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 $n$th space-group operator, and the phase shift $\mathbf{h}^T\mathbf{t}_n$ is expressed in units of $2\pi$ [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 $n$th 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 $n$th 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 $n$th space-group operation. The phase-shift part of an entry is given only if $(p_n q_n r_n)$ is *not* a vector in the direct lattice, since such a vector would give rise to a trivial phase shift (an integer multiple of $2\pi$).

### 1.4.4.3. *Effect of direct-space transformations*

The phase shifts given in Table A1.4.4.1 depend on the translation parts of the space-group operations and these translations are determined, all or in part, by the choice of the space-group origin. It is a fairly easy matter to find the phase shifts that correspond to a given shift of the space-group origin in direct space, directly from Table A1.4.4.1. Moreover, it is also possible to modify the table entries so that a more general transformation, including a change of crystal axes as well as a shift of the space-group origin, can be directly accounted for. We employ here the frequently used concise notation due to Seitz (1935) (see also *IT* A, 1983).

Let the direct-space transformation be given by

$$\mathbf{r}_{\rm new} = \boldsymbol{T}\mathbf{r}_{\rm old} + \mathbf{v}, \qquad (1.4.4.3)$$

where $\boldsymbol{T}$ is a non-singular $3 \times 3$ matrix describing the change of the coordinate system and $\mathbf{v}$ is an origin-shift vector. The components of $\boldsymbol{T}$ and $\mathbf{v}$ are referred to the old system, and $\mathbf{r}_{\rm new}$ ($\mathbf{r}_{\rm old}$) is the position vector of a point in the crystal, referred to the new (old) system, respectively. If we denote a space-group operation referred to the new and old systems by $(\boldsymbol{P}_{\rm new}, \mathbf{t}_{\rm new})$ and $(\boldsymbol{P}_{\rm old}, \mathbf{t}_{\rm old})$, respectively, we have

$$(\boldsymbol{P}_{\rm new}, \mathbf{t}_{\rm new}) = (\boldsymbol{T}, \mathbf{v})(\boldsymbol{P}_{\rm old}, \mathbf{t}_{\rm old})(\boldsymbol{T}, \mathbf{v})^{-1} \qquad (1.4.4.4)$$

$$= (\boldsymbol{T}\boldsymbol{P}_{\rm old}\boldsymbol{T}^{-1}, \mathbf{v} - \boldsymbol{T}\boldsymbol{P}_{\rm old}\boldsymbol{T}^{-1}\mathbf{v} + \boldsymbol{T}\mathbf{t}_{\rm old}). \qquad (1.4.4.5)$$

It follows from (1.4.4.2) and (1.4.4.5) that if the old entry of Table A1.4.4.1 is given by

$$(n)\ \mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t},$$

the transformed entry becomes

$$(n)\ \mathbf{h}^T\boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1} : \mathbf{h}^T\boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1}\mathbf{v} - \mathbf{h}^T\mathbf{v} - \mathbf{h}^T\boldsymbol{T}\mathbf{t}, \qquad (1.4.4.6)$$

and in the important special cases of a pure change of setting ($\mathbf{v} = 0$) or a pure shift of the space-group origin ($\boldsymbol{T}$ is the unit matrix $\boldsymbol{I}$), (1.4.4.6) reduces to

$$(n)\ \mathbf{h}^T\boldsymbol{T}\boldsymbol{P}\boldsymbol{T}^{-1} : -\mathbf{h}^T\boldsymbol{T}\mathbf{t} \qquad (1.4.4.7)$$

or

$$(n)\ \mathbf{h}^T\boldsymbol{P} : \mathbf{h}^T\boldsymbol{P}\mathbf{v} - \mathbf{h}^T\mathbf{v} - \mathbf{h}^T\mathbf{t}, \qquad (1.4.4.8)$$

respectively. The rotation matrices $\boldsymbol{P}$ are readily obtained by visual or programmed inspection of the old entries: if, for example, $\mathbf{h}^T\boldsymbol{P}$ is $khl$, we must have $P_{21} = 1$, $P_{12} = 1$ and $P_{33} = 1$, the remaining $P_{ij}$'s being equal to zero. Similarly, if $\mathbf{h}^T\boldsymbol{P}$ is $kil$, where $i = -h - k$, we have

$$(kil) = (k, -h-k, l) = (hkl)\begin{pmatrix} 0 & \bar{1} & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

The rotation matrices can also be obtained by reference to Chapter 7 and Tables 11.2 and 11.3 in Volume A (*IT* A, 1983).

