Solvation of *tert*-Butyl Alcohol in Water: An Effective Fragment Potential Study

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Recent theoretical and experimental studies of alcohol-water solutions provide evidence for incomplete mixing at the molecular level and retention of the structure of bulk water. To predict the level of mixing and other thermodynamic properties, it is necessary to investigate the intermolecular interactions of liquids. Structure and clustering patterns of tert-butyl alcohol (TBA) aqueous solutions are analyzed using molecular dynamics simulations with the effective fragment potential method (EFP). EFP is a polarizable model potential in which all parameters are obtained from a set of preparatory *ab initio* calculations on isolated fragment molecules. Thus, EFP does not contain any empirical fitted parameters and provides first-principles-based description of intermolecular interactions. TBA solutions with 0.01, 0.03, 0.06 TBA mole fractions are investigated to identify aggregation patterns of TBA molecules and behavior of bulk water as perturbed by the TBA molecules. Radial distribution functions and vibrational frequency calculations are utilized to analyze the results of these simulations.