Hydrogen Bonding in Water-Methanol and Water-Ammonia Clusters

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Large molecular clusters can be considered as intermediate states between gas and condensed phases, and information about them can help us understand condensed phases. In this work, ab initio quantum mechanical methods have been used to examine clusters formed of methanol, ammonium and water molecules. The main goal was to obtain information about the intermolecular interactions and the structure of the clusters at the molecular level. The results of the calculations were compared to the available experimental information regarding the liquid methanol/water and ammonium/water mixtures and to the molecular dynamics and Monte Carlo simulations. The structures, energetics, and vibrational spectra of the first few ($n \leq 6$) water, methanol and ammonia clusters obtained from electronic structure calculations will be presented.