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FOURIER SUMMATIONS FOR SYMMETRICAL CRYSTALS

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ABSTRACT

This paper is concerned with the application of symmetry principles to the reduction of terms in Fourier synthesis. For this purpose two theorems are first given, the reciprocal symmetry theorem and the additivity theorem. To illustrate the use of these in performing summations for symmetrical crystals, the form of the electron density function is derived for Fourier syntheses of projections corresponding to the 17 plane groups. The extension of the method to three-dimensional syntheses is also discussed in sufficient detail so that it can be applied to any space group.

INTRODUCTION

In performing Fourier summations, it appears to be a common practice to disregard the symmetry of the crystal and fit the summation into the classical case of centrosymmetry [1] if possible, otherwise into the non-symmetrical case. Failure to make use of the symmetry of the crystal requires the summation to be made for a great number of unnecessary terms, and thus increases the labor of performing the summation. It also produces a summation in which the errors accumulate in an unsymmetrical way. When symmetry-equivalent segments are selected from such a synthesis, their edges usually do not match, and in order to make the segments fit together, an adjustment of the values in the neighborhood of the edges is necessary.

In this paper, some general devices for utilizing symmetry in performing the summation for symmetrical crystals are discussed. Specific forms for the Fourier summations for the symmetries of the various projections are derived, and the extension of the methods to three-dimensional summations is outlined.

GENERAL FORM OF THE FOURIER SUMMATION

The Fourier summation for electron density has the following form:

$$\rho(xyz) = \frac{1}{V} \sum_{h} \sum_{k=-\infty}^{\infty} \sum_{l} F_{hkl} e^{-2\pi i(hx+ky+lz)}. \tag{1}$$

Since this form involves phases, it is convenient for computational purposes to recast it in such a way that the real and imaginary parts are separated. The decomposition of the complex terms into real and imaginary components is as follows:

$$F_{hkl} = A_{hkl} + iB_{hkl} \tag{2}$$

$$e^{-i\phi} = \cos\phi - i\sin\phi. \tag{3}$$

Making this substitution in (1), it becomes

$$\rho(xyz) = \frac{1}{V}\sum_{h}\sum_{\substack{k\\-\infty}}^{\infty}\sum_{l}\left\{A_{hkl} + iB_{hkl}\right\}\left\{\cos 2\pi(hx + ky + lz) - i\sin 2\pi(hx + ky + lz)\right\}. \tag{4}$$

$$\begin{aligned} = \frac{1}{V}\sum_{h}\sum_{\substack{k\\-\infty}}^{\infty}\sum_{l} & A_{hkl}\cos 2\pi(hx + ky + lz) \\ & - iA_{hkl}\sin 2\pi(hx + ky + lz) \\ & + iB_{hkl}\cos 2\pi(hx + ky + lz) \\ & - i^2B_{hkl}\sin 2\pi(hx + ky + lz). \end{aligned} \tag{5}$$

This summation is made over all indices from $-\infty$ to ∞. If reflections hkl and $\overline{hkl}$ are considered in pairs, then Friedel's law can be applied to the members of the pairs. Friedel's law can be stated in the following form:

$$\begin{aligned} F_{\overline{hkl}} &= A_{\overline{hkl}} + iB_{\overline{hkl}} \\ F_{\overline{hkl}} &= A_{hkl} - iB_{hkl}. \end{aligned} \tag{6}$$

From this statement of the law it is obvious that

$$\begin{aligned} A_{hkl} &= A_{\overline{hkl}} \\ B_{hkl} &= -B_{\overline{hkl}}. \end{aligned} \tag{7}$$

Furthermore, for pairs of reflections hkl and $\overline{hkl}$, the following relations hold in the trigonometric parts of (5):

$$\begin{aligned} \cos 2\pi(hx + ky + lz) &= \cos 2\pi(\bar{h}x + \bar{k}y + \bar{l}z) \\ \sin 2\pi(hx + ky + lz) &= -\sin 2\pi(\bar{h}x + \bar{k}y + \bar{l}z). \end{aligned} \tag{8}$$

In (5), the second line involves the sine, and according to (8) every term in the summation for a particular hkl is exactly cancelled by a similar term for the corresponding $\overline{hkl}$. Similarly, the third line involves a B, and according to (7) every term in the summation for a particular hkl is exactly cancelled by a similar term for the corresponding $\overline{hkl}$. The last line does not cancel for hkl and $\overline{hkl}$, because two sign changes are involved in the relation between hkl and $\overline{hkl}$.

These considerations leave a comparatively simple form for Fourier summation in terms of the real and imaginary components:

$$\rho(xyz) = \frac{1}{V}\sum_{h}\sum_{\substack{k\\-\infty}}^{\infty}\sum_{l} A_{hkl}\cos 2\pi(hx + ky + lz) + B_{hkl}\sin 2\pi(hx + ky + lz). \tag{9}$$

BASIC PRINCIPLES FOR COMBINATION

Introduction. In performing a Fourier summation, it should be possible to limit the actual summation to a representative section of the data and then derive the rest of the summation by principles of symmetry. This derivation, or combination, can be carried on either in reciprocal space or in direct space. If it is carried out in reciprocal space, it is necessary to know the effect of crystal symmetry in reciprocal space. If it is carried out in direct space, it is necessary to know how to make the combination. For these two situations, the following two theorems, respectively, are very useful and are stated without proof [5].

Theorem of Reciprocal Symmetry. *The symmetry of reciprocal space is the same as the isomorphous point-group symmetry of direct space, except that every symmetry element containing the origin produces a phase change in its equivalent space fields of* $e^{2\pi ih/n}$. Here a/n is the translation component of the symmetry operation. Note that the phase shift becomes zero for $n=0$, i.e., for pure reflections and pure rotations.

This theorem makes it unnecessary to derive phase relations between F's by the tedious method of using structure factors [2]. All possible relations for any given space group can be written down by inspection with the aid of the theorem.

