

1.4. Symmetry in reciprocal space

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WITH APPENDIX 1.4.2 BY U. SHMUELI, S. R. HALL AND R. W. GROSSE-KUNSTLEVE

1.4.1. Introduction

Crystallographic symmetry, as reflected in functions on reciprocal space, can be considered from two complementary points of view.

(1) One can assume the existence of a certain permissible symmetry of the density function of crystalline (scattering) matter, a function which due to its three-dimensional periodicity can be expanded in a triple Fourier series (*e.g.* Bragg, 1966), and inquire about the effects of this symmetry on the Fourier coefficients – the structure factors. Since there exists a one-to-one correspondence between the triplets of summation indices in the Fourier expansion and vectors in the reciprocal lattice (Ewald, 1921), the above approach leads to consequences of the symmetry of the density function which are relevant to the representation of its Fourier image in reciprocal space. The symmetry properties of these Fourier coefficients, which are closely related to the crystallographic experiment, can then be readily established.

This traditional approach, the essentials of which are the basis of Sections 4.5–4.7 of Volume I (*IT I*, 1952), and which was further developed in the works of Buerger (1949, 1960), Waser (1955), Bertaut (1964) and Wells (1965), is one of the cornerstones of crystallographic practice and will be followed in the present chapter, as far as the basic principles are concerned.

(2) The alternative approach, proposed by Bienenstock & Ewald (1962), also presumes a periodic density function in crystal space and its Fourier expansion associated with the reciprocal. However, the argument starts from the Fourier coefficients, taken as a discrete set of complex functions, and linear transformations are sought which leave the magnitudes of these functions unchanged; the variables on which these transformations operate are h, k, l and φ – the Fourier summation indices (*i.e.*, components of a reciprocal-lattice vector) and the phase of the Fourier coefficient, respectively. These transformations, or the groups they constitute, are then interpreted in terms of the symmetry of the density function in direct space. This direct analysis of symmetry in reciprocal space will also be discussed.

We start the next section with a brief discussion of the point-group symmetries of associated direct and reciprocal lattices. The weighted reciprocal lattice is then briefly introduced and the relation between the values of the weight function at symmetry-related points of the weighted reciprocal lattice is discussed in terms of the Fourier expansion of a periodic function in crystal space. The remaining part of Section 1.4.2 is devoted to the formulation of the Fourier series and its coefficients (values of the weight function) in terms of space-group-specific symmetry factors, an extensive tabulation of which is presented in Appendix 1.4.3. This is a revised version of the structure-factor tables given in Sections 4.5–4.7 of Volume I (*IT I*, 1952). Appendix 1.4.4 contains a reciprocal-space representation of the 230 crystallographic space groups and some explanatory material related to these space-group tables is given in Section 1.4.4; the latter are interpreted in terms of the two viewpoints discussed above. The tabular material given in this chapter is compatible with the direct-space symmetry tables given in Volume A (*IT A*, 1983) with regard to the space-group settings and choices of the origin.

Most of the tabular material, the new symmetry-factor tables in Appendix 1.4.3 and the space-group tables in Appendix 1.4.4 have been generated by computer with the aid of a combination of numeric and symbolic programming techniques. The algorithm underlying this procedure is briefly summarized in Appendix 1.4.1. Appendix 1.4.2 deals with computer-adapted space-group symbols,

including the set of symbols that were used in the preparation of the present tables.

1.4.2. Effects of symmetry on the Fourier image of the crystal

1.4.2.1. Point-group symmetry of the reciprocal lattice

Regarding the reciprocal lattice as a collection of points generated from a given direct lattice, it is fairly easy to see that each of the two associated lattices must have the same point-group symmetry. The set of all the rotations that bring the direct lattice into self-coincidence can be thought of as interchanging equivalent families of lattice planes in all the permissible manners. A family of lattice planes in the direct lattice is characterized by a common normal and a certain interplanar distance, and these two characteristics uniquely define the direction and magnitude, respectively, of a vector in the reciprocal lattice, as well as the lattice line associated with this vector and passing through the origin. It follows that any symmetry operation on the direct lattice must also bring the reciprocal lattice into self-coincidence, *i.e.* it must also be a symmetry operation on the reciprocal lattice. The roles of direct and reciprocal lattices in the above argument can of course be interchanged without affecting the conclusion.

