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This Week's Citation Classic

Doyle P A & Turner P S. Relativistic Hartree-Fock X-ray and electron scattering factors. *Acta Crystallogr.* **A24**:390-7, 1968. [School of Physics, University of Melbourne, Australia]

This paper **presented tables of kinematic X-ray and electron scattering factors for 76** common **atoms and ions, calculated from relativistic Hartree-Fock atomic fields. Parametric fits to these tables were given. A simple method was proposed to treat forward electron scattering by ionized atoms. [The *SCI*® indicates that this paper has been cited over 885 times since 1968.]**

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The Bragg scattering of X-rays by the periodic electron charge density is usually well described by the so-called structure factor for the unit cell. This structure factor is found using atomic positions in the unit cell plus the Fourier transform of the charge on individual atoms, these transforms are the X-ray scattering factors. The scattering of fast electrons, such as in an electron microscope, by the crystalline potential requires consideration of dynamical interactions Nevertheless, the basic crystal data needed for dynamical calculations are the Fourier coefficients of the crystal potential, which can be written in terms of the electron scattering factors and atomic positions. Therefore, most work in X-ray or electron diffraction by crystals requires atomic scattering factors.

"During the late 1960s, Peter Turner and I were students of John Cowley in the school of physics of Melbourne University Our interest in scattering factors stemmed from our calculations of dynamical electron scattering by the periodic crystal potential, and by the departures from periodicity. Hence when Mike Coulthard,[1] then a student in the atomic physics group at Melbourne, succeeded in writing a computer program to calculate relativistic Hartree-Fock atomic wavefunctions and potentials, I calculated scattering factors from his early results Significant differences occurred by comparison with the then available scattering factors based on less sophisticated atomic models, so Peter and I used the wavefunction program for many more atoms and ions, and calculated scattering factors.

"In those days, the comparatively venerable IBM 7044 took over three hours for one heavy atom, so being unable to take over the University's computer all day as well as all night, we were forced to omit many atoms and ions. The principal sufferers were rare earths and heavy transition metals Our results, together with those of others to make a complete table for all atoms and ions, are now incorporated in the *International Tables for X-ray Crystallography,*[2] many references to our work would now be to these tables rather than to the original 1968 article. The paper also contained data for a parametric fit to the scattering factors, in a form useful for computation, which had become quite conventional, Peter handled this side of the work. In addition, I proposed a simple way to avoid annoying infinities for forward electron scattering by ions.

"This paper owes its wide citation to the underlying relevance of scattering factors to most work on X-ray or electron diffraction by crystals, and perhaps to our care in double- and triple-checking every number, rather than to any fundamentally new concepts introduced. From the vantage point of my present main interest in ultrasonic scattering by defects in materials, I now look back with some nostalgia to this unity in the description of crystal diffraction. The gratitude of Peter and myself is due to Coulthard, who originally wrote his atomic wavefunction program for its relevance to a wide variety of topics, of which X-ray and electron diffraction are but two "

1 **Coulthard M A.** A relativistic Hartree-Fock atomic field calculation. *Proc. Phys. Soc.* **91**:44-9, 1967.
2. **Ibers J A & Hamilton W C,** eds. *International tables for X-ray crystallography volume IV, revised and supplementary tables to volumes II and III.* Birmingham, England: Kynoch Press, 1974.