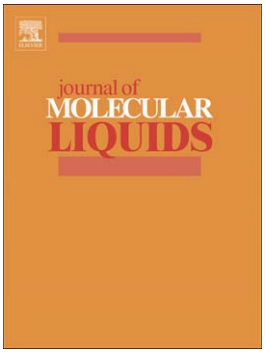

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Microstructures, Interactions and Dynamics Properties Studies of Aqueous Guanidinium Triflate Ionic Liquid from Molecular Dynamics Simulations

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Abstract

In order to understand the phase equilibrium behavior of aqueous ionic liquids (ILs) guanidinium triflate [gua][OTf] solution (binary solvent) at 7 different molar fractions of water ranged from 0.1 to 0.7 at 440.15 K classical molecular dynamic simulations were performed. The simulations measured changes in different properties such as density, structural, bonding properties (radial distribution function, water clustering and hydrogen bonding) and dynamic property (diffusion coefficient). The analysis of radial distribution and spatial distribution functions revealed a significant long-range structural correlation between IL and water. Water molecules intercalated in the coordination shell of both ions, thus