The above elementary considerations recall that for any point group (not necessarily the full point group of a lattice), the operations which leave the lattice unchanged must also leave unchanged its associated reciprocal. This equivalence of point-group symmetries of the associated direct and reciprocal lattices is fundamental to crystallographic symmetry in reciprocal space, in both points of view mentioned in Section 1.4.1.

With regard to the effect of any given point-group operation on each of the two associated lattices, we recall that:

(i) If \mathbf{P} is a point-group rotation operator acting on the direct lattice (*e.g.* by rotation through the angle α about a given axis), the effect of this rotation on the associated reciprocal lattice is that of applying the inverse rotation operator, \mathbf{P}^{-1} (*i.e.* rotation through $-\alpha$ about a direction parallel to the direct axis); this is readily found from the requirement that the scalar product $\mathbf{h}^T \mathbf{r}_L$, where \mathbf{h} and \mathbf{r}_L are vectors in the reciprocal and direct lattices, respectively, remains invariant under the application of a point-group operation to the crystal.

(ii) If our matrix representation of the rotation operator is such that the point-group operation is applied to the direct-lattice (column) vector by *premultiplying* it with the matrix \mathbf{P} , the corresponding operation on the reciprocal lattice is applied by *postmultiplying* the (row) vector \mathbf{h}^T with the point-group rotation matrix. We can thus write, *e.g.*, $\mathbf{h}^T \mathbf{r}_L = (\mathbf{h}^T \mathbf{P}^{-1})(\mathbf{P} \mathbf{r}_L) = [(\mathbf{P}^{-1})^T \mathbf{h}]^T (\mathbf{P} \mathbf{r}_L)$. Note, however, that the orthogonality relationship: $\mathbf{P}^{-1} = \mathbf{P}^T$ is not satisfied if \mathbf{P} is referred to some oblique crystal systems, higher than the orthorhombic.

Detailed descriptions of the 32 crystallographic point groups are presented in the crystallographic and other literature; their complete tabulation is given in Chapter 10 of Volume A (*IT A*, 1983).

1.4.2.2. Relationship between structure factors at symmetry-related points of the reciprocal lattice

Of main interest in the context of the present chapter are symmetry relationships that concern the values of a function defined at the points of the reciprocal lattice. Such functions, of crystal-

1. GENERAL RELATIONSHIPS AND TECHNIQUES

lographic interest, are Fourier-transform representations of direct-space functions that have the periodicity of the crystal, the structure factor as a Fourier transform of the electron-density function being a representative example (see *e.g.* Lipson & Taylor, 1958). The value of such a function, attached to a reciprocal-lattice point, is called the weight of this point and the set of all such weighted points is often termed the weighted reciprocal lattice. This section deals with a fundamental relationship between functions (weights) associated with reciprocal-lattice points, which are related by point-group symmetry, the weights here considered being the structure factors of Bragg reflections (*cf.* Chapter 1.2).

The electron density, an example of a three-dimensional periodic function with the periodicity of the crystal, can be represented by the Fourier series

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{h}} F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T \mathbf{r}), \quad (1.4.2.1)$$

where \mathbf{h} is a reciprocal-lattice vector, V is the volume of the (direct) unit cell, $F(\mathbf{h})$ is the structure factor at the point \mathbf{h} and \mathbf{r} is a position vector of a point in direct space, at which the density is given. The summation in (1.4.2.1) extends over all the reciprocal lattice.

Let $\mathbf{r}' = \mathbf{P}\mathbf{r} + \mathbf{t}$ be a space-group operation on the crystal, where \mathbf{P} and \mathbf{t} are its rotation and translation parts, respectively, and \mathbf{P} must therefore be a point-group operator. We then have, by definition, $\rho(\mathbf{r}) = \rho(\mathbf{P}\mathbf{r} + \mathbf{t})$ and the Fourier representation of the electron density, at the equivalent position $\mathbf{P}\mathbf{r} + \mathbf{t}$, is given by

$$\begin{aligned} \rho(\mathbf{P}\mathbf{r} + \mathbf{t}) &= \frac{1}{V} \sum_{\mathbf{h}} F(\mathbf{h}) \exp[-2\pi i \mathbf{h}^T (\mathbf{P}\mathbf{r} + \mathbf{t})] \\ &= \frac{1}{V} \sum_{\mathbf{h}} [F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T \mathbf{t})] \\ &\quad \times \exp[-2\pi i (\mathbf{P}^T \mathbf{h})^T \mathbf{r}], \end{aligned} \quad (1.4.2.2)$$

