Acta Cryst. (1949). **2**, 322

General Transformation Formulae in Geometric Crystallography

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(*Received* 23 *March* 1949)

For two settings of a crystal, given four sets of corresponding indices, the compatible transformation equations are derived. The four sets may be face indices, edge indices or a mixed group of four sets.

Most text-books on geometric crystallography mention transformation formulae only for a few important particular cases or even none.

Liebisch (1881, p. 55) derived general formulae with the aid of analytic geometrical and Hecht (1893, p. 58) of algebraic methods. These derivations are not easy and their application is not simple.

It is possible, however, to give the derivation in a specific crystallographic way by means of the direct and indirect (reciprocal) lattice.

First we mention the formulae valid for these two lattices (de Jong & Bouman, 1939).

The direct elements may be $a, b, c, \alpha, \beta, \gamma$ and a lattice point $[[uvw]]$; the corresponding indirect elements a^*, b^*, c^*, α^*, β^*, γ^* and a lattice point $[[hkl]]$. After the transition to new direct axes and corresponding new indirect axes the points may be symbolized $[[UVW]]$ and $[[HKL]]$. Then the relevant equations are:

$$\left.\begin{array}{ll} H=u_A h+v_A k+w_A l, & U=h_A u+k_A v+l_A w,\\ K=u_B h+v_B k+w_B l, & V=h_B u+k_B v+l_B w,\\ L=u_C h+v_C k+w_C l, & W=h_C u+k_C v+l_C w,\\ h=h_A H+h_B K+h_C L, & u=u_A U+u_B V+u_C W,\\ k=k_A H+k_B K+k_C L, & v=v_A U+v_B V+v_C W,\\ l=l_A H+l_B K+l_C L, & w=w_A U+w_B V+w_C W,\end{array}\right\} \quad (1)$$

wherein, for example,

$$\left. h_B=\frac{-\begin{vmatrix} v_A & w_A\\ v_C & w_C\end{vmatrix}}{\begin{vmatrix} u_A & v_A & w_A\\ u_B & v_B & w_B\\ u_C & v_C & w_C\end{vmatrix}} \quad\text{and}\quad v_C=\frac{-\begin{vmatrix} h_A & l_A\\ h_B & l_B\end{vmatrix}}{\begin{vmatrix} h_A & k_A & l_A\\ h_B & k_B & l_B\\ h_C & k_C & l_C\end{vmatrix}}.\right\} \quad (2)$$

The coefficients in (1) are the co-ordinates of the points nearest to the origin O, or to O^*, of the old or new axes, described in new or old co-ordinates respectively. This is obvious by inserting

$$\text{old } [[hkl]] \equiv [[100]] \quad \text{becomes} \quad \text{new } [[u_A u_B u_C]], \text{etc.} \quad (3)$$

The symbols $[uvw]$ of crystal edges and (hkl) of faces are not absolute numbers, but they indicate ratios, so that they do not correspond to one point in the lattice concerned but to a row of lattice points, which contain O or O^*. Therefore the edge $[uvw]$ corresponds to $f[[uvw]]$ and the face (hkl) to $f^*[[hkl]]$, wherein f and f^* are whole numbers.

The determination of the nine quantities $u_A \dots w_C$ and the dependent $h_A \dots l_C$ demands three transitions:

$$\begin{array}{ccc} [[u_1v_1w_1]], & [[u_2v_2w_2]], & [[u_3v_3w_3]],\\ \downarrow & \downarrow & \downarrow\\ [[U_1V_1W_1]], & [[U_2V_2W_2]], & [[U_3V_3W_3]].\end{array}$$

The determination demands, however, four transitions of rows:

$$\begin{array}{ccc} f_1[[u_1v_1w_1]] & \dots & f_4[[u_4v_4w_4]],\\ \downarrow & & \downarrow\\ F_1[[U_1V_1W_1]] & \dots & F_4[[U_4V_4W_4]].\end{array}$$

For, from the twelve equalities

$$f_1u_1=u_AF_1U_1+u_BF_1V_1+u_CF_1W_1,$$
$$\vdots$$
$$f_4u_4=w_AF_4U_4+w_BF_4V_4+w_CF_4W_4,$$

nine quantities $u_A \dots w_C$ and three

$$\text{ratios} \qquad \frac{f_1/F_1}{f_2/F_2},\quad \frac{f_2/F_2}{f_3/F_3} \quad\text{and}\quad \frac{f_3/F_3}{f_4/F_4}$$

can be derived.

