

electron density in terms of multipole model are derived to investigate the electron density distribution and chemical bonds. All chemical bonds will be characterized based on atoms in molecule theory, and classified by the location of the bond critical point (BCP) and its associated topological properties. The XAS of Mo K-edge is used to characterize the electronic states of both complexes and the light induced transformation of complex **2**. All experimental observations will be compared with the density functional theory calculation. The different chemical reaction properties between **1** and **2** will be rationalized based on all experimental and theoretical results.

Keywords: charge density; x-ray absorption spectroscopy

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The Molecular Dipole Moment of a Nonlinear Optical Compound (m-Nitrophenol). Fodil Hamzaoui^a, Abdelkader Chouaih^a, Naima Boubagra^a, Mokhtaria Drissi^a. ^aLaboratoire SEA2M-Facultés des Sciences & Technologies-University of Mostaganem, Algeria.

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We present here results of comparative study of electron charge density distribution in the m-Nitrophenol compound from x-ray data experiment en theoretical ab initio investigation. First the electron charge density distribution was obtained from high resolution x-ray experiment thereafter the results obtained were the subject of a comparison to those determined by *ab initio* theoretical calculation.

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-package. The theoretical calculations carried out on the isolated molecule give net atomic charge in good agreement with those found in the experimental investigation. Consequently, the obtained dipole moment is in concord with that deduced from the experiment. The theoretical calculations were carried out using the MOLDEN software. The orientation of the molecular dipole moment shows that the attractive electrostatic potential is around the Nitro en the hydroxyl groups and the repulsive electrostatic potential is found around the C-H groups. The estimation of the molecular dipole moment enables us to measure the influence of the intermolecular forces and to help us to understand the mechanisms of intra molecular charge transfer [2].

Table below gives the average components of the molecular dipole moment in the inertial frame.

Detailed results of the comparative study will be presented in the meeting.

Table 4. Magnitude of the molecular dipole moment

μ_x	μ_y	μ_z	μ (Debye)
-0.032	-0.032	-0.636	5.81 (20)

[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] *International Journal of Molecular Science*, **2007**, *8*, 103-115

Keywords: charge density; XD Software

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Crystal Structure of 2-Nitro-1,3,4,4-tetra-chloro-1-mono(2-methylphenylthio)-1,3-butadiene Compound. Funda Ozkok^a, Cemil Ibis^a. ^aDepartment of Chemistry, Engineering Faculty, Istanbul University, Avcilar, Istanbul-Turkey.

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It is known that some heterocyclic compounds have got biologic activities such as herbicides, insecticides, fungicides etc. from US-patent^[1].

The aim of this work is to synthesis and to determine the crystal structure of 2-Nitro-1,3,4,4-tetrachloro-1-mono(2-methylphenylthio)-1,3-butadiene compound with X-ray diffraction method. Crystal Structure of 2-Nitro-1,3,4,4-tetrachloro-1-mono(2-methylphenylthio)-1,3-butadiene compound was mounted on an Rigaku R-AXIS Rapid-S Diffractometer with a graphite monochromatized MoK α radiation ($\lambda = 0.71073 \text{ \AA}$). The structure was solved by direct method with SIR 92 and refined with crystals^[2].

Crystal data: C₁₁H₇Cl₄NO₂S, triclinic, P-1 (#2), a=6.6525(7) Å b=10.7906(5) Å c= 10.8339(4) Å $\alpha = 72.57(3)^\circ$ $\beta = 84.23(4)^\circ$ $\gamma = 75.81(3)^\circ$ V=719.03(9) Å³ Z=2 D_x=1.658 g/cm³ F(000)= 360.00, $\mu(\text{MoK}\alpha) = 9.61 \text{ cm}^{-1}$

[1] Diamond Alkali Company (Ert.H.Bluestone), U.S. Pat. 3021370 (13 Feb. 1962), *Chem. Abst.*, 57, 3293c [2] A. Altomare, G. Cascarano, C. Giacovazzo, A. Guagliardi, M. Burla, G. Polidori, M. Camalli, SIR92, *J. Appl. Cryst.*, **1994**, *27*, 435.

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Crystal Structure of 1-thiocarboxamide-3-Methyl-4-ethanol-3-pyrazolin-5-one. Z. D. Tomic^a, Z. K. Jacimovic^b, G. Giester^c, A. Galani^d, V. Dokorou^d, D. Kovala Demertzi^d. ^a'Vinča' Institute of Nuclear Sciences Serbia. ^bFaculty of Metallurgy and Technology, University of Montenegro, Montenegro. ^cInstitut für Mineralogie und Kristallographie, Universität Wien, Austria. ^dUniversity of Ioannina, Greece.

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We are currently interested in the structural properties and coordination chemistry of a family of a 3-Methyl-3-pyrazolin-5-one derivatives. It is supposed that these molecules could serve as a versatile ligands, due to the possibility of changing their steric and electronic features by substitution at position 1, 2, and 4 of the pyrazole ring. In this