noting that $\mathbf{h}^T \mathbf{P} = (\mathbf{P}^T \mathbf{h})^T$. Since \mathbf{P} is a point-group operator, the vectors $\mathbf{P}^T \mathbf{h}$ in (1.4.2.2) must range over all the reciprocal lattice and a comparison of the functional forms of the equivalent expansions (1.4.2.1) and (1.4.2.2) shows that the coefficients of the exponentials $\exp[-2\pi i (\mathbf{P}^T \mathbf{h})^T \mathbf{r}]$ in (1.4.2.2) must be the structure factors at the points $\mathbf{P}^T \mathbf{h}$ in the reciprocal lattice. Thus

$$F(\mathbf{P}^T \mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T \mathbf{t}), \quad (1.4.2.3)$$

wherefrom it follows that the magnitudes of the structure factors at \mathbf{h} and $\mathbf{P}^T \mathbf{h}$ are the same:

$$|F(\mathbf{P}^T \mathbf{h})| = |F(\mathbf{h})|, \quad (1.4.2.4)$$

and their phases are related by

$$\varphi(\mathbf{P}^T \mathbf{h}) = \varphi(\mathbf{h}) - 2\pi \mathbf{h}^T \mathbf{t}. \quad (1.4.2.5)$$

The relationship (1.4.2.3) between structure factors of symmetry-related reflections was first derived by Waser (1955), starting from a representation of the structure factor as a Fourier transform of the electron-density function.

It follows that an application of a point-group transformation to the (weighted) reciprocal lattice leaves the moduli of the structure factors unchanged. The distribution of diffracted intensities obeys, in fact, the same point-group symmetry as that of the crystal. If, however, anomalous dispersion is negligibly small, and the point group of the crystal is noncentrosymmetric, the apparent symmetry of the diffraction pattern will also contain a false centre of symmetry and, of course, all the additional elements generated by the inclusion of this centre. Under these circumstances, the diffraction pattern from a single crystal may belong to one of the eleven centrosymmetric point groups, known as Laue groups (*IT I*, 1952).

According to equation (1.4.2.5), the phases of the structure factors of symmetry-related reflections differ, in the general case, by a phase shift that depends on the translation part of the space-group operation involved. Only when the space group is symmorphic, *i.e.* it contains no translations other than those of the Bravais lattice, will the distribution of the phases obey the point-group symmetry of the crystal. These phase shifts are considered in detail in Section 1.4.4 where their tabulation is presented and the alternative interpretation (Bienenstock & Ewald, 1962) of symmetry in reciprocal space, mentioned in Section 1.4.1, is given.

Equation (1.4.2.3) can be usefully applied to a classification of all the general systematic absences or – as defined in the space-group tables in the main editions of *IT* (1935, 1952, 1983, 1987, 1992) – general conditions for possible reflections. These systematic absences are associated with special positions in the reciprocal lattice – special with respect to the point-group operations \mathbf{P} appearing in the relevant relationships. If, in a given relationship, we have $\mathbf{P}^T \mathbf{h} = \mathbf{h}$, equation (1.4.2.3) reduces to

$$F(\mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T \mathbf{t}). \quad (1.4.2.6)$$

Of course, $F(\mathbf{h})$ may then be nonzero only if $\cos(2\pi \mathbf{h}^T \mathbf{t})$ equals unity, or the scalar product $\mathbf{h}^T \mathbf{t}$ is an integer. This well known result leads to a ready determination of lattice absences, as well as those produced by screw-axis and glide-plane translations, and is routinely employed in crystallographic computing. An exhaustive classification of the general conditions for possible reflections is given in the space-group tables (*IT*, 1952, 1983). It should be noted that since the axes of rotation and planes of reflection in the reciprocal lattice are parallel to the corresponding elements in the direct lattice (Buerger, 1960), the component of \mathbf{t} that depends on the location of the corresponding space-group symmetry element in direct space does not contribute to the scalar product $\mathbf{h}^T \mathbf{t}$ in (1.4.2.6), and it is only the intrinsic part of the translation \mathbf{t} (*IT A*, 1983) that usually matters.

