International Tables for Crystallography (2016). Vol. A, Section 3.5.3.3, p. 849.

3.5. NORMALIZERS OF SPACE GROUPS

cannot be mapped onto right-handed quartz by the Euclidean normalizer. The four equivalent descriptions retain the chirality.

More details on Euclidean-equivalent point configurations and descriptions of crystal structures have been given by Fischer & Koch (1983) and Koch & Fischer (2006).

3.5.3.3. Equivalent lists of structure factors

All the different but equivalent descriptions of a crystal structure refer to different but equivalent lists of structure factors. These lists contain the same moduli of the structure factors $|F(\boldsymbol{h})|$, but they differ in their indices $\boldsymbol{h} = (h, k, l)$ and phases $\varphi(\boldsymbol{h})$.

In the previous section, the unit cell (basis and origin) of a space group $\mathcal{G}$ has been considered fixed, whereas the crystal structure or its enantiomorph was embedded into the pattern of symmetry elements at different but equivalent locations. In the present context, however, it is advantageous to regard the crystal structure as being fixed and to let $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ transform the basis and the origin with respect to which the crystal structure is described. This matches the usual approach to resolve the ambiguities in direct methods by fixing the origin and the absolute structure.

Each matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ representing an element of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ describes a unit-cell transformation of $\mathcal{G}$. According to Section 1.5.2 the following equations hold:

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}'), = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}, \quad \begin{pmatrix} \mathbf{a}^{*'} \\ \mathbf{b}^{*'} \\ \mathbf{c}^{*'} \end{pmatrix} = \boldsymbol{P}^{-1} \begin{pmatrix} \mathbf{a}^{*} \\ \mathbf{b}^{*} \\ \mathbf{c}^{*} \end{pmatrix}, \quad \boldsymbol{h}' = \boldsymbol{h}\boldsymbol{P}.$$

As a consequence, the phase $\varphi(\boldsymbol{h})$ of a given structure factor also changes into $\varphi'(\boldsymbol{h}') = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{h}\boldsymbol{p}$.

Similar to equivalent descriptions of a crystal structure, it is possible to derive all equivalent lists of structure factors: The additional generators of $\mathcal{K}(\mathcal{G})$ are pure translations that leave the indices $\boldsymbol{h}$ of all structure factors unchanged but transform their phases according to $\varphi'(\boldsymbol{h}) = \varphi(\boldsymbol{h}) - 2\pi\boldsymbol{h}\boldsymbol{p}$. Therefore, the origin for the description of the crystal structure may be fixed by appropriate restrictions of some phases. The number of these phases equals the number of additional generators of $\mathcal{K}(\mathcal{G})$, given in Tables 3.5.2.3, 3.5.2.4 or 3.5.2.5. These generators [together with the inversion that generates $\mathcal{L}(\mathcal{G})$, if present] also determine the parity classes of the structure factors and the ranges for the phase restrictions.

The inversion that generates $\mathcal{L}(\mathcal{G})$ changes the handedness of the coordinate system in direct space and in reciprocal space and, therefore, gives rise to different absolute crystal structures. The indices of a given structure factor change from $\boldsymbol{h}$ to $\boldsymbol{h}' = -\boldsymbol{h}$, whereas the phase is influenced only if the symmetry centre is not located at $0, 0, 0$.

If no anomalous scattering is observed, Friedel's rule holds and the moduli of any two structure factors with indices $\boldsymbol{h}$ and $-\boldsymbol{h}$ are equal. As a consequence, different absolute crystal structures result in lists of structure factors and indices that differ only in their phases. Therefore, one phase may be restricted to an appropriate range of length π to fix the absolute structure. This is not possible if anomalous scattering has been observed.

If $\mathcal{L}(\mathcal{G})$ differs from $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$, *i.e.* if $\mathcal{G}$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ belong to different Laue classes, the further generators of $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$ always change the orientation of the basis in direct and in reciprocal space. Therefore, the indices of the structure factors are permuted, but their phases are transformed only if $\boldsymbol{p} \neq \boldsymbol{o}$. The choice between these equivalent descriptions of the crystal

Table 3.5.3.1
Changes of structure-factor phases for the equivalent descriptions of a crystal structure in $F222$