Theorem of Additivity. It is convenient to regard the process of Fourier synthesis as a transformation from a space to its reciprocal. For combinations occurring in the new space, the theorem of additivity can be employed. In the present application, the transformation is from reciprocal space to direct space. The following theorem, of course, is valid for either direction of transformation:

The transform of a sum is the sum of the transforms, i.e.,

$$T_{xyz}(M + N) = T_{xyz}(M) + T_{xyz}(N). \tag{10}$$

In the present problem, this can be applied in the following way: If reciprocal space is divided into blocks in any desired way, and if the synthesis is carried out for each block, the complete synthesis is equal to the sum of the separate syntheses of the blocks. In particular, each block of reciprocal space may be one of the unsymmetrical fields related by the several symmetry elements. Actually, since all fields are the same except for orientation, the synthesis need be carried on for only one field. If the resulting transform for this single field is then displaced in accordance with the requirements of the operations of crystal symmetry, and the several results at xyz added, the sum is the complete transform at xyz. An equivalent way of performing the final summation is to start with the transform of a single data field, then add together the value of the transform at xyz and all symmetry-equivalent points, recording the sum at xyz.

This scheme provides a perfectly general way of performing the Fourier synthesis for a symmetrical crystal. If it is pursued blindly, however, it sometimes involves unnecessary labor because in the process of combining, some of the components of symmetrically related fields cancel. For this reason, it is important to first study the consequences of the first theorem, which often reveals the manner in which certain components of the unsymmetrical fields cancel when combined in symmetrical manners.

Additional Aids to Synthesis. By the aid of the two theorems just mentioned, the appropriate form of the synthesis for any plane group or space group can be written down by inspection. If this is to be done in a systematic way for a large number of groups, extensive use may be made of generating operations. Thus, in deriving space groups, a group may be derived from any of its subgroups by adding a generating operation to the subgroup. Similarly, in reciprocal space, a symmetry combination can be derived from a subgroup symmetry by adding a generating operation. This involves an additional phase relation. Therefore, the form for symmetrical Fourier synthesis may be derived from the form appropriate to a subgroup by imposing upon it the appropriate additional phase relationship of the added generating operation.

When the symmetry operations of the crystal transform each axis into itself, then it is also possible to make the form of the synthesis more compact by making use of the symmetrical properties of the trigonometric functions for positive and negative indices with respect to the same axes. For brevity this property is called "interchange symmetry." This kind of compaction is not possible when the symmetry operation does not cause this particular type of transformation. It does not occur, therefore, for trigonal or hexagonal crystals, nor for diagonal reflections.

SYMMETRICAL SYNTHESES FOR THE PLANE PROJECTIONS

Introduction. Since the most common Fourier synthesis is probably the plane projection, the derivation of symmetrical syntheses will be illustrated by deriving the appropriate forms of the summations for plane projections of the several possible plane symmetries. The form of the summation corresponding to the electron density projected on a plane normal to some rational axis is the two-dimensional equivalent of (9). For clearness, suppose specifically that the electron density is desired as projected on a plane normal to the c axis. The form of the summation is then

$$\rho(xy) = \frac{1}{S} \sum_{h}^{\infty}\sum_{k}_{-\infty} A_{hk0} \cos 2\pi(hx + ky) + B_{hk0} \sin 2\pi(hx + ky). \qquad (11)$$

Here S is the area of the section of the cell perpendicular to the direction of the projection, in this case normal to the c axis.

To recast this in a form more convenient for computational procedures, the trigonometric functions of sums of angles are expressed as products, as first suggested by Beevers and Lipson [3] by the use of the identities

$$\begin{aligned}\cos(\alpha+\beta) &= \cos\alpha\cos\beta - \sin\alpha\sin\beta\\ \sin(\alpha+\beta) &= \sin\alpha\cos\beta + \cos\alpha\sin\beta.\end{aligned}\qquad(12)$$

Making these substitutions in (11) it takes the form

$$\begin{aligned}\rho(xy) = \frac{1}{S}\sum_h\sum_k{}_{-\infty}^{\infty}\; & A_{hk0}\cos 2\pi hx\cos 2\pi ky\\ & - A_{hk0}\sin 2\pi hx\sin 2\pi ky\\ & + B_{hk0}\sin 2\pi hx\cos 2\pi ky\\ & + B_{hk0}\cos 2\pi hx\sin 2\pi ky.\end{aligned}\qquad(13)$$

Symmetry *p*1. Friedel's law provides the relation between the phases of any two halves of reciprocal space. For symmetry *p*1, therefore, reciprocal space may be divided into any two halves and the Fourier summation may be expressed in terms of either one. Furthermore, since the symmetry operation 1 transforms each axis into itself, there is a second relation between the indices with respect to positive and negative ends of the same axis which arises due to the symmetrical properties of the trigonometric functions. To take advantage of these two symmetries, divide reciprocal space into four segments along the reciprocal axes. The four segments now contain F's having indices $hk0$, $\bar{h}k0$, $\bar{h}\bar{k}0$, and $h\bar{k}0$, respectively. Now, the summation (13) extends over all reciprocal space. It can be rewritten in terms of the summations over these four segments of reciprocal space. In doing this a precaution should be observed: the division lines of the reciprocal space into four segments occur through the lines $h00$, $0k0$, $\bar{h}00$, and $0\bar{k}0$. Each of these lines, therefore, belong to its two adjoining sectors equally, while the origin point belongs to all four segments. The lines $h00$, $0k0$, $\bar{h}00$, and $0\bar{k}0$ should be counted only at half value for each segment, and the origin point only at quarter value. The special nature of the multiplicity of the edges and point of each segment is indicated by adding a prime to the summation, thus: $\sum'$. With this convention, the expansion of (12) into separate summations for each of the four sectors is

$$\begin{aligned}(xy) = \frac{1}{S}\sum_h{}'\sum_k{}'{}_{0}^{\infty}\\ A_{hk0}\cos 2\pi hx\cos 2\pi ky &+ A_{\bar{h}k0}\cos 2\pi\bar{h}x\cos 2\pi ky + A_{\bar{h}\bar{k}0}\cos 2\pi\bar{h}x\cos 2\pi\bar{k}y + A_{h\bar{k}0}\cos 2\pi hx\cos 2\pi\bar{k}y\\ - A_{hk0}\sin 2\pi hx\sin 2\pi ky &- A_{\bar{h}k0}\sin 2\pi\bar{h}x\sin 2\pi ky - A_{\bar{h}\bar{k}0}\sin 2\pi\bar{h}x\sin 2\pi\bar{k}y - A_{h\bar{k}0}\sin 2\pi hx\sin 2\pi\bar{k}y\\ + B_{hk0}\sin 2\pi hx\cos 2\pi ky &+ B_{\bar{h}k0}\sin 2\pi\bar{h}x\cos 2\pi ky + B_{\bar{h}\bar{k}0}\sin 2\pi\bar{h}x\cos 2\pi\bar{k}y + B_{h\bar{k}0}\sin 2\pi hx\cos 2\pi\bar{k}y\\ + B_{hk0}\cos 2\pi hx\sin 2\pi ky &+ B_{\bar{h}k0}\cos 2\pi\bar{h}x\sin 2\pi ky + B_{\bar{h}\bar{k}0}\cos 2\pi\bar{h}x\sin 2\pi\bar{k}y + B_{h\bar{k}0}\cos 2\pi hx\sin 2\pi\bar{k}y.\end{aligned}\qquad(14)$$

