dass sich die Fluoratome auf der Verbindungslinie Na–Sb befinden. Die SbF_6-Baugruppe ist demnach im $NaSbF_6$ wie der $PtCl_6$-Komplex im K_2PtCl_6 angeordnet; die Lage der Kationen ist natürlich eine andere. Das Maximum der Fluoratome entspricht einem Sb–F-Abstand von 1,78 Å, der in guter Übereinstimmung mit dem Sb–F-Abstand von 1,77 Å ist, den Bode & Voss (1951) im $KSbF_6$ feststellten; aus der Länge der a-Achse berechnet man nach Subtraktion der Na- und F-Ionenradien einen Sb–F-Abstand von 1,782 Å. Schrewelius verwendet in seinem Strukturvorschlag einen Sb–F-Abstand von 1,95 Å und beschreibt die 24 Fluoratome in der allgemeinen Lage x, y, z, da mit dem grösseren Sb–F-Abstand die oben angeführte Struktur nicht möglich ist. Dadurch geht der flächenzentrierte Charakter der Elementarzelle verloren und es müssen schwache Reflexe mit gemischten Indices auftreten. Derartige Reflexe werden jedoch nicht beobachtet, was Schrewelius auf die geringe Intensität der gemischten Reflexe zurückführt; die Möglichkeit, dass die 24 Fluoratome statistisch über eine 96-zählige flächenzentrierte Lage verteilt sind, wird dabei nicht berücksichtigt.

Die Anordnung der Atome erfolgt in der Raumgruppe $Fm3m$–O_h^5 in folgenden Punktlagen:

4 Sb	(a)	0, 0, 0;
4 Na	(b)	$\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$;
24 F	(e)	x, 0, 0, mit $x = 0{,}217$.

Die Exponenten B im Temperaturfaktor für die einzelnen Atome, $\exp(-B \sin^2 \theta/\lambda^2)$, lauten:

$$B(\text{Na}) = B(\text{F}) = 2{,}7 \text{ Å}^2, \ B(\text{Sb}) = 1{,}35 \text{ Å}^2 .$$

Unter Berücksichtigung aller berechneten und experimentellen Strukturfaktoren erhält man einen R-Wert (*reliability index*) von 0,095 — einer befriedigenden Übereinstimmung der berechneten und experimentellen Werte entsprechend.

Aus dem Quotienten Molekulargewicht/Dichte ($d_{\text{röntg.}} = 3{,}134$ g.cm.$^{-3}$) ergibt sich ein experimentell ermitteltes Molvolumen von 82,6 cm.^{3}, während aus den Biltzschen Rauminkrementen (1934) 63,5 cm.^{3} folgt. Diese Diskrepanz lässt sich in der Weise deuten, dass die Fluoratome, die in der Position x, 0, 0 einen F–F-Abstand von 3,27 Å zwischen benachbarten SbF_6-Baugruppen aufweisen, sich durch die Schwingung bis zur gegenseitigen Berührung nähern. Aus dem Temperaturfaktor für die Fluoratome berechnet man nach Artmann (1948) eine Schwingungsamplitude von 0,26 Å; demzufolge können sich die Fluoratome optimal bis auf 2,75 Å nähern. Im $KSbF_6$ beträgt der (konstante) F–F-Abstand zwischen benachbarten SbF_6-Baugruppen 2,78 Å, aus dem Fluorionenradius berechnet man 2,66 Å.

Es ist nun von Interesse, $NaSbF_6$ bei einer Temperatur zu untersuchen, bei der die Schwingung der Fluoratome 'eingeschlafen' ist. Dieser Effekt liegt bei $-40°$ C. vor. Man erhält jedoch ein Röntgendiagramm, das nicht mehr kubisch zu indizieren ist und bisher nicht aufgeklärt werden konnte. Es hat den Anschein, dass die SbF_6-Baugruppe, die nicht genau oktaedrisch gebaut ist, wie im $KSbF_6$ gefunden wurde, beim 'Einschlafen' der Temperaturbewegung der Atome einen Modifikationswechsel verursacht. Bei Zimmertemperatur erscheint jedoch die SbF_6-Baugruppe durch die Schwingung oktaedrisch gebaut und bedingt dadurch die hoch-symmetrische Struktur des $NaSbF_6$.

