MS29-2-4 The role of halogen bonding in sulfonamide co-crystals: π···X preferred over O···X?
#MS29-2-4

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Abstract
Sulfonamides are one of the most important pharmaceutical compound classes.[1] It started in 1935 with Prontosil one of the first synthetic antibacterial drugs which was later honoured with the Nobel Prize.[2] Today there are over 70 active pharmaceutical ingrediencies (APIs) with various applications in use. Herein we present the first systematic study on the role of halogen bonding in sulfonamides multicomponent systems. Co-crystals of four sulfonamides in the range from simple ones to more complex APIs were designed and structurally characterized. Model halogen bond co-formers 1,4-diiodotetrafluorobenzene and/or 1,2-diiodotetrafluorobenzene were used to implement halogen bonds into the systems with N-phenyl-methane sulfonamide, N-methylbenzene sulfonamide, N-phenyl-benzene sulfonamide and Chlorpropamide.[3] In our study we consider general binding patterns, geometrical considerations of the overall crystal packing, perform calculations of lattice energies and energies of intermolecular interaction based on plain wave functions.[4] We finally resolve the question why halogen bonding seems to prefer interactions with π-systems over electron rich N- or O-moieties within these systems.

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