three cross-multiplications show that this is equivalent to

(Naumann) $u(110)$ $p(1\bar{1}0)$ $r(1\bar{1}1)$ $(\bar{1}31)$

  $\downarrow$ $\downarrow$ $\downarrow$ $\downarrow$

(Vom Rath) $(\bar{1}\bar{1}0)$ $(\bar{2}01)$ $(\bar{1}10)$ $(00\bar{1})$.

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

$$u_A = -\tfrac{5}{3}, \quad v_A = -\tfrac{1}{3}, \quad w_A = -\tfrac{2}{3},$$
$$u_B = -1, \quad v_B = -1, \quad w_B = 2,$$
$$u_C = \tfrac{1}{3}, \quad v_C = -\tfrac{1}{3}, \quad w_C = -\tfrac{2}{3}.$$

The dependent coefficients are, from (2),

$$h_A = -\tfrac{1}{6}, \quad k_A = 0, \quad l_A = -\tfrac{1}{12},$$
$$h_B = 0, \quad k_B = -\tfrac{1}{6}, \quad l_B = \tfrac{1}{12},$$
$$h_C = \tfrac{1}{6}, \quad k_C = -\tfrac{1}{2}, \quad l_C = -\tfrac{1}{6}.$$

The transformation formulae are

$$H = -5h - k - 2l, \qquad U = -2u - w,$$
$$K = -3h - 3k + 6l, \qquad V = -2v + w,$$
$$L = h - k - 2l, \qquad W = 2u - 6v - 2w.$$

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

$$[u_A v_A w_A], \quad [\bar{5}1\bar{2}],$$
$$[u_B v_B w_B], \quad [\bar{1}\bar{1}2],$$
$$[u_C v_C w_C], \quad [1\bar{1}\bar{2}].$$

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

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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

a bibliography of this subject and an account of its development. The important contribution of the above report is that the scattering power of a system is not expressed in terms of the frequencies of vibration, but is given directly in terms of the 'dynamical matrix' of the system. In the particular case of crystals, where the normal modes of vibration have the form of waves, the scattering power is a function of the transformed dynamical matrix (in wave-vector space). From this it follows that in order to investigate the scattering, one has to know the value of the transformed dynamical matrix for all wave vectors, or to use a model for which it may be calculated.

Begbie & Born (1947) proposed a model in which the potential energy between the nuclei is assumed to be any arbitrary function of the displacements of the nuclei. All physical properties can be expressed in terms of this function and of its derivatives. In particular, the vibrational properties depend on the second derivatives, which form the dynamical matrix. For a given lattice, the dynamical matrix can be simplified by symmetry considerations. Begbie & Born also assume that the elements of the dynamical matrix are negligibly small except for next neighbours. In this case, the elements of the dynamical matrix can be expressed in terms of a small number of constants (the atomic constants).

The application to a face-centred cubic lattice has been carried out by Begbie (1947). By considering the limiting case of long waves, it is possible to express the elastic constants in terms of the atomic constants (Born, 1923). For the face-centred cubic lattice, it so happens that the number of atomic constants is equal to the number of elastic constants. Thus it follows that the dynamical matrix and its transform in wave-vector space for *all* wave vectors, can be expressed in terms of the elastic constants. The final calculation of the scattering power shows that a considerable intensity with a quite definite structure can be expected in the region between the Laue spots.

This method fails when it is applied to the close-packed hexagonal lattice, because, in this case, the number of atomic constants (seven) is greater than the number of elastic constants (five). In these circumstances, Begbie limited his calculation to the regions in the neighbourhood of the reciprocal-lattice points—the Jahn approximation. Results are given for beryl. The purpose of the present investigation is to extend the work of Begbie into the regions of reciprocal space between the lattice points, by the additional assumption of central forces. In this particular case, the dynamical matrix and the matrix of the elastic constants become proportional to one atomic constant. In this paper, the scattering power of a close-packed hexagonal lattice is obtained as a function of this atomic constant, whose value can be obtained for a particular lattice, if its elastic constants are known.

Born (1942) has shown that, even with the assumption of central forces acting only between first neigh-

bours, the close-packed hexagonal lattice is stable. He has also derived the elastic constants. Beryl is the only hexagonal crystal for which the complete set of elastic constants is known, and in this case the ratio between the constants agrees quite well with that obtained by Born. This suggests that the assumption of central forces is a quite reasonable approximation.

1. The expression for the thermal scattering of X-rays

This section summarizes briefly the results already obtained by Born (1942–3). The lattice cell is described by three elementary vectors a_1, a_2, a_3. Then the position vector of the particles at the vertex of a cell is

$$r^l = l_1 a_1 + l_2 a_2 + l_3 a_3, \qquad (1\cdot1)$$

where l_1, l_2, l_3 are integers. If there are s particles in the unit cell, with masses m_k ($k = 1, 2, ..., s$), and r_k is the position vector of the kth particle from the cell vertex, then

$$r\binom{l}{k} = r^l + r_k \qquad (1\cdot2)$$

defines the position of the particle $\binom{l}{k}$ in equilibrium.

The rectangular components of $r\binom{l}{k}$ are $X_\alpha\binom{l}{k}$ ($\alpha = 1, 2, 3$).

The potential energy Φ of the deformed lattice can be expanded in powers of the rectangular components $u_\alpha\binom{l}{k}$ ($\alpha = 1, 2, 3$) of $u\binom{l}{k}$, where $u\binom{l}{k}$ is a small arbitrary displacement of the particle $\binom{l}{k}$ from equilibrium. The second-order term in the energy, Φ_2, can be written

$$\Phi_2 = \frac{1}{2} \sum_{lk} \sum_{l'k'} \sum_{\alpha\beta} D_{\alpha\beta}\binom{l-l'}{kk'} (m_k m_{k'})^{\frac{1}{2}} u_\alpha\binom{l}{k} u_\beta\binom{l'}{k'}$$

$$(\alpha, \beta = 1, 2, 3). \quad (1\cdot3)$$

The coefficients $D_{\alpha\beta}\binom{l-l'}{kk'}$ are the elements of the dynamical matrix.

The elementary vectors of the reciprocal lattice b_1, b_2, b_3 are defined by the equations

$$a_\alpha . b_\beta = \begin{cases} 1 & \text{if } \alpha = \beta \\ 0 & \text{if } \alpha \neq \beta. \end{cases} \qquad (1\cdot4)$$

If $Q = Q_1 b_1 + Q_2 b_2 + Q_3 b_3$ is a vector in reciprocal space, then

$$Q . r^l = Q_1 l_1 + Q_2 l_2 + Q_3 l_3 = (l, Q).$$

The Fourier transform of the dynamical matrix, or its representation in reciprocal space Q, is a matrix which is diagonal with respect to the Q. The diagonal elements are given by

$$D_{\alpha\beta}\binom{Q}{kk'} = \sum_l D_{\alpha\beta}\binom{l}{kk'} e^{-i(l, Q)}. \qquad (1\cdot5)$$

The quantities (1·5) are considered as elements of the matrix $D(\mathbf{Q})$, the rows and columns being denoted by the pairs (α, k) and (β, k').