Referenzen

ARTMANN, K. (1948). *Z. Phys.* **125**, 298.
BILTZ, W. (1934). *Raumchemie der festen Stoffe.* Leipzig: Voss.
BODE, H. & VOSS, E. (1951). *Z. anorg. Chem.* **264**, 144.
SCHREWELIUS, N. (1938). *Z. anorg. Chem.* **238**, 241.

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 British Co-editor (R. C. Evans, Crystallographic Laboratory, Cavendish Laboratory, Cambridge, England).

Cambridge Summer School in Automatic Computing, 1956

A Summer School in programme design for automatic digital computing machines will be held in the University Mathematical Laboratory at Cambridge, England, during the period 17–28 September 1956. The course will give a basic training in the mathematical use of machines, dealing with the processes employed and their embodiment in programmes which specify the operation in detail. Lectures and practical classes will be held in the design of programmes for the EDSAC, the machine which has been built in the Laboratory. It will be shown how the same principles may be applied in designing programmes for other machines.

A detailed syllabus and form of application for admission may be obtained from G. F. Hickson, Secretary of the Board of Extra-Mural Studies, Stuart House, Cambridge, to whom the completed application form should be returned not later than 15 June 1956.

Twinning in barium titanate crystals

Errors occur in the above Short Communication by E. A. D. White (*Acta Cryst.* (1955), **8**, 845). The three calculated angles for the acute-angled twins should read 37° 52′, 40° 00′ and 38° 56′ respectively.

A note on the calculation of the absorption factors for single crystals with high absorbing power

An error occurs in the above Short Communication by D. Grdenić (*Acta Cryst.* (1952), **5**, 283). In the denominator of the expression for $A(4)$ the sine term should be $\sin \varphi_2/\sin \psi_2$.

Preparation of a new edition of *Crystal Data*

Preparations are now being made for a second edition of the tables of cell constants which first appeared as Part II of *Crystal Data* (J.D.H.Donnay & W. Nowacki, Memoir 60 of the Geological Society of America, 1954) (see *Acta Cryst.* (1954), **7**, 607).

The work of revision will involve correcting errors and omissions in the old material, incorporating all the new material since 1 January 1951 and possibly re-casting the presentation of the data to ensure maximum convenience for all users. It is intended to include all single-crystal data, published or submitted directly to the editors before the closing date (probably middle 1957), for elements, inorganic and organic compounds (excluding fibres and other semi-crystalline high polymers) and minerals. Metallurgical data (alloys) will not be given since they are not considered very suitable for inclusion in a determinative index of this type and they are in any case covered by the *Metals Reference Book* of Smithells (Butterworth) and by a forthcoming publication of W. B. Pearson. The work is being carried out, with the approval of the International Union of Crystallography, by a team consisting of J. D. H. Donnay (editor-in-chief), E. G. Cox (editor of inorganic section) and Olga Kennard (editor of organic section) and their assistants. Crystallographers are invited to help to improve the new edition by sending their own data to the editors (see below).

Data which would not otherwise be published will be particularly welcome, and appropriate acknowledgment will be made. Authors are also invited especially to draw the attention of the editors to any record of crystal data which appears as a minor part of a paper on some other subject and which is thereby liable to be overlooked by abstractors. Although *Crystal Data* is essentially an index of information obtained by single-crystal methods, cell dimensions obtained from reliable and *completely* indexed powder photographs will also be welcome.

It is requested that the information should be submitted as nearly as possible in the same form as the example shown below; blanks for the purpose together with some explanatory notes, can be obtained on application to the editors. It is hoped that crystallographers will not refrain from submitting information because it is incomplete; the crystal system and cell dimensions alone are of sufficient interest to justify an entry in the new edition.

In the case of minerals, authors are requested wherever possible to give locality and chemical analysis, and in the case of new chemical compounds it is desirable to have some information about the source of the material, e.g. a reference to a paper on its preparation or isolation and an analysis of the actual material used for the X-ray work.

