

Des considérations stériques basées sur la taille des groupements ( $XO_4$ ) montrent qu'ils sont très voisins de ceux déterminés par Zachariassen (1948) pour les phosphates correspondants.

Le Tableau 2 reproduit le dépouillement des 16 premières raies d'un diagramme Debye-Scherrer de vana-

date de strontium effectué à la radiation du chrome (2,2909 Å).

#### References

- DURIF, A. (1957a). *C. R. Acad. Sci. Paris*, **244**, 2815.  
 DURIF, A. (1957b). *C. R. Acad. Sci. Paris*, **245**, 1151.  
 ZACHARIASSEN, W. H. (1948). *Acta Cryst.* **1**, 263.

## Notes and News

*Announcements and other items of crystallographic interest will be published under this heading at the discretion of the Editorial Board. Copy should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333 Jay Street, Brooklyn 1, N.Y., U.S.A.) or to the Technical Editor (R. W. Asmussen, Chemical Laboratory B of the Technical University of Denmark, Sølvgade 83, Copenhagen K, Denmark)*

### Crystallographia

The journal '*Crystallographia*' of the Academy of Sciences of the USSR is being published in (complete) translation by the American Institute of Physics. The translation began with the 1957 issues.

There are six issues per year, approximately 1,000 Russian pages. Annually \$25.00 domestic, \$27.00 foreign (\$10.00 and \$12.00 respectively for libraries of nonprofit degree-granting institutions). Subscription orders and inquiries should be addressed to: Translation Journals—American Institute of Physics, 335 East 45 Street, New York 17, N.Y., U.S.A.

### The Electron Microscope Society of America

The 17th Annual Meeting of the *Electron Microscope Society of America* will be held September 9–12, 1959, at Ohio State University, Columbus, Ohio. Information concerning the meeting is obtainable from the Program Chairman Sydney S. Breese, Jr., Plum Island Animal Disease Lab., Greenport, L.I., N.Y. and regarding Scientific and Commercial Exhibits from Walter J. Frajola, N205 North Wing, Univ. Hospital, Ohio State University, Columbus, Ohio. Deadline for 150-word abstracts of contributed papers is June 1, 1959.

### Structure Reports

Volume 14 of *Structure Reports* is now ready. Vol. 14 which is a cumulative index for 1940–50 has been prepared under the general editorship of A. J. C. Wilson, with N. C. Baenziger and C. S. Barrett (Metals), J. M. Bijvoet and J. Wyart (Inorganic Compounds) and J. Monteath Robertson (Organic Compounds) as section editors.

Orders may be placed direct with the publisher:

N. V. A. Oosthoek's Uitgevers Mij.,  
 Domstraat 1–3, Utrecht,  
 Holland,

with the Polycrystal Book Service (G. P. O. Box 620, Brooklyn 1, N.Y., U.S.A.), or with any bookseller. The price is 35 Dutch florins, £3.8.0 or \$9.50.

### L'Académie des sciences

L'Académie des sciences a élu membre titulaire le professeur Jean Wyart, de la Sorbonne.

### Tables of $Q$ as a Function of $2\theta$

*Announcement from the Commission on Crystallographic Data*

1. The parameter  $\sin^2 \theta$  is often used for the indexing of powder diffraction patterns because general linear relations exist between its values for different lines. In published work such values are often listed along with  $d$ , so as to make it easier for the reader to follow the interpretation given. It is known that using  $Q = 1/d^2 = (4/\lambda^2) \sin^2 \theta$  instead of  $\sin^2 \theta$  greatly facilitates both checking and comparison of published data. Not only is  $1/d^2$  independent of the wave-length, but it is also more directly related to unit-cell dimensions.

This function  $Q(2\theta)$  has been given to 5 decimals in  $\text{Å}^{-2}$  (tabulated as  $10^5 Q$ ) for limited but overlapping ranges of  $2\theta$ , for Cu  $K\alpha$  and Cu  $K\alpha_1$  (Donnay & Donnay, 1951). Published in a limited edition, the table was reprinted in 1955 and is still available.

2. New tables have recently been compiled and published (de Wolff, 1959), which give  $Q(2\theta)$  to 5 decimals in  $\text{Å}^{-2}$  (tabulated as  $10^4 Q$ , to one decimal) for  $2\theta = 4^\circ (0.01^\circ) 180^\circ$ . Two volumes have appeared: Vol. I for Cu  $K\alpha_1$  and Vol. II for Fe  $K\alpha_1$ . They can be ordered from the publishers, Technisch Physische Dienst. T.N.O. & T.H., Delft, Netherlands. Price 5 guilders or 10 sh. (U.K.) or \$1.50 per volume. To reduce handling charges all orders must be accompanied by cheque, bank or postal money orders. Banking transactions can be placed through Amsterdamsche Bank N.V., Delft, Netherlands. Tables for other radiations are in preparation.

3. Recently a table of inverse squares especially designed for converting  $d$  into  $Q$  was published (Azaroff & Buerger, 1958). By means of this table the experimentally determined angle  $\theta$  can, indirectly, be converted into  $Q$ , but the procedure results in the accumulation of rounding off errors. This is particularly undesirable because  $Q$ , unlike  $d$ , serves as a starting point for further calculations. It is better, therefore, to use a  $Q(2\theta)$  table for this purpose.

4. Finally there exists an inexpensive table (*National Bureau of Standards*, 1949) that gives  $\sin x$  (and  $\cos x$ ) for  $x = 0 (0.01^\circ) 90^\circ$ . This table will be found serviceable when no  $Q$  table is available for the wave-length used (Donnay & Donnay, 1959).

