International Tables for Crystallography (2010). Vol. B, Section 1.4.4.2, pp. 119–120.

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

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

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:

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

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 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 2π).

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 nonsingular 3×3 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

$$\begin{aligned}(\boldsymbol{P}_{\rm new}, \mathbf{t}_{\rm new}) &= (\boldsymbol{T}, \mathbf{v})(\boldsymbol{P}_{\rm old}, \mathbf{t}_{\rm old})(\boldsymbol{T}, \mathbf{v})^{-1} \qquad (1.4.4.4)\\ &= (\boldsymbol{T}\boldsymbol{P}_{\rm old}\boldsymbol{T}^{-1}, \mathbf{v} - \boldsymbol{T}\boldsymbol{P}_{\rm old}\boldsymbol{T}^{-1}\mathbf{v} + \boldsymbol{T}\mathbf{t}_{\rm old}). \qquad (1.4.4.5)\end{aligned}$$

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 Part 7 and Tables 11.2.2.1 and 11.2.2.2 in Volume A (*IT* A, 2005).

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 entry in Table A1.4.4.1 is (16) *khl* ($\mathbf{t}$ 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 2π 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 4×4 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 2π, 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:

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

where $\boldsymbol{R}$ is a 3×3 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

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

where δ 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 4×4 matrix notation of Bienenstock & Ewald (1962), with the appropriate sign of $\mathbf{t}$.

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:

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

and perform an inverse operation:

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

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.

references