

intermolecular hydrogen-bond interactions. The most promising combinations are then selected for further cocrystallization experiments.

During the cocrystallization screening new pseudopolymorphs of flucytosine were obtained [5]. The flucytosine molecules form ribbons with repeated R₂,2(8) dimer interactions. The solvent molecules adopt related positions with respect to the flucytosine. Depending on the hydrogen bonds formed by the solvent the flucytosine ribbons form layers or tubes.

Moreover we have obtained cocrystals of flucytosine. The interactions with its model receptor molecules resemble the hydrogen-bonding pattern within the GC base pair [Fig. 1]. The complexes are connected into ribbons either by R₂,2(8) or R₄,2(8) interactions, which further show hydrogen-bonded layers or tubes similar to those found in the crystals of flucytosine. We have also observed a conformational change induced by the formation of the cocrystal. In this case, the model receptor molecule adopts a conformation, whose calculated steric energy is 34 kJ/mol above the global minimum.

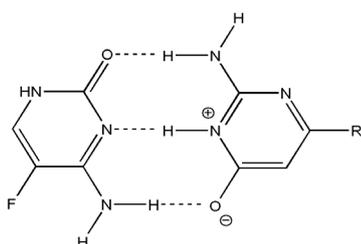


Fig. 1

[1] Morschhäuser J., *Pharm. Unserer Zeit*, 2003, 32, 124-128. [2] Pierrefite-Carle V., Baque P., Gavelli A., Mala M., Chazal M., Gugenheim J., Bourgeon A., Milano G., Staccini P., Rossi B., *J. Natl. Cancer Inst.*, 1999, 91, 2012-2019. [3] Davis A.M., Teague S.J., Kleywegt G.J., *Angew. Chem.*, 2003, 115, 2822-2841. [4] Wagner G., Gemmel E., Beck H., Bolte M., Egert E., MOMO Version 2.00; University of Frankfurt (2006). [5] Tutughamiasro M., Bolte M., Egert E., *Acta Cryst. C*, 2009, 65, o574-o578.

Keywords: Flucytosine, Supramolecular complexes, Drug-receptor interaction

FA4-MS31-P07

Shape Similarity and Chiral Resolution of Tröger's bases Christophe M.L. Vande Velde^a, Sergey Sergeyev^b

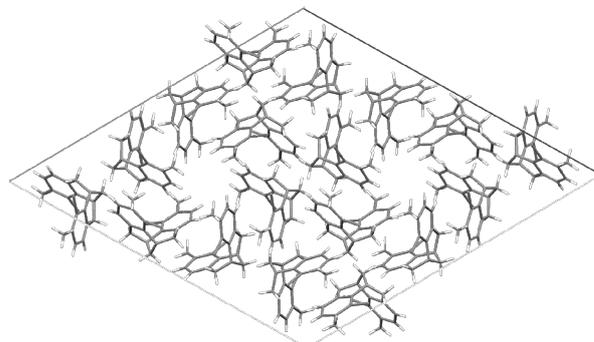
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Tröger's base, or 2,8-dimethyl-6*H*,12*H*-5,11-methanodibenzo[*b,f*][1,5]diazocine, is a V-shaped chiral bicyclic diamine, in which the nitrogen atoms serve as the chiral centres. A recent revival of interest in Tröger's base and its derivatives as a chiral scaffold [1] prompted us to synthesize a number of Tröger's bases. On structure determination, the percentage of structures which exhibited spontaneous resolution seemed conspicuously high, and the determining factor in this, for lack of specific strong or directional interactions, appeared to be the molecular shape. We decided on a formal approach where all possible tetramethyl substituted Tröger's bases would be synthesized, and quantum shape similarity calculations [2] done to verify whether a correlation could be observed. The results indeed

show that the molecules which exhibit spontaneous resolution are the ones with the highest shape dissimilarity. In addition, those molecules with high shape dissimilarity that do not resolve spontaneously, show a number of interesting ways of coping with the stress associated with packing in a racemic crystal. A number of these structures will be presented.



[1]Sergeyev, S. *Helv. Chim. Acta* 2009, 92, 415-422; Dolensky, B et al. *Adv. Het. Chem.* 2007, 93, 1-56 [2] Mestres et al. *J Comp. Chem.* 1994, 15(10), 1113-1120.

