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Ionic liquids based on 1-ethyl-3-methylimidazolium cation and anions of tetrafluoroborate and bis(trifluoromethylsulfonyl)imide: Structural and thermodynamic properties by DFT study

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Influence of Metal Oxides Nanoparticles on Pathogenicity of *Steinernema carpocapsae* Nematodes Ionic liquids based on 1-ethyl-3-methylimidazolium cation and anions of tetrafluoroborate and bis(trifluoromethylsulfonyl)imide: Structural and thermodynamic properties by DFT study

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Abstract

The theoretical study of neutral ion pairs of 1-ethyl-3-methylimidazolium tetrafluoroborate ([EMIM][BF₄]) and 1-ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide ([EMIM][NTf₂]) has been performed. The formation of the neutral ion pairs was considered through inter-ionic reactions involving the [EMIM]⁺ cation and two anions, [BF₄]⁻ and [NTf₂]⁻. Computations were executed by the DFT/6-311++G(d,p) method with B3LYP5 and CAM-B3LYP functionals. The thermodynamic characteristics of the inter-ionic reactions have been determined theoretically for both ion pairs. The thermodynamic stability of the ion pairs was interpreted through analysis of the frontier molecular orbitals (FMOs). In addition, following experimental data available in literature for [EMIM][NTf₂], the enthalpy and entropy of the reaction were

Keywords

Ionic liquids; Density functional theory; 1-Ethyl-3-methylimidazolium tetrafluoroborate; 1-Ethyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide; Geometrical structures Thermodynamic properties