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Disorder in Polymorphic Systems

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Polymorphism is a matter of key importance in the pharmaceutical industry since the properties of polymorphs may vary, including the rate of uptake by the human body of pharmaceutical molecules. In this study we are using diffuse scattering methods to elucidate the disorder in polymorphic systems, with a particular focus on disorder arising from the internal flexibility of molecules. The determination of crystal structures beyond the average structures available from Bragg data provides additional information which may contribute to solving the problem of polymorph prediction and control.

The molecule p-methylbenzylidene-p-methylaniline (MeMe) has three polymorphs, all of which exhibit strong diffuse scattering indicating substantial disorder. Two of the polymorphs (MeMe1 and MeMe3) have orientational disorder in which the orientations are related by end-to-end and/or side-to-side flips of the molecule. Most remarkable is the MeMe2 form which is nominally perfectly ordered and yet its diffraction pattern shows highly structured diffuse scattering indicating the presence of highly correlated displacive disorder. We have produced model crystals of the three polymorphs which reproduce the major features in their diffraction patterns. Exploration of such models provides information on intermolecular interactions.