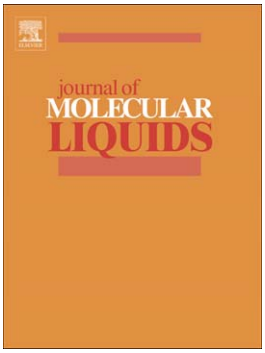

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On the composition dependence of thermodynamic, dynamic and dielectric properties of water - dimethyl sulfoxide model mixtures. NPT molecular dynamics simulation results.

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Abstract

We have systematically examined available molecular dynamics (MD) simulation results for thermodynamic, dynamic and dielectric properties of water - dimethyl sulfoxide (DMSO) mixtures with the purpose of analyzing their discrepancies with experimental data. To get a more profound insight into the behavior of these mixtures, we have performed constant pressure - constant temperature simulations in the entire composition range at 1 bar and 298.15 K and compared the obtained results with experimental data and previous findings. The SPC-E water model was used in combination with the P1, P2 and OPLS united atom models for dimethyl sulfoxide. The dependencies of density, of excess mixing volume and potential energy, of the self-diffusion coefficients of species, and of the dielectric constant on the mixture composition are discussed. The evolution of the hydrogen bonding network was analyzed in terms of the average number of hydrogen bonded molecules and of the distribution of bonding states. In conclusions we discuss the capability of the united atom models for DMSO to adequately reproduce an ample set of properties of these mixtures and outline future work.

Keywords: water models, dimethyl sulfoxide models, thermodynamic properties, self-diffusion coefficient, dielectric constant, molecular dynamics

1. Introduction

It is our great pleasure to dedicate this manuscript to Prof. Vojko Vlachy on the occasion of his 70th birthday. We appreciate his mentorship, friendly

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