Thermodynamics of Ionic Liquids for Separations

S.N.V.K. Aki, J.M. Crosthwaite, J.L. Anthony, E.J. Maginn and J.F. Brennecke [C, S]
Department of Chemical Engineering, University of Notre Dame, South Bend, IN, U.S.A.

Since passage of the Pollution Prevention Act in 1990, there has been a growing emphasis on the development of technologies to prevent the production of pollutants at the source rather than simply treating wastes to reduce their harmful effects when introduced into the environment. Since volatile organic solvents (VOCs), which are pervasive in the chemical processing and pharmaceutical industries, are a major source of both atmospheric and aqueous pollution, the development of alternatives has been a major emphasis. Ionic liquids, which are non-volatile organic salts, are promising potential alternatives. Once environmental constraints are satisfied, the key to the usefulness of these solvents lies in their tunable thermodynamics and phase behavior. Specifically, we will show results from our group on gas solubilities in various classes of ionic liquids, and liquid-liquid equilibria of ionic liquids with water and organics. We will also show how carbon dioxide can be used to induce phase splits in ionic liquid mixtures, and how ionic liquids can be used to perform gas separations. In all these case, molecular thermodynamics is the key to solvent selection and evaluation of the usefulness of these substitute solvents.