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**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 $La_2(H_2O)_8(C_7H_7NO_2)_4Cl_6$.**

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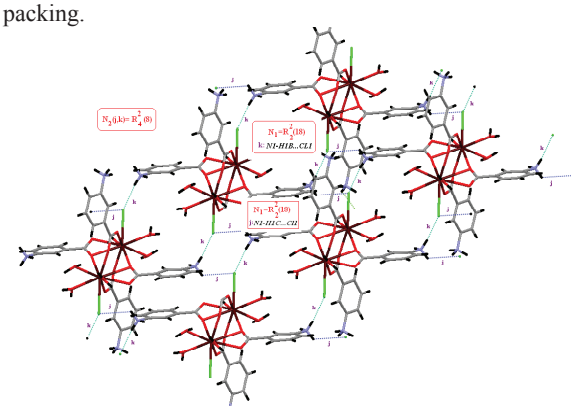
Such complexes can be used as starting materials in a wide range of applications in materials science, including superconductors, magnetic materials, catalysts and luminescent probes [1].In this field much work has been focused on the design and assembly of lanthanide complexes with organic ligands such 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.



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

## FA4-MS05-P20

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

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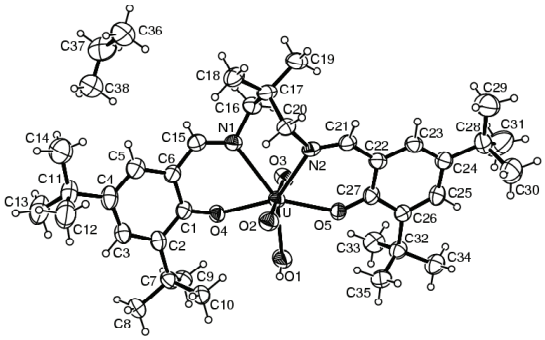
*(N, N'* – bis(3,5-di-*tert*-butylsalicylidene)2-dimethyl 1,3-diaminopropane)uranyl(VII) was synthesized suitable contions. The experimantel data of compound was obtain by Stoe X-ray diffractometer that is graphite monochromatised $MoK_\alpha$(λ=0.7107Å) radiation. Its crystallizes in monoclinic system, 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.**