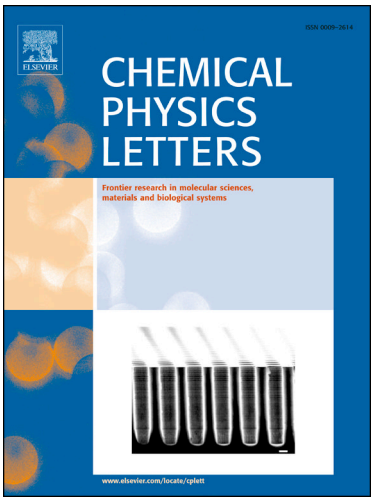

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An X-Ray and Computational Study of Liquid Pentylammonium Nitrate

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Abstract

In this article we report the study of liquid pentylammonium nitrate with Wide Angle X-Ray scattering and AIMD simulations. Static and dynamical features were characterized by comparing the experimental X-ray pattern with *ab initio* molecular dynamics simulation trajectories. From the analysis, we were able to focus our attention on the nature and time duration of the hydrogen bond network established between cation and anion. Such H-bond interactions occur around 2.8 Å, last about 1.55 ps and lead to the loss of degeneracy of the asymmetric stretching normal mode of the anion, with a splitting of about 84 cm^{-1}.

Keywords: X-Ray, Nitrate, Pentylammonium, Vibrations, Ionic Liquids

Ionic liquids (ILs) are salts with a melting point below 100°C, and they are composed of a cation and an anion. The discovery of ionic liquids is generally attributed to Paul Walden(1), who described a series of water-free salts with a melting point below 100 °C. Among the compounds described by Walden was included the widely known ethylammonium nitrate (EAN), melting point 12-14°C, that is commonly defined as RTIL ("Room Temperature Ionic Liquid") in the modern sense. About six decades after Walden's paper, the interest and the scientific literature about these compounds flourished, owing to their peculiar properties, that have been described extensively in several papers, to which the reader is referred for brevity.(2; 3; 4; 5; 6) EAN is one member of

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