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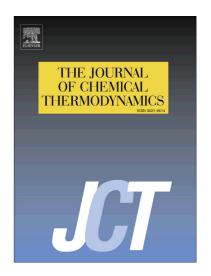
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## ACCEPTED MANUSCRIPT

Experimental densities of 2,2,2-trifluoroethanol with 1-butyl-3-methylimidazolium hexafluorophosphate at high pressures and modelling with PC-SAFT

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#### **HIGHLIGHTS**

- Density measurements at high pressures of TFE + [C<sub>1</sub>C<sub>4</sub>Im][PF<sub>6</sub>].
- Excess molar volumes have a sigmoid shape.
- Apparent molar volumes of IL indicating hydrogen bonding inexistent or scarce.
- PC-SAFT density correlations of 0.3 % for [C<sub>1</sub>C<sub>4</sub>Im][PF<sub>6</sub>] were obtained.
- An ARD of 3.1 % was achieved for PC-SAFT predictions of density for the mixtures.

#### **ABSTRACT**

New data of densities at temperatures in the 288.15-333.15 K range and several pressures, up to 40 MPa, have been measured for 2,2,2-trifluoroethanol + 1-butyl-3methylimidazolium hexafluorophosphate system using a vibrating tube densimeter. The combined expanded uncertainty at the 0.95 confidence level in the density measurements is 2 kg·m<sup>-3</sup>. Excess molar volumes,  $V_m^E$ , and apparent molar volumes,  $V_{\varphi}$ , were determined from the density values of the pure compounds and mixtures. The influence of the temperature, pressure and composition on  $V_m^E$ ,  $V_{\varphi}$ , was studied. In general, the dependence of  $V_m^E$  with the mole fraction is sigmoid showing that there is a competition between the breaking and formation of interactions and the packing effect;  $V_{\varphi}$  was represented using the Redlich-Mayer equation, indicating that hydrogen bonding interactions are inexistent or scarce. Derived properties,  $\kappa_T$  and  $\alpha_p$  were calculated from the analytical differentiation of the Tait equation, and it was observed that the variation with pressure and temperature is very small for 1-butyl-3-methylimidazolium hexafluorophosphate. In addition, PC-SAFT parameters of 1-butyl-3methylimidazolium hexafluorophosphate were optimized using density data at

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