

Solubility of Carbon Dioxide and Ethane in Ionic Liquids Containing the Anion Bis(Trifluoromethylsulfonyl)Amide

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The knowledge of the solubility of gases in liquids is both of fundamental and practical interest. It can contribute to the characterization of solute-solvent interactions and also allows the calculation of vapour-liquid equilibria. The solubility of gaseous solutes in room-temperature ionic liquids (ILs) has been experimentally investigated by our research group using isochoric saturation methods. The quantity of gas dissolved in the liquid phase is determined from the measurement of the equilibrium pressure of the saturated solution produced by the contact of known amounts of dry gas and degassed solvent. Studies^{1,2} on the solubility of eight different gases in 1-butyl-3-methylimidazolium hexafluorophosphate [bmim][PF₆] and 1-butyl-3-methylimidazolium tetrafluoroborate [bmim][BF₄] have shown the higher solubility of carbon dioxide over the other solutes studied. The effect of changing the anion was investigated³ on three imidazolium-based ILs where it was observed that the presence of the bis(trifluoromethylsulfonyl)amide [NTf₂] anion increased the solubility of most solutes.

In the present work, we focus on the effect on the gas solubility of changing the cation of the solvent. Three ILs are considered containing the same anion [NTf₂] and differing in their cation : 1-butyl-methylpyrrolidinium [bmpyrro], 1-ethyl-3-methylimidazolium [emim] and propylcholinium [N113-2-OH]. Ethane and carbon dioxide are chosen as gaseous solutes for their potential technological interest. The solubilities are measured between 303 K and 343 K at pressures close to atmospheric.

Carbon dioxide is more soluble (mole fractions in the liquid phase $1-3 \times 10^{-2}$ in the temperature range studied) than ethane in the three ILs considered. For both solutes, the solubility decreases with temperature. Finally, the presence of the pyrrolidinium cation increases the solubility of the two gases. The thermodynamic properties associated with dissolution are calculated to provide informations about the solute-solvent interactions and the molecular structure of the solutions. Negative enthalpies (exothermic processes) and entropies of solvation are observed for all the studied systems. The variation of these properties with temperature is not the same for all the systems, which probably means that we are in presence of different mechanisms of solvation.

[1] J. Jacquemin, M. F. Costa Gomes, P. Husson, V. Majer, Fluid Phase Equilibria (2006), accepted for publication.

[2] J. Jacquemin, M.F. Costa Gomes, P. Husson, V. Majer, J. Chem. Thermodyn. (2006), in press.

[3] P. Husson, J. Jacquemin, M.F. Costa Gomes, V. Majer (2005), Proceedings 21st European Symposium on Applied Thermodynamics, 168-170.