### Accepted Manuscript

Density and thermodynamic performance of energetic ionic liquids based on 1-alkyl/esteryl-4-amino-1,2,4-triazolium

Tian Tian, Xiaoling Hu, Ping Guan, Shuangjie Wang, Xiaoqi Ding

PII: S0167-7322(17)32029-9

DOI: doi:10.1016/j.molliq.2017.09.024

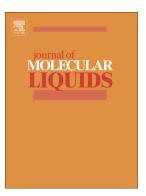
Reference: MOLLIQ 7860

To appear in: Journal of Molecular Liquids

Received date: 10 May 2017 Revised date: 29 August 2017 Accepted date: 7 September 2017

Please cite this article as: Tian Tian, Xiaoling Hu, Ping Guan, Shuangjie Wang, Xiaoqi Ding, Density and thermodynamic performance of energetic ionic liquids based on 1-alkyl/esteryl-4-amino-1,2,4-triazolium. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:10.1016/j.molliq.2017.09.024

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.



# ACCEPTED MANUSCRIPT

## Density and Thermodynamic Performance of Energetic Ionic Liquids Based on 1-alkyl/esteryl-4-amino-1,2,4-triazolium

Tian Tian\*, Xiaoling Hu, Ping Guan, Shuangjie Wang and Xiaoqi Ding

School of Natural and Applied Science, Northwestern Polytechnical University, the Key Laboratory of Space Applied Physics and Chemistry, Ministry of Education, Xi'an 710072, China

**Abstract:** Energetic ionic liquids (EILs) based upon nitrate, perchlorate and dicyandiamide salts of 1-alky/esteryl-4-amino-1,2,4-triazolium are synthesized. The structures are characterized by  $^{1}$ H NMR, FT-IR and element analysis. The density, constant volume combustion heat and specific heat capacity of these EILs are determined through experiment. Their interaction energies of ion pairs, standard molar volume, standard molar heat capacity and standard molar enthalpy of formation are calculated by DFT/B3LYP/6-311+G(d,p) and further researched. The themodynamics function data relative to the reference temperature (298 K) are obtained based on the  $C_p$  from 303-353 K. The influences of temperature, molecular structure and interaction energy of ion pairs on  $\rho$  and  $C_p$  are also discussed systematically. In addition, the density and thermodynamic properties of EILs are deduced from theoretical calculation and experimental evidences. As a result, the physicochemical properties estimation of EILs using theoretical calculation method can be applied in the field of modern military, science, etc.

**Keywords:** energetic ionic liquids; density; specific heat capacity; standard molar enthalpy of formation; DFT/B3LYP/6-311+G(d,p)

#### Introduction

Ionic liquids (ILs), organic salts with melting points less than 300 °C, have recently been the focus of much research owing to the variety of desirable properties<sup>1</sup>. Energetic ionic liquids (EILs) are a kind of functional ionic liquids, which adopting nitrogen-rich triazole-substituted derivatives as cation or anion <sup>2-4</sup> and possessing high

#### Download English Version:

## https://daneshyari.com/en/article/7843504

Download Persian Version:

https://daneshyari.com/article/7843504

<u>Daneshyari.com</u>