Vapor-Liquid-Liquid Equilibria of Ternary Imidazolium-based Ionic Liquids and Water Systems

Alejandra Rocha^{C, S} and Mark Shiflett

Department of Chemical and Petroleum Engineering, The University of Kansas, Lawrence, KS, U.S.A. alejandra.rocha@ku.edu

Edward Maginn

Department of Chemical and Biomolecular Engineering, University of Notre Dame, Notre Dame, IN, U.S.A.

The use of ionic liquids as a potential replacement for organic solvents in reaction and separation processes has attracted great attention over the past years. Fractional extraction has been a commonly investigated separation method in which ionic liquids are employed as a solvent or co-solvent. Some recent studies have considered using partially and miscible ionic liquids, while other studies investigate the use of aqueous ionic liquid biphasic systems as a greener solution. Therefore, it is of interest to probe the phase behavior of ionic liquid mixtures in the presence of water. This study investigates the mutual miscibility of ionic liquid pairs with 1-ethyl-3-methylimidazolium cation as a common ion with different anions (including bis(trifluoromethylsulfonyl)imide, acetate, and chloride). In a wide range of temperatures and compositions, most ionic liquid pairs were found to be purely liquid single phase or solid-liquid biphasic solutions. Molecular simulations predicted vapor-liquid-liquid equilibrium for some of the ionic liquid systems in the presence of water. The influence of water on the phase behavior of the ionic liquid mixtures was verified experimentally at a variety of concentrations and temperatures.