Computational determination of equilibrium geometry and dissociation energy of the water dimer

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The equilibrium geometry and dissociation energy of the water dimer have been determined as accurately as technically possible. Various quantum chemical methods and high-quality basis sets —that is, at the level of a nearly complete basis— have been applied, and both the intermolecular separation and the deformation of the donor and acceptor molecules have been optimized at the level of CCSD(T) theory. The O–O distance is determined to $R = 291.2 \pm 0.5$ pm and the electronic dissociation energy to $D_e = 21.0 \pm 0.2$ kJ mol^{-1}, with respect to dissociation into two isolated water molecules at equilibrium. Accounting for zero-point vibrational energy, the theoretical prediction for the dissociation energy becomes $D_0 = 13.8 \pm 0.4$ kJ mol^{-1}, a result which is open to direct experimental verification.