Friedel's law provides symmetry relations between alternate columns. According to (7) the A's of alternate columns have the same sign, but the B's have opposite signs. Furthermore, the cosines in alternate columns are equal and have the same signs, while the sines are equal but with opposite signs. Note, now, that alternate columns are related by zero or two sign changes in the trigonometric functions if the coefficient is an A, whereas if the coefficient is a B, they are related by one sign change in the trigonometric part. Since B also contributes a sign change according to (7), alternate columns are related by an even number of sign changes, and are, therefore, identical. As a consequence, (14) can be more compactly expressed as twice the sum of the first two columns, namely

$$\begin{aligned}\rho(xy) = \frac{2}{S}\sum_{h}{}'\,{}_{-\infty}^{\infty}\sum_{k}{}' A_{hk0}\cos 2\pi hx \cos 2\pi ky &+ A_{\bar{h}k0}\cos 2\pi\bar{h}x\cos 2\pi ky \\ - A_{hk0}\sin 2\pi hx \sin 2\pi ky &- A_{hk0}\sin 2\pi\bar{h}x \sin 2\pi ky \\ + B_{hk0}\sin 2\pi hx\cos 2\pi ky &+ B_{\bar{h}k0}\sin 2\pi\bar{h}x\cos 2\pi ky \\ + B_{hk0}\cos 2\pi hx \sin 2\pi ky &+ B_{hk0}\cos 2\pi\bar{h}x\sin 2\pi ky. \qquad (15)\end{aligned}$$

The reduction of terms just discussed makes use of Friedel symmetry only. Interchange symmetry is also present in $p1$. To take advantage of this, express $\cos 2\pi\bar{h}x$ as $\cos 2\pi hx$ and express $\sin 2\pi\bar{h}x$ as $-\sin 2\pi hx$. This expresses (15) in terms of functions of positive angles only:

$$\begin{aligned}\rho(xy) = \frac{2}{S}\sum_{h}{}'\,{}_{0}^{\infty}\sum_{k}{}' A_{hk0}\cos 2\pi hx\cos 2\pi ky &+ A_{\bar{h}k0}\cos 2\pi hx\cos 2\pi ky \\ - A_{hk0}\sin 2\pi hx\sin 2\pi ky &- A_{\bar{h}k0}(-\sin 2\pi hx)\sin 2\pi ky \\ + B_{hk0}\sin 2\pi hx\cos 2\pi ky &+ B_{hk0}(-\sin 2\pi hx)\cos 2\pi ky \\ + B_{hk0}\cos 2\pi hx\sin 2\pi ky &+ B_{\bar{h}k0}\cos 2\pi hx \sin 2\pi ky. \qquad (16)\end{aligned}$$

Interchange symmetry provides no relations among A's or among B's. Therefore, although the first and second columns have similar trigonometric forms, they have different coefficients. Nevertheless, a more compact expression, which represents a great reduction in the labor of the synthesis, can be had by combining the trigonometric parts as follows:

$$\begin{aligned}\rho(xy) = \frac{2}{S}\sum_{h}{}'\,{}^{\infty}\sum_{k}{}'(A_{hk0} + A_{\bar{h}k0})&\cos 2\pi hx\cos 2\pi ky \\ - (A_{hk0} - A_{\bar{h}k0})&\sin 2\pi hx\sin 2\pi ky \\ + (B_{hk0} - B_{\bar{h}k0})&\sin 2\pi hx\cos 2\pi ky \\ + (B_{hk0} + B_{\bar{h}k0})&\cos 2\pi hx\sin 2\pi ky. \qquad (17)\end{aligned}$$

Symmetry $p2$. Symmetry* $p2$ may be derived from symmetry $p1$ by adding to it the generating operation 2. According to the reciprocal symmetry theorem, this operation causes the symmetry

$$\begin{aligned} & F_{hk0} = F_{\bar{h}\bar{k}0} \\ \therefore \quad & A_{hk0} + iB_{hk0} = A_{hk0} - iB_{hk0}, \\ \therefore \quad & B_{hk0} = B_{\bar{h}\bar{k}0} = 0, \\ \text{and} \quad & A_{hk0} = F_{hk0}. \end{aligned} \tag{18}$$

Evidently the appropriate form of the symmetrical summation for symmetry $p2$ can be derived from that of symmetry $p1$ by applying the last two conditions of (18) to (17). This provides the following form for $p2$:

$$\begin{aligned} \rho(xy) = \frac{2}{S} \sum_{h}{}' \overset{\infty}{\underset{0}{}} \sum_{k}{}' (F_{hk0} + F_{\bar{h}k0}) \cos 2\pi hx \cos 2\pi ky \\ - (F_{hk0} - F_{\bar{h}k0}) \sin 2\pi hx \sin 2\pi ky. \end{aligned} \tag{19}$$

This is equivalent to the classical form of Beevers and Lipson [1] for projections with centro-symmetry.

Symmetries $pm1$ and $cm1$. Both of the symmetries $pm1$ and $cm1$ have identical symmetries in reciprocal space; these plane groups differ only in the locations of points where the value of the transform does not vanish. These symmetries can be derived from symmetries $p1$ and $c1$, respectively, by the addition of the generating operation m parallel to b. According to the reciprocal symmetry theorem, this imposes the additional relation

$$\begin{aligned} & F_{hk0} = F_{\bar{h}k0}, \\ \therefore \quad & A_{hk0} = A_{\bar{h}k0}, \\ \text{and} \quad & B_{hk0} = B_{\bar{h}k0}. \end{aligned} \tag{20}$$

Under these conditions, the second and third rows of (17) vanish, leaving the simpler form

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* The nomenclature of the plane groups used here differs somewhat from that given inside the covers of the writer's book *X-Ray Crystallography*. The correspondence table is as follows:

