

**FA4-MS06-P01****Synthesis, Structural Characterization, Thermal Stability and Physical Properties of New Hybrid Compound: "Bis(3,4-dimethylanilinium) hexachlorostannate(IV)".**

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Intense research activity during the past few decades in organic-inorganic hybrid materials of formula (R-NH<sub>3</sub>)<sub>n</sub>SnX<sub>n</sub>, where X = F, Cl, Br or I, because for their interesting thermal, optical and electrical properties [1, 2]. In this study we present a new hybrid compound based on tin and derived from anilinium, examine the hydrogen bonding in its crystal structure and explore its thermal decomposition.

The title compound, [SnCl<sub>6</sub>]<sup>2-</sup> · 2(C<sub>8</sub>H<sub>12</sub>N)<sup>+</sup>, crystallized in Triclinic system, with P-1 space group, it has been prepared by slow evaporation of an aqueous solution of 3,4 dimethyl aniline, tin(II) chloride and hydrochloric acid.

The crystal structure consists of alternating layers of hexachlorostannate and 3,4-dimethylanilinium along the c axis. They are linked together by cation-anion hydrogen bonds. This three-dimensional complex network of hydrogen bond reinforces the cohesion of the ionic structure.

We have measured a third-order nonlinear optical susceptibility and electrical conduction. The thermal decomposition of the compound shows that the SnO<sub>2</sub> is obtained after two steps.

[1] Aruta, C., Licci, F. Zappettini, A., Bolzoni, F., Rastelli, F., Ferro, P. & Besagni, *T. Appl. Phys.* **2005**, A 81, 963. [2] Knutson, J. L. & Martin J. D. *Inorg. Chem.* **2005**, 44, 4699.

**Keywords:** single crystal; hydrogen bond; thermal analysis

**FA4-MS06-P02****Unexpected Fragmentation of Phenylthiobenzoate, X-Ray Structure of [μ-η<sup>2</sup>]1,2-(dithio)-1,2(diphenylethylene)-di-iron Hexacarbonyl Complex.**

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The thermal reaction of Fe<sub>2</sub>(CO)<sub>9</sub> with organic substrates containing sulfur atoms is a general synthetic way to various

hexacarbonyliron coordination compounds [1]. When the starting organic ligand is linked to the metal atoms without fragmentation the overall reaction may be rationalized by a stepwise replacement of three carbon monoxide ligand of Fe<sub>2</sub>(CO)<sub>9</sub> by a six-electron one. The reaction of Fe<sub>2</sub>(CO)<sub>9</sub> with dithioesters [2], ethylenetrithiocarbonate [3], or 1,2-dithiol-3-thiones [4], occurs without a ligand fragmentation. However, in some cases the thermal reaction of Fe<sub>2</sub>(CO)<sub>9</sub> with sulfur containing substrates leads to the coordination of binuclear compounds including one or several fragments arising from the organic substrates [5-10]. Surprisingly, we have observed an unusual fragmentation of phenylthiobenzoate PhC(S)SPh (**1**) during its reaction with Fe<sub>2</sub>(CO)<sub>9</sub> leading, besides the expected complexes : [(μ-η<sup>3</sup>(C,S,S)PhCS<sub>2</sub>Ph)]Fe<sub>2</sub>(CO)<sub>6</sub> (**2**) and (μ-S)Fe<sub>3</sub>(CO)<sub>9</sub> (**3**), to the two other complexes (μ-SPh)<sub>2</sub>Fe<sub>2</sub>(CO)<sub>6</sub> (**4**) and [(μ-η<sup>2</sup>)(S,S)PhC(S)=C(S)Ph]Fe<sub>2</sub>(CO)<sub>6</sub> (**5**) (Scheme 1). **4** and **5** compounds or analogous one are unexpected and were never observed during the reaction of Fe<sub>2</sub>(CO)<sub>9</sub> with dithioesters. The X-ray study of **5** establishes that it was a binuclear iron complex. The two iron atoms are maintained at a distance from 2.56Å with a dithiodiphenylethylene group.

