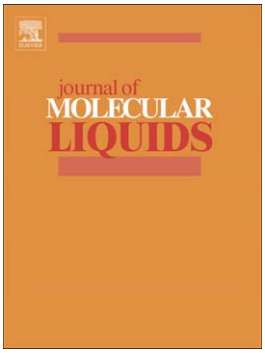

A joint experimental and computational study on ¡!–[INS][E]–¿e¡!–[/INS]–¿thylammonium ¡!–[INS][N]–¿n¡!–[/INS]–¿itrate-¡!–[INS][E]–¿e¡!–[/INS]–¿thylene ¡!–[INS][G]–¿g¡!–[/INS]–¿lycol 1:1 mixture. Structural, kinetic, dynamic and spectroscopic properties

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A joint experimental and computational study on Ethylammonium Nitrate-Ethylene Glycol 1:1 mixture. Structural, kinetic, dynamic and spectroscopic properties

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Abstract

The intrinsic molecular polarity of a molecule, *i.e.* its dipole moment, seems to have an important role in the mixing process of an Ionic Liquid and a Molecular Liquid. In this work we report a complete study on the overall organization of a 1:1 binary mixture of Ethylammonium Nitrate and Ethylene Glycol by means of Wide Angle X-Ray Scattering, Raman Spectroscopy and Far Infrared Spectroscopy. The interpretation of all the experimental data was aided by a variety of computational models obtained via Classical Molecular Dynamics, *ab initio* Molecular Dynamics and DFT calculations. We observe that in the samples examined the Nitrate anion is strongly solvated by glycol molecules. This interaction has notable consequences on experimental observations.

Keywords

Ionic Liquids; Binary Mixture; Wide Angle X-Ray Scattering; Spectroscopy; Computational Simulations

Introduction

The wide potential application of Ionic Liquids (ILs) has a strong appealing in both academy[1] and industry[2,3]. Their characteristic bulk molecular organization[4–7] leads to unique properties that can be tuned by chemical substitutions on the cation and/or the anion[8–10]. The possibility of doing so gave them the fame of "task specific solvents"[11–13]. If within the cation molecular structure is