FA4-MS05-P01

Surface Modification of Calcium Hydroxyapatite and Fluoroapatite by Grafting Methyl Phosphonic Dichloride.

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The calcium hydroxyapatite $Ca_{10}(PO_4)_6(OH)_2$ (CaHAp) and fluoroapatite $Ca_{10}(PO_4)_6(F)_2$ (CaFAp) were prepared by a double decomposition method.Theirs surfaces were modified using different amounts of methylphosphonic dichloride (CH_3POCl_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 cristallinity 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 ν(P-O-P) to 880 cm^{-1} could be allowed to the formation of a covalent bond P_{inorg}-O-P_{org} by intermediary of hydroxyl ion on the surface of apatite (P_{inorg}-OH). The ^{31}P MAS - NMR spectrum for hydroxy and fluoroapatite 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-methylphenylsulfonamido)ethyliminio)ethyl) phenolate.

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The molecular and crystal structure of the title compound, C17H20N2O3S, has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the monoclinic, space group P21/n with unit cell dimensions a=11.4472(6), b=11.1176(4), c=13.4873(7)Å, Mr=332.41, V=1639.36(13)Å3, Z=4, R1=0.034 and wR2=0.097. The molecule adopts a zwitterionic form, stabilized by an intramolecular N+-H…O- type ionic weak hydrogen bond. The molecule pack via intermolecular N-H…O hydrogen bonds which, together with an intramolecular N+-H…O-bond, form an S(6)R24(4)S(6) motif.
Calculational studies were performed by using AM1, PM3 semi-empirical and DFT methods. Geometry optimizations of compound have been carried out by using three semi-empirical methods and DFT method and bond lengths, bond and torsion angles of title compound have been determined. Atomic charge distribution have been obtained from AM1, PM3 and DFT. In order to determine conformational flexibility on the molecule, molecular energy profile of the title compound was obtained with respect to the selected torsion angle T(N1-C9-C10-N2), which is varied from -180o to +180o in every 10 via PM3 semi-empirical method.

Keywords: crystal structure; conformational analysis; DFT

FA4-MS05-P03

The Crystal Structure and Conformational Analyses of 2-[(2-Bromophenylimino) Methyl]-4 –Methoxyphenol.

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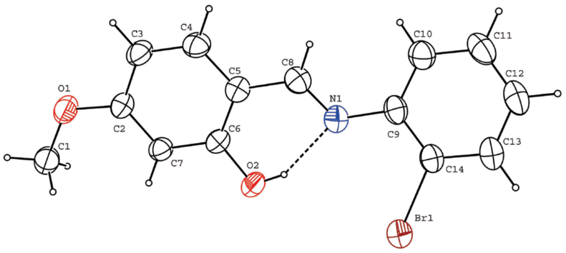
The title compound, $C_{14}H_{12}BrNO_2$, a Schiff base, crystallizes in the phenol-imine tautomeric form. The molecular structure has been confirmed by single crystal X-ray crystallography (monoclinic space group C2/c, a=22.5809(18)Å, b=7.4534(7) Å, c=221394(17)Å and β=136,681(4)˚). The title compound 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-emprical 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 [C14-C9-N1-C8] 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

FA4-MS05-P04

Crystallographic and Conformational Analyses of (E)-4-Methoxy-2-((4-methoxyphenyl imino)

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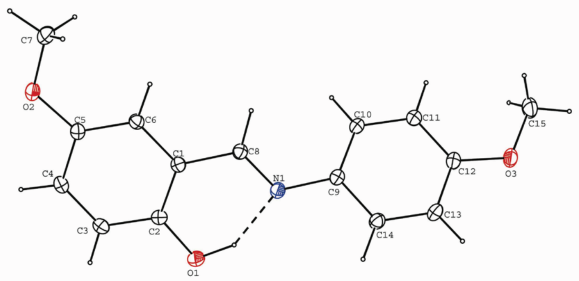
The title compound, ($C_{15}H_{15}NO_3$), crystallizes in the monoclinic space group, $P2_1/c$, with a=14.2603(8)Å, b=14.1478(6)Å, c=6.5745(3)Å, R(F^2)=0.043 for 3046 independent reflections.



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, $C_{19}H_{19}N_3O_3S_3$.

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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···O interactions and weak intramolecular C—H···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.

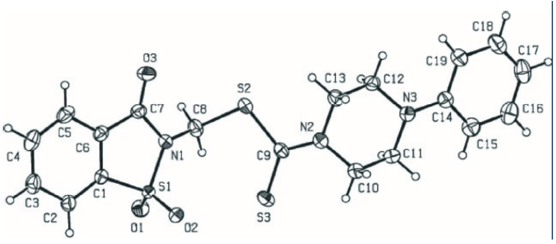

Fig 1: An ORTEP–III view of title compound

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.

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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