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 $\mathcal{N}_{\mathcal{A}}(P112/m)$.