

tensor  $M_{ij}$  has a zero eigenvalue, *i.e.* if the group of atoms being replaced is linear.

It is, of course, necessary to make a good approximation for the matrix  $W$ . For the method described in this paper a meaningful approximation is only possible if the chiralities of the two groups agree. For a linear group the solution is complete if the direction of the principal axis of inertia of minimum value is found for the atoms being replaced. With the correct choice of sign this corresponds to the best estimate of the linear direction. For non-linear groups, the alignment of principal inertial axes is not to be recommended as the choice of sign question remains and accuracy is very doubtful whenever two principal inertial axes are almost equal. The matrix  $W$  transforms three uniquely defined orthonormal directions in one axial system into equivalently defined directions in the other axial system. A sensible choice of three non-collinear atoms is used. Vector  $u_1$  between atoms 1 and 2 and vector  $u_2$  between atoms 1 and 3 define orthonormal vectors  $v_2 = u_2/N_1$ ,  $v_3 = u_1 \times v_2/N_2$  and  $v_1 = v_2 \times v_3$ , where

$N_1$  and  $N_2$  are normalization constants. We say that

$$v_i = \sum_j U_{ij}^A A_j = \sum_k U_{ik}^B B_k,$$

so that

$$W_{jk} = \sum_i U_{ij}^A U_{ik}^B.$$

$U_{ij}^A$  are direction cosines in the orthonormal axial system  $A_j$  defined by three of the atoms being replaced.  $U_{ik}^B$  are direction cosines in the axial system  $B_k$  defined by the corresponding three replacement atoms.

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## Temperature Effect on the Breadth of Powder Pattern Reflections

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A general method is developed for calculating the temperature diffuse intensity for cubic powder patterns. The method is applied to the pattern of an f.c.c. crystal containing  $10^{12}$  atoms. The effect of temperature vibration is a spreading out at the base of the peak. In terms of the integral breadth, there is an increase which may be of the order of several percent. But the main part of the peak is essentially unaltered, and the increase does not relate to what is generally measured as a breadth. The usual observation is better represented by the breadth at half maximum intensity, and for this quantity there is an increase of less than 0.07% for  $2M=1.0$  and less than 0.17% for  $2M=2.0$ . It is concluded that a real temperature broadening of powder pattern peaks will always be too small to be of importance, or to be experimentally observable.

### 1. Introduction

For crystals containing only one kind of atom, the early Debye approximation, involving independent vibration of the atoms, predicted a reduction in the intensity of the Bragg reflections by the factor  $\exp(-2M)$ , and the appearance of a monotonic diffuse intensity equal to  $I_e N f^2 [1 - \exp(-2M)]$ . There was no broadening of a powder pattern reflection, only a reduction in height.

A better approximation represents the atomic vibrations in terms of a system of elastic waves. The first-order temperature diffuse intensity (TDS) for an f.c.c. powder pattern has been evaluated on the basis of the elastic wave model (Warren, 1953) and the contribu-

tion by second-order TDS has been given by Paskin (1958). It is found that the TDS averages closely to the old independent vibration result, but at the position of each of the Bragg reflections, the TDS rises sharply, and the Bragg reflections are superimposed on these peaks in the diffuse intensity. The elastic wave treatment predicts that the temperature vibration of the atoms should produce a broadening in the peaks occurring at the Bragg positions.

However the previous treatment is not satisfactory for predicting the magnitude of the broadening. At the position of each of the Bragg reflections, the TDS rises to infinite values. This unrealistic result came from an integration in the Brillouin zone over the elastic wave vectors  $g$ , including all wave vectors down to  $g=0$ .

But  $g=0$  corresponds to elastic waves of infinite wavelength, and the existence of such waves requires that the crystal be of infinite size. A treatment restricted to crystals of infinite size is not satisfactory for discussing the broadening of reflections, and we look for a more general approach, applicable to crystals of any size.