It may, however, be of interest to note that some screw axes in direct space cannot give rise to any systematic absences. For example, the general Wyckoff position No. (10) in the space group $Pa\bar{3}$ (No. 205) (*IT A*, 1983) has the coordinates $\bar{y}, \frac{1}{2} + z, \frac{1}{2} - x$, and corresponds to the space-group operation

$$(\mathbf{P}, \mathbf{t}) = (\mathbf{P}, \mathbf{t}_i + \mathbf{t}_l) = \left[\begin{pmatrix} 0 & \bar{1} & 0 \\ 0 & 0 & 1 \\ \bar{1} & 0 & 0 \end{pmatrix}, \begin{pmatrix} -\frac{1}{3} \\ \frac{1}{3} \\ \frac{1}{3} \end{pmatrix} + \begin{pmatrix} \frac{1}{6} \\ \frac{1}{6} \\ \frac{1}{6} \end{pmatrix} \right], \quad (1.4.2.7)$$

where \mathbf{t}_i and \mathbf{t}_l are the intrinsic and location-dependent components of the translation part \mathbf{t} , and are parallel and perpendicular, respectively, to the threefold axis of rotation represented by the matrix \mathbf{P} in (1.4.2.7) (*IT A*, 1983; Shmueli, 1984). This is clearly a threefold screw axis, parallel to $[\bar{1}\bar{1}1]$. The reciprocal-lattice vectors which remain unchanged, when postmultiplied by \mathbf{P} (or premultiplied by its transpose), have the form: $\mathbf{h}^T = (h\bar{h}\bar{h})$; this is the special position for the present example. We see that (i) $\mathbf{h}^T \mathbf{t}_i = 0$, as expected, and (ii) $\mathbf{h}^T \mathbf{t}_l = -h$. Since the scalar product $\mathbf{h}^T \mathbf{t}$ is an integer, there are no values of index h for which the structure factor $F(h\bar{h}\bar{h})$ must be absent.

Other approaches to systematically absent reflections include a direct inspection of the structure-factor equation (Lipson & Cochran, 1966), which is of considerable didactical value, and the utilization of transformation properties of direct and reciprocal base vectors and lattice-point coordinates (Buerger, 1942).

Finally, the relationship between the phases of symmetry-related reflections, given by (1.4.2.5), is of fundamental as well as practical importance in the theories and techniques of crystal structure

1.4. SYMMETRY IN RECIPROCAL SPACE

determination which operate in reciprocal space (Part 2 of this volume).

1.4.2.3. Symmetry factors for space-group-specific Fourier summations

The weighted reciprocal lattice, with weights taken as the structure factors, is synonymous with the discrete space of the coefficients of a Fourier expansion of the electron density, or the Fourier space (F space) of the latter. Accordingly, the asymmetric unit of the Fourier space can be defined as the subset of structure factors within which the relationship (1.4.2.3) does not hold – except at special positions in the reciprocal lattice. If the point group of the crystal is of order g , this is also the order of the corresponding factor-group representation of the space group (*IT* A, 1983) and there exist g relationships of the form of (1.4.2.3):

$$F(\mathbf{P}_s^T \mathbf{h}) = F(\mathbf{h}) \exp(-2\pi i \mathbf{h}^T \mathbf{t}_s). \quad (1.4.2.8)$$

We can thus decompose the summation in (1.4.2.1) into g sums, each extending over an asymmetric unit of the F space. It must be kept in mind, however, that some classes of reciprocal-lattice vectors may be common to more than one asymmetric unit, and thus each reciprocal-lattice point will be assigned an occupancy factor, denoted by $q(\mathbf{h})$, such that $q(\mathbf{h}) = 1$ for a general position and $q(\mathbf{h}) = 1/m(\mathbf{h})$ for a special one, where $m(\mathbf{h})$ is the multiplicity – or the order of the point group that leaves \mathbf{h} unchanged. Equation (1.4.2.1) can now be rewritten as

