A Priori Prediction of Phase Equilibria for Ionic Liquid Solutions

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In this work, the dissociation of IL when mixed with a non-dissociative solvent is modeled as a chemical reaction (CA=C+ + A-). The transition of IL in the associated (ion-pairs) and dissociated (free ions) states is a result of minimizing the free energy of the mixture. The concentration dependence of the extent of dissociation (α) of IL thus determined is in good agreement with the experiment. Furthermore, the same model can be used for the prediction of thermodynamic properties and phase behaviors covering high (infinite dilution activity coefficient of solvent), medium (vapor-liquid and liquid-liquid), and low (osmotic coefficient and mean ionic activity coefficient) IL concentrations (a total of 9,857 data points). Therefore, the proposed method not only captures the proper dissociation behavior of IL but also allows for a priori prediction of properties of IL mixtures.