

P.07.04.13*Acta Cryst.* (2005). A61, C308**Inclusion Compounds of Plant Growth Regulators in Cyclodextrins**Athanassios Hountas, Kostas Bethanis, Frantzeska Tsorteki, Dimitris Mentzafos, *Physics Laboratory, Agricultural University of Athens, Greece*. E-mail: hount@aua.gr

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 quantities 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/TM β CD inclusion complex crystallizes in the space group $P2_1$ 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.

[1] Tsorteki F., Bethanis K., Pinotsis N., Giastas P., Mentzafos D., *Acta Cryst. B.*, Accepted 7 February 2005.

Keywords: β -CD, TM β CD, 4CPA**P.07.04.14***Acta Cryst.* (2005). A61, C308**X-ray Structures and Characterizations of Iron Complexes of Thiocalixarenetetrasulfonate**Haru Akashi, Misato Ichikawa, *Research Institute of Natural Sciences, Okayama University of Science, Ridai-cho, Okayama 700-0005, Japan*. E-mail: akashi@high.ous.ac.jp

Recently, we have reported the structure of tetrasodium thiocalix[4]arenetetrasulfonate (H_4TCAS)[1]. Odo and co-workers found that some metal complexes of H_4TCAS 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 $K_2[Fe(H_2O)_6](H_4TCAS) \cdot 8H_2O$, selected for data collection, was mounted in the cold nitrogen stream (105 K) of RAXIS IV(Rigaku Corp.). The compound was found to crystallize in the orthorhombic space group $Pcab$ with $a = 18.552(1)$ Å, $b = 18.7287(8)$ Å, $c = 25.550(2)$ Å, $V = 8863.1(9)$ Å³. The structure analysis of **1** revealed that the iron atom is located in a distorted octahedral site. The iron atom is bound to three oxygen atoms and one sulfur atom of the $TCAS$. This is the first example of the H_4TCAS ligand attached directly to the Fe(III) moiety. Second-sphere coordination compounds, $K[Fe(H_2O)_6](H_4TCAS)$ and $K_2[Fe(H_2O)_6](H_4TCAS)$, will also be reported.

[1] Akashi H., et al., *Acta Cryst.*, 2003, E59, m336. [2] Odo J., et al., *Anal. Sci.*, 2004, 20, 707.

Keywords: thiocalixarene compound, catalytic activity, second-sphere coordination**P.07.04.15***Acta Cryst.* (2005). A61, C308**New Metal Carboxylates prepared at Room Temperature and by Hydrothermal Methods**Graciela Diaz de Delgado, Jines Contreras, Luis León, MarinoGutiérrez, José Miguel Delgado, *Laboratorio de Cristalografía-LNDRX, Universidad de Los Andes, Mérida, Venezuela*. E-mail: diaz@ula.ve

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 $Cmc2_1$, with $a = 28.633(8)$, $b = 9.036(3)$, $c = 7.438(2)$ 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, $P2_1/c$, with $a = 6.1403(6)$, $b = 43.976(4)$, $c = 7.2170(7)$ Å, $\beta = 118.72(1)^\circ$ for the Sr complex and $a = 6.276(2)$, $b = 44.334(8)$, $c = 7.345(2)$ Å, $\beta = 118.74(2)^\circ$ for the Ba complex.

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Keywords: carboxylates, hydrothermal synthesis, coordination compounds**P.07.04.16***Acta Cryst.* (2005). A61, C308**Silver Coordination Polymers with Flexible Ligands. Effect of the Size of the Ligand and the Solvent on the Network Formation**François Brisse, Mohamed Osman Awaleh, Antonella Badia, *Département de chimie, Université de Montréal, Montréal, Canada*. E-mail: francois.brisse@umontreal.ca

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 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 upon the topologies of the supramolecular architectures will be presented.

Keywords: silver, flexible ligand, coordination polymer**P.07.04.17***Acta Cryst.* (2005). A61, C308-C309**Structural Relationships in the Coordination Complexes of Bis(phenylthio)methane (L1) and Bis(phenylthio)propane (L3) with Silver(I) Salts**Mohamed Osman Awaleh, Antonella Badia, François Brisse. *Département de chimie, Université de Montréal, Montréal, Canada*. E-mail: francois.brisse@umontreal.ca.

The structures adopted by coordination polymers formed with flexible ligands are difficult to predict. The factors affecting the framework formation of coordination polymers, such as the ligand length, the stoichiometry, the role of the anion and the solvent were