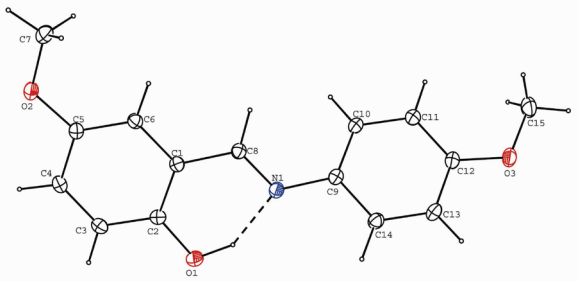
methyl)Phenol. Onur Şahin[a], Orhan Büyükgüngör[a], Mustafa Odabaşoğlu[b], Çiğdem Albayrak[b]. [a]*Department of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey.* [b]*Department of Chemistry, Ondokuz Mayıs University, 55139, Samsun, Turkey.*
E-mail: onurs@omu.edu.tr

The title compound, ($C_{15}H_{15}NO_3$), crystallizes in the monoclinic space group, $P2_1/c$, with a=14.2603(8)Å, b=14.1478(6)Å, c=6.5745(3)Å, $R(F^2)$=0.043 for 3046 independent reflections.



The intramolecular hydrogen bond occurs between the pairs of atom O and N [2.5848(16)Å] and the hydrogen atom is essentially bonded to the oxygen atom. Intermolecular C-H...O hydrogen bonds produce $R_4^4(34)$ ring, which lead two-dimensional chains. An extensive three-dimensional network of C-H...O hydrogen bonds, and C-H...π interactions are responsible for crystal stabilization. Conformations of the title compound were investigated also by semi-empirical quantum mechanical PM3 and AM1 calculations.

Keywords: crystal structure; DFT; conformational analysis

FA4-MS05-P05

Crystal Structure of 1,1,3-Trioxo-2,3-dihydro-1,2-benzisothiazol-2-ylmethyl 4-phenyl Piperazine-1-carbodithioate, $C_{19}H_{19}N_3O_3S_3$. Mehmet Akkurt[a], Şerife Pınar Yalçın[a], Özlen Güzel[b], Aydın Salman[b], Orhan Büyükgüngör[c]. [a]*Erciyes University, Graduate School of Natural and Applied Sciences, Kayseri, Turkey.* [b]*Department of Pharmaceutical Chemistry, Faculty of Pharmacy,Istanbul University, 34116 Istanbul, Turkey.* [c]*Department 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, 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) ^{o}. The piperazine ring has a chair conformation. The crystal structure is stabilized by weak intermolecular C—$H\cdots O$ interactions and weak intramolecular C—$H\cdots S$ interactions.
Using Stoe IPDS II diffractometer system, ıt 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.

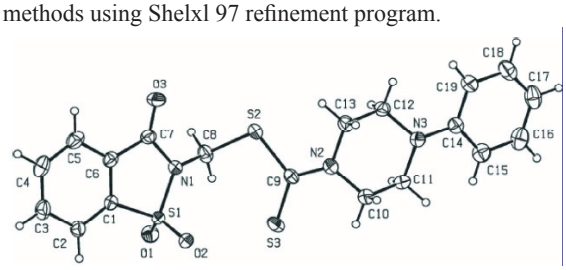


Fig 1: An ORTEP–III view of title compound

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

FA4-MS05-P06

Mono-, di-, poly-nuclear and one-, two- and three-dimensional Ag(I) Saccharinate Complexes with diamine ligands: Syntheses, Thermal Analyses, Crystal Structures and Antimicrobial Properties. Gokhan Kastas[a], Humeyra Pasaoglu[a], Okan Zafer Yesilel[b], Cihan Darcan[c], Aylin Mutlu[b], Orhan Buyukgungor[a]. [a]*Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayis University, Samsun, Turkey.* [b]*Department of Chemistry, Eskişehir Osmangazi University, Eskişehir, Turkey.* [c]*Department of Biology, Dumlupınar University, Kütahya, Turkey.*
E-mail: gkastas@omu.edu.tr

Five new silver(I) complexes, $[Ag_2(sac)_2(tmen)_2]$ (1), $[Ag_2(sac)_2(deten)_2]$ (2), $[Ag_2(sac)_2(dmen)_2]_n$ (3), [Ag(sac)(*N,N*-eten)] (4) and $[Ag(sac)(dmpen)]_n$ (5) (sac: saccharinate, tmen: tetramethylethylenediamine, deten: diethylethylenediamine, dmen: dimethylethylenediamine, *N,N*-eten:*N,N*-diethylethylenediamine and dmpen: 1,3-diamino-2,2-dimethylpropan) have been prepared and characterized by elemental analyses, IR, thermal analyses, single crystal X-ray diffraction and antimicrobial activities. The crystallographic analyses show that all the complexes crystallize in space group $P2_1/c$. In 1, the sac ligand acts as a bridge to connect silver centres through its imino N and carbonyl O atoms, forming an eight-membered bimetallic ring in a chair conformation. The molecular packing of 1 is provided by pi···ring interactions which form two-dimensional network parallel to (100) and a one-dimensional chain running through [100]. Complex 2 has also a dimeric structure in which Ag(sac)(deten) units linked by Ag···Ag interactions. In 3, saccharinate ligand acts as a bridging ligand between two silver(I) centres through sulfonyl group and imino N atom, forming an alternating