Advances in the Parameter Space Concept for Crystal Structure Determination – Linearization of intensity isosurfaces

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As an alternative approach to currently and widely used Fourier transform techniques, a theoretical approach was developed by Fischer, Kirfel and Zimmermann, namely the Parameter Space Concept (PSC), to solve crystal structures by using a minimal number of diffraction intensities\cite{1-6}. We present recent improvements, which target the implementation of linearized intensity isosurfaces and test the routines on numerous randomly generated structures. In the initial stage progress, pairs of sample atomic coordinates are mapped on two- and three-dimensional parameter spaces (P\textsuperscript{2} and P\textsuperscript{3}). The respective intensity isosurfaces, defined by sign and geometrical structure amplitude, where linearized for given reflection orders \textit{l} and converted into systems of linear inequalities and solved to reobtain the atomic coordinates and evaluate the accuracy of the method. Within this framework we utilized Equal Point Atom (EPA) and Non-Equal Point Atom (nEPA) models to treat the scattering power of atoms. Results are given for arbitrary centrosymmetric structures with two (see Fig. 1) as well as three degrees of freedom, and specific challenges are highlighted.


\textbf{Figure 1.} PSC solutions and respective errors as well as spatial uncertainties of randomly generated atomic coordinates for synthetic sample structures. The background color represents the average reduction of spatial uncertainty in the atomic coordinates with increasing order \textit{l}. The red circles present the randomly generated atomic coordinate pairs.

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