Let it be assumed that a beam of X-rays is passing through a crystal, and let $\mathbf{k}$ be the wave vector of the incident beam, and $\mathbf{k}'$ be the wave vector of the scattered beam. Then, if the scattering power is defined as the ratio of the scattered intensity in any direction to the incident intensity, and if $\mathbf{k} - \mathbf{k}' = \mathbf{Q}$, it can be shown (Born, 1942–3) that the scattering produced by the thermal motion is given by

$$\sigma = \sigma_0 N \sum_{k\alpha} \sum_{k\beta} S_{\alpha\beta}\begin{pmatrix} Q \\ kk' \end{pmatrix} w_\alpha(k)\, w^*_\beta(k'), \qquad (1\cdot6)$$

where $S_{\alpha\beta}\begin{pmatrix} Q \\ kk' \end{pmatrix}$ are the elements of a matrix, the scattering matrix, which in first approximation is proportional to the reciprocal of the transformed dynamical matrix

$$S(\mathbf{Q}) = kT D(\mathbf{Q})^{-1}. \qquad (1\cdot7)$$

Here, k is Boltzmann's constant† and T is the absolute temperature.

The other symbols have the following meaning:

$$\mathbf{w}(k) = \frac{f_k}{\sqrt{m_k}}\, e^{i\mathbf{Q}.\mathbf{r}_k}\mathbf{Q}; \qquad (1\cdot8)$$

f_k, the modified scattering factor dependent on T;
N, the number of cells in the crystal;

σ_0, the Thomson factor $\left[= \left(\dfrac{e^2}{mc^2}\dfrac{1}{r}\right)^2 \frac{1}{2}(1 + \cos^2 \chi)\right]$;

e, the electronic charge;
m, the mass of the electron;
c, the velocity of light;
r, the distance of the small scattering volume from the point of observation;
χ, the angle of deflexion of the X-ray beam.

2. The dynamical matrix and its reciprocal

In the work of Begbie & Born, all the elements of the dynamical matrix are assumed to be arbitrary constants, and then relations are found between them by applying the symmetry transformations of the lattice.

In the case of central forces, the elements of the dynamical matrix are given explicitly in terms of the atomic constants, and hence already satisfy the necessary symmetry relations. The dynamics of a crystal lattice under the assumption of central forces has been completely worked out by Born (1923). Here it is assumed that the potential energy between any two particles, $Q\begin{pmatrix} l \\ kk' \end{pmatrix}$, depends only on the nature of the particles and on $\left| \mathbf{r}\begin{pmatrix} l \\ kk' \end{pmatrix} \right|$, the distance between them.

————

† The fact that k is also used as a suffix is not likely to cause confusion.

Accordingly, the elements of the dynamical matrix are determined by

$$\left. \begin{aligned} -(m_k m_{k'})^{\frac{1}{2}} D_{\alpha\beta}\begin{pmatrix} l \\ kk' \end{pmatrix} &= \delta_{\alpha\beta} P\begin{pmatrix} l \\ kk' \end{pmatrix} \\ &\quad + X_\alpha\begin{pmatrix} l \\ kk' \end{pmatrix} X_\beta\begin{pmatrix} l \\ kk' \end{pmatrix} Q\begin{pmatrix} l \\ kk' \end{pmatrix} \quad \begin{pmatrix} l \neq 0 \\ k \neq k' \end{pmatrix}, \\ m_k D_{\alpha\beta}\begin{pmatrix} 0 \\ kk \end{pmatrix} &= -\sum_{lk'}{}' (m_k m_{k'})^{\frac{1}{2}} D_{\alpha\beta}\begin{pmatrix} l \\ kk' \end{pmatrix}, \end{aligned} \right\} \quad (2\cdot1)$$

where the dash over the summation sign means the term $\begin{pmatrix} 0 \\ kk \end{pmatrix}$ is to be omitted,

$$\left. \begin{aligned} P\begin{pmatrix} l \\ kk' \end{pmatrix} &= \left[\frac{1}{r}\frac{d\phi}{dr}\right]_0, \\ Q\begin{pmatrix} l \\ kk' \end{pmatrix} &= \left[\frac{1}{r}\frac{d}{dr}\left(\frac{1}{r}\frac{d\phi}{dr}\right)\right]_0, \end{aligned} \right\} \quad (2\cdot2)$$

and $[\;]_0$ means the values of the variables are to be taken at the equilibrium position.

The conditions for equilibrium (Born, 1923), are

$$\left. \begin{aligned} \sum_{lk'} P\begin{pmatrix} l \\ kk' \end{pmatrix} X_\alpha\begin{pmatrix} l \\ kk' \end{pmatrix} &= 0 \quad (\alpha = 1, 2, 3), \\ \sum_{lkk'} P\begin{pmatrix} l \\ kk' \end{pmatrix} X_\alpha\begin{pmatrix} l \\ kk' \end{pmatrix} X_\beta\begin{pmatrix} l \\ kk' \end{pmatrix} &= 0 \quad (\alpha, \beta = 1, 2, 3). \end{aligned} \right\} \quad (2\cdot3)$$

Now, in the special case where only first neighbours are considered to act on one another, and all the particles are of the same kind, one obtains from the last equation

$$P\begin{pmatrix} l \\ kk' \end{pmatrix} \sum_{lk'} X_\alpha^2\begin{pmatrix} l \\ kk' \end{pmatrix} = 0 \qquad (2\cdot4)$$

$(\alpha = 1, 2, 3;\ l$ restricted to first neighbours). So it follows that, if P^1 represents $P\begin{pmatrix} l \\ kk' \end{pmatrix}$ for first neighbours,

$$P^1 = 0, \qquad (2\cdot5)$$

and the elements of the dynamical matrix reduce to

$$D_{\alpha\beta}\begin{pmatrix} l \\ kk' \end{pmatrix} = -(m_k m_{k'})^{-\frac{1}{2}} X_\alpha\begin{pmatrix} l \\ kk' \end{pmatrix} X_\beta\begin{pmatrix} l \\ kk' \end{pmatrix} Q\begin{pmatrix} l \\ kk' \end{pmatrix} \quad (2\cdot6)$$

(l restricted to first neighbours). The value of the remaining atomic constant, Q^1 say, can be obtained by comparison with the matrix (c_{rs}) of the elastic constants (see (2·11)). Now the elements of the dynamical matrix can be written down as soon as the form of the lattice is known.

