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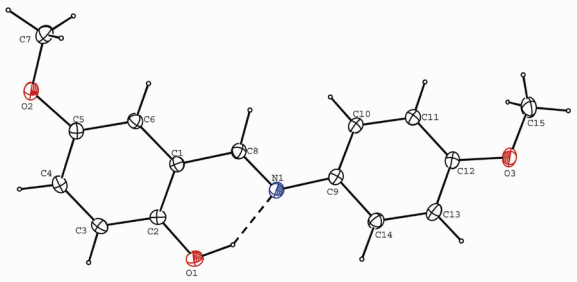
The title compound, ($C_{15}H_{15}NO_3$), crystallizes in the monoclinic space group, $P2_1/c$, with a=14.2603(8)Å, b=14.1478(6)Å, c=6.5745(3)Å, $R(F^2)$=0.043 for 3046 independent reflections.



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.*
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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.

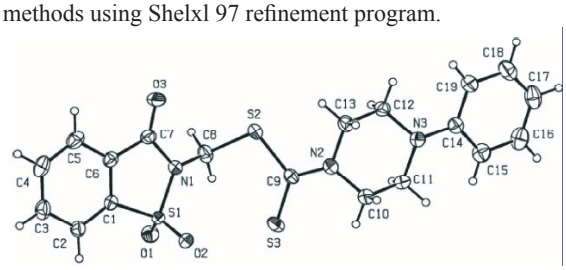

Fig 1: An ORTEP–III view of title compound

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.*
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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

polymeric chain through [010]. In addition, the silver(I) ions in 3 are four- and five-coordinated in individual polymeric chains. In 4, the inter-molecular N-H···O hydrogen bonds form one-dimensional polymeric chains through the *a* axis. These linear chains are inter-connected to each other by N-H···O hydrogen bonds. The molecular packing is also supported by pi···ring interactions, leading to a sheet structure parallel to *bc* plane. Complex 5 is a coordination polymer, in which the monomeric $[Ag(dmpen)(sac)]_n$ units are linked by Ag···Ag interactions and the dmpen ligand acts as a bridge between the silver(I) ions, forming a two-dimensional network parallel to the plane (100). For all of the compounds, antimicrobial activity was studied against selected wild type and clinical microorganisms in vitro by using Minimum inhibitory concentration (MIC) and the disc diffusion method. MIC values of complexes 1-5 were determined in range 13.5-55 µg/ml. These MIC values were approximately the same as those of standard medicinal antibiotics. Therefore, these complexes could be a new candidate for the treatment of microbial diseases.

Keywords: saccharinate complexes; silver(I) complexes; antimicrobial properties

FA4-MS05-P07

Diaquabis(3-Hydroxybenzoato-κO)Bis (Nicotinamide-κN)Zinc(II). Onur Şahin[a], Orhan Büyükgüngör[a], Dursun Ali Köse[b], Hacali Necefoğlu[c]. *[a]Department of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. [b]Department of Chemistry, Hacettepe University, 06800, Ankara, Turkey. [c]Department of Chemistry, Kafkas University, 06100, Kars, Turkey.*
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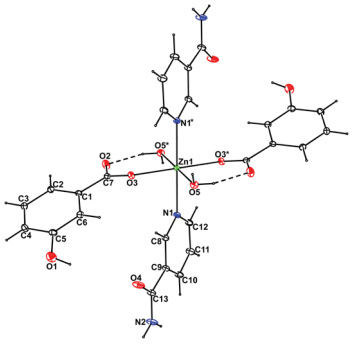
The title compound, $[Zn(C_7H_5O_3)_2(C_6H_6N_2O)_2(H_2O)_2]$, is a two-dimensional hydrogen-bonded supramolecular complex. The Zn^{II} ion resides on the centre of symmetry and is in an octahedral coordination environment comprising two pyridyl N atoms, two carboxylate O atoms and two O atoms from water molecules. Intermolecular N-H...O and O-H...O hydrogen bonds produce $R_1^1(6)$, $R_2^2(7)$, $R_2^2(8)$, $R_2^2(16)$, $R_2^2(20)$, $R_2^2(22)$ and $R_3^3(30)$ rings which lead to a one-dimensional polymeric chains. An extensive two-dimensional network of N-H...O, O-H...O, C-H...O hydrogen bonds, and C-H...π interactions are responsible for crystal stabilization.



Keywords: zinc complex; crystal structure analysis; hydrogen bond

FA4-MS05-P08

Bis[µ-(acesulfamato-N,O:O)(acesulfamato-N,O) bis(2-methylpyridine)cadmium(II)]. Zarife Sibel Şahin[a], Hasan İçbudak[b], Şamil Işık[a]. *[a]Department of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. [b]Department of Chemistry, Ondokuz Mayıs University, 55139, Samsun, Turkey.*
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The title compound, $(C_{40}H_{44}Cd_2N_8O_{16}S_4)$, is a three-dimensional hydrogen-bonded supramolecular complex, which crystallizes in the monoclinic space group C2/c with unit-cell parameters a=14.9475(12)Å, b=16.5004(11)Å, c=21.4067(15)Å and Z = 4. Within the dinuclear complex, two Cd(II) ions are bridged by two carboxylate O atoms. Each Cd(II) ion is coordinated by two N and three O atoms of the acesulfamato ligands and two N atoms of the 2-methylpyridine ligands, resulting in a distorted pentagonal bipyramidal coordination. Intermolecular C-H...O hydrogen bonds produce $R_1^1(8)$ and $R_2^2(20)$ rings which lead to a two-dimensional polymeric chains. An extensive three-dimensional network of C-H...O hydrogen bonds, and π...π interactions are responsible for crystal stabilization.

Keywords: cadmium complex; crystal structure analysis; hydrogen bond

FA4-MS05-P09

(E)-2-[(2-Chlorophenyl)iminomethyl]-4-Methylphenol. Özlem Deveci[a], Şamil Işık[a], Ferda Erşahin[b], Erbil Ağar[b]. *[a]Department of Physics, Ondokuz MayısUniversity, Samsun. [b]Department of Chemistry, Arts and Sciences Faculty, Ondokuz MayısUniversity, Samsun.*
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The molecule of the title compound, $C_{14}H_{12}ClNO$, adopts the enol–imine tautomeric form, with an intramolecular O—H…N hydrogen bond. In the molecule, the two benzene rings are twisted with respect to each other by 30.6 $(2)^0$. The crystal structure is stabilized by intermolecular C—H…π interactions.

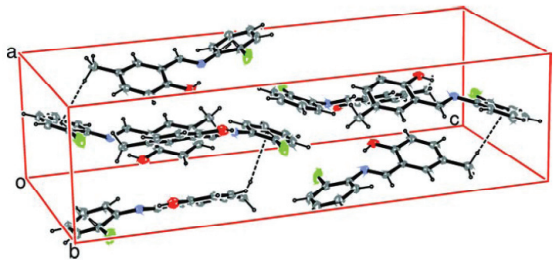

Figure 1. A perspective view of the molecular packing of compound. Dashed lines indicate hydrogen bonds and C-H…π interactions.

In STOE IPDS-II diffractometer system, diffraction data