As a part of a systematic investigation of the inclusion compounds of plant growth regulators in Cyclodextrins (CDs) we report here the crystal structures of the complexes of 4-chlorophenoxyacetic acid (4CPA) encapsulated in β-CD (4CPA/β-CD) and in heptakis(2,3,6-tri-O-methyl)-β-CD (4CPA/TM β-CD). 4CPA is considered as a sufficiently safe plant growth regulator, exhibiting only slightly toxic qualities and it is fairly used in the food industry.

The 4CPA/β-CD complex crystallizes as a dimer in the space group C2 in the Tetrad packing mode. A review on the packing modes of the dimeric β-CD inclusion compounds indicates that close correspondence of unit-cell dimensions is a necessary, but not a sufficient condition for isostructurality.

The 4CPA/TMβ-CD inclusion complex crystallizes in the space group P21 and its asymmetric unit contains two crystallographically independent complexes exhibiting different orientations. These complexes exhibit also different conformations related to the different orientation of the guests inside the cavities. It is noted that the complexation process induces striking differences between the hosts of the two complexes though the guest molecules retain the same conformation. Thus, we conclude that the same guest having the same conformation does not inevitably cause a definite conformation of the host.

Recently, we have reported the structure of tetrasodium thiacalix[4]arenetetraysulfonate (H4TCAS)[1]. Odo and co-workers found that some metal complexes of H4TCAS attached on ion-exchangers showed peroxidase-like catalytic activity[2]. This prompted us to make single crystals of metal complexes of TCAS for the structure analyses. We succeeded in the preparation of micro crystals of Fe(III) complex of TCAS. A blue thin plate-like crystal of K3[Fe(H2TCAS)(H2O)2].8H2O was obtained, which is the Sr Fe(III) complex of TCAS. A blue thin plate-like crystal of Fe(III) complex of TCAS for the structure analyses. We succeeded in the preparation of micro crystals of Fe(III) complex of TCAS. A blue thin plate-like crystal of K3[Fe(H2TCAS)(H2O)2].8H2O was obtained. The authors wish to thank Dr. Lee Daniels and Dr. Ron Benson from Rigaku MSC for data collection. We also thank FONACIT-Venezuela for support through grant LAB-9700821.

Keywords: carboxylates, hydrothermal synthesis, coordination compounds

In metal-organic crystal engineering, when flexible ligands are involved in the supramolecular networks, predicting the topology of the coordination polymer is more difficult since several factors such as the kind of solvent, the metal coordination, the counter-anion, the metal-to-ligand ratio and the degree of flexibility of the ligand affect the framework formation. In order to gain some insight into the influence of those factors, we report here the effect of the size of the ligand, its symmetry and degree of flexibility, as well as the influence of the anion, upon the supramolecular architecture when diarylthioether ligands are used as building blocks in silver(I) complexes. Only ligands with an even number of methylene groups will be discussed here. The non-coordinating anions favor the formation of cationic three-dimensional networks. As these anions serve as terminal ligands, the anions, which are usually located within the channel, are relatively free to move, the anion-exchange properties of those complexes will be examined. The weakly coordinating anions give rise to 1D-coordination polymers. As these anions serve as terminal ligands, the formation of two or three dimensional networks is ruled out. The more strongly coordinating acetate anions yield 2 or 3-dimensional networks. Weak silver-silver interactions are noted. In some cases, those interactions are retained in the 2D-network. The details of these 2D, 3D-networks and the silver-silver interactions will be described and illustrated. A rationalization of the influence of the various parameters on the topologies of the supramolecular architectures will be presented.

Keywords: silver, flexible ligand, coordination polymer

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Keywords: thiacalixarene compound, catalytic activity, second-sphere coordination

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New Metal Carboxylates prepared at Room Temperature and by Hydrothermal Methods

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New alkaline-earth metal derivatives of nicotinic, isonicotinic, and cis-4-cyclohexene dicarboxylic (CDCA) acid have been prepared at room temperature and/or by hydrothermal methods. They have been characterized by spectroscopic, thermal, and X-ray diffraction techniques in polycrystalline and single crystal samples.

Layered structures are obtained in all cases. However, it should be noted that the Ba derivative of CDCA prepared under hydrothermal conditions crystallizes in an orthorhombic unit cell, space group Cmc21, with a = 28.63(4), b = 0.936(3), c = 7.43(2) Å. This is a completely different structure from the one obtained previously at room temperature. The Sr and Ba complexes of isonicotinic acid are monoclinic, P21/c, with a = 6.1403(6), b = 43.976(4), c = 7.2107(7) Å, β = 118.72(1)° for the Sr complex and a = 6.276(2), b = 44.338(4), c = 7.345(2) Å, β = 118.74(2)° for the Ba complex.

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