Quantification of the Solubility of Ionic Liquids in Water by Electrospray Ionization Mass Spectrometry

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Low melting organic salts or ionic liquids (ILs) have been extensively investigated in the last decade. Ionic liquids are salts composed of large ions that cannot easily form an ordered crystal and thus remain liquid at or near room temperature. Their intrinsic thermophysical properties, their high solvating ability and their negligible vapor pressures make them interesting solvents in conventional organic liquid-phase reactions and in separation processes. In particular, knowledge of their mutual solubilities with water is very important in their application in the extraction of organic products from chemical reactions that proceed in aqueous media and liquid-liquid extractions from aqueous phases, since ILs with low solubility in water are required.

The solubility of pyridinium and imidazolium-based ILs in water is easily determined by UV spectroscopic absorption, since the IL has a significant absorbance at a characteristic wavelength. If the IL is aliphatic, another method to determine its solubility in water is required. In this work, Electrospray Ionization Mass Spectrometry is proposed to experimentally determine solubilities of pyrrolidinium and piperidinium-based ILs in water, between (288.15 and 318.15) K and at atmospheric pressure. This work is an extension of our previous contributions in characterizing the IL-water liquid phase behavior [1,2].

[1] Freire, M.G.; Carvalho, P.J.; Gardas, R.L.; Marrucho, I.M.; Santos, L.M.N.B.F. and Coutinho, J.A.P.; *J. Phys. Chem. B* 112 (2008) 1604.
[2] Freire, M. G.; Neves, C. M. S. S.; Carvalho, P. J.; Gardas, R. L.; Fernandes, A. M.; Marrucho, I. M.; Santos, L. M. N. B. F. and Coutinho, J. A. P.; *J. Phys. Chem. B* 111 (2007) 13082.