Laboratory Notes


A miniature Peltier-effect goniometer-head attachment

Fraase Storm & Tuinstra (1986) have described an attachment for a single-crystal head in which the crystal is maintained anywhere in the range between 248 and 353 K by means of a temperature-controlled air stream. The air passes through a labyrinth, cooled (or heated) by a ring-shaped Peltier device mounted immediately below the crystal. The advantages of the arrangement are that only thin-walled flexible tubes for air and water and electrical leads for the Peltier device carrying 9 A need to be attached to the device. The labyrinth is thermally insulated by a hard form cover. We have appreciably reduced the size of the device by making the air labyrinth in the form of a hollow rod of square cross section. Four Peltier elements are mounted between this rod and four water-cooled brass pieces. In this way the room-temperature parts are on the outside and the cooled (or heated) parts are on the inside, so that no external heat insulation is required. Consequently, the device can be made very compact (see Fig. 1), so that it can be mounted either on an XYZ head or a standard eucentric goniometer head, although in the latter case the crystal is above the centre of the arcs. The semi-angle of the blind cone subtended at the crystal is only 25° and the attachment imposes no additional restrictions to the accessible angles in the \( \kappa \) geometry. Furthermore, by connecting the four Peltier elements (Melcor, type FC073205L) electrically in series the maximum supply current is only 1.5 A.

As in the original design the crystal is mounted in a capillary tube which in turn is glued to a thin steel tube. The latter is pushed into the central hole in the nylon part at the bottom of the device. A 'perspex' tube is then inserted in the recess turned in the top of the water-cooled brass assembly to act as a guide for lowering the concentric Mylar tubes attached to nylon bushes at both ends. The tubes, made by welding from 0.04 mm foil, are sufficiently strong to allow the screw thread to be started. The tube assembly is screwed down after removing the guiding tube.

The performance of our device is very similar to that described by Fraase Storm & Tuinstra (1986).

U. W. ARNDT
S. J. STUBBINGS

MRC Laboratory of Molecular Biology
Hills Road
Cambridge CB2 2QH
England

(Received 23 March 1987; accepted 20 May 1987)

Reference

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].


EASY-REFINE, X-ray powder diffraction refinement program.
By J. L. GAUTIER, S. ZAPATA and J. ORTIZ, Departamento de Química, Facultad de Ciencia, Universidad de Santiago de Chile, Casilla 5659, Santiago 2, Chile

(Received 26 June 1985; accepted 28 April 1987)

The crystallographic problem: EASY-REFINE refines crystal structural parameters against data obtained from integrated Bragg intensities measured by means of X-ray diffraction on powder samples. Ease of use has been one of its design features.

Method of solution: X-ray powder intensities are generated with an adaption of the LAZY-PULVERIX program (Yvon, Jeitschko & Parthé, 1977) from an initial set of atomic and crystal parameters. An adaption of the ANDEGE (Zapata, 1985) program is then used to perform multiple linear regression of the calculated against the observed integrated intensities. The parameter shifts are controlled by using the Fischer test and normalized residual plots (Draper & Smith, 1981).

Software environment: Operating system VM/CMS. Programming language Fortran IV. No overlays. Subroutine libraries: Global TXTLIB VFORTLIB.

Hardware environment: IBM 4331 model L02 Computer of the Computing Centre, University of Santiago of Chile. The program requires 750 kbytes of memory, eight bits per word. The peripherals used are virtual IBM disks and IBM 3262 printer.

Program specification: The restrictions on the complexity of the calculation are the same as for the LAZY-PULVERIX program. The program has 4000 source code lines and is written in modular form using top-down concepts. A typical run