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Lorenzo Gontrani, Ruggero Caminiti, Umme Salma, Marco Campetella

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

Lorenzo Gontrani^{*a}, Ruggero Caminiti^{a,b}, Umme Salma^a, Marco Campetella^{*a,c}

^aUniversità degli Studi di Roma “La Sapienza”, P. le Aldo Moro 5, I-00185, Roma, Italy

^bCentro di Ricerca per le Nanotecnologie Applicate all’Ingegneria CNIS, Università di Roma, “La Sapienza”, P. le Aldo Moro 5, I-00185 Roma, Italy

^cChimie ParisTech, PSL Research University, CNRS, Institut de Recherche de Chimie Paris, F-75005 Paris, France

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 structure 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,

Email addresses: lorenzo.gontrani@uniroma1.it (Lorenzo Gontrani*), marco.campetella@uniroma1.it (Marco Campetella*)

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