

MS15 O1

Constructing, deconstructing, and reconstructing molecular cocrystals Christer B. Aakeröy *Department of Chemistry, Kansas State University, Manhattan, KS, 66506, U.S.A.* E-mail: aakeroy@ksu.edu

Keywords: hydrogen bonds; co-crystals; molecular recognition

The design, properties and even definitions of cocrystals continue to receive considerable attention. Our understanding of the way in which molecules communicate and assemble is still incomplete, which means that supramolecular synthesis of discrete or extended molecular assemblies held together by non-covalent forces, remains a major fundamental scientific challenge. In this presentation, we outline a hypothesis-driven three-step protocol for the construction of ternary cocrystals and supermolecules where stoichiometry and primary intermolecular interactions can be readily rationalized [1-5].

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New Avenues in Co-crystal Studies: Boronic Acids in Supramolecular Chemistry V. R. Pedireddi, *Division of Organic Chemistry, Solid State & Supramolecular Structural Chemistry Unit, National Chemical Laboratory, Pune 411 008, India.* E-mail: vr.pedireddi@ncl.res.in

Keywords: boronic acids, co-crystals, supramolecular Synthesis

Supramolecular synthesis employing noncovalent bonds such as hydrogen bonds is the major focus of contemporary research in the solid state studies, for the creation of assemblies of exotic architectures with tailor-made properties. For this purpose, co-crystallization of molecular entities possessing various acceptor-donor functional groups like -COOH, -CONH₂, etc. were thoroughly explored because of their ability to yield robust hydrogen bonds. However, boronic acids, with a general formula of R-B(OH)₂, which have been found to be highly versatile organic moieties in various conventional synthetic and application arenas have not been explored in the supramolecular synthesis despite their ability to form hydrogen bonds, until recently. In this connection, our first report employing boronic acids for the creation of ladder type of architectures followed by the elegant examples evolved from others lead to the systematic exploration of this novel functional group for the creation of exotic assemblies by co-crystallizing with numerous organic components as well as metal ions. Salient features of design and synthetic strategies would be discussed in detail in the presentation.

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MS15 O3

Absorption and adsorption of ETBE and mesitylene in and on ice Martin U. Schmidt^a, Sonja M. Hammer^a and Elke Fries^b ^a*Institute of Inorganic and Analytical Chemistry, University of Frankfurt, Max-von-Laue-Str. 7, D-60438 Frankfurt am Main, Germany.* ^b*Institute of Environmental Systems Research, University of Osnabrueck, Barbarastraße 12, D-49069 Osnabrueck, Germany*
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The absorption and adsorption of ETBE (ethyl-*tert*-butylether) and mesitylene (1,3,5-trimethylbenzene) in and on ice I_h were simulated by force field calculations and measured in laboratory experiments.

Clouds in the upper troposphere consist mainly of ice. Ice I_h is the only stable ice polymorph at atmospheric conditions^[1]. When ice crystals begin to form in the troposphere, volatile organic compounds (VOCs) can adsorb at the surface or be incorporated into the ice crystals. Thereby VOCs may be removed from the atmosphere and pollute snow and water on the earth's surface.

Two representative VOCs are ETBE and mesitylene. ETBE is produced industrially in large amounts since a few years. It is used as antiknock compound in fuel. Because of production, storage and use, it is contaminating the atmosphere^[2]. Mesitylene is produced industrially as well. It has been found in snow samples^[3]. Recent laboratory investigations show that mesitylene is taken up by growing ice crystals^[4]. The same is assumed for ETBE. From the experiments it is not yet clear, if the organic compounds only adsorb on the ice surfaces, or if they are included in the ice bulk.

For the simulation of the adsorption and absorption of ETBE and mesitylene on and in ice crystals, three cases were investigated: the adsorption on the (0001) surface of ice I_h, the absorption into bulk ice (by substituting one or more water molecules, as a point defect), and the absorption on a small-angle grain boundary (as an example for a lattice defect).

For the force field calculations a modified Dreiding force field^[5] was used. All calculations were made with periodic boundary conditions with up to 768 water molecules and a single organic molecule.

At the surface, as well as in the bulk ice or at a small-angle grain boundary, the ETBE molecules form hydrogen bonds with water molecules. When ETBE enters the bulk ice it replaces one water molecule and distorts the surrounding ice lattice. When ETBE adsorbs at a small-angle grain boundary it replaces two water molecules. The adsorption at the surface is energetically more favourable than an absorption in the bulk ice. Absorption at a grain boundary is in between.

For the adsorption of mesitylene on ice surfaces we found the energetically best structure with the mesitylene molecule being almost parallel to the ice surface.

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