

theory. First the electron charge density distribution was obtained from high resolution X-ray experiment at low temperature using XD package [1]. The crystal structure was refined using the multipolar model of Hansen and Coppens (1978) [2]. The study of the molecular electron charge density distribution reveals the nature of inter-molecular interactions including charge transfer [3]. Thereafter the results obtained were the subject of a comparison to those determined by theoretical calculation.

The agreement between the experimental and theoretical results such as: atomic net charge, molecular dipole moment, electrostatic potential and electron density was satisfactory. Table and figure below gives the molecular dipole obtained with different models and the orientation of the X-ray diffraction dipole moment in the molecule of DMACB, respectively.

Table: Magnitude of the molecular dipole moment

| Models | X-ray diffraction | AM1 | HF/6-31G** | DFT/B3LYP/6-31G** |
|-----------|-------------------|--------|------------|-------------------|
| μ (D) | 5.80 | 5.1999 | 6.5974 | 8.4973 |

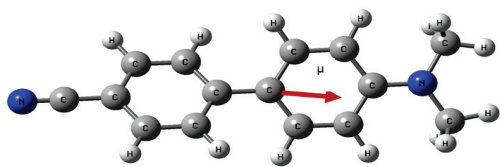


Figure: Orientation of dipole moment in DMACB

[1] Koritsanszky, T.; Howard, S.; Richter, T.; Su, Z.; Mallinson, P.R.; Hansen, N.K. XD a Computer Program Package, University of Berlin 2003. [2] Hansen & Coppens, Acta Cryst. (1978), A34, 909-921. [3] Coppens, P. X-ray Charge Densities and Chemical Bonding. New York: Oxford, 1997.

Keywords: Charge density, XD and Gaussian Software

FA4-MS28-P04

On the the use of single crystal diffractometer data necessary for performing the 2nd and 4th restricted moment method. Prabal Dasgupta, Bholanath Mondal

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With the advent of epoch-making paper by Groma & Borbely [1] & Borbely et al [2] renaissance of 2nd & 4th restricted moment method for evaluation of crystallite size has taken place. Above mentioned authors have reported that they have made use of high resolution XRD data. Present work aims to explore if the same technique may be applied to commonly used double crystal diffractometer data? To probe this, background & instrumental broadening corrected 111 & 200 line of commercial grade Ni (in continuous as well as in step-scan mode) were subjected to such analysis. M_2 & M_4/q^2 plots suggest that peak broadening in these materials are mainly crystallite size-related broadening. Different step-widths varying from 0.005 to 0.03 and scan rate varying from 0.2 to 2.5 sec were chosen so as to ascertain the quality of data that yields more or less same crystallite size (within 5%) from the 2nd & 4th moment plot. It was revealed that XRD data

with stepwidth of 0.01deg or less and scan speed of at least 2.0 sec step⁻¹ in the step-scan mode as well as in continuous mode yields satisfactory convergence.

[1] Borbely A. & Groma I. Appl. Phys. Lett. 79 p-1772-1774, 2001

[2] Borbely A., Revesz A. & Groma I., Z. Krist., Suppl., 23, p-87, 2006

Keywords: applied crystallography materials, powder method, crystallite size strain

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Theoretical and Crystallographic calculations on meta-Nitrophenol: a non linear optical compound.

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We investigated, in the present work, theoretically and experimentally the electron density distribution and electrostatic potential around the molecule m-Nitrophenol (m-NPH). The experimental determination and results of the molecule have been calculated from a high-resolution X-ray diffraction study. The X-ray experiment showed that there is an important accumulation of the electronic density around the connections of hydroxyl and nitro groups. Moreover, the lone pairs of the oxygen atoms were perfectly localized [1]. The x-ray data refinements were holed by using the XD software. XD uses the multipolar pseudo-atom model for the electron-density refinement [2]. The experimental charge density of the molecule m-NPH obtained by the multipolar model of Hansen and Coppens [3] is compared to the theoretical charge density determined from ab initio calculation. Theoretical calculations were performed with the Gaussian package at the density-functional (DFT) level of theory and semi empirical methods. The theoretical calculations carried out on the isolated molecule give results (net atomic charge, dipole moment, electrostatic potential ...) in good agreement with those found in the experimental investigation.

Table below gives the molecular dipole moment in the inertial frame obtained with different models.

Table 1. Magnitude of the molecular dipole moment

| Models | Multipolar refinement | AM1 | MNDO | Ab initio |
|-----------|-----------------------|------|------|-----------|
| μ (D) | 5.80 | 6.03 | 6.12 | 5.89 |

[1] Hamzaoui, F.; Baert, F.; Wojcik, G. Electron-density study of m-nitrophenol in the orthorhombic structure. Acta Cryst. B 1996, 52, 159-164. [2] Hansen & Coppens, Acta Cryst. (1978), A34, 909-921. [3] Hamzaoui F., Drissi M., Chouaih A., Vergoten G., International Journal of molecular Sciences, 2007, 8, 103-115

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PPDock-Portal Patch Dock: a web server for drug virtual screen and visualizing the docking structure by GP and X-Score. Po-Tsang Huang, Pei-Hua Lo,

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