



Fig. 1. Intensities of four reflections of  $\text{CuIn}_5\text{S}_8$ , taken with the  $\theta$ - $2\theta$  scan technique at various angles,  $\psi$ , around their scattering vectors, with  $\Delta\psi = 0.1^\circ$ . The continuous curve represents the integrated intensity  $I_0$ , corrected for the background, and the dotted line indicates the  $3\sigma(I)$  value.

arises from the fact that these reflections are affected by the Renninger effect. Since low-angle reflections (e.g. 200) are affected more in X-ray diffraction than in other techniques, we have examined some high-angle forbidden reflections.

Debye-Scherrer powder films of  $\text{CuIn}_5\text{S}_8$  and  $\text{AgIn}_5\text{S}_8$  showed that both have cubic spinel-type structures. For precise determination of lattice constants a Philips camera with the asymmetric Straumanis film mounting was used. Four reflections with  $\theta > 65^\circ$  gave the following final cell constants:  $\text{AgIn}_5\text{S}_8$ :  $a = 10.8268(5) \text{ \AA}$ ;  $\text{CuIn}_5\text{S}_8$ :  $a = 10.6858(3) \text{ \AA}$  (the Nelson-Riley function was plotted). Single crystals were mounted on a four-circle Syntex  $P2_1$  diffractometer;  $\text{Mo } K\alpha$  ( $\lambda = 0.71073 \text{ \AA}$ ) radiation was used ( $\mu = 11.54$  and  $12.21 \text{ mm}^{-1}$  respectively). The crystal was rotated about the scattering vector of each reflection ( $\psi$  angle) and a  $\theta$ - $2\theta$  scan collection carried out at fixed intervals ( $0.1^\circ$ ) of  $\psi$ . Two background values were measured at  $1^\circ$  below and  $1^\circ$  above the  $K_{\alpha_1}$  and  $K_{\alpha_2}$  peaks respectively.

The copper compound shows the presence of a considerable number of forbidden reflections, even at relatively high  $\theta$  values. Four of these, chosen for their remarkable intensities, are plotted in Fig. 1. There are many Renninger peaks, separated by approximately flat regions, where the intensity variations are of the order of three or four times  $\sigma(I)$ .

The diagrams show, from top to bottom, two plots for each reflection: the intensity  $I_0$  corrected for the background, and the  $3\sigma(I)$  level.

On the basis of these results  $\text{CuIn}_5\text{S}_8$  can be assigned to space group  $F\bar{4}3m$ . However, these results could be explained by a non-random distribution of copper and indium ions in the two tetrahedral sites  $4(a)$  and  $4(c)$ , so a complete structural determination of this compound has been undertaken.

No forbidden reflections were detected for the silver compound, so we believe that, on the basis of the X-ray diffraction analysis, it must be assigned to the conventional space group  $Fd\bar{3}m$ .

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#### Reference

THOMPSON, P. & GRIMES, N. V. (1977). *J. Appl. Cryst.* **10**, 369-371.

## International Union of Crystallography

*Acta Cryst.* (1979). B35, 2284

### Radiation leakage around X-ray tube shields

The Union's Commission on Crystallographic Apparatus recommends that the radiation level around X-ray tube shields should be carefully checked, because considerable leakage has been detected in some laboratories. Particular care should be taken when high-energy tubes are used and when tubes made by one manufacturer are enclosed in shields made by a different manufacturer.

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### Commission on Journals

#### Submission of Crystal Structure Manuscripts

Chemical-connectivity relationships in all recent crystal structure manuscripts have been checked by the Co-editors of *Acta Crystallographica* for internal consistency with the corresponding crystallographic data. As many as 35% of the manuscripts have been found by some Co-editors to contain

at least one important error. The Commission on Journals has now decided that the burden of keypunching the atomic coordinates, lattice constants and crystal symmetry in order that bond lengths, bond angles and torsion angles may be computed and compared with the values quoted in the manuscripts may reasonably be reduced with the author's cooperation. In future, all crystal structure papers must be accompanied by the *connected* computer output of the author's program that lists all final input data together with the output bond lengths and angles. All numerical information on the computer output must be clearly labelled. In addition, the first sheet of the structure factor listing should be given as part of the continuous listing if possible.

