MS048.O01

Hydrogen bonds and halogen bonds: solid-state, solution-phase and theory

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Hydrogen bonds, and more recently halogen bonds, have played a prominent role in crystal engineering, notably with respect to the directed assembly of molecular crystals. Both types of interactions have been subject to recent definition or redefinition by IUPAC. Establishing the preferred geometries [1] and the most common (reliable) patterns of such interactions and quantifying their strength [2] is important in making best use of these interactions in the design and construction of solid state assemblies from molecular building blocks. Examples will be presented from our work that illustrate the combination of the two types of interaction in crystal engineering. The examples will focus on determining, and on tuning, the strength of the interactions, in the pursuit of control of supramolecular assembly in molecular crystals [3]. The influence of the strength of interactions on directing the final crystal structure will be examined, including consideration of the effect of solvent on the formation of intermolecular interactions and on the assembly of crystals where hydrogen bonds or halogen bonds are prominent [3d] or even in competition [3c].

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Keywords: hydrogen bond, halogen bond