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{s=1}^g \sum_{\mathbf{h}_a} q(\mathbf{h}_a) F(\mathbf{P}_s^T \mathbf{h}_a) \exp[-2\pi i (\mathbf{P}_s^T \mathbf{h}_a)^T \mathbf{r}], \quad (1.4.2.9)$$

where the inner summation in (1.4.2.9) extends over the reference asymmetric unit of the Fourier space, which is associated with the identity operation of the space group. Substituting from (1.4.2.8) for $F(\mathbf{P}_s^T \mathbf{h}_a)$, and interchanging the order of the summations in (1.4.2.9), we obtain

$$\rho(\mathbf{r}) = \frac{1}{V} \sum_{\mathbf{h}_a} q(\mathbf{h}_a) F(\mathbf{h}_a) \sum_{s=1}^g \exp[-2\pi i \mathbf{h}_a^T (\mathbf{P}_s \mathbf{r} + \mathbf{t}_s)] \quad (1.4.2.10)$$

$$= \frac{1}{V} \sum_{\mathbf{h}_a} q(\mathbf{h}_a) F(\mathbf{h}_a) [A(\mathbf{h}_a) - iB(\mathbf{h}_a)], \quad (1.4.2.11)$$

where

$$A(\mathbf{h}) = \sum_{s=1}^g \cos[2\pi \mathbf{h}^T (\mathbf{P}_s \mathbf{r} + \mathbf{t}_s)] \quad (1.4.2.12)$$

and

$$B(\mathbf{h}) = \sum_{s=1}^g \sin[2\pi \mathbf{h}^T (\mathbf{P}_s \mathbf{r} + \mathbf{t}_s)]. \quad (1.4.2.13)$$

The symmetry factors A and B are well known as geometric or trigonometric structure factors and a considerable part of Volume I of *IT* (1952) is dedicated to their tabulation. Their formal association with the structure factor – following from direct-space arguments – is closely related to that shown in equation (1.4.2.11) (see Section 1.4.2.4). Simplified trigonometric expressions for A and B are given in Tables A1.4.3.1–A1.4.3.7 in Appendix 1.4.3 for all the two- and three-dimensional crystallographic space groups, and for all the parities of hkl for which A and B assume different functional forms. These expressions are there given for general reflections and can also be used for special ones, provided the occupancy factors $q(\mathbf{h})$ have been properly accounted for.

Equation (1.4.2.11) is quite general and can, of course, be applied to noncentrosymmetric Fourier summations, without neglect of dispersion. Further simplifications are obtained in the centrosym-

metric case, when the space-group origin is chosen at a centre of symmetry, and in the noncentrosymmetric case, when dispersion is neglected. In each of the latter two cases the summation over \mathbf{h}_a is restricted to reciprocal-lattice vectors that are not related by real or apparent inversion (denoted by $\mathbf{h}_a > 0$), and we obtain

$$\rho(\mathbf{r}) = \frac{2}{V} \sum_{\mathbf{h}_a > 0} q(\mathbf{h}_a) F(\mathbf{h}_a) A(\mathbf{h}_a) \quad (1.4.2.14)$$

and

$$\rho(\mathbf{r}) = \frac{2}{V} \sum_{\mathbf{h}_a > 0} q(\mathbf{h}_a) |F(\mathbf{h}_a)| [A(\mathbf{h}_a) \cos \varphi(\mathbf{h}_a) + B(\mathbf{h}_a) \sin \varphi(\mathbf{h}_a)] \quad (1.4.2.15)$$

for the dispersionless centrosymmetric and noncentrosymmetric cases, respectively.

1.4.2.4. Symmetry factors for space-group-specific structure-factor formulae

The explicit dependence of structure-factor summations on the space-group symmetry of the crystal can also be expressed in terms of symmetry factors, in an analogous manner to that described for the electron density in the previous section. It must be pointed out that while the above treatment only presumes that the electron density can be represented by a three-dimensional Fourier series, the present one is restricted by the assumption that the atoms are isotropic with regard to their motion and shape (*cf.* Chapter 1.2).

Under the above assumptions, *i.e.* for isotropically vibrating spherical atoms, the structure factor can be written as

$$F(\mathbf{h}) = \sum_{j=1}^N f_j \exp(2\pi i \mathbf{h}^T \mathbf{r}_j), \quad (1.4.2.16)$$

where $\mathbf{h}^T = (hkl)$ is the diffraction vector, N is the number of atoms in the unit cell, f_j is the atomic scattering factor including its temperature factor and depending on the magnitude of \mathbf{h} only, and \mathbf{r}_j is the position vector of the j th atom referred to the origin of the unit cell.

