

Thermal decomposition of the title compounds has been studied. Final products of thermal decomposition are single-phase hexagonal closed-packed metal solid solutions  $Rh_{0.25}Re_{0.75}$  (a = 2.749(2), c = 4.395(3)) and  $Ir_{0.25}Re_{0.75}$  (a = 2.758(2), c = 4.393(3)).  $Ru_{0.25}Re_{0.75}$  (a = 2.756(2), c = 4.414(3) Å).

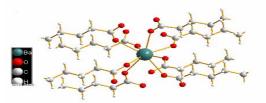
### MS13 P22

Synthesis And Structures Of Dicarboxylato-Bridged Earth-Alcaline Polymers <sup>1)</sup>Aliouane. K., <sup>(1)</sup>Guehria-Laidoudi A., <sup>(2)</sup>Dahaoui S. and <sup>(2)</sup>Lecomte C. <sup>a</sup> Laboratoire de cristallographie appliquée, Institut de Chimie, U.S.T.H.B., B.P. 32, El-Alia 16111, Bab-Ezzouar, Alger, Algérie <sup>(2)</sup> LCM<sup>3</sup>B-CNRS UMR 7036, Faculté des Sciences Université Henri Poincaré BP 239, 54506 Vandoeuvre-lès-Nancy, France.

## Keywords: polymeric structure, earth-alcaline, dicarboxylate

The binding of earth-alcaline ions to dicarboxylate ligands partially  $[CO_2(CH_2)_nCO_2H]^-$  or completely  $[(CH_2)_n - (CO_2)_2]^2$  deprotonated often lead to polymeric structures. The resulting model complexes are designed to permit the significance of interactions in such extended structures which are used in several fields, particularly in biology and medecine. An extensive polymeric arrays involving earth-alcaline ion depends on the geometric constraints of the metal ion. It is well known that barium, calcium and strontium exhibit a great flexibility if compared to magnesium, in which a rigid requirement of octahedral geometry is invariably found, preventing aggregation. However, in its hydrated  $\alpha$ ,  $\omega$  dicarboxylates, Mg realizes chain structure for small values of n (1 to 3) and layer structure for higher values<sup>1</sup>.

The three anhydrous Ba, Ca and Sr sebasate, have been synthesized. Single X-ray diffraction studies, carried out at (293K) and (120K), show that they contain partially deprotonated legands. Their space groups, centrosymmetric for Sr (P4<sub>2</sub>/nbc) and Ca (P-1) complexes and non centrosymmetric for Ba (P-4b2) point to the invalidity of n parity criteria in the centrosymmetry. In the two tetragonal symmetries, the values of cell parameters, particularly c parametrer, provide evidence that this later, is not related to the lengthening of carbon backbone. The metals are eight-coordinated, and µ-1, 3 oxo-bridges, lead to a two-dimensional layered structure, exhibiting wide empty channels. The general structural features are very similar to those lanthanum complexes, obtained with a relatively long alkyl chain<sup>2</sup> ( $n \ge 5$ ), even though, the tetragonal symmetry seems to be, in the series, particular to anhydrous barium complexes whatever n values<sup>3</sup>.



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### MS13 P23

The Study of Unprecedented Tubular Channels Formation in Alkyl-Substituted Oxamide Oxime Metal Complexes <u>Yurii Chumakov<sup>a,b</sup></u>, Dominique Luneau<sup>a</sup>, Fatma Yuksel<sup>a,c</sup>, Vefa Ahsen<sup>c,d</sup>, Gulay Gumus<sup>d</sup>, Ilke Gurol<sup>d</sup>. <sup>a</sup>Université Claude Bernard Lyon 1, France, <sup>b</sup>Institute of Applied Physics of Academy of Science of Moldova, <sup>c</sup>Gebze Institute of Technology, <sup>d</sup>TUBITAK-Marmara Research Center, Turkey E-mail: <u>iurii.ciumacov@univ-lyon1.fr</u>

## Keywords: oxamide oxime metal complexes, tubular channels, conformational analysis

It was found that nickel(II) and palladium(II) complexes of hexyl- substituted oxamide oxime are self-assembled through hydrogen bonds involving the oximic oxygens and amino nitrogen atoms to afford metal-organic frameworks with tubular channels partly filled by the hexyl chains [1]. But whether the chains cooperate in the formation of these structures, or simply fill the empty space, was unclear. Therefore, the nickel (II) (1a-3a) and palladium(II) (1b-3b, 5b,6b) complexes of oxamide oximes substituted with alkyl chains of different length (C3-C8) were synthesized and characterized by X-ray and spectroscopic methods as well as their conformational analysis was carried out in order to understand the role of chains in formation of the tubular channels in the crystals. All studied molecules are centrosymmetric at the metal center forming the perfectly planar central cores containing the metal ion  $[M{O1-N1-C1(N3)-C2(N4)-N2-O2}2]$ [M=Ni(II), Pd(II)]. It was found that only palladium(II) (1b-3b, 5b,6b) complexes form the infinite tubular channels filled by the chains. The channels in these ones, as well as in nickel(II) (4a) and palladium(II) (4b) complexes [1], are walled by the central cores which are self-assembled via N-H...O hydrogen bonds involving the oximic oxygens and amino nitrogen atoms. The building blocks which form the crystal packing of **2b-6b** and **4a** have been extracted in order to perform the quantitative analysis of channels topology and they were characterized by the packing indexes. It was shown that the space in the channels which is filled by chains in compounds of 2b, 3b, 5b and 6b is greater in 2.6-3.6 times then in 4a and 4b. On the base of conformational analysis using the module Conformational Search implemented in HyperChem 6.03 it was found that the formation of infinite tubular channels in the crystals of alkyl-substituted oxamide oxime nickel (II) and palladium (II) complexes depends on the orientation of the chains relatively to the fragments of  $[M{O1-N1-C1(N3)-C2(N4)-N2-O2}]$ . In order to understand the role of metal in the channel formation the intermolecular metal-chains interaction energies have been calculated according to the empirical consistent valence force field (CVFF).

