

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.

Keywords: crystallography in chemistry; organic compounds chemical crystallography; sulfur compounds

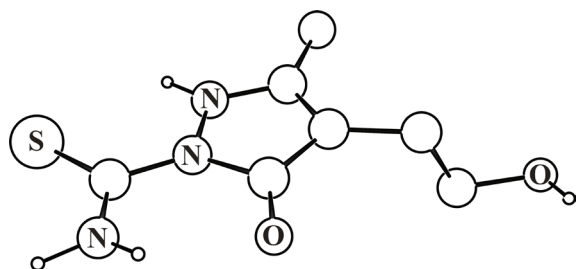
FA4-MS05-P38

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

work we present the crystal structure of the potential ligand molecule where $R1=(CS)NH_2$, $R2=H$, and $R4=CH_2CH_2OH$, with emphasis on the mode of molecular association in the crystal lattice. The crystal structure of the parent 3-Methyl-3-pyrazolin-5-one was reported in two polymorphic forms [1,2]. Comparison of the title compound with the structure of the parent molecule, shows that the most significant difference in the pyrazole ring geometry is extension of the N1-C5 bond for $\approx 0.1\text{\AA}$. This difference could be attributed to the perturbation in the electronic structure caused by the presence of thiocarboxamide substituent on the N1. The pyrazole ring is nearly planar: the largest deviation from the mean plane of the ring is $0.010(2)$. The mean planes of the thiocarboxamide substituent and of the pyrazole ring form dihedral angle of $4.0(2)^\circ$. Hydroxyl group is placed so that the normal distance between the mean plane of the pyrazole ring and the O atom is $1.485(2)\text{\AA}$ (Fig). Association of molecules in the crystal lattice is determined by the spatial relationships between the hydrogen bond donors and acceptors, which are placed in a neighbouring positions. This enable extension of dimeric hydrogen bonded units into the molecular chains. These chains are connected by weaker $N(\text{pyr})\cdots H\cdots OH$ bond. Due to stereochemical properties of the title molecule, the neighbouring chains are positioned in the approximately orthogonal fashion.



- [1] De Camp W.H., Stewart J.M., *Acta Cryst.*, **1971**, B27, 1227.
 [2] Zhang Z., Jin S., Wang S., Liu B., Guo J., *Acta Cryst.* **2004**, E60, 315.

Keywords: pyrazolon; X-ray structure

FA4-MS05-P39

Calculation of the Raman spectra of the polymorphic forms of $Y_2Si_2O_7$. Daniel M. Töbrens^a, Reinhard Kaindl^a, Volker Kahlenberg^a. ^a*Institute of Mineralogy and Petrography, University of Innsbruck, Austria.*

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$Y_2Si_2O_7$ forms a number of polymorphs. Three building principles can be distinguished based on the conformation of the silicate groups. Forms β and γ are composed of Si_2O_7 dihedra with the SiO_4 tetrahedra in staggered orientation. In δ , ϵ , and ζ the two tetrahedra in the dihedra are in eclipsed orientation. The forms α and η contain both monohedra and eclipsed trihedra. Experimental Raman spectra were obtained for the forms α , β , γ , η . Calculations of the vibrational spectra were conducted for all forms but η , which has a very large unit cell. For the *ab initio* calculations the

program CRYSTAL06 [1] was used. Calculations were done using DFT with both local and hybrid functionals. Various basis sets taken from the CRYSTAL website were tested (www.crystal.unito.it). For the simple spectrum of form β , unequivocal assignment of all lines was possible. From this, a simple correction of the calculated frequencies could be derived, which helped in the assignment of the more complex spectra. After application of these corrections, the different basis sets give very similar results. Basis sets specifically optimized for this problem reached a slightly better agreement with the observed line positions without correction. However, the calculation times necessary for this are disproportionally longer, and no qualitative changes result. For all polymorphs, the most characteristic lines of the Raman spectra are observed in the range $600 - 900\text{ cm}^{-1}$. In all cases, these are Si-O stretching and bending modes. An inspection of the underlying structural mechanisms shows the crucial influence of the different conformations of the silica groups especially in this region of the spectra. Pure O-Y-O bending modes were found to be located below 200 cm^{-1} . The lines in the range from 200 cm^{-1} to 520 cm^{-1} are generally O-Y-O bending modes, but contain some degree of distortion of the SiO_4 tetrahedra. Those observed modes involving Y-O stretching were found to be weak.

[1] Dovesi, R. *et al.* Crystal06 User's Manual. Università di Torion, Torino, 2006.

Keywords: rare-earth compounds; raman spectroscopy; ab-initio calculations

FA4-MS05-P40

Structure de Di(4,4',5,5'-Tetramethyl-1,3-Dithia-1',3'-Diselenafulvalene) Tetrafluoroborate: (TMDTSDF)2BF4. Mhanni Allal^a, Ouahab Lahcen^a.

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$(C_{10}H_{12}S_2Se_2)_2 BF_4$, Mr = 795.31, triclinic, P1, a = 7.208 (16), b = 7.571 (5), c = 13.068 (4) Å, $\alpha = 85.65 (4)^\circ$, $\beta = 86.88 (7)^\circ$, $\gamma = 70.46 (8)^\circ$, V = 669.9 Å³, Z = 1, Dx = 1.971 g cm⁻³, F(000) = 385. (Mo K) = 0.71073 Å, = 57.59 cm⁻¹, = 293K, = 0.044 based on 1206 observed reflections with. The F atoms of the tetrahedral BF₄ unit are disordered as already observed in such an union. However, the B atom is located at the origin of the unit cell, in contrast with its distribution on both sides of the origin in (TMTCF)2BF₄, C=S and Se. The heteroatoms (S and Se) also present a statistical disorder. The bond distances (specially C-S/Se: 1.80 - 1.85 Å), The interplanar separation (3.59 and 3.62 Å) between adjacent organic molecules and the intermolecular heteroatom contacts are midway between those observed in (TMTTF)2BF₄ and (TMTSF)2BF₄.

Keywords: electrocrystallisation; magnétisme; crystallography