Crystal Structure and DFT Calculations of Two Derivatives of Phthalimide. Serap YAZICI1, Nalan Turkoz1, Halil Kutuk1, Ismet Senel1, Orhan Buyukgungor1. 1Department of Physics, Ondokuz Mayis University, TR-55139, Samsun, Turkey. 2Department of Chemistry, Ondokuz Mayis University, TR-55139, Samsun, Turkey. E-mail: vsrap@omu.edu.tr.

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.


Keywords: phthalimide; DFT; structural analysis

The Crystal Structure of (E)-5-Phenyl-N-(thiophen-2-ylmethylene)-1,3,4-thiadiazole-2-amine. Günes DEMİRTAŞ1, Necmi Dege2, Memet Şekerçi3, Süleyman Servi3, Muharrem Dinçer4. 1Ondokuz Mayis University, Department of Physics, Samsun, Turkey. 2Firat University, Department of Chemistry, Elazığ, Turkey. E-mail: gunesd@omu.edu.tr

The crystal structure of the title compound, C14H14S2N, is determined 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

Synthesis and Characterizations of Some New Triazol-3-one Derivatives. N. Burcu ARSLAN1, Canan KAZAK1, Yasemin ÜNVER1, Kemal SANCAK2. 1Department of Physics, Ondokuz Mayis University, Samsun, Turkey. 2Department of Chemistry Faculty of Arts and Sciences Karadeniz Teknik University, Trabzon, Turkey. E-mail: barslan@omu.edu.tr

Compound 4-[3-(phenyl- aliliden 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 cinnamaldehyde. 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 identified by IR, 1H-NMR, 13C-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 bonds and in addition to these interactions crystal structure presents C-H...π stacking.

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

ExperimentalandDFTStudiesofN-2-Methoxyphenyl-2-oxo-5-nitro-1-benzylidenemethyamine: In Gas Phase and Solvent Media. Hasan TANAK1, Metin Yavuz2, Orhan Büyüküngör3, Ferda Erşahin4, Erbil Ağar5. 1Department of Physics, Faculty of Arts and Sciences, Ondokuz Mayis University, Kurupelit, 55139 Samsun, Turkey. 2Gerze Sinop Vocational School, Sinop University, Sinop, Turkey. 3Department of Chemistry, Faculty of Arts and Sciences, Ondokuz Mayis University, Kurupelit, 55139 Samsun, Turkey. E-mail: htanak@omu.edu.tr

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-benzylidenemethyamine obtained from single-crystal X-ray diffraction was compared with those obtained from DFT method 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.