#### References

- AZAROFF, L. V. & BUERGER, M. J. (1958). 'The Powder Method in X-ray Crystallography' McGraw Hill, New

York. Appendix 2, Table of 'Conversion of  $d$  to  $Q$ '. Interval in  $d = 0.001 \text{ \AA} \cdot Q$  given to four decimal places for  $d = 1-4$ , to six decimal places for  $d = 4-10$ .

DONNAY, G. & DONNAY, J. D. H. (1951). Tables for the interpretation of X-ray diffraction data, giving the square of the reciprocal lattice vector to 5 decimals in terms of the deviation angle  $2\theta$  for every hundredth of a degree from  $10.00^\circ$  to  $49.99^\circ$  for  $\text{Cu } K\alpha$  and from  $25.00^\circ$  to  $69.00^\circ$  for  $\text{Cu } K\alpha_1$ . Publication of the Crystallographic Laboratory, The Johns Hopkins University, Baltimore 18, Maryland (1951). Limited edition. (Reprinting, 1955). Price \$5.00.

DONNAY, J. D. H. & DONNAY, G. (1959). Sine table for indexing powder patterns. Amer. Min. (In press).

DE WOLFF, P. M. (1959). Tables of  $10^4 Q$  ( $10^4/d^2$ ) as a function of diffraction angle. Technisch Physische Dienst. T.N.O. & T.H., Delft, Netherlands. Hfl. 5 or 10 sh. (U.K.) or \$1.00 per volume.

National Bureau of Standards (1949). Table of sines and cosines to fifteen decimal places at hundredths of a degree. U.S. Department of Commerce, National Bureau of Standards, Applied Mathematics Series 5. U.S. Govt. Printing Office, Washington, D.C. Price 45 cents.

### CaTaO<sub>3</sub>: Un nouveau composé de type pérovskite

La formule du composé CaTaO<sub>3</sub> décrit dans l'article de M. Gasperin (*Acta Cryst.* (1958), **11**, 739) est erronée: l'auteur a pu, depuis cette publication, fabriquer assez de produit pour faire deux analyses chimiques, et toutes deux ont montré, sans ambiguïté, que le composé étudié répond à la formule CaTa<sub>2</sub>O<sub>6</sub>.

La densité calculée à partir de la formule exacte est  $7,07 \text{ g.cm.}^{-3}$  et correspond mieux à la densité mesurée:  $7,0 \text{ g.cm.}^{-3}$ . Il n'est plus nécessaire de supposer une réduction de la valence du tantale pour expliquer cette pérovskite: elle est d'un type nouveau:  $AB_2O_6$ , et sa structure s'interprète en supposant que les atomes  $y$  occupent les mêmes positions que dans les pérovskites classiques  $ABO_3$ , mais qu'un atome  $A$  sur deux est manquant. Les positions  $A$  laissées libres peuvent être ordonnées, ce qui expliquerait les raies de surstructure observées sur le cliché.

### La méthode statistique dans le cas d'une structure partiellement connue

Dans le mémoire par E. F. Bertaut (*Acta Cryst.* (1957), **10**, 670), une erreur de transcription s'est produite. Au lieu de  $\alpha$  (5) il faut lire

$$\alpha = 1 + \frac{1}{2} \frac{\sum (\mathcal{R}_k^2 - 1) \mathcal{R}_l (\mathcal{A}_k^2 - 1) \mathcal{A}_l}{\sum \mathcal{R}_k \mathcal{R}_l \mathcal{R}_m \mathcal{A}_k \mathcal{A}_l \mathcal{A}_m + \dots} \quad (5')$$

Par conséquent, on doit remplacer  $(1 + \alpha)$  (4),  $[1 + \alpha^+]$  (6),  $[1 + \alpha^-]$  (7), respectivement par  $\alpha$ ,  $\alpha^+$ ,  $\alpha^-$ .

Toutes les autres relations restent inchangées.

### An improved method for determining the relative positions of molecules

Errors occur in the above article by C. A. Taylor & K. A. Morley (*Acta Cryst.* (1959), **12**, 101). In the expressions for  $G(h, k)$  when  $h+k$  is even (equation (2)) and for  $P(h, k)$  and  $Q(h, k)$  when  $h+k$  is even (equation (3)) for  $+B$  substitute  $-C$  and for  $+C$  substitute  $-B$ .

## Book Reviews

*Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 333, Jay Street, Brooklyn 1, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.*

**Zone Melting.** By W. G. PFANN. Pp. 236 with 127 figs. New York: Wiley; London: Chapman & Hall. 1958. Price 60s.

It is fitting that the first book on zone-melting should come from the author of the first paper on the subject; and the resulting volume goes far to meet the claim on the dust-jacket—'complete coverage of the theory and practice of this new way of using the freezing process for high purity and control of crystal composition'. After outlining the relationship between zone-melting and fractional crystallisation, and emphasising the significance of the distribution coefficient in both these processes, the author gives a clear account of the theory of zone-refining. It is unfortunate that the rigorous theoretical treatment by Braun and Marshall appeared too late for inclusion in this chapter, and perhaps surprising to find here experimental details of a 'do-it-yourself' analogue computer. In later chapters the techniques and applications of zone-refining are enumerated

in great detail, and these must prove invaluable to anyone faced with the problem of preparing material of very high purity, or with controlled distribution of specific impurities.

One of the greatest difficulties in practical zone-refining is to determine the success of the operation. In most applications, the remaining impurity concentrations are so small as to lie beyond the limit of detection by conventional means. New techniques, often of great intricacy, have to be devised, and these are dismissed in this book in less than one page. In view of the importance of this aspect of the subject, one chapter would seem more appropriate.

The book upholds in every way the high standard of production associated with the Wiley Series on the Science and Technology of Materials.

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