BOOK REVIEWS

ADVANCES IN STRUCTURE RESEARCH BY DIFFRACTION METHODS; FORTSCHRITTE DER STRUKTURFORSCHUNG MIT BEUGUNGSMETHODEN. Volume 1, Edited by R. Brill, Berlin, with contributions of G. E. Bacon, B. K. Vainshtein, J. Karle, W. Hoppe, H. Jagodzinski, A. Niggli. Interscience Publishers, N. Y., London. viii+221 pp., 102 figs. $13.50.

This first volume of a series of progress reports is a praiseworthy international effort. Contributions from an Englishman, a Russian, an American and a Swiss are given in English; two German contributors use their mother tongue. The editor is the director of the Fritz-Haber Institute in West Berlin. He explains in the preface that future volumes may be somewhat less technical and will be written in English only, " . . . the language which is rapidly becoming the *lingua franca* of science." Each contributor is an outstanding man in his field and is excellently qualified to present a survey of his specialty. There is, however, no attempt made to unify the separate contributions which range far and wide, and some of which are presented in a very technical manner. One cannot help wondering how many of today's highly specialized scientists will be able to appreciate the book *as a whole* (especially in view of its high cost).

Dr. Bacon's chapter is entitled "The determination of crystal structures by neutron-diffraction measurements," which is somewhat misleading since it excludes the large field of magnetic structures. The author concentrates on the location and thermal motion of light atoms, especially hydrogen in inorganic and organic crystalline compounds. Many of the results reported were obtained by the author himself and his coworkers. The presentation is simple and clear, structural mineralogists will profit greatly from reading these 23 pages. The second chapter by Dr. Vainshtein, head of the Institute of Crystallography in Moscow, is written in good English on "Fourier synthesis of potential in electron diffraction structure analysis and its applications to the study of hydrogen atoms." The underlying theory, much of it developed by the author, is considerably more complex than that of x-ray or neutron diffraction, so that the summary given here is perhaps more intriguing than informative to the non-expert. Various procedures for obtaining experimental data are given. The last half of this contribution deals with the results obtained and can be enjoyed by all. "The determination of phase angles" is presented by J. Karle. The introduction and historical survey make excellent reading. The going gets tougher in the part that deals with the Karle-Hauptman method, based on the theory of probabilities. This chapter with its extensive bibliography (135 titles), will prove particularly useful to structural crystallographers who have already applied the method and to those who would like to try it.

By far the longest chapter, 76 pages, is authored by W. Hoppe of Munich and deals with thermal diffuse scattering and its application to the structural investigation of molecular crystals. A brief historical review is followed by a discussion of the theory, which occupies two-thirds of the text and appears, at least in part, to be an original contribution. It is highly technical and whatever attempt was made at simplifying the approach is not apparent. The discussion of the experimental procedures and the presentation of the conclusions are equally difficult to follow. This is a great pity, because the subject matter is of vital interest to all structure analysts. An extended monograph might have been needed to do this contribution justice. Another cause of diffuse reflections, namely disorder in crystals, is discussed in general terms by H. Jagodzinski. His treatment, an admittedly original contribution, is limited to crystals that give diffuse reflections in addition to sharp reflections. (It is not clear how these diffuse intensities can, in practice, be distinguished from those due to thermal motion of the previous chapter.) The theory is lucidly presented: the

treatment is carried out in Patterson space, and theoretical Patterson functions are derived for various types of disorders. The classification of the latter is based on the number of dimensions in which disorder extends (Fehlordnung). Qualitative agreement with observations is pointed out.

Diffraction data which became disturbingly diffuse in the previous two chapters have disappeared completely in the last one, where A. Niggli of Zürich gives a strictly theoretical discussion of "Antisymmetry, colour symmetry and degenerate symmetry." A reader familiar with group theory will have no trouble following this excellent treatment, which places the many different contributions, especially those of the last fifteen years, in clear perspective. A listing of the limited number of present-day applications of generalized symmetry, including the artistic ones by M. C. Escher, concludes the chapter.

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MATHEMATICAL THEORY OF *X*-RAY POWDER DIFFRACTOMETRY. A. J. C. WILSON. Philips Technical Library, Eindhoven, 1963. ix+128 pp., $4.25.

A great deal of information has been published in recent years, dealing with aberrations in powder diffractometry instrumentation. Heretofore this information was available only in piecemeal form and unavailable, in a practical sense, for many workers involved with routine laboratory applications. This book is the first of a series of two, the second being prepared by W. P. Parrish. In this work the emphasis is on the theory behind aberrations in diffractometry, while the second is being designed to cover more practical aspects.

The line profile observed with a diffractometer is the convolution of the aberration functions with the scattering function of the specimen. This leads directly to the use of the centroid and variance as the most conveniently handled measures of profile position and dispersion, respectively. Aberrations are conveniently divided into two categories: geometrical and physical. Under geometrical aberrations are included such factors as the effects of finite focal spot size, errors in specimen alignment, gear mis-setting, specimen transparency, and combinations of various source and receiver slit systems. Changes in both centroid position and variance are derived for each. Similar discussions are given for physical aberrations such as refraction, dispersion, and factors affecting the intensity of the emission profile as a function of wavelength.

