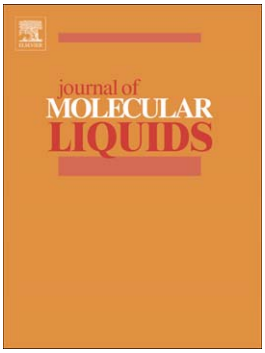

Structural effects on dynamic and energetic properties of mixtures of ionic liquids and water

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Structural effects on dynamic and energetic properties of mixtures of ionic liquids and water

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Abstract

The aim of this study is to improve our understanding of the microscopic and macroscopic properties of mixtures of ionic liquids with water, in the context of working pairs for absorption heat cycles. We report a molecular dynamics study of dynamic properties (viscosity and diffusion coefficients), water solvation (free energy and local solvation environments) and hydrogen bonding in mixtures of six ionic liquids with water, at two concentrations $x_{H_2O} = 0.104$ and $x_{H_2O} = 0.900$. Three anions, methanesulfonate, dicyanamide and acetate; and two cations, N-ethylpyridinium and cholinium, were chosen due to their potential for water absorption and halogen-free structures. Simulation results capture the trends of experimental data, and were interpreted in terms of the molecular structures and interactions. The strength of hydrogen bonding is a major criterion determining the affinity of an ionic liquid towards water. In particular, the cholinium cations compete with water establishing hydrogen bonds with the acetate anions and this is not favorable in terms of water affinity. Dicyanamide anions lead to the systems with lower viscosity.

Keywords: ionic liquids, water, molecular simulation, solvation, hydrogen bonding, transport properties

1. Introduction

Ionic liquids (ILs) are among the most promising classes of solvents, reaction or separation media or technological fluids of the XXI century [1, 2]. Due to their tuneable physical and chemical properties, and recyclability, ionic liquids appear as alternatives for many applications [3–5], within the trend of sustainable chemistry, reduce the environmental footprint of chemical and processes. Concerns of sustainability are central when choosing alternatives to traditional industrial processes.

Among the potential uses of ionic liquids, absorption heat pumps present an opportunity to reduce the emissions of greenhouse gases in heating/cooling systems. The advantages and challenges of this technology was already treated in detail [6, 7]. The scientific community is seeking alternatives to improve the performance of traditional working pairs of refrigerant/absorbent and amidst the most promising working pairs are those based on ILs together with water as refrigerant [8, 9].

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