In the close-packed hexagonal lattice there are two identical particles of mass m in the unit cell, distinguished by $k = 1$, $k = 2$. The cell vectors $\mathbf{a}_1$, $\mathbf{a}_2$, $\mathbf{a}_3$ can be chosen in such a way that the angle between $\mathbf{a}_1$ and $\mathbf{a}_2$ is $\frac{2}{3}\pi$ and $\mathbf{a}_3$ is at right angles to the plane of $\mathbf{a}_1$ and $\mathbf{a}_2$ in the direction that makes the system of axes right-

handed. The lengths of the lattice vectors are given by

$$|\mathbf{a}_1| = |\mathbf{a}_2| = a, \quad |\mathbf{a}_3| = c = (\sqrt{\tfrac{8}{3}})\,a. \qquad (2\cdot7)$$

The Cartesian co-ordinate system used is so orientated that x_1 lies along the positive direction of $\mathbf{a}_2$, and x_3
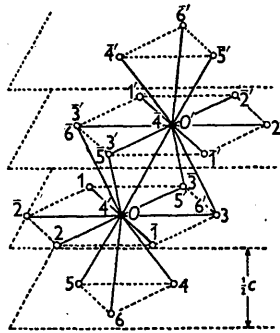

Fig. 1. First neighbours of the two points in the unit cell of the close-packed hexagonal lattice.
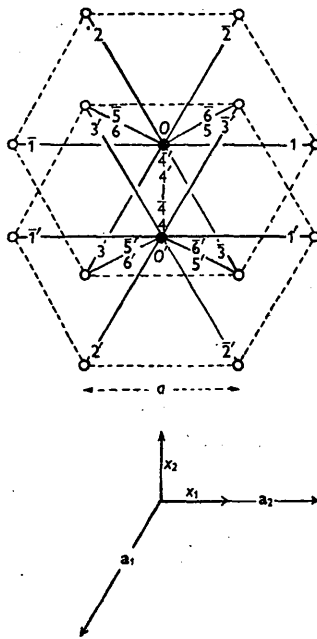

Fig. 2. Projection of the structure in Fig. 1 on to a plane perpendicular to the lattice vector $\mathbf{a}_3$.

along the positive direction of $\mathbf{a}_3$ (Fig. 2). For simplicity, it is assumed that the base vector of the particles of the type $k=1$ is zero, while that of the type $k=2$ is given by

$$\mathbf{r}_2 = \mathbf{r}_{21} = \tfrac{2}{3}\mathbf{a}_1 + \tfrac{1}{3}\mathbf{a}_2 + \tfrac{1}{2}\mathbf{a}_3, \qquad (2\cdot8)$$

or, in rectangular co-ordinates, by

$$\mathbf{r}_{21} = (0,\ -\tfrac{1}{3}a,\ \tfrac{1}{2}c). \qquad (2\cdot9)$$

Particles of the same type lie in alternate planes, perpendicular to the $\mathbf{a}_3$ axis.

It is only necessary to consider those matrices $D\!\begin{pmatrix} l \\ kk' \end{pmatrix}$ which arise from the first neighbours of the two particles in a chosen unit cell. These two particles are labelled O

and O' in Figs. 1 and 2. Each point has twelve first neighbours, six in a plane containing the point, and three above and three below this plane. The line joining O or O' to a neighbouring point $\begin{pmatrix} l \\ kk' \end{pmatrix}$ is labelled by the letter p, and Dp is written for $D\!\begin{pmatrix} l \\ kk' \end{pmatrix}$. The twelve neighbours of O are again split into two groups $p, \bar{p}$, those of O' into $p', \bar{p}'$, as indicated by the following scheme:

$$\left.\begin{array}{l} p \to 1, 2, 3, 4, 5, 6 \\ \bar{p} \to \bar{1}, \bar{2}, \bar{3}, \bar{4}, \bar{5}, \bar{6} \end{array}\right\} \text{ neighbours of } O,$$

$$\left.\begin{array}{l} p' \to 1', 2', 3', 4', 5', 6' \\ \bar{p}' \to \bar{1}', \bar{2}', \bar{3}', \bar{4}', \bar{5}', \bar{6}' \end{array}\right\} \text{ neighbours of } O'.$$

The symbols p and the Cartesian co-ordinates X_α^p are connected to $\begin{pmatrix} l \\ kk' \end{pmatrix}$ as given in Tables 1 and 2.

Table 1. *Connexion between the symbols p and $\begin{pmatrix} l \\ kk' \end{pmatrix}$*

(The notation is due to Begbie (1947).)

p	1	2	3	4	5	6	$\bar{1}$	$\bar{2}$	$\bar{3}$	$\bar{4}$	$\bar{5}$	$\bar{6}$
l_1	0	-1	1	0	-1	-1	0	-1	1	0	-1	-1
l_2	1	-1	0	0	0	-1	-1	0	1	0	-1	0
l_3	0	0	0	-1	-1	-1	0	0	0	0	0	0
(kk')	(11)	(11)	(11)	(21)	(21)	(21)	(11)	(11)	(11)	(21)	(21)	(21)

p	$1'$	$2'$	$3'$	$4'$	$5'$	$6'$	$\bar{1}'$	$\bar{2}'$	$\bar{3}'$	$\bar{4}'$	$\bar{5}'$	$\bar{6}'$
l_1	0	1	-1	0	1	1	0	1	-1	0	1	1
l_2	1	0	-1	0	1	0	-1	1	0	0	0	1
l_3	0	0	0	0	0	0	0	0	0	1	1	1
(kk')	(22)	(22)	(22)	(12)	(12)	(12)	(22)	(22)	(22)	(12)	(12)	(12)

The elements of the dynamical matrix, given by

$$D_{\alpha\beta}^p = -\frac{1}{m} X_\alpha^p X_\beta^p Q^1, \qquad (2\cdot10)$$

can be read off immediately from Table 2. They are given in Table 3. All the elements have to be multiplied by the factor $-a^2 Q^1/m$.

The elements of $D\!\begin{pmatrix} l \\ kk \end{pmatrix}$, $l=(0,0,0)$, obtained from the second equation of $(4\cdot1)$, are

$$D^0 = \begin{bmatrix} -4 & 0 & 0 \\ 0 & -4 & 0 \\ 0 & 0 & -4 \end{bmatrix} = D^{0'}.$$

The elastic constants of the close-packed hexagonal lattice have been considered by Born (1942) in an investigation of the stability of such a lattice. The matrix (c_{rs}) of the elastic constants (case of first neighbours only) can be written in the form

$$(c_{rs}) = \frac{a^4 Q^1}{12\Delta} \begin{bmatrix} 29 & 11 & 8 & 0 & 0 & 0 \\ 11 & 29 & 8 & 0 & 0 & 0 \\ 8 & 8 & 32 & 0 & 0 & 0 \\ 0 & 0 & 0 & 8 & 0 & 0 \\ 0 & 0 & 0 & 0 & 8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 9 \end{bmatrix}, \qquad (2\cdot11)$$

