

## DENSITY OF THE REFERENCE IONIC LIQUID [C6mim][NTf<sub>2</sub>] AT HIGH PRESSURES

João C. F. Diogo<sup>1</sup>, Fernando J. P. Caetano<sup>1,2</sup> and João M. N. A. Fareleira<sup>1\*</sup>

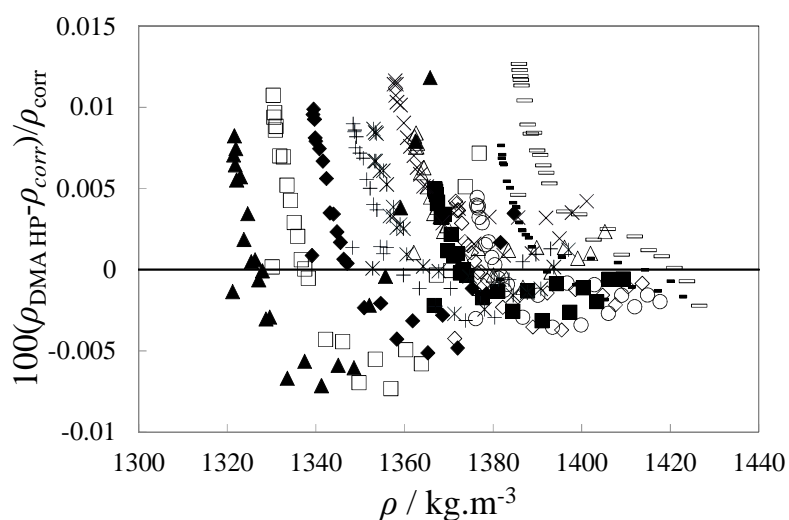
<sup>1</sup>Centro de Química Estrutural, Instituto Superior Técnico, Universidade Técnica de Lisboa, Av. Rovisco Pais, 1049-001 Lisbon, Portugal

<sup>2</sup>Universidade Aberta, R. da Escola Politécnica, 147, 1269-001 Lisbon, Portugal

\*Corresponding author: j.fareleira@ist.utl.pt

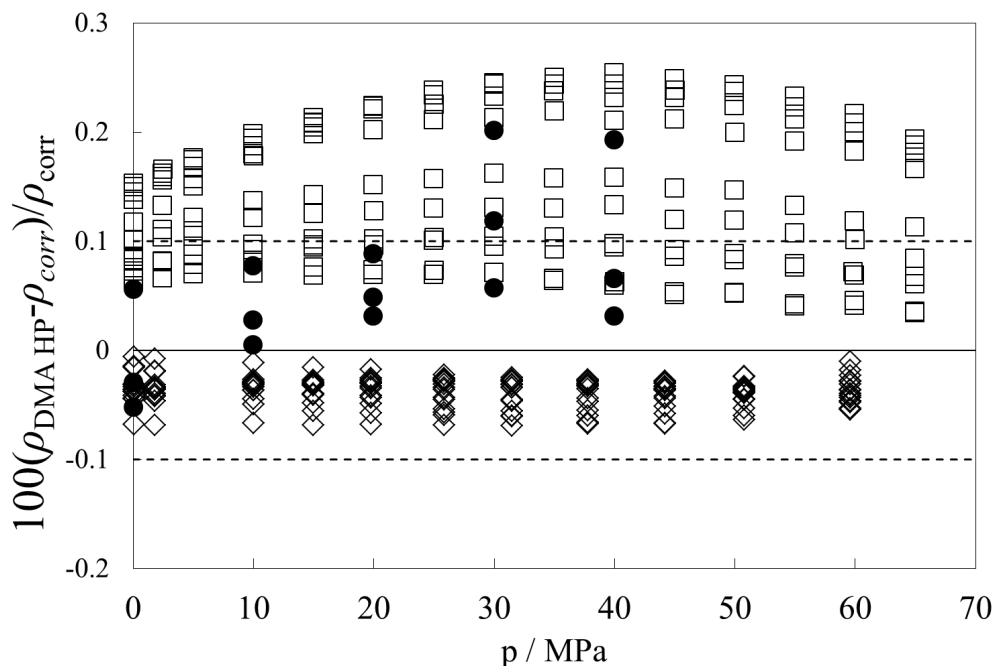
**Keywords:** Density, Ionic Liquid, [C6mim][NTf<sub>2</sub>], High pressure, U-tube densimeter.

