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 $m_{\rm p}$ and the multiplicity of its Bravais lattice is $m_{\rm L}$, there are $g' = m_{\rm p} \times m_{\rm L}$ 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 Their applications to modern crystallographic computing have been largely superseded by fast Fourier techniques, in reciprocal space, and by direct use of matrix and vector representations of space-group operators, in direct space, especially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.