

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.

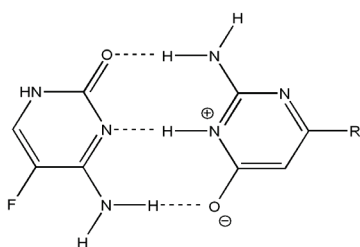


Fig. 1

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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^a, Sergey Sergeev^b

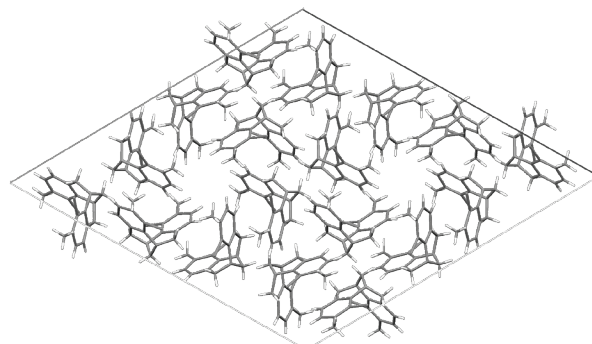
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Tröger's base, or 2,8-dimethyl-6*H*,12*H*-5,11-methanodibenzo[*b,f*][1,5]diazocine, is a V-shaped chiral bicyclic diamine, in which the nitrogen atoms serve as the chiral centres. A recent revival of interest in Tröger's base and its derivatives as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

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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.