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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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.

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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 $\mu_{-1,3}$ 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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