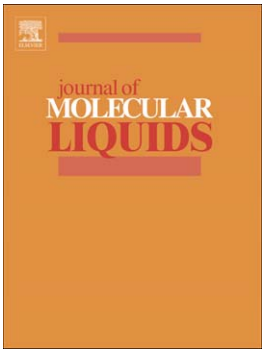

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Rheological behavior of Ionic Liquids: analysis of the H-bonds formation by Molecular Dynamics

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Abstract

Equilibrium and Non-Equilibrium Molecular Dynamics simulations were performed with the aim to deepen in the understanding of Ionic Liquids molecular interactions. Hydrogen Bonds (HBs) and the structure of ions for 1-butyl-3-methylimidazolium bis(trifluorometilsulfonil) imide ([bmim][TF_2N]) were studied. The SLLOD equation of motion in an NVT ensemble at room conditions were solved to obtain the rheological behavior. The flow curve shows two regions: a first Newtonian plateau and a second shear thinning. We found that HBs play an important role in the shear viscosity for this ionic liquid, since the reduction in viscosity is in proportion to the reduction in the number of HBs. Results for viscosity are in good agreement with those reported experimentally.

Keywords: Ionic Liquids, Molecular Dynamics, Rheological behavior, Hydrogen Bonds, Structure

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