1.26123074 2.3769768 2.310626
H -1.22530895 2.33442905 3.2692117
H -0.81289113 1.56242053 2.01759024
O 2.71148056 0.00580992 2.32264346
H 2.79059137 0.81862817 2.82818407

H 1.79236635 0.0200714 1.99876032
O -1.3313117 -2.24984041 2.37512133
H -0.95436794 -2.93229834 2.93740311
H -2.24454279 -2.51205777 2.22985758

**Doubly solvated monomer (*N* = 17)**

51
-1297.77823496 a.u. (MP2/aVTZ)

| | | | |
|---|---|---|---|
| O | -0.06849174 | -0.02143682 | -0.00638088 |
| H | -0.52608217 | 0.77020930 | -0.32510728 |
| H | -0.49768733 | -0.85461657 | -0.24985935 |
| O | -0.08228775 | 0.04010825 | 2.78593789 |
| H | 0.84119378 | 0.05499565 | 3.07686630 |
| H | -0.04943812 | 0.02248963 | 1.81831731 |
| O | 2.56869058 | -0.00784720 | -0.92622160 |
| H | 2.66518802 | 0.75980439 | -1.50852598 |
| H | 1.65041768 | 0.01265619 | -0.61957262 |
| O | -1.38834476 | 2.26195126 | -0.92570081 |
| H | -1.69513465 | 2.17686263 | -1.84020559 |
| H | -0.76696479 | 3.00462158 | -0.92831569 |
| O | -1.27881133 | -2.37728993 | -0.89300643 |
| H | -0.69573358 | -2.91352255 | -1.44992117 |
| H | -2.03588051 | -2.15048475 | -1.45254621 |
| O | 2.54568416 | 0.09478621 | 3.73028749 |
| H | 3.20180089 | 0.08742357 | 3.01815285 |
| H | 2.83452606 | -0.58499094 | 4.35650829 |
| O | -1.35099575 | -2.27684292 | 3.69320828 |
| H | -0.78947422 | -2.65973950 | 4.38296395 |
| H | -0.89198000 | -1.47646415 | 3.39930783 |
| O | -1.52197638 | 2.28126514 | 3.62589903 |
| H | -2.17420445 | 1.97672627 | 4.27361326 |
| H | -1.03609950 | 1.48886644 | 3.35440857 |
| O | 2.95334539 | 2.17781009 | -2.62208868 |
| H | 2.15504971 | 2.71502393 | -2.73073670 |
| H | 3.28722785 | 2.02471807 | -3.51805991 |
| O | 2.99951783 | -2.37529320 | -2.34418125 |
| H | 3.67510026 | -2.19007349 | -3.01273277 |
| H | 2.87186175 | -1.54274144 | -1.86643592 |
| O | 4.28522177 | 0.08601123 | 1.27508109 |
| H | 4.93238867 | -0.62575737 | 1.16444844 |
| H | 3.70674743 | 0.03372335 | 0.50028271 |
| O | -2.21780413 | 1.86133611 | -3.56246529 |
| H | -1.97329563 | 0.98948600 | -3.90564466 |
| H | -1.94402494 | 2.49413857 | -4.24238081 |
| O | 0.41102596 | 4.39591813 | -0.82837305 |

| | | | |
|---|---|---|---|
| H | 1.28236043 | 4.13859861 | -0.49334765 |
| H | 0.16820716 | 5.19304126 | -0.33510552 |
| O | -3.55062683 | 2.78793689 | 0.76216695 |
| H | -3.51024466 | 2.29029313 | 1.59186513 |
| H | -2.75942691 | 2.53101206 | 0.26651444 |
| O | 0.52244595 | -3.81381915 | -2.47189156 |
| H | 1.38755191 | -3.38437863 | -2.54154522 |
| H | 0.27278366 | -4.04347709 | -3.37886735 |
| O | -3.50831367 | -1.67823367 | -2.42325539 |
| H | -3.65258683 | -0.72153081 | -2.46305495 |
| H | -4.36937411 | -2.06166677 | -2.20137006 |
| O | -2.10015135 | -3.85468181 | 1.33044496 |
| H | -2.09537223 | -3.33720109 | 2.14890081 |
| H | -1.80501439 | -3.24659573 | 0.63704421 |

