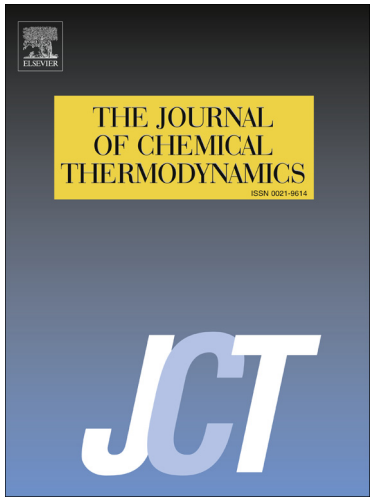

Measurement and thermodynamic modelling of ternary liquid-liquid equilibrium for extraction of (1R,2R)-(-)-1,2-Diaminocyclohexane from aqueous solution with C4–C5 alcohols at different temperatures

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Measurement and thermodynamic modelling of ternary liquid-liquid equilibrium for extraction of (1R,2R)-(-)-1,2-Diaminocyclohexane from aqueous solution with C4–C5 alcohols at different temperatures

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Abstract: (Liquid + liquid) equilibrium data for the ternary systems of {(2-Methyl-1-propanol or 3-Methyl-1-butanol) + (1R,2R)-(-)-1,2-Diaminocyclohexane + water } were measured at (288.2- 318.2)K under atmospheric pressure. The Othmer-Tobias and Hand equations were employed to verify the reliability of the experimental data. Besides, the distribution coefficients and selectivity factors calculated from the experimental tie-line data were applied to evaluate the extraction performance of separating (1R,2R)-(-)-1,2-Diaminocyclohexane from aqueous solution and 3-Methyl-1-butanol was proved to be very promising. Furthermore, the binary interaction parameter values were obtained by correlating the experimental data with NRTL and UNIQUAC models. All the *RMSD* values were less than 0.0184, indicating that both models can be used to describe the liquid-liquid equilibrium behaviour of the studied systems.

Keywords: Ternary (liquid + liquid) equilibrium; (1R,2R)-(-)-1,2-Diaminocyclohexane; Extraction; Thermodynamic models

1. Introduction

(1R,2R)-(-)-1,2-Diaminocyclohexane((-)-1,2-DACH) is a building-block for chiral ligands, which is widely used as pharmaceutical and chemical intermediate[1]. For example, oxaliplatin, which is on the basis of (-)-1,2-DACH, is extensively applied in the treatment of malignant tumours [2-3]. Furthermore, it plays a crucial part in asymmetric synthesis and is widely employed as a chiral catalyst which can induce cyclopropanation, epoxidation and hydrolysis of epoxy compounds [4-5]. However, (-)-1,2-DACH usually presents as the enantiomers of ((±)-1,2-DACH), and the resolution of (±)-1,2-DACH is usually performed by using L-(+)-tartaric acid as an efficient chiral resolving agent [6-7]. And in the resolution process, one of the most important step is the separation of (-)-1,2-DACH from aqueous solution. There is no