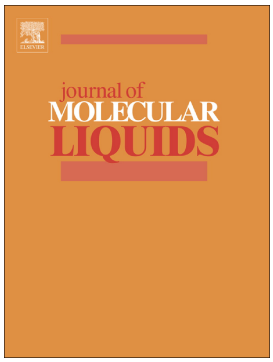

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Thermodynamic Modelling of Liquid-Liquid Extraction Systems involving Ionic Liquids: A New Approach

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Abstract

In this study, a new approach is introduced for the thermodynamic correlation of liquid-liquid extraction (LLE) systems involving ionic liquids (ILs). The model incorporates the effect of local composition and ion solvation in the liquid-liquid equilibrium. Margules excess Gibbs energy model was used to express the short-range molecule-molecule forces whereas the ion solvation theory of modified three characteristic parameter correlation (TCPC) model was employed to characterize the ion-molecule short range forces. With this proposed approach, better results were obtained for the correlation of experimental tie line data and activity coefficients for LLE systems involving ILs. Moreover, the new approach imparted theoretical improvements over previously used thermodynamic models for the correlation of said systems. A wide range of published experimental data for ternary liquid-liquid extraction systems was examined and the new interaction parameters were optimized. A very low root mean square deviation (RMSD) was observed for all the ternary systems, indicating the proficiency of the proposed model.

1. Introduction

Ionic liquids (ILs) have found immense applications in academic research and industry. They can be purposely designed for specific uses. Properties like very low vapour pressure, high thermal and chemical stability and non-flammability are some of the desirable traits for green and environmental friendly processes [1]. Hence, ILs are more acceptable in areas where conventional solvents underperform or cannot be used due to safety implications or