

Figure 1. Physical scales and the related modifications due to the spin crossover in a molecular crystal (adapted from ref [6])

Keywords: X-ray diffraction, structure-properties relationship, spin-crossover, iron, molecular materials

MS30 Hydrogen bonding from theory to applications

Chairs: László Fábián, Nikolett Bathori

MS30-O1 Molecular Cups and Capsules Through Hydrogen Bonding

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An exciting research challenge in crystal engineering and supramolecular chemistry is to design, synthesize, and characterize nano-sized architectures with applications in biology, chemistry, and materials science.¹ Predicting and designing non-covalently bound supramolecular complexes and assemblies is difficult because of the weakness of the interactions involved, thus the resulting superstructure is often a compromise between the geometrical constraints of the building blocks and the competing weak intermolecular interactions.²

Our research interest has been focused on the studies of weak non-covalent intermolecular, viz. supramolecular interactions as the driving force in self-assembly and molecular recognition, especially in the solid state by single crystal X-ray diffraction. The lecture will highlight some of our recent studies on a new family of macrocyclic host molecules, derived from well-known resorcinarenes, namely tetra-N-alkylammonium resorcinare salts (Fig. 1a), NARXs.³ The NARXs exhibit a rich host-guest chemistry and self-assembling properties, exemplified by an inclusion complex 3a (Fig. 1b), a deep cavity cavitand based on hydrogen and halogen bonding 3d (Fig. 1c) and the first halogen bonded dimeric resorcinare capsule 3i (Fig. 1d).

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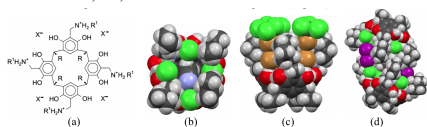


Figure 1. The chemical structure of a NARX (a), acetonitrile inclusion (b), deep cavity cavitand (c) and XB based dimeric capsule (d).

Keywords: hydrogen bonding, cavitands, resorcinaranes

MS30-O2 Organic Hydrates: Chemistry, H-Bonding & Packing

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The occurrence and understanding of hydrates (water-containing crystals) is of particular importance in the field of pharmaceutical research and industry. Hydrate formation is common for Active Pharmaceutical Ingredients (API), with one experimental polymorph screening study [1] reporting that 38% of molecules screened form hydrates and another account [2] indicating hydrates to occur for as many as 75% of drugs. This presentation will address the topic of hydration likelihood and water coordination patterns in organic hydrates, in particular with reference to pharmaceutical hydrates. We focus on the relative frequencies of hydration of specific types of molecules, re-evaluate the frequencies of occurrence and types of water coordination environment in these subsets and comment on the onward use of this information for structure evaluation and prediction.

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