

shown in Fig. 1.

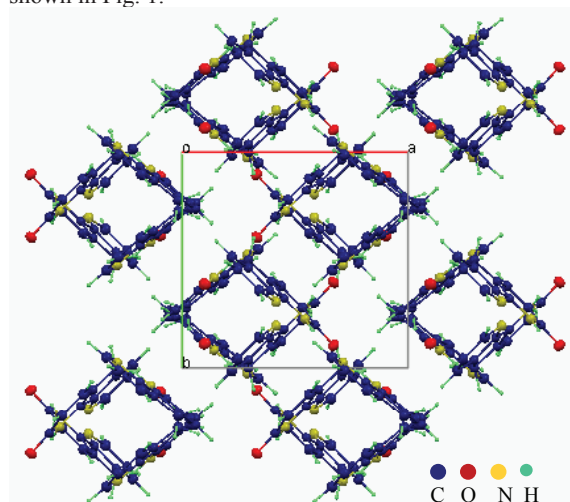


Fig.1. Packing diagram of the title compound.

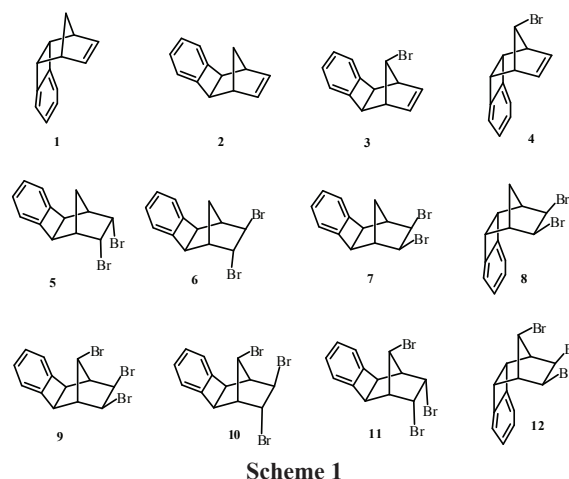
[1] M. Riklin, A. von Zelewsky, A. Bashall, M. McPartin, A. Baysal, J.A. Connor, J.D. Wallis, *Helv. Chim. Acta*, **1999**, 82, 1666. [2] A. Baysal, F. Durap, B. Gümgüm, L. T. Yıldırım, D. Ülkü, D. A. Boğa, S. Özkar, *Helv. Chim. Acta*, **2007**, 90, 1211. [3] L. J. Henderson, Jr., F. R. Fronczek, W. 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*-Benzocyclobutenonorbornene-Dibromides by Using ^1H , ^{13}C NMR and X-Ray Diffraction Techniques. Ertan Şahin^a, Baris Anıl^a, Arif Daştan^a, Cavit Kazaz^a. ^aAtatürk University, Faculty of Sciences, Department of Chemistry, 25240-Erzurum Turkey. E-mail: ertan@atauni.edu.tr

Several monobromides, dibromides and tribromides derived from *endo*- and *exo*-benzocyclobutenonorbornene 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 correlating exact conformations obtained by X-ray diffraction analysis. ^1H -NMR, ^{13}C -NMR, DEPT, gCOSY, gHMBC 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*-Benzocyclobutenonorbornene 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, $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3\text{S}_3$ Mehmet Akkurt^a, Serife Pinar Yalçın^a, Özlen Güzel^b, Aydın Salman^b, Orhan Büyükgüngör^c. ^aErciyes University, Graduate School of Natural and Applied Sciences, Kayseri, Turkey. ^bDepartment of Pharmaceutical Chemistry, Faculty of Pharmacy, Istanbul University, 34116 Istanbul, Turkey. ^cDepartment of Physics, Faculty of Arts and Sciences, Ondokuz Mayıs University, 55139 Samsun, Turkey. E-mail: serifepinar@gmail.com

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 $\text{C}_{19}\text{H}_{19}\text{N}_3\text{O}_3\text{S}_3$ was Triclinic, space group

$P\bar{1}$, $a = 8.0390(5)\text{Å}$, $b = 11.7619(7)\text{Å}$, $c = 11.8796(8)\text{Å}$, $\alpha = 109.029(5)^\circ$, $\beta = 103.791(5)^\circ$, $\gamma = 102.326(5)^\circ$, $Z = 2$, $D = 1.472 \text{ Mgm}^{-3}$, $\mu = 0.41 \text{ mm}^{-1}$, $R = 0.0291$, $wR_2 = 0.0764$, $S = 1.04$.