its temperature factor and depending on the magnitude of **h** only, and $\mathbf{r}_j$ is the position vector of the jth 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 $g' = m_\mathrm{p} \times m_\mathrm{L}$ 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

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

where $\boldsymbol{P}_s$ and $\mathbf{t}_s$ are the rotation and translation parts of the sth space-group operation respectively. The inner summation in (1.4.2.17) contains the dependence of the structure factor of reflection **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

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

where

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

and

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

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 Their applications to modern crystallographic computing have been largely superseded by fast Fourier techniques, in reciprocal space, and by direct use of matrix and vector representations of space-group operators, in direct space, especially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:

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

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

$$\begin{aligned} A = 8[&\cos(2\pi hx)\cos(2\pi ky)\cos(2\pi lz) \\ &+ \cos(2\pi hy)\cos(2\pi kz)\cos(2\pi lx) \\ &+ \cos(2\pi hz)\cos(2\pi kx)\cos(2\pi ly)], \end{aligned} \tag{1.4.3.2}$$

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

$$\begin{aligned} 8[&\cos(2\pi hx)\cos(2\pi kz)\cos(2\pi ly) \\ &+ \cos(2\pi hz)\cos(2\pi ky)\cos(2\pi lx) \\ &+ \cos(2\pi hy)\cos(2\pi kx)\cos(2\pi lz)] \end{aligned} \tag{1.4.3.3}$$

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 *noncyclic* 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 each of its three terms (triple products). This is not surprising since each of the above space groups contains threefold axes of rotation along [111] and related directions, and such permutations of *xyz* for fixed *hkl* (or *vice versa*) are expected. It was therefore possible to introduce two permutation operators and represent *A* and *B* in terms of the following two basic blocks:

$$\begin{aligned} \mathrm{Epqr} = {}&\mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky)\mathrm{r}(2\pi lz) + \mathrm{p}(2\pi hy)\mathrm{q}(2\pi kz)\mathrm{r}(2\pi lx) \\ &+ \mathrm{p}(2\pi hz)\mathrm{q}(2\pi kx)\mathrm{r}(2\pi ly) \end{aligned} \tag{1.4.3.4}$$

and

$$\begin{aligned} \mathrm{Opqr} = {}&\mathrm{p}(2\pi hx)\mathrm{q}(2\pi kz)\mathrm{r}(2\pi ly) + \mathrm{p}(2\pi hz)\mathrm{q}(2\pi ky)\mathrm{r}(2\pi lx) \\ &+ \mathrm{p}(2\pi hy)\mathrm{q}(2\pi kx)\mathrm{r}(2\pi lz), \end{aligned} \tag{1.4.3.5}$$

where each of p, q and r can be a sine or a cosine, and appears at the same position in each of the three terms of a block. The capital prefixes E and O were chosen to represent even and odd permutations of the coordinates *xyz*, respectively.

For example, the trigonometric structure factor for the space group $Pa\bar{3}$ (No. 205, *IT* I, 1952, *IT* A, 1983) can now be tabulated as follows:

A	*B*	$h+k$	$k+l$	$h+l$
8Eccc	0	even	even	even
−8Ecss	0	even	odd	odd
−8Escs	0	odd	even	odd
−8Essc	0	odd	odd	even

(*cf.* Table A1.4.3.7), where the sines and cosines are abbreviated by s and c, respectively. It is interesting to note that the only maximal non-isomorphic subgroup of $Pa\bar{3}$, not containing a threefold axis, is the orthorhombic *Pbca* (see *IT* A, 1983, p. 621), and this group–subgroup relationship is reflected in the functional forms of the trigonometric structure factors; the representation of *A* and *B* for *Pbca* is in fact analogous to that of $Pa\bar{3}$, including the parities of *hkl* and the corresponding forms of the triple products, except that the prefix E – associated with the threefold rotation – is absent from *Pbca*. The expression for *A* for the space group $Pm\bar{3}m$ [the sum of (1.4.3.2) and (1.4.3.3)] now simply reads: $A = 8(\mathrm{Eccc} + \mathrm{Occc})$.

As pointed out above, the permutation operators also apply to rhombohedral space groups that are referred to rhombohedral axes (Table A1.4.3.6), and the corresponding expressions for *R*3 and $R\bar{3}$ bear the same relationship to those for *P*1 and $P\bar{1}$ (Table A1.4.3.2), respectively, as that shown above for the related $Pa\bar{3}$ and *Pbca*.

