# 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 follow the standard format given on page 189 of the June 1985 issue of the Journal [J. Appl. Cryst. (1985). **18**, 189–190].*

## *LAUEX*: a user-friendly program for the simulation and indexation of Laue diagrams on UNIX systems

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**The crystallographic problem:** The use of computer programs has considerably simplified the determination of unknown crystal orientation, avoiding the classical method using stereographic projection and Wulff nets. Simulations may also be useful for teaching purposes.

Since the first simulation of a Laue pattern by Krahl-Urban, Butz & Preuss (1973), many programs have been written for the simulation and/or indexation of Laue diagrams. Some of them are referenced by Marín, Cintas & Diéguez (1994).

Up to now, it seems that no modern general program dedicated to the processing of diffraction data has been available on UNIX workstations, except the *LAUEGEN* package of Campbell (1995). However, *LAUEGEN* is a large program, requiring a lot of disk space, involved in a suite whose aim is the computation of integrated intensities with a view to structure resolution, while *LAUEX* is only a small simulation/indexation program for everyday work.

**Method of solution:** *LAUEX* is a user-friendly program, with an X Window graphical interface. The user enters data in the menus and chooses options by clicking on buttons or moving sliders with the mouse. The data may be saved for later use.

*LAUEX* performs the following tasks:

(i) Simulation of a Laue diagram, from knowledge of the orientation of the crystal, the cell parameters and the position of the detector. Note that *LAUEX* is not limited to the transmission and reflection cases, but that the position of the detector may be located anywhere on a sphere centred on the crystal. This feature has been introduced especially for work carried out at a synchrotron. If the structure of the crystal is known, the program may evaluate the intensities of the Laue spots and draws them as spots whose size is proportional to their intensity. The parameters taken into account for this computation are those described by Preuss (1979) (except for the crystal shape), plus the response curve of the detector.

(ii) Indexation of an experimental Laue diagram, by the knowledge of the cell parameters and the position of a number of spots of low index. The indexation procedure has been suggested by Riquet & Bonnet (1979) and has already been used by Laugier & Filhol (1983).

(iii) Alignment of a crystallographic direction along an axis of the apparatus (usually the one pointing towards the X-ray source), or rotation of the crystal.

(iv) Storing of the simulated diagram as a PostScript file, or printing directly to a laser printer.

On-line help is available if a World Wide Web (WWW) browser is installed on the machine.

**Software environment:** *LAUEX* is designed for small UNIX workstations. It has been developed under AIX but may run with other UNIX operating systems. It is written in the C language. An X Window system (Xlib and Xt libraries) and OSF-Motif widgets (Xm library) are required for the graphical user interface.

**Hardware environment:** The program is used on an IBM RS 6000 workstation. It runs on other UNIX computers: it has been successfully compiled on an HP 9000/735 and a Silicon Graphics Indigo2. An X Windows display is mandatory, but colour is not necessary.

The memory requirements of *LAUEX* depend on the maximum number of spots for the simulation; with 3000 spots, a memory size of about 2 Mbytes is needed. The disk space required for the installation of the software is about 6 Mbytes.

For paper output, a PostScript printer must be available.

**Program specification:** Typical run times for normal utilization are of the order of a few seconds of CPU time on an IBM RS 6000/560. The source code consists of approximately 22 000 lines.

**Documentation:** Documentation of about 1300 lines describes the program use, two examples and the installation procedure. It is available in French as well as in English, as HTML files. It may also be accessed *via* the WWW from the software section of the Serveur d'Information National en Cristallographie (SINCRIS) at http://www.lmcp.jussieu.fr/sincris/logiciel/.

### References

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## Crystallographers

*This section is intended to be a series of short paragraphs dealing with the activities of crystallographers, such as their changes of position, promotions, assumption of significant new duties, honours etc. Items for inclusion, subject to the approval of the Co-editors, should be sent to The Executive Secretary, 2 Abbey Square, Chester CH1 2HU, England.*

### Reginald C. G. Killean 1934–1995

Dr R. C. G. Killean, Senior Lecturer in Physics at the University of St Andrews, died in Edinburgh on 26 September 1995 after a short illness. Apart from one year in school teaching, Reg spent his entire post-school life at the University of St Andrews, as an undergraduate, an assistant lecturer at Queens College, Dundee (then a college of St Andrews, now Dundee University) and, from 1963, as ICI research fellow, lecturer and senior lecturer.

His first work on X-ray diffraction was with small organic molecules. In the late sixties, he was responsible for setting up in St Andrews one of the first computer-controlled diffractometers and the accuracy obtained from this instrument enabled him to develop accuracy studies and useful weighting schemes for diffractometer data. These studies were based on his formidable mathematical abilities. Further interests were developed in polarization studies, anharmonic studies in metals and instrumentation.

Latterly, his interests moved to digital electronics and he built up at St Andrews a small but active unit engaged in the design of digital communication devices. He also worked with advanced electronics companies in Glenrothes and set up his own small company. At the same time, he was more than willing to share his electronic and computing expertise with his colleagues at St Andrews.

Reg was a man of independent thought and action. He committed himself completely to the task at hand, whether at work or in his varied pastimes, of which climbing Munros was the one that gave him most pleasure. Many students have reason to be grateful for the high standards he set himself as a teacher and the staff and students, past and present, have been much saddened by his untimely death.

J. L. LAWRENCE

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*J. Appl. Cryst.* (1996). **29**, 510

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