International Tables for Crystallography (2016). Vol. A, Section 3.5.3.4, pp. 849–850.

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:

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

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 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.

Table 3.5.3.1
Changes of structure-factor phases for the equivalent descriptions of a crystal structure in *F*222

	$h+k+l=$			
*F*222	$4n$	$4n+2$	$4n+1$	$4n+3$
$t(0, 0, 0)$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$
$t(\frac{1}{4}, \frac{1}{4}, \frac{1}{4})$	$\varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi + \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi + \varphi(\boldsymbol{h})$
$t(\frac{1}{2}, \frac{1}{2}, \frac{1}{2})$	$\varphi(\boldsymbol{h})$	$\varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$
$t(\frac{3}{4}, \frac{3}{4}, \frac{3}{4})$	$\varphi(\boldsymbol{h})$	$\pi + \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi + \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi + \varphi(\boldsymbol{h})$
$\bar{1}$ 0, 0, 0	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$
$\bar{1}$ $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$	$-\varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi - \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi - \varphi(\boldsymbol{h})$
$\bar{1}$ $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$	$-\varphi(\boldsymbol{h})$	$-\varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$
$\bar{1}$ $\frac{3}{8}, \frac{3}{8}, \frac{3}{8}$	$-\varphi(\boldsymbol{h})$	$\pi - \varphi(\boldsymbol{h})$	$\frac{3}{2}\pi - \varphi(\boldsymbol{h})$	$\frac{1}{2}\pi - \varphi(\boldsymbol{h})$

Example

According to Table 3.5.2.4, eight equivalent descriptions exist for each crystal structure with symmetry *F*222. 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 $\pi/2 \le \varphi(\boldsymbol{h}_1) < \pi$, 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 $-\pi/4 \le \varphi(\boldsymbol{h}_1) < 3\pi/4$, 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) normalizer of $\mathcal{G}$, *i.e.* if they are conjugate subgroups of the Euclidean (affine) normalizer.

In the following, the term 'equivalent subgroups (supergroups)' is used if a statement is true for Euclidean-equivalent *and* affine-equivalent subgroups (supergroups), and $\mathcal{N}(\mathcal{G})$ is used to designate the Euclidean as well as the affine normalizer.

The knowledge of Euclidean-equivalent subgroups is necessary in connection with the possible deformations of a crystal structure due to symmetry reduction. Affine-equivalent subgroups play an important role for the derivation and classification of black-and-white groups (magnetic groups) and of colour groups (*cf.* for example Schwarzenberger, 1984). Information on equivalent supergroups is useful for the determination of the idealized type of a crystal structure.

For any pair of space groups $\mathcal{G}$ and $\mathcal{H}$ with $\mathcal{H} < \mathcal{G}$, the relation between the two normalizers $\mathcal{N}(\mathcal{G})$ and $\mathcal{N}(\mathcal{H})$ controls the subgroups of $\mathcal{G}$ that are equivalent to $\mathcal{H}$ and the supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. The intersection group of both normalizers, $\mathcal{M}(\mathcal{G},\mathcal{H}) = \mathcal{N}(\mathcal{G}) \cap \mathcal{N}(\mathcal{H}) \geq \mathcal{H}$ may or may not coincide with $\mathcal{N}(\mathcal{G})$ and/or with $\mathcal{N}(\mathcal{H})$. The following two statements hold generally:

(i) The index i_g of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ equals the number of subgroups of $\mathcal{G}$ which are equivalent to $\mathcal{H}$. Each coset of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{G})$ maps $\mathcal{H}$ onto another equivalent subgroup of $\mathcal{G}$.

(ii) The index i_h of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ equals the number of supergroups of $\mathcal{H}$ equivalent to $\mathcal{G}$. Each coset of $\mathcal{M}(\mathcal{G},\mathcal{H})$ in $\mathcal{N}(\mathcal{H})$ maps $\mathcal{G}$ onto another equivalent supergroup of $\mathcal{H}$.

