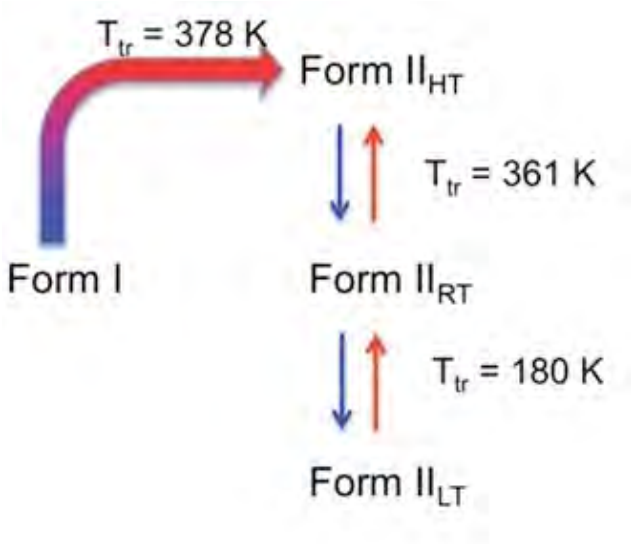

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Keywords: 2-propyl-1H-benzimidazole, polymorphism

MS31-P08

Understanding supramolecular interactions with hydrogen bond propensities

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The variety of supramolecular interactions in the solid state can lead to substantial risk or untold opportunity. Lack of control of such interactions can lead to crystal form polymorphism and can have a critical impact on formulated product robustness, with pharmaceuticals having been withdrawn from the market upon the unexpected appearance of a more stable polymorph. However, a detailed understanding of those same interactions can provide an opportunity to generate materials with desired properties through crystal engineering.

The Cambridge Structural Database contains over 940,000 crystal structures, and data points from many millions of individual supramolecular interactions. We can use this data from every crystal structure ever published to understand the solid form landscape of a novel material. What are the risks of polymorphism, and can we engineer specific packing motifs?

The Hydrogen Bond Propensity method makes use of statistics derived from hydrogen bonds observed in similar crystal structures, along with an understanding of the chemistry of a molecule, to make predictions on the likelihood of forming specific interactions in the solid state.[1] When combined with a knowledge of the coordination environment of the functional groups of that molecule, we can generate a landscape of likely hydrogen bonding networks.[2] By understanding the supramolecular interactions that occur in a crystal structure, we are able to understand the risk of polymorphism resulting from variations in these interactions.

In this presentation, we will describe the Hydrogen Bond Propensity method and its application to understanding polymorphism in the organic solid state. We will highlight improvements that we are making to the method and discuss how it can be applied to the design of novel multi-component systems.[3]

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Keywords: hydrogen bonding, polymorphism, co-crystals