STRUCTURE, ENERGETICS AND FINITE TEMPERATURE OH-STRETCH SPECTROSCOPY OF THE WATER HEXAMER

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We use a newly developed and recently reparameterized classical empirical simulation model for water that involves explicit three-body interactions to study the water hexamer. The lowest energy isomer is found to be one of the cage structures, in agreement with vibration-rotation-tunneling experiments. Furthermore, the relative energy ordering of the different isomers is in good agreement with CCSD(T) calculations. The OH-stretch spectra calculated for the low-energy structures is compared to *ab initio* and density functional theory calculations. Finally, replica-exchange molecular dynamics were performed from 40 to 194 K, showing the cage isomer has the lowest free energy from 0 to 70 K, and the book isomer has the lowest free energy from 70 to 194 K. The OH-stretch spectra were calculated from these simulations, leading to a re-assignment of the peaks in recent experimental spectra.