

## The Literature of Crystallography

by John S. Kasper

In recent years there has been an evident increase of interest in crystallography among workers in a variety of disciplines, such as solid-state physics, chemistry, metallurgy and biology. At least there has occurred a greater recognition in these disciplines of the importance and need of the results of crystallographic research. It does appear, however, that the nonspecialist may encounter some difficulty in an attempt either to use the results of crystallography or to learn more of its techniques, methods and practice. Actually, there is an extensive literature of crystallography, well known to crystallographers, but probably not sufficiently known by interested nonspecialists. It is in the hope that the latter may benefit from a better acquaintance with that literature that this article is written.

### IUC PUBLICATIONS

The basic library of almost every practicing crystallographer contains certain publications that are sponsored by the International Union of Crystallography (IUC). This organization, reflecting the traditional international interaction of crystallographers, holds congresses and symposia every three years and provides a variety of services for all crystallographers, among which is the publication of three major works. These are *Acta Crystallographica*, a monthly journal covering current research in crystallography; *Structure Reports*, a detailed compilation of the

structure determinations reported for a given year; and *International Tables of Crystallography*, a three-volume collection of tables and basic information needed by the crystallographer. All three works involve a continuing active participation of crystallographers from all parts of the world, all of whom serve without pay.

The three projects began with the establishment of IUC in 1946 and reflect the desire of the union's organizers to continue three eminently successful projects, all of German origin but international in character, that were ended by World War II. Thus, *Acta Crystallographica* was to serve in the capacity of the *Zeitschrift für Kristallographie*, which was essentially the only journal of crystallography prior to 1941. Similarly, *Structure Reports* was to continue the reporting of structure determinations that was done before 1941 by *Strukturbericht*; the *International Tables* were to be a revised and up-to-date replacement for the two-volume *Internationale Tabellen zur Bestimmung von Kristallstrukturen*.

*Acta Crystallographica* is now in its twentieth year of publication and has been the main medium for reporting structure determinations, methods and theory of structure analysis, and diffraction theory and practice. Although other areas are represented, the majority of the papers are in the aforementioned fields where high standards of quality have been maintained. Papers are accepted in English, French, German or Russian and participation is international, although contributions from the Soviet Union are conspicuous by their absence.

*Structure Reports*, printed in English, presents in elegant fashion reports on the crystal-structure determinations of a given year. Sufficient detail, including illustrations, is given

to enable the crystallographer in most cases to understand or reconstruct the structure without recourse to the original literature. The task of producing *Structure Reports* has been a difficult one ever since it began after World War II. First, there were the years since 1939, the last year of publication of *Strukturbericht*, to be made up as well as the ever increasing amount of work for current years. At present 18 volumes have been issued bringing the continuity through volume 21 (1957), with volumes 22 (1958) and 24 (1960) due to appear soon—volume 23 (1959) is already available. There had been seven volumes of *Strukturbericht* and hence the earliest volume of *Structure Reports* (for 1940–41) is volume 8. The combined works, *Strukturbericht* (vols. 1–7) and *Structure Reports* (vols. 8–), are then a convenient and indispensable reference for essentially all the structures that have ever been determined. One particular point to note is that a systematic classification scheme for structure types was started in *Strukturbericht* and that this is the most prevalent scheme used today. Unfortunately, as more and more complex structures were reported, the scheme was no longer applicable and no such scheme is attempted for new structure types in *Structure Reports*.

The *International Tables for X-Ray Crystallography* (Kynoch Press, Birmingham, England) consist of three volumes: volume 1, Symmetry Groups; volume 2, Mathematical Tables; and volume 3, Physical and Chemical Tables. The largest part of volume 1 is devoted to space-group tables. For the 230 space groups and the 17 plane groups, diagrams illustrate the location of equivalent positions and of the various symmetry elements; the analytical expression of the coordinates of equivalent positions

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with their point symmetry and the number of positions; the conditions limiting possible reflections; and structure-factor expressions. Other topics related to symmetry are also included. Volume 2 includes not only purely mathematical tables but also a treatment of mathematical topics especially pertinent to crystallography and diffraction; for example, crystal geometry, Fourier series and Fourier transforms, statistics. Among the contents of volume 3 are x-ray wavelengths, atomic-scattering factors, absorption coefficients, and atomic radii. Each volume is quite comprehensive and is extensively used by all practicing crystallographers. The first editions of 4000 copies have been sold out for vols. 1 and 2; vol. 3 is about to be sold out; and new editions with corrections are now available.

In addition to the three main publication activities of IUC, there are other special books and booklets that are of immense value to crystallographers. One of these is the *World List of Crystallographic Computer Programs*, which is to appear in its second edition very soon. Modern computing facilities have become essential for certain crystallographic endeavors, particularly structure analysis, and some crystallographers have been at the forefront of advances in computer and programming activities. The extensive list is obviously beneficial to the increasing number of people who use computers.

