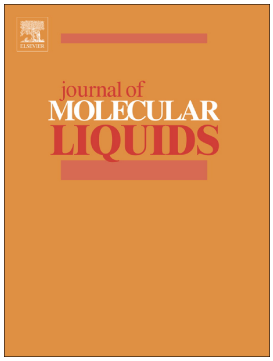

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Theoretical Study on Interactions between Trifluoromethanesulfonate (Triflate) Based Ionic Liquid and Thiophene

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Abstract

Density functional theory was employed to investigate the interactions between 1-ethyl-3-methylimidazolium ($[EMIM]^+$)/ 1-ethylpyridinium ($[EPY]^+$)/ 1-ethyl-1-methylpyrrolidinium ($[EPYRO]^+$)/ 1-ethyl-1-methylpiperidinium ($[EPIP]^+$) cations and trifluoromethanesulfonate ($[OTf]^-$) anion, as well as the interactions between trifluoromethanesulfonate ($[EMIM]^+[OTf]^-$/ 1-ethylpyridinium trifluoromethanesulfonate ($[EPY]^+[OTf]^-$/ 1-ethyl-1-methylpyrrolidinium trifluoromethanesulfonate ($[EPYRO]^+[OTf]^-$/ 1-ethyl-1-methylpiperidinium trifluoromethanesulfonate ($[EPIP]^+[OTf]^-$) and thiophene. The ionic liquids and complexes formed between $[EMIM]^+[OTf]^-$/ $[EPY]^+[OTf]^-$/ $[EPYRO]^+[OTf]^-$/ $[EPIP]^+[OTf]^-$ and thiophene were analyzed by natural bond orbital, atoms in molecules, and noncovalent interaction, HOMO-LUMO overlap integral analyses, and electron density difference analysis. The calculated results show that thiophene ring is parallel to $[EMIM]^+$/ $[EPY]^+$ ring, beneficial to π-π interaction, while $[EPYRO]^+$ / $[EPIP]^+$ branched chains tend to form C-H···π interactions with thiophene. The interactions between $[EMIM]^+$/ $[EPY]^+$ / $[EPYRO]^+$ / $[EPIP]^+$ and thiophene are stronger than that of $[OTf]^-$ and thiophene proposed by interaction energy and electron density differences. The HOMO-LUMO overlap integral analyses demonstrate the different charge transfer direction and interacting nature of frontier orbitals.

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