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Modeling Amphiphilic Solutes in a Jagla Solvent ZHIQIANG SU, Center for Polymer Studies and Dept of Physics, Boston University, SERGEY V. BULDYREV, Dept of Physics, Yeshiva University, PABLO G. DEBENEDETTI, Dept of Chemical and Biological Engineering, Princeton University, PETER J. ROSSKY, Dept of Chemistry and Biochemistry, College of Natural Science, The University of Texas at Austin, H.EUGENE STANLEY, Center for Polymer Studies and Dept of Physics, Boston University — Methanol is an amphiphilic solute whose aqueous solutions exhibit distinctive physical properties. The volume change upon mixing, for example, is negative across the entire composition range, indicating strong association. We explore the corresponding behavior of a Jagla solvent, which has been previously shown to exhibit many of the anomalous properties of water. We consider two models of an amphiphilic solute: (i) a "dimer" model, which consists of one hydrophobic hard sphere linked to a Jagla particle with a permanent bond, and (ii) a "monomer" model, which is a limiting case of the dimer, formed by concentrically overlapping a hard sphere and a Jagla particle. Using discrete molecular dynamics, we calculate the thermodynamic properties of the resulting solutions. We systematically vary the set of parameters of the dimer and monomer models and find that one can readily reproduce the experimental behavior of the excess volume of the methanol-water system as a function of methanol volume fraction. We compare the pressure and temperature dependence of the excess volume and the excess enthalpy of both models with experimental data on methanol-water solutions and find qualitative agreement in most cases. We also investigate the solute effect on the temperature of maximum density and find that the effect of concentration is orders of magnitude stronger than measured experimentally.

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