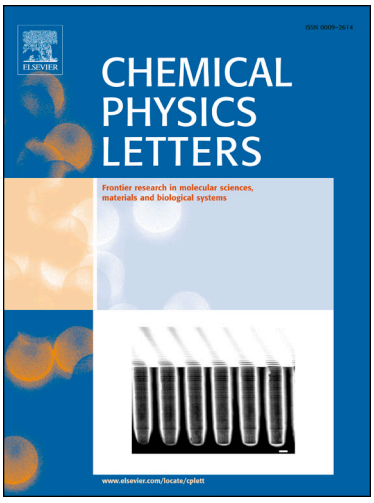

Research paper

Molecular dynamics simulation of the ionic liquid N-octylpyridinium tetrafluoroborate and acetonitrile: Thermodynamic and structural properties

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Molecular dynamics simulation of the ionic liquid N-octylpyridinium tetrafluoroborate and acetonitrile: Thermodynamic and structural properties

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Abstract: Using molecular dynamics simulation, the research obtained the thermodynamic properties and microstructures of the mixture of N-octylpyridinium tetrafluoroborate and acetonitrile, including density, self-diffusion coefficients, excess properties, radial distribution functions (RDFs) and spatial distribution functions (SDFs). Both RDFs and SDFs indicate that the local microstructure of the polar region is different from the nonpolar region with different mole fraction of ionic liquids. Acetonitrile could increase the order of the polar regions. While with acetonitrile increasing, the orderliness of the nonpolar region increases firstly and then decreases. In relatively dilute solution, ionic liquids were dispersed to form small aggregates wrapped by acetonitrile.

Keywords: N-octylpyridinium tetrafluoroborate; Molecular dynamics simulation; Thermodynamic property; Microstructure.

1. Introduction

Room temperature ionic liquids (RTILs) are special ionic compounds that are liquid at room temperature or near room temperature, which generally consists of organic cation and inorganic anion [1]. In recent years, more and more researchers pay attention to ionic liquids that are a new kind of green solvent [2-6].

Compared with traditional solvent, ionic liquids have many superior characteristics,

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