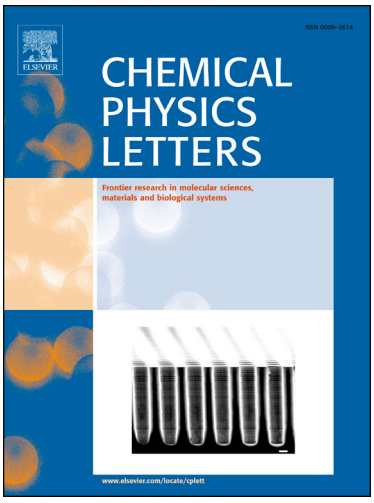

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A Structural and Theoretical Study of the Alkylammonium Nitrates Forefather: Liquid Methylammonium Nitrate

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Abstract

We present here a structural and vibrational analysis of melted methylammonium nitrate, the simplest compound of the family of alkylammonium nitrates. The static and dynamical features calculated were endorsed by comparing the experimental X-ray data with the theoretical ones. A reliable description cannot be obtained with classical molecular dynamics owing to polarization effects. Contrariwise, the stucture factor and the vibrational frequencies obtained from *ab initio* molecular dynamics trajectories are in very good agreement with the experiment. A careful analysis has provided additional information on the complex hydrogen bonding network that exists in this liquid.

Keywords: X-Ray, Nitrate, Methylammonium, Melted, AIMD

1. Introduction

The latvian/russian/german chemist Paul Walden is generally recognized as one of the "fathers" of that class of (organic) molten salts that most contemporary chemists would call "ionic liquids". As a matter of fact, Walden,

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