This paper	X. R. C.	This paper	X. R. C.
*p*1	*P*1	*p*3	*C*3
*pm*1	*Pl*	*p*3*m*1	*C*3*l*1
*pg*1	*Pb*	*p*31*m*	*C*31*l*
*cm*1	*Cl*	*p*4	*P*4
*p*2	*P*2	*p*4*mm*	*P*4*ll*
*p*2*mm*	*Pll*	*p*4*gg* (origin on 4)	*P*4*bl*
*p*2*gg*	*Pba*	*p*6	*P*6
*p*2*gm*	*Pbl*	*p*6*mm*	*C*6*ll*
*c*2*mm*	*Cll*		

$$\rho(xy) = \frac{4}{S}\sum_{h}{}'\sum_{\substack{k\\0}}^{\infty}{}'\; A_{hk0}\cos 2\pi hx \cos 2\pi ky$$

$$+\; B_{hk0}\cos 2\pi hx \sin 2\pi ky \tag{21}$$

$$= \frac{4}{S}\sum_{h}{}'\left[\sum_{\substack{k\\0}}^{\infty}{}' A_{hk0}\cos 2\pi kx + B_{hk0}\sin 2\pi ky\right]\cos 2\pi hx. \tag{22}$$

The latter form implies a considerable saving in labor. It indicates that for each available value of *h*, a summation over *k* can be made for *h* constant. This first summation requires both a cosine and a sine summation. But once this preliminary summation is complete, the resulting coefficient requires only a cosine summation over the available values of *h*.

Symmetry *pg*1. Symmetry *pg*1 can be derived from *p*1 by the addition of a generating operation *g* parallel to *b*. According to the reciprocal symmetry theorem, this symmetry element gives rise to the additional relation

$$F_{hk0} = e^{2\pi ik/2}\,F_{\bar{h}k0}. \tag{23}$$

Therefore, the reflections can be grouped into two classes:

$$\begin{aligned} &\text{for } k \text{ even:} \quad F_{hk0} = F_{\bar{h}k0}\\ &\text{for } k \text{ odd:} \quad F_{hk0} = -\,F_{\bar{h}k0}. \end{aligned} \tag{24}$$

This circumstance requires the summation to be split into two summations, one with *k* even and the other with *k* odd. For *k* even, the conditions are exactly the same as in the last section, and consequently (22) holds for this half of the summation. For *k* odd, substitution of the real and imaginary parts of the second half of (24) into (17) causes the first and last rows to vanish, leaving

$$\underset{k\ \text{odd}}{\rho(xy)} = \frac{4}{S}\sum_{h}{}'\sum_{\substack{k\\0}}^{\infty}{}' - A_{hk0}\sin 2\pi hx \sin 2\pi ky$$

$$+\; B_{hk0}\sin 2\pi hx \cos 2\pi ky$$

$$= \frac{4}{S}\sum_{\substack{h\\0}}{}'\left[\sum_{\substack{k\\0}}^{\infty}{}' - A_{hk0}\sin 2\pi ky + B_{hk0}\cos 2\pi ky\right]\sin 2\pi hx. \tag{25}$$

The entire summation includes summation over both *k* even and *k* odd, namely an expression like (22) for *k* even, plus (25) for *k* odd. The complete form is

$$\rho(xy) = \frac{4}{S}\sum_{\substack{0\\h}}^{\infty}{}'\left[\sum_{\substack{0\\k\ \text{even}}}^{\infty}{}' A_{hk0}\cos 2\pi ky + B_{hk0}\sin 2\pi ky\right]\cos 2\pi hx$$

$$-\left[\sum_{\substack{0\\k\ \text{odd}}}^{\infty}{}' A_{hk0}\sin 2\pi ky - B_{hk0}\cos 2\pi ky\right]\sin 2\pi hx. \tag{26}$$

This form looks somewhat formidable, but by appropriate selection of masks for the Patterson-Tunell method [4], or Beevers-Lipson method [1], it is no more difficult than (22). It merely requires different treatment of even and odd terms.

For computations of projections having this symmetry, the preferred form of the summation is (26). For the subsequent derivation of *p2gg*, however, it is desirable to have the origin of the plane group chosen halfway between neighboring glide-lines, the glides remaining parallel to *b*. It can be easily shown [5] that a change of origin of a reflection parallel to *b* by amount a/m produces a phase change of $e^{2\pi i 2h/m}$. For the new origin shifted $a/4$ from the first origin, (23) is, therefore, replaced by

$$\begin{aligned} F_{hk0} &= e^{2\pi ih/2}\, e^{2\pi ik/2}\, F_{\bar{h}k0} \\ &= e^{2\pi i(h+k)/2}\, F_{\bar{h}k0}. \end{aligned} \tag{27}$$

By imposing this condition on (17) in exactly the same way it was done for the first origin, the following form of the synthesis results:

$$\begin{aligned} \rho(xy) = \frac{4}{S}\Bigg\{ &\sum_{\substack{0\\h\\h+k\text{ even}}}^{\infty}{}' \left[\sum_{\substack{0\\k}}^{\infty}{}' A_{hk0}\cos 2\pi ky + B_{hk0}\sin 2\pi ky\right]\cos 2\pi hx \\ - &\sum_{\substack{0\\h\\h+k\text{ odd}}}^{\infty}{}' \left[\sum_{\substack{0\\k}}^{\infty}{}' A_{hk0}\sin 2\pi ky - B_{hk0}\cos 2\pi ky\right]\sin 2\pi hx.\Bigg\} \end{aligned} \tag{28}$$

Symmetries *p2mm* and *c2mm*. These symmetries have subgroups *p*2 and *pm*1, or *c*2 and *cm*1, respectively. They can, therefore, be derived from the first subgroup by adding *m* parallel to *b*, or from the second by adding the operation 2. Either derivation may be used to find the appropriate form of the Fourier summation. In the first derivation, conditions (20) are imposed on (19), which causes the vanishing of the second line; in the second derivation, conditions (18) are imposed on (22), which causes the *B* parts to vanish. By either route, the Fourier summation reduces to the very simple form

$$\rho(xy) = \frac{4}{S}\sum_{h}{}' \sum_{\substack{k\\0}}^{\infty}{}' F_{hk0}\cos 2\pi hx\cos 2\pi ky. \tag{29}$$

Symmetry *p2gm*. This symmetry can be derived from its subgroup *pg*1 by adding the generating operation 2. This imposes conditions (18) on (26), causing the *B* terms to vanish. The summation then assumes the simpler form

$$\begin{aligned} \rho(xy) = \frac{4}{S}\Bigg\{ &\sum_{h}{}' \sum_{\substack{k\text{ even}\\0}}^{\infty}{}' F_{hk0}\cos 2\pi hx\cos 2\pi ky \\ - &\sum_{h}{}' \sum_{\substack{k\text{ odd}\\0}}^{\infty}{}' F_{hk0}\sin 2\pi hx\sin 2\pi ky\Bigg\}. \end{aligned} \tag{30}$$