The attention of authors is also drawn to notices concerning stereofigures [*Acta Cryst.* (1978), B34, 3846], dimensions of material for deposition [*Acta Cryst.* (1979), B35, 792] and estimated standard deviations, SI units and anisotropic thermal parameters [*Acta Cryst.* (1979), B35, 1302].

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### Standard Crystallographic File Structure

At the Eleventh IUCr Congress held in Warsaw in August 1978 the Union's Commissions on Crystallographic Data and Crystallographic Computing set up a working party to propose a standard computer-readable file structure that would simplify the interchange of crystallographic data between laboratories. The working party has now produced an interim report, outlining the criteria to be met by such

a file structure and proposing a trial version containing formats for the more basic types of crystallographic data. A final report will be submitted to the parent Commissions at the Twelfth IUCr Congress in Ottawa in 1981. In the meantime anyone interested in the interim report should write to the Chairman of the working party, Dr I. D. Brown, Institute for Materials Research, McMaster University, Hamilton, Ontario, Canada L8S 4M1.

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### Molecular Structures and Dimensions

The International Union of Crystallography and the Cambridge Crystallographic Data Centre announce the publication of the latest volume in this series: Volume 10, entitled *Bibliography 1977-78, Organic and Organometallic Crystal Structures*. It contains bibliographic information on 3018 structures published during 1977-1978. As in previous volumes the entries are arranged in 86 chemical classes and cover organic compounds, complexes and organometallic compounds. There are extensive indexes for authors, compound names and formulae.

The price of the new volume is 100 Netherlands guilders (about US \$50 at current rates of exchange). Personal copies may be purchased at a reduced price of 75 Netherlands guilders. Copies are available directly from Bohn, Scheltema & Holkema, PO Box 23, 7400 GA Deventer, The Netherlands. Alternatively, orders may be placed with Polycrystal Book Service, PO Box 11567, Pittsburgh, PA 15238, USA, or with any bookseller.

## Book Review

*Works intended for notice in this column should be sent direct to the Book-Review Editor (J. H. Robertson, School of Chemistry, University of Leeds, Leeds LS2 9JT, England). As far as practicable books will be reviewed in a country different from that of publication.*

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**Scientific information transfer: the editor's role.** Edited by MIRIAM BALABAN. Pp. xxxii + 686. Dordrecht: Reidel, 1978. Price Dfl 70.00, US \$34.50

It is impossible to write a review, in the ordinary sense of the word, of a book consisting of approximately 75 papers (with discussion), presented at what was described as the 'First International Conference of Scientific Editors', held in Jerusalem, 24-29 April 1977. The book is reproduced from typescript of varying quality and different typefaces, so that it presents a very uneven appearance. The inherent quality of the papers is also variable; some are the result of original research, and others are good reviews; some seem to have been prepared simply as a justification for attending the conference, and one or two can be regarded only as elaborate jokes.

Among the papers that caught my interest was that of Anthony Woodward, of ASLIB, on the economics of an idea that has been much canvassed both in the USA and the

United Kingdom: Editorial Processing Centres. The idea is that one office could serve the needs of the publications of a number of learned societies, providing secretarial services, processing and technical editing of typescripts, and photocomposition (probably computer-controlled). According to Woodward's analysis, under European conditions the claimed financial savings would arise almost entirely from the photocomposition stage, and this is something that can just as well be provided by the printer, without the additional complication and bureaucracy of an editorial processing centre. His figures were not challenged, possibly because no one else had bothered to do the calculations, and had simply assumed that the arrangement would be advantageous. However, Dorothy Mizoguchi, of the Japanese Cancer Association in Tokyo, describes two centres for scientific publications in Japan. One published 45 journals on behalf of scientific societies, some in Japanese and some in English. The other was a business centre, which undertook the collection of membership fees, mailing of notices and journals, preparing membership lists, and similar duties for about 80 societies. The special problems of publishing in English in Japan obviously provided a situation quite