## 2. Intensity theory

We consider an f.c.c. crystal with four atoms in the cubic cell. The crystals are assumed to be spherical with  $N$  atoms per crystal, and there are  $W$  crystals in the powder sample. To avoid including a structure factor, we start out using the rhombohedral axes which define a unit cell containing only one atom. Allowing for thermal vibrations, the intensity from one crystal is given by equation (11.16) of Warren (1969):

$$I = I_e f^2 \sum_m \sum_n \exp [2\pi i (\mathbf{S}/\lambda) \cdot \mathbf{r}_{mn}] \exp [-\langle P_{mn}^2 \rangle / 2].$$

From equation (11.14)

$$\langle P_{mn}^2 \rangle = 16\pi^2 (\sin \theta / \lambda)^2 \langle (u_{ms} - u_{ns})^2 \rangle$$

where  $u_{ms}$  is the component of displacement of atom  $m$  along the diffraction vector  $\mathbf{S}$ . An expression for the average  $\langle (u_{ms} - u_{ns})^2 \rangle$  is given on p. 205 of Warren (1969)

$$\langle (u_{ms} - u_{ns})^2 \rangle = 2\langle u_s^2 \rangle [1 - \text{Si}(2\pi g_m r_{mn}) / 2\pi g_m r_{mn}]$$

where  $g_m$  is the radius of the sphere of equal volume which replaces the Brillouin zone, and the approximation has been made that all elastic waves have the same velocity. The Debye temperature factor is given by

$$2M = 16\pi^2 \langle u_s^2 \rangle (\sin \theta / \lambda)^2.$$

Combining these equations, we express the effect of temperature vibration on the intensity from one crystal.

$$I = I_e f^2 \sum_m \sum_n \exp [2\pi i (\mathbf{S}/\lambda) \cdot \mathbf{r}_{mn}] \times \exp \left[ -2M \left\{ 1 - \frac{\text{Si}(2\pi g_m r_{mn})}{2\pi g_m r_{mn}} \right\} \right]. \quad (1)$$

Let  $\mathbf{q}$  be a vector in reciprocal space, directed to the position of measurement from the nearest  $hkl$  point

$$\mathbf{S}/\lambda = h\mathbf{b}_1 + k\mathbf{b}_2 + l\mathbf{b}_3 + \mathbf{q}.$$

It follows that

$$\exp [2\pi i (\mathbf{S}/\lambda) \cdot \mathbf{r}_{mn}] = \exp (2\pi i \mathbf{q} \cdot \mathbf{r}_{mn}) = \exp (2\pi i q r_{mn} \cos \varphi).$$

It is now possible to replace the double sum in equation (1) by an integration in which  $r_{mn}$  is replaced by the continuous variable  $r$ . In the spherical crystal there are displacements of magnitude  $r$  in all orientations relative to  $\mathbf{q}$ , and we can first average over all orientations.

$$\langle \exp (2\pi i q r \cos \varphi) \rangle = \frac{\sin (2\pi q r)}{2\pi q r}. \quad (2)$$

By adding and subtracting  $\exp(-2M)$ , equation (1) is conveniently divided into a Bragg intensity  $I_B$ , and a diffuse intensity  $I_D$

$$I_B(q) = I_e f^2 e^{-2M} \sum_m \sum_n \frac{\sin (2\pi q r)}{2\pi q r} \quad (3)$$

$$I_D(q) = I_e f^2 e^{-2M} \sum_m \sum_n V(r) \frac{\sin (2\pi q r)}{2\pi q r} \quad (4)$$

where

$$V(r) = \exp [2M \text{Si}(2\pi g_m r) / 2\pi g_m r] - 1.$$

## 3. The diffuse intensity

In using equation (4) for the diffuse intensity in an  $hkl$  zone, we neglect the small variation in  $2M$  and use a constant value appropriate to the zone center. Fig. 1 shows a sphere of radius  $R$  which cuts the  $hkl$  Brillouin sphere. The powder pattern intensity for  $R = 2 \sin \theta / \lambda$  is obtained by integrating  $I(q)$  over that part of the surface of the sphere of radius  $R$  which is within the Brillouin sphere, adding the contributions from all zones which are cut by the sphere of radius  $R$ , dividing by  $4\pi R^2$ , and multiplying by  $W$  the number of crystals in the sample. With  $p(hkl)$  as the cubic multiplicity

$$I(R) = \frac{W}{4\pi R^2} \sum_{hkl} p(hkl) \int_{\alpha=0}^{\alpha_m} I(q) 2\pi R^2 \sin \alpha d\alpha.$$