Table 2. *Connexion between the components of the distances between neighbours and* $\begin{pmatrix} l \\ kk' \end{pmatrix}$

p	1	2	3	4	5	6	$\bar{1}$	$\bar{2}$	$\bar{3}$	$\bar{4}$	$\bar{5}$	$\bar{6}$
X_1^p	a	$-\dfrac{a}{2}$	$-\dfrac{a}{2}$	0	$\dfrac{a}{2}$	$-\dfrac{a}{2}$	$-a$	$\dfrac{a}{2}$	$\dfrac{a}{2}$	0	$-\dfrac{a}{2}$	$\dfrac{a}{2}$
X_2^p	0	$\dfrac{\sqrt{3}a}{2}$	$-\dfrac{\sqrt{3}a}{2}$	$-\dfrac{a}{\sqrt{3}}$	$\dfrac{a}{2\sqrt{3}}$	$\dfrac{a}{2\sqrt{3}}$	0	$\dfrac{\sqrt{3}a}{2}$	$-\dfrac{\sqrt{3}a}{2}$	$-\dfrac{a}{\sqrt{3}}$	$\dfrac{a}{2\sqrt{3}}$	$\dfrac{a}{2\sqrt{3}}$
X_3^p	0	0	0	$-\dfrac{c}{2}$	$-\dfrac{c}{2}$	$-\dfrac{c}{2}$	0	0	0	$\dfrac{c}{2}$	$\dfrac{c}{2}$	$\dfrac{c}{2}$
(kk')	(11)	(11)	(11)	(21)	(21)	(21)	(11)	(11)	(11)	(21)	(21)	(21)

p	$1'$	$2'$	$3'$	$4'$	$5'$	$6'$	$\bar{1}'$	$\bar{2}'$	$\bar{3}'$	$\bar{4}'$	$\bar{5}'$	$\bar{6}'$
X_1^p	a	$-\dfrac{a}{2}$	$-\dfrac{a}{2}$	0	$\dfrac{a}{2}$	$-\dfrac{a}{2}$	$-a$	$\dfrac{a}{2}$	$\dfrac{a}{2}$	0	$-\dfrac{a}{2}$	$\dfrac{a}{2}$
X_2^p	0	$-\dfrac{\sqrt{3}a}{2}$	$\dfrac{\sqrt{3}a}{2}$	$\dfrac{a}{\sqrt{3}}$	$-\dfrac{a}{2\sqrt{3}}$	$-\dfrac{a}{2\sqrt{3}}$	0	$-\dfrac{\sqrt{3}a}{2}$	$\dfrac{\sqrt{3}a}{2}$	$\dfrac{a}{\sqrt{3}}$	$-\dfrac{a}{2\sqrt{3}}$	$-\dfrac{a}{2\sqrt{3}}$
X_3^p	0	0	0	$-\dfrac{c}{2}$	$-\dfrac{c}{2}$	$-\dfrac{c}{2}$	0	0	0	$\dfrac{c}{2}$	$\dfrac{c}{2}$	$\dfrac{c}{2}$
(kk')	(22)	(22)	(22)	(12)	(12)	(12)	(22)	(22)	(22)	(12)	(12)	(12)

Table 3. *Elements of the dynamical matrix*

$$D^1 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = D^{\bar{1}'}, \qquad D^{\bar{1}} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{bmatrix} = D^{1'},$$

$$D^2 = \begin{bmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} & 0 \\ -\frac{\sqrt{3}}{4} & \frac{3}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix} = D^{\bar{2}'}, \qquad D^{\bar{2}} = \begin{bmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} & 0 \\ \frac{\sqrt{3}}{4} & \frac{3}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix} = D^{2'},$$

$$D^3 = \begin{bmatrix} \frac{1}{4} & \frac{\sqrt{3}}{4} & 0 \\ \frac{\sqrt{3}}{4} & \frac{3}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix} = D^{\bar{3}'}, \qquad D^{\bar{3}} = \begin{bmatrix} \frac{1}{4} & -\frac{\sqrt{3}}{4} & 0 \\ -\frac{\sqrt{3}}{4} & \frac{3}{4} & 0 \\ 0 & 0 & 0 \end{bmatrix} = D^{3'},$$

$$D^4 = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{3} & \frac{\sqrt{2}}{3} \\ 0 & \frac{\sqrt{2}}{3} & \frac{2}{3} \end{bmatrix} = D^{\bar{4}'}, \qquad D^{\bar{4}} = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \frac{1}{3} & -\frac{\sqrt{2}}{3} \\ 0 & -\frac{\sqrt{2}}{3} & \frac{2}{3} \end{bmatrix} = D^{4'},$$

$$D^5 = \begin{bmatrix} \frac{1}{4} & \frac{1}{4\sqrt{3}} & -\frac{1}{\sqrt{6}} \\ \frac{1}{4\sqrt{3}} & \frac{1}{12} & -\frac{\sqrt{2}}{6} \\ -\frac{1}{\sqrt{6}} & -\frac{\sqrt{2}}{6} & \frac{2}{3} \end{bmatrix} = D^{\bar{5}'}, \qquad D^{\bar{5}} = \begin{bmatrix} \frac{1}{4} & -\frac{1}{4\sqrt{3}} & -\frac{1}{\sqrt{6}} \\ -\frac{1}{4\sqrt{3}} & \frac{1}{12} & \frac{\sqrt{2}}{6} \\ -\frac{1}{\sqrt{6}} & \frac{\sqrt{2}}{6} & \frac{2}{3} \end{bmatrix} = D^{5'},$$

$$D^6 = \begin{bmatrix} \frac{1}{4} & -\frac{1}{4\sqrt{3}} & \frac{1}{\sqrt{6}} \\ -\frac{1}{4\sqrt{3}} & \frac{1}{12} & -\frac{\sqrt{2}}{6} \\ \frac{1}{\sqrt{6}} & -\frac{\sqrt{2}}{6} & \frac{2}{3} \end{bmatrix} = D^{\bar{6}'}, \qquad D^{\bar{6}} = \begin{bmatrix} \frac{1}{4} & \frac{1}{4\sqrt{3}} & \frac{1}{\sqrt{6}} \\ \frac{1}{4\sqrt{3}} & \frac{1}{12} & \frac{\sqrt{2}}{6} \\ \frac{1}{\sqrt{6}} & \frac{\sqrt{2}}{6} & \frac{2}{3} \end{bmatrix} = D^{6'}.$$

where Voigt's form for the elastic energy per unit volume is

$$\Phi_2 = \tfrac{1}{2}\sum_{\rho\sigma} c_{\rho\sigma} X_\rho X_\sigma, \tag{2.12}$$

and Δ is the volume of the unit cell. Thus Q^1 can be obtained by a determination of the elastic constants.

