

Metal-organic motif found using ligand L and silver salts

[1] Brito, I.; Vallejos, J.; Lopez-Rodriguez, M.;Cardenas, A., *Acta Cryst.*, 2010, o114 [2] Huang, Z.; Du, M.; Song, H.; Bu, X., *Cryst. Growth Des.*, 2004, 71. [3] Liu, Y.; P. Yang, P.; Hou, G.; Gao, J.; Lu, J. Y., *Cryst. Growth Des.* 2010, 1623.

Keywords: Coordination Polymers, Silver salts, X-ray diffraction.

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The Crystal Structure of a Mixed-Metal Basic Trifluoroacetate of Aluminium and Zinc:

 $[AlZn(\mu^4-O(O_2CCF_3)_3]_4.$ <u>Georgi Genchev</u>^a, Walter Frank^a, ^aInstitut für Anorganische und Strukturchemie II, Heinrich-Heine Universität Düsseldorf, Germany E-mail: <u>wfrank@uni-duesseldorf.de</u>

M₄X₄ molecular cages where M is a metal and X is an element of group 15, 16 or 17 are quite common [1, 2]. All these cages have the cube geometry as found in the well known Fe₄S₄ ferredoxins [3]. Here we report on the synthesis and the crystal structure of $[AlZn(\mu^4-O)(O_2CCF_3)_3]_4$ (1). This exceptional compound was discovered during a study on the thermal behaviour of aluminiumtris(trifluoroacetate). Crystals were obtained by the thermolysis of Al(O₂CCF₃)₃ in the presence of zinc powder. The reaction was carried out at 200-220 °C under static vacuum. 1 crystallizes in the monoclinic space group $P2_1/c$ with lattice parameters of a = 19.906(4) Å, b =14.490(3) Å, c = 18.384(4) Å and $\beta = 98.02(3)$ ° and with Z =8. In the crystal each of the Al_4 tetrahedrons is capped by a zinc atom resulting in Al₃Zn pyramids that contain an oxygen atom. All of the 12 Al-Zn edges are bridged by trifluoroacetate The aluminium atoms have an octahedral ligands. coordination. Two of the four zinc atoms have tetrahedral and the other two have trigonal bipyramidal coordination. Due to secondary Zn-O interactions compound 1 is a chain polymer. On the molecular level the structure of 1 has a close relationship to the structure of spinel. Indicative for this similarity is the M₄O₄ core, the presence of di- and tri-positive metal cations and the equal mode of coordination of the atoms in both structures.

Sarasa J. P., Poblet J. M., Benard M., Organometallics, 2000, 19,
Cotton A. F., Duraj S. A., Roth W. J., Inorg. Chem., 1984,
4042. [3] Hahn F. E., Jocher C., Lügger T., Z. Naturforsch., 2004,
59b, 855.

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FA4-MS31-P10

Hydrogen-bonded networks within dicarboxylates and guanidine assemblies. Samir Habi-Benhariz^a, Khadidja Aliouane^a, <u>Achoura Guehria-Laïdoudi</u>^a, Slimane Dahaoui^b, Claude Lecomte^b, ^aLaboratoire Cri-Ther Faculty of Chemistry USTHB Algiers, Algeria ^bCRM2 UMR-CNRS Nancy University, France E-mail:guehria_laidoudi@yahoo.fr

In extended frameworks, the carboxylate anions can act as linking ligands and hydrogen-bond acceptors. By varying the cations which can be used as potential H-donors, we can control the factors that govern the overall ordered assembly and building blocks' interactions. In this context, we investigate the competitive effect of non-covalent and coordination bonds in supramolecular architecture, by using metallic oxides and guanidine as connectors or template's cations and dicarboxylates as ditopic anionic ligands.

This work presents three new guanidine derivativesdicarboxylate crystals, where only short-range interactions are present in the lack of any metal. The hydrogen-bonded motifs, the supramolecular chemistry of CO_2 and NH_2 functional groups, the synthon flexibility, the nature of the components and their basic features in the crystals are discussed:

The three compounds belong to the same space group $(P2_1/c)$, often encountered in this kind of materials.

 $[(CH_2)_3(CO_2)_2][C(NH_2)_3]$ and [(NH₂)₂C(NH)CH₂COOH] [(CH₂)₅CO₂CO₂H] are based on two charged entities. The glutarate's formulation indicates a proton transfer. The specific geometry of the hydrogenpimelate builds up wide cavities running in zig-zag, and the resulting 3D packing can be very probably porous, as in metal-organic-frameworks. $[(CO_2H)_2][C_3H_5N_3O]$ is based on two neutral units. Within it, the guanidine has been converted to an imidazol derivative. These three compounds display H-bond patterns with several kinds of motifs, giving two-dimensional networks or noncatemeric chains. Their major "element of structural design"are heterosynthons involving acid-amine or acid-amide interactions with bifurcated bonds. The three compounds are anhydrous, exhibiting empty, more or less wide channels. In the two ionic ones, this can be explained by the hydrophobic character of the cavities surrounded by protuberant methylen groups. The glutarate can be related to superacid salts, and the dihydrogenoxalate and hydrogenpimelate to cocrystals. However, in the controversial debate occurring around salts and cocrystals, these new results show that, when we use the approach introduced in metal-organic-frameworks and coordination polymers, these materials can be affiliated to MOFs or CPs, as it is the case in the hydroxonium polymer recently published.

 Li H., Eddaoudi M., Groy T.L., Yaghi O.M. J.Am.Chem. Soc. 1998, 120, 8571.
Bernstein J. Chemm. Commun. 2005, 40, 5007.
Videnova-Adrabinska V., Obara R., Lis T. New J.Chem. 2007, 31, 287.
Kherfi H., Hamadène M., Guehria-Laïdoudi A., Dahaoui S., Lecomte C. Materials 2010, 3, 1281.

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