**FA4-MS05-P01**

**Surface Modification of Calcium Hydroxyapatite and Fluorapatite by Grafting Methyl Phosphoninic Dichloride.**

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The calcium hydroxyapatite \(\text{Ca}_10(\text{PO}_4)_6(\text{OH})_2\) (CaHAp) and fluorapatite \(\text{Ca}_10(\text{PO}_4)_6(F)\) (CaFAp) were prepared by a double decomposition method. Their surfaces were modified using different amounts of methylphosphoninic dichloride \((\text{CH}_3\text{POCl}_2)\) in dichloromethane. Evidence of grafting was performed by elemental analysis, infrared spectroscopy, X-ray diffraction and \(^{31}\)P MAS - NMR.

The X-ray powder analysis showed that the crystallinity was not affected by the presence of organic moieties. The IR spectroscopy showed new vibration modes appearing essentially at 2950, 1200, 880, and 780 cm\(^{-1}\) related to phosphonate groups. The presence of the band v(P-O-P) to 880 cm\(^{-1}\) could be allowed to the formation of a covalent bond \(\text{P}---\text{O}---\text{P}\) by intermediary of hydroxyl ion on the surface of apatite \(\text{P}---\text{O}---\text{H}\). The \(^{31}\)P MAS - NMR spectrum for hydroxy and fluorapatite exhibits a single signal at 2.8 ppm. After reaction with methylphosphonic dichloride the spectra show the presence of new signals, assigned to the organic phosphorus.

**Keywords:** surface modification; phosphonate

**FA4-MS05-P02**

**Experimental and Semi-empirical and DFT Calculational Studies on (E)-2-(1-(2-(4-methoxyphenylsulfonyl)ethyliminio)ethyl)phenolate.**

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The molecular and crystal structure of the title compound, \(\text{C}_17\text{H}_{20}\text{N}_2\text{O}_3\text{S}\), has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group \(P2_1/n\) with unit cell dimensions \(a=11.4472(6)\), \(b=11.1176(4)\), \(c=13.4873(7)\) Å, \(\alpha=90^\circ\), \(\beta=92.03^\circ\), \(\gamma=90^\circ\). The title molecule contains two intermolecular C-H…π interactions.

**Keywords:** X-ray crystallography; DFT; conformation analyses

**FA4-MS05-P04**

**Crystallographic and Conformational Analyses of (E)-4-Methoxy-2-(4-methoxyphenylimino)ethanol.**

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The title compound, \(\text{C}_17\text{H}_{12}\text{BrNO}_2\), a Schiff base, crystallizes in the phenol-imine tautomeric form. The molecular structure has been confirmed by single crystal X-ray crystallography (monoclinic space group \(C2/c\), \(a=22.5809(18)\) Å, \(b=7.4534(7)\) Å, \(c=221394(17)\) Å and \(β=136.681(4)^\circ\)). The title compound is not planar and the angle between the benzene rings is 23.76(3)°. It also contains two intermolecular C-H…π interactions.

The molecular geometry of the title compound in the ground state has been calculated using PM6 semi-empirical method and density functional method (B3LYP) with 6-31G basis set. The optimized geometric bond lengths and bond angles are in good agreement with the experimental values.

In order to define the conformational flexibility of the title compound, semi empirical calculations using the AM1 and PM3 molecular orbital method were carried out. Minimum energy conformation was calculated as a function of the \([\text{C}14-\text{C}9-\text{N}1-\text{C}8]\) torsion angle varied every 10 degrees. The optimized geometry of the crystal structure corresponding to the non-planar conformation is the most stable conformation in all calculations. Besides, the total energy, heat of formation and dipole moments are calculated by DFT for X-ray starting geometry of the title molecule.

**Keywords:** X-ray crystallography; DFT; conformation analyses
methyl)Phenol. Onur Sahin a, Orhan Büyükşengör a, Mustafa Odabaso lu b, Çiğdem Albayrak b, a Department of Physics, Ondokuz Mayis University, 55139, Samsun, Turkey. b Department of Chemistry, Ondokuz Mayis University, 55139, Samsun, Turkey. E-mail: onurs@omu.edu.tr

The title compound, \( \left( \text{C}_{19} \text{H}_{15} \text{NO}_{3} \right) \), crystallizes in the monoclinic space group, \( P2_1/c \), with \( a = 14.2603(8) \AA, b = 14.1478(6) \AA, c = 6.5745(3) \AA, R(F^2) = 0.043 \) for 3046 independent reflections.

The intramolecular hydrogen bond occurs between the pairs of atom O and N [2.5848(16)\( \AA \)] 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

Crystal Structure of 1,1,3-Trioxo-2,3-dihydro-1,2-benzisothiazol-2-ylmethyl 4-phenyl Piperazine-1-carbodiithioate, \( \left( \text{C}_{19} \text{H}_{15} \text{N}_{3} \text{O}_{3} \text{S}_{3} \right) \), Mehmet Akkurt a, Serife Pinar Yalcın b, Özlen Güzel b, Aydin Salman b, Orhan Büyükşengör b. 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. E-mail: serifeyparan@gmail.com

Crystal system of \( \text{C}_{19} \text{H}_{15} \text{N}_{3} \text{O}_{3} \text{S}_{3} \) was Triclinic, space group \( P_1 \), \( a = 8.0390(5) \AA, b = 11.7619(7) \AA, c = 11.8796(8) \AA, \alpha = 109.025(9)^\circ, \beta = 103.791(5)^\circ, \gamma = 102.326(5)^\circ \), \( Z = 2, D = 1.472 \text{ Mgm}^{-1}, \mu = 0.41 \text{ mm}, R = 0.0291, wR = 0.0764, S = 1.04 \).

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

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 diamin ligands: Syntheses, Thermal Analyses, Crystal Structures and Antimicrobial Properties. Gokhan Kastas a, Yesilcebili b, Cihan Darcanc b, Aylin Mutla 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. E-mail: gkastas@omu.edu.tr

Five new silver(I) complexes, \( [\text{Ag} \text{(sac)}(\text{tmen})]_2 \) (1), \( [\text{Ag} \text{(sac)}(\text{dmen})]_2 \) (2), \( [\text{Ag} \text{(sac)}(\text{dmpen})]_2 \) (3), \( [\text{Ag} \text{(sac)}(\text{N,N-eten})]_2 \) (4) and \( [\text{Ag} \text{(sac)}(\text{dmpen})]_2 \) (5) (sac: saccharinate, tmen: tetramethylethylenediamine, dmen: diethylhydelyenediamine, 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 \( \text{Ag} \text{(sac)}(\text{dten}) \) units linked by \( \text{Ag}--\text{Ag} \) 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...