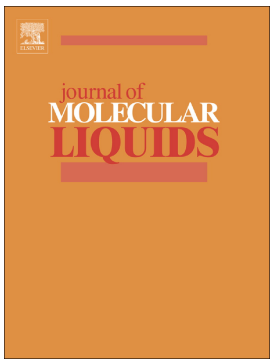

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Microscopic Characterization of Mixtures of Amino Acid Ionic Liquids and Organic Solvents

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ABSTRACT: The properties of aminoacid – based ionic liquids mixed with a set of eight different protic and aprotic ionic liquids are studied using molecular dynamics simulations. Intermolecular forces, dynamic properties, clustering and additional microscopic features are studied in the full composition range as a function of the type of ionic liquid and the considered organic solvent. The intermolecular anion-cation and ionic liquid – organic solvent hydrogen bonding, especially for protic organic solvents, is also analysed in this work. The changes in ion-ion self-aggregation and the competing effect of the ion – organic solvent interactions is analysed in terms of fluids structure. The reported results show that anion-cation self – aggregation through hydrogen bonding is maintained even for highly diluted solutions of ionic liquid, and thus, the properties of these ionic liquids can be tuned through the selection of suitable organic solvents.