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Halogen-bonded co-crystals for ferroelectric materials: synthesis, crystal growth and structural investigations

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In crystal engineering, intermolecular interactions play a crucial role, and give the possibility to create co-crystals. One of these interactions is halogen bond. As an analogue to the hydrogen bonding, it is a non-covalent interaction between covalently bounded halogen atom and Lewis base. This interaction is essentially of electrostatic nature. Indeed, the electron cloud around halogen atom is anisotropically distributed, leading to a depletion of charge (+δ) in the prolongation of the C–Hal bond, called σ-hole, and a concentration of charge (–δ) in the equatorial zone. This polarization effect is strongest with iodine, with I > Br » Cl

> F.[1] Accordingly, strong and linear interactions are found between iodinated molecules and Lewis bases acting as halogen bond acceptors. In order to vary the strength of halogen bonding, different iodinated molecules can be evaluated, as well as different Lewis base acceptors.[1-3]

During the master thesis, series of co-crystals of two halogen bond donors, namely, N-iodosuccinimide and N-iodosaccharin[4,5] investigated by single-crystal X-ray diffraction. An intermolecular N–I•••N' interaction was identified in different co-crystals involving primary aliphatic, and aromatic amines. In all samples, the N–I•••N' interaction is linear and notably shorter than the sum of van der Waals radii. Depending on the donor and acceptor molecules, the N–I and I•••N' distances vary up to a point where they are almost equal. Co-crystals with N-iodosaccharin exhibit indeed strong halogen bonding, with the possibility for a neutral to ionic transition at low temperatures.

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