The elements of the dynamical matrix in the reciprocal-lattice space (which for a hexagonal lattice is another hexagonal lattice) are obtained from the $D_{\alpha\beta}\begin{pmatrix} l \\ kk' \end{pmatrix}$ by means of (1.5). Before doing this, however, it is convenient to denote the co-ordinates of a wave vector $\mathbf{Q}$ in reciprocal space by four symbols instead of three. This is done in order to utilize fully the symmetry of the lattice and corresponds to the fact that in a hexagonal direct lattice there are three symmetry lines in the plane $l_3 = 0$, any two of which may be taken for the direction of the cell vectors. The co-ordinates of the

point $\mathbf{Q}$ are thus denoted by (Q_1, Q_2, Q_3, Q_4), where Q_3 denotes the new co-ordinate and the one previously called Q_3 now becomes Q_4. As a point is now specified by four co-ordinates instead of three, a relation must hold between them. This is given by

$$Q_1 + Q_2 + Q_3 = 0. \qquad (2\cdot13)$$

The elements of the matrix are thus given by

$$D_{\alpha\beta}\binom{Q}{kk'} = \sum_l D_{\alpha\beta}\binom{l}{kk'} e^{-i(\mathbf{Q}\cdot\mathbf{r}^l)}$$

$$(\mathbf{Q}\cdot\mathbf{r}^l = Q_1 l_1 + Q_2 l_2 + Q_4 l_3). \qquad (2\cdot14)$$

It is not necessary to calculate all the matrices, as it is easily seen that

$$D\binom{Q}{11} = D\binom{-Q}{22}, \quad D\binom{Q}{21} = D\binom{-Q}{12}. \qquad (2\cdot15)$$

Thus, only the cases $D\binom{Q}{11}$ and $D\binom{Q}{21}$ are worked out in detail. The corresponding l values can be obtained from the upper half of Table 1. The resultant matrices are given by

$$D\binom{Q}{11} = D^1 e^{-iQ_2} + D^2 e^{-iQ_3} + D^3 e^{-iQ_1}$$
$$\qquad + D^{\overline{1}} e^{iQ_2} + D^{\overline{2}} e^{iQ_3} + D^{\overline{3}} e^{iQ_1} + D^0,$$
$$D\binom{Q}{21} = D^4 e^{iQ_4} + D^5 e^{i(Q_1+Q_4)} + D^6 e^{i(Q_4-Q_3)}$$
$$\qquad + D^{\overline{4}} + D^{\overline{5}} e^{-iQ_3} + D^{\overline{6}} e^{iQ_1}. \qquad (2\cdot16)$$

In this paper, as in Begbie's the calculation is confined to the plane $Q_4 = 0$. With this condition, the non-vanishing elements reduce to

$$D_{11}\binom{Q}{11} = -\frac{a^2 Q^1}{m}\{2c_2 + \tfrac{1}{2}(c_1 + c_3) - 4\},$$

$$D_{22}\binom{Q}{11} = -\frac{a^2 Q^1}{m}\{\tfrac{3}{2}(c_1 + c_3) - 4\},$$

$$D_{12}\binom{Q}{11} = -\frac{a^2 Q^1}{m}\left\{\frac{\sqrt{3}}{2}(c_1 - c_3)\right\} = D_{21}\binom{Q}{11},$$

$$D_{33}\binom{Q}{11} = -\frac{a^2 Q^1}{m}\{-4\},$$

$$D_{11}\binom{Q}{21} = -\frac{a^2 Q^1}{m}\{\tfrac{1}{2}(e^{iQ_1} + e^{-iQ_3})\}, \qquad (2\cdot17)$$

$$D_{22}\binom{Q}{21} = -\frac{a^2 Q^1}{m}\{\tfrac{2}{3} + \tfrac{1}{6}(e^{iQ_1} + e^{-iQ_3})\},$$

$$D_{12}\binom{Q}{21} = -\frac{a^2 Q^1}{m}\left\{\frac{1}{2\sqrt{3}}(e^{iQ_1} - e^{-iQ_3})\right\} = D_{21}\binom{Q}{21},$$

$$D_{33}\binom{Q}{21} = -\frac{a^2 Q^1}{m}\{\tfrac{4}{3}(1 + e^{iQ_1} + e^{-iQ_3})\},$$

where $\qquad c_\alpha = \cos Q_\alpha. \qquad (2\cdot18)$

The matrix $D(Q)$ is of order 6×6, corresponding to the six possible values of the pair of indices α, k. If the

rows and columns are so ordered that the elements $D_{\alpha\beta}\binom{Q}{kk'}$ which occur in the fifth and sixth rows and columns have at least one of the indices $\alpha, \beta = 3$, then the matrix can be written in the form

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}. \qquad (2\cdot19)$$

Here the A_{rs} are submatrices. A_{11} consists of the sixteen elements for which α and β are equal to 1 or 2, A_{22}, the four elements for which both α and β are equal to 3, and A_{12}, A_{21} are composed of the remaining terms for which one of the indices α, β is equal to 3. From (2·17) it follows that the submatrices A_{12}, A_{21} are zero matrices.

Now, if the reciprocal matrix is partitioned in a corresponding manner, the submatrices being denoted by B_{rs}, it will have the same form as the original matrix, and the submatrices B_{11}, B_{22} are the reciprocals of A_{11}, A_{22}, respectively. A glance at the scattering formula, (1·6), shows that the submatrix B_{22} always acts on the component Q_3, or, as it is now called Q_4. Since the calculation is confined to the plane $Q_4 = 0$, this submatrix will contribute nothing to the scattering. Hence, in the sequel, the term-transposed dynamical matrix, $D(Q)$, will be applied to the 4×4 submatrix A_{11}.

The reciprocal of the 4×4 submatrix can be written

$$D^{-1}(Q) = -\frac{m}{a^2 Q^1 \Delta} \begin{bmatrix} \Delta_{11} & -\Delta_{21} & \Delta_{31} & -\Delta_{41} \\ -\Delta_{12} & \Delta_{22} & -\Delta_{32} & \Delta_{42} \\ \Delta_{13} & -\Delta_{23} & \Delta_{33} & -\Delta_{43} \\ -\Delta_{14} & \Delta_{24} & -\Delta_{34} & \Delta_{44} \end{bmatrix}, \qquad (2\cdot20)$$

where Δ is the determinant

$$\begin{vmatrix} D_{11}\binom{Q}{11}' & D_{12}\binom{Q}{11}' & D_{11}\binom{Q}{12}' & D_{12}\binom{Q}{12}' \\ D_{21}\binom{Q}{11}' & D_{22}\binom{Q}{11}' & D_{21}\binom{Q}{12}' & D_{22}\binom{Q}{12}' \\ D_{11}\binom{Q}{21}' & D_{12}\binom{Q}{21}' & D_{11}\binom{Q}{22}' & D_{12}\binom{Q}{22}' \\ D_{21}\binom{Q}{21}' & D_{22}\binom{Q}{21}' & D_{21}\binom{Q}{22}' & D_{22}\binom{Q}{22}' \end{vmatrix},$$

and $\qquad D_{\alpha\beta}\binom{Q}{kk'}' = D_{\alpha\beta}\binom{Q}{kk'} \bigg/ \left(-\frac{a^2 Q^1}{m}\right). \qquad (2\cdot21)$