Symmetry $p2gg$. If the origin of this group is placed at a 2-fold rotor› with glide lines parallel to a and b, the glides are located at $a/4$ and $b/4$. A subgroup of this is $pg1$. The form of the Fourier summation for this subgroup with the glide line removed from the origin by an amount $a/4$ was given in (28). The appropriate form for $p2gg$ can be derived from (28) by imposing the conditions of the generating operation 2 on (28). These conditions are given in (18). They cause the B terms in (28) to vanish, leaving the simpler form

$$\rho(xy) = \frac{4}{S}\left\{\sum_{\substack{h \\ \\ h+k \text{ even}}}{}' \overset{\infty}{\underset{0}{}} \sum_{k}{}' F_{hk0} \cos 2\pi hx \cos 2\pi ky \right.$$

$$\left. - \sum_{\substack{h \\ \\ h+k \text{ odd}}}{}' \overset{\infty}{\underset{0}{}} \sum_{k}{}' F_{hk0} \sin 2\pi hx \sin 2\pi ky \right\}. \tag{31}$$

Symmetry $p4$. According to the reciprocal symmetry theorem, the reciprocal to a crystal of symmetry $p4$ also has 4-fold symmetry. Therefore, the following relations hold

$$F_{hk0} = F_{\bar{k}h0} = F_{\bar{h}\bar{k}0} = F_{k\bar{h}0}. \tag{32}$$

Since alternate terms of (32) correspond to symmetry 2, conditions (18) can be imposed at once on the general form of the Fourier summation (13) causing the last two lines involving B components to vanish. The summation then involves only A components, but the summation limits extend over all reciprocal space. To take advantage of the 4-fold symmetry, reciprocal space is divided along the h and k axes into four equivalent parts and the entire summation split into four summations, one for each of these quadrants. The summation then has a somewhat similar form to (14), but with the B terms eliminated and A's replaced by the first two coefficients of (32). Using the arguments outlined following equation (14), the summations of opposite quadrants can be added, giving a form somewhat similar to (15), specifically

$$\rho(xy) = \frac{2}{S} \sum_{h}{}' \overset{\infty}{} \sum_{k}{}' F_{hk0} \cos 2\pi hx \cos 2\pi ky + F_{\bar{k}h0} \cos 2\pi \bar{k}x \cos 2\pi hy$$

$$- F_{hk0} \sin 2\pi hx \sin 2\pi ky - F_{\bar{k}h0} \sin 2\pi \bar{k}x \sin 2\pi hy. \tag{33}$$

All the F's in this summation are equal, according to (32). The trigonometric functions can also be changed into functions of positive angles, as follows:

$$\rho(xy) = \frac{2}{S} \sum_{h}{}' \overset{\infty}{\underset{0}{}} \sum_{k}{}' F_{hk0} \cos 2\pi hx \cos 2\pi ky + F_{hk0} \cos 2\pi kx \cos 2\pi hy$$

$$- F_{hk0} \sin 2\pi hx \sin 2\pi ky + F_{hk0} \sin 2\pi kx \sin 2\pi ky. \tag{34}$$

The summation is now expressed in terms of the positive quadrant of reciprocal space. Because of the equivalence of the a_1 and a_2 axes, it is possible to reduce the number of terms in this summation still further. To accomplish this, each column of (34) is split into two columns, one for each half-quadrant. The two halves of the quadrant are related by interchange of h and k indices. The limits of the original summation were from 0 to ∞, but with the split summation, the lower limit becomes the diagonal (labelled D) of the positive quadrant. This effectively reduces the number of terms in the summation by half. Let this summation be represented by $\sum_{D}^{\infty}{}'$. Then the Fourier expression is

$$\rho(xy) = \frac{2}{S}\underset{D}{\overset{\infty}{\sum_{h}{}'\sum_{k}{}'}}$$

$$\begin{aligned}&F_{hk0}\cos 2\pi hx\cos 2\pi ky + F_{kh0}\cos 2\pi kx\cos 2\pi hy + F_{hk0}\cos 2\pi kx\cos 2\pi hy + F_{kh0}\cos 2\pi hx\cos 2\pi ky\\ -\,&F_{hk0}\sin 2\pi hx\sin 2\pi ky - F_{kh0}\sin 2\pi kx\sin 2\pi hy + F_{hk0}\sin 2\pi kx\sin 2\pi hy + F_{kh0}\sin 2\pi hx\sin 2\pi ky.\end{aligned} \tag{35}$$

It will be observed that, although the F's are of two kinds, the trigonometric parts of columns 1 and 4 are the same, and that the trigonometric parts of columns 2 and 3 are the same. The summation can, therefore, be more compactly expressed as

$$\begin{aligned}\rho(xy) = \frac{2}{S}\underset{D}{\overset{\infty}{\sum_{h}{}'\sum_{k}{}'}}&(F_{hk0}+F_{kh0})\cos 2\pi hx\cos 2\pi ky + (F_{hk0}+F_{kh0})\cos 2\pi hy\cos 2\pi kx\\ &-(F_{hk0}-F_{kh0})\sin 2\pi hx\sin 2\pi ky + (F_{hk0}-F_{kh0})\sin 2\pi hy\sin 2\pi kx.\end{aligned} \tag{36}$$

The form of (36) looks rather formidable. Actually the summation is easy to perform. Since the parts of first and second columns are identical except for interchange of x and y, (and the sign of the second row) only the summations of the first column need be performed. The summations of the second column can then be derived from them by interchanging the axes of x and y. The entire summation consists of adding the results of the two summations and recording them at coordinates xy.

Symmetry $p4mm$. Plane group $p4mm$ can be derived from $p4$ by the addition of the generating operation m parallel to a diagonal and through the origin. According to the reciprocal symmetry theorem, this entails the condition

$$F_{hk0} = F_{kh0}. \tag{37}$$

If this is applied to (36), it causes the sine terms to vanish, leaving only

$$\rho(xy) = \frac{4}{S}\underset{D}{\overset{\infty}{\sum_{h}{}'\sum_{k}{}'}}F_{hk0}\cos 2\pi hx\cos 2\pi ky + F_{hk0}\cos 2\pi hy\cos 2\pi kx. \tag{38}$$

To perform the summation, only the first term need be summed. The second term is derived from it by interchange of x and y. The entire summation is the sum of these two summations.