**Water cluster with ~3 solvation shells (*N* = 53)**

159
-4044.87096279 a.u. (PBE96-D3/def2-svpd)

| | | | |
|---|---|---|---|
| O | 2.18558230 | 5.77592379 | -2.07874456 |
| H | 2.39928169 | 4.83484978 | -2.33032124 |
| H | 2.30833397 | 5.77676499 | -1.09241134 |
| O | -0.71612465 | 1.47694471 | -5.27216547 |
| H | -0.55709098 | 2.32882874 | -4.79501053 |
| H | -1.60415878 | 1.19617083 | -4.95879869 |
| O | -3.19919493 | 2.23376064 | 4.76575176 |
| H | -3.26979162 | 2.36267425 | 3.76823957 |
| H | -3.76605662 | 2.90417352 | 5.18048650 |
| O | 0.08817339 | 6.57943766 | 1.96805230 |
| H | 0.13922929 | 5.96266707 | 2.72912766 |
| H | 0.99930648 | 6.52863664 | 1.60343140 |
| O | -0.31629346 | 6.02012814 | -2.50273107 |
| H | 0.71424969 | 6.00777794 | -2.34584158 |
| H | -0.51086127 | 6.80409777 | -3.04182947 |
| O | -2.12130006 | -4.79011075 | 1.25355844 |
| H | -1.25103520 | -5.20499358 | 1.44702311 |
| H | -1.94762602 | -3.83213240 | 1.09630886 |
| O | 3.52840925 | -1.82770124 | 2.87917689 |
| H | 3.29558761 | -1.98466232 | 3.81899243 |
| H | 4.18761998 | -2.56791971 | 2.54373330 |
| O | 1.46438435 | -1.72145378 | -0.74601330 |
| H | 1.39743721 | -2.12240256 | 0.17446546 |
| H | 2.37570571 | -1.30716441 | -0.83003799 |
| O | 5.48571044 | 1.50540997 | -0.71104425 |
| H | 5.16761542 | 2.21234601 | -0.07541659 |
| H | 6.40258261 | 1.29836876 | -0.46739602 |

| | | | |
|---|---|---|---|
| O | 0.05068094 | -2.74063572 | -4.36839087 |
| H | -0.02505958 | -3.28303022 | -5.16888694 |
| H | 0.57180481 | -3.27370231 | -3.65673404 |
| O | -0.10007826 | 3.43703257 | -3.42968565 |
| H | -0.26803108 | 4.39889796 | -3.25114761 |
| H | 0.87952352 | 3.29128367 | -3.25526875 |
| O | 5.45675570 | -3.04892154 | -0.60583025 |
| H | 4.96223828 | -2.22356780 | -0.82377735 |
| H | 4.92420971 | -3.76781919 | -1.05279670 |
| O | -5.38047363 | 0.50099642 | 1.68635030 |
| H | -5.17268537 | -0.35936697 | 1.25070935 |
| H | -4.51804466 | 0.98604083 | 1.80541631 |
| O | 4.13935129 | 3.28088848 | 0.79596497 |
| H | 4.01680086 | 3.09543891 | 1.76178781 |
| H | 3.36423378 | 2.79008857 | 0.38578787 |
| O | -1.96298818 | -1.74241719 | -2.90441955 |
| H | -1.26859206 | -2.14119406 | -3.50476603 |
| H | -1.47380122 | -1.38407081 | -2.12294143 |
| O | -2.68895979 | -5.69966238 | -1.22139578 |
| H | -2.61238756 | -5.37143207 | -0.27675431 |
| H | -3.18469181 | -4.98923825 | -1.71911435 |
| O | 2.41945350 | 3.10168789 | -2.65178826 |
| H | 2.31142767 | 2.52857145 | -1.85413545 |
| H | 3.29794488 | 2.79343099 | -3.05670082 |
| O | -6.02582048 | -1.85421398 | -1.98195532 |
| H | -6.97553060 | -2.03091924 | -2.08316988 |
| H | -5.86309139 | -0.93624686 | -2.37222726 |
| O | -3.21864911 | 2.06981933 | 2.14589745 |
| H | -2.36897536 | 1.57569436 | 1.96400597 |
| H | -3.23348219 | 2.71968519 | 1.38482851 |
| O | 0.96872987 | -0.17359948 | -3.94415121 |
| H | 0.65829804 | -1.06870259 | -4.22167401 |
| H | 0.41271236 | 0.46829380 | -4.47913005 |
| O | -1.53029416 | 1.90812895 | -1.83424045 |
| H | -2.08681586 | 2.46278811 | -1.21641646 |
| H | -0.95739865 | 2.53640073 | -2.38437374 |
| O | 4.97477478 | -3.69023320 | 1.93138234 |
| H | 4.34612373 | -4.43372812 | 1.77976021 |
| H | 5.25106936 | -3.42397283 | 0.99209661 |
| O | -1.81612028 | -1.54863348 | 3.34633750 |
| H | -1.99850339 | -1.70106218 | 2.37318921 |
| H | -2.66311215 | -1.15836277 | 3.72229951 |
| O | -5.51771270 | 2.27946653 | -0.58956964 |
| H | -5.65280958 | 1.67356957 | 0.18243616 |
| H | -5.54262204 | 1.69660355 | -1.38608709 |
| O | -4.91276462 | -1.99160302 | 0.45377172 |

