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**Keywords: copper compounds-1, biomimetics-2, catalyst structure -3**

#### FA4-MS31-P04

##### Defect Engineering in Colloidal Photonic Crystals.

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Imaging of lattice defects in crystalline materials has captured the attention of the scientific community for many decades. Because the size of typical defects is of the order of the lattice period of a crystal, techniques to image stacking faults, dislocations and vacancies have never been able to resolve their structure down to the core level. By crystallizing micron-sized colloidal particles into close-packed structures, we are now able to study crystal structures and defects in real and reciprocal space. We use synchrotron microradian X-ray diffraction to image the average crystal structure over large crystalline areas. Through confocal microscopy, we also have access to the local crystal structure on a single particle level. The combination of these techniques enables us to identify the global crystal structure and explain it through the presence of local defects. Using this approach, we have identified a large concentration of intrinsic stacking faults in colloidal crystals that were previously thought to be pure face-centred cubic in structure. Through confocal microscopy we found Lomer-Cottrell dislocations to be responsible for the nucleation of these stacking faults. Exploiting this growth mechanism, we were able to selectively grow stacking faults into colloidal crystals by sedimentation onto a structured template containing a 2D projection of a Lomer-Cottrell dislocation. This is of interest for the applicability of colloidal crystals as photonic materials.

**Keywords: defects, colloids, photonic crystals**

#### FA4-MS31-P05

##### Magnetic Exchange Interactions through H-bonds in Copper(II) Carboxylates.

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Hydrogen bonds and coordination bonds are used as interesting tools for inorganic crystal engineering to build up building blocks that possess their application in supramolecular structures [1]. Some copper(II) complexes, as examples, have shown that the intermolecular hydrogen bonds can modified their magnetic properties [2]. Similar system of hydrogen bonds have been found in some supramolecular isomers [3] of the other copper(II) carboxylate complexes.

We have recently published dinuclear complex  $[\text{Cu}(\mu\text{-nia})(5\text{-MeSal})_2(\text{H}_2\text{O})_2]_2$  (nia = nicotinamide, 5-MeSal = 5-methoxysalicylate anions) [4] and mononuclear complex  $[\text{Cu}(\text{nia})(3\text{-NO}_2\text{Bz})_2(\text{H}_2\text{O})_2]$  (3-NO<sub>2</sub>Bz = 3-nitrobenzoate anion) [5], which exhibit similar magnetic properties. Very similar magnetic properties of mononuclear and binuclear complexes could be explained by the presence of very similar supramolecular synthons that are pathway for the magnetic exchange interactions. The hydrogen bonds, described by supramolecular synthons, formed by coordinated water molecule and two carboxylatogroups on each copper atom could create supramolecular dimers of two mononuclear complex molecules [4] and supramolecular chains of dinuclear complex molecules [5]. In this report we present series of 1-D coordination polymers of general formula  $[\text{Cu}(\mu\text{-dena})(\text{RCO}_2)_2(\text{H}_2\text{O})_n]$  (RCO<sub>2</sub> are substituted benzoate or salicylate anions, dena = N,N-diethylnicotinamide) with similar magnetic properties, that are explained as a consequence of the supramolecular synthons allowing to create two dimensional layer structures based on the 1-D coordination polymers bonded by hydrogen bonds. This could be given as the proof, that the hydrogen bonds described above are the main path for observed magnetic exchange and for that reason the similarity in magnetic properties (maximum of susceptibility at similar temperature and the value of antiferromagnetic interactions  $2J$ ) are observed in all complexes, despite they are of different crystal structures, and different dimensionality (monomeric, dimeric, or polymeric).

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**Keywords: crystal structure, hydrogen bonds, magnetic exchange interactions**

#### FA4-MS31-P06

##### Cocrystals of flucytosine: Models for drug-receptor interactions.

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Flucytosine (5-fluorocytosine) is a systemic antifungal drug. It is intrafungally converted into 5-fluorouracil and inhibits RNA and DNA synthesis [1]. Furthermore, it has a novel application as a prodrug active against liver tumours [2]. The interaction between flucytosine and its receptor, as well as the base pairing, can be imitated by hydrogen-bonded complexes [3]. In order to examine these interactions we cocrystallized flucytosine together with several model compounds containing complementary functional groups and studied the preferred conformations adopted by the model compounds.

Since the cocrystallization of supramolecular complexes is not a straightforward procedure, we have developed a concept for designing these structures. After selection of model compounds, we calculate the structures and energies of a multitude of alignments ("constellations") by our force-field program MOMO [4]. Various analytical tools (especially IR spectroscopy and powder diffraction) are used to identify the

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 R<sub>2</sub>,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 R<sub>2</sub>,2(8) or R<sub>4</sub>,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.

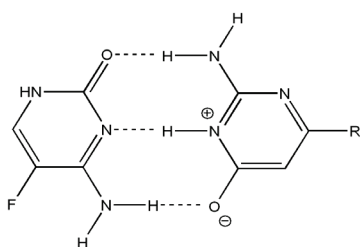


Fig. 1

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**Keywords: Flucytosine, Supramolecular complexes, Drug-receptor interaction**

#### FA4-MS31-P07

#### Shape Similarity and Chiral Resolution of Tröger's bases Christophe M.L. Vande Velde<sup>a</sup>, Sergey Sergeyev<sup>b</sup>

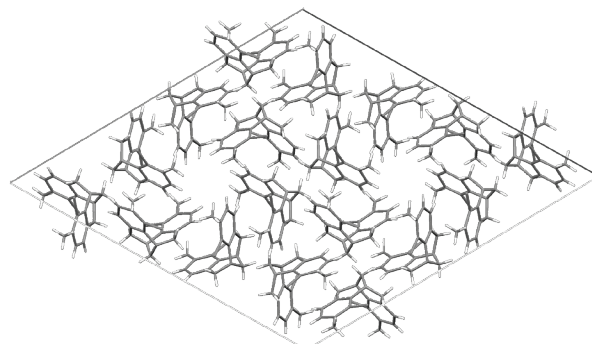
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Tröger's base, or 2,8-dimethyl-6*H*,12*H*-5,11-methanodibenzo[*b,f*][1,5]diazocine, is a V-shaped chiral bicyclic diamine, in which the nitrogen atoms serve as the chiral centres. A recent revival of interest in Tröger's base and its derivatives as 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.



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**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)(CF<sub>3</sub>SO<sub>3</sub>)<sub>n</sub>]}<sub>n</sub> (1), {[Ag(L)(BF<sub>4</sub>)<sub>n</sub>]}<sub>n</sub> (2), {[Ag(L)(NO<sub>3</sub>)<sub>n</sub>]}<sub>n</sub> (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 CF<sub>3</sub>SO<sub>3</sub><sup>-</sup>, BF<sub>4</sub><sup>-</sup> and NO<sub>3</sub><sup>-</sup> 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 NO<sub>3</sub><sup>-</sup> 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.