MS25-01 **Value and Perspectives of Multicomponent Crystals in Pharmaceutical Development.** Ulrich J. Griesser,[a] [a]*Institute of Pharmacy, University of Innsbruck, Innrain 52c, 6020 Innsbruck, Austria*
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Though muticomponent crystals have long been a strategic component in pharmaceutical development the current interest in so called "co-crystals" triggered a renaissance in research on supra-molecular aggregation in binary and multinary crystals. These research activities are accompanied by an on-going and often controversial debate on what comprises the term co-crystal and what is something else. This situation highlights the complex nature of multi-component crystals and the fact that the boundaries between established classes of solid state forms are blurred. For economically important materials such as pharmaceutical compounds this problem is critical and affects the work of regulatory agencies and decisions that are concerned with the protection of intellectual properties. At the same time it pushes us to the limits of understanding supramolecular aggregation as well as of chemical bonding and stimulates innovative research in this field.

Given that new drug substances increasingly exhibit solubility problems, it is understandable that the improvement of solubility is a main motivation for producing salts or crystalline molecular complexes with non-ionic excipients. Undesired properties such as low storage stability, bad particle properties, bad crystallization behavior and hygroscopicity are other examples that justify efforts to design multicomponent crystals with better properties compared to single component phases of the drug. Moreover, the increasing size and molecular complexity of novel drug candidates means that crystalline adducts with water and organic solvents (hydrates / solvates) more often occur. This issue usually adds complications in drug development, requires a broader analytical spectrum and offers specific challenges for crystallography, which often provides the key informations for a profound understanding of complex multicomponent systems. The occurrence of non-stoichiometric combinations of the solid-solution type, mixed solvates, isostructural phases, disorder phenomena, chirality and polymorphism add further challenges and levels of complexity that need to be resolved with a combination of suitable strategies and experimental techniques.

In general, drug development is faced with a strongly increasing number of multicomponent crystals in future – a perspective that should encourange science, regulatories and industry to elaborate clearer definitions and concepts for such adducts. Here an overview and a discussion of the critical and beneficial aspects of multi-component crystals will be presented using illustrative examples.

Keywords: multi-component crystals; crystalline pharmaceuticals; industrial and physical pharmacy

MS25-02 **Hybrid salt-cocrystals and exotic stoichiometries in host-guest compounds: troubles in nomenclature!** Gerard Coquerel, S. Petit, *SMS EA 3233 Université de Rouen, F-76821 Mont Saint Aignan Cedex France*
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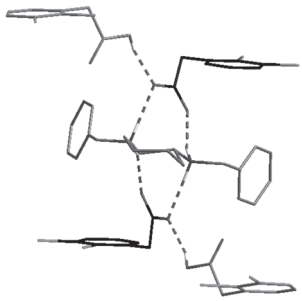
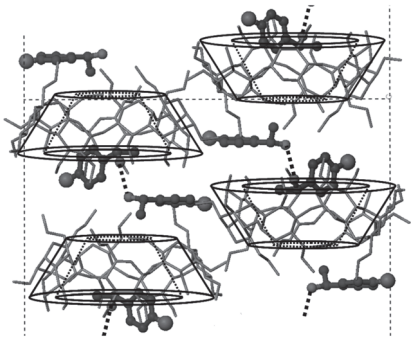
In almost every domain of knowledge, 'Classification' has always been a spontaneous and primary activity of experts in the field. Unfortunately, whatever the criteria chosen, exceptions and/or limitations appear soon or later!..... The concept of co-crystal does not escape this fact. A long controversy arose quickly after this new term has been proposed [1].

The lecture will focus on hybrid cases of salt - cocrystal and host guest inclusions.

Trans-N,N'-dibenzyldiaminocyclohexane (B) is a chiral dibase$(BH_2)^{2+}$ crystallizingas a stable conglomerate with two deprotonated acids A^- and two protonated 2,3-dichlorophenylacetic acid AH (see figure below).



Enantiomers of (±) Para-Fluoro-phenylethanol[3] are discriminated via the crystallization of an odd metastable phase with permethylated beta cyclodextrine in a (2-1) ratio.



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Keywords: Co-crystals, Host Guest-Inclusions, Hybrids, Chiral Discrimination