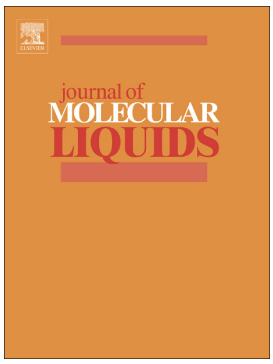

COSMO-RS screening for ionic liquid to be applied in extraction of 2-phenylethanol from aqueous solutions

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COSMO-RS screening for ionic liquid to be applied in extraction of 2-phenylethanol from aqueous solutions

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Abstract

Conductor-like screening model for real solvents (COSMO-RS) is presented as thermodynamic predictive tool for calculating liquid-liquid equilibrium (LLE) phase diagrams in ternary mixtures {ionic liquid (IL) + 2-phenylethanol (PEA) + water} — a model system of extractive recovery of PEA bioproduced using yeast. Overview of the performance of the model is demonstrated by using the experimental LLE data available in the literature. An effect of quantum chemical theory level (BP-TZVP-COSMO vs. BP-TZVPD-FINE) on accuracy of thermodynamic data prediction is discussed. Capacity of the COSMO-RS approach in capturing effect of chemical structure of IL on LLE as well as LLE-derived properties (distribution ratio of PEA and PEA/water selectivity) is presented. Infinite dilution PEA/water selectivity is adopted to carry out the COSMO-RS-based screening of approximately 9000 ILs to find possibly the most effective extracting agent. On the basis on presented methodology, some general guidelines on a proper selection of IL for extraction of PEA form aqueous solutions are proposed and discussed.

Keywords: ionic liquids, 2-phenylethanol, extraction, screening, COSMO-RS

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