

Heteromolecular Structure Formation in Aqueous Solutions of Ethanol, Tetrahydrofuran and Dimethylformamide

Authors : Sh. Gofurov, O. Ismailova, U. Makhmanov, A. Kokhkharov

Abstract : The refractometric method has been used to determine optical properties of concentration features of aqueous solutions of ethanol, tetrahydrofuran and dimethylformamide at the room temperature. Changes in dielectric permittivity of aqueous solutions of ethanol, tetrahydrofuran and dimethylformamide in a wide range of concentrations (0÷1.0 molar fraction) have been studied using molecular dynamics method. The curves depending on the concentration of experimental data on excess refractive indices and excess dielectric permittivity were compared. It has been shown that stable heteromolecular complexes in binary solutions are formed in the concentration range of 0.3÷0.4 mole fractions. The real and complex part of dielectric permittivity was obtained from dipole-dipole autocorrelation functions of molecules. At the concentrations of $C = 0.3 / 0.4$ m.f. the heteromolecular structures with hydrogen bonds are formed. This is confirmed by the extremum values of excessive dielectric permittivity and excessive refractive index of aqueous solutions.

Keywords : refractometric method, aqueous solution, molecular dynamics, dielectric constant

Conference Title : ICPMDMM 2017 : International Conference on Physics, Molecular Dynamics and Molecular Modeling

Conference Location : Venice, Italy

Conference Dates : April 13-14, 2017