MS19 Experimental and theoretical advances in quantum crystallography

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Tackling anomalous X-ray scattering via Waller's dispersion formula

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Abstract

In standard X-ray refinements, the effects due to anomalous dispersion are routinely mitigated using tabulated dispersion values (the real (dispersive) and imaginary (absorptive) parameters f' and f'') for each element. These tabulated values can be unreliable for X-rays with wavelengths near absorption edges and do not take any bonding into account.

One approach is to include these dispersion parameters as refinement parameters within the refinement process. This has recently been verified in [1] by comparison with an experimentally measured absorption spectrum for the determination of f'' and using the Kramers-Kronig relationship for the derivation of f'.

Another approach is to calculate the dispersion parameters f' and f'' quantum mechanically, for example, by employing Waller's dispersion formula [2]. Waller's dispersion formula takes excitation phenomena of electrons via the incoming X-rays into account, extending classical Thomson scattering. This method of deriving the contributions to the dispersion parameters from the electrons in the K- and L-shell of atoms (viewing them as hydrogen-like) has been discussed in the classical papers by Hoenl [3] and Eisenlohr-Mueller[4]. Mathematically this is done via the inclusion of energy-dependent matrix coefficients into the scattering moment.

The aim of this work is to extend the theorical aspects of the approach in [3,4] to the M-shell and to prepare the ground for a successful implementation in *Olex2*. By this approach, we will calculate specific dispersion parameters for each atom in any given structure. This is in some sense akin to modern refinement procedures in which specific form factors are calculated quantum mechanically, for example in Hirshfeld atom refinement (HAR) as implemented in *Olex2* via NoSpherA2 [5,6].

References

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