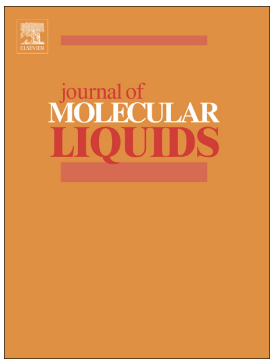

Theoretical study of the second-order nonlinear optical properties of ionic liquids

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PII: S0167-7322(18)32516-9
DOI: doi:10.1016/j.molliq.2018.08.057
Reference: MOLLIQ 9502

To appear in: *Journal of Molecular Liquids*

Received date: 15 May 2018
Revised date: 8 August 2018
Accepted date: 10 August 2018

Please cite this article as: J.E. Castellanos Águila, M. Trejo-Durán , Theoretical study of the second-order nonlinear optical properties of ionic liquids. Molliq (2018), doi:10.1016/j.molliq.2018.08.057

Theoretical study of the second-order nonlinear optical properties of ionic liquids.

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Abstract

The second-order nonlinear optical properties of ionic liquids formed by $[EMIM]^+$, $[BMIM]^+$, $[MePyrr]^+$, and $[BuPy]^+$ cations in conjunction with four anions, $[BF_4]^-$, $[NO_3]^-$, $[CF_3COO]^-$, and $[PF_6]^-$, were carried out at the framework of the Density Functional Theory. First, we determinate the first hyperpolarizability for all ions and later, we study the local interactions between the ions to find the key factor that determine their nonlinear optical properties of ionic liquids. The results show that $[BuPy]^+[CF_3COO]^-$, $[BuPy]^+[NO_3]^-$, $[BuPy]^+[BF_4]^-$, and $[BMIM]^+[NO_3]^-$ systems have large first hyperpolarizabilities and can be treated as a good candidate for nonlinear optical devices.

Keywords: DFT, Ionic Liquids, Nonlinear Optical Properties

1. Introduction

Nonlinear optical (NLO) materials have attracted great interest among scientists due to their potential applications such as frequency doublers [1], photorefractive media [2] and electrooptic modulators [3]. It is know that if a material presents nonlinear optical properties, the incident light will induce different responses depending on the intensity of the electromagnetic field at the surrounding regions. In general, NLO properties of organic materials, such as the hyperpolarizability, increase when strong donor/acceptor groups are attracted and their orbitals overlap. In ionic liquids, it is possible to have strong acceptors and donors in the cation and anionic parts, respectively. Moreover, it is possible to tune the structural geometry of anions, cations and their combinations. These characteristics make the NLO properties of ionic liquid designable for different requirements in chemical industry, for example.

Recently, it has been shown that large second-order NLO responses in ionic liquids are capable to decrease the response time of electrooptic switching elements for optical information processing and telecommunications [4, 5]. Besides, it has been investigated the optical nonlinearity with nonlocal character [6]. This last characteristic makes the ionic liquids to have large thermo-optical responses owing to the change of the refractive index as a consequence of the heat conduction process. Such feature could provide a better medium for thermal lens measurements than water [7]. This and other interesting NLO properties make ionic liquids to be among the most promising materials for applications in optical holographic recording [8], catalysis [9], and to create electrical-controlled memory systems and switching in continuous low intensity lasers [10].

Futhermore, an ionic liquid commonly used in chemical synthesis is composed by imidazolium cation ($[IM]^+$) and hexafluorophosphate anion ($[PF_6]^-$) [11]. This compound presents good second-order NLO properties, however, its degradation is not easy and it represents an environment problem. Imidazolium compounds have been studied extensively in chemical area,