Algebraically, however, this calculation is cumbersome, and we choose the following method.

Four transitions of edges may be given:

$$\begin{array}{cccc} [u_1v_1w_1], & [u_2v_2w_2], & [u_3v_3w_3], & [u_4v_4w_4],\\ \downarrow & \downarrow & \downarrow & \downarrow\\ [U_1V_1W_1], & [U_2V_2W_2], & [U_3V_3W_3], & [U_4V_4W_4],\end{array}$$

and we desire to know the formulae for the transition of an arbitrary edge $[uvw] \rightarrow [UVW]$, in other words the quantities $u_A \dots w_C$.

We consider the corresponding rows in the direct lattice and apply the property that it is always possible to indicate a row-point on each of the first three rows in such a manner that the vectorial sum of the radius vectors from O to these points determines the radius vector from O to a point of the fourth row; these points may be $[[\lambda_1u_1, \lambda_1v_1, \lambda_1w_1]]$, etc. Then

$$\left.\begin{array}{rl} & \lambda_4u_4=\lambda_1u_1+\lambda_2u_2+\lambda_3u_3,\\ & \lambda_4v_4=\lambda_1v_1+\lambda_2v_2+\lambda_3v_3,\\ & \lambda_4w_4=\lambda_1w_1+\lambda_2w_2+\lambda_3w_3,\\ \text{and} & \Lambda_4U_4=\Lambda_1U_1+\Lambda_2U_2+\Lambda_3U_3,\\ & \Lambda_4V_4=\Lambda_1V_1+\Lambda_2V_2+\Lambda_3V_3,\\ & \Lambda_4W_4=\Lambda_1W_1+\Lambda_2W_2+\Lambda_3W_3.\end{array}\right\} \quad (4)$$

From Fig. 1 it follows that

$$\frac{\lambda_1 r_1}{\Lambda_1 R_1}=\frac{\lambda_2 r_2}{\Lambda_2 R_2} \quad \text{and} \quad \frac{\lambda_1 r_1}{\Lambda_1 R_1}=\frac{\lambda_3 r_3}{\Lambda_3 R_3}.$$

Now $r_1=R_1$, $r_2=R_2$ and $r_3=R_3$, so that

$$\frac{\lambda_1}{\Lambda_1}=\frac{\lambda_2}{\Lambda_2}=\frac{\lambda_3}{\Lambda_3}. \tag{5}$$

Analogously

$$\left.\begin{aligned} \mu u&=\mu_1 u_1+\mu_2 u_2+\mu_3 u_3,\\ \mu v&=\mu_1 v_1+\mu_2 v_2+\mu_3 v_3,\\ \mu w&=\mu_1 w_1+\mu_2 w_2+\mu_3 w_3,\\ MU&=M_1 U_1+M_2 U_2+M_3 U_3,\\ MV&=M_1 V_1+M_2 V_2+M_3 V_3,\\ MW&=M_1 W_1+M_2 W_2+M_3 W_3,\end{aligned}\right\} \tag{6}$$

and

$$\frac{\mu_1}{M_1}=\frac{\mu_2}{M_2}=\frac{\mu_3}{M_3}. \tag{7}$$

From (5) and (7) it follows that

$$\frac{\lambda_1/\Lambda_1}{\mu_1/M_1}=\frac{\lambda_2/\Lambda_2}{\mu_2/M_2}=\frac{\lambda_3/\Lambda_3}{\mu_3/M_3}=G, \tag{8}$$

where G is a number.

We derive from (4)

$$\lambda_1=\frac{\lambda_4\begin{vmatrix} u_4 & u_2 & u_3\\ v_4 & v_2 & v_3\\ w_4 & w_2 & w_3\end{vmatrix}}{\begin{vmatrix} u_1 & u_2 & u_3\\ v_1 & v_2 & v_3\\ w_1 & w_2 & w_3\end{vmatrix}}, \quad \Lambda_1=\frac{\Lambda_4\begin{vmatrix} U_4 & U_2 & U_3\\ V_4 & V_2 & V_3\\ W_4 & W_2 & W_3\end{vmatrix}}{\begin{vmatrix} U_1 & U_2 & U_3\\ V_1 & V_2 & V_3\\ W_1 & W_2 & W_3\end{vmatrix}},$$

and, from (6), analogous expressions for μ_1 and M_1.

