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Density and Thermodynamic Performance of Energetic Ionic Liquids Based on 1-alkyl/esteryl-4-amino-1,2,4-triazolium

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Abstract: Energetic ionic liquids (EILs) based upon nitrate, perchlorate and dicyandiamide salts of 1-alkyl/esteryl-4-amino-1,2,4-triazolium are synthesized. The structures are characterized by ^1H NMR, FT-IR and element analysis. The density, constant volume combustion heat and specific heat capacity of these EILs are determined through experiment. Their interaction energies of ion pairs, standard molar volume, standard molar heat capacity and standard molar enthalpy of formation are calculated by DFT/B3LYP/6-311+G(d,p) and further researched. The thermodynamics function data relative to the reference temperature (298 K) are obtained based on the C_p from 303-353 K. The influences of temperature, molecular structure and interaction energy of ion pairs on ρ and C_p are also discussed systematically. In addition, the density and thermodynamic properties of EILs are deduced from theoretical calculation and experimental evidences. As a result, the physicochemical properties estimation of EILs using theoretical calculation method can be applied in the field of modern military, science, etc.

Keywords: energetic ionic liquids; density; specific heat capacity; standard molar enthalpy of formation; DFT/B3LYP/6-311+G(d,p)

Introduction

Ionic liquids (ILs), organic salts with melting points less than 300 °C, have recently been the focus of much research owing to the variety of desirable properties¹. Energetic ionic liquids (EILs) are a kind of functional ionic liquids, which adopting nitrogen-rich triazole-substituted derivatives as cation or anion²⁻⁴ and possessing high

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