

Poster Presentation

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Exploring the structural landscape in nia derivatives and their Cd(II) complexes

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Constant need for design of new materials with desired and pre-determined bulk properties necessitates much improved understanding of competition and balance between non-covalent interactions. In order not to rely on serendipity when targeting synthesis of new solids with pre-determined connectivity and topology, as this offers a path towards the design of materials with pre-determined bulk properties, it is imperative to map out the reliability and robustness of supramolecular synthons. In this contribution, we want to delineate the effect of the counter ion accommodation in the supramolecular assembly on the synthon formation. We opted for positively charged pyridine-based organic molecules that are encoded with two functionalities, caboxamide and carboxylic acid moieties, which both proved as robust and reliable self-complementary reagents, accompanied with one of the three halide counter ions (Cl⁻, Br⁻, I⁻). The study thus focuses on the competition and hierarchy of supramolecular synthons in organic systems of the ligands themselves as well as in the Cd(II)-containing architectures (upon the ligand coordination) depending on the polarizability of the present halide ion. Furthermore, the most prominent intermolecular contacts in the crystal structures will be visualized by Hirshfeld surface analysis and their contributions to the Hirshfeld surface area will be determined. Bader's QTAIM (Quantum Theory of Atoms in Molecules) analysis will be used to characterize the nature and strength of intermolecular interactions based on the DFT calculations started from X-ray determined geometries. The computationally determined data will be compared with the experimental results to get unbiased analysis about the role of specific intermolecular interactions on crystal packing of examined compounds.



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