

Accepted Manuscript

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PII: S0167-7322(18)32928-3
DOI: doi:[10.1016/j.molliq.2018.08.031](https://doi.org/10.1016/j.molliq.2018.08.031)
Reference: MOLLIQ 9476
To appear in: *Journal of Molecular Liquids*
Received date: 5 June 2018
Accepted date: 6 August 2018



Please cite this article as: J.L. Trenzado, R. Alcalde, M. Atilhan, S. Aparicio , Molecular dynamics and experimental characterization of [BMIM][BF₄] and [BMIM][PF₆] with ether cosolvent binary mixtures. Molliq (2018), doi:[10.1016/j.molliq.2018.08.031](https://doi.org/10.1016/j.molliq.2018.08.031)

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Molecular Dynamics and Experimental Characterization of [BMIM][BF₄] and [BMIM][PF₆] with Ether Cosolvent Binary Mixtures

J. L. Trenzado,^{*a} R. Alcalde,^b M. Atilhan,^{c,d} S. Aparicio^{*b}

^a Departamento de Física, Universidad de Las Palmas de Gran Canaria, 35017 Las Palmas G.C., Spain

^b Department of Chemistry, University of Burgos, 09001 Burgos, Spain

^c Department of Chemical Engineering, Texas A&M University at Qatar, Doha, Qatar

^d Gas and Fuels Research Center, Texas A&M University, College Station, TX, USA

*Corresponding authors: jtrenzado@dfis.ulpgc.es (J. L. T.), sapar@ubu.es (S. A.)

ABSTRACT: The properties of binary liquid mixtures of 1-butyl-3-methylimidazolium [BF₄] / [PF₆] with diethylene glycol methyl ether or diethylene glycol dimethyl ether were studied in the full composition range as a function of temperature. Excess and mixing properties were obtained from experimental density and viscosity data and analysed in terms of intermolecular forces and non-ideal mixing behaviour. The microscopic features were analysed with molecular dynamics simulations, which allowed characterizing intermolecular forces, hydrogen bonding, and liquid structuring as a function of the involved molecules and ions together with the effect of mixtures mole fraction. The joint experimental and computational study enables both microscopic and macroscopic characterization of the studied mixed fluids, thus this work contributes to the knowledge of the effect of molecular solvents for tuning ionic liquid properties in terms of the involved intermolecular forces and microscopic features.

Keywords: Alkylimidazolium ionic liquids, Mixtures, Ether, Molecular simulation, Thermophysics.

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