

This Week's Citation Classic

Cruickshank D W J, Pilling D E, Bujosa A, Lovell F M & Truter M R. Crystallographic calculations on the Ferranti Pegasus and Mark I computers. (Pepinsky R, Robertson J M & Speakman J C. eds.) *Computing methods and the phase problem in X-ray crystal analysis*. New York: Pergamon Press, 1961. p. 32-78. [Sch. Chemistry, Univ. Leeds, Leeds, England]

The paper described crystallographic programs for two early computers. The crystallographic least-squares and Fourier-synthesis equations were analyzed so as to allow very efficient programs. Various useful procedures were also given. [The SC[®] indicates that this paper has been cited over 905 times since 1961.]

Durward W.J. Cruickshank
Department of Chemistry
University of Manchester
Institute of Science and Technology
Manchester M60 1QD
England

October 23, 1979

"This paper described methods developed in the Leeds University chemistry department for crystallographic calculations in the early days of electronic computers, 1952-1960. Curiously the paper has been cited most often for a simple though practically useful formula, a weighting scheme for structure factors in least-squares calculations. This is sometimes called 'Cruickshank et al.'s weighting scheme,' a credit not entirely deserved, since the paper stated clearly that the scheme was a modification of one due to Gene Carpenter of Brown University.

"Actually the paper contained much more significant material, especially a description of how to design efficient programs for crystallographic calculations of any symmetry and with anisotropic atomic vibrations. The methods of analysis of anisotropic vibrations and accurate structure determination had been developed in earlier articles in *Acta Crystallographica*, several of which were featured in Garfield's 1974 study of frequently cited *Acta Crystallographica* papers.¹ Indeed the first article² from 1949 on the accuracy of electron density maps was listed by Garfield³ in 1977 as among the highly cited physical science papers of the 1940s.

"A computer in service in the late 1950s, the Pegasus, had a fast store of 48 words (not 48K!) with a backing store of 4K on a magnetic drum. Programming was in a neat machine code. Multiplication took 2 msec. These factors compelled extremely efficient coding and algorithm design, but in consequence surprisingly large calculations were run and the geometrical structures of many molecules determined.

"The predecessor of Pegasus was the Ferranti Mark I, which ran in Manchester from 1951 and incorporated the famous Williams storage tubes. This machine helped in some calculations on vitamin B₁₂ done for Dorothy Hodgkin of Oxford, who won the Nobel Chemistry Prize in 1964. By the standards of the day the B₁₂ calculations were vast, a single cycle of structure factors followed by a Fourier synthesis took about 30 hours. I well remember a day-night-day session in 1957 which my co-author Diana Pilling and I operated jointly. Since the Mark I had a mean time between errors of only a few minutes, the programs had to assume a dodgy computer. However by 1957 reliability was much better than in 1952. Our first all-night session had been accomplished only by compensating a broken return spring on the teleprinter carriage with an electric kettle hung as a counterweight on a piece of electric flex. The kettle bobbed up and down until dawn!

"Crystallographers were well into computing before that. In the 1930s Beevers-Lipson strips made practical the hand calculation of two-dimensional Fourier syntheses, and the need for three-dimensional maps took the pioneers on to punched-card machines in the 1940s. At present, whether the problem is a protein with 10⁶ items in its data set or an instrument controlled by a chip, the need for sound analysis and efficient programming remains the same as in the 1950s. Pleasingly, some of the old methods remain useful."

1. Garfield E. Journal citation studies. XIII. *Acta Crystallographica*. *Current Contents* (37):5-10, 11 September 1974.*
2. Cruickshank D W J. The accuracy of electron-density maps in x-ray analysis with special reference to dibenzyl. *Acta Cryst.* 2:65-82, 1949.
3. Garfield E. Highly cited articles. 36. Physics, chemistry and mathematics papers published in the 1940s. *Current Contents* (10):5-11, 7 March 1977.*

* Reprinted in: Garfield E. *Essays of an information scientist*. Philadelphia: ISI Press, 1980. 3 vols.