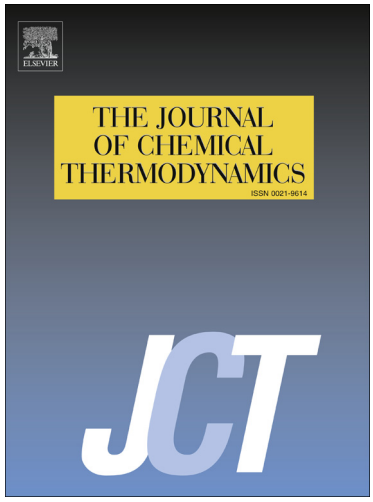

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Extraction of *o*-, *m*- and *p*-cresol from aqueous solution with methyl isopropyl ketone: equilibrium, correlations, and COSMO-RS predictions

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ABSTRACT: In this work, methyl isopropyl ketone (MIPK) was studied to extract *o*-, *m*-, *p*-cresol from water at 333.2 and 343.2 K. The liquid-liquid equilibrium (LLE) data for the ternary systems, MIPK + *o*-, *m*-, *p*-cresol + water, were determined at 101.3 kPa. The extraction performance of MIPK for cresols was evaluated by the distribution coefficient and selectivity. High distribution coefficients and selectivity values indicate MIPK is a promising extractant to separate cresols from wastewater. The experimental LLE data were accurately correlated by using the NRTL and UNIQUAC activity coefficient models, with root mean square deviation (RMSD) values below 1%. The conductor-like screening model for real solvent (COSMO-RS) model was used to predict the phase diagrams of the studied systems, and the RMSD from the experimental data are ~5% (*o*-cresol), ~3% (*m*-cresol), ~2.5% (*p*-cresol) respectively. Furthermore, molecular dynamics (MD) simulations were employed to study the effect of temperature on the hydrogen bonds in the studied systems. The results were used to adjust the hydrogen-bonding parameter of the COSMO-RS model, yielding phase diagram closer to the experiments.

Keywords: Liquid-liquid equilibrium; MIPK; cresol; thermodynamic models; COSMO-RS; MD simulation