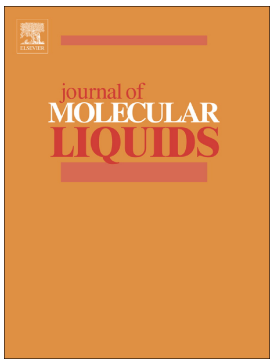

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Intermolecular Forces in 1-Butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide + Ethanol Mixtures

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ABSTRACT: The characteristics of intermolecular forces in 1-butyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide + ethanol mixtures were studied in the full composition range using a combined experimental and theoretical approach. Molecular clusters were used to model the short-range interactions between the ionic liquid and the primary alcohol, studied using density functional theory calculations, inferring preferred interaction sites, strength of interactions and topological characteristics of intermolecular forces. Dynamic viscosity and refraction index were measured as a function of mixture composition and temperature and analysed in terms of evolution of intermolecular forces. Raman IR studies were carried out and the analysis of selected spectral regions allowed to characterize hydrogen bonding evolution for all the possible interacting sites.

Highlights

- Imidazolium ionic liquids.
- Mixtures.
- Experimental and theoretical study.
- Intermolecular forces.
- Hydrogen bonding.

KEYWORDS: ionic liquid, imidazolium, molecular solvent, mixtures, DFT, Raman, hydrogen bonding.