Solubilities and Liquid-Liquid Equilibria at Various Temperatures of Aqueous Ternary Mixtures Containing Halogenated Hydrocarbons with Isopropanol

Fouzia Amireche *
Cristallorgaphy-Thermodynamics Laboratory, Faculty of Chemistry, University of Sciences and Technology Houari Boumediene, PO Box 32 El Alia, 16111 Bab Ezzouar, Algiers, Algeria

Malika Chaou
Cristallorgaphy-Thermodynamics Laboratory, Faculty of Chemistry, University of Sciences and Technology Houari Boumediene, PO Box 32 El Alia, 16111 Bab Ezzouar, Algiers, Algeria

Abstract

Liquid-liquid equilibrium (LLE) is a key phenomenon in numerous industrial applications involving systems where two immiscible or partially miscible liquid phases coexist. Accurate measurement of LLE is essential for optimizing processes such as solvent extraction, separation, purification, and chemical synthesis. Reliable LLE data enable the development of efficient and energy-saving separation strategies, thereby minimizing waste and enhancing product quality. Consequently, LLE measurements are indispensable for the design and optimization of industrial processes. In this study, the solubility and LLE data of ternary mixtures composed of (water + isopropanol + tetrachloroethane, iodomethane, or trifluorotoluene) were determined at three temperatures: T = (288.15, 298.15, and 308.15) K under atmospheric pressure (P = 101.2 kPa). Solubility measurements were performed using a thermostated equilibrium cell, while the compositions of the coexisting liquid phases were analyzed via gas-liquid chromatography. The consistency of the experimental binodal curves and phase diagrams was evaluated using the Hand and Othmer-Tobias empirical correlations. Critical solution compositions, distribution coefficients, and selectivity values of the halogenated compounds in the ternary systems are reported. The experimental results were satisfactorily correlated using two activity coefficient models: UNIQUAC and NRTL, and the outcomes were further compared with predictions obtained from DFT-based calculations.