Symmetry $p4gg$. Plane group $p4gg$ can be derived from $p4$ by the addition of glide through the origin and diagonal to the axes. The glide component is $a/2+b/2$. According to the reciprocal symmetry theorem, this gives rise to the reciprocal symmetry

$$F_{hk0} = e^{2\pi i(h+k)/2}F_{kh0}. \tag{39}$$

There are, therefore, two classes of reflections:

$$\begin{aligned} &\text{for } h+k \text{ even:} \quad F_{hk0} = F_{kh0} \\ &\text{for } h+k \text{ odd:} \quad F_{hk0} = -\,F_{kh0}. \end{aligned} \tag{40}$$

For the first class of reflections, the second line of (36) vanishes, and for the second class of reflections, the first line vanishes. Therefore, the entire summation for $p4gg$ is

$$\begin{aligned} \rho(xy) = \frac{4}{S}\Bigg\{ &\underset{h+k\text{ even}}{\underset{D}{\sum_h{}'^{\infty}\sum_k{}'}} F_{hk0}\cos 2\pi hx\cos 2\pi ky + F_{hk0}\cos 2\pi hy\cos 2\pi kx \\ &+ \underset{h+k\text{ odd}}{\underset{D}{\sum_h{}'^{\infty}\sum_k{}'}} -\,F_{hk0}\sin 2\pi hx\sin 2\pi ky + F_{hk0}\sin 2\pi hy\sin 2\pi kx \Bigg\}. \end{aligned} \tag{41}$$

As before, Fourier summations need be made only for the parts of the first column of (41). The summations of the second column are derived from the first by interchanging the axes of x and y. The summation is completed by adding together the separate summations.

Symmetry $p3$. The symmetry of trigonal crystals is best displayed by choosing axes a_1, a_2, and a_3 at 120° intervals. With respect to these axes the indices are h, k, and i, such that $h+k+i=0$. According to the reciprocal symmetry theorem, the relations between F's is

$$F_{hk0} = F_{ki0} = F_{ih0}. \tag{42}$$

According to the additivity theorem, the Fourier synthesis can be written as the sum of three syntheses, one for each of the symmetrically equivalent sectors of the trigonally symmetrical reciprocal structure. Since each sector is nonsymmetrical, the summation for a sector has the form of (13) but with summation limits 0 to ∞. The entire summation is

$$\begin{aligned} \rho(xy) = \frac{1}{S} &\underset{0}{\sum_h{}'^{\infty}\sum_k{}'} \\ &A_{hk0}\cos 2\pi hx\cos 2\pi ky + A_{ki0}\cos 2\pi kx\cos 2\pi iy + A_{ih0}\cos 2\pi ix\cos 2\pi hy \\ &- A_{hk0}\sin 2\pi hx\sin 2\pi ky - A_{ki0}\sin 2\pi kx\sin 2\pi iy - A_{ih0}\sin 2\pi ix\sin 2\pi hy \\ &+ B_{hk0}\sin 2\pi hx\cos 2\pi ky + B_{ki0}\sin 2\pi kx\cos 2\pi iy + B_{ih0}\sin 2\pi ix\cos 2\pi hy \\ &+ B_{hk0}\cos 2\pi hx\sin 2\pi ky + B_{ki0}\cos 2\pi kx\sin 2\pi iy + B_{ih0}\cos 2\pi ix\sin 2\pi hy. \end{aligned} \tag{43}$$

The symmetry of this summation is not appropriate for utilizing interchange symmetry of the trigonometric parts, so (43) is the final form of the summation for trigonal crystals. It has a formidable appearance. Actually, however, only the summation represented by the first column need be carried out. The summations represented by the other two columns are identical with that of the first column except for rotation of axes by 120° and 240° respectively. To perform the summation represented by (43), therefore, it is only necessary to make a Fourier summation of the first column, then add values for symmetrically equivalent points, recording the sum of the values at *xy*.

Symmetry *p*31*m*. Plane group *p*31*m* can be derived from *p*3 by the addition of a symmetry line diagonally between the axes. According to the reciprocal symmetry theorem, this causes the additional relation

$$F_{hk0} = F_{kh0}. \tag{44}$$

To take advantage of this in reducing the number of terms involved in the summation, reciprocal space is divided into the three sectors of the summation (43), then each sector is divided into two segments along the diagonal. The appearance of the summation is twice as large as (43), since each column has a corresponding column with interchanged indices. The summation has a formidable appearance. Actually, the Fourier part of the summation need be performed on only one of these six columns. The final part of the summation consists of recording at coordinate *xy*, the sum of the results for this one summation which appear at the six sets of coordinates related to *xy* by the symmetry of the projection, namely 31*m*.

A convenient way of performing the summation is to choose new axes for the purposes of the summation. Instead of using a_1 and a_2 as axes for the synthesis, the axes a_1 and *D* (the diagonal) are used. The work of the Fourier summation then consists of summing over indices *h* and *k'*, where *k'* is the index on *D*, namely,

$$\begin{aligned}\sum_h{}' \sum_{k'}{}'{}_0^{\infty} A_{hk'0} &\cos 2\pi hx \cos 2\pi k'y \\ - A_{hk'0} &\sin 2\pi hx \sin 2\pi k'y \\ + B_{hk'0} &\sin 2\pi hx \cos 2\pi k'y \\ + B_{hk'0} &\cos 2\pi hx \sin 2\pi k'y.\end{aligned} \tag{45}$$

Symmetry *p*3*m*1. Plane group *p*3*m*1 can be derived from *p*3 by the addition of a reflection parallel to the long diagonal of the cell. This causes a_1 and $-a_2$ to become equivalent. According to the reciprocal symmetry theorem, the following symmetry arises in reciprocal space:

$$F_{hk0} = F_{\overline{kh}0}. \tag{46}$$

To reduce the number of terms of the summation, reciprocal space is divided into the three sectors of (43), then each sector subdivided into segments along the two long diagonals extending from the origin. A convenient way to perform the actual summation is to choose these two diagonals in reciprocal space as new axes, h' and k'. The actual Fourier part of the summation then consists of the single summation

$$\begin{aligned}\overset{\infty}{\underset{0}{\sum_{h'}{}'\sum_{k'}{}'}} A_{h'k'0} &\cos 2\pi h'x \cos 2\pi k'y \\ &- A_{h'k'0} \sin 2\pi h'x \sin 2\pi k'y \\ &+ B_{h'k'0} \sin 2\pi h'x \cos 2\pi k'y \\ &+ B_{h'k'0} \cos 2\pi h'x \sin 2\pi k'y. \qquad (47)\end{aligned}$$

The summation is completed by adding the values of this summation at the six points related by the symmetry $3m1$ and recording the sum at xy.