Equivalent subgroups are *conjugate* in $\mathcal{G}$ if and only if $\mathcal{G} \cap \mathcal{N}(\mathcal{H}) \neq \mathcal{G}$. In this case, $\mathcal{G}$ contains elements not belonging to $\mathcal{N}(\mathcal{H})$ and the cosets of $\mathcal{G} \cap \mathcal{N}(\mathcal{H})$ in $\mathcal{G}$ refer to the different conjugate subgroups.

Examples

(1) $\mathcal{G} = Cmmm$ has four monoclinic subgroups of type $P2/m$ with the same orthorhombic metric and the same basis as $Cmmm$: $\mathcal{H}_1 = P2/m11$, $\mathcal{H}_2 = P12/m1$, $\mathcal{H}_3 = P112/m$ ($\bar{1}$ at $0,0,0$), $\mathcal{H}_4 = P112/m$ ($\bar{1}$ at $\frac{1}{4},\frac{1}{4},0$). According to Table 3.5.2.4, the Euclidean normalizer of $\mathcal{G}$ is $Pmmm$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$. Because of the orthorhombic metric of all four subgroups, their Euclidean normalizers $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_1)$, $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_2)$, $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_3)$ and $\mathcal{N}_{\mathcal{E}}(\mathcal{H}_4)$ are enhanced in comparison with the general case and coincide with $\mathcal{N}_{\mathcal{E}}(\mathcal{G})$. Hence, no two of the four subgroups are Euclidean-equivalent.

(2) $\mathcal{G} = I\bar{4}m2$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, $\mathcal{H} = P\bar{4}$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$.
$\mathcal{N}(\mathcal{G}) = I4/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ is a supergroup of index 2 of $\mathcal{N}(\mathcal{H}) = P4/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}) = \mathcal{M}(I\bar{4}m2, P\bar{4})$. Therefore, $I\bar{4}m2$ has two equivalent subgroups $P\bar{4}$ that are mapped onto one another by a centring translation of $\mathcal{N}(\mathcal{G})$, *e.g.* by $t(0,\frac{1}{2},\frac{1}{4})$. Both subgroups are not conjugate in $I\bar{4}m2$ because $\mathcal{G} \cap \mathcal{N}(\mathcal{H})$ equals $\mathcal{G}$. As $\mathcal{N}(\mathcal{H})$ coincides with $\mathcal{M}(\mathcal{G},\mathcal{H})$, no further supergroups of $P\bar{4}$ equivalent to $I\bar{4}m2$ exist.

(3) $\mathcal{G} = Fm\bar{3}$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, $\mathcal{H} = F23$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$.
$\mathcal{N}(\mathcal{H}) = Im\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ is a supergroup of index 2 of $\mathcal{N}(\mathcal{G}) = Pm\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c}) = \mathcal{M}(Fm\bar{3}, F23)$. Therefore, $F23$ has two equivalent supergroups $Fm\bar{3}$ that differ in their locations with site symmetry $m\bar{3}$ by a centring translation of $Im\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$, *e.g.* by $t(\frac{1}{4},\frac{1}{4},\frac{1}{4})$. As $\mathcal{N}(\mathcal{G})$ coincides with $\mathcal{M}(\mathcal{G},\mathcal{H})$, no further subgroups of $Fm\bar{3}$ equivalent to $F23$ exist.

(4) $\mathcal{G} = Pmma$ $(\mathbf{a}, \mathbf{b}, \mathbf{c})$, $\mathcal{H} = Pmmn$ $(\mathbf{a}, 2\mathbf{b}, \mathbf{c})$.
The intersection of $\mathcal{N}_{\mathcal{A}}(Pmma) = Pmmm$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ and $\mathcal{N}_{\mathcal{A}}(Pmmn) = P4/mmm$ $(\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$ is the group $\mathcal{M}(Pmma, Pmmn) = Pmmm$ $(\frac{1}{2}\mathbf{a}, \mathbf{b}, \frac{1}{2}\mathbf{c})$, which is a proper subgroup of both normalizers. As i_g equals 2, $Pmma$ has two affine-equivalent subgroups of type $Pmmn$ that are mapped onto each other by the additional translation $t(0,\frac{1}{2},0)$ of the normalizer of $\mathcal{G}$. As i_h also equals 2, $Pmmn$ has two affine-equivalent supergroups, $Pmma$ and $Pmmb$, that are mapped onto each other, *e.g.* by the affine 'reflection' at a diagonal 'mirror plane' of $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$.

