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

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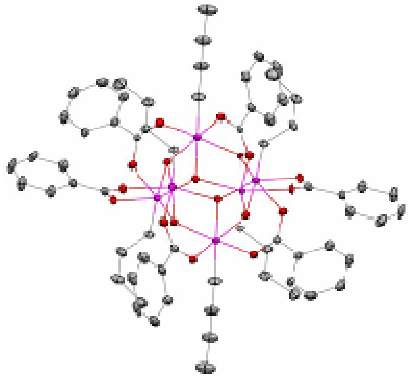
Keywords: Organooxotin, Self-assembly, Fullerene

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 n-butylstannonic 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_{60} 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 ^{119}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.

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

Reactions of Cu(II) halides ($CuCl_2$ and $CuBr_2$) with simple pyridine based alcohols: (2-hydroxymethyl)-pyridine, (2-hydroxyethyl)-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 $[Cu_4L_4Br_4]$ 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

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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),* and *syn- (Z,Z).*

Three different nickel complexes of *vic*-dioximes are known in literature. Orange-red, square planar, and diamagnetic (*E,E*)-bis(dioximato)nickel(II) {[(*E,E*)-$Ni(HL)_2$]} complexes are most common type. Moreover, in the literature there are few examples of green, octahedral, paramagnetic (*E,E*)-tris(dioximato) nickel(II) dichloride {[(*E,E*)-$Ni(LH_2)_3]Cl_2$} [6] and green tetrahedral, paramagnetic (*E,Z*)-bis(dioximato)nickel(II) ([(*E,Z*)-$Ni(HL)_2$]) [7] complexes.

In this work, we use x-ray to clarify the structural confusion between three different forms of Ni (II) complexes of oxamide oximes. We synthesized [(*E,E*)-$Ni(HL)_2$] and [(*E,E*)-$Ni(LH_2)_3]Cl_2$ complexes of three different *(E,E)*-oxamide oxime derivatives and investigated their behaviors dependence of pH by UV spectra. All complexes are novel and characterized by single crystal x-ray diffraction and other spectroscopic techniques.

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MS13 P27

Intra-cavity cyclodextrin monomer in a new complex of Ag (I)

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In the supramolecular host-guest system, cyclodextrins (CDs) seem to be an important class of cavity-shaped hosts. Their chemical modifications give access to a wide range of cavity-shaped molecules that find applications in many areas of contemporary chemistry [1]. We have modified CDs by substituting four hydroxyl groups present at the surface of the macrocycle in order to get new ligands [2] which can yield interesting complexes having potential applications in catalysis. With this attempt, we have synthesized and structurally studied a novel complex of Ag (I) based on sulfur-capped α-CD. We report in this communication, the crystal engineering and the single crystal structure of C108H190Ag2B2F8O57S4. This material has been obtained by low temperature route after mixing in organic medium, a metallic precursor and the dissolved ligand initially synthesized in powder form. The single crystals belong to monoclinic system, space group P21 and parameters a = 16.4968(2) Å, b = 15.7557(2) Å, c = 27.3215(4) Å, β = 102.994 (1) °. The Flack parameter is equal to -0.030(16). In the molecule, the silver cation points toward the CD interior. Differently from the complexes of Pd (II) and Pt (II) recently obtained [3], the sulfur lone pairs point in a fashion that brings about an intra-cavity orientation. Moreover, these electronic pairs are involved in the coordination around the Ag connector, as like as one molecule of butanone which was trapped in the CD-cavity. In addition, this metallo-cavitand is a monomer where the metal is near the macrocycle.

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Keywords: α-cyclodextrins; thiacavitands; intra-cavity monomer.

MS13 P28

Single crystal study of $H_3O(HC_2O_4)(H_2C_2O_4)(H_2O)$

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Keywords: single crystal structure, hydrogen bond network, bridged oxalate

In the continuation of our work dealing with polymeric frameworks, large single crystals were obtained from conventional method. The structure determination, using Kappa CCD diffractometer, has revealed that the compound was hydronium tetroxalate dihydrate. The symmetry is triclinic with P-1 space group and parameters a= 6,3387(4)Å, b=7,2260(4)Å, c=10,5118(6)Å, α=94,208(4)° β=100,296(5)° and γ=97,767(5)°, and is isostructural with previously reported alkali tetroxalates [1][2][3][4]. All hydrogen atoms have been located from Fourier-differences map.

The hydronium ion is coordinated to nine oxygen atoms from three monoprotonated ligands, three oxalic acid molecules and two water molecules, displaying various coordination modes of the oxalate ligands, as chelating -bridging μ_4-η^4, monodentate μ_2-bridging and tetradentate μ_4-bridging. In the coordination polyhedron, which can be described as monocapped dodecahedron, the strongest O-O interactions are between the central ion and the oxalate ligands and the weaker ones with water molecules. The three dimensional structure is composed of isolated polyhedra bridged by organic moieties. All the hydrogen atoms are involved in hydrogen bonds which are responsible of the polymeric structure as well as μ-$_{1,3}$ conventional carboxylate bridges.

The hydrogen bond network of the investigated complex involving water molecules, oxalate ligands as well as hydronium ion, is the most important in the $MH_3(C_2O_4)_2(H_2O)_2$ (M=K, Rb, Cs, NH_4^+) compound series.

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