FA4-MS05-P15

Crystal Structure and DFT Calculations of Two Derivatives of Phthalimide. Serap Yazici[a], Nalan Turkoz[b], Halil Kutuk[b], Ismet Senel[a], Orhan Buyukgungor[a]. [a]*Department of Physics, Ondokuz Mayis University, TR-55139, Samsun, Turkey.* [b]*Department of Chemistry, Ondokuz Mayis University, TR-55139, Samsun, Turkey.*
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Phthalimides exhibit various biological properties and have been reported as antipsychotics [1], anti-inflammatory agents [2] and herbicides [3]. Here we report the molecular and crystal structure of N-(p-Methoxyphenylthio) phthalimide and N-(p-Toluenethio) phthalimide. The crystal structures have been determined by single crystal X-ray diffraction analysis. The optimized molecular structures of these compounds have been obtained with DFT calculations, and then the corresponding geometric parameters were compared with those of X-ray crystallography.

[1] Norman, M. H., Minick, D. J. & Rigdon, G. C., **1996**. J. Med. Chem. 39, 149-157. [2] Collin, X., Robert, J.-M., Wielgosz., G., Le Baut, G., Bobin- Dubigeon, C.,Grimaud, N. & Petit, J.-Y., **2001**. Eur. J. Med. Chem. 36, 639-649 [3] Kawaguchi, S. & Ilkeda, O., **2001**. Jpn Pat. Appl. JP 2001 328 911.

Keywords: phthalimide; DFT; structural analysis

FA4-MS05-P16

The Crystal Structure of (E)-5-Phenyl-N-(thiophen-2-ylmethylene)-1,3,4-thiadiazole-2-amine. Güneş Demirtaş[a], Necmi Dege[a], Memet Şekerci[b], Süleyman Servi[b], Muharrem Dinçer[a]. [a]*Ondokuzmayıs University, Department of Physics, Samsun, Turkey.* [b]*Fırat University, Department of Chemistry, Elazığ, Turkey.*
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The crystal structure of the titile compound, $C_{13}H_9S_2N_3$, determinated at 293 K. The structure contain three ring. In the crystal structure intramolecular C---H...S hydrogen bonds and intermolecular C---H...Cg interactions may be effective in the stabilization of the crystal structure. The molecule is almost planar.

Keywords: intramolecular interactions; intermolecular interactions; 1,3,4-thiadiazole

FA4-MS05-P17

Synthesis and Characterizations of Some New Triazol–3-one Derivatives. N. Burcu Arslan[a], Canan Kazak[a], Yasemin Ünver[b], Kemal Sancak[b]. [a]*Department of Physics, Ondokuz Mayıs University, Samsun, Turkey.* [b] *Department of Chemistry Faculty of Arts and Sciences Karadeniz Teknik University, Trabzon, Turkey.*
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Compound *4-[(3-phenyl- alliden amino) -5- thiophen -2-yl- methyl-2,4-dihydro-[1,2,4]triazol-3-one* (2) was synthesized via the reaction of 4-amino-5-thiophen-2-yl methyl 2,4-dihydro-[1,2,4] triazol-3-one (1) with cinnam aldehyde. Other compounds(3, 4) were obtained from compound 2 with bromo acetophenon and bromo ethyl acetate respectively. The synthesis of compounds 2,3 and 4 and crystal structure of compound 2 are being reported. The molecular structure was identifed by IR, ^{1}H-NMR, ^{13}C-NMR and MS analysis. Analysis of the crystal packing of the compound 2 reveals that the molecule is linked by means of intermolecular and intramolecular hydrogen bondings and in addition to these interactions crystal structure presents C-H ....π stacking.

Keywords: synthesis inorganic; X-ray diffraction crystallography; crystallography in chemistry

FA4-MS05-P18

Experimental and DFT Studies of N-2-Methoxyphenyl-2-oxo-5-nitro-1-benzylidenemethylamine: In Gas Phase and Solvent Media. Hasan Tanak[a], Metin Yavuz[a], Orhan Büyükgüngör[a], Ferda Erşahin[b], Erbil Ağar[c]. [a]*Department of Physics,Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey.* [b]*Gerze Sinop Vocational School, Sinop University, Sinop, Turkey.* [c]*Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayıs University, Kurupelit, 55139 Samsun, Turkey.*
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Schiff bases are of interest because they are known to show photochromism and thermochromism in the solid state; this may involve reversible proton transfer from the hydroxyl-O atom to the imine-N atom. In general, O-hydroxy Schiff bases exhibit two possible tautomeric forms, the phenol-imine (or benzenoid) and keto-amine (or quinoid) forms. Depending on the tautomers, two types of intra-molecular hydrogen bonds are possible: O—H···N in benzenoid and N—H···O in quinoid tautomers. The H atom in title compound (I) is located on atom N1, thus the keto-amine tautomer is favored over the phenol-imine form, as indicated by the C11—O2, C14—N1, C10—C11 and C11—C12 bond lengths. These values are in good agreement with the related compound [1].There are two molecules in the asymmetric unit. In the structure, there are N–H…O intramolecular hydrogen bonds (graph set S(5) and S(6)) and C–H…O intermolecular hydrogen bonds.
The experimental geometry of N-2-Methoxyphenyl-2-oxo-5-nitro-1-benzylidenemethylamine obtained from single-crystal X-ray diffraction was compared with those obtained from DFT methot in gas phase. In order to evaluate the energetic and atomic charge behavior of the title compound in solvent, we carried out optimization calculations in the three kinds of solvent (chloroform, ethanol and water). The methodology used in this investigation is centered on Onsager's reaction field theory.