

Molecular Modelling of Physicochemical Properties of Molecular Mixtures

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The results on modelling supramolecular ordering and macroscopic properties of molecular mixtures have been reviewed. The main attention is paid to the unified approach based on a quasichemical model for thermodynamic, dielectric and optical properties of mixtures, self-organized by specific bonding [1,2].

The hierarchy of models of molecular aggregates is considered. The nonideal mixture of molecular aggregates, polyvariant as regard structure and composition, has been discussed. Interrelations between a set of the thermodynamic, dielectric, and optical properties of liquids, reflecting different molecular parameters, and the characteristics of quasichemical processes are presented. Applications for thermodynamic functions of mixing (Gibbs energy, enthalpy, entropy), permittivity, coefficients of isotropic and anisotropic Rayleigh light scattering for alcohols, amides, amines, and their mixtures with non-polar and polar inert and solvating solvents (hydrocarbons, halohydrocarbons, ketones, etc.) are presented. New features of the aggregation in liquids, including long-range molecular correlations have been discussed in terms of the integral and differential parameters of aggregation. Comparison with computer simulation of methanol has been given [3]. Macroscopic manifestations of supramolecular ordering in the physicochemical properties of mixtures are also discussed.

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