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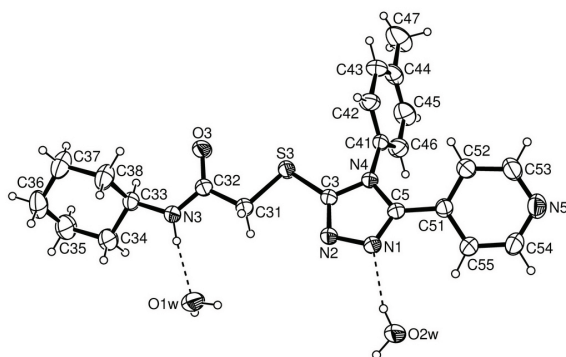
Keywords: powder diffraction; structure solution; DFT calculations

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