As an example, consider the phase shifts corresponding to the operation No. (16) of the space group $P4/nmm$ (No. 129) in its two origins given in Volume A (*IT* A, 1983). For an Origin 2-to-Origin 1 transformation we find there $\mathbf{v} = (\frac{1}{4}, -\frac{1}{4}, 0)$ and the old Origin 2



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entry in Table A1.4.4.1 is (16) *khl* (**t** is zero). The appropriate entry for the Origin 1 description of this operation should therefore be $\mathbf{h}^T\boldsymbol{P}\mathbf{v} - \mathbf{h}^T\mathbf{v} = k/4 - h/4 - h/4 + k/4 = -h/2 + k/2$, as given by (1.4.4.8), or $-(h+k)/2$ if a trivial shift of $2\pi$ is subtracted. The (new) Origin 1 entry thus becomes: (16) *khl*: $-110/2$, as listed in Table A1.4.4.1.

### 1.4.4.4. *Symmetry in Fourier space*

As shown below, Table A1.4.4.1 can also be regarded as a collection of the general equivalent positions of the symmetry groups of Fourier space, in the sense of the treatment by Bienenstock & Ewald (1962). This interpretation of the table is, however, restricted to the underlying periodic function being real and positive (see the latter reference). The symmetry formalism can be treated with the aid of the original $4 \times 4$ matrix notation, but it appears that a concise Seitz-type notation suits better the present introductory interpretation.

The symmetry dependence of the fundamental relationship (1.4.2.5)

$$\varphi(\mathbf{h}^T\boldsymbol{P}_n) = \varphi(\mathbf{h}) - 2\pi\mathbf{h}^T\mathbf{t}_n$$

is given by a table entry of the form: $(n)\ \mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}$, where the phase shift is given in units of $2\pi$, and the structure-dependent phase $\varphi(\mathbf{h})$ is omitted. Defining a combination law analogous to Seitz's product of two operators of affine transformation:

$$[\mathbf{a}^T : b](\boldsymbol{R}, \mathbf{r}) = [\mathbf{a}^T\boldsymbol{R} : \mathbf{a}^T\mathbf{r} + b], \tag{1.4.4.9}$$

where $\boldsymbol{R}$ is a $3 \times 3$ matrix, $\mathbf{a}^T$ is a row vector, $\mathbf{r}$ is a column vector and $b$ is a scalar, we can write the general form of a table entry as

$$[\mathbf{h}^T : \delta](\boldsymbol{P}, -\mathbf{t}) = [\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t} + \delta], \tag{1.4.4.10}$$

where $\delta$ is a constant phase shift which we take as zero. The positions $[\mathbf{h}^T : 0]$ and $[\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}]$ are now related by the operation $(\boldsymbol{P}, -\mathbf{t})$ *via* the combination law (1.4.4.9), which is a shorthand transcription of the $4 \times 4$ matrix notation of Bienenstock & Ewald (1962), with the appropriate sign of **t**.

