THERMODYNAMIC MODELLING OF LIQUID CRYSTALLINE PHENYLBENZOATE-SOLVENT SYSTEMS

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Liquid crystals (LCs) have found a wide application in various fields of modern technology, primarily in display technologies. The development of new materials requires data on the nature of intermolecular interactions between components in systems containing LCs.

Binary systems based on nematic and smectic–nematic phenylbenzoates R_1-C_6H_4-COO-C_6H_4-R_2 (R = n-alkyl-, alkoxy-) and the nematic compound C_4H_9OCOO-C_6H_4-COO-C_6H_4-OC_2H_5 (H-23) with nonmesogens were studied by thermal analysis methods (DTA, visual polythermal analysis, and the solubility method).

T–*x* diagrams of H-23 systems with butyl acetate and 1-propanol were obtained. Polytherms of LC solubility in solvents of different classes were investigated; the enthalpy, entropy, and Gibbs energy of LC dissolution ($\Delta_{dissol}H$, $\Delta_{dissol}S$, $\Delta_{dissol}G$) were calculated according to the scheme [1]. In almost all systems, the calculated enthalpies of dissolution exceed the melting enthalpy of LC (for H-23 – 25.1 kJ/mol). The largest positive deviations from ideality were observed in LC systems with n-alkanes. For H-23 systems, $\Delta_{dissol}H$ increases with increasing alkyl chain length: with n-alkanes - from 43.8 (n-hexane) to 64.4 kJ/mol (n-octane), and with alcohols - from 41.9 (ethanol) to 57.6 kJ/mol (1-propanol). Phase demixing is observed in H-23 systems with alcohols and alkanes, which is confirmed by differences in Hildebrand solubility parameters and the Teas triangle diagram [1].

Activity coefficients of LC components were calculated using the Hildebrand and Hansen solubility parameters [2] (for LCs calculated by the group contribution method) and the UNIFAC equation.

The best agreement between calculated and experimental solubility polytherms was obtained using the UNIFAC equation (Dortmund modification).

1. Guo F., Ren Y., Sha J. Solubility, molecular simulation, Hansen solubility parameter and thermodynamic properties of citiolone in thirteen organic pure solvents at different temperatures // J. Chem. Thermodyn. 2022. Vol. 164, 106624

2. Hansen solubility parameters. A user's Handbook. 2 Ed. / ed. Hansen C.M. Boca Raton: CRC Press, 2007. 544 p.