

P.09.01.1*Acta Cryst.* (2005). A61, C353**Investigating Weak Interactions in Pharmaceutical Co-Crystal Systems**Pauline Gavan^a, Nick Blagden^a, Colin Seaton^a, Ian Grimsey^a, Pete Marshall^b, ^a*The School of Pharmacy, University of Bradford, UK.* ^b*Pfizer Ltd., Sandwich, UK.* E-mail: P.T.Gavan@Bradford.ac.uk

Pharmaceutical co-crystallisation is emerging as a possible alternative to polymorphs, salts and solvates in the modification of an active pharmaceutical ingredient (API) during dosage form. It may alter the physico-chemical properties of the API (e.g. melting point and solubility), and also have intellectual property implications.

Traditionally, co-crystallisation research has involved robust synthons with strong interactions and rarely involved pharmaceutically acceptable co-crystallising agents and conditions. Our current work has focused on the co-crystallisation of sulfathiazole with sugar excipients, [1], where moderate to weak interactions were expected to dominate.

Co-crystallisation was investigated by solution and solid-state methods (including solvent mediated grinding). Co-crystallisation of sulfathiazole with lactose, mannitol and sorbitol was unsuccessful from solution or the solid-state. However, sulfathiazole-glucose co-crystals were produced from ethanol and propanol solutions.

[1] Gavan P.T., Blagden N., Seaton C.C., Grimsey, I.M., Marshall, P., *CrystEngComm.*, 2005, submitted.

Keywords: cocrystals, weak interactions, pharmaceuticals

P.09.01.2*Acta Cryst.* (2005). A61, C353**Design and Synthesis of Co-crystals: From Molecular Sense to Supramolecular Sensibility**Christer B. Aakeröy, *Department of Chemistry, Kansas State University, Manhattan, KS, 66506, U.S.A.* E-mail: aakeroy@ksu.edu

What is most likely going to happen when a homogeneous solution containing two different molecular solutes is allowed to evaporate to dryness? Unless a chemical reaction driven by the formation of covalent bonds takes place between the two solutes one would, as a rule, expect the appearance of two separate molecular solids. This is a manifestation of the inherent structural selfishness of molecules, something that is relied upon every time recrystallization is employed as a method of purification. Recrystallization processes are essential in most covalent synthetic procedures and are performed on a regular basis in every synthetic laboratory. In the supramolecular laboratory, however, the very same process also provides an opportunity to move in the opposite direction – a co-crystallization is a deliberate attempt at bringing together different molecular species in one crystalline lattice without making or breaking covalent bonds. Recrystallization and co-crystallization processes are, in essence, only distinguishable by their intents. The goal of the former is a homomeric product, the goal of the latter is a heteromeric product. Since the odds are stacked firmly in favor of a homomeric product, how do we go about developing reliable and versatile synthetic methods for the directed assembly of co-crystals? This presentation will attempt to answer the question by outlining several modular hydrogen-bond driven strategies for the design and synthesis of binary and ternary supermolecules and co-crystals.

Keywords: hydrogen bond, cocrystals, molecular recognition

P.09.01.3*Acta Cryst.* (2005). A61, C353**Crystal Engineering of Arylammonium Perhalometallates**Melanie Rademeyer, Christos Tsouris, *School of Chemistry, University of KwaZulu-Natal, Durban, South Africa.* E-mail: rademeyerm@ukzn.ac.za

The ultimate aim of crystal engineering is the design of crystal structures, and as a result, materials with desired properties. A fundamental requirement of crystal engineering is the understanding of the role of non-covalent interactions occurring in the solid-state structure.

A number of crystal engineering studies have focused on the identification of interaction synthons in compounds of the type LMX₄ where L is the 4,4'-bipyridinium cation [1] or the pyridinium cation [2].

This study focuses on the identification of non-covalent interactions in a family of primary arylammonium perhalometallate organic-inorganic hybrid materials. A number of novel crystal structures, some isostructural, will be reported.

The hydrogen bonding- and aromatic interactions present in these crystal structures will be highlighted, and their influence on the molecular packing illustrated. Crystal engineering synthons will be identified, and compared to synthons identified in related structures.

[1] Gillon A.L., Orpen A.G., Starbuck J., Wang X., Rodriques-Martin Y., Ruiz-Perez C., *Chem. Comm.*, 1999, 2287-2288.

[2] Felloni M., Huberstep P., Wilson C., Schroder M., *CrystEngComm.*, 2004, 6, 87-95.

Keywords: non-covalent interactions, organic-inorganic hybrids, crystal engineering

P.09.01.4*Acta Cryst.* (2005). A61, C353**Towards Electrochemical Artificial Muscles: A Supramolecular Machine Based on One-dimensional Copper-containing Organophosphonate System**Shu-Juan Fu, K. J. Lin, *Department of Chemistry, National Chung-Hsing University, Taichung, Taiwan.* E-mail: d9051010@mail.nchu.edu.tw

The development of artificial system is a field which is currently being intensively explored. In particular, interest is being focused on transition-metal-containing system. In our laboratory, we have created a new supramolecular machine, exhibited reversible electromechanical actuators based on sheets of water-soluble one-dimensional copper-centred ethylenephosphonate (1DOP-Cu) chains, described for the first time. Like natural muscles, the macroscopic sheet actuators are composed of mats of individual nanofiber bundles joined by mechanical entanglement and pi-pi interaction forces along the crystallographic a-axis. The lithium inserted state, upon electrochemical charge injection into 1DOP-Cu, exhibits a reversible contraction/ stretched process by oxidizing or reducing the copper center to Cu(II) or Cu(I) whose coordinated geometries will be changed at will by a redox process, as characterized by x-ray diffraction patterns, solid state NMR, and XANE spectra.

[1] Gu G., Schmid M., Chiu P. W., Minett A., Frayse J., Kim G. T., Roth S., Kozlov M., Muñoz E., Baughman R. H., *Nature materials*, 2003, 2, 316. [2] Fu S. J., Cheng C. Y., Chen W. H., Lin K. J., Kao H. M., *Angew. Chem. Int. Ed.*, 2004, 43, 4186.

Keywords: copper, artificial muscles, supramolecular chemistry

P.09.02.1*Acta Cryst.* (2005). A61, C353-C354**Molecularly Designed Functional Materials; Can We Really Control their Supramolecularity?**Solhe F. Alshahateet, Emily H. E. Lau, Fathi Kooli, Reginald B. H. Tan, Pui Shan Chow, *Institute of Chemical and Engineering Sciences, 1 Pesek Road, Jurong Island, Singapore 627833.* E-mail: solhe_alshahateet@ices.a-star.edu.sg

Supramolecular chemistry can be simply defined as the chemistry of multicomponent molecular assemblies in which the component structural units are typically held together by a variety of weaker (noncovalent) interactions (chemistry beyond molecules). A specific example of such supermolecules is inclusion compounds. Inclusion compounds are formed by the noncovalent insertion of guest molecules into the host lattice during the crystallization process.

Supramolecules present great potential industrial applications in separation of isomers, purification of solvents, drug delivery, catalysis, molecular recognition and many other fields. Recently, we have been working on design and synthesis of new host molecules such as V-shape diquinolines and arene derivatives and investigating their self assembly as well as their potential applications. Although the