shown in Fig. 1.

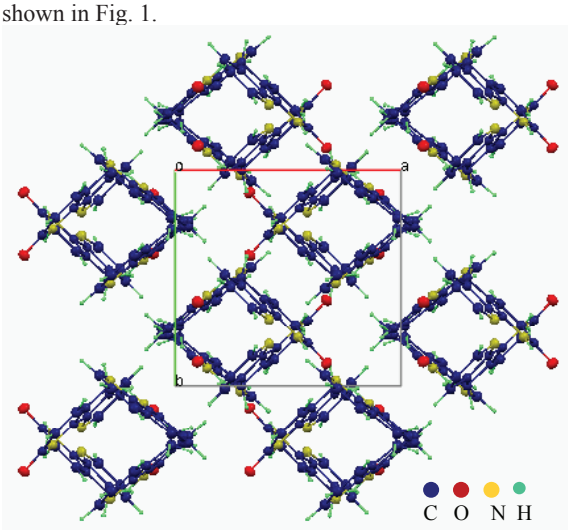

Fig.1. Packing diagram of the title compound.

[1] M. Riklin, A. von Zelewsky, A. Bashall, M. McPartin, A. Baysal, J.A. Connor, J.D. Wallis, *Helv. Chim. Acta*, **1999**, 82, 1666. [2] A. Baysal, F. Durap, B. Gümgüm, L. T. Yıldırım, D. Ülkü, D. A. Boğa, S. Özkar, *Helv. Chim. Acta*, **2007**, 90, 1211. [3] L. J. Henderson, Jr., F. R. Fronczek, W. R. *Cherry, J. Am. Chem. Soc.*, **1984**, 106, 5876. [4] D. E. Marx, A. J. Lees, *Inorg. Chem.*, **1987**, 26, 620.

Keywords: diazafluorene; bipy; phen; crystal packing

FA4-MS05-P29

Structural Analysis of *endo*- and *exo*-Benzocylcobutenonorbornene-Dibromides by Using ^{1}H, ^{13}C NMR and X-Ray Diffraction Tecniques.

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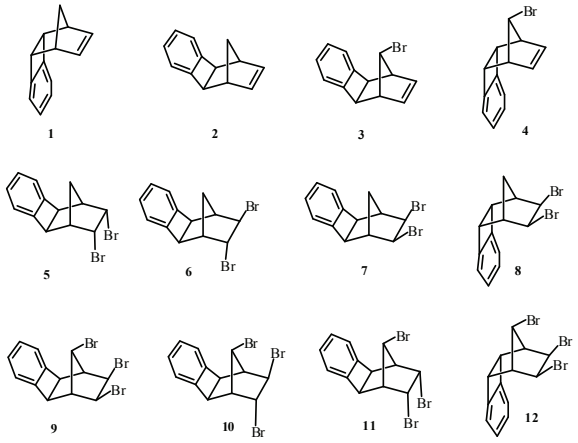
Several monobromides, dibromides and tribromides derived from endo- and exo-benzocylcobutenonorbornene were synthesised and published by Daştan co-worker for several purposes [1]. This kind of products are also important to investigate "the γ-gauche effect" in NMR spectroscopy [2]. In this study, we study on spectroscopic data of isomeric compounds by corelatting exact conformotions obtained by X-ray diffraction analysis. ^{1}H-NMR, ^{13}C-NMR, DEPT, gCOSY, gHMQC and GHMBC and double resonance techniques were used to determine the exact signal for each nucleus.



Scheme 1

[1] a) E. Uzundumlu, Bromination of *Endo*- and *Exo*-Benzocylcobutenonorbornene at different conditions. Master Thesis, Atatürk University Graduate School of Natural and Applied Sciences Department of Chemistry, Erzurum 2003. b) A. Dastan, E. Uzundumlu, M. Balci, F. Fabris, O. De Lucchi *Eur. J. Org. Chem.* 2004, 183-192. [2] a) M. D. Gheorghiu, E.Olteanu, *J. Org. Chem.* **1987**, *52*, 5158-5162. b) C. Kazaz, A. Dastan, M. Balci. *Magn. Reson. Chem*. **2005**, *43*, 75-81.

Keywords: isomeric compounds; dibromides; single crystal

FA4-MS05-P30

Crystal Structure of 1,1,3-Trioxo-2,3-dihydro-1,2-benzisothiazol-2-ylmethyl 4-phenyl piperazine-1-carbodithioate, $C_{19}H_{19}N_3O_3S_3$

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Title compound (Fig 1) is imported that Dithiocarbamates which found in its structure are appreciated as fungicidal [1-4], antibacterial and anticancer agents. In this compound, the mean planes of the benzisothiazole system and the phenyl ring make a dihedral angle of 8.87 (8)^{0}. The piperazine ring has a chair conformation. The crystal structure is stabilized by weak intermolecular C-H···O interactions and weak intramolecular C-H···S interactions.
Using Stoe IPDS II diffractometer system, it was found that Crystal system of $C_{19}H_{19}N_3O_3S_3$ was Triclinic, space group $P\bar{1}$, a = 8.0390(5)Å, b = 11.7619(7)Å, c = 11.8796(8)Å, α = 109.029(5)°, β = 103.791(5)°, γ = 102.326(5)°, Z = 2, D = 1.472 Mgm^{-3}, μ = 0.41 mm^{1}, R = 0.0291, wR_2 = 0.0764, S = 1.04.

Data of these crystal was collected by the use of. Stoe IPDS II diffractometer system. Crystal structure were solved by direct methods. Sır97 structure solution program was used. A refinement was carried out by full – matrix least – squares methods using Shelxl 97 refinement program.

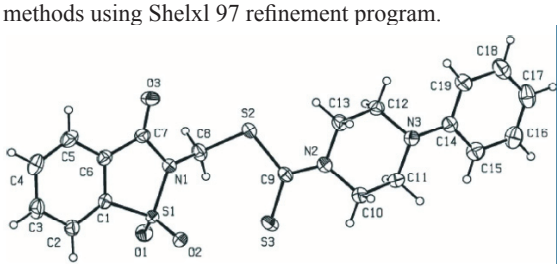

Fig 1: An ORTEP–III view of title compound

[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^{O}. This conformation for DNBP has also been confirmed using density functional theory (Guassian) 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], Andrew N. Fitch[a], Lee Brooks[c], Graeme R. Jones[c]. [a]*European Synchrotron Radiation Facility, BP 220, 38043 Grenoble cedex, France.* [b]*ILL Institut Laue-Langevin, BP 156, 38042 Grenoble cedex 9, France.* [c]*School of Chemistry and Physics, Keele University, Staffordshire, England.*
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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.