

MS34-O4 From versatile hydrogen- and halogen-bond acceptors to elastic bending of metal-containing architectures

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In order to use weak interactions as effective tools in deliberate synthesis of desired metal-containing supramolecular assemblies a very detailed understanding of the importance of different noncovalent interactions is required [1,2]. Thanks to their comparable strengths and directionalities, hydrogen and halogen bonds have emerged as key synthetic tools in this context [3].

To establish similarities and possible mimicry of the two types of interactions we have carried out a structural examination of a series of metal-based halide complexes with pyridine-type ligands equipped with functionalities capable of forming of either hydrogen or halogen bonds. Our results indicate that synthon-transferability from system to system, regardless of the building-block dimensionality, is a genuine possibility. Some surprising physical properties, including elastic bending (Fig.1), will be discussed against a backdrop of weak interactions using a combination of experiment and theory.

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Figure 1. Elastic bending in crystals of $[\text{CdBr}_2(\text{L-pz})_2]_n$.

Keywords: hydrogen bond, halogen bond, elastic bending

MS34-O5 Mechanisms of Guest Exchange and Selectivity in Host-Guest Systems

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Halogenated organic host-guest compounds have been exposed to organic guest vapours in order to elucidate the mechanism of guest exchange. In the case of the inclusion compound tetrakis(4-bromophenyl)ethylene (H1) with dichloroethane (DCE), the kinetics of guest exchange with methyl iodine (MeI) vapour was monitored and the crystal structure of the intermediate product elucidated. The latter contains both guests DCE and MeI in distinct positions in an expanded unit cell. When the guests exchanged are Benzene and Piperidine, the guests occupy the same sites and the mechanism is one of isomorphous replacement.

The mechanism controlling synergistic effects of enhanced selectivity in host-guest chemistry have yielded interesting results. This is when two similar host compounds are exposed simultaneously to a target mixture of similar guests with a view to separating one particular guest. We have investigated the isomers of xylene, picolines and lutidines and explained the results in terms of the non-bonded interactions that occur in the crystal structures.

Keywords: Mechanism, Guest-exchange, Selectivity