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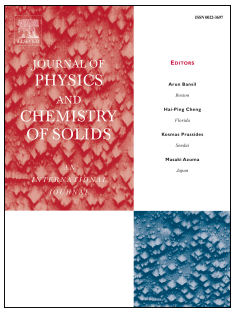

Hydrogen bonded 2-methyl-1H-imidazol-3-ium 3,5-dinitrobenzoate 3,5-dinitrobenzoic acid, a new optical crystal: Evaluation of properties by structural, spectral, quantum chemical calculations, Z-scan and Hirshfeld studies

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Hydrogen bonded 2-methyl-1H-imidazol-3-ium 3,5-dinitrobenzoate 3,5-dinitrobenzoic acid, a new optical crystal: Evaluation of properties by structural, spectral, quantum chemical calculations, Z-scan and Hirshfeld studies.

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Abstract

A new hydrgen bonded proton transfer complex, 2-methyl imidazolium 3, 5-dinitrobenzoate 3,5-dinitro benzoic acid (MIDB) was synthesised by the reaction between 2-methyl imidazole with 3,5-dinitro benzoic acid (1:2) in methanol solvent at room temperature. The crystals were subjected to FT-IR spectral analysis to confirm the functional groups of the new compound. Single crystal XRD analysis reveals that MIDB belongs to monoclinic system with $P2_1/c$ space group. The asymmetric unit consists of one 2-methyl imidazolium cation, one 3, 5-dinitrobenzoate anion and one uncharged 3,5-dinitro benzoic acid moiety. Experimental NMR spectroscopic data and theoretically calculated NMR data correlated very well to estabilish the exact carbon skeleton and hydrogen environment in the molecular structure of MIDB. The thermal stability of the compound was investigated by thermogravimetry and differential thermal analysis (TG-DTA). Computational studies such as optimisation of molecular geometry, natural bond analysis (NBO), Mulliken population analysis and HOMO-LUMO analysis were performed using Gaussian 09 software by B3LYP method at 6-31g basis set level. The calculated first-order polarizability (β) of MIDB from computational studies is 4.1752 $X10^{-30}$ esu, which is 32 times greater than that of urea. UV-vis-NIR spectral studies revealed that the MIDB has a large optical transparency window.The optical nonlinearities of MIDB have been investigated by Z-scan technique with He-Ne laser radiation of wavelength 632.8 nm. Hirshfeld analysis indicate O…H/H…O interactions are the superior interactions confirming excessive hydrogen bond net work in the molecular structure.

Keywords: Spectroscopic studies, single crystal XRD, HOMO-LUMO, hyperpolarizabiity, Hirshfeld surface

1 Introduction