The equality of the first and fourth term of (8) then becomes

$$\frac{\lambda_4\begin{vmatrix} u_4 & u_2 & u_3\\ v_4 & v_2 & v_3\\ w_4 & w_2 & w_3\end{vmatrix}}{\begin{vmatrix} u_1 & u_2 & u_3\\ v_1 & v_2 & v_3\\ w_1 & w_2 & w_3\end{vmatrix}}\times\frac{M\begin{vmatrix} U & U_2 & U_3\\ V & V_2 & V_3\\ W & W_2 & W_3\end{vmatrix}}{\begin{vmatrix} U_1 & U_2 & U_3\\ V_1 & V_2 & V_3\\ W_1 & W_2 & W_3\end{vmatrix}}$$

$$\times\frac{\begin{vmatrix} u_1 & u_2 & u_3\\ v_1 & v_2 & v_3\\ w_1 & w_2 & w_3\end{vmatrix}}{\mu\begin{vmatrix} u & u_2 & u_3\\ v & v_2 & v_3\\ w & w_2 & w_3\end{vmatrix}}\times\frac{\begin{vmatrix} U_1 & U_2 & U_3\\ V_1 & V_2 & V_3\\ W_1 & W_2 & W_3\end{vmatrix}}{\Lambda_4\begin{vmatrix} U_4 & U_2 & U_3\\ V_4 & V_2 & V_3\\ W_4 & W_2 & W_3\end{vmatrix}}=G,$$

or

$$\frac{M\lambda_4}{\Lambda_4\mu G}\begin{vmatrix} U & U_2 & U_3\\ V & V_2 & V_3\\ W & W_2 & W_3\end{vmatrix}=\frac{\begin{vmatrix} U_4 & U_2 & U_3\\ V_4 & V_2 & V_3\\ W_4 & W_2 & W_3\end{vmatrix}}{\begin{vmatrix} u_4 & u_2 & u_3\\ v_4 & v_2 & v_3\\ w_4 & w_2 & w_3\end{vmatrix}}\begin{vmatrix} u & u_2 & u_3\\ v & v_2 & v_3\\ w & w_2 & w_3\end{vmatrix}.$$

We call the fraction P_1, and have further in the same manner P_2 and P_3. Hence

$$P_1\equiv\frac{\begin{vmatrix} U_2 & U_3 & U_4\\ V_2 & V_3 & V_4\\ W_2 & W_3 & W_4\end{vmatrix}}{\begin{vmatrix} u_2 & u_3 & u_4\\ v_2 & v_3 & v_4\\ w_2 & w_3 & w_4\end{vmatrix}}, \quad P_2\equiv\frac{\begin{vmatrix} U_1 & U_3 & U_4\\ V_1 & V_3 & V_4\\ W_1 & W_3 & W_4\end{vmatrix}}{\begin{vmatrix} u_1 & u_3 & u_4\\ v_1 & v_3 & v_4\\ w_1 & w_3 & w_4\end{vmatrix}},$$

$$P_3\equiv\frac{\begin{vmatrix} U_1 & U_2 & U_4\\ V_1 & V_2 & V_4\\ W_1 & W_2 & W_4\end{vmatrix}}{\begin{vmatrix} u_1 & u_2 & u_4\\ v_1 & v_2 & v_4\\ w_1 & w_2 & w_4\end{vmatrix}}.$$

Then, from the three equalities (8),

$$\frac{M\lambda_4}{\Lambda_4\mu G}\begin{vmatrix} U & U_2 & U_3\\ V & V_2 & V_3\\ W & W_2 & W_3\end{vmatrix}=P_1\begin{vmatrix} u & u_2 & u_3\\ v & v_2 & v_3\\ w & w_2 & w_3\end{vmatrix},$$

$$\frac{M\lambda_4}{\Lambda_4\mu G}\begin{vmatrix} U_1 & U & U_3\\ V_1 & V & V_3\\ W_1 & W & W_3\end{vmatrix}=P_2\begin{vmatrix} u_1 & u & u_3\\ v_1 & v & v_3\\ w_1 & w & w_3\end{vmatrix},$$

$$\frac{M\lambda_4}{\Lambda_4\mu G}\begin{vmatrix} U_1 & U_2 & U\\ V_1 & V_2 & V\\ W_1 & W_2 & W\end{vmatrix}=P_3\begin{vmatrix} u_1 & u_2 & u\\ v_1 & v_2 & v\\ w_1 & w_2 & w\end{vmatrix}.$$

