MS44-P4 Cross-correlation functions used for structure determination from powder patterns – Method development and application scenarios

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A new method for the determination of organic crystal structures from powder diffraction data has been developed and implemented in the program FIDEL (FIt with DEviating Lattice parameters) [1]. The approach taken relies on a robust fitting algorithm, which uses the normalized integral of a weighted cross-correlation function for the comparison of powder patterns. This generalized similarity measure, originally introduced by de Gelder *et. al* [2] has been successfully deployed for fitting, clustering and comparison of crystal structures. The lattice parameters, molecular position, molecular orientation and selected intramolecular degrees of freedom of a start structure are fitted to the powder pattern in a robust and scalable procedure that is suited both for visibly strongly deviating structure models and experimental patterns of very low quality. This allows for a wide range of highly automated applications:

1) Testing the similarity of powder patterns and crystal structures with different space group settings

2) Preprocessor for Rietveld refinements starting with significantly deviating structural models, e.g. from (a) structure data of an isostructural chemical derivative; (b) structure data of an isostructural hydrate or solvate; (c) structure data from measurements at another temperature. FIDEL includes capabilities for an automatic Rietveld refinement sequence using the program TOPAS [3].

3) Automated clustering and screening of large numbers of possible structure candidates. This has been demonstrated using the results from crystal structure predictions based on lattice-energy minimizations by force-field methods.

4) Structure determination from unindexed powder patterns from scratch using an iterative fitting procedure in various space groups based on a Monte Carlo approach. The method can even be applied to powder patterns of disordered structures or non-phase-pure samples providing best matching structural candidates for further analysis.

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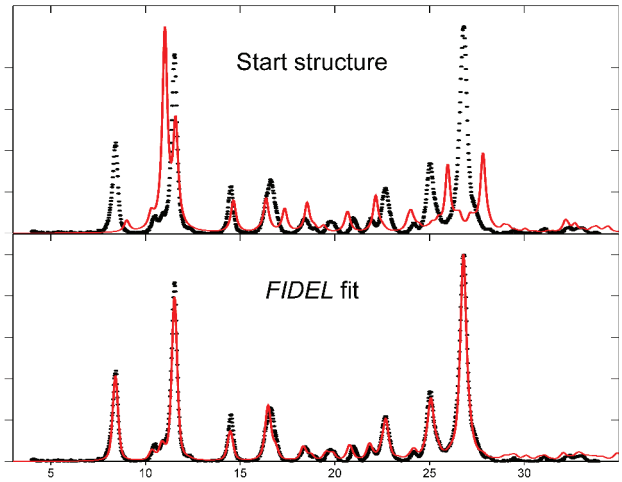

Figure 1. Background corrected X-ray powder diagram of Pigment Yellow 14 (dots) and simulated diagrams (red lines) of a strongly deviating structural model (a) before optimization with FIDEL, (b) after optimization with FIDEL

Keywords: cross-correlation functions, similarity measure, crystal structure fitting, SDPD, powder diffraction, organic compounds