

Structural features of selected protic ionic liquids based on a super-strong base.

Alessandro Triolo^{1,*}, Fabrizio Lo Celso², Carlo Ottaviani¹, Pengju Ji³, Giovanni Battista Appetecchi⁴, Francesca Leonelli⁵, Dean S. Keeble⁶ and Olga Russina^{7,*}.

¹ Laboratorio Liquidi Ionici, Istituto Struttura della Materia, Consiglio Nazionale delle Ricerche, (ISM-CNR) Rome, Italy

² Department of Physics and Chemistry, Università di Palermo, Palermo, Italy.

³ Center of Basic Molecular Science (CBMS), Department of Chemistry, Tsinghua University, Beijing 100084, China

⁴ ENEA, SSPT-PROMAS-MATPRO Technical Unit, Rome, Italy.

⁵ Department of Environmental Biology, University of Rome Sapienza, Rome, Italy

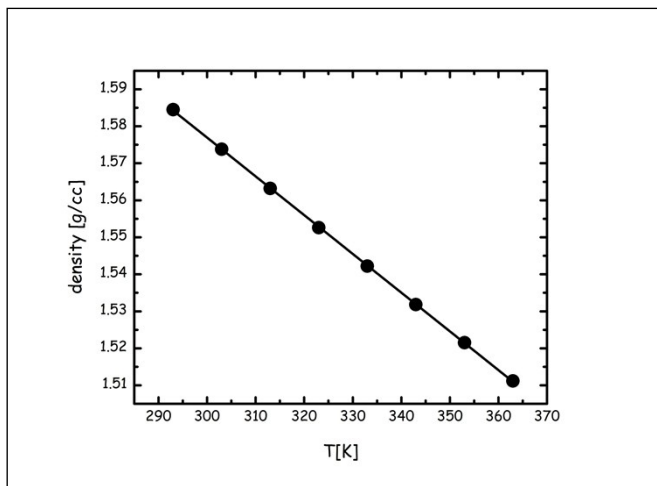
⁶ Diamond Light Source, Harwell Campus, Didcot OX11 0DE UK

⁷ Department of Chemistry, University of Rome Sapienza, Rome, Italy

Corresponding Authors: A. T. (triolo@ism.cnr.it); O.R. (olga.russina@uniroma1.it)

Supporting information

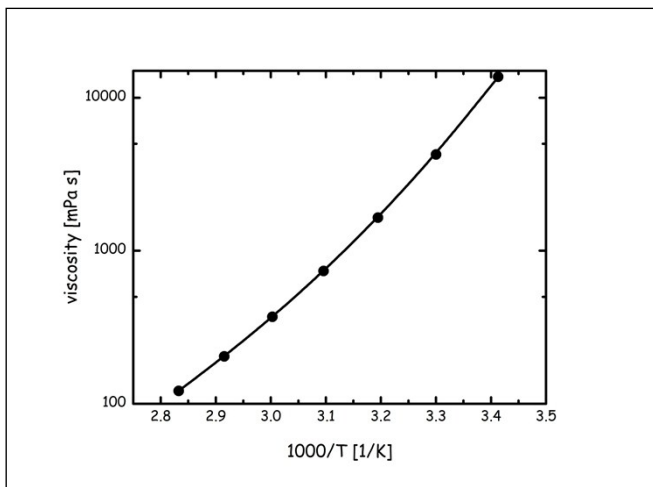
Density.



Density of [DBUH][IM14]. Experimental data have been modelled with a linear trend (continuous line):

$$\rho \text{ [g/cc]} = a \cdot T \text{ [K]} + b, \text{ with } a = 0.001047 \text{ (} 3 \cdot 10^{-6} \text{) K}^{-1} \text{ and } b = 1.891 \text{ (} 1 \cdot 10^{-3} \text{) (} R^2 = 0.99994 \text{)}$$

Viscosity.

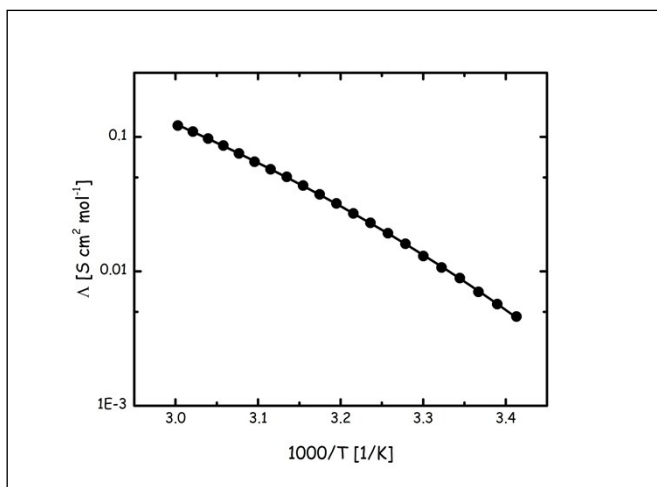


Viscosity of [DBUH][IM14]. Experimental data have been modelled with the trend (continuous line):

$$\eta(\text{mPa s}) = \eta_0 \exp [B/(T-T_0)]; \text{ with } \eta_0 = 0.070 (0.001) \text{ mPa s, } B=1172 (1) \text{ K}^{-1}, T_0=197 (1) \text{ K.}$$

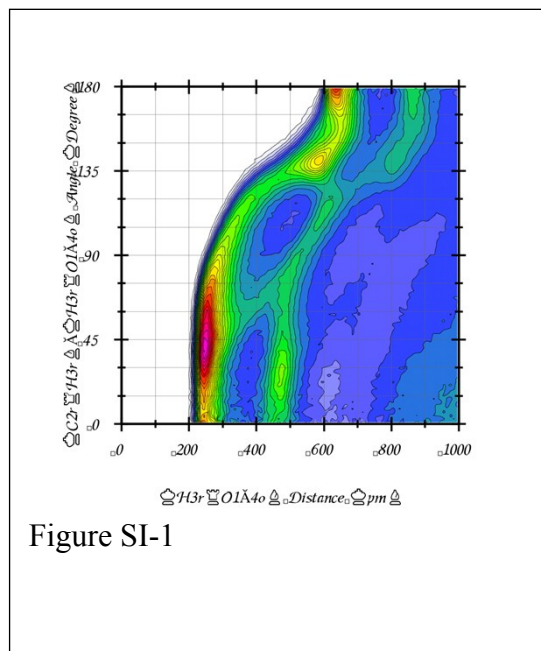
($R^2=0.99992$)

Molar conductance.



Molar conductance of [DBUH][IM14]. Experimental data have been modelled with the trend (continuous line):

$$\Lambda \text{ (S cm}^2 \text{ mol}^{-1}\text{)} = \Lambda_0 \exp [-B/(T-T_0)]; \text{ with } \Lambda_0 = 139 \text{ (3) S cm}^2 \text{ mol}^{-1}, B=890 \text{ (2) K}^{-1}, T_0=208 \text{ (2) K. (R}^2=0.99985\text{)}$$



Combined Distribution Function obtained from the MD study of an aprotic IL based on the [IM14] anion and the 1-octyl,3-methylimidazolium cation ([C8mim][IM14]), highlighting the structural features of the hydrogen bonding interactions therein between the anion and the acidic H atom between the two imidazolium Nitrogen atoms.