| | | | |
|---|---|---|---|
| H | -5.37020234 | -1.98770812 | -0.43860812 |
| H | -5.21914920 | -2.79018777 | 0.91664551 |
| O | 3.90967820 | -0.75322072 | -1.20997112 |
| H | 4.39459910 | 0.05176076 | -0.90143319 |
| H | 3.83526843 | -0.64505896 | -2.20042131 |
| O | -2.21590601 | -2.06188961 | 0.75316539 |
| H | -1.72745437 | -1.45794454 | 0.13899638 |
| H | -3.17921122 | -2.01374771 | 0.51568146 |
| O | -5.46860298 | 0.58893559 | -2.87840053 |
| H | -6.00959332 | 0.94734999 | -3.60248287 |
| H | -4.49053888 | 0.60891501 | -3.22424584 |
| O | 1.28005594 | -3.85212773 | -2.41312691 |
| H | 1.33429441 | -3.09863836 | -1.75309782 |
| H | 0.70991297 | -4.57577530 | -2.02301871 |
| O | 3.11634119 | 2.70076614 | 3.29971522 |
| H | 3.55511531 | 2.72857623 | 4.16519131 |
| H | 2.26915611 | 3.27614714 | 3.38453395 |
| O | 3.53680128 | -0.32353370 | -3.85307873 |
| H | 3.81646459 | -0.98140713 | -4.50983226 |
| H | 2.51720663 | -0.21407688 | -3.95452195 |
| O | -0.84811774 | 1.10537440 | 1.49954826 |
| H | -0.73563731 | 0.44347920 | 0.75484019 |
| H | -0.40389998 | 0.75956213 | 2.30766615 |
| O | 2.32622108 | 0.36601464 | 2.07701093 |
| H | 2.93443049 | -0.40895520 | 2.28209396 |
| H | 2.67997319 | 1.14013164 | 2.59234561 |
| O | 0.32028448 | -0.10694700 | 3.79690029 |
| H | -0.45827206 | -0.72507105 | 3.57351576 |
| H | 1.03264237 | -0.09982198 | 3.08814728 |
| O | -0.07131944 | -3.65340462 | 3.70220639 |
| H | 0.52891074 | -3.30680648 | 4.39864951 |
| H | -0.86546322 | -3.06453279 | 3.74521730 |
| O | 2.06338283 | 1.87512254 | -0.21300550 |
| H | 2.12098393 | 1.12980353 | 0.44159813 |
| H | 1.28351205 | 2.42320264 | 0.06471129 |
| O | 0.10707366 | 3.46628350 | 0.77901941 |
| H | -0.53810306 | 4.12561492 | 0.36700933 |
| H | -0.38609092 | 2.63241432 | 1.02751526 |
| O | 1.79836335 | -1.96688205 | 5.17481412 |
| H | 1.87923242 | -1.86526111 | 6.13682076 |
| H | 1.25946795 | -1.19168495 | 4.85618257 |
| O | 2.31055902 | 5.37897598 | 0.62550840 |
| H | 1.62719387 | 4.67566556 | 0.67466701 |
| H | 3.15381832 | 4.87423708 | 0.75313050 |
| O | -3.84960119 | -3.69089580 | -2.59320456 |
| H | -4.69869869 | -3.22018518 | -2.47257711 |

