446d Estimating Solubility of Organic Salts with Enrtl-Sac Model

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The NonRandom Two-Liquid segment activity coefficient model of Chen and Song (2004) has shown to be a simple and practical tool for chemists and engineers to estimate solubilities of organic nonelectrolytes in support of chemical and pharmaceutical process design. In this paper, the model is extended to facilitate computation of ionic activity coefficients and solubilities of electrolytes, organic and inorganic, in common solvents and solvent mixtures. In addition to the three molecular parameters defined for organic nonelectrolytes, i.e., hydrophobicity X, polarity Y, and hydrophilicity Z, an additional molecular parameter, e, is introduced to characterize both local and long-range ion-ion and ion-molecule interactions attributed to charged segments of electrolytes. Successful representations on mean ionic activity coefficients and solubilities of electrolytes, inorganic and organic, in aqueous and nonaqueous solvents are presented.