Please send information as follows:

1. Corrections to entries in, and omissions from, the first edition to Prof. J. D. H. Donnay, Crystallographic Laboratory, The Johns Hopkins University, Baltimore 18, Md., U.S.A.
2. New information on elements, inorganic compounds and minerals to Prof. E. G. Cox, School of Chemistry, The University, Leeds 2, England.
3. New information on organic compounds to Dr Olga Kennard, National Institute for Medical Research, The Ridgeway, Mill Hill, London N.W. 7, England.

Example

Substance: *iso*-CORYDINE (ARTABOTRINE; 4-HYDROXY-3,5,6-TRIMETHOXYAPORPHINE)　　　　Formula: $C_{20}H_{23}O_4N$

System: Orthorhombic　　　Space group: $P2_12_12_1$　　　No. of formula-weights per cell: 4
Wavelength used: $\lambda = 1\cdot539$ kX.　　　Crystal structure: unknown

$a = 23\cdot13 \pm 0\cdot08$　　$b = 9\cdot89 \pm 0\cdot05$　　$c = 7\cdot51 \pm 0\cdot05$ kX.　　Density (obs.): $1\cdot29$ g.cm.$^{-3}$
$\alpha = \quad\pm$　　$\beta = \quad\pm$　　$\gamma = \quad\pm$　　Density (calc.): $1\cdot32$ g.cm.$^{-3}$

$(a : b : c)_{\text{X-ray}} = 2\cdot339 : 1 : 0\cdot759$　　$(a : b : c)_{\text{gon.}} = 2\cdot364 : 1 : 0\cdot7837$

Source: Analysed specimen supplied by Barger & Sargent　　M.p. 185–186° C.
　　　　(see ref. 1)

Habit: Tabular on {100}; other forms {210} and {201}
　　　　see ref. 1 for illustration

Optical properties:
　　(all for NaD)　　$n(\alpha) = 1\cdot50$ approx., $n(\beta) = 1\cdot67$, $n(\gamma) = 1\cdot75$
　　　　$2V = 70°$ approx. Acute bisectrix [a], plane of optic axes (001).

References: (1) Barger & Sargent, *J. Chem. Soc.*, p. 991, 1939 (with crystallographic measurements by C. J. Brown & E. G. Cox.)
　　　　(2) Schlittler & Huber, *Helv. Chim. Acta*, **35**, 111, 1952
Remarks:
　　　　According to ref. 2 the artabotrine of ref. 1 is identical with *iso*-corydine

Date: 30-4-56　　　　　　　　　　　　　　　　　　Signature: E. G. Cox.

Name & Address (block capitals): E. G. COX, SCHOOL OF CHEMISTRY,
　　　　　　　　　　THE UNIVERSITY, LEEDS 2, ENGLAND.

International Tables for X-ray Crystallography

The Editors give notice of the following corrections to *International Tables for X-ray Crystallography*, vol. 1 (1952, Birmingham: Kynoch Press).

p. 1.   End of 4th paragraph: Axel, not Alex.

p. 2.   Column 1, line 22: 76, not 16.

p. 14.   Fig. 2·4·1 is not quite geometrically exact; in particular the direction 000–110 should be normal to the (110) planes.

p. 24.   Tertiary position, hexagonal system: Mirror lines, parallel, not Mirror lines at 90°.

p. 208. No. 118 should be $P\bar{4}n2$, not $P4n2$.

p. 294. Some copies only have the bar over the 6 in $P\bar{6}m2$ missing (large type, top left corner of page).