Δ_{rs} are the minors of the elements in the rth row and the sth column. They satisfy the relations

$$\Delta_{11} = \Delta_{33}, \quad \Delta_{22} = \Delta_{44}, \quad \Delta_{12} = \Delta_{34}^*, \quad \Delta_{23} = \Delta_{41}^*, \quad \Delta_{rs} = \Delta_{sr}^*. \qquad (2\cdot22)$$

Instead of working out the elements of the reciprocal matrix in detail, the calculation is simplified by taking certain linear combinations, which, being related to the symmetry of the lattice, simplify the expression of the

scattering power. This will be shown in detail in the next section. The symbol R before a quantity means that the real part of that quantity has to be taken. The required linear combinations are defined as follows

$$\left.\begin{aligned}\Delta_1 &= \mathrm{R}(\sqrt{3}\Delta_{21} - \Delta_{22}),\\ \Delta_2 &= \tfrac{1}{2}(3\Delta_{11} - \Delta_{22}),\\ \Delta_3 &= \mathrm{R}(\sqrt{3}\Delta_{21} + \Delta_{22}),\end{aligned}\right\} \quad (2\cdot23)$$

$$\left.\begin{aligned}\Delta_1' &= \mathrm{R}(\Delta_{24} - \sqrt{3}\Delta_{23})\exp\left[i(Q_1 - Q_3)/3\right],\\ \Delta_2' &= \mathrm{R}(\tfrac{3}{2}\Delta_{13} - \tfrac{1}{2}\Delta_{24})\exp\left[i(Q_1 - Q_3)/3\right],\\ \Delta_3' &= \mathrm{R}(\Delta_{24} + \sqrt{3}\Delta_{23})\exp\left[i(Q_1 - Q_3)/3\right].\end{aligned}\right\} \quad (2\cdot24)$$

A somewhat lengthy calculation shows the values of these quantities, and of the determinant Δ, to be given by

$$\left.\begin{aligned}3\Delta_1 &= \alpha_1\gamma - c_1^2 + c_2^2 + c_3^2 - 4c_2c_3 + 3(c_2 + c_3) - 8c_1 + 8,\\ 3\Delta_2 &= \alpha_2\gamma + c_1^2 - c_2^2 + c_3^2 - 4c_3c_1 + 3(c_3 + c_1) - 8c_2 + 8,\\ 3\Delta_3 &= \alpha_3\gamma + c_1^2 + c_2^2 - c_3^2 - 4c_1c_2 + 3(c_1 + c_2) - 8c_3 + 8;\end{aligned}\right\} \quad (2\cdot25)$$

$$\left.\begin{aligned}3\Delta_1' = &-\alpha_1(\alpha_1 + \alpha_2)\cos\tfrac{1}{3}(Q_2 - Q_1) + \alpha_2\alpha_3\cos\tfrac{1}{3}(Q_3 - Q_2)\\ &-\alpha_1(\alpha_1 + \alpha_3)\cos\tfrac{1}{3}(Q_1 - Q_3) + \cos\tfrac{1}{3}(Q_2 - Q_1)\\ &+\cos\tfrac{1}{3}(Q_1 - Q_3) + \cos\tfrac{2}{3}(Q_2 - Q_3),\\ 3\Delta_2' = &-\alpha_2(\alpha_1 + \alpha_2)\cos\tfrac{1}{3}(Q_2 - Q_1)\\ &-\alpha_2(\alpha_2 + \alpha_3)\cos\tfrac{1}{3}(Q_3 - Q_2) + \alpha_1\alpha_3\cos\tfrac{1}{3}(Q_1 - Q_3)\\ &+\cos\tfrac{1}{3}(Q_3 - Q_2) + \cos\tfrac{1}{3}(Q_2 - Q_1) + \cos\tfrac{2}{3}(Q_3 - Q_1),\\ 3\Delta_3' = &\;\alpha_1\alpha_2\cos\tfrac{1}{3}(Q_2 - Q_1) - \alpha_3(\alpha_2 + \alpha_3)\cos\tfrac{1}{3}(Q_3 - Q_2)\\ &-\alpha_3(\alpha_1 + \alpha_3)\cos\tfrac{1}{3}(Q_1 - Q_3) + \cos\tfrac{1}{3}(Q_1 - Q_3)\\ &+\cos\tfrac{1}{3}(Q_3 - Q_2) + \cos\tfrac{2}{3}(Q_1 - Q_2);\end{aligned}\right\} \quad (2\cdot26)$$

$$\begin{aligned}9\Delta = &\;\gamma^2 - 2(c_1^3 + c_2^3 + c_3^3) - 48c_1c_2c_3 - 34(c_1^2 + c_2^2 + c_3^2)\\ &+ 46(c_1c_2 + c_2c_3 + c_3c_1) + 66(c_1 + c_2 + c_3) - 189; \end{aligned} \quad (2\cdot27)$$

where

$$\left.\begin{aligned}\alpha_1 &= 2(c_2 + c_3) - c_1 - 4, \quad \alpha_2 = 2(c_3 + c_1) - c_2 - 4,\\ \alpha_3 &= 2(c_1 + c_2) - c_3 - 4,\\ \gamma &= 9(c_1c_2 + c_2c_3 + c_3c_1) - 24(c_1 + c_2 + c_3) + 48.\end{aligned}\right\} \quad (2\cdot28)$$

3. The scattering power and isodiffusion lines

Since all the atoms in the hexagonal lattice are of the same kind, the formula for the scattering power (1·6) reduces to

$$\sigma = \sigma_0 N k T \frac{|f|^2}{m} \sum_{k\alpha}\sum_{k'\beta} D_{\alpha\beta}^{-1}\!\begin{pmatrix}Q\\kk'\end{pmatrix}\exp\left[-i\mathbf{Q}\cdot\mathbf{r}_{kk'}\right] Q_\alpha' Q_\beta'. \quad (3\cdot1)$$