[1] W.P.Fehlhammer, H. Stolzenberg, in *Comprehensive Organometallic Chemistry* (G. Wilkinson, Ed.), Pergamon Press, Vol. 4, **1982**, 513. [2] E.A. Koerner Von Gustorf, F.W. Grevels, I. Fischler, (Ed.), *The organic Chemistry of Iron*, vol. 2, Academic Press, New-York, **1981**. [3] A. Benoit, J.Y. Le Marouille, C. Mahé, H. Patin, *J. Organometal. Chem.*, 218, **1981**, C6. [4] P.H. Bird, U. Siniwardane, A. Shaver, O. Lopez D.N. Harpp., *J. Chem Soc. Chem. Commun.*, **1981**, 513. [5] H. Patin, G. Mignani, A. Benoit, *J. Organometal. Chem.*, 168, **1979**, C21. [6] H. Patin, G. Mignani, A. Benoit, J.Y. Le Marouille D. Grandjean, *Inorg. Chem.*, 20, **1981**, 4351. [7] A. Lagadec, R. Dabard, B. Misterkiewicz, A. Le Rouzic, H. Patin, *J. Organometal. Chem.*, 326, **1987**, 381. [8] M. Bouzid, J. P. Pradere, P. Palvadeau, J.P. Venien, L. Toupet, *J. Organometal. Chem.*, 369, **1981**, 205. [9] E.K. Lhadi, H. Patin and A.Darchen, *organometallics*, 3, **1984**, 1128. [10] A. Darchen, E.K. Lhadi, H. Patin, *Nouv. J. Chim.*, 12, **1988**, 377.

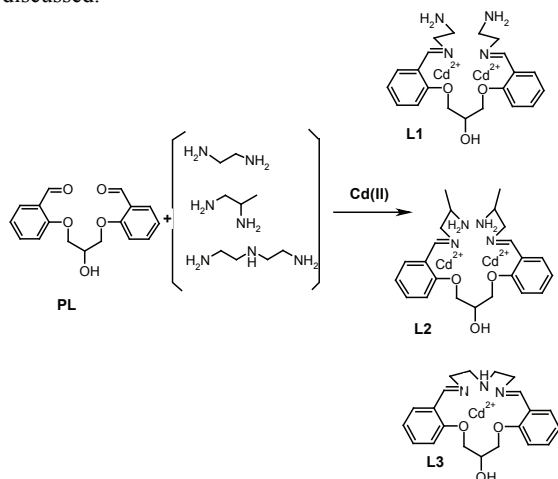
**Keywords:** dithioester; iron; complex; X-ray

**FA4-MS06-P03****Is the Chain Length of Diamine Sufficient to Span Dialdehyde to Form a Macrocyclic? Leila Noohinejad**

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Uncontrolled condensation reactions, e.g. of diamines with dialdehydes lead inevitably to a mixture of oligomers and various size macrocycles as the reaction products. The use of metal ions as templates is able to somewhat steer these kind of condensation reactions towards the formation of macrocyclic Schiff bases, but even with the

metal ion templates the prediction of the outcome of such a condensation reaction is still a largely empirical enterprise. It is thus clearly desirable to improve our understanding of the sequence of the stepwise macrocycle formation reactions in such template reactions, which then might be applied to the synthesis of new macrocycles with particular desired coordination properties. Some insight into the nature of these reactions has been gained by the isolation of complexes of open-chain ligands. The isolation of these only halfway reacted ligands indicate that the course of the reaction is strongly depend on the flexibility and spacer length of the diamines used in the synthesis. Reaction of two diamines, 1,2-diaminoethane and 1,2-diaminopropane, with 2-[3-(2-formylphenoxy)-2-hydroxypropoxy]benzaldehyde (PL) [1] in the presence of  $\text{Cd}^{2+}$  ions yielded the dinuclear complexes  $\text{Cd}_2\text{L}^1(\text{NO}_3)_3$ ,  $\text{H}_2\text{O}$  and  $\text{Cd}_2\text{L}^2(\text{NO}_3)_3$  where  $\text{L}^1$  and  $\text{L}^2$  are the open chain ligands derived from the condensation of one molecule of dialdehyde with two molecules of the amine. The same reaction with diethylenetriamine, however, yielded the macrocyclic  $\text{CdL}^3(\text{NO}_3)_3$  complex. Spectroscopic and X-ray structural data as well as a possible reason for the failure or success of the ring closure reactions are discussed.



