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.*
E-mail: yserap@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.

[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.*
E-mail: gunesd@omu.edu.tr

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.*
E-mail: barslan@omu.edu.tr

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.*
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-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.

[1] A. Özek, S. Yüce, Ç. Albayrak, M. Odabasoğlu, and O. Büyükgüngör, Acta Crystallogr., **2005**, E61, o3179.

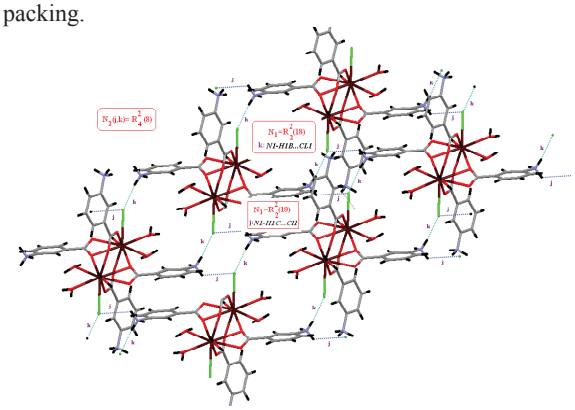
Keywords: X-ray diffraction; DFT; dielectric media

FA4-MS05-P19

Hydrogen bonding motifs, Crystal Structure of the Polymeric chloride of tetrakis(3-aminobenzoato-O,O') hexaquadichloride lanthanium(III). dihydrate $La_2(H_2O)_8(C_7H_7NO_2)_4Cl_6$.

Meriem Benslimane[a], Hocine Merazig[a]. [a]*Laboratory of Molecular Chemistry, Control of the Environment and Measures Phisico-chemical, Department of Sciences Mentouri University of Constantine. 25000 Algérie.*
E-mail:benslimane_meriem@yahoo.fr

Such complexes can be used as starting materials in a wide range of applications in materials science, including superconductors, magnetic materials, catalysts and luminescent probes [1].In this field much work has been focused on the design and assembly of lanthanide complexes with organic ligands such as aromatic carboxylic acids, *β*-dicetones, crypltands, calixarenes and heterocyclic ligands. In particular, lanthanide complexes with aromatic carboxylic acids have been studied because of their novel features and potential applications in a number of areas. The present contribution deals with the synthesis and the crystal structure of the dimeric lanthanum compound, $La_2(H_2O)_8(C_7H_7NO_2)_4Cl_6$ (I). The complexes (I), consists of dimeric units related by an inversion center. The two La^{III} atoms are linked by two bridging bidentate carboxylate groups and two monodentate carboxylate groups. Each La^{III} atom is nine-coordinated by five O atoms from carboxylate groups of the 3-aminobenzoate, three from water molecules and chloride ion, they adopt a distorted tricapped trigonal-prismatic arrangement. The modeling of the various existing types of connections in the two structures by using the theory of Bernstein [2] enabled us to build the various binary graphs, which were used to understand the crystal packing.



[1] Quiche, A., Suzuki, Y., Ohki, Y. & Koizumi, Y., **1988**. *Coord. Chem. Rev.* 92,29±43. [2] Bernstein, J.,R.E. Davis, L. Shimoni, and N. –L. Chang. Patterns in hydrogen bonding: Functionality and graph set analysis in crystal. Angew Chem int ED Engl 34: 1555-73, **1995**.

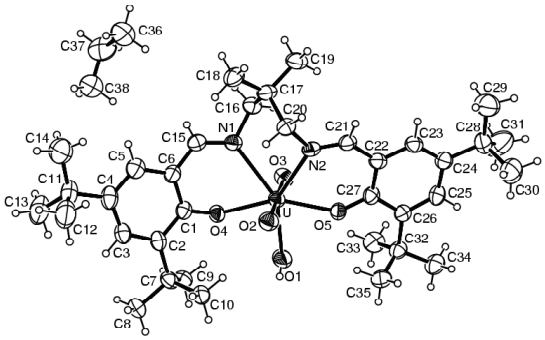
Keywords: amino acids; lanthanide ions; graph-set theory

FA4-MS05-P20

Syntesis, Crystallographic Structure and Semiempirical Studies of a Novel Complexes of Uranyl(VII).

Ahmed Arif Tek[a], Ömer Çelik[a], Mahmut Ulusoy[b], Nazan Ocak İskeleli[c], Erol Eroğlu[a], Eşref Taş[d]. [a]*Department of Physics, Faculty of Science & Art, Harran University 63300, Şanlıurfa,Turkey.* [b]*Department of Chemistry, Faculty of Science, Ege University, 35100 Bornova, İzmir, Turkey.* [c]*Ondokuz Mayis University, Department of Science Education, 55200, Samsun Turkey.* [d]*Department of Chemistry, Faculty of Science & Art, Siirt University, 56100, Siirt, Turkey.*
E-mail: ahmedariftek@gmail.com

(N, N' – bis(3,5-di-*tert*-butylsalicylidene)2-dimethyl 1,3-diaminopropane)uranyl(VII) was synthesized suitable contions. The experimantel data of compound was obtain by Stoe X-ray diffractometer that is graphite monochromatised MoK_α(λ=0.7107Å) radiation. Its crystallizes in monoclinic system, space group P21/n, with lattice parameters a=15.5501(6) Å, b=12.0559(5) Å, c=21.5158(8) Å, β=103.186(3)°, Z=4, μ=4.174 mm^{-1}, S=1.011, R=0.0418 and wR=0.0704 for 7667 observed reflections. The equatorial geometry surrounding the uranyl centres is distorted pentagonal bipyramidal. The U atom is coordinated by two N and five O atoms. The structures were solved by direct methods using the SHELX-97 program package and refined on F^2. The data were treated and corrected for Lorentz-polarisation effects. The equatorial geometry surrounding the uranyl centres is distorted pentagonal bipyramidal. The U atom is coordinated by two N and five O atoms. The compound has a lof of intramoleculer and four intermolecular interaction. Also bond lengths and angles is calculated for both X-ray and model starting geometry of molecule by semiempirical of Gaussien3 programme. Values of bond length and angle of the both X-ray and semiemprical canputations were compared.



Keywords: uranyl; gaussian3; crystal structure

FA4-MS05-P21

Experimental and Semi-empirical and DFT Calculational Studies on (E)-4-(2-((4-chloro phenylimino)methyl)phenoxy)Phthalonitrile.