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## Crystal structure prediction of organic pigments

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The present work investigates the feasibility of predicting crystal structures of industrially important pigments when only low quality XRPD patterns are available.
Despite the commercial significance of organic pigments only few crystal structures of these materials have been reported. Pigments are practically insoluble in most solvents and, therefore, it is difficult to grow a single crystal of good enough quality for the structure determination. In industry, pigments are produced by precipitation reactions leading to very fine powders. The crystallites are often so small that they cause a considerable line broadening in X-ray powder diffraction. Therefore, a powder pattern of limited quality is usually the only information available.
The structures of organic pigments PV19, PV23 and PR202 were successfully predicted using the Polymorph Predictor of Cerius$^2$ in combination with XRPD patterns of limited quality. After generation and energy minimization of the possible structures, their powder patterns were compared to the experimental ones. On this basis, structures of pigments were chosen from the list of all the structures. Rietveld refinement was used to validate the right choice of the structures.

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## The Influence of Disorder on Polymorphism

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Polymorphism is a matter of key importance in the pharmaceutical industry [1,2] since the properties of polymorphs may vary, including the rate of uptake by the human body of pharmaceutical molecules [3]. 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. Recent attempts to predict such polymorphic structures *ab initio* have been quite unsuccessful [4]. The determination of crystal structures beyond the average structures which are available from Bragg data may provide 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 that is nominally perfectly ordered, and yet its diffraction pattern shows highly structured scattering indicating the presence of highly correlated displacive disorder. We have produced model crystals of the three polymorphs that reproduce the major features in their diffraction patterns. Exploration of such models provides detailed information on intra- and intermolecular interactions and shows how the motion of a given fragment of a molecule is correlated to motions of different fragments of the same molecule or of neighbouring molecules.

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