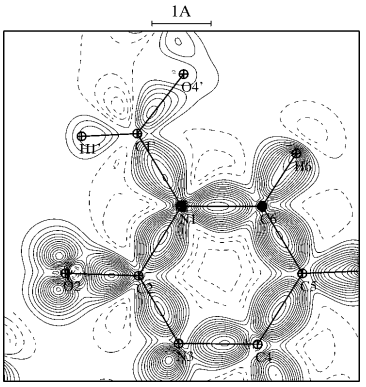

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Keywords: Z-DNA, sub-atomic resolution, deformation density

MS41.P19

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Charge density studies on N-n-butyltetrachlorophthalimide

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The charge density distribution in N-n-butyltetrachloro-phthalimide has been determined by means of high-resolution X-ray diffraction at 100K. The supramolecular structure of the title compound is stabilized by intermolecular halogen bonds C-Cl···O and intermolecular Cl···Cl interactions [1]. In the current presentation the deformation density distribution of electron density and topological analysis of electron density for the title compound crystal are shown. The deformation density clearly indicates a significantly anisotropic distribution of electrons in the halogen atom with less of them in the direction of C-Cl bond and more in the other two directions (see Figure 1 below). The topological analysis confirms conclusions derived from the deformation density distribution.

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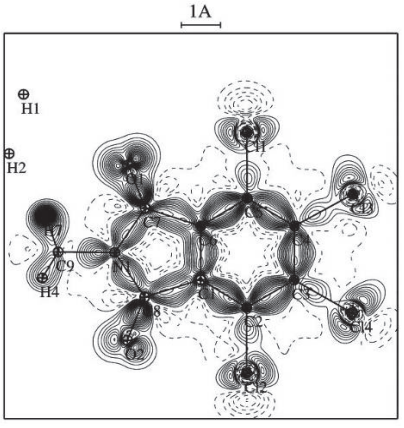

Fig. 1. Deformation density distribution for N-n-butyltetrachlorophthalimide

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Keywords: halogen bonding, electron density, electron density topology

MS41.P20

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Electrostatics of fluoroquinolone antibiotics derived from crystal structures

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A comparison of nine fluoroquinolone antibiotics [1] with respect to their solid-state electrostatic properties is reported. Molecular electrostatic potentials and dipole moments were derived from the electron density distribution after crystal structure refinement with *Invarioms*. The comparison of molecular electrostatic potentials has important implications on their function as anti-infective agents. Molecular electrostatic potentials for the same protonation states show a striking degree of similarity for the whole class of compounds. The relevance of this similarity for rational drug design and optimization of lead structures is discussed. The rapid calculation of electrostatic potentials directly from the invariom database makes the procedure suitable for high-throughput screening.

Deposited, newly determined and re-measured single-crystal diffraction data of varying quality were evaluated in this manner. The structure of lomefloxacin hydrochloride tetrahydrate is reported for the first time and the structural model of enoxacin methanol solvate as reported by Yoon *et al.* [2] needed revision: it turns out to be a water solvate. An *in silico* validation procedure for invariom database entries [3] is presented.

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Keywords: ntibacterial, electrostatics, charge density

MS41.P21

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Dipole moment determination in push-pull chromophores from charge density data

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Push-pull chromophores find use in organic optical materials and for many applications their ground state dipole moment and polarizability are important properties. [1] In the condensed phase intermolecular interactions influence these properties and may lead to an enhancement of the dipole moment. The crystalline state provides a rigid surrounding for the intermolecular interactions, thus maximizing the effects.

Experimental charge density studies facilitate the determination of molecular "in-crystal" dipole moments. However, the dipole moment values determined in this way have to be examined critically and are prone to systematic errors. [2] In this study dipole moments obtained from multipole refinements of structure factor amplitudes determined experimentally by diffraction and theoretically by *ab-initio* calculations are compared. The applicability of the invariom model [3]

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

MS41.P22

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

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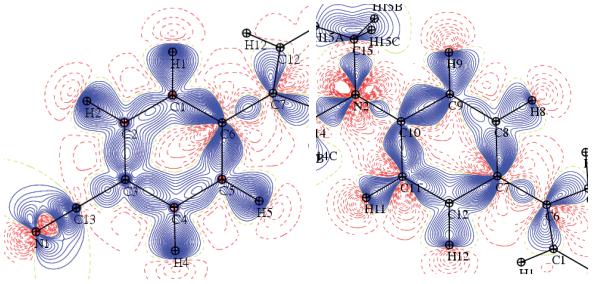
In recent years an intense worldwide effort has been focused on the design and development of organic conjugated materials with large optical non-linearities due to their potential applications in various optical devices [1–5]. Materials with high non-linear optical (NLO) activities are useful as electro-optic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

MS41.P23

Acta Cryst. (2011) A**67,** C515

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

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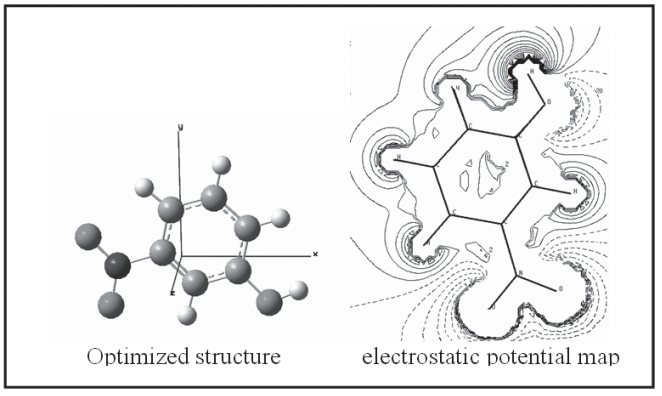
A combined experimental and theoretical study of the non linear optical compound, m-Nitrophenol was made on the basis of the electron density distribution and topological analysis. Accurate single-crystal diffraction data were measured on a suitable crystal with MoK α radiation at 125 K. Parallel MO 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)

MS41.P24

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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