VIBRATIONAL SPECTRA AND ENERGETICS OF THE WATER HEPTAMER ANION

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In this work we analyze the vibrational spectra of the $(H_2O)_7^-$ cluster obtained by the Yale part of the team. The spectrum is interesting due to the appearance of different $(H_2O)_7^-$ isomers depending on the number of attached Ar atoms. Parallel tempering Monte Carlo simulations performed using a one-electron model Hamiltonian with Drude oscillators to account for the polarization effects and dispersion interactions[a] are used to identify low-lying isomers of $(H_2O)_7^-$. Selected low-energy isomers are then characterized by means of the all-electron Becke3LYP, MP2, and CCSD(T) methods. We propose an assignment of the observed spectra based on comparison of calculated harmonic spectra and electron binding energies with the corresponding experimental values.

[a] Wang, F.; Jordan, K. D. *J. Chem. Phys.* **2001**, *114*, 10717.