A very useful booklet is the *World Directory of Crystallographers*, listing crystallographers and their addresses with information as to field of specialization, professional background, and date of birth. A third edition (1965) contains over 5000 entries.

A *Crystallographic Book List*, edited by H. D. Megaw and issued in 1965, contains information on about 800 books that cover peripheral subjects of interest to crystallographers as well as strictly crystallographic topics. In addition to the usual pertinent information, books are graded as to elementary, undergraduate, or more advanced level; and a subject classification is provided.

A commemorative volume, *Fifty Years of X-Ray Diffraction*, edited by Paul P. Ewald, on the occasion

(1962) of the fiftieth anniversary of the discovery of x-ray diffraction by Max von Laue, was also sponsored by IUC. It gives an interesting account not only of the early historical experiments and the subsequent development of diffraction and structure analysis but also of the development of schools and centers of research in different nations and regions of the world, with the inclusion of personal reminiscences by many of the pioneers in this relatively young branch of science. The book is a delight to crystallographers but can be recommended to anyone with a peripheral interest.

While the IUC publications serve crystallographers very well in their various capacities, they do not, of course, represent the only literature. This is particularly true of publications containing crystallographic information.

#### JOURNALS

As mentioned previously, *Acta Crystallographica* assumed in 1947 the role fulfilled before World War II by the *Zeitschrift für Kristallographie*. Actually, the latter journal was revived in 1954 and has been successful as another international crystallography journal. There is overlap in the kinds of articles in *Acta* and in the new *Zeitschrift* but there is a higher proportion of papers on minerals and morphology to be found in the latter.

Although the Soviet Union has adhered to IUC and Soviet crystallography has been very active, essentially no Russian papers have appeared in the international journals. Instead, the Soviet journal *Krystallographiya*, started in 1951, has served in the same capacity for the Soviet Union as *Acta* for the Western world. Fortunately

for American crystallographers this journal is translated into English under the auspices of the American Institute of Physics and is entitled *Soviet Physics—Crystallography*. The translations have appeared regularly and with only a few months lag after the original has appeared.

In recent years an increasing number of crystallographic papers has appeared in less specialized journals. In the US, for example, the *Journal of Chemical Physics* and the *Journal of Inorganic Chemistry* have contained a significant number of papers on crystal structures, and many neutron-diffraction papers have been published in *The Physical Review*.

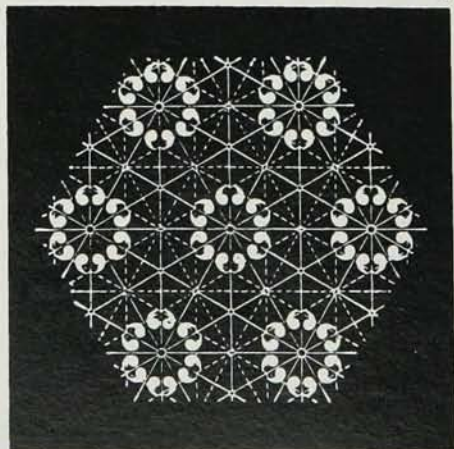
#### CRYSTAL-STRUCTURE DATA

In addition to *Structure Reports*, which presents results on an annual basis, there are several collections of crystal-structure data that are frequently used as references. A particularly popular and good one is *Crystal Structures* by Ralph W. G. Wyckoff (Interscience, New York). The most recent edition (1963, 1964) is in hard cover in three volumes, replacing a looseleaf edition that had lacked an index. The structures are described in the standard language of crystallography—space-group, atomic coordinates, interatomic distances, atomic coordinations, with frequent good illustrations and often a more descriptive text. Structures of the same type are collected together, and the succeeding chapters are in order of increasing complexity of substance composition.

The Wyckoff work is quite exhaustive for inorganic and organic structures, but not so for metals and alloys. An especially good reference for the latter is *A Handbook of Lattice Spacings of Metals and Alloys* by W. B. Pearson (Pergamon Press, Oxford, 1958), which is rather complete to the date of publication.

Another good systematic collection of crystal structures is in *Landolt-Bornstein: Zahlenwerte und Funktionen aus Physik, Chemie, Astronomie, Geophysik und Technik*, Vol. 1, Part 4, *Kristalle* (Springer-Verlag, Berlin, 1955).

A very useful reference of basic crystallographic data (space group, lattice parameters, density, etc.) is *Crystal*



*Data: Part II, Determinative Tables* by J. D. H. Donnay and G. Donnay (American Crystallographic Association Special Monograph No. 5).

#### ACA PUBLICATIONS

##### Monographs

The American Crystallographic Association (ACA) sponsors special monographs from time to time to fulfill the desire of the membership for specialized treatment of certain topics of particular pertinence to crystallography but which may not be conveniently available in the literature. In addition to *Crystal Data*, mentioned above, the following monographs are available:

No. 1 *The Photography of the Reciprocal Lattice*. By M. J. Buerger.