p. 360. Formula at top of page should read

$$A = 16 \cos 2\pi \frac{h+k+l}{4}$$

$$\times \left\{ \cos 2\pi \left(hx + \frac{l}{4} \right) \cos 2\pi \left(ky + \frac{h}{4} \right) \cos 2\pi \left(lz + \frac{k}{4} \right) \right.$$

$$+ \cos 2\pi \left(hz + \frac{l}{4} \right) \cos 2\pi \left(kx + \frac{h}{4} \right) \cos 2\pi \left(ly + \frac{k}{4} \right)$$

$$+ \cos 2\pi \left(hy + \frac{l}{4} \right) \cos 2\pi \left(kz + \frac{h}{4} \right) \cos 2\pi \left(lx + \frac{k}{4} \right)$$

$$+ \cos 2\pi \left(h + k + \frac{l}{4} \right)$$

$$\times \left[\cos 2\pi \left(hx + \frac{k}{4} \right) \cos 2\pi \left(ly + \frac{h}{4} \right) \cos 2\pi \left(kz + \frac{l}{4} \right) \right.$$

$$+ \cos 2\pi \left(hy + \frac{k}{4} \right) \cos 2\pi \left(lz + \frac{h}{4} \right) \cos 2\pi \left(kx + \frac{l}{4} \right)$$

$$\left. \left. + \cos 2\pi \left(hz + \frac{k}{4} \right) \cos 2\pi \left(lx + \frac{h}{4} \right) \cos 2\pi \left(ky + \frac{l}{4} \right) \right] \right\}.$$

p. 435. End of 5th line from bottom: $|(Fhkl)|$ should be $|F(hk\bar{l})|$.

p. 454. $P4/mnm$ should be $P4_2/mnm$.

p. 461. D_{4h}^{02} (top right-hand corner) should be D_{4h}^{20}.

p. 505. Interchange   (9) and (13),
                       (12) and (16),
                       (11) and (15),
                       (10) and (14)

at the ends of appropriate rows.

p. 520. (6) The formula should read

$$A = 32 \{ \cos 2\pi lz \cos \pi(h+k)(x+y) \cos \pi(h-k)(x-y)$$

$$+ \sin 2\pi lz \sin \pi(h-k)(x+y) \cos \pi(h+k)(x-y)$$

$$+ \cos 2\pi lx \cos \pi(h+k)(y+z) \cos \pi(h-k)(y-z)$$

$$+ \sin 2\pi lx \sin \pi(h-k)(y+z) \cos \pi(h+k)(y-z)$$

$$+ \cos 2\pi ly \cos \pi(h+k)(z+x) \cos \pi(h-k)(z-x)$$

$$+ \sin 2\pi ly \sin \pi(h-k)(z+x) \cos \pi(h+k)(z-x) \}$$

$$F(hkl) = F(\bar{h}k\bar{l}) = F(\bar{h}kl) = -F(h\bar{k}l) = F(hk\bar{l})$$

(7) should read
    Change $h \to k \to l \to h$ in formulae (6).

(8) should read
    Change $h \to l \to k \to h$ in formulae (6).

$$F(hkl) = F(\bar{h}k\bar{l}) = -F(\bar{h}kl) = F(h\bar{k}l) = F(hk\bar{l}).$$

p. 529. Last line: $x, 0, \frac{1}{3}$ should be $\bar{x}, 0, \frac{1}{2}$.

p. 534. Table 5·1·1. The diagrams for the 2nd and 6th case of the monoclinic system should be interchanged. The text is correct.

Book Reviews

Works intended for notice in this column should be sent direct to the Editor (P. P. Ewald, Polytechnic Institute of Brooklyn, 99 Livingston Street, Brooklyn 1, N.Y., U.S.A.). As far as practicable books will be reviewed in a country different from that of publication.

Diffusion in Metallen. By W. SEITH and T. HEUMANN. Pp. vi+306 with 238 figs. Berlin, Göttingen, Heidelberg: Springer. 2nd ed. 1955. Price DM. 39.

Since publication of the first edition of Seith's book in 1939 many new results have been obtained and considerable progress in understanding diffusion phenomena in metals has been made. The second edition has, therefore, been considerably enlarged. It gives a well balanced summary of experimental methods, numerical values of diffusion coefficients, theoretical interpretation, and applications. Although other authors have published excellent and more detailed reviews on the theory of metallic diffusion, this book is especially recommended as a helpful introduction and a valuable reference work because it covers practical and theoretical aspects.

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