

Data of these crystal was collected by the use of. Stoe IPDS II diffractometer system. Crystal structure were solved by direct methods. SIR97 structure solution program was used. A refinement was carried out by full – matrix least – squares methods using Shelxl 97 refinement program.

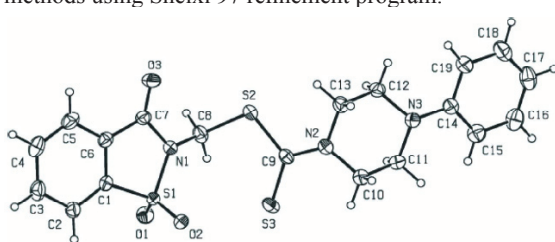


Fig 1: An ORTEP–III view of title compound

[1] Ates, Ö., Cesur, N., Güner, H., Uzun, M., Kiraz, M. & Kaya, D., *Farmaco*, **1995**, 50, 361–364. [2] Günay, N. S., Çapan, G., Ulusoy, N., Ergenç, N., Öztürk, G. & Kaya, D., *Farmaco*, **1999**, 54, 826–831. [3] Farghaly, A. O. & Moharram, A. M., *Boll. Chim. Farm.* **1999**, 138, 280–289. [4] Xu, L. Z., Jiao, K., Zhang, S. S. & Kuang, S. P., *Bull. Korean Chem. Soc.* **2002**, 23, 1699–1701.

Keyword: crystal structure; 1,2- benzisothiazol; 4-phenyl piperazine

FA4-MS05-P31

Structural Studies of Molecular Complexes of 4,4'-Dinitrobiphenyl. Peet H. van Rooyen^a, David Liles^a, Eric Modau^a. ^a*Department of Chemistry, University of Pretoria, Pretoria, South Africa.*

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Complexes of para disubstituted and 4-monosubstituted biphenyl formed with 4,4'-dinitrobiphenyl (DNBP), demonstrate intense colours, from pale yellow to dark red, upon formation. These colours are dissimilar to the colour combination of the parent compounds. The focus of this study was to investigate the nature of these molecular donor-acceptor interactions in the solid state, using spectroscopic techniques such as IR, Raman, UV-Vis, NMR and X-ray crystallography. Typical interactions observed in such molecular complexes include π - π interactions, hydrogen bonding, charge transfer and van der Waals interactions. There are no significant localized interactions between the guest molecule and the DNBP, except for the weak H-bond observed in the hydroxybiphenyl complex [1]. Complexes of DNBP, as acceptor, studied included a variety of mono- and disubstituted donors, such as dihalo, diamino, di- and monohydroxy groups. The crystal structures of these complexes showed retention of the non-planar conformation of DNBP with a dihedral angle of around 35°. This conformation for DNBP has also been confirmed using density functional theory (Gaussian) calculations that showed good agreement between the theoretically calculated and experimentally observed IR and Raman spectra in the solid state. In non-complexed DNBP, adjacent stacks of DNBP imolecules form a herring-bone pattern when viewed from above. On forming complexes with planar guest molecules, the stacks open out to form a checker-board pattern (as viewed from above) forming slots between

the stacks which are occupied by the guest molecules. The packing is generally similar in all the complexes with planar guest molecules and is determined by the stacking of the DNBP molecules - with the substituted biphenyls, urea [2] or thiourea guest molecules slotting in between the stacks. It appears as if the packing of the complexes in the solid state is directed mainly by the similar packing of DNBP units in these complexes. Some of the molecular ratios for these complexes that vary, depending on the electronic properties of the donor molecules, were determined using NMR spectroscopy. The ratio of guest to DNBP depends on the size (length) of the guest molecule.

[1] C.P. Brock, K.L. Haller *Acta Crystallogr. Sect. C, C: Cryst. Struct. Commun.*, **1984**, 40, 1387. [2] R. Thaimattam, D.S. Reddy, Feng Xue, T.C.W. Mak, A. Nangia, G.R. Desiraju (1998) *J. Chem. Soc., Perkin Trans. 2*, **1998**, 1783.

Keywords: molecular complexes; density functional theory; spectroscopy and molecular structure

FA4-MS05-P32

Study of the Crystal Structure of Three Synthetic Insect Pheromones Using X-ray Powder Diffraction and DFT Calculations. Michela Brunelli^b,

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Pheromones are widely recognised as being extremely important among social insects as a means of communication [1]. They can be both volatile and non-volatile chemicals, which can act by simple detection in the air or by direct contact, respectively. The pheromones that this study focuses on fall in the second category ("recognition pheromones"), and in particular on methyl branched alkanes. Whilst evidence suggests that methyl-branched alkanes have an effect as recognition pheromones, straight chain alkanes have regularly been shown to have no effect, despite having very similar chemical properties. This has led to the suggestion that the conformation of the compounds may have an effect which leads to the distinction. Previous theoretical calculations [2] have suggested that the lowest energy conformation of a methyl-branched alkane is a "paperclip" conformation. In this study three enantiomerically pure methyl-branched alkanes were investigated, namely 11-methyl nonacosane C29Me(11), 9-methyl nonacosane C29Me(9) and 11-methyl heptacosane C27Me(11). Their structures were derived from high resolution X-ray powder diffraction data and subsequently optimized by a geometry optimization by energy minimization in solid state using DFT approach. The aim is to attempt to ascertain how the stereochemistry associated with the methyl group, or the conformation of the molecule imposed by this group, may affect the binding of the molecule to the receptors in an insect's antennae.

[1] Vander Meer, Breed, Espelie, Winston. Pheromone communication in Social insects. Westview, Oxford. [2] Goodman. *J. Chem. Inf. Comput. Sci.* **1997**, 37, 876-878; Gummow R.J., Liles D.C., *Mat. Res. Bull.*, **1993**, 28, 1293.

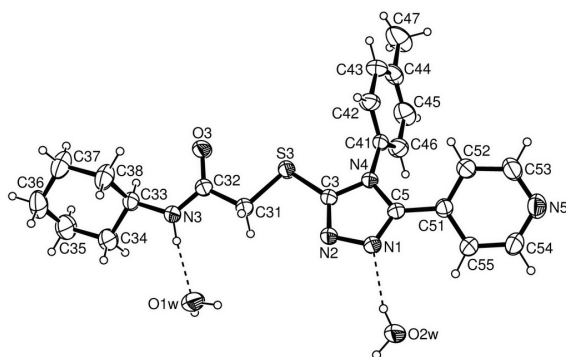
Keywords: powder diffraction; structure solution; DFT calculations

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].



[1] Abbas, A. A. & Khalil, N. S. A. M., **2005**. *Nucleosides, Nucleotides and Nucleic Acids*, 24 (9), 1353–1372. [2] Li, B.

-Z., Liu, X. -G., Peng, Y. -F., Li, B. -L. & Zhang, Y., **2006**. *Acta Cryst.* C62, m41-m44. [3] Frisch, M. J. et al. **2004**. GAUSSIAN03, Revision E.01. Gaussian, Inc., Wallingford CT 06492, USA.

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