Omitting the common factor and solving for U, V and W, we find the ratios $U:V:W$, wherein

$$\begin{aligned} U=&\left[\begin{vmatrix} v_2 & w_2\\ v_3 & w_3\end{vmatrix}P_1 U_1+\begin{vmatrix} v_3 & w_3\\ v_1 & w_1\end{vmatrix}P_2 U_2+\begin{vmatrix} v_1 & w_1\\ v_2 & w_2\end{vmatrix}P_3 U_3\right]u\\ &+\left[\begin{vmatrix} w_2 & u_2\\ w_3 & u_3\end{vmatrix}P_1 U_1+\begin{vmatrix} w_3 & u_3\\ w_1 & u_1\end{vmatrix}P_2 U_2+\begin{vmatrix} w_1 & u_1\\ w_2 & u_2\end{vmatrix}P_3 U_3\right]v\\ &+\left[\begin{vmatrix} u_2 & v_2\\ u_3 & v_3\end{vmatrix}P_1 U_1+\begin{vmatrix} u_3 & v_3\\ u_1 & v_1\end{vmatrix}P_2 U_2+\begin{vmatrix} u_1 & v_1\\ u_2 & v_2\end{vmatrix}P_3 U_3\right]w,\end{aligned}$$

$$\begin{aligned} V=&\left[\begin{vmatrix} v_2 & w_2\\ v_3 & w_3\end{vmatrix}P_1 V_1+\begin{vmatrix} v_3 & w_3\\ v_1 & w_1\end{vmatrix}P_2 V_2+\begin{vmatrix} v_1 & w_1\\ v_2 & w_2\end{vmatrix}P_3 V_3\right]u\\ &+\left[\begin{vmatrix} w_2 & u_2\\ w_3 & u_3\end{vmatrix}P_1 V_1+\begin{vmatrix} w_3 & u_3\\ w_1 & u_1\end{vmatrix}P_2 V_2+\begin{vmatrix} w_1 & u_1\\ w_2 & u_2\end{vmatrix}P_3 V_3\right]v\\ &+\left[\begin{vmatrix} u_2 & v_2\\ u_3 & v_3\end{vmatrix}P_1 V_1+\begin{vmatrix} u_3 & v_3\\ u_1 & v_1\end{vmatrix}P_2 V_2+\begin{vmatrix} u_1 & v_1\\ u_2 & v_2\end{vmatrix}P_3 V_3\right]w,\end{aligned}$$

$$\begin{aligned} W=&\left[\begin{vmatrix} v_2 & w_2\\ v_3 & w_3\end{vmatrix}P_1 W_1+\begin{vmatrix} v_3 & w_3\\ v_1 & w_1\end{vmatrix}P_2 W_2+\begin{vmatrix} v_1 & w_1\\ v_2 & w_2\end{vmatrix}P_3 W_3\right]u\\ &+\left[\begin{vmatrix} w_2 & u_2\\ w_3 & u_3\end{vmatrix}P_1 W_1+\begin{vmatrix} w_3 & u_3\\ w_1 & u_1\end{vmatrix}P_2 W_2+\begin{vmatrix} w_1 & u_1\\ w_2 & u_2\end{vmatrix}P_3 W_3\right]v\\ &+\left[\begin{vmatrix} u_2 & v_2\\ u_3 & v_3\end{vmatrix}P_1 W_1+\begin{vmatrix} u_3 & v_3\\ u_1 & v_1\end{vmatrix}P_2 W_2+\begin{vmatrix} u_1 & v_1\\ u_2 & v_2\end{vmatrix}P_3 W_3\right]w.\end{aligned}$$

Disregarding a common factor, the expressions between the square brackets are

$$\begin{matrix} h_A & k_A & l_A,\\ h_B & k_B & l_B,\\ h_C & k_C & l_C,\end{matrix}$$

and the quantities $u_A \ldots w_C$ may be calculated from (2).

