VARIATION OF THE LOCAL STRUCTURE OF WATER DUE TO DISSOLUTION OF PROPANOL

N.O. Atamas', O.O. Atamas', L.A. Bulavin

Taras Shevchenko Kyiv National University
(*2, Academician Glushkov Prosp., Kyiv 03027*)

S u m m a r y

The work presents the results of Monte-Carlo calculations of radial distribution functions (RDF) for a "water–propyl alcohol" solution at T=300 K in a wide range of concentrations, as well as analysis of the interaction of water molecules with one another. Hydrogen bond lengths and dimensions of the first and second hydration spheres were obtained at various mole concentrations of propanol. We also established the concentration ranges within which the local structure of the solution is reconstructed.