If the crystal belongs to a point group of order m_p and the multiplicity of its Bravais lattice is m_L , there are $g' = m_p \times m_L$ general equivalent positions in the unit cell of the space group (*IT* A, 1983). We can thus rewrite (1.4.2.16), grouping the contributions of the symmetry-related atoms, as

$$F(\mathbf{h}) = \sum_j f_j \sum_{s=1}^{g'} \exp[2\pi i \mathbf{h}^T (\mathbf{P}_s \mathbf{r} + \mathbf{t}_s)], \quad (1.4.2.17)$$

where \mathbf{P}_s and \mathbf{t}_s are the rotation and translation parts of the s th space-group operation respectively. The inner summation in (1.4.2.17) contains the dependence of the structure factor of reflection \mathbf{h} on the space-group symmetry of the crystal and is known as the (complex) geometric or trigonometric structure factor.

Equation (1.4.2.17) can be rewritten as

$$F(\mathbf{h}) = \sum_j f_j [A_j(\mathbf{h}) + iB_j(\mathbf{h})], \quad (1.4.2.18)$$

where

$$A_j(\mathbf{h}) = \sum_{s=1}^{g'} \cos[2\pi \mathbf{h}^T (\mathbf{P}_s \mathbf{r}_j + \mathbf{t}_s)] \quad (1.4.2.19)$$

and

$$B_j(\mathbf{h}) = \sum_{s=1}^{g'} \sin[2\pi \mathbf{h}^T (\mathbf{P}_s \mathbf{r}_j + \mathbf{t}_s)] \quad (1.4.2.20)$$

1. GENERAL RELATIONSHIPS AND TECHNIQUES

are the real and imaginary parts of the trigonometric structure factor. Equations (1.4.2.19) and (1.4.2.20) are *mathematically* identical to equations (1.4.2.11) and (1.4.2.12), respectively, apart from the numerical coefficients which appear in the expressions for A and B , for space groups with centred lattices: while only the order of the point group need be considered in connection with the Fourier expansion of the electron density (see above), the multiplicity of the Bravais lattice must of course appear in (1.4.2.19) and (1.4.2.20).

Analogous functional forms are arrived at by considerations of symmetry in direct and reciprocal spaces. These quantities are therefore convenient representations of crystallographic symmetry in its interaction with the diffraction experiment and have been indispensable in all of the early crystallographic computing related to structure determination. Their applications to modern crystallographic computing have been largely superseded by fast Fourier techniques, in reciprocal space, and by direct use of matrix and vector representations of space-group operators, in direct space, especially in cases of low space-group symmetry. It should be noted, however, that the degree of simplification of the trigonometric structure factors generally increases with increasing symmetry (see, *e.g.*, Section 1.4.3), and the gain of computing efficiency becomes significant when problems involving high symmetries are treated with this 'old-fashioned' tool. Analytic expressions for the trigonometric structure factors are of course indispensable in studies in which the knowledge of the functional form of the structure factor is required [*e.g.* in theories of structure-factor statistics and direct methods of phase determination (see Chapters 2.1 and 2.2)].

Equations (1.4.2.19) and (1.4.2.20) are simple but their expansion and simplification for all the space groups and relevant hkl subsets can be an extremely tedious undertaking when carried out in the conventional manner. As shown below, this process has been automated by a suitable combination of symbolic and numeric high-level programming procedures.

1.4.3. Structure-factor tables

1.4.3.1. Some general remarks

This section is a revised version of the structure-factor tables contained in Sections 4.5 through 4.7 of Volume I (*IT I*, 1952). As in the previous edition, it is intended to present a comprehensive list of explicit expressions for the real and the imaginary parts of the trigonometric structure factor, for all the 17 plane groups and the 230 space groups, and for the hkl subsets for which the trigonometric structure factor assumes different functional forms. The tables given here are also confined to the case of general Wyckoff positions (*IT I*, 1952). However, the expressions are presented in a much more concise symbolic form and are amenable to computation just like the explicit trigonometric expressions in Volume I (*IT I*, 1952). The present tabulation is based on equations (1.4.2.19) and (1.4.2.20), *i.e.* the numerical coefficients in A and B which appear in Tables A1.4.3.1–A1.4.3.7 in Appendix 1.4.3 are appropriate to space-group-specific structure-factor formulae. The functional form of A and B is, however, the same when applied to Fourier summations (see Section 1.4.2.3).

