MONTE CARLO CALCULATIONS OF STRUCTURAL FEATURES OF AQUEOUS SOLUTIONS OF ETHYL ALCOHOL AT VARIOUS CONCENTRATIONS AND TEMPERATURES

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S u m m a r y

The Monte Carlo method has been used for studying the processes of hydrophobic hydration of ethyl alcohol in water within the temperature interval from 5 to 35 °C and at the mole fraction of ethyl alcohol from 0.005 to 0.5. Employing the method of computer simulation, the radial distribution functions for interactions between the molecules of different solution components have been obtained and used to analyze the influence of the temperature and the concentration of ethyl alcohol molecules on the local structure modifications in the solution.