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Halogen, chalcogen and pnictogen bonding: other bricks in the wall

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The understanding of the relative importance and effect of intermolecular interactions in the solid state is highly valuable in a range of applied research areas, not least in the pharmaceutical industry where control of polymorph stability is crucial. Within pharmaceutical crystal structures, hydrogen bonding tends to dominate - for these interactions there are already a range of established methodologies [1,2] to help understand the most probable outcomes and assess the stability or risk of polymorphism. How important in this context are other intermolecular interactions though? What is likely to be the effect of halogen bonds, chalcogen bonds or pnictogen bonds? This presentation will review the statistics on some typical halogen, chalcogen and pnictogen bonds in the CSD in the context of other intermolecular interactions in organic crystals. We focus on the impact of these interactions for an organic crystal designer or engineer. There are nearly a million structures in the CSD – what do they tell us about the significance of these interactions and do we have enough data?

References:

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