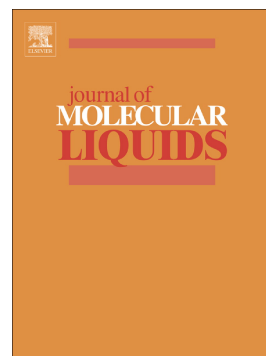


Accepted Manuscript

Insights into interactions between 1-butyl-3-methylimidazolium dicyanamide and molecular solvents: γ -valerolactone, γ -butyrolactone and propylene carbonate. Volumetric properties and MD simulations



Nebojša Zec, Abdenacer Idrissi, Marija Bešter-Rogač, Milan Vraneš, Slobodan Gadžurić

PII: S0167-7322(18)32375-4
DOI: doi:[10.1016/j.molliq.2018.07.079](https://doi.org/10.1016/j.molliq.2018.07.079)
Reference: MOLLIQ 9400
To appear in: *Journal of Molecular Liquids*
Received date: 8 May 2018
Revised date: 18 June 2018
Accepted date: 17 July 2018

Please cite this article as: Nebojša Zec, Abdenacer Idrissi, Marija Bešter-Rogač, Milan Vraneš, Slobodan Gadžurić, Insights into interactions between 1-butyl-3-methylimidazolium dicyanamide and molecular solvents: γ -valerolactone, γ -butyrolactone and propylene carbonate. Volumetric properties and MD simulations. *Molliq* (2018), doi:[10.1016/j.molliq.2018.07.079](https://doi.org/10.1016/j.molliq.2018.07.079)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

Insights into interactions between 1-butyl-3-methylimidazolium dicyanamide and molecular solvents: γ -valerolactone, γ -butyrolactone and propylene carbonate. Volumetric properties and MD simulations

Nebojša Zec^{1,2*}, Abdenacer Idrissi³, Marija Bešter-Rogač⁴, Milan Vraneš² and Slobodan Gadžurić²

¹German Engineering Materials Science Centre (GEMS) at Heinz Maier-Leibnitz Zentrum (MLZ) Helmholtz-Zentrum Geesthacht GmbH, Lichenbergstr. 1, 85748 Garching bei München, Germany

²Faculty of Science, Department of Chemistry, Biochemistry and Environmental Protection, University of Novi Sad, Trg Dositeja Obradovića 3, 21000 Novi Sad, Serbia

³University of Lille, Science and Technology, LASIR (UMR CNRS A8516), Bât. C5, Cité Scientifique, 59655 Villeneuve d'Ascq Cedex, France

⁴Faculty of Chemistry and Chemical Technology, University of Ljubljana, Večna pot 113, 1000 Ljubljana, Slovenia

Abstract

Experimental densities of the binary mixtures containing 1-butyl-3-methylimidazolium dicyanamide ionic liquid, [C₁C₄im][DCA] and molecular solvent: γ -valerolactone (γ VL) or propylene carbonate (PC) were measured at temperatures from (293.15 to 313.15) K and at a pressure of 0.1 MPa over the whole composition range. Related excess molar volumes were calculated and fitted using Redlich-Kister's polynomial equation and compared with previously measured IL + γ -butyrolactone (γ BL) mixture. Obtained values are negative in the whole range of ionic liquid mole fraction and at all temperatures. Molecular dynamics simulations were applied to quantify the intermolecular interactions in pure liquids and binary mixtures, hydrogen bond, dipole-dipole and stacking interactions. Excess molar volumes obtained from MD simulations follow the trend observed in the experiment. Orientational correlations were characterized by several combined angular and distance distribution functions between first neighbour molecules. Results suggest that strength of solvent-solvent interactions plays a significant role in the observed difference in volumetric properties of these binary mixtures. Calculated hydrogen bond geometry indicates that the hydrogen bond interaction in the three molecular solvents is weak and follows the order PC > γ BL > γ VL.

* Corresponding author: Tel: +49 89 289 10748; E-mail: nebojsa.zec@hzg.de

Download English Version:

<https://daneshyari.com/en/article/7841763>

Download Persian Version:

<https://daneshyari.com/article/7841763>

[Daneshyari.com](https://daneshyari.com)