

Thermoelectric and optoelectronic properties of a heterocyclic isoxazolone nucleus compound



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ABSTRACT

The density of states, electronic charge density distribution and the optical susceptibilities of 3-methyl-4-[3-(5-benzyloxy-1H-indole)methylene]-isoxazol-5(4H)-one (C₂₀H₁₆N₂O₃) single crystal have been investigated using density functional theory. The exchange–correlation potential was treated within local density approximation (LDA) and the generalized gradient approximation of Perdew–Burke and Ernzerhof (PBE-GGA). In addition, the Engel–Vosko generalized gradient approximation (EV-GGA) was also applied to improve the electronic structure calculations. From the calculated total and partial density of states we concluded that the valence band is dominated by p state of N and C atoms while the conduction band is dominated by p state of N, O and C atoms. We have calculated the optical properties, namely, the real and imaginary parts of the dielectric function, refractive index, extinction coefficient, reflectivity, and energy loss function for radiation up to 14.0 eV. We also calculated the thermoelectric properties of the investigated compound, in order to better understand the temperature dependent, thermal conductivity, the temperature dependence of the Seebeck coefficients and the electrical conductivity for this compound.

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1. Introduction

The field of organic electronics has experienced in a few years a rapid development moving from a basic research level to the construction of molecule-based devices that are already commercially viable [1]. These devices have in common that their performance depends on how efficiently the charge carriers are injected and transported in the different organic active layers. Therefore, important advances achieved in this field have been connected to the enhancement of the charge carrier mobility of the organic molecules. However the incorporation of organic

molecules in the electronic devices shows still serious stability and processability limitations. At this stage one of the main demands is to find new stable organic semiconducting materials [2].

Isoxazolone nucleus is considered as the best proaromatic acceptor, when associated to aromatic donors, for conjugated donor–acceptor (D–π–A) merocyanine dye [3,4]. Due to their well tunable absorption spectra, molar extinction coefficients, and large first molecular hyperpolarizabilities (β), the merocyanine dyes with an isoxazolone nucleus are being used for the nonlinear optical and optical (recording) research [5]. In 2012 Zhang et al. [6] synthesized, two merocyanine dyes, all with an isoxazolone nucleus. In the two dyes, X-ray crystal structures were correlated with the IR spectra, particularly illustrating the molecular configurations and intra- and inter-molecular

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connections. The details through the X-ray crystallography resulting about the molecular configuration (or intermolecular interactions) relating to the cyanine and merocyanine dyes are still effective and are a view to their practical application [7]. Interestingly, the derivatives of isoxazolone can be present in three tautomeric forms i.e. in the OH, C=O and also in the NH form. These mixture can be always obtained but usually the most important form is ketonic [8]. The canine derivatives are of particular interest for the chiroptical effects [9]. Zhang et al. [6] focused on the effect of the solvent on the electrical devices absorption of the dyes through experimental and theoretical procedures. The solvatochromism of the dyes was reproduced through the time dependent density functional theory (TDDFT) parallel with the self-consistent reaction field (SCRf) approach, which hinged on the adjacent solvent molecules and a polarizable continuum. This has proved that the theoretical calculations of organic dyes on the chromophoric properties are inevitable apparatus for practical applications and are probably helpful in forecasting and clarifying the structure–property relationships of the dyes [10–13]. Thus, for the IR spectra of the dyes, the resonance frequency calculations were conducted for initial studies. In experimental study the vibrational spectroscopy depicts a directly relation in the spectra and the structure, but the theoretical calculations of vibrational spectra are of practical value for the recognition of identified and unidentified compounds [14–16].

In view of $C_{20}H_{16}N_2O_3$ we found that there is a scarcity of theoretical information. In the past the B3LYP method was used in investigating the vibrational data and electronic spectra of this compound [6]. To the best of our knowledge, no electronic structure, chemical bonding, optical properties and thermal properties of $C_{20}H_{16}N_2O_3$ have been yet reported in literature. Therefore, it stimulates us to deal with the electronic structure, chemical bonding, optical properties and thermal properties of $C_{20}H_{16}N_2O_3$ in the present paper.

The rest of the manuscript has been divided in three parts. In Section 2, we momentarily explain the computational techniques used in this study. In Section 3, which belongs to the results and discussion, the most pertinent results obtained for the electronic structure, chemical bonding, optical properties and the thermoelectric properties of $C_{20}H_{16}N_2O_3$ are presented. In Section 4 we summarized the work.

2. Methodology

The results were carried out within all electron full potential linear augmented plane wave (FP-LAPW) method based on DFT [17,18] as implemented in the WIEN2k code [19]. The crystallographic data of the 3-methyl-4-[3-(5-benzyloxy-1H-indole)methylene]-isoxazol-5(4H)-one ($C_{20}H_{16}N_2O_3$) was taken from Cambridge Crystallographic Data Centre, the CCDC number 729689 [20]. The unit cell's

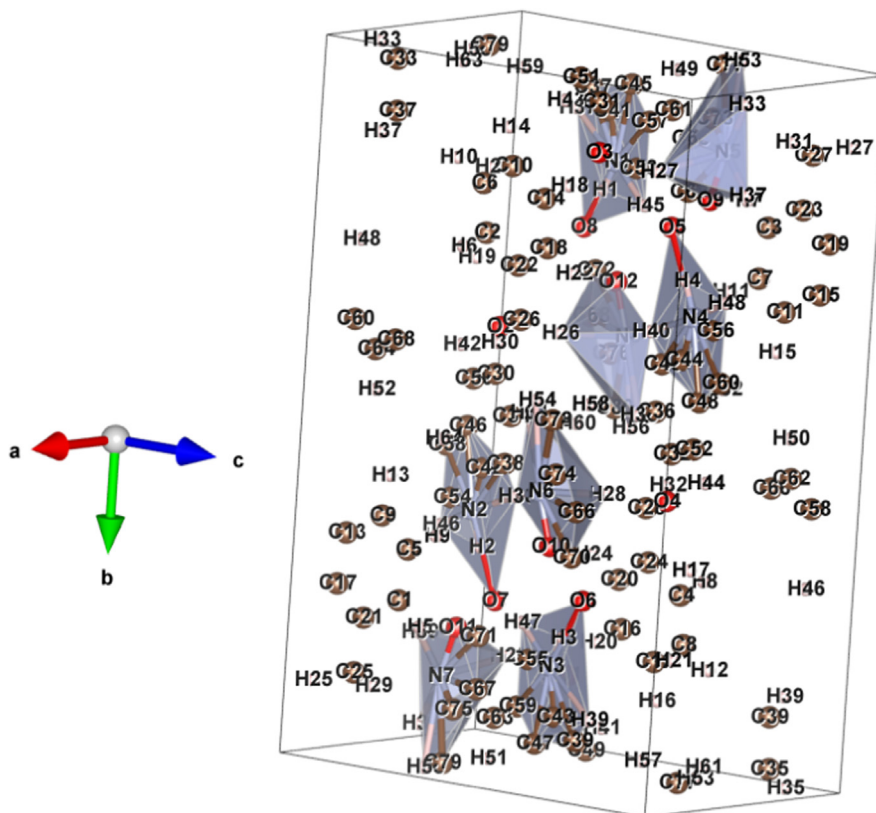


Fig. 1. Unit cell structure of $C_{20}H_{16}N_2O_3$.

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