Let us evaluate the result of a successive application of two such operators, say $(\boldsymbol{P}, -\mathbf{t})$ and $(\boldsymbol{Q}, -\mathbf{v})$ to the reference position $[\mathbf{h}^T : 0]$ in Fourier space:

$$\begin{aligned}[\mathbf{h}^T : 0](\boldsymbol{P}, -\mathbf{t})(\boldsymbol{Q}, -\mathbf{v}) &= [\mathbf{h}^T : 0](\boldsymbol{PQ}, -\boldsymbol{P}\mathbf{v} - \mathbf{t}) \\ &= [\mathbf{h}^T\boldsymbol{PQ} : -\mathbf{h}^T\boldsymbol{P}\mathbf{v} - \mathbf{h}^T\mathbf{t}],\end{aligned} \tag{1.4.4.11}$$

and perform an inverse operation:

$$\begin{aligned}[\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}](\boldsymbol{P}, -\mathbf{t})^{-1} &= [\mathbf{h}^T\boldsymbol{P} : -\mathbf{h}^T\mathbf{t}](\boldsymbol{P}^{-1}, \boldsymbol{P}^{-1}\mathbf{t}) \\ &= [\mathbf{h}^T\boldsymbol{P}\boldsymbol{P}^{-1} : \mathbf{h}^T\boldsymbol{P}\boldsymbol{P}^{-1}\mathbf{t} - \mathbf{h}^T\mathbf{t}] \\ &= [\mathbf{h}^T : 0].\end{aligned} \tag{1.4.4.12}$$

These equations confirm the validity of the shorthand notation (1.4.4.9) and illustrate the group nature of the operators $(\boldsymbol{P}, -\mathbf{t})$ in the present context.

Following Bienenstock & Ewald, the operators $(\boldsymbol{P}, -\mathbf{t})$ are symmetry operators that act on the positions $[\mathbf{h}^T : 0]$ in Fourier space, provided they satisfy the following requirements: (i) the application of such an operator leaves the magnitude of the (generally) complex Fourier coefficient unchanged, and (ii) after $g$ successive applications of an operator, where $g$ is the order of its rotation part, the phase remains unchanged up to a shift by an integer multiple of $2\pi$ (a trivial phase shift, corresponding to a translation by a lattice vector in direct space).

If our function is the electron density in the crystal, the first requirement is obviously satisfied since $|F(\mathbf{h})| = |F(\mathbf{h}^T\boldsymbol{P})|$, where $F$ is the structure factor [*cf.* equation (1.4.2.4)]. In order to make use of the second requirement in deriving permissible symmetry operators on Fourier space, all the relevant transformations, *i.e.* those which have rotation operators of the orders 1, 2, 3, 4 and 6, must be individually examined. A comprehensive example, covering most of the tetragonal system, can be found in Bienenstock & Ewald (1962).

It is of interest to illustrate the above process for a simple particular instance. Consider an operation, the rotation part of which involves a mirror plane, and assume that it is associated with the monoclinic system, in the second setting (unique axis $b$). We denote the operator by $(\boldsymbol{m}, -\mathbf{u})$, where $\mathbf{u}^T = (uvw)$, and the permissible values of $u$, $v$ and $w$ are to be determined. The operation is of order 2, and according to requirement (ii) above we have to evaluate

$$\begin{aligned}[\mathbf{h}^T : 0](\boldsymbol{m}, -\mathbf{u})^2 &= [\mathbf{h}^T : 0](\boldsymbol{I}, -\boldsymbol{m}\mathbf{u} - \mathbf{u}) \\ &= [\mathbf{h}^T : -\mathbf{h}^T(\boldsymbol{m} + \boldsymbol{I})\mathbf{u}] \\ &= [hkl : -2(hu + lw)],\end{aligned} \tag{1.4.4.13}$$

where

$$\boldsymbol{m} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \bar{1} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

is the matrix representing the operation of reflection and $\boldsymbol{I}$ is the unit matrix. For $(\boldsymbol{m}, -\mathbf{u})$ to be an admissible symmetry operator, the phase-shift part of (1.4.4.13), *i.e.* $-2(hu + lw)$, must be an integer (multiple of $2\pi$). The smallest non-negative values of $u$ and $w$ which satisfy this are the pairs: $u = w = 0$, $u = \frac{1}{2}$ and $w = 0$, $u = 0$ and $w = \frac{1}{2}$, and $u = w = \frac{1}{2}$. We have thus obtained four symmetry operators in Fourier space, which are identical (except for the sign of their translational parts) to those of the direct-space monoclinic mirror and glide-plane operations. The fact that the component $v$ cancels out simply means that an arbitrary component of the phase shift can be added along the $b^*$ axis; this is concurrent with arbitrary direct-space translations that appear in the characterization of individual types of space-group operations [see *e.g.* Koch & Fischer (1983)].