A short discussion is given of the application of the derived centroid shifts to the accurate determination of lattice parameters. Included here is a discussion of peak displacements, peak positions being more easily determined than centroid positions. The remainder of the text is devoted to the interpretation of the broadening of diffraction profiles as a function of small particle size and crystal imperfections.

The style of writing is clear and concise. The comprehensive reference list provides ready access to supplementary information. This book provides the much needed service of bringing together the wealth of recently acquired information on the theory of diffractometry, authored by one of the principal contributors to the field. It should be read by all those with interest in diffractometry, to acquire at least an appreciation, if not a working knowledge, of the subject.

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DATA FOR X-RAY ANALYSIS. CHARTS FOR SOLUTION OF BRAGG'S EQUATION; (d *vs.* θ and 2θ); Vol. I, Cu K-rad. (125 pages, 108 charts, $4.50); Vol. II, Mo K-, Co K- and W L-rad. (141 pages, 118 charts, $5.50); Vol. III, Fe K- and Cr K-rad.

(137 pages, 112 charts, $5.50). WILLIAM PARRISH AND MARIAN MACK, Philips' Technical Library, Eindhoven, Holland, 1963, 2nd Edition.

Anyone who has frequent need to convert values of θ or 2θ into d or vice versa will welcome these volumes.

This is a greatly expanded version of a similar work with the same title by Parrish and Irwin published in 1953, these three volumes replacing the original Volume I of 100 pages. The original scale of 1 degree 2θ equal 5 cm has been retained for Co, Mo, W, Fe and Cr, and expanded to 1 degree equal 10 cm for Cu Kα. However, for all radiations, the scale of the ordinate has been expanded for higher 2θ angles to keep the slope of the curves near 45 degrees so that values can be easily and accurately read. This means that d always can be read to the same precision as the 2θ angles. Thus for Cu Kα radiation, 2θ values can be read to 0.01 degree 2θ (and interpolated to about one-half this value), and the precision of the corresponding d's ranges from 0.1 Å near 1 degree to 0.00001 near 180 degrees. Thus the precision for Cu Kα is comparable to and the precision for Fe Kα about half that which is obtained by interpolating between tenths of degrees 2θ in the widely used U. S. Geological Survey Circular 29. The advantage of the charts lies in the ease and speed of graphic methods.

The *x*-ray wavelengths are those used in the *International Tables for X-ray Crystallography* (1959). Ranges of 2θ values are as follows: Cu K-rad., α 0–90; α_1 and α_2 20–180; β 0–180; Mo K-rad., α 1–45, α_1 and α_2 15–90, β_1 3.7–87.5; Co K-rad., α 1.9–110, α_1 and α_2 20–180, β 2.9–175, W L-rad., α_1 2.7–175, α_2 12.5–112.5, β_1 2.4–175; Fe K-rad., α2–120, α_1 and α_2 20–180, β 3–175; Cr K-rad., α 2–130, α_1 and α_2 30–180, β 3–175.

To facilitate reading the graphs, the grid coordinates (smallest division, one mm) have been printed in light blue and the curves and numbers in black. The authors warn the reader that where the black check marks do not coincide with the blue grid, the curves are displaced a similar amount. In most cases this difference is much less than one-third mm. and can be ignored. The maximum displacement observed by this reader was one mm. Where necessary, corrections can be easily made by the reader, but one should either habitually check each chart before reading it or else make a note of the charts that need such adjustments. Thus this minor flaw detracts very little from the general usefulness of these charts.

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MINERALY, SPRAVOCHNIK. Tom. I. Native elements, intermetallic compounds, carbides, nitrides, phosphides, arsenides, antimonides, bismuthides, sulfides, selenides, tellurides: Izdatel'stvo Akad. Nauk. SSSR, Moscow, 1960, 616 pp. 363 figures, price 3 rubles, 50 kopecks (about $3.75). Tom. II, No. 1, Halides, 1963, 295 pp., 141 figures, price 1 ruble, 65 kopecks (about $1.80) (both in Russian).

These are the first two sections of a comprehensive reference work on mineralogy comparable to Dana's System of Mineralogy, to be published under the editorship of F. V. Chukhrov, with the assistance of E. M. Bonshtedt-Kupletskaya, G. P. Barsanov, and N. V. Belov. The work is to comprise seven volumes: II Halides and oxides, III and IV, Silicates, V and VI Remaining oxygen compounds, VII Mineralogical phase equilibrium diagrams. The authors listed include 21 for v. I, and 15 for v. II, No. 1.

Detailed review is not possible, but the scope may perhaps be indicated. The treatment is very similar to that of Dana's System, but includes *x*-ray powder data, some representations of crystal structure, and some DTA curves, in addition. In vol. I the sulfosalts are included with the sulfides. A rough indication of the scope may be indicated by comparison with Dana's System: Tom. I—contains material covered in p. 87–488 of Dana, Vol. I