From here on, we shall be using cubic axes with  $a$  the edge of the cubic unit cell. From Fig. 1,

$$q^2 = R^2 + R_{hkl}^2 - 2RR_{hkl} \cos \alpha$$

and hence

$$RR_{hkl} \sin \alpha d\alpha = q dq.$$

The new limits are  $q = R - R_{hkl}$  and  $q = g_m$ . Introducing the notation  $X = aR = 2a \sin \theta / \lambda$ ,  $X_{hkl} = aR_{hkl}$ , and  $\varepsilon = X - X_{hkl}$ ,

$$I_D(X) = \frac{W I_e f^2 e^{-2M}}{8\pi^2 X} \sum_{hkl} \frac{p(hkl)}{X_{hkl}} \times \sum_m \sum_n V(r) \left[ \frac{\cos 2\pi \varepsilon r / a - \cos 2\pi g_m r}{(r/a)^2} \right]. \quad (5)$$

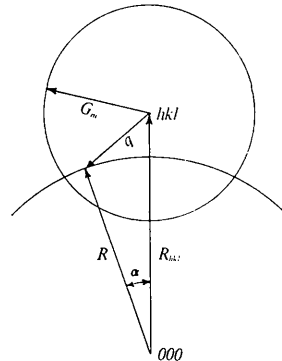


Fig. 1. Construction for obtaining the contribution from the zone  $hkl$  to the powder pattern intensity at  $R = 2 \sin \theta / \lambda$ .

The volume of the Brillouin zone is the reciprocal of the volume per atom

$$\frac{4\pi}{3} g_m^3 = \frac{4}{a^3}, \quad a g_m = 0.985, \quad \gamma = 2\pi g_m a = 6.19.$$

We now replace the double sum by an integral. For a spherical crystal of radius  $\varrho$  containing  $N$  atoms, the number of terms corresponding to pairs of atoms with separation between  $r$  and  $r+dr$  is

$$n(r)dr = NG(r) \frac{4}{a^3} 4\pi r^2 dr$$

where

$$G(r) = 1 - \frac{3r}{4\varrho} + \frac{r^3}{16\varrho^3}.$$

The integration is from  $r=0$  to  $r=2\varrho$ , and  $\varrho$  is determined by

$$\frac{4\pi}{3} \varrho^3 \left( \frac{4}{a^3} \right) = N.$$

It is convenient to introduce a dimensionless variable with the following changes

$$r/a = u, \quad \varrho/a = U, \quad G(u) = 1 - \frac{3u}{4U} + \frac{u^3}{16U^3},$$

$$V(u) = \exp [2M \text{Si}(\gamma, u)/\gamma, u] - 1.$$

With these changes equation (5) becomes

$$I_D(X) = WNI_e f^2 e^{-2M} \frac{2}{\pi X} \sum_{hkl} \frac{p(hkl)}{X_{hkl}} \times \int_{u=0}^{2U} G(u)V(u) [\cos 2\pi\epsilon u - \cos \gamma u] du. \quad (6)$$

To evaluate the integral in equation (6), we divide it into two parts. For  $u > 5$ ,  $\text{Si}(\gamma, u)/\gamma, u$  is well approximated by  $\pi/2\gamma, u$ , the exponential in  $V(u)$  can be expanded, and we can write  $V(u) = \pi M/\gamma u$ .

$$\int_{u=0}^{2U} G(u)V(u) \cos 2\pi\epsilon u du = Y(\epsilon) = Y_1(\epsilon) + Y_2(\epsilon)$$

where

$$Y_1(\epsilon) = \int_{u=0}^5 G(u)V(u) \cos 2\pi\epsilon u du,$$

$$Y_2(\epsilon) = \frac{\pi M}{\gamma} \int_{u=5}^{2U} \left( 1 - \frac{3u}{4U} + \frac{u^3}{16U^3} \right) \frac{\cos 2\pi\epsilon u}{u} du.$$

The first integral  $Y_1(\epsilon)$  is readily evaluated numerically. The integral  $Y_2(\epsilon)$  can be expressed in terms of tabulated functions such as  $\text{Ci}(z)$  and  $\sin z/z$ . Discarding terms in  $1/U^3$  and restricting to values of  $\epsilon$  for which  $\epsilon > (1/U)$

$$Y_2(\epsilon) = \frac{\pi M}{\gamma} \left[ -\text{Ci}(2\pi\epsilon 5) + \frac{15}{4U} \frac{\sin 2\pi\epsilon 5}{2\pi\epsilon 5} - \frac{\sin 4\pi\epsilon U}{(4\pi\epsilon U)^3} \right].$$

