

Influence of Complex Formation on Mutual Diffusion in Benzene-Chloroform

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Peculiarities of diffusion in the mixture of molecular liquids are connected with intermolecular interactions. Theory of nonlinear diffusion takes into account the effect of molecular complexes formation in liquid mixtures. Process of diffusion mass-transfer is described by the following system of equations [1]:

$$\frac{\partial \varphi_n}{\partial t} + \operatorname{div} \vec{J}_n = S_n, \quad \vec{J}_n = \sum_m d_{nm} \cdot [\varphi_n \nabla \varphi_m - \varphi_m \nabla \varphi_n]. \quad (1)$$

$$\sum_n \varphi_n = 1, \quad \sum_n \vec{J}_n = 0, \quad \sum_n S_n = 0. \quad (2)$$

Here φ_n is a relative volume of the n -th component; S_n is the source functions (determined by interactions between molecules in the solution).

Under some conditions (matter-transfer is slow, but generation of the complex is fast), Fick's law of diffusion takes place. However, the coefficients of diffusion become dependent on the component concentrations. For example, if two liquids are mixed, then total flow of the 1st component is: $\vec{J}_1^{tot} = -D_1^{ef}(\varphi_1^{tot}) \cdot \nabla \varphi_1^{tot}$ (here $\varphi_1^{tot} = \varphi_1 + \alpha_{13}\varphi_3$, where φ_3 - relative volume of chemical complex, α_{13} - share of the 1st component in the complex "3").

We investigated mutual diffusion in liquid benzene-chloroform mixture at 25 °C. Initial binary mixture is considered as ternary which consists of pure benzene, pure chloroform and equimolecular complex. Concentration dependence of the effective diffusion coefficient $D_1^{ef}(\varphi_1^{tot})$ was explained using the set of equations (1) and (2). Also this theory provides obtaining of the concentrations of mixture components.

1. V. Obukhovskiy, V. Nikonova, *Ukr. J. Phys.* **55**, 891 (2010).