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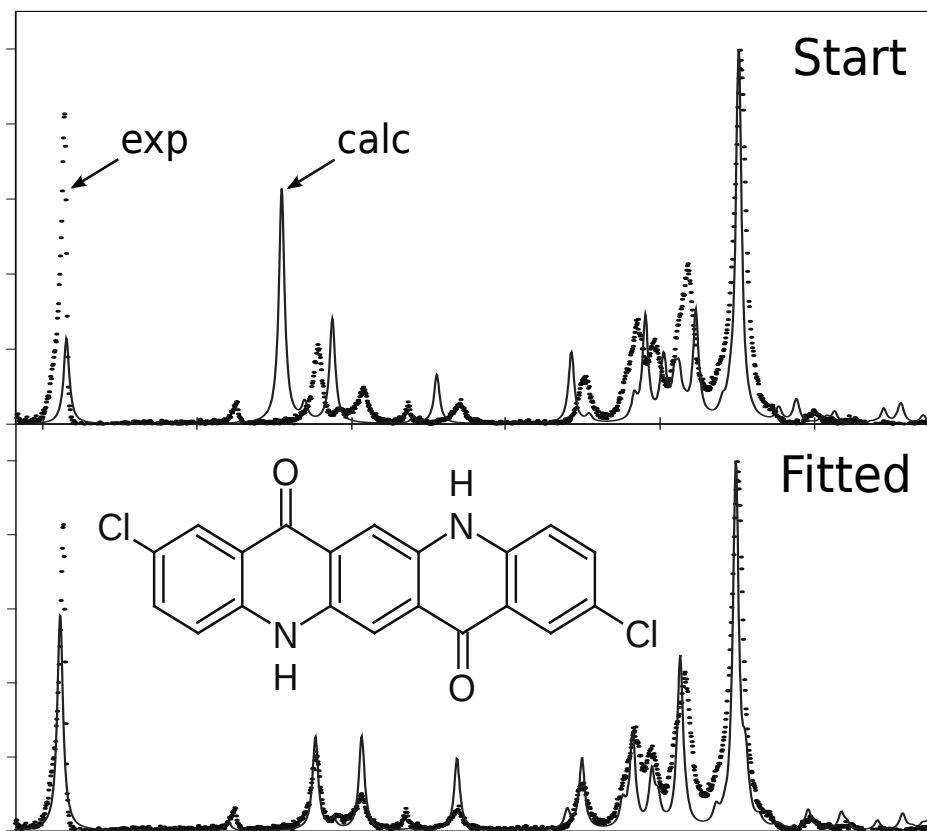
*FIDEL: A new method for SDPD of nanocrystalline organic compounds*

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Rietveld refinements generally fail, if the lattice parameters of the structural model differ more than slightly from the correct lattice parameters and the simulated reflections do not overlap with the experimental ones. For molecular crystals, we have developed a more robust fitting algorithm, which uses the cross-correlation function of calculated and experimental powder patterns, and allows a Fit with DEviating Lattice parameters (FIDEL). The method is also successful for nanocrystalline organic compounds showing only 10-20 peaks in their powder diagrams. The FIDEL method has proven to be useful for various applications, including refinements starting from (1) structure data of an isostructural chemical derivative; (2) structure data of an isostructural hydrate or solvate; (3) structure data from measurements at another temperature (e.g. for fitting a room-temperature powder diagram starting with a structure determined from a single-crystal measurement at 100K). FIDEL is also used for determining crystal structures from non-indexed powder diagrams of nanocrystalline organic compounds. Three steps are performed: (1) Prediction of possible crystal structures in various space groups using global lattice-energy minimizations by force-field methods. (2) FIDEL fit of 100 to 600 low-energy structures to the experimental powder pattern. The structure candidate leading to the correct structure results in a significantly better fit than all other structures. (3) Rietveld refinement. The FIDEL method was used to determine the hitherto unknown crystal structure of the nanocrystalline alpha-phase of 2,9-dichloroquinacridone (C<sub>20</sub>H<sub>10</sub>Cl<sub>2</sub>N<sub>2</sub>O<sub>2</sub>). The upper part of the figure shows the experimental powder pattern and the simulated powder diagram of one of the predicted low-energy structures before any fitting. The lower part displays the result of the FIDEL fit, before the Rietveld refinement.

[1] Habermehl, S., Mörschel, P., Eisenbrandt, et al, M.U. (2014). *Acta Cryst. B70*, doi:10.1107/S2052520613033994



**Keywords:** crystal structure prediction, fit with deviating lattice parameters, structure determination from powder data