Furthermore we would like to present our first experiences with the implementation of remote access to a single crystal CCD X-ray diffractometer at Youngstown State University (YSU) in the United States by users from University of Tabriz in Tabriz, Iran by way of which the data were collected.

[1] Khandar A.A., Hosseini- Yazdi S. A., *Polyhedron*, **2003**, *22*, 1481-1487.

**Keywords:** macrocycle; cadmium complexes; remote data collection

#### FA4-MS06-P04

**Polymorphism and Isomorphism in Silver Coordination Compounds.** Katharina M. Fromm. *Department of Chemistry, University of Fribourg, Fribourg Switzerland.*

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Coordination polymer networks, respectively metal organic frameworks (MOFs) are currently in the focus of interest for their fascinating properties, e. g. luminescence, porosity, magnetism, which occur due to the combination of metal ions or metal cluster compounds as nodes, and organic molecules as ligands. [1]

Silver and its compounds are known to have antimicrobial properties, [2, 3] however, they can be toxic in too high concentrations. We have therefore investigated the formation of coordination polymer networks containing silver ions. For the possible medical applications, it is important to tune the solubility, structure and light stability of these compounds. In this presentation, the different structures obtained with a certain ligand system will be presented, and how these structures differ in terms of their properties. A number of polymorphs and isomorphs will be shown, together with their physical, chemical and microbiological properties.

[1] A. Y. Robin, K. M. Fromm, *Coord. Chem. Rev.* **2006**, *250*, 2127-2157. [2] P. S. Brunetto, K. M. Fromm, *Chimia*, **2008**, *62(4)*, 249-252. [3] T. Vig Slenters, I. Hauser-Gerspach, A. U. Daniels, K. M. Fromm, *J. Mat. Chem.*, **2008**, *18*, 5359-5362.

**Keywords:** coordination polymers; polymorphism; isomerism

#### FA4-MS06-P05

**Study of the Interaction of T-shaped Tricarboxylate Ligands with Copper(II) Ions.** Ana Belén Lago<sup>a</sup>, Laura Cañadillas-Delgado<sup>a</sup>, Mariadel Déniz<sup>a</sup>, Óscar Fabelo<sup>a</sup>, Jorge Pasán, Catalina Ruiz-Pérez<sup>a</sup>. <sup>a</sup>Laboratorio de Rayos X y Materiales Moleculares, Departamento de Física Fundamental II, Facultad de Física, Universidad de La Laguna. La Laguna, Tenerife. Spain.

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In recent years a great deal of effort has focused on the design and synthesis of extended frameworks of coordination compounds which have a wide variety of network topologies and potential applications in several fields[1]. Many of the architectures reported to date are based upon rigid linear linker ligands, with less efforts focusing on the use of ligands showing conformational flexibility. The use of flexible ligands can lead to the formation of interesting architectures without loss of control in the self-assembly process. We have performed an investigation on the formation of copper(II) coordination compounds based on the use of two tricarboxylic acids and auxiliary ligands such as 1,10-phenanthroline or 2,2'-bipyridine. The use of T-shaped ligands like the aconitic (*trans*-1,2,3-propanetricarboxylic) ( $\text{H}_3\text{L}_1$ ) or the tricarballylic (1,2,3-propanetricarboxylic) acid ( $\text{H}_3\text{L}_2$ ) lets us exert some control over the self-assembly process, i.e. only specific network topologies can be formed. The use of blocking ligands limits the coordination orientation of the carboxylic acids and facilitates the formation of suitable crystals for X-ray analysis.