Symmetry $p6$. Plane group $p6$ can be derived from $p3$ by the addition of the operation 2. Therefore, the appropriate form of the symmetrical Fourier summation can be found by imposing conditions (18) on the form of (43). To take full advantage of the hexagonal symmetry, however, it is more convenient to rewrite (43) in six parts, which is equivalent to dividing reciprocal space into six sectors which are equivalent by hexagonal symmetry. The edges of each sector are an a axis and a diagonal, D. These edges may be chosen as axes on which the indices are h and k'. If the sectors are considered in centrosymmetrical pairs, one member of the pair has indices like $hk0$, while the other has the corresponding negative indices, $\overline{hk}0$. Thus the summation consists of three columns, each column including opposite sectors, with summation limits from $-\infty$ to ∞, namely

$$\rho(xy) = \frac{1}{S} \overset{\infty}{\underset{-\infty}{\sum_{h}{}'\sum_{k'}{}'}}$$

$$\begin{aligned} &A_{h\bar{i}0} \cos 2\pi hx \cos 2\pi\bar{i}y + A_{k\bar{h}0} \cos 2\pi kx \cos 2\pi\bar{k}y + A_{i\bar{k}0} \cos 2\pi ix \cos 2\pi\bar{k}y \\ &- A_{h\bar{i}0} \sin 2\pi hx \sin 2\pi\bar{i}y - A_{k\bar{h}0} \sin 2\pi kx \sin 2\pi\bar{k}y - A_{i\bar{k}0} \sin 2\pi ix \sin 2\pi\bar{k}y \\ &+ B_{h\bar{i}0} \sin 2\pi hx \cos 2\pi\bar{i}y + B_{k\bar{h}0} \sin 2\pi kx \cos 2\pi\bar{k}y + B_{i\bar{k}0} \sin 2\pi ix \cos 2\pi\bar{k}y \\ &+ B_{h\bar{i}0} \cos 2\pi hx \sin 2\pi\bar{i}y + B_{k\bar{h}0} \cos 2\pi kx \sin 2\pi\bar{k}y + B_{i\bar{k}0} \cos 2\pi ix \sin 2\pi\bar{k}y. \qquad (48)\end{aligned}$$

The number of terms in this summation may be reduced by a factor of 4 by applying conditions (18) for the two-fold operation. This eliminates the B terms and doubles up the A terms, changing the summation limits from $-\infty$ to ∞, to 0 to ∞. The simplified summation appropriate to $p6$ is therefore

$$\rho(xy) = \frac{2}{S} \overset{\infty}{\underset{0}{\sum_{h}{}'\sum_{k'}{}'}}$$

$$\begin{aligned} &A_{h\bar{i}0} \cos 2\pi hx \cos 2\pi\bar{i}y + A_{k\bar{h}0} \cos 2\pi kx \cos 2\pi\bar{h}y + A_{i\bar{k}0} \cos 2\pi ix \cos 2\pi\bar{k}y \\ &- A_{h\bar{i}0} \sin 2\pi hx \sin 2\pi\bar{i}y - A_{k\bar{h}0} \sin 2\pi kx \sin 2\pi\bar{h}y - A_{i\bar{k}0} \sin 2\pi ix \sin 2\pi\bar{k}y. \qquad (49)\end{aligned}$$

As in the case of the trigonal summations, only the Fourier summation for the first column of (49) need be performed. The summation is completed by adding together the results found for three coordinate positions separated by 120° and recording the sum at the first of the three points.

Symmetry *p6mm*. Plane group *p6mm* can be derived from its subgroup *p6* by the addition of a reflection parallel to an axis. This provides the additional relation

$$F_{hk0} = F_{kh0}. \tag{50}$$

This permits changing the summation limits of (49) from 0 to ∞, to *D* to ∞. Otherwise the form of the summation is the same. To perform the summation, the Fourier part consists of summing for the first column only. The summation is completed by adding together at coordinates *xy* the six results found at points related to *xy* by symmetry *3mm*.

THREE DIMENSIONAL SUMMATIONS

Introduction. The computation of three-dimensional summations, one level at a time, can be referred to the pattern established for two-dimensional summations. In the following discussion, it is assumed, for sake of clearness, that it is desired to compute the electron density at level z_1. The value of z is, therefore, constant for the level.

The form of the Fourier summation for the general, non-symmetrical case was given in (9). Since z_1 is constant for the level, it is convenient to separate the trigonometric parts of (9) into constant and variable portions. This can be done by utilizing relations (12). Making these substitutions, (9) becomes

$$\begin{aligned}\rho(xyz_1) = \frac{1}{V}\sum_h \sum_{k=-\infty}^{\infty} \sum_l & A_{hkl}\cos 2\pi(hx+ky)\cos 2\pi lz_1 - A_{hkl}\sin 2\pi(hx+ky)\sin 2\pi lz_1 \\ & + B_{hkl}\sin 2\pi(hx+ky)\cos 2\pi lz_1 + B_{hkl}\cos 2\pi(hx+ky)\sin 2\pi lz_1. \end{aligned}\tag{51}$$

Now, for any selected level, z_1, the values of

$$\begin{aligned} C_{A,hkl} &= \sum_l A_{hkl}\cos 2\pi lz_1 \\ S_{A,hkl} &= \sum_l A_{hkl}\sin 2\pi lz_1 \\ C_{B,hkl} &= \sum_l B_{hkl}\cos 2\pi lz_1 \\ S_{B,hkl} &= \sum B_{hkl}\sin 2\pi lz \end{aligned}\tag{52}$$

are fixed, and can be computed in advance of making the Fourier summation proper. Therefore, the summations over l can be eliminated in (51) and it assumes the simpler form

$$\begin{aligned}\rho(xyz_1) = \frac{1}{V}\sum_h \sum_{k=-\infty}^{\infty} & C_{A,hkl}\cos 2\pi(hx+ky) - S_{A,hkl}\sin 2\pi(hx+ky) \\ & + S_{B,hkl}\cos 2\pi(hx+ky) + C_{B,hkl}\sin 2\pi(hx+ky) \end{aligned}\tag{53}$$

$$= \frac{1}{V} \sum_{h} \sum_{k}{}_{-\infty}^{\infty} (C_A + S_B)_{hkl} \cos 2\pi(hx + ky) + (C_B - S_A) \sin 2\pi(hx + ky). \quad (54)$$

