

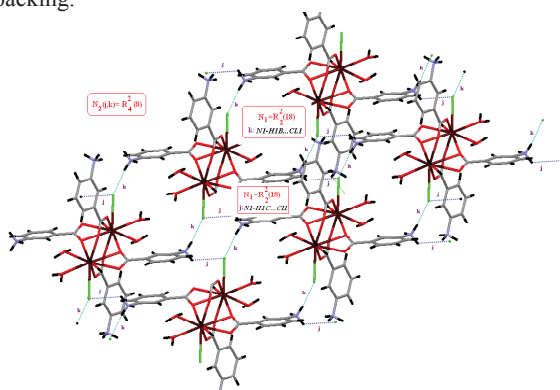
[1] A. Özek, S. Yüce, Ç. Albayrak, M. Odabasoğlu, and O. Büyükgüngör, *Acta Crystallogr.*, **2005**, E61, o3179.

**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 lanthanum(III) dihydrate  $\text{La}_2(\text{H}_2\text{O})_8(\text{C}_7\text{H}_7\text{NO}_2)_4\text{Cl}_6$ .** Meriem Benslimane<sup>a</sup>, Hocine Merazig<sup>a</sup>. <sup>a</sup>Laboratory of Molecular Chemistry, Control of the Environment and Measures Physico-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,  $\beta$ -diketones, cryptand, 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,  $\text{La}_2(\text{H}_2\text{O})_8(\text{C}_7\text{H}_7\text{NO}_2)_4\text{Cl}_6$  (I). The complex (I), consists of dimeric units related by an inversion center. The two  $\text{La}^{\text{III}}$  atoms are linked by two bridging bidentate carboxylate groups and two monodentate carboxylate groups. Each  $\text{La}^{\text{III}}$  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. Shimon, and N. -L. Chang. Patterns in hydrogen bonding: Functionality and graph set analysis in crystal. *Angew Chem int ED Engl* 34: 1555-73, **1995**.

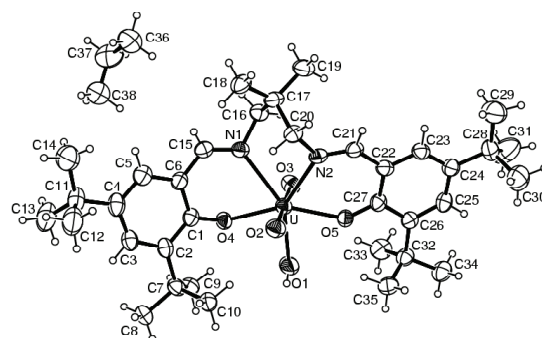
**Keywords:** amino acids; lanthanide ions; graph-set theory

#### FA4-MS05-P20

**Synthesis, Crystallographic Structure and Semiempirical Studies of a Novel Complexes of Uranyl(VII).** Ahmed Arif Tek<sup>a</sup>, Ömer Çelik<sup>a</sup>, Mahmut Ulusoy<sup>b</sup>, Nazan Ocak İskeleli<sup>c</sup>, Erol Eroğlu<sup>a</sup>, Eşref Taş<sup>d</sup>. <sup>a</sup>Department of Physics, Faculty of Science & Art, Harran University 63300, Şanlıurfa, Turkey. <sup>b</sup>Department of Chemistry, Faculty of Science, Ege University, 35100 Bornova, İzmir, Turkey. <sup>c</sup>Ondokuz Mayıs University, Department of Science Education, 55200, Samsun Turkey. <sup>d</sup>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 conditions. The experimental data of compound was obtained by Stoe X-ray diffractometer that is graphite monochromatised  $\text{MoK}_\alpha$  ( $\lambda=0.7107\text{Å}$ ) radiation. It crystallizes in monoclinic system, space group P21/n, with lattice parameters  $a=15.5501(6)\text{Å}$ ,  $b=12.0559(5)\text{Å}$ ,  $c=21.5158(8)\text{Å}$ ,  $\beta=103.186(3)^\circ$ ,  $Z=4$ ,  $\mu=4.174\text{mm}^{-1}$ ,  $S=1.011$ ,  $R=0.0418$  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 lot of intramolecular and four intermolecular interactions. Also bond lengths and angles are calculated for both X-ray and model starting geometry of molecule by semiempirical of Gaussian3 programme. Values of bond length and angle of the both X-ray and semiempirical calculations were compared.



