

Accepted Manuscript

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

Apramita Chand, Snehasis Chowdhuri

PII: S0167-7322(16)30958-8
DOI: doi:[10.1016/j.molliq.2016.10.129](https://doi.org/10.1016/j.molliq.2016.10.129)
Reference: MOLLIQ 6533

To appear in: *Journal of Molecular Liquids*

Received date: 21 April 2016
Revised date: 20 October 2016
Accepted date: 28 October 2016



Please cite this article as: Apramita Chand, Snehasis Chowdhuri, Behaviour of aqueous *N*-methylacetamide solution in presence of ethanol and 2,2,2 tri-fluoroethanol: Hydrogen bonding structure and dynamics, *Journal of Molecular Liquids* (2016), doi:[10.1016/j.molliq.2016.10.129](https://doi.org/10.1016/j.molliq.2016.10.129)

This is a PDF file of an unedited manuscript that has been accepted for publication. As a service to our customers we are providing this early version of the manuscript. The manuscript will undergo copyediting, typesetting, and review of the resulting proof before it is published in its final form. Please note that during the production process errors may be discovered which could affect the content, and all legal disclaimers that apply to the journal pertain.

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

Apramita Chand and Snehasis Chowdhuri*

School of Basic Sciences, Indian Institute of Technology, Bhubaneswar 751013, India

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 CH₃-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.

* Telephone number: +91-674-2576052, E-mail: snehasis@iitbbs.ac.in

Download English Version:

<https://daneshyari.com/en/article/5409620>

Download Persian Version:

<https://daneshyari.com/article/5409620>

[Daneshyari.com](https://daneshyari.com)