

عنوان مقاله:

A Structural Study on Bulk of Imidazolium Base Amino Acid Ionic Liquid

محل انتشار:

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خلاصه مقاله:

An imidazolium based amino acid ionic liquid (AAIL) was studied to obtain effect of imidazolium ring of anion on structural properties by molecular dynamics simulation. In current study, possible hydrogen bond and its structure are investigated. Oxygen of anion was the more accessible site of hydrogen bond. Spatial orientation of the hydrogen bond is responsible for this observation. It was also observed that self-interaction of anion is also probable. The intermolecular and intramolecular hydrogen bonds affect spatial structure of. Anion-cation and anion-anion imidazolium rings are capable to form π - π stacking to each other. However, cation-cation correlation is not a possible interaction.

کلمات کلیدی:

Amino Acid Ionic Liquid, Spatial orientation, hydrogen bond, Molecular Dynamics Simulation

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