



DEPARTMENT OF CHEMISTRY

DEPARTMENTAL SEMINAR

Professor Christer Aakeröy

Kansas State University

"Constructing co-crystals using molecular sense and supramolecular sensibility"

Co-crystallization brings together different molecular species within one heteromeric crystal. In general, the process of crystallization yields, however, a homomeric product. How do we go about developing reliable, effective, and versatile synthetic methods for the directed assembly of heteromeric co-crystals? This presentation will (a) outline practical strategies for modular and directed assembly of co-crystals and (b) demonstrate how different physical properties of an active ingredient (such as a pharmaceutically relevant compound) can be altered through co-crystal synthesis.

Christer Aakeröy received MSc from Uppsala U-ty (Sweden, 1986) and PhD from the U-ty of Sussex (UK, 1990). He was a Lecturer at the Queen's U-ty of Belfast (Northern Ireland, 1993-6). He joined Chemistry Department at Kansas State U-ty in 1996 where became Professor in 2006. Prof Aakeröy's research interests focus on fundamental and pharmaceutical application aspects of crystal engineering, supramolecular and structural chemistry, intermolecular forces and host-guest chemistry. He serves as the regional editor (Americas) for the RSC journal CrystEngComm. Recently he was appointed to a four-year term on the board of governors of the Cambridge Crystallographic Data Centre. He is one of eight distinguished scientists on the board and is the only member from North America.

NEW SCIENCE COMPLEX, Room 1511

Thursday, February 18th, 2010, at 10:45 am

Coffee and Timbits will be served at 10:30 am in SCIE-1511

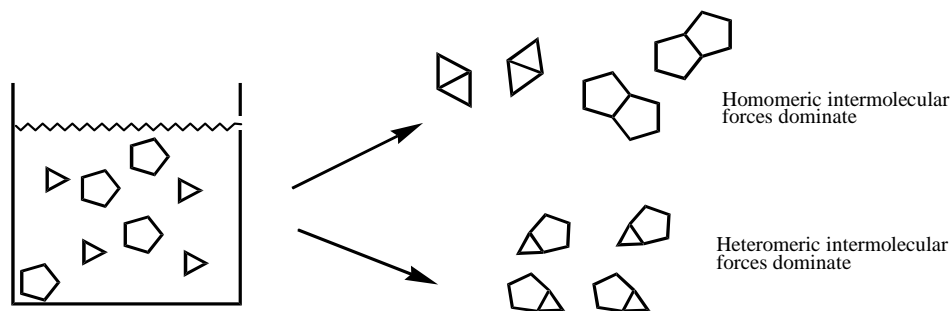
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Constructing co-crystals using molecular sense and supramolecular sensibility

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What is the most likely outcome 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 – the equivalent of a simple recrystallization. In the supramolecular laboratory, however, the very same process provides an opportunity to move in a completely different direction – a co-crystallization is a deliberate attempt at bringing together different molecular species within one periodic 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, whereas the latter procedure strives for a heteromeric product and, in general, the odds are stacked firmly in favor of a homomeric product, Scheme 1, so how do we go about developing reliable, effective, and versatile synthetic methods for the directed assembly of heteromeric co-crystals?



This presentation will (a) outline practical strategies for modular and directed assembly of co-crystals and (b) demonstrate how different physical properties of an active ingredient (such as a pharmaceutically relevant compound) can be altered through co-crystal synthesis.

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- [1] C.B. Aakeröy, J. Desper, M. Fasulo, I. Hussain, B. Levin and N. Schultheiss, *CrystEngComm*, 10, 1816, (2008).
 - [2] C.B. Aakeröy, J. Desper and M.M. Smith, *Chem. Commun.* 3936, (2007).
 - [3] C.B. Aakeröy, M. Fasulo, S. Schultheiss, J. Desper and C. Moore, *J. Am. Chem. Soc.*, 129, 13772, (2007).
 - [4] C.B. Aakeröy, J. Desper, B.A. Helfrich, P. Metrangolo, T. Pilati, G. Resnati, and A. Stevenazzi, *Chem. Commun.*, 4236, (2007).
 - [5] C.B. Aakeröy, J. Desper and B.M.T. Scott, *Chem Commun*, 1445, (2006).