In this equation, dashes are placed over the Q_α, in order to show that they are co-ordinates in the Cartesian system. If now the dashed co-ordinates of $\mathbf{Q}$, (Q_1', Q_2', Q_3') in the Cartesian system are replaced by the hexagonal system (Q_1, Q_2, Q_3, Q_4) referred to the basic

vectors of the reciprocal lattice, by means of the transformation

$$Q_1' = \frac{Q_2}{a}, \quad Q_2' = \frac{Q_3 - Q_1}{\sqrt{3}a} \quad (Q_4 = 0), \quad (3\cdot2)$$

and use is made of

$$D^{-1}\!\begin{pmatrix}Q\\11\end{pmatrix} = D^{-1}\!\begin{pmatrix}Q\\22\end{pmatrix}^{*}, \quad D^{-1}\!\begin{pmatrix}Q\\12\end{pmatrix} = D^{-1}\!\begin{pmatrix}Q\\21\end{pmatrix}^{*}, \quad (3\cdot3)$$

the scattering power can be written in the form

$$\sigma = \tfrac{4}{3}\sigma_0 N k T \frac{|f|^2}{a^4 Q^1} \sum_\alpha - \frac{B_\alpha Q_\alpha^2}{\Delta}. \quad (3\cdot4)$$

The coefficients B_α are given by

$$\left.\begin{aligned}B_1 &= \mathrm{R}\{\Delta_{22} - \sqrt{3}\Delta_{21} + (\Delta_{24} - \sqrt{3}\Delta_{23})\\ &\qquad\exp\left[-i(Q_1 - Q_3)/3\right]\} = \Delta_1 + \Delta_1',\\ B_2 &= \mathrm{R}\{\tfrac{1}{2}(3\Delta_{11} - \Delta_{22}) + \tfrac{1}{2}(3\Delta_{13} - \Delta_{24})\\ &\qquad\exp\left[-i(Q_1 - Q_3)/3\right]\} = \Delta_2 + \Delta_2',\\ B_3 &= \mathrm{R}\{\Delta_{22} + \sqrt{3}\Delta_{21} + (\Delta_{24} + \sqrt{3}\Delta_{23})\\ &\qquad\exp\left[-i(Q_1 - Q_3)/3\right]\} = \Delta_3 + \Delta_3',\end{aligned}\right\} \quad (3\cdot5)$$

or, more explicitly, by

$$\left.\begin{aligned}3B_1 = &\;\alpha_1\gamma - c_1^2 + c_2^2 + c_3^2 - 4c_2c_3 + 3c_2 + 3c_3 - 8c_1 + 8\\ &-\alpha_1(\alpha_1 + \alpha_2)c_{21} + \alpha_2\alpha_3 c_{32} - \alpha_1(\alpha_1 + \alpha_3)c_{13} + c_{21}\\ &+c_{13} + \cos\tfrac{2}{3}(Q_2 - Q_3),\\ 3B_2 = &\;\alpha_2\gamma + c_1^2 - c_2^2 + c_3^2 - 4c_3c_1 + 3c_3 + 3c_1 - 8c_2 + 8\\ &-\alpha_2(\alpha_2 + \alpha_3)c_{32} + \alpha_3\alpha_1 c_{13} - \alpha_2(\alpha_2 + \alpha_1)c_{21} + c_{32}\\ &+c_{21} + \cos\tfrac{2}{3}(Q_3 - Q_1),\\ 3B_3 = &\;\alpha_3\gamma + c_1^2 + c_2^2 - c_3^2 - 4c_1c_2 + 3c_1 + 3c_2 - 8c_3 + 8\\ &-\alpha_3(\alpha_3 + \alpha_1)c_{13} + \alpha_1\alpha_2 c_{21} - \alpha_3(\alpha_3 + \alpha_2)c_{32} + c_{13}\\ &+c_{32} + \cos\tfrac{2}{3}(Q_1 - Q_2),\\ &\qquad c_{\alpha\beta} = \cos\frac{Q_\alpha - Q_\beta}{3}.\end{aligned}\right\} \quad (3\cdot6)$$

If the formula (3·1) for the scattering power is written in the form

$$\sigma = \sigma_0 N k T \frac{|f|^2}{m} d(\mathbf{Q}), \quad (3\cdot7)$$

where

$$d(\mathbf{Q}) = \sum_{k\alpha}\sum_{k'\beta} D_{\alpha\beta}^{-1}\!\begin{pmatrix}Q\\kk'\end{pmatrix}\exp\left[-i\mathbf{Q}\cdot\mathbf{r}_{kk'}\right] Q_\alpha' Q_\beta', \quad (3\cdot8)$$

the function $d(\mathbf{Q})$ is known as the 'diffusion function' (Born, 1942–3) since it describes the diffusion of scattered intensity about a Laue spot, in virtue of the thermal motion. The so-called 'surfaces of isodiffusion', $d(\mathbf{Q}) = \text{const.}$, give a graphical representation of the scattering.

In the present case, the isodiffusion function is given from (3·4) by

$$d(\mathbf{Q}) = \frac{4m}{3a^4 Q^1} \sum_\alpha - \frac{B_\alpha Q_\alpha^2}{\Delta}. \quad (3\cdot9)$$

The process of calculating this function can be considerably reduced on account of various symmetry relations. In the first place, the determinant Δ and the three coefficients Δ_α are periodic in the Q_α. Then it is easily shown that replacing the point (Q_1, Q_2, Q_3) by $(-Q_2, -Q_3, -Q_1)$ corresponds to a rotation of 60° in the plane $Q_4 = 0$. Δ is invariant under such substitution and the triad (B_1, B_2, B_3) becomes (B_2, B_3, B_1). Thus it follows that $d(\mathbf{Q})$ is invariant under 60° rotations in the plane $Q_4 = 0$, and so it is only necessary to evaluate it in one sextant. Further, replacing the point

$$(x - \tfrac{1}{2}y, \; y, \; -x - \tfrac{1}{2}y) \quad \text{by} \quad (-x - \tfrac{1}{2}y, \; y, \; x - \tfrac{1}{2}y)$$

corresponds to a reflexion in the line $Q_2 + 2Q_1 = 0$. Inspection shows that (B_1, B_2, B_3) becomes (B_3, B_2, B_1), so that $d(\mathbf{Q})$ is invariant with respect to reflexions in the six lines of the type $Q_2 + 2Q_1 = 0$, and so it is only necessary to calculate it for a sector of 30°.

The isodiffusion function $d(\mathbf{Q})$ is calculated from (3·9) for a network of points lying in the plane $Q_4 = 0$. They form a lattice which has unit vectors in the plane $Q_4 = 0$ of magnitude one-sixth of the reciprocal-lattice vectors. In order to check the accuracy of the calculation, the points were taken in a sector of 60°, so that each value is evaluated twice. The results, which include the sixteen reciprocal-lattice points $(0, 0)$, $(0, 1)$, $(-1, 0)$, $(-1, 1)$, $(-1, 2)$, $(-2, 0)$, $(-2, 1)$, $(-2, 2)$, $(0, 2)$, $(0, 3)$, $(-3, 0)$, $(-1, 3)$, $(-3, 1)$, $(-2, 3)$, $(-3, 2)$, $(-3, 3)$, where the co-ordinates refer to the axes Q_1, Q_2, are shown in Fig. 3. The numbers plotted are actually the values of $-\dfrac{120}{4\pi^2}\sum_\alpha \dfrac{B_\alpha Q_\alpha^2}{\cdot \Delta}$ and to get the true diffusion function, have to be multiplied by the factor $\dfrac{4m}{3a^4 Q^1} \times \dfrac{4\pi^2}{120}$, where, of course, Q^1 is obtained from the elastic constants in the manner already described.

