

Excess Gibbs free energy models for studying ionic liquid-H₂O binary system

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Abstract

In this work, the excess Gibbs free energy models, i.e., non-random two-liquid (NRTL) model, electrolyte NRTL model, and electrolyte NRTL model including new strategies (association or hydration), were used to describe the macroscale properties and interpret the microstructure, clarifying the role of association and hydration in model development, and the enthalpy of mixing of three imidazolium-based IL-H₂O systems containing the same cation but different sizes of anions, i.e., Cl⁻, Br⁻, and I⁻ were measured for the first time to provide systematic data for model development. The models were developed and evaluated based on the newly measured data and the osmotic coefficient from the literature. The model reflecting the intrinsic mechanism of dissociation and hydration competition gives the best modeling results. The real ionic strength predicted from the identified model was quantitatively correlated with the electrical conductivities.

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