No. 2 *Fourier Transforms and Structure Factors*. By D. Wrinch.

No. 3 *The Solution of the Phase Problem: I, The Centrosymmetric Crystal*. By H. Hauptman, J. Karle.

No. 4 *On the Systems Formed by Points Regularly Distributed on a Plane or in Space*. By M. A. Bravais. English translation of a classic work.

##### Transactions of symposia

A recently instituted policy of ACA is the sponsorship of symposia with publication of papers and discussion as *Transactions*. Volume 1 (1965) is entitled *Accuracy in X-Ray Intensity Measurement*. Volume 2 (1966) is *Proceedings of the Symposium on Machine Interpretations of Patterson Functions and Alternative Direct Approaches and the Austin Symposium on Gas Phase Molecular Structure*. The *Transactions* are free to the current membership of ACA and are available at a nominal price to non-members.

#### BOOKS

Although a generation ago it could be said that there did not exist many textbooks and introductory books on crystallography, today there are a good number of such books as well as advanced and specialized treatises. The Crystallographic Book List, mentioned above, contains a comprehensive compilation. A more restricted list, representing to some extent books in greater demand in the US, is that carried

by Polycrystal Book Service, which will be discussed subsequently.

This article is not intended to be a book review in the usual sense and no attempt is made to appraise critically the numerous books available. It may be helpful to the reader, however, to indicate some examples in various branches of crystallography that have found wide use by American crystallographers.

##### Elementary, general textbooks

*Elementary Crystallography*. By M. J. Buerger. Wiley, New York, 1956.

*Chemical Crystallography*. (Second ed.) By C. W. Bunn. Oxford University Press, Oxford, 1961.

*Elements of X-Ray Diffraction*. By B. D. Cullity. Addison-Wesley, Reading, Mass., 1956.

##### Geometry and symmetry

*An Introduction to Crystallography*. (Third ed.) By F. C. Phillips. Longmans, London, 1963.

*Colored Symmetry*. By A. V. Shubnikov, N. V. Belov et al. Trans. from Russian. Pergamon Press, Oxford, 1964.

##### Structure analysis

*The Determination of Crystal Structures*. By H. Lipson, W. Cochran. Bell, London, 1953.

*Crystal Structure Analysis*. By M. J. Buerger. Wiley, New York, 1960.

##### Diffraction theory

*Theory of X-Ray Diffraction in Crystals*. By W. H. Zachariasen. Wiley, New York, 1946.

*Direct Analysis of Diffraction by Matter*. By R. Hosemann, S. N. Bagchi. North-Holland, Amsterdam, 1962.

##### Physics of diffraction

*The Optical Principles of the Diffraction of X-Rays*. (Second ed.) By R. W. James. Bell, London, 1963.

##### Diffraction techniques and applications

*X-Ray Procedures for Polycrystalline and Amorphous Materials*. By H. P. Klug, L. E. Alexander. Wiley, New York, 1954.

*Structure of Metals* (Second ed.) By C. S. Barrett. McGraw-Hill, New York, 1952.

##### Crystal chemistry and structural principles

*The Nature of the Chemical Bond*. (Third ed.) By L. Pauling. Cornell University Press, Ithaca, New York, 1960.

*Structural Inorganic Chemistry*. (Third ed.) By A. F. Wells. Oxford University Press, Oxford, 1962.

*Organic Chemical Crystallography*. By A. I. Kitaigorodskii. Trans. from Russian. Consultants Bureau, New York, 1961.

##### Neutron diffraction

*Neutron Diffraction*. (Second ed.) By G. E. Bacon. Oxford University Press, Oxford, 1962.

##### Mineral structures

*Crystals and Crystal Growing*. By W. L. Bragg, G. F. Claringbull. Bell, London, 1965.

##### Optical crystallography

*Optical Crystallography*. (Third ed.) By E. E. Wahlstrom. Wiley, New York, 1960.

##### Popular books

*Crystals and Crystal Growing*. By A. Holden, P. Singer. Doubleday, New York, 1960.

*The Third Dimension in Chemistry*. By A. F. Wells. Oxford University Press, Oxford, 1956.

#### POLYCRYSTAL BOOK SERVICE

American crystallographers are fortunate to have available the Polycrystal Book Service (P.O. Box 11567, Pittsburgh, Pa. 15238), which makes available all the publications discussed here as well as many others. In particular it is the most convenient source of ACA and IUC publications. It provides, in addition, charts, models and atlases, which have not been discussed here, as well as many books on crystallography and related subjects, which may be difficult to obtain because they are low-volume items whose sources are not well known. A list of available publications can be obtained from Polycrystal.