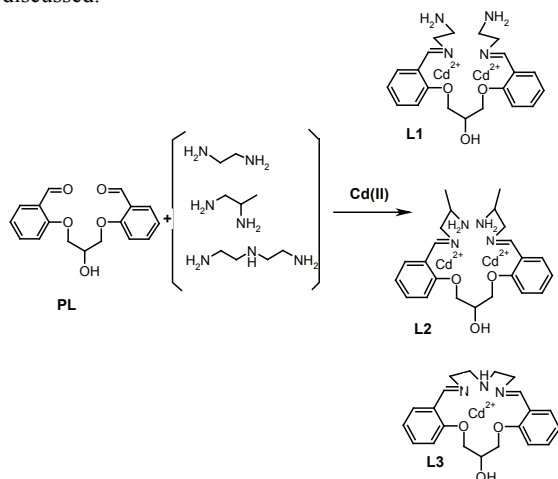


metal ion templates the prediction of the outcome of such a condensation reaction is still a largely empirical enterprise. It is thus clearly desirable to improve our understanding of the sequence of the stepwise macrocycle formation reactions in such template reactions, which then might be applied to 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 Cd^{2+} ions yielded the dinuclear complexes $\text{Cd}_2\text{L}^1(\text{NO}_3)_3$, H_2O and $\text{Cd}_2\text{L}^2(\text{NO}_3)_3$ where L^1 and 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.

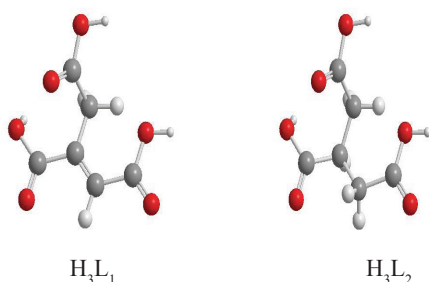
Keywords: coordination polymers; polymorphism; isomerism

FA4-MS06-P05

Study of the Interaction of T-shaped Tricarboxylate Ligands with Copper(II) Ions. Ana Belén Lago^a, Laura Cañadillas-Delgado^a, Mariadel Déniz^a, Óscar Fabelo^a, Jorge Pasán, Catalina Ruiz-Pérez^a. ^aLaboratorio 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) (H_3L_1) or the tricarballylic (1,2,3-propanetricarboxylic) acid (H_3L_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.



The use of ligands with carboxylate groups makes that the first supramolecular association is organized by the effect of OH...O hydrogen bonds. The π ... π stacking interactions between blocking ligands can cooperate in the formation of the whole crystal structure. All of these interactions can link low-dimensional complexes to give high-dimensional supramolecular structures and further stabilize the crystal structures in the solid state.

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Keywords: copper complexes; crystal structures; coordination chemistry

FA4-MS06-P06

Crystal Structures of Double Oxygen-bridged Tetranuclear and Polynuclear Metal Complexes.

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The [N,N'-bis(salicylidene)-1,3-propane-diamine, (SALPD), (C₁₇H₁₆N₂O₂)] ligand forms different complexes with metal salts in nonaqueous media. These compounds are of interest because of their magnetic super-exchange interactions between bridged metal ions[1]. Various combinations of metal ions are possible[2]. Magnetic interactions depend on the immediate environment of the bridge as well as on the ligand arrangement around the metal atoms. Oxygen, nitrogen, acetate or nitrite anions may constitute the μ -bridges. We report here two new structures of this group of compounds:

(I) [Cu₂(SALPD)(C₄H₈O₂)(N₃)₂]_n, P 2₁/n, a=11.2922(12), b=15.4136(11), c=13.6107(13) Å, β =97.402(5)°, Z=2, Dx=1.64 g.cm⁻³, λ =0.71073 Å, I > 2 σ 2575, N_{par}=293, R, R_w→0.07, 0.16, $\Delta\rho_{max}$, $\Delta\rho_{min}$ → 1.2, -1.1 e Å³. Two doubly oxygen-bridged dinuclear Cu complexes are bridged in a head-on fashion via two azido groups to build a centrosymmetrical tetranuclear complex. The terminal Cu ion has a distorted square-pyramidal coordination,

involving two bridging O and two N atoms from a (SALPD) and one O atom from a dioxane molecule. The inner Cu ions also have an irregular square-pyramidal coordination, consisting of two bridging O atoms from a SALPD ligand, two bridging N atoms from two azido groups, and one N atom from the third azido group. Whether the coordination sphere around the metal atoms is a trigonal-bipyramide or square-pyramide was decided on the basis of τ value calculations. $\phi_{bridge}(Cu-N-Cu) = 102.1(3)^\circ$, $\phi_{bridge}(Cu-O-Cu) = 105.6(2)^\circ$.

(II) [ZnHg(SALPD)(C₄H₄N₂S₂)_n]_n, P 2₁2₁2₁, a=8.6824(12), b=16.1222(12), c=16.3339(11) Å, Z=4, D_x=2.01 g.cm⁻³, λ =0.71073 Å, I > 2 σ 1951, N_{par}=276, R, R_w→0.031, 0.075, $\Delta\rho_{max}$, $\Delta\rho_{min}$ → 0.80, -0.88 e Å³. Doubly oxygen-bridged dinuclear ZnHg complexes are bridged via SCN groups in an end to end fashion to build a polynuclear chain. The coordination around Zn ion is a distorted square-pyramide involving two O and two N atoms from a SALPD and one N atom from a SCN group. The Hg atom has a tetrahedral environment consisting of two O atoms from a (SALPD) and two S atoms from two SCN groups. The S and N atoms of the SCN bridge between the dinuclear ZnHg complexes are coordinated to Hg and Zn atoms, respectively. This results in a polymeric chain structure. The bridging SCN groups are almost linear. S-C-N angle is 176.5(2)°, $\phi_{bridge}(Zn-O-Hg) = 105.5(2)^\circ$ to 106.5(2)°.

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Keywords: organometallic crystal structures; metalloorganic structures; coordination compounds

FA4-MS06-P07

Magnesium(II) phthalocyanine Coordination Compounds with 3,4- and 3,5-lutidines.

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Magnesium phthalocyanine (MgPc) and its MgPcL and MgPcL₂ coordination complexes (4+1 and 4+2) with N and O donor ligands deserve attention because of similarity with chlorophyll, thus being its synthetic models. Due to their electrochemical properties they find application in solar energy conversion, are used as pigments in optical disks, laser printers, display devices and chemical sensors. As a continuation of the series of works concerned with MgPc coordination with N- and O- donor ligands we present the results of syntheses and structural investigation of a number of coordination compounds of MgPc with 3,5-lutidine (3,5-lut) and 3,4-lutidine (3,4-lut).

All of the compounds were obtained by recrystallization of purified MgPc (Sigma) from solution of the appropriate lutidine. Four compounds were obtained, as presented on the reaction schemes below:

