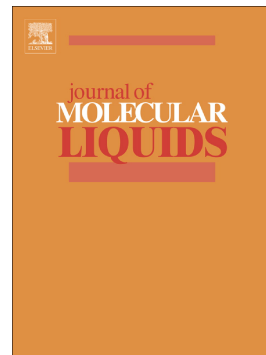


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Microscopic Characterization of Amino Acid Ionic Liquids - Water Mixtures

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Abstract

The properties of ionic liquids containing glycinate anion and 1-ethyl-3-methylimidazolium or cholinium or methylpiperazinium cation mixed with water were studied in the full composition range in this manuscript. Relevant thermodynamic properties, such as excess molar volume or self-diffusion coefficients, were predicted to infer deviations from ideality. Nanostructuring and intermolecular forces in the mixed fluids were also analysed together with dynamic properties. The behaviour of these liquid mixtures at vacuum interfaces were also presented in this work. Likewise, the effect of static and dynamic external electric fields on fluid's dynamics and intermolecular forces were analysed.

Keywords: ionic liquids; water; mixtures: molecular dynamics, external electric fields; vacuum interfaces.

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