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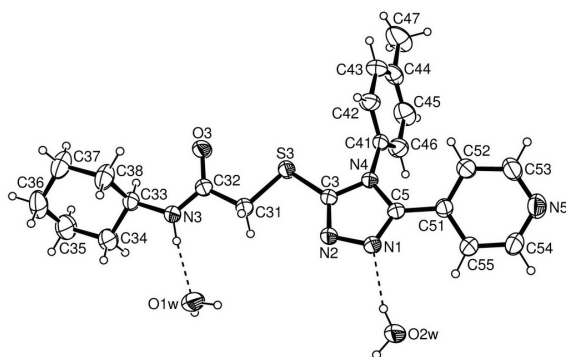
Keywords: powder diffraction; structure solution; DFT calculations

FA4-MS05-P33

Experimental and Theoretical Investigation of the Molecular and Electronic Structure of *N*-Cyclohexyl-2-[5-(4-pyridyl)-4-(*p*-tolyl)-4*H*-1,2,4-triazol-3-ylsulfanyl]acetamide Dihydrate. Muharrem Dinçer^a, Namık Özdemir^a, Ahmet Çetin^b, Tekin Keser^c. ^aDepartment of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. ^bDepartment of Chemistry, Bingöl University, 12000, Bingöl, Turkey. ^cDepartment of Chemistry, Firat University, 23119, Elazığ, Turkey.

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1,2,4-triazoles and its derivatives represent one of the most biologically active classes of compounds, possessing a wide spectrum of activities including antibacterial, antifungal, antiviral, *anti*-inflammatory, anticonvulsant, antidepressant, antihypertensive, analgesic, and hypoglycemic properties [1]. In addition, substituted 1,2,4-triazoles have been actively studied as bridging ligands coordinating through their vicinal N atoms [2]. In the title compound, C₂₂H₂₅N₅OS·2H₂O, the molecules are stacked in columns running along the *b* axis. In this arrangement, the molecules are linked to each other by a combination of one two-centre N—H···O hydrogen bond and four two-centre O—H···O hydrogen bonds containing two types of ring motif, viz. R₄⁴(10) and R₃³(11). In the crystal structure, centrosymmetric π — π interactions between the triazole rings, with a distance of 3.691 (2) Å between the ring centroids, also affect the packing of the molecules. The experimental geometry of title compound (I) obtained from single-crystal X-ray diffraction was compared with those obtained from quantum-mechanical calculations, together with IR and ¹H-NMR spectra. Theoretical calculations were performed by means of GAUSSIAN 03W [3].



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Keywords: single-crystal X-ray diffraction; quantum mechanics; theoretical crystal calculations

FA4-MS05-P34

Bis(acesulfamato- κ O⁴)diaquabis-(3-methylpyridine- κ N)nickel(II). Necmi Dege^a, Hasan İçbudak^a, Elif Adıyaman^a. ^aDepartment of Physics, Ondokuz Mayıs University, Samsun, Turkey.

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In the crystal structure of the title compound [systematic name: diaquabis(6-methyl-2,2-dioxo-1,2,3-oxathiazin-4-olato- κ O⁴)bis(3-methylpyridine- κ N)nickel(II)], [Ni(C₄H₄NO₄S)₂(C₆H₇N)₂(H₂O)₂], the Ni^{II} centre resides on a centre of symmetry and has a distorted octahedral geometry. The basal plane is formed by two carbonyl O atoms of two monodentate *trans*-oriented acesulfamate ligands and two *trans* aqua ligands. The axial positions in the octahedron are occupied by two N atoms of two *trans* pyridine ligands. Molecules are stacked in columns running along the *a* axis. There are π - π stacking interactions between the molecules in each column, with a distance of 3.623(2) Å between the centroids of the pyridine rings. There are also O—H...O interactions between the columns.

Keywords: saccharinato complexes; methylpyridine; acesulfamate

FA4-MS05-P35

Chemical Bonding and Electronic Configuration of Phosphido-bridged Mo and W Complexes. I-Jui Hsu^a, Chi-Rung Lee^b, Hsiu-Mei Lin^c, Yu Wang^d, Shin-Guang Shyu^e. ^aDepartment of Molecular Science and Engineering, National Taipei University of Technology. ^bDepartment of Chemical Engineering, Minghsin University of Science and Technology. ^cInstitute of Bioscience and Biotechnology, National Taiwan Ocean University. ^dDepartment of Chemistry, National Taiwan University. ^eInstitute of Chemistry, Academia Sinica, Taiwan.

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Charge density and x-ray absorption spectroscopy (XAS) are applied to characterize the chemical bonding and electronic structures of the heterobimetallic phosphido-bridged complexes, CpW(CO)₃(μ -PPh₂)Mo(CO)₅ (**1**) with W-Mo distance 3.1723(4) Å and CpW(CO)₃(μ -PPh₂)Mo(CO)₅ (**2**) with W-Mo distance 4.510(4) Å. Both have been reported with special chemical reaction properties because of the interaction between W and Mo: complex **2** can be converted into **1** after irradiation with UV or heating at reflux temperature. In order to correlate how the chemical bond of Mo-W affect the chemical reaction in complex **1** and **2**, the accurate single crystal diffraction data of both complexes at 100 K are collected and the experimental

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

FA4-MS05-P36

The Molecular Dipole Moment of a Nonlinear Optical Compound (m-Nitrophenol). Fodil Hamzaoui^a, Abdelkader Chouaih^a, Naima Bouabgra^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

FA4-MS05-P37

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, $\mu(\text{MoK}\alpha) = 9.61 \text{ cm}^{-1}$

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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