platform at the rear supports an auxiliary beam stop, *S*, of tungsten, mercury or other heavy element that may be required if hard radiation is present in the incident beam.

Minor features of the design can be deduced from the drawings. The prototype allowed 2θ values from 0 to 60°; it entirely contained unwanted Laue reflections and tracked accurately over the wavelength range tested. It has been used when scattering in the horizontal plane but can be oriented in any direction without loss of performance.

The authors thank Henry Barber and the mechanical workshop of the Department of Physics, Aberdeen University for their care in constructing the prototype and the Science and Engineering Research Council who supported the work for which this monochromator was developed.

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Computer Program Abstracts

The category Computer Program Abstracts provides a rapid means of communicating up-to-date information concerning both new programs or systems and significant updates to existing ones. Following normal submission, a Computer Program Abstract will be reviewed by one or two members of the IUCr Commission on Crystallographic Computing. It should not exceed 500 words in length and should use the standard format given on page 189 *of the June* 1985 *issue of the Journal* [*J. Appl. Cryst.* (1985), **18**, 189–190].

J. Appl. Cryst. (1988). **21**, 993

QUIDCRYST-87, a software package for X-ray data collection using a two-circle computer-controlled diffractometer.

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The crystallographic problem: A software package has been written for use with a Stoe Stadi-2 two-circle equi-inclinational diffractometer. This package includes programs for alignment, data collection, simulation, presentation and photography.

Method of solution: The programs include: (1) *QUIDCRYST*-87†, the controlling program, which is menu driven and allows the user to enter the system. 'FILE' contains cell dimensions, space group, *etc.* It may be modified. (2) *UB MATRIX DETERMINATION* program finds two intense reflections at ψ between 5 and 40° and approximately 90° between their φs. It determines an orientation matrix. Checks are made to verify the correctness of the cell selected. The program stores intensity scans for subsequent inspection. (3) *LEVEL* finds two standards used in data collection and helps in the manual adjustment of μ and ν. It finds suitable scan ranges and creates a suitable 'WORKING FILE'. (4) *QUID DATA COLLECTION* takes information from FILE and WORKING FILE. It controls data collection and operates the Stoe Stadi-2 two-circle equi-inclinational diffractometer with a φ scan. Markers are added to the data file when peaks are asymmetric/unobserved. The output is stored on disk in the *SHELX* format (3I4, 2I8) (Sheldrick, 1976). (5) *QUID TO RECIPROCAL LATTICE* takes QUID data collection output and plots it in a two-dimensional array. (6) *PEAK ANALYSIS* graphs peak profiles obtained from *LEVEL* and *DEBYE–SCHERRER POWDER DIFFRACTOMETER* programs. (7) *WEISSENBERG SIMULATOR* uses FILE and produces a simulated Weissenberg with space-group absences. Intensities are not displayed. (8) *DEBYE–SCHERRER POWDER DIFFRACTOMETER* program allows QUID to be used as a powder diffractometer with a $2\theta/\omega$ step scan. (9) *OSCILLATION PHOTO* enables QUID to take oscillation photographs of a suitably mounted single crystal. A film cassette is placed on the diffractometer and the program controls the rotation of φ through a given angle.

Software environment: All programs are in Applesoft Basic and run on the Apple II series of computers or clones. A machine language, Timer, controls the real-time clock necessary for the system.

Hardware environment: Apple II type computer is used with two floppy disk drives, a printer (Epson FX80), plotter (Roland DXY 880), real-time clock (Sundox), A/D interface (ETI), machine interface (custom built) and stepping-motor controller (custom built). Drawings and photographs are available.

Documentation: A manual outlining hardware modifications, listings of all programs and a typical run is available.

Availability: The program source and documentation are available from C. H. L. Kennard. The cost is US$100, with special arrangements possible for developing countries. Users are not entitled to redistribute the package.

PEAK ANALYSIS is based on software originally written by Peter Farrington, Department of Chemistry, University of Queensland, Australia.

Keywords: Two-circle diffractometer, Weissenberg, simulation.

Reference

Sheldrick, G. M. (1976). *SHELX*76. Program for crystal structure determination. Univ. of Cambridge, England.

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†QUID stands for Queensland University Inclinational Diffractometer.

Letter to the Editor

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Programs distributed without sources

Sir,

It is not uncommon that crystallographic software does not perform quite the way its originator intended. These inadequacies are often of no serious import. Sometimes, however, they affect fundamental aspects such as reflection centering, cell reduction, profile analysis, data reduction or Patterson-map calculations. Knowing this, we are concerned that there is a growing tendency for crystallographic software, for both diffractometer control and the subsequent analysis, to be distributed as object or executable modules only.

We wish to point out here that this trend can only harm scientific progress. The user has to rely on the program description to find out what the software *ought* to do, and does not have the option of examining the source code to find out what it *is* doing. This is in contradiction with the first of the four precepts put forward by Descartes (1637), which are at the base of scientific knowledge:

> Le premier [précepte] était de ne recevoir jamais aucune chose pour vraie, que je ne la connusse évidemment être telle: c'est-à-

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dire d'éviter soigneusement la précipitation et la prévention; et de ne comprendre rien de plus en mes jugements, que ce qui se présenterait si clairement et si distinctement à mon esprit, que je n'eusse aucune occasion de le mettre en doute.

The usual justification put forward is the protection of intellectual property. In our opinion, in view of the very small number of authors of original crystallographic software, all well known to each other, a simple copyright claim in the sources should be just as effective.

Executable code may be difficult to prove incorrect, and cannot be rectified without the sources. If, in fact, the code is incorrect or deficient, only the originator can modify it, a procedure which is usually lengthy or even non-existent. With sources available, exchange of corrections and improvements to the program is made possible within the group of registered users. The practice of exchange of this information within this group would seem neither to violate any copyright nor jeopardize any commercial interests of the originator.

In the case of complex instruments like diffractometers, the source code is probably the only detailed technical information on the hardware control. Without this code, it is impossible to make any improvements. Should the manufacturer withdraw support for the instrument, as has happened, there is then no way any changes can be made.

We feel that sources are an integral part of any scientific software. Crystallographers should ponder this point before buying or otherwise acquiring any software, especially if it constitutes the only way of driving an expensive and long-lived piece of hardware.

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Reference

Descartes, R. (1637). *Discours de la Méthode*. Reprinted 1977. Paris: Union Générale d'Editions.

International Union of Crystallography

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