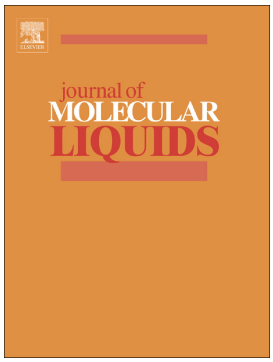

Hydrogen-bond network in liquid Formamide Methanol mixture as studied by neutron scattering and density functional theory

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Hydrogen-bond network in liquid Formamide Methanol mixture as studied by neutron scattering and density functional theory

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Abstract

In this work, a hydrogen-bond network in an equimolar formamide-Methanol (FA-MeOH) mixture was investigated by means of neutron scattering combined with Density Functional Theory (DFT). Original neutron scattering data were analyzed in order to deduce the structure factor $S_M(Q)$ and the intermolecular pair correlation function $g_L(r)$. To describe the intermolecular associations in this mixture liquid, different H-bonded clusters: dimer, trimers and tetramer are considered. Our investigation shows that the local order of FA-MeOH mixture is better described by a trimer T1 and tetramer T3 where two FA molecules are connected to one or two methanol molecules. Topological analysis AIM was performed to examine the electronic densities and the strength of hydrogen-bond network involved in the more probable clusters T1 and T3. Good correlations have been obtained between hydrogen bond lengths versus AIM topological parameters like electron density $\rho(r)$ and its correspondent Laplacian $\nabla^2\rho(r)$ at the bond critical points. Natural Bond Orbital (NBO) analysis was performed in order to explore interactions and charge transfer among different orbitals and lone pairs taking place within the T1 and T3 clusters.

Keywords: FA-MeOH mixture; hydrogen-bond network; neutron scattering; DFT calculation

1. Introduction

Understanding of H-bonding interactions calls for experimental as well as theoretical investigations. Amides have attracted great attention due to the importance of H-bonding interactions in determining the structures and properties of biological systems, such as proteins and polypeptides [1-3].