

STRUCTURE EFFECTS IN CONCENTRATED AQUEOUS SOLUTIONS OF ETHANOL

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S u m m a r y

The Monte Carlo method has been used to calculate structure and energy properties of the concentrated aqueous solutions of ethanol with mole fraction of ethanol from 0.5 to 0.9. On the basis of analysis of the concentration dependences of the radial distribution functions and energy properties of the solution, a model that describes intermolecular interaction mechanisms between water molecules in concentrated aqueous solutions of ethanol has been developed.