



Fig. 1. Details of apparatus: (a) perspective view, (b) vertical plan.

can be grown inside the apparatus or introduced into it [watch glass (A)] inside a dry box. (B) and (C) are containers for the drying agent and glue respectively. (D) is a rod in a tightly fitting grease-filled cylinder pierced through the rubber seal. A circular plate attached to the rod carries glass capillary tubes (Lindemann glass tubes) held by plasticine. (E) represents rods which have glass fibres attached and are used for selecting and mounting crystals. A considerable degree of lateral movement is possible because of the flexibility of the 'Suša-Seal' cap. Crystals are delivered into the tubes and the open ends are then sealed with glue before being removed from the apparatus. (F) is a spare side arm which could be used for fitting a vacuum line to the apparatus, or for some other purpose.

The attractive features are the easy manoeuvrability of the apparatus for selecting and mounting crystals that have been grown in an inert environment and the ability to view the crystals in an unimpaired manner under a microscope during mounting.

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## Letter to the Editor

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### The proper description of low-temperature X-ray diffraction apparatus\*

Sir,

The purpose of this comment is to detail the minimum information which should be included in describing any low-temperature X-ray diffraction (LTXRD) device. In addition, a computer-based coded bibliography of LTXRD apparatus, which will be useful in reducing duplication of effort in the construction of future devices, is described.

Since 1916, when the first (LTXRD) apparatus was constructed, eight methods of cooling have been used in the construction of over 400 different types of LTXRD systems and components (Rudman, 1976). However, very often the LTXRD device was not completely described in the literature. This is particularly true when the primary focus of the paper is on the analysis of diffraction data, but it has also been noted in many papers whose sole purpose is to describe LTXRD apparatus. As a result, a number of very similar instruments have been developed over the years, at a great expense in both manpower and money.

There are six basic points which should be included in all descriptions of LTXRD instruments.

- (1) Type of sample that can be studied.
- (2) Type of cooling system used.
- (3) Method of preventing frost formation.
- (4) Minimum temperature attainable.
- (5) Type of X-ray instrument used.
- (6) Other special characteristics.

A schematic diagram should be included in the report. However, if space limitations preclude the publication of a diagram, then instructions should be given describing how it may be obtained, preferably by having it deposited as a Supplementary Publication, as are structure factor tables.

Other details concerning the construction and operation of the device that should be included in the paper (where applicable) are as follows.

\* Presented, in part, at the Open Commission Meeting on Crystallographic Measurements at Controlled Pressures and Temperatures, jointly sponsored by the Commission on Crystallographic Apparatus and the Commission on Crystallographic Studies at Controlled Temperatures and Pressures at the Tenth IUCr Congress, 1975.

(7) The dimensions and cryogen capacity of the apparatus.

(8) A list of manufacturers of any special components used in the construction of the device (can be presented as an Appendix).

(9) Rate of cryogen consumption and frequency of refill.

(10) Accuracy of temperature measurement.

(11) Long- and short-range temperature fluctuations.

(12) Temperature gradient in the vicinity of the crystal.

All of these points should be covered so as to furnish a complete description of any previously unreported LTXRD apparatus. At the very least, the code number (see below) should be given for identification purposes.

Finally, in order to facilitate retrieval of this information, the abstract should mention that a low-temperature device is described in the article.

During the course of developing the computer-based bibliography of low-temperature apparatus and techniques (Rudman, 1976), a method was developed for coding the primary characteristics of each device (items 1–6 above). Each low-temperature instrument appearing in the bibliography is assigned a six-digit code number (as shown in Table 1) which gives a concise summary of its major features.

As the bibliographic data are read into the computer, arrays are formed so that it is possible to sort the code-numbers in several ways. First, the six-digit apparatus code-number is listed, in order of increasing magnitude, together with the serial number of the reference(s) in which the device is described. In subsequent listings the references are sorted on the basis of the individual digits of the code-number. Thus, it is possible to identify all references to a specific type of apparatus (six-digit code-number) or to a specific aspect of low-temperature apparatus.

Examples of the usefulness of the bibliography and sorted listings include the following.

(a) The code number 111312 means that the device described in that article *can be used* with any type of sample, *cools the sample* with a cold stream of gas, *prevents ice condensation* by means of a concentric warm outer gas stream, can reach a *minimum temperature* somewhere between 78 and 200 K, and was *designed for use* with a Debye-Scherrer camera having a vertical sample axis.

