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This Week's Citation Classic®

Berghuis J, Haanappel IJ M, Potters M, Loopstra B O, MacGillavry C H & Veenendaal A L. New calculations of atomic scattering factors. *Acta Crystallogr.* 8:478-83, 1955.
[Mathematical Centre, Amsterdam, and Laboratory for General and Inorganic Chemistry, University of Amsterdam, The Netherlands]

Atomic scattering factors describe the self-interference of electrons in an atom when scattering radiation such as X-rays. Scattering factors are essential for calculating the intensities of the X-ray reflections from a crystal in order to compare the correctness of a structural model with observed X-ray crystallographic data. These scattering-factor calculations represented a major improvement over older data. [The *SCI*® indicates that this paper has been cited in over 1,015 publications.]

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In 1953 MacGillavry was engaged as an editor in the preparation of Volume III of the *International Tables for X-ray Crystallography*.[1] These tables were intended to be the successors to the then old—and by now antique—*Internationale Tabellen zur Bestimmung von Kristallstrukturen*, published in 1935.[2] In the old tables, scattering factors were based on Hartree wave function for a few light atoms, interpolations between these for others, and Thomas-Fermi models for all atoms from K on upwards.

Soon after publication of the old tables, a vast amount of new wave-function calculations had become available, and hence it was decided to recalculate the scattering factors with a smaller interval and a higher numerical precision than before. Working in MacGillavry's lab as a graduate student engaged in solving the crystal structure of vitamin A acid—with no success at all due to a data set that turned out to be too limited—I immediately grabbed a task that would at least yield tangible results even though the computing effort involved in calculating scattering factors for 23 atoms surpassed our powers by far. Fourier inversion of wave functions to scattering factors, however trivial nowadays, represented no mean task then. It was finally arranged that we would supply the data and that the computations would be performed at the nearby Mathematical Centre, which had at its disposal the automatic computing equipment Amsterdam (ARRA), punched-card tabulating equipment (IBM) with an electronic extension, and 24 human computers. Scattering-factor calculations were mostly done on the IBM equipment because of the large volume of the output, and because it was available.

A major problem was checking all of the operations of the machines and the operators. A scheme was devised satisfying this requirement for all operations but one: printing the final tables. The operator happened to punch a new card at this stage by reading the information from the debris of one that had jammed in the machine, and this introduced an error.

The way it was detected seems to defy Murphy's Law. I had picked the wave functions of K^+ to transform by hand on a Monroe calculator in many long evenings and an occasional free afternoon. Eager to check myself when the final results appeared, I compared the sets. The line through my own points was just a shade smoother than the corresponding line through the points of the full data set. And although with reluctance, I suggested that there might be, notwithstanding everything.... Sure enough, there was.

The calculations survived to about 1974. In that year, Volume IV of the *International Tables for X-ray Crystallography*[3] presented new calculations, again on a finer interval and with higher precision, and again based on a much more elaborate set of wave-function data. In practice, this accuracy is rarely used. Instead, a polynomial approximation with nine constants[4] or even one with only five constants[5] is used.

In a sense, it is astonishing that the paper has been cited so often. The work was intended to be embedded in the *International Tables*, and I had expected that it would be cited by reference to the *Tables*. Obviously, authors prefer to cite papers. During the two decades of their effective lifetime, the data of the cited paper filled a gap the way they were intended to.

Another cause of wonder is the development of computing over the past 30 years. I am grateful to J. Berghuis for a clear description of how our computing actually was performed, but one is stunned by the thought of ever having operated the way we did: it cannot possibly be a thing to be proud of!

From this little piece of history one might conclude that "great leaps forward" in the field of atomic scattering factors take 20 years. If we are allowed to generalize this, what a sight it will be to look at these factors in the year 2000!

1. **MacGillavry C H & Rieck G D,** eds. *International tables for X-ray crystallography. Volume III. Physical and chemical tables.* Birmingham: Kynoch Press, 1962. 354 p.
2. **Hermann C,** ed. *Internationale Tabellen zur Bestimmung von Kristallstrukturen.* Berlin: Gebrüder Borntraeger, 1935. 2 vols.
3. **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: Kynoch Press, 1974. 357 p.
4. *Ibid.* p. 99-101.
5. **Cromer D T & Mann J B.** X-ray scattering factors from numerical Hartree-Fock wave functions. *Acta Crystallogr.* A24:321-4, 1986.

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