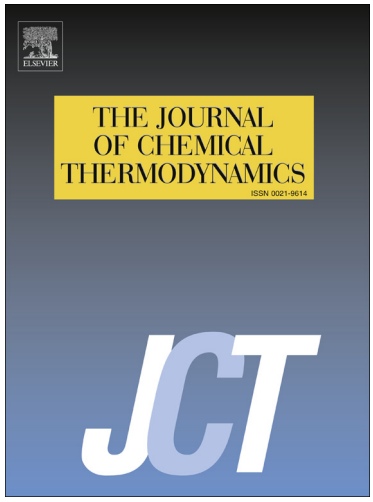

Phase equilibrium measurements and thermodynamic modelling of {water + phenol + [Hmim][NTf_2]} ionic liquid system at several temperatures

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Phase equilibrium measurements and thermodynamic modelling of {water + phenol + [Hmim][NTf_2]} ionic liquid system at several temperatures

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ABSTRACT

Experimental liquid–liquid equilibrium (LLE) data of the ternary chemical system of {water + phenol + 1-hexyl-3-methylimidazolium bis(trifluoromethanesulfonyl)imide, [Hmim][NTf_2], ionic liquid (IL)} were obtained under different temperatures of (293.2, 298.2 and 308.2) K and ambient pressure of 81.5 kPa. The cloud point method, based on refractive index measurement, was employed. The results indicate that the solubility of phenol in the IL is considerably higher than in water, especially at high level concentrations. Meanwhile, due to very low miscibility of the IL in water and strong hydrogen bonding between the IL and phenol, high level solute distribution coefficient and separation factor were obtained within (5.586 - 25.001) and (105.05 - 1476.23), respectively. The reliability of the tie-line data was examined with Hand and Bachman equations. Further, the well-known NRTL and UNIQUAC models were used to correlate the experimental data. For this aim, the thermodynamic properties of the IL were determined by the Density Functional Theory (DFT) calculations, carried out at the M05-2X/6-311++G** level of theory. Low levels of root mean square deviations indicate the capability of the both models to correlate data with a preference for NRTL model.

Keywords: Experimental LLE; Ionic liquid; Phenol; Separation factor; LLE correlation

1. Introduction

Phenols are known as recalcitrant organic compounds or persistent organic pollutants with high toxicity and harmful effects. The maximum acceptable concentration of phenol in

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