

INTERNATIONAL TABLES
FOR
X-RAY CRYSTALLOGRAPHY
VOLUME III
PHYSICAL AND CHEMICAL TABLES

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FOR
X-RAY CRYSTALLOGRAPHY

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Volume III
PHYSICAL AND CHEMICAL TABLES

Editors

CAROLINE H. MACGILLAVRY and GERARD D. RIECK

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(continued) *Table 1* continued

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p.1. Column 1, line 9. B (rom.) *should be* B (ital.).

p. 9. Section 2.1.6; example 1(b). The author has supplied the following correction:

The statement "If the u_i, u_j, u_k are relative prime, at least one pair among them must be relative prime . . ." is incorrect. The general form for three relative prime integers is

$$u_i = d_{ij} d_{ik} e_i$$

in which d_{ij} is the highest common factor of u_i and u_j . Thus the sets d_{ij} and e_i are each within themselves pair-wise relative prime, but e_i may have one factor in common with d_{ij} and another (relative prime to the first) in common with d_{jk} .

Under these conditions one must first find all vectors U which are reciprocal to u with relative prime components satisfying

$$u_1 U_1 + u_2 U_2 + u_3 U_3 = 1$$

The general solution for this equation can be expressed as

$$U_i = r_{ki}(q_k - u_k g_k) + d_{jk} e_j h_k$$

$$U_j = r_{ki}(q_k - u_k g_k) - d_{ki} e_i h_k$$

$$U_k = p_k + d_{ij} g_k$$

In these expressions g_k, h_k are arbitrary integers (positive or negative) or zero. The relative prime pair of integers p_k, q_k are a solution of the equation

$$p_k u_k + q_k d_{ij} = 1$$

and the relative prime pair of integers r_{ki}, r_{kj} are a solution of the equation

$$r_{ki} u_i + r_{kj} u_j = d_{ij}$$

There are three representations of the same set of vectors U which may be obtained by cyclic permutation of the subscripts in the above expressions.

In the second stage of the calculation one must obtain sets of two vectors

$$A_1 = a_{11} a_1 + a_{21} a_2 + a_{31} a_3$$

$$A_2 = a_{12} a_1 + a_{22} a_2 + a_{32} a_3$$

(with relative prime components a_{i1}, a_{i2}) whose vector product generates the vector U . Since the components U_i of this vector are relative prime, they have the same general form as the u_i , i.e.

$$U_i = D_{ki} D_{ij} E_i$$

A particular solution is

$$A'_1 = m_{ki} D_{jk} E_k a_i + m_{kj} D_{ki} E_k a_j - D_{ij} a_k$$

$$A'_2 = -D_{jk} E_j a_i + D_{ki} E_i a_j$$

in which $m_{ki} E_i + m_{kj} E_j = 1$.

The general solution is then

$$A_1 = s_1 A'_1 + t_1 A'_2$$

$$A_2 = s_2 A'_1 + t_2 A'_2$$

provided that $s_1 t_2 - s_2 t_1 = 1$.

The undersigned is indebted to Mr. J. F. Nicholas of the Division of Tribophysics, CSIRO, Australia, who pointed out the error in the tables, and to Dr. P. Du Val of University College London for comments on the present solution.

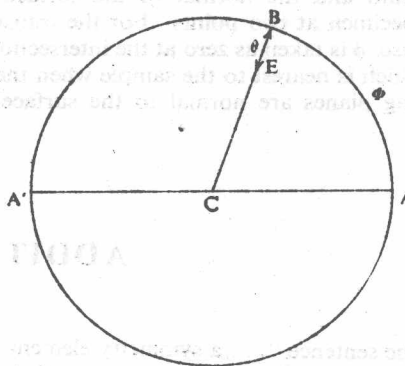
A. L. PATTERSON

p. 46. Correction to previous erratum. Last sentence: the last two cases *should be* cases (c)–(g).

p. 82. NOTE 1. $\int \dots dx$ *should be* $\int \dots du$.

p. 162. Last line. Shiebold *should be* Schiebold.

p. 168. Fig. 4.2.1.2(2) *should be replaced by* the accompanying diagram; with the same legend but adding "The pole of projection is O (cf. Fig. 4.2.1.2(1))."



p. 175. Definition of σ , line 5. *Delete and before* σ ; *insert* d^*_{hki} *before by* Henry . . .

p. 194. Equation (3) *should be* $d^* = \cot \bar{\mu} - s/\sqrt{(r_1^2 + s^2)}$.

