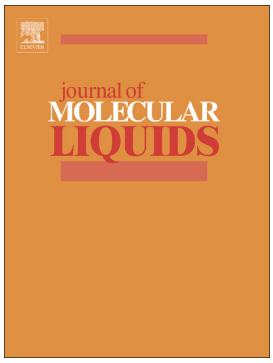

Atomistic insights into the thermodynamics, structure, and dynamics of ionic liquid 1-hexyl-3-methylimidazolium hexafluorophosphate via molecular dynamics study

Zeinab Pouramini, Ali Mohebbi, Mohammad Hossein Kowsari

PII: S0167-7322(17)33010-6
DOI: doi: 10.1016/j.molliq.2017.09.043
Reference: MOLLIQ 7880

To appear in: *Journal of Molecular Liquids*

Received date: 8 July 2017
Revised date: 13 September 2017
Accepted date: 13 September 2017

Please cite this article as: Zeinab Pouramini, Ali Mohebbi, Mohammad Hossein Kowsari , Atomistic insights into the thermodynamics, structure, and dynamics of ionic liquid 1-hexyl-3-methylimidazolium hexafluorophosphate via molecular dynamics study, *Journal of Molecular Liquids* (2017), doi: 10.1016/j.molliq.2017.09.043

Atomistic Insights into the Thermodynamics, Structure, and Dynamics of Ionic Liquid 1-Hexyl-3-methylimidazolium Hexafluorophosphate via Molecular Dynamics Study

Zeinab Pouramini [a], Ali Mohebbi [a,*], Mohammad Hossein Kowsari [b]

[a] Department of Chemical Engineering, Faculty of Engineering, Shahid Bahonar University of Kerman, Kerman, Iran

[b] Department of Chemistry and Center for Research in Climate Change and Global Warming (CRCC), Institute for Advanced Studies in Basic Sciences (IASBS), Zanjan, Iran

Abstract

Molecular dynamics (MD) simulations were performed to compute the properties of the ionic liquid 1-hexyl-3-methylimidazolium hexafluorophosphate, [hmim][PF_6], at three different temperatures (298, 323, and 348 K) and atmospheric pressure. Thermodynamic, structural, and dynamical properties, such as average density, isobaric thermal expansion coefficient, isothermal compressibility factor, radial distribution function (RDF), spatial distribution function (SDF), mean square displacement (MSD) and velocity autocorrelation function (VACF) were computed and interpreted. The ionic self-diffusion coefficients were calculated using both the Einstein and Green–Kubo formulas and it was found that the cation diffuses faster than the anion and contributes more in the electric current. The ionic self-diffusion coefficients obtained from the Green-Kubo method agreed reasonably well with the experimental data in compared to the Einstein method. Also, the self-diffusion coefficients obtained from the two methods were used to calculate the ionic conductivity from the Nernst−Einstein equation. The effects of the system size and simulation run-time on

* Corresponding author: Tel./Fax: +98 3432118298

E-mail addresses: amohebbi2002@yahoo.com, amohebbi@uk.ac.ir