

Poster Presentation

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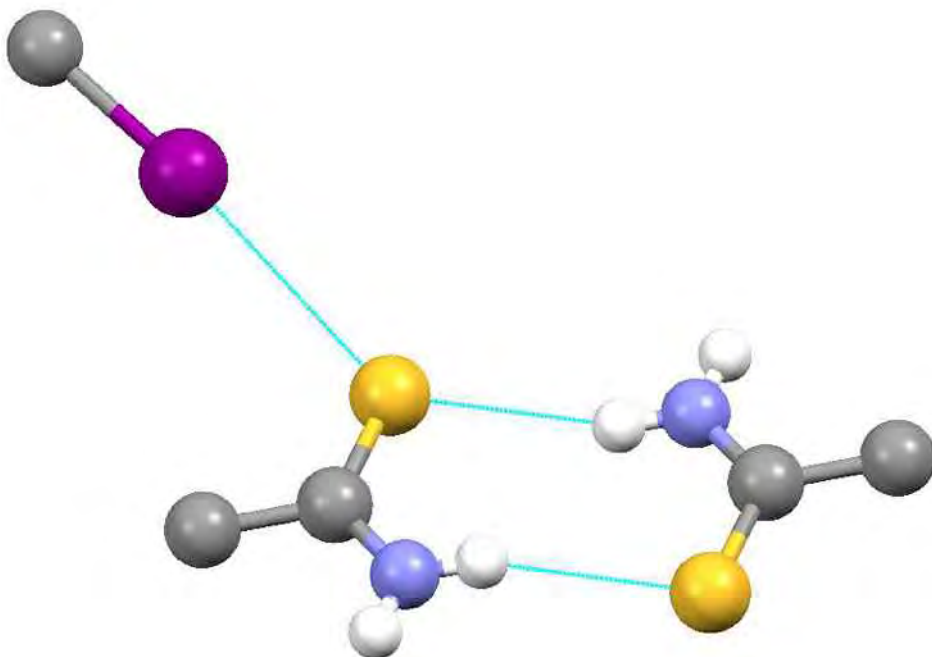
Halogen Bonding with Sulfur Functional Groups

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Crystal engineering has been defined as “the understanding of intermolecular interactions in the context of crystal packing and the utilisation of such understanding in the design of new solids with desired physical and chemical properties”. [1] Halogen bonding is a significant type of intermolecular interaction involving a halogen atom with neutral or anionic components which has recently been exploited for the formation of multicomponent crystalline materials. Sulfur can exist in a variety of different oxidation states, giving rise to a wide variety of different functional groups that are potentially available for halogen bonding. We have recently reported our investigations with sulfoxide, [2] sulfone [2] and sulfinamide functional groups. [3] Herein we extend this work to include the thioamide functional group and compare it with its more extensively studied amide analogue. Investigation into the propensity for primary aromatic thioamides to form halogen interactions through the thiocarbonyl (C=S) functional group. A range of substituent aromatic primary thioamides containing different electronic substituents on the aromatic ring were synthesized and investigated for cocrystallisation. These cocrystals are held together by a combination of weak hydrogen bonding (N–H⋯S=C) and strong halogen interactions (C–X⋯S=C).

[1] Desiraju G. R., *Crystal Engineering – The design of organic solids*, Elsevier, Amsterdam, 1989., [2] Eccles, K. S.; Morrison, R. E.; Stokes, S. P.; et al., *Cryst. Growth Des.*, 2012, 12, 2969–2977., [3] Eccles, K. S.; Morrison, R. E.; Daly, C. A.; et al., *CrystEngComm*, 2013, 15, 7571–7575 .



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