MS32-P03 | INFLUENCE OF THE BASICITY OF HALOGEN BOND ACCEPTORS ON STOICHIOMETRY OF COCRYSTALS WITH 1,3,5-TRIIODO-2,4,6-TRIFLUOROBENZENE

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Perfluorinated halogenobenzenes are group of halogen bond donors that include a wide range of compounds with different number of donor atoms, what ultimately allows to synthesize halogen bonded cocrystals with various stoichiometries and crystal packing motifs [1]. In many crystal structures can be observed that molecules that are potential donors of more halogen bonds, participate in bonding with a smaller number of donor atoms [2]. Related to our previous research [3], in this study we have prepared cocrystals of 1,3,5-triiodo-2,4,6-trifluorobenzene (**titfb**) with a series of organic nitrogen bases with different basicities to investigate the influence of the basicity, sterics and topicity of halogen bond acceptors to form cocrystals with 3:1 stoichiometry. Out of the 12 used compounds, 3 the most basic acceptors form cocrystals of 3:1 stoichiometry, 2 moderate bases gave cocrystals with 2:1 stoichiometry, while the 7 cocrystals with weak bases have one acceptor bonded to **titfb** molecule. These preliminary results indicate that along with the efficiency of crystal packing, also basicity of the halogen bond acceptor is an important factor in the supramolecular synthesis of compounds with high acceptor:donor ratio [4].

[1] Metrangolo *et. al.*, *Chem. Rev.* **116** (2016) 2478 – 2601.
[2] M. E. van der Boom *et. al.*, *Cryst. Growth Des.* **7** (2007) 386 – 392.
[3] Bedeković et. al., *New J. Chem.* **42** (2018) 10584 – 10591.
[4] W. Bruce *et. al.*, *Cryst. Growth Des.***10** (2010) 3710 – 3720.