1.4.3.2. Preparation of the structure-factor tables

The lists of the coordinates of the general equivalent positions, presented in *IT A* (1983), as well as in earlier editions of the *Tables*, are sufficient for the expansion of the summations in (1.4.2.19) and (1.4.2.20) and the simplification of the resulting expressions can be performed using straightforward algebra and trigonometry (see, *e.g.*, *IT I*, 1952). As mentioned above, the preparation of the present structure-factor tables has been automated and its stages can be summarized as follows:

- (i) Generation of the coordinates of the general positions, starting from a computer-adapted space-group symbol (Shmueli, 1984).
- (ii) Formation of the scalar products, appearing in (1.4.2.19) and (1.4.2.20), and their separation into components depending on the rotation and translation parts of the space-group operations:

$$\mathbf{h}^T(\mathbf{P}_s, \mathbf{t}_s)\mathbf{r} = \mathbf{h}^T\mathbf{P}_s\mathbf{r} + \mathbf{h}^T\mathbf{t}_s \quad (1.4.3.1)$$

for the space groups which are not associated with a unique axis; the left-hand side of (1.4.3.1) is separated into contributions of the relevant plane group and unique axis for the remaining space groups.

- (iii) Analysis of the translation-dependent parts of the scalar products and automatic determination of all the parities of hkl for which A and B must be computed and simplified.

- (iv) Expansion of equations (1.4.2.19) and (1.4.2.20) and their reduction to trigonometric expressions comparable to those given in the structure-factor tables in Volume I of *IT* (1952).

- (v) Representation of the results in terms of a small number of building blocks, of which the expressions were found to be composed. These representations are described in Section 1.4.3.3.

All the stages outlined above were carried out with suitably designed computer programs, written in numerically and symbolically oriented languages. A brief summary of the underlying algorithms is presented in Appendix 1.4.1. The computer-adapted space-group symbols used in these computations are described in Section A1.4.2.2 and presented in Table A1.4.2.1.

1.4.3.3. Symbolic representation of A and B

We shall first discuss the symbols for the space groups that are not associated with a unique axis. These comprise the triclinic, orthorhombic and cubic space groups. The symbols are also used for the seven rhombohedral space groups which are referred to rhombohedral axes (*IT I*, 1952; *IT A*, 1983).

The abbreviation of triple products of trigonometric functions such as, *e.g.*, denoting $\cos(2\pi hx) \sin(2\pi ky) \cos(2\pi lz)$ by csc , is well known (*IT I*, 1952), and can be conveniently used in representing A and B for triclinic and orthorhombic space groups. However, the simplified expressions for A and B in space groups of higher symmetry also possess a high degree of regularity, as is apparent from an examination of the structure-factor tables in Volume I (*IT I*, 1952), and as confirmed by the preparation of the present tables. An example, illustrating this for the cubic system, is given below.

The trigonometric structure factor for the space group $Pm\bar{3}$ (No. 200) is given by

$$A = 8[\cos(2\pi hx) \cos(2\pi ky) \cos(2\pi lz) + \cos(2\pi hy) \cos(2\pi kz) \cos(2\pi lx) + \cos(2\pi hz) \cos(2\pi kx) \cos(2\pi ly)], \quad (1.4.3.2)$$

and the sum of the above nine-function block and the following one:

$$8[\cos(2\pi hx) \cos(2\pi kz) \cos(2\pi ly) + \cos(2\pi hz) \cos(2\pi ky) \cos(2\pi lx) + \cos(2\pi hy) \cos(2\pi kx) \cos(2\pi lz)] \quad (1.4.3.3)$$

is the trigonometric structure factor for the space group $Pm\bar{3}m$ (No. 221, *IT I*, 1952, *IT A*, 1983). It is obvious that the only difference between the nine-function blocks in (1.4.3.2) and (1.4.3.3) is that the permutation of the coordinates xyz is *cyclic* or *even* in (1.4.3.2), while it is *non-cyclic* or *odd* in (1.4.3.3).

It was observed during the generation of the present tables that the expressions for A and B for all the cubic space groups, and all the relevant hkl subsets, can be represented in terms of such 'even' and 'odd' nine-function blocks. Moreover, it was found that the order of the trigonometric functions in each such block remains the same in