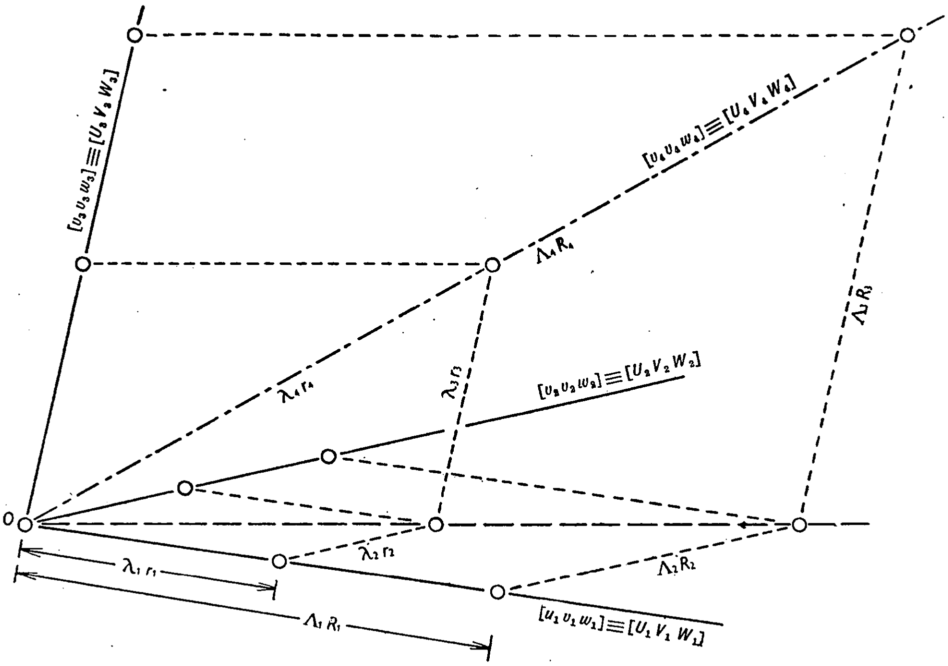

Fig. 1. The composition of radius vectors to the row-points $\lambda_4[[u_4v_4w_4]]$ and $\Lambda_4[[U_4V_4W_4]]$, from three other vectors to the row-points $\lambda_1[[u_1v_1w_1]]$, etc. r_1 is the length of the radius vector from O to the point $[[u_1v_1w_1]]$, etc.

When four transitions of crystal faces $(h_1k_1l_1) \to (H_1K_1L_1)$, etc., are given, we can derive analogous formulae with the aid of the indirect lattice. Indicating

$$P_1^* \equiv \frac{\begin{vmatrix} H_2 & H_3 & H_4 \\ K_2 & K_3 & K_4 \\ L_2 & L_3 & L_4 \end{vmatrix}}{\begin{vmatrix} h_2 & h_3 & h_4 \\ k_2 & k_3 & k_4 \\ l_2 & l_3 & l_4 \end{vmatrix}}, \quad P_2^* \equiv \frac{\begin{vmatrix} H_1 & H_3 & H_4 \\ K_1 & K_3 & K_4 \\ L_1 & L_3 & L_4 \end{vmatrix}}{\begin{vmatrix} h_1 & h_3 & h_4 \\ k_1 & k_3 & k_4 \\ l_1 & l_3 & l_4 \end{vmatrix}},$$

$$P_3^* \equiv \frac{\begin{vmatrix} H_1 & H_2 & H_4 \\ K_1 & K_2 & K_4 \\ L_1 & L_2 & L_4 \end{vmatrix}}{\begin{vmatrix} h_1 & h_2 & h_4 \\ k_1 & k_2 & k_4 \\ l_1 & l_2 & l_4 \end{vmatrix}},$$

we have

$$\begin{aligned} H = & \left[\begin{vmatrix} k_2 & l_2 \\ k_3 & l_3 \end{vmatrix} P_1^* H_1 + \begin{vmatrix} k_3 & l_3 \\ k_1 & l_1 \end{vmatrix} P_2^* H_2 + \begin{vmatrix} k_1 & l_1 \\ k_2 & l_2 \end{vmatrix} P_3^* H_3 \right] h \\ & + \left[\begin{vmatrix} l_2 & h_2 \\ l_3 & h_3 \end{vmatrix} P_1^* H_1 + \begin{vmatrix} l_3 & h_3 \\ l_1 & h_1 \end{vmatrix} P_2^* H_2 + \begin{vmatrix} l_1 & h_1 \\ l_2 & h_2 \end{vmatrix} P_3^* H_3 \right] k \\ & + \left[\begin{vmatrix} h_2 & k_2 \\ h_3 & k_3 \end{vmatrix} P_1^* H_1 + \begin{vmatrix} h_3 & k_3 \\ h_1 & k_1 \end{vmatrix} P_2^* H_2 + \begin{vmatrix} h_1 & k_1 \\ h_2 & k_2 \end{vmatrix} P_3^* H_3 \right] l, \end{aligned}$$

