This Week's Citation Classic®

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Sheldrick G M. *SHELX76, program for crystal structure determination.*
Cambridge, England: University of Cambridge, 1976. (Computer program.)

This citation references a computer program widely used for the determination of crystal structures from X-ray diffraction data. This technique is essentially interdisciplinary and finds application in biochemistry, physics, materials science, mineralogy, and chemistry. [The *SCI*® indicates that this "paper" has been cited in over 4,260 publications.]

Program for Crystal Structure Determination—SHELX76

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The above citation must be one of the most frequently cited *unpublished* works in the *Science Citation Index*® (*SCI*®). Computer programs employed in crystal structure determination used to be referenced (or not) in a variety of ways.

A few years ago, the editors of *Acta Crystallographica*, a very exacting journal that provides its authors with extremely precise and exhaustive instructions[1] for the preparation of their manuscripts, decided (with some justification) to bring some order into this chaos. They decreed that all computer programs employed should be referenced and that there should be a standard form of words for referencing each program, usually *not* involving a journal or book reference (since there frequently wasn't one). The same

form of words then began to appear in other journals, possibly fueled by papers that had been rejected by *Acta Crystallographica*, even when—as in this case—the author had subsequently made several attempts to describe his or her program in print. The *Journal of the Chemical Society* goes a step further and gives the above reference as an example in its "Notes to Authors."

Budding computer programmers aspiring to immortality in the *SCI* ranking list may find the following suggestions helpful: (a) The program should be sufficiently robust that it will produce sensible looking (and thus eminently publishable) numbers even when used for purposes for which it was not intended by someone who has lost the instructions (if there were any). (b) The only truly transportable and efficient language is FORTRAN. Pascal, C, ADA, Modula-2, and so on, are far too ephemeral for serious scientific applications. (c) "Comments" in a program and "structured programming" are superfluous and make it easy for users to "improve" a program. After a time they will change the name of the program and forget who wrote the original. (d) NEVER publish the original algorithms employed (if any), or you will encourage cheap imitations. (e) Make sure that the program contains one or two undocumented "features" or even "bugs." The users will feel dependent on you for the final, fully "debugged" and so perfected version of the program and its documentation and so will feel obliged to cite you in their publications. By definition, the final version is always six months from completion, and so it never can be released.

For a recent nontechnical account of the SHELX program, reference 2 may be consulted.

1. International Union of Crystallography. Notes for authors. *Acta Crystallogr. A—Found. Crys.* 39:174-86, 1983.
2. Robinson W & Sheldrick G M. SHELX. (Isaacs N W & Taylor M R, eds.) *Crystallographic computing 4: techniques and new technologies.* Oxford, England: Oxford University Press, 1988. p. 366-77.

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