When in any given standard space-group setting one of the coordinate axes is parallel to a unique axis, the point-group rotation matrices can be partitioned into 2×2 and 1×1 diagonal blocks, the former corresponding to an operation of the plane group resulting from the projection of the space group down the unique axis. If, for example, the unique axis is parallel to **c**, we can decompose the scalar product in (1.4.2.19) and (1.4.2.20) as follows:

$$\begin{aligned} \mathbf{h}^T(\boldsymbol{P}_s\mathbf{r} + \mathbf{t}_s) = {}&\begin{pmatrix} h & k \end{pmatrix}\left[\begin{pmatrix} P_{11} & P_{12} \\ P_{21} & P_{22} \end{pmatrix}\begin{pmatrix} x \\ y \end{pmatrix} + \begin{pmatrix} t_1 \\ t_2 \end{pmatrix}\right] \\ &+ l(P_{33}z + t_3), \end{aligned} \tag{1.4.3.6}$$

where the first scalar product on the right-hand side of (1.4.3.6) contains the contribution of a plane group and the second product is the contribution of the unique axis itself. The above decomposition often leads to a convenient factorization of *A* and *B*, and is applicable to monoclinic, tetragonal and hexagonal families, the latter including rhombohedral space groups that are referred to hexagonal axes.

The symbols used in Tables A1.4.3.3, A1.4.3.5 and A1.4.3.6 are based on such decompositions. In those few cases where explicit expressions must be given we make use of the convention of replacing $\cos(2\pi u)$ by $\mathrm{c}(u)$ and $\sin(2\pi u)$ by $\mathrm{s}(u)$. For example, $\cos[2\pi(hy + kx)]$ *etc.* is given as $\mathrm{c}(hy + kx)$ *etc.* The symbols are defined below.

Monoclinic space groups (Table A1.4.3.3)

The following symbols are used in this system:

$$\begin{aligned} \mathrm{c}(hl) &= \cos[2\pi(hx + lz)], \quad & \mathrm{c}(hk) &= \cos[2\pi(hx + ky)] \\ \mathrm{s}(hl) &= \sin[2\pi(hx + lz)], \quad & \mathrm{s}(hk) &= \sin[2\pi(hx + ky)] \end{aligned} \tag{1.4.3.7}$$

so that any expression for *A* or *B* in the monoclinic system has the form $K\mathrm{p}(hl)\mathrm{q}(ky)$ or $K\mathrm{p}(hk)\mathrm{q}(lz)$ for the second or first setting, respectively, where p and q can each be a sine or a cosine and *K* is a numerical constant.

Tetragonal space groups (Table A1.4.3.5)

The most frequently occurring expressions in the summations for A and B in this system are of the form

$$\mathrm{P(pq)} = \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky) + \mathrm{p}(2\pi kx)\mathrm{q}(2\pi hy) \qquad (1.4.3.8)$$

and

$$\mathrm{M(pq)} = \mathrm{p}(2\pi hx)\mathrm{q}(2\pi ky) - \mathrm{p}(2\pi kx)\mathrm{q}(2\pi hy), \qquad (1.4.3.9)$$

where p and q can each be a sine or a cosine. These are typical contributions related to square plane groups.

Trigonal and hexagonal space groups (Table A1.4.3.6)

The contributions of plane hexagonal space groups to the first term in (1.4.3.6) are

$$\begin{aligned} p_1 &= hx + ky, \quad p_2 = kx + iy, \quad p_3 = ix + hy, \\ q_1 &= kx + hy, \quad q_2 = hx + iy, \quad q_3 = ix + ky, \end{aligned} \qquad (1.4.3.10)$$

where $i = -h - k$ (*IT* I, 1952). The symbols which represent the frequently occurring expressions in this family, and given in terms of (1.4.3.10), are

$$\begin{aligned} \mathrm{C}(hki) &= \cos(2\pi p_1) + \cos(2\pi p_2) + \cos(2\pi p_3) \\ \mathrm{C}(khi) &= \cos(2\pi q_1) + \cos(2\pi q_2) + \cos(2\pi q_3) \\ \mathrm{S}(hki) &= \sin(2\pi p_1) + \sin(2\pi p_2) + \sin(2\pi p_3) \\ \mathrm{S}(khi) &= \sin(2\pi q_1) + \sin(2\pi q_2) + \sin(2\pi q_3) \end{aligned} \qquad (1.4.3.11)$$

and these quite often appear as the following sums and differences:

$$\begin{aligned} \mathrm{PH(cc)} &= \mathrm{C}(hki) + \mathrm{C}(khi), \quad \mathrm{PH(ss)} = \mathrm{S}(hki) + \mathrm{S}(khi) \\ \mathrm{MH(cc)} &= \mathrm{C}(hki) - \mathrm{C}(khi), \quad \mathrm{MH(ss)} = \mathrm{S}(hki) - \mathrm{S}(khi). \end{aligned} \qquad (1.4.3.12)$$

The symbols defined in this section are briefly redefined in the appropriate tables, which also contain the conditions for vanishing symbols.

