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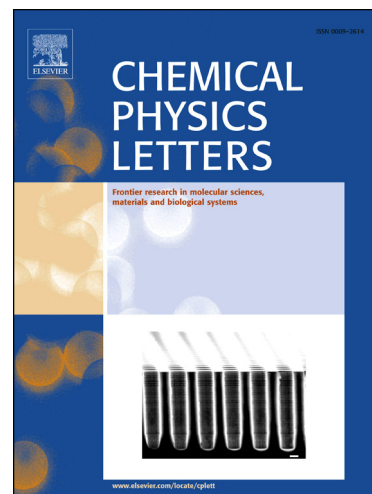
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Second hyperpolarizability of the calcium-doped lithium salt of pyridazine $\text{Li-H}_3\text{C}_4\text{N}_2 \cdots \text{Ca}$

Suélio Marques^{a,b}, Marcos A. Castro^{a,*}, Salviano A. Leão^a, Tertius L. Fonseca^a

^a*Instituto de Física, Universidade Federal de Goiás, Campus Samambaia, 74690-900 Goiânia, GO, Brasil*

^b*Instituto Federal Goiano, Campus Iporá, Av. Oeste nº 350, Santa Catarina, 76200-000 Iporá, GO, Brazil*

Abstract

In this work we report results of coupled cluster calculations for the second hyperpolarizability of the calcium-doped lithium salt of pyridazine ($\text{Li-H}_3\text{C}_4\text{N}_2 \cdots \text{Ca}$) molecule. In the static limit an unusual value of 4.34×10^6 au was obtained at the CCSD level of calculation. Results obtained for the dc-Kerr effect through SCF, CCS and CCSD methods show that $\gamma(-\omega; \omega, 0, 0)$ is strongly dependent of the electron correlation treatment. Dynamic results obtained at the CCSD level are also reported for the IDRI, dc-SHG and THG nonlinear optical processes.

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1. Introduction

Nowadays there is an intensive search for molecules with large hyperpolarizabilities as they are potential units to obtain materials with large macroscopic optical nonlinearities, a desirable feature for applications in many fields of science [1, 2]. Among systems with large hyperpolarizabilities are noteworthy inorganic noncentrosymmetric crystals [3], organic π -conjugate molecules [4] and organic molecules with incorporated donor and acceptor groups [5–7]. The substitution or incorporation of alkali or alkaline-earth metal atoms in organic or inorganic compounds has also been used as strategy to enhance the nonlinear optical responses [8–13].

In recent years has gained prominence electrides and alkalides, systems having loosely bound electrons that contribute decisively to enhance the nonlinear optical responses. In alkalides, alkali metal atoms are changed into anions after catching an electron from a ligand. The extra electron remains loosely bound because of the

small electron affinity of the alkali atom. In electrides, loose electrons behave as anions. Typically a valence electron of an alkali metal atom is pushed by the lone pair of a nitrogen (or fluorine) atom present in a complexant to which the alkali atom is bound, becoming a diffuse excess electron. Many electrides and alkalides have been synthesized [14–17] and great theoretical effort has been devoted for designing materials with these characteristics [18–29]. Electrides and alkalides are frequently unstable and strategies as encapsulation [30–32] and the use of rigid inorganic complexants [33] have been proposed to enhance their stability.

Two molecules based on lithium salt of pyridazine with unusual first hyperpolarizabilities were recently designed [34, 35]. Ma et al. [34] calculated the first hyperpolarizability of the lithium salt of pyridazine at the MP2 level and obtained the value of 859 au. They also showed that the addition of two sodium atoms to this lithium salt yields a new electride molecule with a pair of excess electrons and extraordinary first hyperpolarizability (1.4×10^6 au). Wang et al. [35] investigated how doping a calcium atom in pyridazine or alkaline-substituted pyridazine affects the optical properties of

*Corresponding author. Phone/Fax +55 62 3521 1014

Email address: mcastro1@ufg.br (Marcos A. Castro)

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