H -3.17134243 -2.97135906 -2.67170338
O -0.40984287 2.32513794 4.94807419
H -1.39679699 2.32582758 5.00490469
H -0.16127035 1.42325648 4.62801644
O -3.01678103 0.61129650 -3.64607940
H -2.66162812 -0.31420552 -3.49287307
H -2.51709040 1.15477299 -2.96156117
O 0.26308232 -6.45169703 1.02972612
H -0.03311058 -7.33935287 1.28869924
H 0.11604869 -6.38535939 0.04108463
O -1.40348986 5.46116755 -0.07653203
H -1.05317347 5.79569798 -0.94950480
H -0.99819573 6.02249522 0.64249008
O -0.20951797 -5.96575036 -1.59310974
H -0.03759475 -6.69069855 -2.21694408
H -1.25880503 -5.84569626 -1.54586497
O 2.72794009 -5.18952382 1.04863746
H 2.21744485 -4.34854465 1.20594048
H 2.03187934 -5.87740539 1.16768884
O -4.09252236 -0.40320680 4.23118112
H -4.72829024 -0.19740072 3.50880977
H -3.86599223 0.48158230 4.60556814
O -0.72892167 -0.36478696 -0.75206953
H 0.21361780 -0.73342684 -0.86300451
H -0.86658987 0.50437796 -1.24049565
O 1.38631369 -2.86692677 1.62694085
H 0.74335322 -3.17951031 2.34088158
H 2.15465551 -2.46651456 2.13183888
O 4.73084568 2.12266396 -3.42669291
H 5.15128638 1.96563492 -2.54968157
H 4.42627041 1.22618426 -3.71918240
O -3.14088478 3.34261608 -0.18320151
H -4.09635336 3.13092888 -0.43576641
H -2.91715206 4.30100583 -0.21655093
O 0.86207793 4.02830263 3.38129949
H 0.30070707 3.45008437 3.99403382
H 0.52480149 3.83911033 2.46761514
O 3.77081741 -5.00213033 -1.51400382
H 3.00906979 -4.62086731 -2.00463513
H 3.39119235 -5.17683029 -0.61239138

**Water cluster with ~4 solvation shells (*N* = 102)**

306
-7784.512904675292 a.u. (PBE96-D3/def2-svpd; 26 lin dep.)
O -4.51217055 5.68730278 -3.07824506

