to extended delocalized π–electron systems and the intrinsic neglect of intermolecular interactions are investigated.

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Keywords: charge density, dipole moment, chromophore

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Charge density study of an nonlinear optical compound – A combined experimental and theoretical study.

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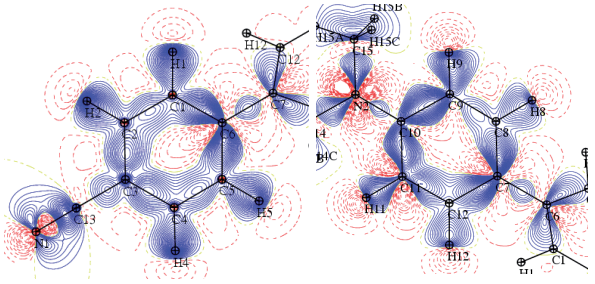
In recent years an intense worldwide effort has been focused on the design and development of organic conjugated materials with large optical non-linearities due to their potential applications in various optical devices [1–5]. Materials with high non-linear optical (NLO) activities are useful as electro-optic switching elements for telecommunication and optical information processing.

We present here a comparative study of a quantum-chemical analysis and X-ray diffraction study of a nonlinear optical material structure. The molecular optimized and experimental geometries are obtained via B3LYP/6-31G (d, p) level and X-ray diffraction respectively. The agreement between the experimental and theoretical results was satisfactory. The multipolar refinement was performed using Hansen-Coppens model implemented in the Mopro program [6]. The molecular electron charge density distribution is described accurately. The study reveals the nature of inter-molecular interactions including charge transfer and hydrogen bonds. More results about electrostatic properties will be presented at the meeting.



charge density of the studied compound

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Key words: Organic compounds, nonlinear optical properties, X-ray diffraction, DFT, charge density.

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Topological Analysis and Charge Density Studies of m-Nitrophenol compound. A Combined Experimental and Theoretical Study.

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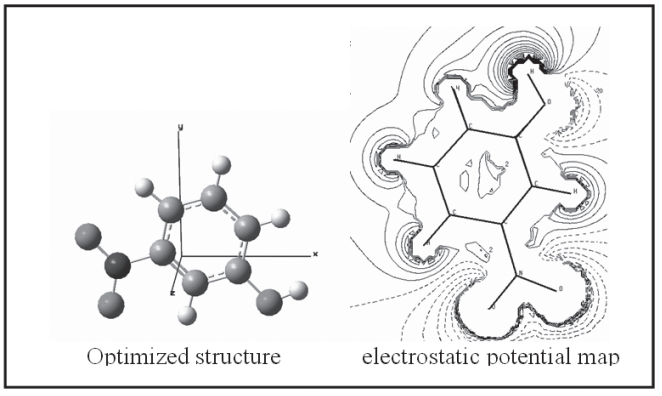
A combined experimental and theoretical study of the non linear optical compound, m-Nitrophenol was made on the basis of the electron density distribution and topological analysis. Accurate single-crystal diffraction data were measured on a suitable crystal with MoK α radiation at 125 K. Parallel MO calculations were made at UHF and DFT/UB3LYP. The agreement between experiment and theory is reasonably good. A charge density analysis, including the multipole refinement based on the Hansen – Coppens formalism [1], deformation density, topological analysis of ρ(r) according to the AIM theory [2] was carried out with the program Mopro [3]. The results of the topological analysis of ρ(r) at the bond critical points enable a quantitative description of the bonds. The chemical bonding characterization is presented in terms of the topological properties associated with bond critical points and the natural bond orbital (NBO) analysis as well. The asphericity in electron density is nicely demonstrated by the Laplacian of electron density in both experimental and theoretical results.



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Keywords: Structural Study, Electron charge density, m-Nph, Mopro program, nonlinear optical compound (NLO)

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Experimental charge density study of the [RuCl(κ³-*N,N,O*-bdmpza)(η⁴-cod)] complex

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The [RuCl(κ³-*N,N,O*-bdmpza)(η⁴-cod)] (bdmpza = bis(3,5-dimethylpyrazol-1yl)acetate) complex is a versatile catalyst precursor in some specific organic reactions. We have carried out a detailed experimental