MS21-P102 - LATE | NON-SPHERICAL FORM FACTORS AND CRYSTALLOGRAPHIC REFINEMENT

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Standard crystallographic refinement relies on tabulated form factors [1] – carefully calculated and confirmed functions derived from single-atom electron densities. These spherical form factors have been used for decades, but are necessarily an approximation to the true form factors. My recent work has focused on the viability of using alternative form factors of improved accuracy, such as from quantum mechanical calculations.

In its simplest iteration, the form factor is the Fourier transform of the electron density associated with a particular atom. In the standard tables, this electron density is taken as a spherically symmetric function around an atom, leading to a spherically symmetric form factor dependent only on the magnitude of the vector ha*+kb*+lc*. However, in reality, bonding and other factors lead to an electron density which is influenced by its neighbours – that is, the atoms of the whole molecule affect the electron density, and thus, in turn, the form factor.

In this contribution, I cover the theoretical backing behind the use of such form factors, consider the information required, and discuss the adjustments and considerations made to the crystallographic refinement process needed to properly employ this information. Additionally, I will mention further investigations needed into the limits of viability of these form factors, the limits of inaccuracy of the model under which they become less accurate than standard spherical approximations.

[1] International tables for crystallography. Vol. C. Mathematical, physical and chemical tables, Bryan, RF