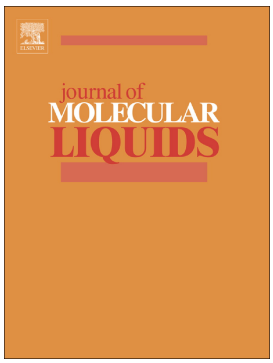

Physicochemical properties, NMR, Ab initio calculations and the molecular interactions in a binary mixture of N-methylimidazole and water

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
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

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 *x*N-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 ^{1}H-NMR and ^{13}C-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 ($\Delta_{mix}H_m$), ^{1}H-NMR chemical shift changes of *N*-mim and water protons ($\Delta\delta_H$), ^{13}C-NMR chemical