Aspherical Scattering Factors from Multipole Model for X-Ray and Electron Crystallography

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To interpret experimental diffraction data, it is necessary to use appropriate atomic scattering factors. Commonly, they are computed from the independent atom model (IAM) based on assumption that atoms are spherical and do not interact with each other. In reality, electron densities and electrostatic potentials of atoms in molecules or crystals are not spherical, and the associated with them point charges rarely resemble the formal one. Nowadays, with better equipment, the shortcomings of IAM are clearly visible in routine X- ray crystallography, pointing to the need for more accurate scattering factors. The same is happening with electron crystallography.

The Transferable Aspherical Atom Model (TAAM), built of atoms in the multipolar formalism and parameterized with a data bank of pseudoatoms (e.g. UBDB or MATTS), is one of the alternative models for IAM. Systematic studies on refinements of organic crystal structures with X-ray or 3D electron diffraction (3D ED) data show that TAAM is able to fit to the data much better than IAM and the obtained atomic models of crystal structures are of increased accuracy and precision. The most spectacular is improved localization of hydrogen atoms in the case of X-ray diffraction, approaching the accuracy of neutron diffraction. In addition, the time and effort needed to do TAAM refinement is almost the same as for IAM, including crystals with disorder or twinning. Thus we advocate that routine crystal structure refinement should never be stopped at IAM.

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