**Introduction:** Density of the ionic liquid [C6mim][NTf<sub>2</sub>] – a reference ionic liquid for thermophysical properties, as proposed by IUPAC8[1,2] was measured using an Anton Paar density meter DMA HP. The basic experimental setup was described previously [3], and the modifications introduced in order to avoid water contamination of the sample are described in the presentation. The measurements were performed in the temperature range ( $283.15 \leq T \leq 353.15$ ) K and at pressures ( $0.1 \leq p \leq 65$ ) MPa. The water content of the samples was measured by Karl-Fisher coulometry, both before and after the measurements. As the viscosity of that ionic liquid is much higher than the viscosity of the fluids used in the calibration of the densimeter, a correction of the results became necessary, to account for the consequent error in the period of oscillation of the U-tube. For this purpose, the viscosity effect on the density measurements on the Anton Paar DMA HP was quantified using the viscosity standard specimen (200GW) from ZMK, GmbH. The experimental determination of the viscosity correction to the measured density is described and also the preliminary results of the density of [C6mim][NTf<sub>2</sub>] are compared with literature values[4-6].



**Figure 1.** Relative deviations,  $\Delta\rho = \rho_{\text{exp}} - \rho_{\text{corr}}$ , of the density of [C6mim][NTf<sub>2</sub>],  $\rho_{\text{exp}}$ , corrected for the viscosity effect, as a function of density. 283.15 K – open rectangles;

288.15 K – small black rectangles; 293.15 K – open circles; 298.15 K – open diamonds;  
 303.15 K – black squares; 308.15 K – open triangles; 313.15 K – x crosses; 318.15 K – stars;  
 323.15 K – crosses; ; 333.15 K – black diamonds; 343.15 K – open squares; 353.15 K – black triangles.



**Figure 2.** Relative density deviation of the [C6mim][NTf<sub>2</sub>] from literature density data, as a function of pressure. Open diamonds: Azevedo et al. [4] (DMA 512P, no viscosity correction); black circles - Kandil et al.[5] (DMA 512P, viscosity corrected); open squares - Esperança et al.[6] (DMA 512P, viscosity corrected).

**Conclusions:** Viscosity effect corrections were made to the [C6mim][NTf<sub>2</sub>] density data, measured in this work. The maximum correction was less than  $-0.11\%$ . The deviations of selected literature data<sup>4-6</sup> from the results obtained in this work are under  $\pm 0.3\%$  for [C6mim][NTf<sub>2</sub>] over the measurement temperature and pressure ranges.

#### References:

1. Marsh, K.; Bremmecke, J. F.; Chirico, R. D.; Frenkel, M.; Heintz, A.; Magee, J. W.; Peters, C. J.; Rebelo, L. P. N.; and Seddon, K. R., Thermodynamic and thermophysical properties of the reference ionic liquid: -hexyl-3-methylimidazolium bis(trifluorosulfonyl)imide (including mixtures). part 1. experimental methods and results (IUPAC Technical Report), *Pure Appl. Chem.* 81 (2009) 781–790.
7. Chirico, R. D.; Diky, Vladimir; Magee, J. W.; Frenkel, M.; and Marsh, K., Thermodynamic and thermophysical properties of the reference ionic liquid: -hexyl-3-methylimidazolium bis(trifluorosulfonyl)imide (including mixtures). Part

2. Critical evaluation and recommended property values (IUPAC Technical Report), *Pure Appl. Chem.* 81(2009) 791–828.
8. Abreu, S. B. E.; Avelino, H.; Caetano, F. J. P.; and Fareleira, J., Density of diisodecyl phthalate at temperatures from (283.15 to 363.15) K and pressures from (0.1 to 65) MPa, *J. Chem. Eng. Data* 55 (2010) 3525-3531.
9. de Azevedo, R. G.; Esperanca, J.; Szydowski, J.; Visak, Z. P.; Pires, P. F.; Guedes, H. J. R.; and Rebelo, L. P. N., Thermophysical and thermodynamic properties of ionic liquids over an extended pressure range: bmim NTf(2) and hmim NTf(2), *J. Chem. Thermodyn.* 37 (2007) 888-899.
10. Kandil, M. E.; Marsh, K. N.; and Goodwin, A. R. H., Measurement of the viscosity, density, and electrical conductivity of 1-hexyl-3-methylimidazolium bis(trifluorosulfonyl)imide at temperatures between (288 and 433) K and pressures below 50 MPa, *J. Chem. Eng. Data* 52 (2007) 2382-2387.
11. Esperança, J. M. S. S.; Guedes, H. J. R.; Lopes, J. N. C.; and Rebelo, L. P. N., Pressure-Density-Temperature (p-G-T) surface of [C6mim][NTf2], *J. Chem. Eng. Data* 53 (2008) 867–870.