(b) If one wishes to locate all devices in which Joule-Thomson expansion

Table 1. *Code numbers used in classifying low-temperature X-ray diffraction apparatus and techniques*

First digit: type of sample that can be studied

- (1) Any type
- (2) Single crystal
- (3) Powder
- (4) Metal
- (5) Protein
- (6) Neutron diffraction

Second digit: type of cooling used

- (1) Cold-gas stream
- (2) Conduction (cryogenic fluid as coolant)
- (3) Conduction (thermoelectric cooling)
- (4) Conduction (mechanical refrigeration)
- (5) Joule-Thomson expansion
- (6) Immersion of sample
- (7) Immersion of camera
- (8) Use of cold room

Third digit: method of frost prevention

- (1) Dry gas stream
- (2) Dry chamber
- (3) Evacuated chamber
- (4) Not given
- (5) None

Fourth digit: minimum temperature attainable (Kelvin)

- (1) Less than 20
- (2) 20–78
- (3) 78–200
- (4) 200–260
- (5) Greater than 260
- (6) Not available

Fifth digit: type of X-ray instrument mentioned

- (0) Any type
- (1) Debye-Scherrer camera (includes back-reflection)
- (2) Flat-cassette and Laue cameras
- (3) Guinier camera
- (4) Oscillation-rotation camera
- (5) Weissenberg goniometer
- (6) Precession camera
- (7) Diffractometer
- (8) Small-angle
- (9) Topographic studies

Sixth digit: special characteristics

- (0) None
- (1) Horizontal
- (2) Vertical
- (3) Back-reflection
- (4) High-temperature also
- (5) High-pressure also
- (6) Weissenberg goniometer accessories
- (7) Cold-working at low temperatures

cooling is used, category 5 in the list where the references are sorted on the

basis of the *second* digit of the code number would be examined.

(c) If one has a need for a particular kind of LTXRD device, it is possible to 'design' this instrument by constructing the suitable six-digit code number. A check of the six-digit listing will reveal whether or not a similar instrument has actually been constructed.

Proper reporting of LTXRD apparatus and the use of this bibliography should greatly reduce duplication of effort and wasted man-hours in the design and construction of LTXRD instrumentation.

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#### Reference

Rudman, R. (1976). *Low-Temperature X-ray Diffraction: Apparatus and Techniques*. New York: Plenum.

### 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 Editorial Board, should be sent to the Executive Secretary of the International Union of Crystallography (J. N. King, International Union of Crystallography, 13 White Friars, Chester CH1 1NZ, England).*

Sir **Alan Cottrell**, Master of Jesus College, University of Cambridge, has been appointed a Vice-President of the Royal Society. He has also been awarded the 1977 Guthrie Medal and Prize of the Institute of Physics for his many contributions to the science of metals.

Professor **Dorothy Hodgkin**, Wolfson Research Professor of the Royal Society and Immediate Past President of the IUCr, received the Fankuchen Award of the American Crystallographic Association at the ACA's spring meeting held in Asilomar, California, in February 1977. The award, which is given every three years, was made to Professor Hodgkin for her 'outstanding contributions to the teaching of crystallography and for fundamental and fruitful investigations in the many areas of crystal-structure analysis'. The award was established in 1970 by former students and friends of Professor

**Isidor Fankuchen** (1904–1964) to honour his memory and his many contributions in a way in which he, himself, would have thought to be particularly appropriate. In addition to presenting her lecture *Water and Protein Molecules: The Case of Insulin* at the ACA meeting, Professor Hodgkin also presented it at the Polytechnic Institute of Brooklyn, where Professor Fankuchen was Professor of Physics (1942–1964).

Sir **James Menter**, Principal of Queen Mary College, University of London, has been awarded the 1977 Glazebrook Medal and Prize of the Institute of Physics for his contributions to industrial research.

Dr **R. F. Pearson** of Mullard Research Laboratories, Redhill, England, has been awarded the 1977 Duddell Medal and Prize of the Institute of Physics for his contribution to the understanding of the crystal anisotropy and other single crystal properties of substituted ferrimagnetic substances.

Professor **D. C. Phillips**, Professor of Molecular Biology at the University of Oxford, has been appointed a Vice-President of the Royal Society. He has also been elected Biological Secretary of the Royal Society, to succeed Sir **Bernard Katz**.

### Erratum

We regret the unfortunate error in the announcement (*Crystallographers*, December 1976 issue) concerning the **Bertram E. Warren Award** presented to Dr **S. Iijima** and Professor **J. M. Cowley**. The award is *not* sponsored by IBM, a corporate entity, but by the individual personal contributions of Professor Warren's students and friends on the occasion of his retirement from Massachusetts Institute of Technology in 1967. The fund is wholly managed by the American Crystallographic Association and the earnings from it permit the giving of this award every third year.

### International Union of Crystallography

#### Establishment of a President's Fund

At the Tenth General Assembly of the Union, held in Amsterdam in August