

Liquid-Liquid Phase Separation of Ionic Liquid-Toluene Mixtures using CO₂

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Ionic liquids (ILs) are low melting point salts (below 100 °C) with high thermal stability and negligible vapor pressures at ambient temperature [1]. One of the interesting applications of ILs is for performing separations as shown by Scurto et al. [2] where an initial binary IL + organic compound system is mixed with high pressure CO₂. Increasing pressure increases the CO₂ concentration in the liquid phase and causes the liquid volume to expand until a second liquid phase appears. This liquid-liquid-vapor equilibrium consists of an IL-rich phase, an organic-rich phase and a CO₂ + organic gas phase. The objective of this work is to determine the composition and volume expansion of the liquid phase for the ternary system IL + toluene + CO₂ as a function of CO₂ pressure along several isotherms. In addition, we have determined the pressures at which the second organic-rich liquid phase appears (i.e., the cloud point). Investigations have focused on 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonyl) imide ([hmim][Tf₂N]) and 1-hexyl-3-methylpyridinium bis(trifluoromethylsulfonyl) imide ([hmpy][Tf₂N]). The ternary IL/toluene/CO₂ systems were measured at 25, 40 and 60 °C and pressures up to 80 bar, with initial liquid compositions of 30, 50 and 70 mole% IL in the mixtures with toluene. Solubility isotherms indicate higher CO₂ compositions at lower temperatures and higher pressures, as expected. Cloud point pressures are lower at lower initial IL compositions and lower temperatures. Volume expansion is higher in systems with higher initial composition of toluene and at lower temperatures. In addition, we will compare the results for the imidazolium and the pyridinium ILs.

[1] Fredlake, C.P., Crosthwaite, J.M., Hert, D.G., Aki, S.N.V.K., Brennecke, J.F., "Thermophysical Properties of Imidazolium-Based Ionic Liquids", *J. Chem. Eng. Data*, 49, 954 (2004)

[2] Scurto, A.M., Aki, S.N.V.K., Brennecke, J.F., "CO₂ as a Separation Switch for Ionic Liquid/Organic Mixtures", *J. Am. Chem. Soc.*, 124, 10276 (2001)