In equation (6), the contribution from the term  $\cos \gamma u$  is small. Neglecting this term, the contribution to the powder pattern diffuse intensity from the zone  $hkl$  is given by

$$I_D(\epsilon) = WNI_e f^2 e^{-2M} \frac{p(hkl)}{X X_{hkl}} \frac{2}{\pi} Y(\epsilon). \quad (7)$$

#### 4. Intensity distribution in the Bragg reflections

The Bragg intensity from one crystal is given by equation (3). It is identical to the  $I_D(\varrho)$  of equation (4) if we set  $V(r)=1$ . The powder pattern intensity distribution in a Bragg reflection is obtained by following the same procedure used in obtaining equations (5) and (6). By setting  $V(u)=1$  in equation (6) and making the approximation  $X=X_{hkl}$  we obtain

$$I_B(\epsilon) = WNI_e f^2 e^{-2M} \frac{p(hkl)}{X_{hkl}^2} \times \frac{2}{\pi} \int_{u=0}^{2U} G(u) [\cos 2\pi\epsilon u - \cos \gamma u] du.$$

The contribution from the term  $\cos \gamma u$  is small enough to neglect. With an integration by parts, the powder pattern intensity distribution in a Bragg reflection is given by

$$I_B(\epsilon) = WNI_e f^2 e^{-2M} \frac{p(hkl)}{X_{hkl}^2} \frac{3U}{2\pi} Z(2\pi\epsilon U) \quad (8)$$

where

$$Z(t) = \frac{1}{t^2} \left[ 1 + \left( \frac{\sin t}{t} \right)^2 - \frac{2 \sin 2t}{2t} \right]. \quad (9)$$

The function  $Z(t)$  has the properties

$$Z(0) = 1, \quad \int_0^\infty Z(t) dt = 2\pi/3.$$

#### 5. Peak broadening by temperature vibration

To compare the diffuse intensity related to an  $hkl$  Brillouin zone, with the intensity in the same  $hkl$  Bragg reflection, it is convenient to introduce reduced intensities  $I'_D(\epsilon)$  and  $I'_B(\epsilon)$ . For  $I'_D(\epsilon)$  we make the approximation  $X=X_{hkl}$ .

$$I'_D(\epsilon) = \frac{I_D(\epsilon) X_{hkl}^2}{WNI_e f^2 p(hkl)} = e^{-2M} \frac{2}{\pi} Y(\epsilon), \quad (10)$$

$$I'_B(\epsilon) = \frac{I_B(\epsilon) X_{hkl}^2}{WNI_e f^2 p(hkl)} = e^{-2M} \frac{3U}{2\pi} Z(2\pi\epsilon U). \quad (11)$$

The broadening of the reflection at a Bragg position by inclusion of the diffuse intensity is illustrated by a numerical example. We choose the values  $2M=1.0$  and  $N=10^{12}$  from which  $U=3910$ . Fig. 2 shows the Bragg intensity  $I'_B(\epsilon)$ , the diffuse intensity  $I'_D(\epsilon)$ , and the sum

$I'_B(\varepsilon) + I'_D(\varepsilon)$ . The major effect of adding  $I'_D(\varepsilon)$ , is to spread out the base of the Bragg peak. For this unusual kind of broadening, it makes a difference whether we discuss the broadening in terms of the integral breadth or the half maximum intensity breadth.

We first consider the broadening in terms of the integral breadth  $\beta$ . Calling  $A_B$  the area of the  $I'_B(\varepsilon)$  peak,

$$A_B = \int_{-\infty}^{+\infty} I'_B(\varepsilon) d\varepsilon = e^{-2M} \frac{3U}{2\pi} \int_{-\infty}^{+\infty} Z(2\pi U\varepsilon) d\varepsilon = \frac{1}{\pi} e^{-2M}.$$