For compactness, if one takes

$$(C_A + S_B)_{hkl} = A'_{hkl}$$

and

$$(C_B - S_A)_{hkl} = B'_{hkl} \quad (55)$$

then (54) has the form

$$\rho(xyz_1) = \frac{1}{V} \sum_{h} \sum_{k}{}_{-\infty}^{\infty} A'_{hkl} \cos 2\pi(hx + ky) + B'_{hkl} \sin 2\pi(hx + ky). \quad (56)$$

This is exactly the same form as (11) for the non-symmetrical two-dimensional summation. Obviously, therefore, the three-dimensional summation can be handled exactly like the two-dimensional one after the coefficients (55) have been computed from (52). In practical summation, (56) should be recast into product form exactly the same as (13) except for primes indicating the composite nature of the coefficients in (55).

SYMMETRY BETWEEN UPPER AND LOWER RECIPROCAL SPACE

If the upper and lower halves of the crystal are related by any symmetry, the upper and lower halves of reciprocal space have a corresponding symmetry according to the reciprocal symmetry theorem. This specializes the forms of the coefficients in (55). To see how this affects (54), split each coefficient into a part pertaining to the upper half of reciprocal space and another pertaining to the lower half. Then (54) becomes

$$\rho(xyz_1) = \frac{1}{V} \sum_{h} \sum_{k}{}_{-\infty}^{\infty} (C_{A+} + C_{A-} + S_{B+} + S_{B-})_{hkl} \cos 2\pi(hx + ky)$$

$$+ (C_{B+} + C_{B-} - S_{A+} - S_{A-})_{hkl} \sin 2\pi(hx + ky). \quad (57)$$

Under the following headings, the way in which these coefficients are related in important cases, according to the reciprocal symmetry theorem, are tabulated. The simplified form of (57) is also listed:

Inversion center:

$$F_{\overline{hkl}} = F^*_{hkl},$$

$$\therefore \quad A_+ = A_- \qquad C_+ = C_-$$

and

$$B_+ = -B_- \qquad S_+ = -S_-$$

$$\therefore \quad C_{A+} = C_{A-},$$
$$C_{B+} = -C_{B-},$$
$$S_{B+} = S_{B-},$$
$$S_{A+} = -S_{A-}.$$

$$\rho(xyz_1) = \frac{2}{V} \sum_{h} \sum_{k} (C_{A+} + S_{B-}) \cos 2\pi(hx + ky). \quad (58)$$

Reflection:

$$F_{hkl} = F_{hk\bar{l}},$$

$$\therefore \quad A_+ = A_-$$

and

$$B_+ = B_-.$$

$$\rho(xyz_1) = \frac{2}{V} \sum_h \sum_k C_{A+} \cos 2\pi(hx + ky) + C_{B+} \sin 2\pi(hx + ky). \tag{59}$$

Glide, translation-component a/2:

$$\begin{array}{lll} & h \text{ even} & h \text{ odd} \\ & F_{hkl} = F_{h\overline{kl}}, & F_{hkl} = -F_{hk\bar{l}} \\ \therefore & A_{hkl} = A_{hk\bar{l}}, & A_{hkl} = -A_{hk\bar{l}} \\ \text{and} & B_{hkl} = B_{hk\bar{l}}, & B_{hkl} = -B_{hk\bar{l}}. \end{array}$$

$$\rho(xyz_1) = \frac{2}{V} \left\{ \sum_{\substack{h \\ \text{even}}} \sum_k C_{A+} \cos 2\pi(hx + ky) + C_{B+} \sin 2\pi(hx + ky) \right.$$

$$\left. + \sum_{\substack{h \\ \text{odd}}} \sum_k S_{B+} \cos 2\pi(hx + ky) - S_{A+} \sin 2\pi(hx + ky) \right\}. \tag{60}$$

2-fold rotation $\|$ *a:*

$$F_{hkl} = F_{h\overline{kl}},$$

$$\therefore \quad A_{hkl} = A_{hkl},$$

and

$$B_{hkl} = B_{h\overline{kl}}.$$

$$\rho(xyz_1) = \frac{2}{V} \sum_h \sum_k C_{A+} \cos 2\pi(hx + ky) + C_{B+} \sin 2\pi(hx + ky). \tag{61}$$

2-fold screw $\|$ *a, translation-component a/2:*

$$\begin{array}{lll} & h \text{ even} & h \text{ odd} \\ & F_{hkl} = F_{h\overline{kl}}, & F_{hkl} = -F_{h\overline{kl}} \\ \therefore & A_{hkl} = A_{h\overline{kl}}, & A_{hkl} = -A_{h\overline{kl}} \\ \text{and} & B_{hkl} = B_{hkl}, & B_{hkl} = -B_{h\overline{kl}}. \end{array}$$

$$\rho(xyz_1) = \frac{2}{V} \left\{ \sum_{\substack{h \\ \text{even}}} \sum_k C_{A+} \cos 2\pi(hx + ky) + C_{B+} \sin 2\pi(hx + ky) \right.$$

$$\left. + \sum_{\substack{h \\ \text{odd}}} \sum_k S_{B+} \cos 2\pi(hx + ky) - S_{A+} \sin 2\pi(hx + ky) \right\}. \tag{62}$$

Computation. The computation of a three-dimensional summation has the symmetry of the section at which the summation is made. This is usually lower than the symmetry of the projection on a plane parallel to the section. On the other hand, the trigonometric part of the summation may have the same symmetry as that of the projection. In any case, when it is necessary to utilize the symmetry of the section, the same system can be followed which was discussed in detail for the projections, except that the coefficients involved are those shown in detail in (57) instead of A_{hkl} and B_{hkl}.

The additivity theorem suggests a general method of computing which can be used for three dimensional summations; the Fourier synthesis is performed at z_1 and $-z_1$ for data contained in a representative unsymmetrical block of the reciprocal structure. (In this synthesis, terms which the previous section indicates will cancel on combination may be omitted.) This gives the Fourier transform at xyz_1 and $xy\bar{z}_1$ for one block of the reciprocal structure. The summation is completed by adding together at xyz_1 the results obtained for the several points equivalent by symmetry to xyz_1.

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