Hydrogen bonding motifs, Crystal Structure of the Polymeric chloride of tetrais(3-aminobenzoato-O-O’) hexaquadichloride lanthanum(III). dihydrate La₄(H₂O)₂(C₇H₇NO₂)₄Cl₄, Meriem Benslimane¹, Hocine Merazig², 'Laboratory of Molecular Chemistry, Control of the Environment and Measures Phisico-chemical, Department of Sciences Mentoouri 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, cryptands, 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 features and potential applications in a number of areas. 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].

Keywords: X-ray diffraction; DFT; dielectric media


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

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Keywords: X-ray diffraction; DFT; dielectric media

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Syntesis, Crystallographic Structure and Semiempirical Studies of a Novel Complexes of Uranyl(VII). Ahmed Ari˚Tek⁰, Ömer Çelik⁰, Mahmut Ulusoy⁰, Nazan O€ak Isk€el€el⁰, Erol Ero€glü⁰, Esref Taş⁰. 'Department of Physics, Faculty of Science & Art, Harran University 63300, Şanlurfa,Turkey. 'Department of Chemistry, Faculty of Science, Ege University, 35100 Bornova, İzmir, Turkey. 'Onadokuz Mayis University, Department of Science Education, 55200, Samsun Turkey. 'Department of Chemistry, Faculty of Science & Art, Siirt University, 56100, Siirt, Turkey.

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(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(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 F². 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 lot of intramolecualer 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 semiempirical canputations were compared.

Keywords: uranyl; gaussian3; crystal structure

FA4-MS05-P21

Experimental and Semi-empirical and DFT Calculation Studies on (E)-4-(2-((4-chloro phenylimino)methyl)phenoxy)Phthalonitrile.
FA4-MS05 Structure and Reactivity in Molecular Crystals by Crystallographic, Spectroscopic and Computational Methods

Marife Tüfekçi, Gökhan Alpaslan, Erbil Ağar, Ferda Erşahin, Ahmet Erdönmez. 

The molecular and crystal structure of the title compound, 

\[ C_{15}H_{20}Cl_4FeN_5P_3 \] 

has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the triclinic, space group \( P\overline{1} \) with unit cell dimensions \( a = 8.8342(9), b = 10.2301(8), c = 11.2401(9), \alpha = 76.473(6)^\circ, \beta = 84.912(7)^\circ, \gamma = 64.419(6)^\circ, V = 890.74(13)\,\text{Å}^3, Z = 2, R = 0.045 \) and \( wR \) = 0.130. The crystal structure of the title compound was obtained with respect to the selected flexibility on the molecule, molecular energy profile of the 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 have been carried out by using three 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 \( \text{T(C21-C16-N3-C15)} \), which is varied from \(-180^\circ\) to \(+180^\circ\) in every 10 via PM3 semi-empirical method.

Keywords: single crystals; crystallographic analysis; DFT

FA4-MS05-P22


In this study, crystal structures of two ferrocenyl-phosphazene derivatives, \( C_{15}H_{20}ClFeN_5P_3 \), (I), and \( C_{15}H_{12}FeN_4P_3 \), (II), are investigated. The data have been collected with Mo K\(_\alpha\) radiation on an Enraf-Nonius CAD-4 diffractometer.

\( \text{spiro} \text{-Butane-1,4-diamino} \)-[N-(1-ferrocenyl-methyl)-4,4,6,6-tetrachloro-cyclophosphazatriene] (I) is a monofunctional \( \text{spiro} \)-cyclic phosphazene derivative and it belongs to the space group \( P\overline{1} \) with cell parameters \( a = 16.027(3), b = 11.8348(8), c = 24.1114(4)\,\text{Å} \). It has \( \pi-\pi \) contact between cyclopentadiene rings \( \text{centroid-centroid distance} = 3.278(4)\,\text{Å} \). The N-H\ldots N intermolecular hydrogen bonds links the molecules, forming infinite one dimensional chains running approximately parallel to \( c \) axis and the intramolecular C-H\ldots N H bonds form a dimerization.

\( \text{spiro} \)-[Butane-1,4-diamino]-[N,N'-bis(1-ferrocenyl-methyl)]-4,4,6,6-tetrakispyrroldino-cyclotriphosphazatriene (II) is a bis-ferrocenyl \( \text{spiro} \)-cyclic phosphazene derivative including two ferrocenes and it belongs to the space group \( P\overline{1} \) with cell parameters \( a = 11.494(4), b = 15.259(3), c = 15.293(3)\,\text{Å} \) and \( \alpha = 60.98(1)^\circ, \beta = 75.49(2)^\circ, \gamma = 71.33(2)^\circ \). It also has \( \pi-\pi \) contact between cyclopentadiene rings and C-H\ldots N contacts between \( H \) atoms of \( \text{C13}, \text{C19}, \text{C34} \) and cyclopentadiene rings (C6/ C7/C8/C9/C10) and (C1/C2/C3/C4/C5) and phosphazene ring (P1/P2/N2/P3/N3).

Keywords: phosphazenes; ferrocenyl-phosphazenes; hydrogen bonds

FA4-MS05-P23


For the first time, high-resolution data on geometry of semiquinone radicals not participating in charge-transfer interactions (such as coordination bonds or low-barrier hydrogen bonds) has been experimentally obtained. Geometry of the quinoid rings and C-O bond lengths \( (1.25 – 1.26\,\text{Å}) \) differs slightly from the hydrogen bonded semiquinone (chloranil) radical anions are well-known for their stability. They were extensively studied by EPR, IR and Raman spectroscopies and theoretical methods; an X-ray crystallographic study was also attempted. The crystal structures, however, remained elusive. Freshly prepared semiquinone crystals are red, but turn green in a few minutes at RT. The colour change is due to disproportionation of the radicals into a quinhydrone-like substance \[1\]. All previous studies of tetrachlorosemiquinone radical anions were done using a green compound. For the first time, high-resolution data on geometry of semiquinone radicals not participating in charge-transfer interactions (such as coordination bonds or low-barrier hydrogen bonds) has been experimentally obtained. Geometry of the quinoid rings and C-O bond lengths \( (1.25 – 1.26\,\text{Å}) \) differs slightly from the hydrogen bonded semiquinone (C-O bond lengths of 1.29–1.30 Å \[1\]), and these results agree well with quantum chemical models.

Keywords: radical salts; accurate geometry; low-temperature data collection

FA4-MS05-P24

Crystal Structure of 2,4,4-Tris(benzylsulfanyl)-1,1-dichloro-3-nitrobuta-1,3-diene. Cigdem Savil, Goksin Aydinli, Cemil Ibisi. 

The molecule of the title compound, \( C_{15}H_{12}NO_3S_3 \), is not planar. The three phenyl rings and the butadiene group are inclined at angles of \( 85.9(1), 61.9(1), 81.4(1)\)


Keywords: radical salts; accurate geometry; low-temperature data collection