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 La₃(H₂O)₇(C₇H₇NO₂)₆Cl₄, Meriem Benslimane, Hocine Merazig. \textsuperscript{a}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 \cite{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, \(\beta\)-dicetones, cryptands, calixarenes and heterocyclic ligands. In particular, lanthanide complexes with aromatic carboxylic acids have been studied because of their novel ligands. In particular, lanthanide complexes with aromatic carboxylic acids, \(\beta\)-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 crystal structure of the dimer lanthanum compound, \(La_2(H_2O)_6(C_7H_7NO_2)_4Cl_4\) (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 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 \cite{2} enabled us to build the various binary graphs, which were used to understand the crystal packing.

FA4-MS05-P20

\textbf{Synthesis, Crystallographic Structure and Semiempirical Studies of a Novel Complexes of Uranyl(VII).} Ahmed Arit Tek, Ömer Çelik, Mahmut Ulusoy, Nazan Ocan Iskeli, Erol Ereğli, Esref Taş. \textsuperscript{a}Department of Physics, Faculty of Science & Art, Harran University, 63300, Şanlıurfa, Turkey. \textsuperscript{b}Department of Chemistry, Faculty of Science, Ege University, 35100 Bornova, İzmir, Turkey. \textsuperscript{c}Ondokuz Mayis University, Department of Science Education, 55200, Samsun Turkey. \textsuperscript{d}Department of Chemistry, Faculty of Science & Art, Siirt University, 56100, Siirt, Turkey. E-mail: ahmedarittek@gmail.com

\(\text{(N, N} - \text{bis(3,5-di-tert-butylsalicylidene)}-2\text{-dimethyl 1,3-diaminopropane})\text{uranyl(VII)}\) was synthesized suitable conditions. The experimantel data of compound was obtain by Stoe X-ray diffractometer that is graphite monochromatised MoK\(\lambda\)\(=0.7107\) radiation. Its crystallizes in monoclinic system, space group \(P2_1/n\), 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 SHELEX-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 interaction. Also bond lengths and angles is 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 calulations were compared.

Keywords: uranyl; gaussian3; crystal structure

FA4-MS05-P21

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


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