Keywords: chiral resolution, ab initio calculations, crystal engineering

FA4-MS31-P08

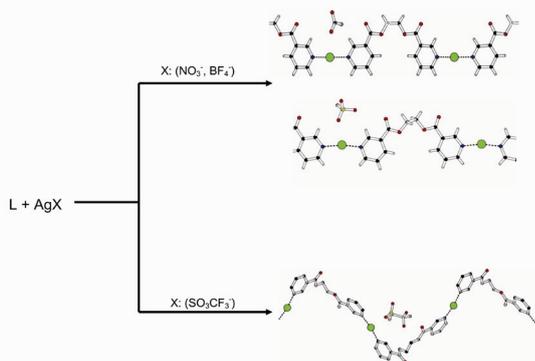
Counter Ion and Conformation Ligand Effect on the Crystal structure of Novel Ag(I) Coordination

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The reaction of the flexible ligand ethane-1,2-diyl-bis-(pyridyl-3-carboxylate) (L) and various inorganic silver (I) salts, under same conditions lead to the formation of three coordination polymers with different motif; {[Ag(L)(CF₃SO₃)_n]}_n (1), {[Ag(L)(BF₄)_n]}_n (2), {[Ag(L)(NO₃)_n]}_n (3). In all compounds, the ethylene moiety of L retains the gauche conformation [1], however, the nitrogen of the aromatic ring in (1) are pointing to the different side compared to the conformation of the ligand in (2) or (3). This is important factor in the generation of helicity motif in (1), compared with the lineal motif of (2) and (3). Concerning the coordination abilities of CF₃SO₃⁻, BF₄⁻ and NO₃⁻ anions to the silver cation, they exhibit differences in the mode and strength coordination [2,3]. The stronger coordination of the silver cation by the counter ion is related for the distortion of the bend N-Ag-N and the weakening of the distance Ag-N. The atomic parameters in the obtained complexes are consistent with these relations; the compound (3) presents the lowest values of the N-Ag-N angle (158°) and longer value of the Ag-N distance (2.18Å), with the NO₃⁻ anion strongly coordinated with the silver cation. For (1) and (2) the counter ions are weakly coordinated with the metal cation, in accordance with the above, we find the longer value of the N-Ag-N angle (168 and 169°) and shorter value of the Ag-N distance (2.15 and 2.16Å) respectively. These results indicate that the nature of the ligands and counter ions plays the critical role in construction of these novel coordination polymers.



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.

FA4-MS31-P09

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

$[AlZn(\mu^4-O(O_2CCF_3))_3]_4$. Georgi Genchev^a, Walter Frank^a, ^a*Institut für Anorganische und Strukturchemie II, Heinrich-Heine Universität Düsseldorf, Germany*
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M_4X_4 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 Fe_4S_4 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 $Al(O_2CCF_3)_3$ 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 $\beta = 98.02(3)^\circ$ and with $Z = 8$. In the crystal each of the Al_4 tetrahedrons is capped by a zinc atom resulting in Al_3Zn pyramids that contain an oxygen atom. All of the 12 Al-Zn edges are bridged by trifluoroacetate ligands. The aluminium atoms have an octahedral 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 M_4O_4 core, the presence of di- and tri-positive metal cations and the equal mode of coordination of the atoms in both structures.

[1] Sarasa J. P., Poblet J. M., Benard M., *Organometallics*, 2000, 19, 2264. [2] Cotton A. F., Duraj S. A., Roth W. J., *Inorg. Chem.*, 1984, 23, 4042. [3] Hahn F. E., Jocher C., Lügger T., *Z. Naturforsch.*, 2004, 59b, 855.

Keywords: aluminium compounds, single-crystal X-ray diffraction, thermal behaviour

FA4-MS31-P10

Hydrogen-bonded networks within dicarboxylates and guanidine assemblies. Samir Habi-Benhariz^a, Khadidja Aliouane^a, Achoura Guehria-Laïdoudi^a, Slimane Dahaoui^b, Claude Lecomte^b, ^a*Laboratoire Criter Ther Faculty of Chemistry USTHB Algiers, Algeria*
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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 derivatives-dicarboxylate 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 $[(NH_2)_2C(NH)CH_2COOH][C(NH_2)_3]$ 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 non-catemic 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.

[1] Li H., Eddaoudi M., Groy T.L., Yaghi O.M. *J. Am. Chem. Soc.* 1998, 120, 8571. [2] Bernstein J. *Chem. Commun.* 2005, 40, 5007. [3] Videnova-Adrabsinska V., Obara R., Lis T. *New J. Chem.* 2007, 31, 287. [4] Kherfi H., Hamadène M., Guehria-Laïdoudi A., Dahaoui S., Lecomte C. *Materials* 2010, 3, 1281.

Keywords: supramolecular frameworks, heterosynthons, guanidine