Molecular signatures in the 3D-Δ-PDF

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The 3D-Δ-PDF [1] is obtained as the inverse Fourier transform of the single crystal diffuse scattering. As such its signal describes the deviation of the full Patterson function of the actual crystal structure from the Patterson function of the average structure. The latter, the classical Patterson function, is obtained by the inverse Fourier transform of the integrated Bragg intensities only. As detailed in the original work by Weber and Simonov, the maxima in the 3D-Δ-PDF have characteristic shapes and sign, which depend on the local defect type. Simple positive or negative maxima indicate substitutional atomic disorder, while maxima that are accompanied by small subsidiary maxima of opposite sign typically correspond to displacement order.

For highly disordered molecular compounds additional features are observed like very broad regions of negative density in the 3D-Δ-PDF. A further feature characteristic signature of molecular signals in the 3D-Δ-PDF is possibility that some of the intramolecular Patterson vectors may be absent in the 3D-Δ-PDF, even though the molecule itself is disordered. The presentation will provide a systematic case study of molecular signatures in the 3D-Δ-PDF and recent advances in the initial data processing.

[1] Weber T, Simonov A. The three-dimensional pair distribution function analysis of disordered single crystals: basic concepts. Z Kristallogr. 227, 238 (2012)