

FA4-MS05-P01

Surface Modification of Calcium Hydroxyapatite and Fluoroapatite by Grafting Methyl Phosphonic Dichloride. Hassen Agougui^a, Abdallah Aissa^a, Mongi Debbabi^a. *^aLaboratoire de physico-chimie des Matériaux, Faculté des Sciences de Monastir, 5019 Monastir, Tunisie.*

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The calcium hydroxyapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{OH})_2$ (CaHAp) and fluoroapatite $\text{Ca}_{10}(\text{PO}_4)_6(\text{F})_2$ (CaFAp) were prepared by a double decomposition method. Their 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 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 $\nu(\text{P-O-P})$ to 880 cm^{-1} could be allowed to the formation of a covalent bond $\text{P}_{\text{inorg}}-\text{O}-\text{P}_{\text{org}}$ by intermediary of hydroxyl ion on the surface of apatite ($\text{P}_{\text{inorg}}-\text{OH}$). 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

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Experimental and Semi-empirical and DFT Computational Studies on (E)-2-(1-(2-(4-methylphenylsulfonamido)ethyliminio)ethyl) phenolate. Gökhan Alpaslan^a, Erbil Ağar^b, Ferda Erşahin^b, Şamil Işık^a, Ahmet Erdönmez^a. *^aOndokuz Mayıs Univ., Department of Physics, Samsun-Turkey. ^bOndokuz Mayıs Univ., Department of Chemistry, Samsun-Turkey.*

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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 $\text{P}21/n$ with unit cell dimensions $a=11.4472(6)$, $b=11.1176(4)$, $c=13.4873(7)\text{Å}$, $M_r=332.41$, $V=1639.36(13)\text{Å}^3$, $Z=4$, $R_1=0.034$ and $wR_2=0.097$. The molecule adopts a zwitterionic form, stabilized by an intramolecular $\text{N}^+-\text{H}\cdots\text{O}^-$ type ionic weak hydrogen bond. The molecule pack via intermolecular $\text{N}-\text{H}\cdots\text{O}$ hydrogen bonds which, together with an intramolecular $\text{N}^+-\text{H}\cdots\text{O}^-$ bond, form an $\text{S}(6)\text{R}24(4)\text{S}(6)$ 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 $\text{T}(\text{N1}-\text{C9}-\text{C10}-\text{N2})$, which is varied from -180o to +180o in every 10 via PM3 semi-empirical method.

Keywords: crystal structure; conformational analysis; DFT

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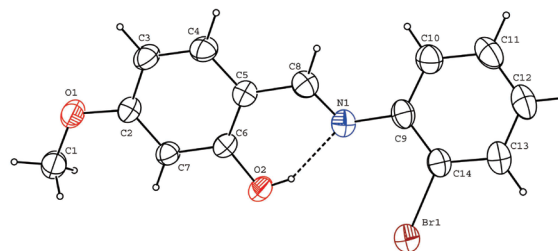
The Crystal Structure and Conformational Analyses of 2-[(2-Bromophenylimino) Methyl]-4-Methoxyphenol. Zariye Sibel Şahin^a, Ferda Erşahin^b, Erbil Ağar^b, Şamil Işık^a. *^aDepartment of Physics, Ondokuz Mayıs University, 55139, Samsun, Turkey. ^bDepartment of Chemistry, Ondokuz Mayıs University, 55139, Samsun, Turkey.*

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The title compound, $\text{C}_{14}\text{H}_{12}\text{BrNO}_2$, 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 $\text{C}2/c$, $a=22.5809(18)\text{Å}$, $b=7.4534(7)\text{Å}$, $c=221394(17)\text{Å}$ and $\beta=136,681(4)^\circ$). The title compound is not planar and the angle between the benzene rings is $23.76(3)^\circ$. It also contains two intermolecular $\text{C}-\text{H}\cdots\pi$ 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; conformational analyses

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