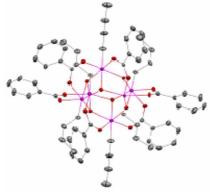
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### MS13 P24

Self-assembled fullerene-rich stannoxane derivatives Carine Duhayon, Uwe Hahn, A. Gégout, Y. Coppel, A. Saquet, J.-F. Nierengarten Laboratoire de Chimie de Coordination du CNRS, 205 route de Narbonne, 31077 Toulouse Cedex, France. E-mail: <u>duhayon@lcc-toulouse.fr</u>

#### Keywords: Organooxotin, Self-assembly, Fullerene

Organooxotin cages have received considerable attention in view of their structural diversity [1]. Importantly, these compounds can be self-assembled in almost quantitative yields under very mild reaction conditions. Therefore, organotin chemistry appears to be an attractive tool for the preparation of multi-functional nanostructures. Indeed, Chandrasekhar and co-workers have already reported the self-assembly of a robust, thermally stable hexaferrocene assembly in quantitative yield by reaction of nbutylstannonic acid with ferrocene monocarboxylic acid [2]. By using a similar approach, the same group has also described the synthesis of a hexaporphyrin assembly with promising DNA cleavage activity [3]. Herein, we show that C<sub>60</sub> derivatives bearing a carboxylic acid function undergo self-assembly with n-butylstannonic acid (nBuSn(O)OH) to produce fullerene-rich nanostructures with a stannoxane core in nearly quantitative yields. The reaction conditions have been first tested with several model compounds and the structure of the stannoxane core confirmed by X-ray crystal structure analysis.



Further investigations with fullerene derivatives have also been successful. The fullerene-rich derivatives were obtained in quantitative yields and their structure confirmed by the observation of a single resonance in their <sup>119</sup>Sn NMR spectra [4]. The self-assembly of fullerene-containing components reported herein is an efficient tool for the preparation of fullerene-rich nanostructures. Such compounds are thus easier to produce and the range of systems that can be prepared is not severely limited by the synthetic route. In this way, in-depth investigations of their properties is possible and one can really start to envisage the use of fullerene-rich materials for specific applications.

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## MS13 P25

**Copper(II) halide complexes with simple pyridine based alcohols.** <u>Ivan Leban</u> and Nina Lah, Faculty of Chemistry and Chemical Technology, University of Ljubljana, Askerceva 5, 1000-Ljubljana, Slovenia; E-mail: <u>ivan.leban@fkkt.uni-lj.si</u>

## Keywords: Cu(II) coordination polymer, alkoxide, pyridine alcohol ligands

Reactions of Cu(II) halides (CuCl<sub>2</sub> and CuBr<sub>2</sub>) with simple pyridine based alcohols: (2-hydroxymethyl)-pyridine, (2hydroxyethyl)-pyridine and (2-hydroxypropyl)-pyridine afford a series of new Cu(II) alkoxide complexes, all having a similar dinuclear  $Cu_2O_2$  structural motif [1]. The structures of six new complexes will be presented, spanning diverse architectures from discrete dinuclear complex  $[Cu_2L_2Br_2],$ an ionic compound  $[Cu_2Cl_2(HL)_4]Cl_2 \cdot 2H_2O$ , to two tetranuclear complexes of a defect dicubane-like type structure,  $[Cu_4L_4Cl_4]$  and [Cu<sub>4</sub>L<sub>4</sub>Br<sub>4</sub>] and two polymeric chain compounds with the  $[Cu_2L_2Cl_2]_n$  and  $[Cu_2(HL)_2Cl_4]_n$  composition (L and HL are deprotonated and neutral forms of simple pyridine alcohol ligans). In addition to the synthesis and structural description, their magnetic properties will be presented and correlated with their structural features.

Additionally, the crystal structures of two mononuclear compounds of the  $CuBr_2(HL)_2$  and  $CuBr(HL)_2]Br$  will be also presented.

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## MS13 P26

Benefits of X-ray on Characterization of vic-Dioxime Nickel(II) Complexes <u>Fatma Yuksel</u><sup>a,b</sup>, Ayse Gul Gurek<sup>a</sup>, Erwan Jeanneau<sup>b</sup>, Ilke Gurol<sup>c</sup>, Mahmut Durmus<sup>a</sup>, Dominique Luneau<sup>b</sup>, Vefa Ahsen<sup>a,c</sup>. <sup>a</sup>Gebze Institute of Technology, Turkey. <sup>b</sup>Université Claude Bernard Lyon 1, France <sup>c</sup>TUBITAK-Marmara Research Center, Turkey E-mail: <u>fatma@gyte.edu.tr</u>

# Keywords: metalloorganic complexes, coordination chemistry, *vic*-dioxime

*vic*-Dioximes have been used as chelating agent in coordination chemistry since early 1900s [1-3]. Because of mildly acidic hydroxyl groups and slightly basic nitrogen atoms, *vic*-dioximes are amphoteric ligands which form square planar, square pyramidal and octahedral complexes with transition metal cations such as nickel (II), copper (II) palladium (II) and cobalt (III) [4-5]. *vic*-Dioximes give rise to several geometrical isomers. When the molecule is formally symmetric, three forms are possible: *anti-* (*E*,*E*), *amphi-* (*E*,*Z*).