Poster Presentation

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Diffuse scattering in the polymorphs of p(N-methylbenzylidene)-p-methylaniline

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Polymorphism refers to the ability of a solid to exist in more than one crystal structure. Apart from being of scientific interest, it is of practical importance in the pharmaceutical and chemical manufacturing industries. In pharmaceuticals the polymorphic form of the substance can affect the ease of manufacture or the rate of uptake by the human body [1]. There is consequently a great need to be able to understand, predict and control polymorphism. This work is part of a larger study using diffuse scattering methods to investigate the role of molecular flexibility and disorder in polymorphism. Diffuse scattering is sensitive to two-body correlations so can provide information about the intermolecular interactions that cannot be obtained from the Bragg peaks, such as how the displacement or orientation of a molecule is correlated with that of its neighbours. p-(N-methylbenzylidene)-p-methylaniline (MeMe) is a model system for studying polymorphic behaviour. The system is trimorphic with all three polymorphs exhibiting highly structured diffuse scattering patterns [2]. The short-range order has been modelled using the program ZMC in which the molecules are allowed to interact via Hooke's law springs and brought to thermal equilibrium using a Monte Carlo algorithm [3]. Here we present a comparison of the diffuse scattering in the different forms of MeMe and assess how successfully different models for the intermolecular interactions reproduce the observed diffuse scattering data.

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