| | | | |
|---|---|---|---|
| H | -3.69199651 | 5.26589269 | -3.45968355 |
| H | -4.23166511 | 6.17815086 | -2.26852086 |
| O | -4.23636362 | 0.13010929 | -5.93817484 |
| H | -4.33901712 | 0.91931005 | -5.33787745 |
| H | -4.70944617 | -0.59309407 | -5.48511050 |
| O | -6.61652486 | 2.57868405 | 2.78853065 |
| H | -6.76060274 | 2.67787711 | 3.74311793 |
| H | -5.70097685 | 2.20340316 | 2.69834945 |
| O | -4.01227252 | 0.98366051 | 4.96345855 |
| H | -4.11611178 | 0.97325330 | 3.96434518 |
| H | -4.22089706 | 0.04661066 | 5.22360437 |
| O | -2.66128654 | -6.53327679 | -2.61867247 |
| H | -2.56364466 | -5.56477412 | -2.38415640 |
| H | -1.74183194 | -6.80679811 | -2.84751440 |
| O | -7.39356864 | -5.34248077 | -2.52212558 |
| H | -8.16870280 | -5.67880860 | -2.99419195 |
| H | -6.66183210 | -6.01754687 | -2.63790105 |
| O | -5.44487544 | -7.18093496 | -2.68202595 |
| H | -4.53167061 | -6.95067640 | -2.97138339 |
| H | -5.30362832 | -7.47675994 | -1.75919926 |
| O | -5.54108461 | 4.86005563 | 0.71765678 |
| H | -5.51105219 | 5.00730054 | 1.69323524 |
| H | -5.12077806 | 5.65808962 | 0.30682642 |
| O | -6.21951348 | 3.77674049 | -3.10665499 |
| H | -5.58222613 | 4.59014353 | -3.02839160 |
| H | -6.97019018 | 4.07630042 | -3.64588506 |
| O | 4.87616204 | 4.96717973 | -1.86116927 |
| H | 4.54523843 | 5.46528402 | -2.65322759 |
| H | 5.49880461 | 4.26162360 | -2.22990397 |
| O | 0.37102889 | -3.77229942 | 2.36971744 |
| H | 1.17513215 | -3.87586237 | 1.76646396 |
| H | 0.31935890 | -2.81180673 | 2.56041654 |
| O | 3.18996674 | 2.90724294 | -1.06545605 |
| H | 3.64700530 | 3.74148253 | -1.32519445 |
| H | 3.62241761 | 2.19837547 | -1.60988809 |
| O | 0.99533847 | 0.56578709 | -1.87003312 |
| H | 1.56227709 | 0.69113615 | -1.06600731 |
| H | 1.13226100 | 1.33917279 | -2.49752056 |
| O | 3.99254482 | 5.70545967 | -4.31984152 |
| H | 4.23480292 | 6.45697811 | -4.88483505 |
| H | 4.42341669 | 4.87129750 | -4.73307179 |
| O | 2.12500764 | -6.47793689 | 5.59691829 |
| H | 1.21472901 | -6.16189607 | 5.39998416 |
| H | 2.27456329 | -7.15953527 | 4.88212949 |
| O | 1.38029634 | 5.03822773 | -3.76928584 |
| H | 0.99300419 | 5.54998210 | -2.98870701 |

| | | | |
|---|---|---|---|
| H | 2.27603967 | 5.39469632 | -3.98983207 |
| O | -0.62482514 | -1.98999336 | -4.99171480 |
| H | -0.18118330 | -2.64131340 | -5.56613812 |
| H | 0.06569333 | -1.81392940 | -4.25186202 |
| O | -4.26506629 | 2.16038104 | -4.13289923 |
| H | -5.07287120 | 2.66885391 | -3.85051242 |
| H | -3.54673563 | 2.86577908 | -4.22539982 |
| O | 3.49810158 | 1.39927965 | -4.91762976 |
| H | 2.67295220 | 1.79731905 | -4.50104624 |
| H | 3.17487557 | 0.75584249 | -5.61101066 |
| O | -5.38910013 | -2.26444943 | 2.99353458 |
| H | -4.59524508 | -2.59113072 | 2.48715226 |
| H | -5.97726491 | -1.84292601 | 2.31497199 |
| O | -0.05019248 | 6.12280879 | -1.85421534 |
| H | 0.22957249 | 6.17805174 | -0.91004796 |
| H | -0.59795218 | 5.29736152 | -1.85217734 |
| O | -2.75022603 | -2.17248272 | -3.37018178 |
| H | -2.02155376 | -2.15537734 | -4.04988334 |
| H | -2.89757996 | -1.24726330 | -3.05207486 |
| O | 1.00558423 | -2.59513526 | 5.43457586 |
| H | 0.12728624 | -2.19940046 | 5.21788650 |
| H | 1.53495402 | -1.81694586 | 5.77749007 |
| O | 1.61371011 | 4.85972704 | 5.26828795 |
| H | 2.61606486 | 5.01759373 | 5.39391438 |
| H | 1.15252899 | 5.39289608 | 5.93600294 |
| O | 4.22372445 | 5.05621065 | 5.31301991 |
| H | 4.37635051 | 4.13990602 | 5.65437091 |
| H | 4.36743581 | 4.96394107 | 4.33854185 |
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