Invited Lecture

Advancing refinements on 3D electron diffraction data with multipolar scattering factors

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In recent years, we have seen remarkable progress in the field of 3D Electron Diffraction (3D ED). These improvements encompass various aspects, including instrumentation, data collection strategies, mitigation of radiation damage, data processing, handling of dynamical scattering, and refinement. During the refinement stage, it seems to be essential to use appropriate atomic scattering factors. These are usually calculated based on the Independent Atom Model (IAM), which presumes atoms are spherical and do not interact with each other. However, in reality, the electron densities and electrostatic potentials of atoms within molecules or crystals are not perfectly spherical, and the point charges associated with them deviate from the formal charge.

Advanced electron density models have been utilized in X-ray crystallography for many years [1, 2]. When high-quality and high-resolution X-ray data is available, these models allow for the extraction of detailed information about electron density directly from the experimental data [3]. Even with more routine X-ray data of standard resolution, it is still possible to benefit from using more sophisticated models. This can be achieved by using scattering factors based on advanced models, which are either obtained from theoretical calculations [4] or transferred from appropriate databanks [5].

More complex models of electrostatic potential have also been incorporated into electron crystallography. During the lecture, I will provide a summary of what we have recently learned from applying the Transferable Aspherical Atom Model (TAAM) [6, 7, 8], based on the MATTS databank, and other multipole models to the currently available 3D ED data for organic crystals. I will attempt to answer the question of what benefits we gain by using these models in the case of data of varying quality, different resolution, and the use of kinematical or dynamical refinement.

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