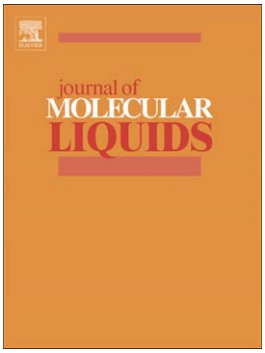

Behaviour of aqueous *N*-methylacetamide solution in presence of ethanol and 2,2,2 tri-fluoroethanol: Hydrogen bonding structure and dynamics

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Behavior of aqueous N-methylacetamide solution in presence of ethanol and 2,2,2 tri-fluoroethanol: Hydrogen bonding structure and dynamics

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Abstract

Effects of ethanol (EtOH) and 2,2,2-trifluoroethanol (TFE) on the hydrogen bonding structure and dynamics in aqueous N-methylacetamide (NMA) solution are investigated by classical molecular dynamics simulations. The interactions between NMA and water in presence of ethanol or 2,2,2-trifluoroethanol molecules are depicted here by different site-site radial distribution functions and the average interaction energies between these species in the solution. It is observed that the aqueous peptide hydrogen bond interaction is preferably stronger with increasing alcohol concentration in the solution, whereas hydrophobic solvation of CH_3-groups of NMA decreases significantly. **The $O_{NMA}…H_{NMA}$ hydrogen-bond interaction is better maintained in TFE solution than in EtOH.** TFE prefers to donate the hydrogen-bond towards water or NMA, whereas EtOH shows the hydrogen bond accepting ability. The lifetimes of NMA-water, water-water hydrogen bonds are found to increase with alcohol concentration in the solution and it is more significant in case of EtOH than TFE. Our calculated self-diffusion coefficients and orientational relaxation times shows slower dynamics of water in concentrated EtOH solution compared to TFE due to formation of preferable water-ethanol hydrogen bonds.

Keywords: Aqueous NMA, 2,2,2-trifluoroethanol, Hydrogen-bond lifetime, Structural relaxation times, Self-diffusion coefficients, Orientational relaxation times.

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