On an  $\varepsilon$  scale, the integral breadth of the  $I'_B(\varepsilon)$  peak is

$$\beta_B = A_B / I'_B(0) = 2/3U.$$

Suppose that areas are measured above a background line which cuts through the curve  $I'_B(\varepsilon) + I'_D(\varepsilon)$  of Fig. 2 at  $\varepsilon = \pm\eta$ . The area contributed by the diffuse intensity  $I'_D(\varepsilon)$  is

$$A_D(\eta) = \frac{4}{\pi} e^{-2M} T(\eta)$$

where

$$T(\eta) = \int_0^\eta Y(\varepsilon) d\varepsilon - \eta T(\eta).$$

Let  $\beta'(\eta)$  be the integral breadth of that part of  $I'_B(\varepsilon) + I'_D(\varepsilon)$  above the background level

$$\begin{aligned} \beta'(\eta) &= \frac{A_B + A_D(\eta)}{I'_B(0) + I'_D(0) - I'_D(\eta)} \\ &= \frac{1 + 4T(\eta)}{(3U/2) \{1 + (4/3U) [Y(0) - Y(\eta)]\}}. \end{aligned} \quad (12)$$

The broadening produced by temperature vibration is conveniently represented by the ratio  $\beta'(\eta)/\beta_B$ . Calling this ratio  $\alpha$ , we have

$$\alpha = \frac{\beta'(\eta)}{\beta_B} = \frac{1 + 4T(\eta)}{1 + (4/3U) [Y(0) - Y(\eta)]}. \quad (13)$$

Values of the ratio are given in Table 1, for various values of  $2M$  and  $\eta$ .

Table 1. Values of  $\alpha$  for  $N = 10^{12}$

|            | $\eta = 0.01$ | $\eta = 0.02$ | $\eta = 0.05$ |
|------------|---------------|---------------|---------------|
| $2M = 1.0$ | 1.010         | 1.020         | 1.052         |
| $2M = 2.0$ | 1.021         | 1.042         | 1.107         |

In terms of the integral breadth, the temperature vibration of the atoms has produced an increase in peak breadth which amounts to several percent. However this increase is due to inclusion of the area increase resulting from the spreading out at the base of the peak. The main part of the peak is essentially unaltered, and it is questionable whether it is realistic

to consider this as truly representative of a peak broadening.

The breadth at half maximum intensity probably represents more closely the quantity observed when comparing peak breadths, and we now consider this kind of breadth. For  $2M = 1.0$ , the curves of interest are those of Fig. 2. For the Bragg reflection alone, at half maximum intensity,  $\varepsilon = 7.0 \times 10^{-5}$  and  $dI'_B(\varepsilon)/d\varepsilon = -67 \times 10^5$ . The value of  $I'_D(\varepsilon)$  decreases very little in a range of  $\varepsilon$  several times that corresponding to the half maximum breadth of  $I'_B(\varepsilon)$ , and in this range of  $\varepsilon$ , the curve  $I'_B(\varepsilon) + I'_D(\varepsilon)$  is essentially just  $I'_B(\varepsilon)$  raised by  $I'_D(0) = 0.68$ . If the background level is taken at the zero ordinate of Fig. 2, the half maximum breadth of  $I'_B(\varepsilon) + I'_D(\varepsilon)$  will be that of the half maximum position on  $I'_B(\varepsilon)$  lowered by  $0.68/2 = 0.34$ . The increase in  $\varepsilon$  is given by  $0.34 (67 \times 10^5) = 0.0050 \times 10^{-5}$ , and the fractional increase in breadth is  $\Delta\varepsilon/\varepsilon = 0.0050 \times 10^{-5} / (7.0 \times 10^{-5}) = 0.0007$ . For the extreme case, where the background is taken at the zero level of Fig. 2, the increase is 0.07%. A similar calculation for  $2M = 2.0$  gives an upper limit of 0.17% for the increase in breadth. Since the background level will always be taken well above the zero level of Fig. 2, the increase in the half maximum intensity breadth will be less than the upper limit values of 0.07 and 0.17% which have been computed. In practice the peak will be broadened by a convolution with the various sources of instrumental broadening, and this will further decrease the observable broadening by temperature vibration.

