عنوان مقاله:

A Quantum Chmistry Study on Structures and Interactions of Biodegradable Aromatic CBNILS

محل انتشار:

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خلاصه مقاله:

Biodegradable ionic liquids (bio-ILs) have attracted intensive attention due to toxicologicaland ecological reasons. Yu et al. [1] synthesized cholinium-based ionic liquids with naphtenicbasedanions; among the compounds studied, those including benzoate and salicylate anionsshowed very good biodegradability properties. In this study, we focus on the molecularinteractions of two aromatic choline based naphthenic acid ionic liquids (CBNAILs), namely,choline benzoate ([CH][BE]) and choline salicylate ([CH][SA]). Structures, electronic properties,and intermolecular interactions in two aromatic CBNAILs were investigated by quantumchemistry calculations. Hydrogen bonds were analyzed by quantum theory of atoms in molecules(AIM) and reduced density gradient (RDG) function [2,3]. The analysis of short-rangeanion–cation interactions showed that interionic interactions are developed between the COOanionicgroup and the hydrogen of hydroxyl group of cation with less important interactionthrough the anion hydroxyl group for salicylate anion. The strength of these interactions for[CH][SA] is weaker than that of the [CH][BE] in agreement with its weaker interaction energies.Analysis of frontier orbitals for isolated anions and cations by density of states (DOSs) showsthat the HOMO-LUMO energy gaps follow the order of [CH][BE] (4.482 eV) > [CH][SA](3.786 eV) which is in agreement with the binding energies. These conclusions will be helpfulfor in depth understanding of the biodegradable CBNAILs .and further contribute to designingand preparing ILs in a task specific way

کلمات کلیدی:

Aromatic CBNAILs, Hydrogen bond, AIM analysis, RDG analysis, DOSs analysis