$F222$	$h+k+l=$			
	$4n$	$4n+2$	$4n+1$	$4n+3$
$t(0,0,0)$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$
$t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi+\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi+\varphi(\boldsymbol{h})$
$t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$
$t(\frac{3}{4},\frac{3}{4},\frac{3}{4})$	$\varphi(\boldsymbol{h})$	$\pi+\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi+\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi+\varphi(\boldsymbol{h})$
$\bar{1}\ \ 0,0,0$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$
$\bar{1}\ \ \frac{1}{8},\frac{1}{8},\frac{1}{8}$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi-\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi-\varphi(\boldsymbol{h})$
$\bar{1}\ \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$
$\bar{1}\ \ \frac{3}{8},\frac{3}{8},\frac{3}{8}$	$-\varphi(\boldsymbol{h})$	$\pi-\varphi(\boldsymbol{h})$	$\frac{3}{2}\pi-\varphi(\boldsymbol{h})$	$\frac{1}{2}\pi-\varphi(\boldsymbol{h})$

structure is made when indexing the reflection pattern. In the case of anomalous scattering, the similar choice between the absolute structures is also combined with the indexing procedure.

Example

According to Table 3.5.2.4, eight equivalent descriptions exist for each crystal structure with symmetry $F222$. Four of them differ only by an origin shift and the other four are enantiomorphic to the first four. $t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ transforms all phases according to $\varphi'(\boldsymbol{h}) = \varphi(\boldsymbol{h}) - (\pi/2)(h+k+l)$, which gives rise to four parity classes of structure factors: $h+k+l = 4n$, $4n+1$, $4n+2$ and $4n+3$ (n integer). As $t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$ generates all additional translations of $\mathcal{K}(F222)$, restriction of one phase $\varphi(\boldsymbol{h}_1)$ to a range of length $\pi/2$ fixes the origin. Restriction of a second phase $\varphi(\boldsymbol{h}_2)$ to an appropriately chosen range of length π discriminates between pairs of enantiomorphic descriptions in the absence of anomalous scattering. For inversion through the origin $\bar{1}\ 0, 0, 0$, the corresponding change of phases is $\varphi'(\boldsymbol{h}) = -\varphi(\boldsymbol{h})$. Table 3.5.3.1 shows, for structure factors from all parity classes, how their phases depend on the chosen description of the crystal structure. Only phases from parity classes $h+k+l = 4n+1$ or $4n+3$ determine the origin in a unique way. The phase $\varphi(\boldsymbol{h}_2)$ that fixes the absolute structure may be chosen from any parity class but the appropriate range for its restriction depends on the parity classes of $\varphi(\boldsymbol{h}_1)$ and $\varphi(\boldsymbol{h}_2)$ and, moreover, on the range chosen for $\varphi(\boldsymbol{h}_1)$. If, for instance, $\varphi(\boldsymbol{h}_1)$ with $h+k+l = 4n+1$ is restricted to $\pi/2 \leq \varphi(\boldsymbol{h}_1) < \pi$, one of the following restrictions may be chosen for $\varphi(\boldsymbol{h}_2)$: $0 < \varphi(\boldsymbol{h}_2) < \pi$ for $h+k+l = 4n$; $-\pi/2 < \varphi(\boldsymbol{h}_2) < \pi/2$ for $h+k+l = 4n+2$; $-\pi/4 < \varphi(\boldsymbol{h}_2) < 3\pi/4$ for $h+k+l = 4n+1$; $-3\pi/4 < \varphi(\boldsymbol{h}_2) < \pi/4$ for $h+k+l = 4n+3$. If, however, the phase $\varphi(\boldsymbol{h}_1)$ of the same first reflection was restricted to $-\pi/4 \leq \varphi(\boldsymbol{h}_1) < 3\pi/4$, the possible restrictions for the second phase change to: $0 < \varphi(\boldsymbol{h}_2) < \pi$ for $h+k+l = 4n$ or $4n+2$; $-\pi/2 < \varphi(\boldsymbol{h}_2) < \pi/2$ for $h+k+l = 4n+1$ or $4n+3$ (for further details, *cf.* Koch, 1986).

3.5.3.4. Euclidean- and affine-equivalent sub- and supergroups

The Euclidean or affine normalizer of a space group $\mathcal{G}$ maps any subgroup or supergroup of $\mathcal{G}$ either onto itself or onto another subgroup or supergroup of $\mathcal{G}$. Accordingly, these normalizers define equivalence relationships on the sets of subgroups and supergroups of $\mathcal{G}$ (Koch, 1984*b*):

Two *subgroups* or *supergroups* of a space group $\mathcal{G}$ are called *Euclidean-* or $\mathcal{N}_{\mathcal{E}}$-*equivalent* (*affine-* or $\mathcal{N}_{\mathcal{A}}$-*equivalent*) if they are mapped onto each other by an element of the Euclidean (affine)

references