

# Accepted Manuscript

Research paper

Molecular dynamics simulation of the ionic liquid N-octylpyridinium tetrafluoroborate and acetonitrile: Thermodynamic and structural properties

Siwen Zhou, Guanglai Zhu, Xianqu Kang, Qiang Li, Maolin Sha, Zhifeng Cui, Xinsheng Xu

PII: S0009-2614(18)30313-0  
DOI: <https://doi.org/10.1016/j.cplett.2018.04.028>  
Reference: CPLETT 35584

To appear in: *Chemical Physics Letters*

Received Date: 10 February 2018  
Revised Date: 10 April 2018  
Accepted Date: 12 April 2018

Please cite this article as: S. Zhou, G. Zhu, X. Kang, Q. Li, M. Sha, Z. Cui, X. Xu, Molecular dynamics simulation of the ionic liquid N-octylpyridinium tetrafluoroborate and acetonitrile: Thermodynamic and structural properties, *Chemical Physics Letters* (2018), doi: <https://doi.org/10.1016/j.cplett.2018.04.028>

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.



# Molecular dynamics simulation of the ionic liquid N-octylpyridinium tetrafluoroborate and acetonitrile: Thermodynamic and structural properties

Siwen Zhou<sup>a</sup>, Guanglai Zhu<sup>a,\*</sup>, Xianqu Kang<sup>a</sup>, Qiang Li<sup>a</sup>, Maolin Sha<sup>b</sup>, Zhifeng Cui<sup>a</sup>, Xinsheng Xu<sup>a</sup>

<sup>a</sup>*Institute of Atomic and Molecular Physics, Anhui Normal University, Wuhu 241000, China*

<sup>b</sup>*Department of Chemistry and Chemical Engineering, Hefei Normal University, Hefei 230061, China*

**Abstract:** Using molecular dynamics simulation, the research obtained the thermodynamic properties and microstructures of the mixture of N-octylpyridinium tetrafluoroborate and acetonitrile, including density, self-diffusion coefficients, excess properties, radial distribution functions (RDFs) and spatial distribution functions (SDFs). Both RDFs and SDFs indicate that the local microstructure of the polar region is different from the nonpolar region with different mole fraction of ionic liquids. Acetonitrile could increase the order of the polar regions. While with acetonitrile increasing, the orderliness of the nonpolar region increases firstly and then decreases. In relatively dilute solution, ionic liquids were dispersed to form small aggregates wrapped by acetonitrile.

**Keywords:** N-octylpyridinium tetrafluoroborate; Molecular dynamics simulation; Thermodynamic property; Microstructure.

## 1. Introduction

Room temperature ionic liquids (RTILs) are special ionic compounds that are liquid at room temperature or near room temperature, which generally consists of organic cation and inorganic anion [1]. In recent years, more and more researchers pay attention to ionic liquids that are a new kind of green solvent [2-6].

Compared with traditional solvent, ionic liquids have many superior characteristics,

---

\* Corresponding author, E-mail address: zhglai@mail.ahnu.edu.cn

Download English Version:

<https://daneshyari.com/en/article/7837680>

Download Persian Version:

<https://daneshyari.com/article/7837680>

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