International Tables for Crystallography (2010). Vol. B, Section 1.4.4.3, p. 120.

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

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

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

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

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

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

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

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

or

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

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) $\bar{k}\bar{h}l$ ($\mathbf{t}$ 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) $\bar{k}\bar{h}l$: $-110/2$, 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:

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

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

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

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:

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

and perform an inverse operation:

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

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.