In terms of the integral breadth, the temperature vibration of the atoms produces an increase in peak

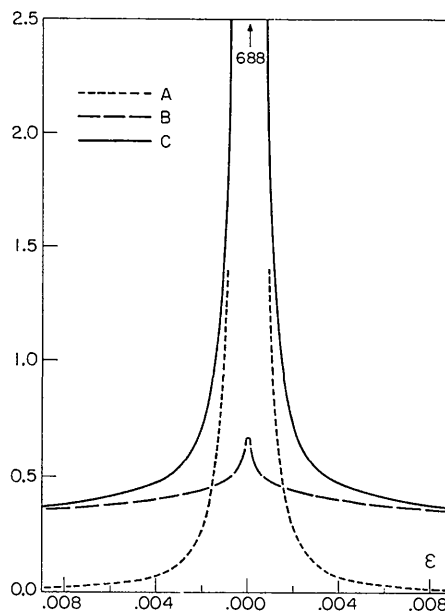


Fig. 2. Contributions to a Bragg peak for  $N = 10^{12}$  and  $2M = 1.0$ . A is the Bragg peak  $I'_B(\varepsilon)$ , B is the diffuse intensity  $I'_D(\varepsilon)$ , C is the sum  $I'_B(\varepsilon) + I'_D(\varepsilon)$ .

breadth which may amount to several percent. However this is an increase which results from a spreading out at the base of peak, it is not the kind of increase in breadth which we normally look for in comparing two peaks. The breadth at half maximum intensity represents more closely the quantity which is used in practice. Although there is a small increase in this kind of breadth, the magnitude is too small to be of importance or to be experimentally observable.

I am indebted to Dr B. D. Cullity for a preliminary discussion of powder pattern broadening by temperature vibration.

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## Some Comments on and *Addenda* to the Tables of Irreducible Representations of the Classical Space Groups Published by S. C. Miller and W. F. Love

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A summary is given of some work which has been performed to identify those special points, lines, and planes of symmetry that have been omitted from published tables of irreducible representations of space groups. In order to have a complete set of all the irreducible representations of every space group, it is necessary to determine the irreducible representations for these additional wave vectors in order to supplement the existing published sets of tables. The generation of these supplementary tables is reported.

### 1. Introduction

The irreducible representations of space groups have been used for many years for labelling the electronic band structures of crystalline solids. More recently, their use has been extended to labelling phonon dispersion relations and the energy eigenstates for other particles or quasi-particles. In addition to providing a useful scheme for labelling energy bands or dispersion relations, the irreducible representations of the space groups can also be used to predict essential degeneracies, to simplify the calculation of electronic band structures or of phonon dispersion relations, and in the determination of selection rules for processes involving electrons or phonons in crystalline solids; for details see, for example, Cracknell (1974, 1975).

Tables of irreducible representations were first published for three important symmorphic space groups,  $Pm3m(O_h^1)$ ,  $Fm3m(O_h^5)$ , and  $Im3m(O_h^9)$  by Bouckaert, Smoluchowski & Wigner (1936) and for two of the more important non-symmorphic space groups,  $P6_3/mmc(D_{6h}^4)$  and  $Fd3m(O_h^7)$ , by Herring (1942). Since then, many papers have been published giving tables of the irreducible representations of various selections of space groups. During the last few years there have been several systematic attempts to publish complete sets of tables of irreducible representations for all the

230 classical space groups (Faddeyev, 1964; Kovalev, 1965; Miller & Love, 1967; Zak, Casher, Glück & Gur, 1969; Bradley & Cracknell, 1972). Some recent work which we have been doing, in connexion with the reduction of Kronecker products of space-group representations, has made us realize that each of these published sets of tables contains some deficiencies. We shall concern ourselves primarily with the tables of Miller & Love (1967), which we shall refer to hereafter as M & L, because they are the most explicit tables and also, being computer-generated, they are in the most convenient form for use in further computer-based calculations.

The points that we wish to make concern (i) the completeness of the identification of special points and lines of symmetry, without restrictions being imposed on the axial ratios for certain space groups (see § 2), (ii) the systematic identification of planes of symmetry in all space groups (see § 3), and (iii) the determination of the irreducible representations for all distinct wave vectors in the 'representation domain',  $\Phi$ , which for many space groups is larger than the 'basic domain',  $\Omega$ .

In the space available in this journal we shall only be able to summarize our work on these topics. There are, inevitably, a considerable number of new diagrams and tables that we have had to construct but which cannot be included here.\*

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\* The diagrams and tables are all included in a paper. *On the completeness of tables of irreducible representations of the classical space groups* (Davies & Cracknell, 1976).