$$\begin{aligned} K = & \left[\begin{vmatrix} k_2 & l_2 \\ k_3 & l_3 \end{vmatrix} P_1^* K_1 + \begin{vmatrix} k_3 & l_3 \\ k_1 & l_1 \end{vmatrix} P_2^* K_2 + \begin{vmatrix} k_1 & l_1 \\ k_2 & l_2 \end{vmatrix} P_3^* K_3 \right] h \\ & + \left[\begin{vmatrix} l_2 & h_2 \\ l_3 & h_3 \end{vmatrix} P_1^* K_1 + \begin{vmatrix} l_3 & h_3 \\ l_1 & h_1 \end{vmatrix} P_2^* K_2 + \begin{vmatrix} l_1 & h_1 \\ l_2 & h_2 \end{vmatrix} P_3^* K_3 \right] k \\ & + \left[\begin{vmatrix} h_2 & k_2 \\ h_3 & k_3 \end{vmatrix} P_1^* K_1 + \begin{vmatrix} h_3 & k_3 \\ h_1 & k_1 \end{vmatrix} P_2^* K_2 + \begin{vmatrix} h_1 & k_1 \\ h_2 & k_2 \end{vmatrix} P_3^* K_3 \right] l, \end{aligned}$$

$$\begin{aligned} L = & \left[\begin{vmatrix} k_2 & l_2 \\ k_3 & l_3 \end{vmatrix} P_1^* L_1 + \begin{vmatrix} k_3 & l_3 \\ k_1 & l_1 \end{vmatrix} P_2^* L_2 + \begin{vmatrix} k_1 & l_1 \\ k_2 & l_2 \end{vmatrix} P_3^* L_3 \right] h \\ & + \left[\begin{vmatrix} l_2 & h_2 \\ l_3 & h_3 \end{vmatrix} P_1^* L_1 + \begin{vmatrix} l_3 & h_3 \\ l_1 & h_1 \end{vmatrix} P_2^* L_2 + \begin{vmatrix} l_1 & h_1 \\ l_2 & h_2 \end{vmatrix} P_3^* L_3 \right] k \\ & + \left[\begin{vmatrix} h_2 & k_2 \\ h_3 & k_3 \end{vmatrix} P_1^* L_1 + \begin{vmatrix} h_3 & k_3 \\ h_1 & k_1 \end{vmatrix} P_2^* L_2 + \begin{vmatrix} h_1 & k_1 \\ h_2 & k_2 \end{vmatrix} P_3^* L_3 \right] l. \end{aligned}$$

The expressions between the square brackets are proportional to

$$\begin{matrix} u_A & v_A & w_A, \\ u_B & v_B & w_B, \\ u_C & v_C & w_C, \end{matrix}$$

and $h_A \ldots l_C$ may be derived from (2).

If we are given, for example, three transitions of edges and one of a face, or another combination of four transitions, the easiest method is to reduce the case to one of those treated above by a few cross-multiplications.

The directions of the old and new axes follow immediately from (3).

Example*

Axinite, triclinic pinacoidal.

We call the setting after Naumann the old and after Vom Rath the new. Given

$$\begin{matrix} \text{(Naumann)} & [1\bar{1}\bar{2}] & [001] & [110] & (\bar{1}31) \\ & \downarrow & \downarrow & \downarrow & \downarrow \\ \text{(Vom Rath)} & [001] & [\bar{1}1\bar{2}] & [\bar{1}\bar{1}\bar{2}] & (00\bar{1}), \end{matrix}$$

* Cf. Liebisch (1881, p. 60) and *Encycl. d. math. Wiss* (1905) V, **1**, 410.

three cross-multiplications show that this is equivalent to

$$\begin{array}{lcccc} \text{(Naumann)} & u(110) & p(1\bar{1}0) & r(1\bar{1}1) & (\bar{1}31) \\ & \downarrow & \downarrow & \downarrow & \downarrow \\ \text{(Vom Rath)} & (\bar{1}\bar{1}0) & (\bar{2}01) & (\bar{1}10) & (00\bar{1}). \end{array}$$