**Keywords:** uranyl; gaussian3; crystal structure

#### FA4-MS05-P21

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

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The molecular and crystal structure of the title compound, C<sub>21</sub>H<sub>12</sub>ClN<sub>3</sub>O, has been determined by X-ray single crystal diffraction technique. The compound crystallizes in the triclinic, space group *P-1* with unit cell dimensions  $a=8.8342(9)$ ,  $b=10.2301(8)$ ,  $c=11.2401(9)$ ,  $\alpha=76.473(6)^\circ$ ,  $\beta=84.912(7)^\circ$ ,  $\gamma=64.419(6)^\circ$ ,  $V=890.74(13)\text{Å}^3$ ,  $Z=2$ ,  $R_f=0.045$  and  $wR_2=0.130$ . The crystal structure of the title compound phthalonitrile derivatives, C<sub>21</sub>H<sub>12</sub>ClN<sub>3</sub>O, is stabilized by  $\pi$ - $\pi$  stacking interactions.

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 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

**Crystal Structures of Ferrocenyl- Phosphazene Derivatives.** Asli Ozturk<sup>a</sup>, Nuran Asmafiliz<sup>b</sup>, Tuncer Hokelek<sup>a</sup>, Zeynel Kilic<sup>b</sup>. <sup>a</sup>*Hacettepe University, Department of Physics Engineering, 06800 Ankara, Turkey.* <sup>b</sup>*Ankara University, Department of Chemistry, 06100 Ankara, Turkey.*

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In this study, crystal structures of two ferrocenyl-phosphazene derivatives, C<sub>15</sub>H<sub>20</sub>Cl<sub>4</sub>FeN<sub>5</sub>P<sub>3</sub>, (I), and C<sub>42</sub>H<sub>62</sub>Fe<sub>2</sub>N<sub>9</sub>P<sub>3</sub>, (II), are investigated. The data have been collected with Mo K <sub>$\alpha$</sub>  radiation on an Enraf-Nonius CAD-4 diffractometer.

*spiro*(Butane-1,4-diamino)-[N-(1-ferrocenyl-methyl)]-4,4,6,6-tetrachloro-cyclotriphosphazatriene (I) is a mono-ferrocenyl *spiro*-cyclic phosphazene derivative and it belongs to the space group *P bca* with cell parameters  $a=16.027(3)$ ,  $b=11.834(8)$ ,  $c=24.111(4)$  Å. It has  $\pi$ - $\pi$  contact between cyclopentadiene rings [centroid-centroid distance = 3.278(4) Å]. The N-H...N intermolecular hydrogen bonds<sup>[1]</sup> link the molecules, forming infinite one dimensional chains running approximately parallel to *c* axis and the intramolecular C-H...N H bonds form a dimerization.

*spiro*-(Butane-1,4-diamino)-[N,N'-bis(1-ferrocenyl-methyl)]-4,4,6,6-tetrakispyrrolidino-cyclotrip

hosphazatriene (II) is a bis-ferrocenyl *spiro*-cyclic phosphazene derivative including two ferrocenes and it belongs to the space group *P-1* with cell parameters  $a=11.494(4)$ ,  $b=15.259(3)$ ,  $c=15.293(3)$  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... $\pi$  contacts between H atoms of C13, C19, C34 and cyclopentadiene rings (C6/C7/C8/C9/C10) and (C1/C2/C3/C4/C5) and phosphazene ring (P1/N1/P2/N2/P3/N3).

[1] İltter, E. E., Asmafiliz, N., Kılıç, Z., Işıklan, M., Hökelek, T., Çaylak, N. and Şahin, E., *Inorg. Chem.*, 46, 9931-9944, 2007.

**Keywords:** phosphazenes; ferrocenyl-phosphazenes; hydrogen bonds

#### FA4-MS05-P23

**Solid State Chemistry of Tetrabromo-and Tetrachlorosemiquinone Radical Anions.** Krešimir Molčanov<sup>a</sup>, Biserka Kojić-Prodić<sup>a</sup>. <sup>a</sup>*Rudjer Bošković Institute, Zagreb, Croatia.*

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*p*-Tetrabromosemiquinone (bromanil) and *p*-tetrachlorosemiquinone (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 anion salts 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 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.

[1] K. Molčanov, B. Kojić-Prodić, M. Roboz, *Acta Cryst. B*, 2006, 62, 1051.

**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 Sayil<sup>a</sup>, Goksin Aydinli<sup>a</sup>, Cemil Ibis<sup>a</sup>. <sup>a</sup>*Istanbul University, Faculty of Engineering, Department of Chemistry, 34320 Avcılar-Istanbul, Turkey.*

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The molecule of the title compound, C<sub>25</sub>H<sub>21</sub>Cl<sub>2</sub>NO<sub>2</sub>S<sub>3</sub>, 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)