Each of the 230 space groups, which leaves invariant a (real and non-negative) function with the periodicity of the crystal, thus has its counterpart which determines the symmetry of the Fourier expansion coefficients of this function, with equivalent positions given in Table A1.4.4.1.

### 1.4.4.5. *Relationships between direct and reciprocal Bravais lattices*

Centred Bravais lattices in crystal space give rise to systematic absences of certain classes of reflections (*IT* I, 1952; *IT* A, 1983) and the corresponding points in the reciprocal lattice have accordingly zero weights. These absences are periodic in reciprocal space and their 'removal' from the reciprocal lattice results in a lattice which – like the direct one – must belong to one of the fourteen Bravais lattice types. This must be so since the point group of a crystal leaves its lattice – and also the associated reciprocal lattice – unchanged. The magnitudes of the structure factors (the weight functions) are also invariant under the operation of this point group.

The correspondence between the types of centring in direct and reciprocal lattices is given in Table 1.4.4.1.

Notes:

(i) The vectors $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$, appearing in the definition of the multiple unit cell in the reciprocal lattice, define this lattice *prior to*

Table 1.4.4.1. *Correspondence between types of centring in direct and reciprocal lattices*

| Direct lattice | | Reciprocal lattice | | |
|---|---|---|---|---|
| Lattice type(s) | Centring translations | Lattice type(s) | Restriction on *hkl* | Multiple unit cell |
| *P*, *R* | | *P*, *R* | | $\mathbf{a}^*$, $\mathbf{b}^*$, $\mathbf{c}^*$ |
| *A* | $0, \frac{1}{2}, \frac{1}{2}$ | *A* | $k+l=2n$ | $\mathbf{a}^*$, $2\mathbf{b}^*$, $2\mathbf{c}^*$ |
| *B* | $\frac{1}{2}, 0, \frac{1}{2}$ | *B* | $h+l=2n$ | $2\mathbf{a}^*$, $\mathbf{b}^*$, $2\mathbf{c}^*$ |
| *C* | $\frac{1}{2}, \frac{1}{2}, 0$ | *C* | $h+k=2n$ | $2\mathbf{a}^*$, $2\mathbf{b}^*$, $\mathbf{c}^*$ |
| *I* | $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$ | *F* | $h+k+l=2n$ | $2\mathbf{a}^*$, $2\mathbf{b}^*$, $2\mathbf{c}^*$ |
| *F* | $0, \frac{1}{2}, \frac{1}{2}$<br>$\frac{1}{2}, 0, \frac{1}{2}$<br>$\frac{1}{2}, \frac{1}{2}, 0$ | *I* | $k+l=2n$<br>$h+l=2n$<br>$h+k=2n$ | $2\mathbf{a}^*$, $2\mathbf{b}^*$, $2\mathbf{c}^*$ |
| $R_{\rm hex}$ | $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$<br>$\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ | $R_{\rm hex}$ | $-h+k+l=3n$ | $3\mathbf{a}^*$, $3\mathbf{b}^*$, $3\mathbf{c}^*$ |

*the removal* of lattice points with zero weights (absences). All the restrictions on *hkl* pertain to indexing on $\mathbf{a}^*$, $\mathbf{b}^*$ and $\mathbf{c}^*$.

(ii) The centring type of the reciprocal lattice refers to the multiple unit cell given in the table.

(iii) The centring type denoted by $R_{\rm hex}$ is a representation of the rhombohedral lattice *R* by a triple hexagonal unit cell, in the obverse setting (*IT* I, 1952), *i.e.* according to the transformation

$$\begin{aligned}\mathbf{a} &= \mathbf{a}_R - \mathbf{b}_R \\ \mathbf{b} &= \mathbf{b}_R - \mathbf{c}_R \\ \mathbf{c} &= \mathbf{a}_R + \mathbf{b}_R + \mathbf{c}_R,\end{aligned} \qquad (1.4.4.14)$$

where $\mathbf{a}_R$, $\mathbf{b}_R$ and $\mathbf{c}_R$ pertain to a primitive unit cell in the rhombohedral lattice *R*.