This factor will, naturally, only change the scale of the isodiffusion lines, but not their form. The isodiffusion lines in Fig. 3 are drawn from the numbers plotted.

From this chart of the isodiffusion lines in the plane $Q_4 = 0$, it is seen that the most intense scattering is represented by those areas which lie close to the points of the reciprocal lattice. These areas of intense scattering are, of course, the so-called 'extra spots', which are surrounded by a weak background. Nevertheless, although the background is relatively weak, it possesses a considerable amount of fine structure. The 'extra spots' associated with the first ring of reciprocal-lattice points are almost isolated by regions of very low scattering power. However, there are ridges of higher scattering power connecting the second ring of reciprocal-lattice points.

Further general features of the chart are that it is invariant for 60° rotations about the origin, and for reflexions in any of the twelve lines joining the second ring of reciprocal-lattice points to the origin. Since it can be shown that these features follow from general symmetry considerations, they must be a general consequence of the close-packed arrangement, and not of the particular assumption of central forces. Another feature of the close-packed arrangement is that the isodiffusion function itself, apart from the factors Q_α^2, is periodic for displacements of three cells in the reciprocal lattice.

It is rather difficult to see what features are general consequences of the assumption of central forces. In the general case, the equation for an isodiffusion line will contain the seven atomic constants. By the assumption of central forces, these seven atomic constants can be expressed in terms of one independent constant, Q^1.
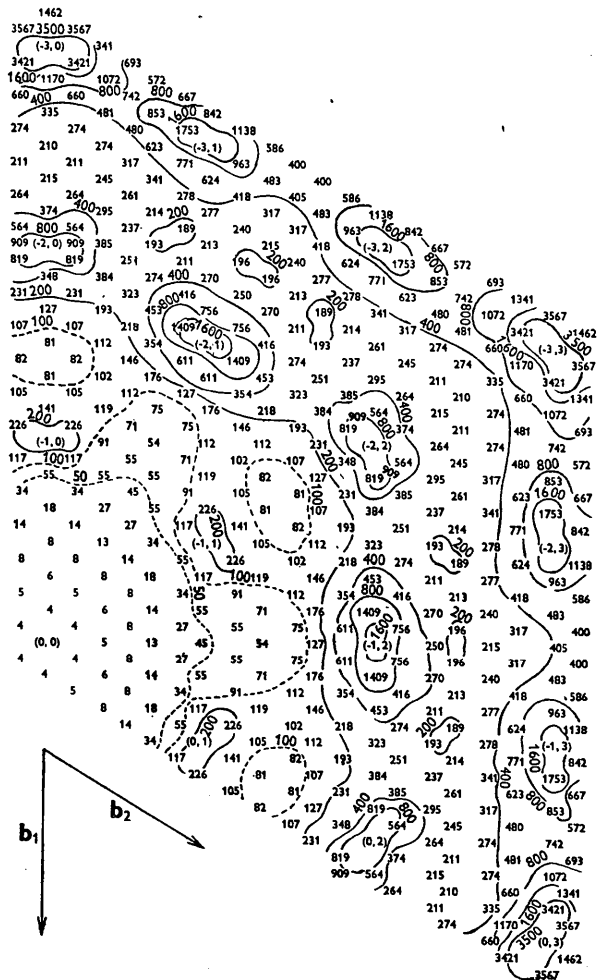

Fig. 3. The isodiffusion lines of a close-packed hexagonal lattice in the plane $Q_4 = 0$.

Thus, the particular form of the isodiffusion lines within the general framework of the features discussed above, is a direct result of the assumption of central forces.

The innermost contour around each reciprocal-lattice point of the chart approximates very closely to the isodiffusion lines obtained by Begbie (1947), for the limiting case of the Jahn approximation. This is only to be expected, since Begbie used the elastic constants of

beryl, which, as has been stated earlier, satisfy approximately the conditions required for central forces. The general shape of the contours changes as one proceeds outwards from a reciprocal-lattice point.

There are no signs of the very strong streaks connecting the Laue spots, which have been reported by Lonsdale (1946) for the case of ice and ammonium fluoride. This would suggest that the origin of these streaks (Born, 1946) is not due to the ordinary thermal motion, but to the existence, in these crystals, of atoms, which have two possible positions of equilibrium. In the case of ice, the hydrogen atoms are assumed to lie on a line joining two oxygen atoms. The equilibrium position of the hydrogen atom is not at the midpoint of this line, but nearer to either one or the other of the oxygen atoms. A survey of the evidence for this is given in a paper by Penny (1947). A statistical distribution of the hydrogen atoms over these two positions would, as Born has shown, give rise to a continuous distribution of scattering power in reciprocal space.

It is to be noted that the chart cannot be extended indefinitely in Q-space, for the general formula (1·6), for the scattering power, is valid only for points of Q-space which are not too far from the origin. This distance depends on the temperature. A full discussion of the validity of the general theory is given in the report by Born (1942–3).

Finally it should be remembered that the calculation has been made using a model in which only the forces between next neighbours are considered. The neglect of long-range forces will be of little influence for long waves (corresponding Q-vectors will lie near a reciprocal-lattice point), but will be very essential for waves of the same order of length as the lattice constant. Thus, in the case of an ionic lattice, where long-range forces are important, the value obtained above for the isodiffusion function for those wave vectors Q which lie in the region between the reciprocal-lattice points can be regarded only as a first approximation. As has been stated by Begbie (1947), the reason for using a model, which certainly is not a good picture of reality, is that the method of next neighbours can be generalized; it can be used for all kinds of substances, and all kinds of symmetry.

I wish to take this opportunity of expressing my gratitude to Prof. Born for suggesting this problem to me and for his advice during the progress of the work.

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Morphological and Dielectric Studies of some Crystals of the Rochelle Salt Type

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Observations have been made on the morphology of crystals of the Rochelle salt type, with particular reference to the effects of added impurities. Certain noteworthy changes of habit have been recorded. Measurements have also been made on the inductivities of about ninety specimens of these crystals, at room temperature, throughout the range of frequency from 650 to 2650 kcyc.sec.$^{-1}$.

While individual values were found not to vary at these frequencies, the inductivities showed a marked dependence on composition and on the presence of cupric ions, boric acid, or the ammonium radical.

Introduction

The crystals of the type of Rochelle salt, with whose inductivities this paper is concerned, may be considered as being derivatives of the original sodium potassium tartrate tetrahydrate (Rochelle salt), in which either the relative amounts of sodium and potassium have been changed or one of these metals has been substituted by a new metallic radical. Crystals of each type were also grown with a habit-modifying addition in the solution.