

عنوان مقاله:

Investigation of Stability of Some Ionic Liquids as Green Solvents and Safe Materials

محل انتشار:

اولین همایش ملی تکنیک های نوین در تجهیزات و مواد آزمایشگاهی صنعت نفت ایران (سال: 1394)

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خلاصه مقاله:

Stability of ionic liquids Ethylammonium nitrate (EAN), 1-Ethyl-3-methylimidazolium chloride (EMIC), 1-Butyl-3-methylimidazolium hexafluorophosphate (BMIHP), and 1-Ethyl-3-methylimidazolium dicyanamide (EMIDC) was studied using computational quantum chemistry methods. The order of stability of the above mentioned ionic liquids is EAN EMIDC EMIC BMIHP. Arrangement of atoms in molecule BMIHP which makes ring critical points (RCPs) and cage critical points (CCPs) in the molecular graphs of it, leads to more stable geometry for this ionic liquid in comparison with other ionic liquids. Also, some of atomic charges in cationic part of BMIHP is 0.87 e which is higher than those for other ionic liquids. As a result, high stability of ionic liquids, which arises from values of total atomic charges in cationic and anionic parts of these new materials together with magnitude of electron charge density values at RCPs make them safe solvents for many applications such as synthesis of new drugs.

کلمات کلیدی:

ionic liquid, green solvent, Ethylammonium nitrate, EMIC, BMIHP

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