The corresponding multiple reciprocal cell, with centring denoted by $R_{\rm hex}$, contains nine lattice points with coordinates 000, 021, 012, 101, 202, 110, 220, 211 and 122 – indexed on the usual reciprocal to the triple hexagonal unit cell defined by (1.4.4.14). Detailed derivations of these correspondences are given by Buerger (1942), and an elementary proof of the reciprocity of *I* and *F* lattices can be found, *e.g.*, in pamphlet No. 4 of the Commission on Crystallographic Teaching (Authier, 1981). Intuitive proofs follow directly from the restrictions on *hkl*, given in Table 1.4.4.1.

## Appendix 1.4.1.

## Comments on the preparation and usage of the tables

(U. SHMUELI)

The straightforward but rather extensive calculations and text processing related to Tables A1.4.3.1 through A1.4.3.7 and Table A1.4.4.1 in Appendices 1.4.3 and 1.4.4, respectively, were performed with the aid of a combination of FORTRAN and REDUCE (Hearn, 1973) programs, designed so as to enable the author to produce the table entries directly from a space-group symbol and with a minimum amount of intermediate manual intervention. The first stage of the calculation, the generation of a space group (coordinates of the equivalent positions), was accomplished with the program *SPGRGEN*, the algorithm of which was described in some detail elsewhere (Shmueli, 1984). A complete list of computer-adapted space-group symbols, processed by *SPGRGEN* and not given in the latter reference, is presented in Table A1.4.2.1 of Appendix 1.4.2.

The generation of the space group is followed by a construction of symbolic expressions for the scalar products $\mathbf{h}^T(\boldsymbol{P}\mathbf{r}+\mathbf{t})$; *e.g.* for position No. (13) in the space group $P4_132$ (No. 213, *IT* I, 1952, *IT* A, 1983), this scalar product is given by $h(\frac{3}{4}+y)+k(\frac{1}{4}+x)+l(\frac{1}{4}-z)$. The construction of the various table entries consists of expanding the sines and cosines of these scalar products, performing the required summations, and simplifying the result where possible. The construction of the scalar products in a FORTRAN program is fairly easy and the extremely tedious trigonometric calculations required by equations (1.4.2.19) and (1.4.2.20) can be readily performed with the aid of one of several available computer-algebraic languages (for a review, see *Computers in the New Laboratory – a Nature Survey*, 1981); the REDUCE language was employed for the above purpose.

Since the REDUCE programs required for the summations in (1.4.2.19) and (1.4.2.20) for the various space groups were seen to have much in common, it was decided to construct a FORTRAN interface which would process the space-group input and prepare automatically REDUCE programs for the algebraic work. The least straightforward problem encountered during this work was the need to 'convince' the interface to generate *hkl* parity assignments which are appropriate to the space-group information input. This was solved for all the crystal families except the hexagonal by setting up a 'basis' of the form: $h/2, k/2, l/2, (k+l)/2, \ldots, (h+k+l)/4$ and representing the translation parts of the scalar products, $\mathbf{h}^T\mathbf{t}$, as sums of such 'basis functions'. A subsequent construction of an automatic parity routine proved to be easy and the interface could thus produce any number of REDUCE programs for the summations in (1.4.2.19) and (1.4.2.20) using a list of space-group symbols as the sole input. These included trigonal and hexagonal space groups with translation components of $\frac{1}{2}$. This approach seemed to be too awkward for some space groups containing threefold and sixfold screw axes, and these were treated individually.

There is little to say about the REDUCE programs, except that the output they generate is at the same level of trigonometric complexity as the expressions for *A* and *B* appearing in Volume I (*IT* I, 1952). This could have been improved by making use of the pattern-matching capabilities that are incorporated in REDUCE, but



references