p. 221. Table 4.7.3, row Flat Specimen, columns 5 and 6: $\cos \theta$ and $\cos \theta \cot \theta$ *should be* $\cot \theta$ and $\cot^2 \theta$.

p. 237. Definition of f_0 : at absolute zero *should be* for atom at rest.

p. 267. Column 1, line 8 from bottom. *Replace the second* = sign *by* – *and the symbol* μ *by* $\bar{\mu}$. This brings the equation into agreement with the definition of $\bar{\mu}$ given in Section 5.2.5.3. It should be noted that $\bar{\mu} = 90^\circ - \mu$, where μ is as defined in Table 4.3.1,

P.T.O.

p. 175, and again in Section 5.2.5.1. Hence the formula may be written

$$1/L^2 = \xi^2 \sin^2 \mu - \frac{1}{4}(\xi^2 - 2\xi \cos \mu + \xi^2)^2$$

$$\text{or } 1/L^2 = \xi^2 \cos^2 \mu - \frac{1}{4}(\xi^2 - 2\xi \sin \mu + \xi^2)^2$$

The reference to A. L. Mackay's publication is *Acta Cryst.*, 13, 240 (1960).

p. 301, Section 5.3.8. In the first sentence: "variation in absorption" *should be* "variation in diffracting volume and absorption."

Add two notes to the figures, as follows

1. Note that Fig. 5.3.8(1) must be seen from the back to be consistent with Figs. 5.3.8(2) and 5.3.8(3).
2. Note that Figs. 5.3.8(2) and 5.3.8(3) define the convention for the direction of the diffracted beam.

p. 306. Column 1. *Change definitions* as follows:

γ = acute angle between the sheet normal and the incident beam

ϕ = azimuthal angle around the diffraction ring; this ring intersects the plane containing the incident beam and the normal to the surface of the specimen at two points. For the transmission case, ϕ is taken as zero at the intersection point which is nearest to the sample when the reflecting planes are normal to the surface of the

sheet. For the reflection case, $\phi = 0$ at the intersection point contained in the reflection region.

α = acute angle between the sheet normal and the diffracting plane. The sign of α is defined as shown in Figs. 5.3.8(2) and 5.3.8(3).

p. 313. Column 1, line 20, below equation (1): *and this line with a full stop and replace the following line "and consequently . . . weakened."* by "Although within a very narrow angular range there is total reflection, the integrated intensity of the reflected beam is weakened compared with the reflection from a mosaic crystal."

Then after "primary extinction," add "This simple picture is reasonably adequate for the so-called Bragg case; but when both incident and reflected beams emerge on the same side of the crystal (the so-called Laue case) or when the crystal is completely bathed in the primary beam, the situation is more complicated."

p. 314. Equation (10): $(\cos^2 \phi - \sin^2 \theta)$ *should be* $(\cos^2 \phi - \sin^2 \theta)$, where ϕ is the angle between the axis of rotation and the reflecting plane.

p. 324. Equation (9) *should be* $\rho_s(r) = N \left(\frac{r}{\pi} \right)^2 e^{-r^2}$

p. 364. Entry for $x=10.43$ *should be* 2954, not 3954.

Volume I

ADDITIONAL ERRATA

(January 1962)

pp. 46-7. The sentence "... a symmetry element at a distance t along any direction necessarily involves a repetition of this element at a distance $(\frac{1}{2} + t)$ along the same direction" *should read* "... a twofold symmetry element at a primitive translation t ..."

p. 49. The similar phrase "... a symmetry operator at any primitive translation t ..." *should read* "... a twofold symmetry operator t ..."

p. 75. Top left. Triclinic 1 *should be* Triclinic $\bar{1}$.

p. 387. Space group No. 23 (I222)

$$B = -8 \sin 2\pi hx \cos 2\pi ky \cos 2\pi lz \text{ should be}$$

$$B = -8 \sin 2\pi hx \sin 2\pi ky \sin 2\pi lz$$

p. 507. The formula for $c(XYZ)$ *should have* three +

signs at the right-hand side *instead of* three - signs.

p. 550. 85 C_4/n *should be* C_4/a .

86 C_4/n *should be* C_4/a .

88 F_4/a *should be* F_4/d .

There is also some ambiguity in using the notation C_4mb for space group 100 when it is referred to the C lattice because the glide plane parallel to (110) now involves a translation of $(a+b)/4$ for which there is at present no separate symbol. Similarly in space group 102, now called C_4mn , the glide after reflection across (110) is $[(a+b)/4 + c/2]$. Corresponding glides occur in space groups 104, 106, 117, 118, 125, 126, 127, 128, 133, 134, 135, 136 when referred to a C lattice.

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