3.5.3.5. Reduction of the parameter regions to be considered for geometrical studies of point configurations

Each point configuration with space-group symmetry $\mathcal{G}$ may be described by its metrical and coordinate parameters. To cover all point configurations belonging to a certain space-group type exactly once, the metrical parameters of $\mathcal{G}$ have to be varied without restrictions, whereas the coordinate parameters x, y and z must be restricted to one asymmetric unit of $\mathcal{G}$. For the study of the geometrical properties of point configurations (*e.g.* sphere-packing conditions or types of Dirichlet domains *etc.*), the Euclidean normalizers (*cf. e.g.* Laves, 1931; Fischer, 1971, 1991; Koch, 1984*a*) as well as the affine normalizers (*cf.* Fischer, 1968) of the space groups allow a further reduction of the parameter regions that have to be considered.

Examples

(1) $\mathcal{G} = P4/m$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$: A geometrical consideration may be restricted to one asymmetric unit of $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P4/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$, *i.e.* to the region $0 \leq x \leq \frac{1}{2}$, $y \leq \min(x, \frac{1}{2} - x)$, $0 \leq z \leq \frac{1}{4}$. All metrical parameters are unrestricted.

(2) $\mathcal{G} = P4$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 < y < \frac{1}{2}$, $0 \leq z < 1$: The normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = \mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P^14/mmm$ $(\frac{1}{2}\mathbf{a} - \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{b}, \varepsilon\mathbf{c})$ restricts the parameter region to be considered to $0 \leq x \leq \frac{1}{2}$, $y \leq \min(x, \frac{1}{2} - x)$, $z = 0$. Again, no restriction exists for the metrical parameters.

(3) $\mathcal{G} = Pmmm$ with asymmetric unit $0 \leq x \leq \frac{1}{2}$, $0 \leq y \leq \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$: The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = Pmmm$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ reduces the parameter region to be considered to $0 \leq x \leq \frac{1}{4}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z \leq \frac{1}{4}$. All metrical parameters are unrestricted. The affine normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G}) = Pm\bar{3}m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ enables a further reduction of the parameter region that has to be studied. For this, two different possibilities exist:
   (i) the metrical parameters remain unrestricted but the coordinate parameters are limited to one asymmetric unit of $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$, *i.e.* to $0 \leq x \leq \frac{1}{4}$, $0 \leq y \leq x$, $0 \leq z \leq y$;
   (ii) the coordinate parameters are not further restricted, but the metrical parameters have to obey *e.g.* the relation $a \leq b \leq c$, *i.e.* $a/c \leq b/c \leq 1$.

(4) $\mathcal{G} = P112/m$ with asymmetric unit $0 \leq x < 1$, $0 \leq y \leq \frac{1}{2}$, $0 \leq z \leq \frac{1}{2}$. The Euclidean normalizer $\mathcal{N}_{\mathcal{E}}(\mathcal{G}) = P112/m$ $(\frac{1}{2}\mathbf{a}, \frac{1}{2}\mathbf{b}, \frac{1}{2}\mathbf{c})$ reduces the region that has to be considered for the coordinate parameters to $0 \leq x < \frac{1}{2}$, $0 \leq y \leq \frac{1}{4}$, $0 \leq z \leq \frac{1}{4}$, but it does not impose restrictions on the metrical parameters. These may be restricted, however, to the range $a/b \leq 1$ and $0 \leq 2\cos\gamma \leq -a/b$ (as shown in Fig. 3.5.2.1) by means of the affine normalizer $\mathcal{N}_{\mathcal{A}}(P112/m)$.

references