1.4.3.4. Arrangement of the tables

The expressions for A and B are usually presented in terms of the short symbols defined above for all the representations of the plane groups and space groups given in Volume A (*IT* A, 1983), and are fully consistent with the unit-cell choices and space-group origins employed in that volume. The tables are arranged by crystal families and the expressions appear in the order of the appearance of the corresponding plane and space groups in the space-group tables in *IT* A (1983).

The main items in a table entry, not necessarily in the following order, are: (i) the conventional space-group number, (ii) the short Hermann–Mauguin space-group symbol, (iii) brief remarks on the choice of the space-group origin and setting, where appropriate, (iv) the real (A) and imaginary (B) parts of the trigonometric structure factor, and (v) the parity of the hkl subset to which the expressions for A and B pertain. Full space-group symbols are given in the monoclinic system only, since they are indispensable for the recognition of the settings and glide planes appearing in the various representations of monoclinic space groups given in *IT* A (1983).

1.4.4. Symmetry in reciprocal space: space-group tables

1.4.4.1. Introduction

The purpose of this section, and the accompanying table, is to provide a representation of the 230 three-dimensional crystallographic space groups in terms of two fundamental quantities that characterize a weighted reciprocal lattice: (i) coordinates of point-symmetry-related points in the reciprocal lattice, and (ii) phase shifts of the weight functions that are associated with the translation parts of the various space-group operations. Table A1.4.4.1 in Appendix 1.4.4 collects the above information for all the space-group settings which are listed in *IT* A (1983) for the same choice of the space-group origins and following the same numbering scheme used in that volume. Table A1.4.4.1 was generated by computer using the space-group algorithm described by Shmueli (1984) and the space-group symbols given in Table A1.4.2.1 in Appendix 1.4.2. It is shown in a later part of this section that Table A1.4.4.1 can also be regarded as a table of symmetry groups in Fourier space, in the Bienenstock–Ewald (1962) sense which was mentioned in Section 1.4.1. The section is concluded with a brief description of the correspondence between Bravais-lattice types in direct and reciprocal spaces.

1.4.4.2. Arrangement of the space-group tables

Table A1.4.4.1 is subdivided into point-group sections and space-group subsections, as outlined below.

(i) *The point-group heading.* This heading contains a short Hermann–Mauguin symbol of a point group, the crystal system and the symbol of the Laue group with which the point group is associated. Each point-group heading is followed by the set of space groups which are isomorphic to the point group indicated, the set being enclosed within a box.

(ii) *The space-group heading.* This heading contains, for each space group listed in Volume A (*IT* A, 1983), the short Hermann–Mauguin symbol of the space group, its conventional space-group number and (in parentheses) the serial number of its representation in Volume A; this is also the serial number of the explicit space-group symbol in Table A1.4.2.1 from which the entry was derived. Additional items are full space-group symbols, given only for the monoclinic space groups in their settings that are given in Volume A (*IT*, 1983), and self-explanatory comments as required.

(iii) *The table entry.* In the context of the analysis in Section 1.4.2.2, the format of a table entry is: $\mathbf{h}^T\boldsymbol{P}_n : -\mathbf{h}^T\mathbf{t}_n$, where $(\boldsymbol{P}_n, \mathbf{t}_n)$ is the nth space-group operator, and the phase shift $\mathbf{h}^T\mathbf{t}_n$ is expressed in units of 2π [see equations (1.4.2.3) and (1.4.2.5)]. More explicitly, the general format of a table entry is

$$(n)\, h_n k_n l_n : -p_n q_n r_n/m. \qquad (1.4.4.1)$$

In (1.4.4.1), n is the serial number of the space-group operation to which this entry pertains and is the same as the number of the general Wyckoff position generated by this operation and given in *IT* A (1983) for the space group appearing in the space-group heading. The first part of an entry, $h_n k_n l_n$:, contains the coordinates of the reciprocal-lattice vector that was generated from the reference vector (hkl) by the rotation part of the nth space-group operation. These rotation parts of the table entries, for a given space group, thus constitute the set of reciprocal-lattice points that are generated by the corresponding point group (*not Laue group*). The second part of an entry is an abbreviation of the phase shift which is associated with the nth operation and thus

$$-p_n q_n r_n/m \quad \text{denotes} \quad -2\pi(hp_n + kq_n + lr_n)/m, \qquad (1.4.4.2)$$

where the fractions p_n/m, q_n/m and r_n/m are the components of the translation part $\mathbf{t}_n$ of the nth space-group operation. The

references