Then

$$P_1^* = \frac{\begin{vmatrix} \bar{2} & 0 & 1 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{vmatrix}}{\begin{vmatrix} 1 & \bar{1} & 0 \\ 1 & \bar{1} & 1 \\ \bar{1} & 3 & 1 \end{vmatrix}} = -1, \quad P_2^* = \frac{\begin{vmatrix} \bar{1} & \bar{1} & 0 \\ \bar{1} & 1 & 0 \\ 0 & 0 & \bar{1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & 0 \\ 1 & \bar{1} & 1 \\ \bar{1} & 3 & 1 \end{vmatrix}} = -\tfrac{1}{3},$$

$$P_3^* = \frac{\begin{vmatrix} \bar{1} & \bar{1} & 0 \\ \bar{2} & 0 & 1 \\ 0 & 0 & \bar{1} \end{vmatrix}}{\begin{vmatrix} 1 & 1 & 0 \\ 1 & \bar{1} & 0 \\ \bar{1} & 3 & 1 \end{vmatrix}} = -1,$$

$$u_A = \begin{vmatrix} \bar{1} & 0 \\ \bar{1} & 1 \end{vmatrix} (-1)(-1) + \begin{vmatrix} \bar{1} & 1 \\ 1 & 0 \end{vmatrix} (-\tfrac{1}{3})(-2) + \begin{vmatrix} 1 & 0 \\ \bar{1} & 0 \end{vmatrix} (-1)(-1) = -\tfrac{5}{3}.$$

In the same way we find

$$\begin{array}{lll} u_A = -\tfrac{5}{3}, & v_A = -\tfrac{1}{3}, & w_A = -\tfrac{2}{3}, \\ u_B = -1, & v_B = -1, & w_B = 2, \\ u_C = \tfrac{1}{3}, & v_C = -\tfrac{1}{3}, & w_C = -\tfrac{2}{3}. \end{array}$$

The dependent coefficients are, from (2),

$$\begin{array}{lll} h_A = -\tfrac{1}{6}, & k_A = 0, & l_A = -\tfrac{1}{12}, \\ h_B = 0, & k_B = -\tfrac{1}{6}, & l_B = \tfrac{1}{12}, \\ h_C = \tfrac{1}{6}, & k_C = -\tfrac{1}{2}, & l_C = -\tfrac{1}{6}. \end{array}$$

The transformation formulae are

$$\begin{array}{ll} H = -5h - k - 2l, & U = -2u - w, \\ K = -3h - 3k + 6l, & V = -2v + w, \\ L = h - k - 2l, & W = 2u - 6v - 2w. \end{array}$$

Vom Rath chose his axes along the edges, which Naumann symbolized

$$\begin{array}{ll} [u_A v_A w_A], & [\bar{5}1\bar{2}], \\ [u_B v_B w_B], & [\bar{1}\bar{1}2], \\ [u_C v_C w_C], & [1\bar{1}\bar{2}]. \end{array}$$

I am greatly indebted to Dr J. Bouman for his revision of the manuscript.

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Acta Cryst. (1949). **2**, 325

Thermal Scattering of X-rays by a Close-packed Hexagonal Lattice

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(*Received* 2 *June* 1949)

The dynamical properties of a crystal for small vibrations can be described by the set of coefficients of the potential energy forming the dynamical matrix. The elastic constants and many other observable quantities can be calculated in terms of the elements of the dynamical matrix, but, in general, the reverse does not hold. On the assumptions that only central forces need to be considered, and that only next-neighbour atoms act on one another, the dynamical matrix for a close-packed hexagonal lattice is expressed in terms of one atomic constant, which can be determined by comparing the expressions for the elastic constants with experiment. The Fourier transform of the dynamical matrix and its reciprocal, which in first approximation is proportional to the scattering matrix, are then calculated. A diagram of the equidiffusion lines, which covers a part of reciprocal space containing sixteen lattice points, is drawn. The diagram shows that the 'extra spots' are surrounded by a weak background which exhibits considerable fine structure. The equidiffusion lines constructed for the vicinity of the selective reflexions (Jahn case) agree with those calculated by Begbie for beryl. No trace is found of the intense star pattern observed by Lonsdale for ice and ammonium fluoride.

Introduction

The general theory of the thermal scattering of X-rays has been given by several physicists. The most important publication is probably that of Waller (1925). A condensed presentation of this theory appeared in *Reports on Progress in Physics* (Born, 1942–3), which contains