

Accepted Manuscript

Physicochemical properties, NMR, Ab initio calculations and the molecular interactions in a binary mixture of N-methylimidazole and water

Haiyun Hou, Baojuan Jiao, Qingzhong Li, Xinlu Lin, Min Liu, Haojun Shi, Li Wang, Songtao Liu



PII: S0167-7322(17)35578-2
DOI: doi:[10.1016/j.molliq.2018.02.098](https://doi.org/10.1016/j.molliq.2018.02.098)
Reference: MOLLIQ 8740
To appear in: *Journal of Molecular Liquids*
Received date: 19 November 2017
Revised date: 28 January 2018
Accepted date: 21 February 2018

Please cite this article as: Haiyun Hou, Baojuan Jiao, Qingzhong Li, Xinlu Lin, Min Liu, Haojun Shi, Li Wang, Songtao Liu , Physicochemical properties, NMR, Ab initio calculations and the molecular interactions in a binary mixture of N-methylimidazole and water. The address for the corresponding author was captured as affiliation for all authors. Please check if appropriate. Molliq(2017), doi:[10.1016/j.molliq.2018.02.098](https://doi.org/10.1016/j.molliq.2018.02.098)

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.

Physicochemical Properties, NMR, Ab initio Calculations and the Molecular Interactions in a Binary Mixture of *N*-methylimidazole and Water

Haiyun Hou^{a*}, Baojuan Jiao^b, Qingzhong Li^c, Xinlu Lin^a, Min Liu^a, Haojun Shi^a, Li Wang^a, Songtao

Liu^a

^a College of Environmental and Chemical Engineering, Xi'an Polytechnic University, Xi'an, 710048, China

^b School of Chemical Engineering, Xi'an University, Xi'an, 710065, China

^c Laboratory of Theoretical and Computational Chemistry, School of Chemistry and Chemical Engineering, Yantai University, Yantai, 264005, China

ABSTRACT: For a binary mixture of *xN*-methylimidazole (hereafter abbreviated to *N*-mim) + (1-*x*) water, over a full molar fraction range, the mass density, sound velocity, refractive index, viscosity, mixing enthalpy, conductivity, and pH at (298.15, 308.15, 318.15) K and 0.1 MPa, and ¹H-NMR and ¹³C-NMR at room temperature combined with Ab initio calculations, were measured and carried out. The excess molar volume (V_m^E), sound deviation (Δu), refractive index deviation (Δn_D), viscosity deviation ($\Delta \eta$), excess Gibbs energy of activation of viscous flow (ΔG^{*E}), molar mixing enthalpy ($\Delta_{\text{mix}}H_m$), ¹H-NMR chemical shift changes of *N*-mim and water protons ($\Delta \delta_H$), ¹³C-NMR chemical

Download English Version:

<https://daneshyari.com/en/article/7842685>

Download Persian Version:

<https://daneshyari.com/article/7842685>

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