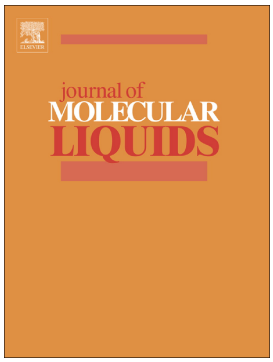

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Multiscale simulations to Uncover the Relationship between Hydrogen Bond and Viscosity for Ammonium-based Ionic Liquids

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Abstract

The knowledge of viscosity about ionic liquids is important for their large scale-up application. Although some theoretical models and experimental methods are developed to evaluate the viscosity, there are some common disadvantages for them including complexity, time consuming, and unreliable. It is necessary to develop a simple method to evaluate the viscosity. Even if the accurate value of viscosity could not be obtained, the relative sequence for a series of ionic liquids with similar structures is still beneficial for their applications. The relationship between hydrogen bond and viscosity for TBA pyruvate, TBA L-lactate, and TBA L-malate are studied by combination of molecular dynamics simulation and quantum chemistry methods. The strength of hydrogen bond in TBA L-malate is the larger resulting in the larger viscosity. In contrast, the number of hydrogen bond has a minor influence on the viscosity. It is expected that this study would provide some useful information to build the relationship between hydrogen bond and viscosity for task functionalized ionic liquids.

Keywords: Ionic liquid, Viscosity, Hydrogen bond, Molecular dynamics, Quantum

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