International Tables for Crystallography (2011). Vol. A1, Section 2.1.7, pp. 86–90.

2.1.7. Derivation of the minimal supergroups from the subgroup tables

The minimal supergroups of the space groups, in particular the *translationengleiche* or *t*-supergroups, are not fully listed in the tables. However, with the exception of the *translationengleiche* supergroups of triclinic and monoclinic space groups $\mathcal{H}$, the listing is sufficient to derive the supergroups with the aid of the subgroup tables. For this derivation the coset decomposition $(\mathcal{X} : \mathcal{T}(\mathcal{X}))$ of a space group $\mathcal{X}$ relative to its translation subgroup $\mathcal{T}(\mathcal{X})$ as well as the normalizers $\mathcal{N}(\mathcal{H})$ and $\mathcal{N}(\mathcal{G})$ of the space groups $\mathcal{H}$ and $\mathcal{G}$ play a decisive role. The coset decomposition of a group relative to a subgroup has been defined in Section 1.2.4.2; the coset decomposition of a space group relative to its translation subgroup in Sections 1.2.5.1 and 1.2.5.4. The notions of the affine and the Euclidean normalizer have been introduced in Section 1.2.6.3.

In the next Sections 2.1.7.1 and 2.1.7.2 the minimal *k*-supergroups including the isomorphic supergroups will be derived by inversion of the subgroup data. In Section 2.1.7.3 one minimal *t*-supergroup of each type will be found from the corresponding subgroup data, also by inversion. Starting from this supergroup other minimal *t*-supergroups can be obtained. This procedure is described in Sections 2.1.7.4 and 2.1.7.5.

2.1.7.1. Determination of the non-isomorphic minimal k-supergroups by inverting the subgroup data

All non-isomorphic *klassengleiche* maximal subgroups of a space group $\mathcal{G}$ are listed individually, whereas the infinite number of isomorphic *k*-subgroups of $\mathcal{G}$ are listed essentially by series. Therefore, it is more transparent to deal with the isomorphic supergroups separately (in Section 2.1.7.2). The non-isomorphic *klassengleiche* supergroups are considered here.

The procedure for deriving the *k*-supergroups $\mathcal{G}_j$ of a space group $\mathcal{H}$ is simpler than that for the derivation of the *t*-supergroups, described in Sections 2.1.7.3, 2.1.7.4 and 2.1.7.5. The data for *k*-supergroups of $\mathcal{H}$ are more detailed and, unlike the *t*-supergroups, there is only one *k*-supergroup per entry for the supergroup data of $\mathcal{H}$.

To show this, one considers the coset decomposition of the group $\mathcal{H}$ with respect to the normal subgroup $\mathcal{T}(\mathcal{H})$ of all its translations, *cf.* Section 8.1.6 of *IT* A. The set of cosets with respect to this decomposition forms a group, the factor group $\mathcal{H}/\mathcal{T}(\mathcal{H})$. Each coset, *i.e.* each element of the factor group $\mathcal{H}/\mathcal{T}(\mathcal{H})$, consists of all those elements (symmetry operations) of $\mathcal{H}$ which have the same matrix part in common and differ in their translation parts only.

In a *klassengleiche* supergroup $\mathcal{G} > \mathcal{H}$ the coset decomposition of $\mathcal{H}$ is retained; only the set of translations is increased in $\mathcal{G}$ relative to $\mathcal{H}$, $\mathcal{T}(\mathcal{G}) > \mathcal{T}(\mathcal{H})$. With the additional translations, each coset of $\mathcal{H}$ is extended to a coset of $\mathcal{G}$. The cosets are independent of the chosen coset representatives. Thus, as the coset representatives of $\mathcal{H}$ always belong to the elements of $\mathcal{G}$, the coset representatives of $\mathcal{H}$ can be taken as the coset representatives of $\mathcal{G}$ and the elements of $\mathcal{G}$ are uniquely determined.

It follows that for each maximal *k*-subgroup $\mathcal{H}$ which is listed among the subgroups of $\mathcal{G}$, $\mathcal{G}$ is the only minimal *k*-supergroup for the corresponding extension of the lattice translations (there may be other lattice extensions in addition which result in other supergroups). If different *k*-subgroups $\mathcal{H}_j$ of $\mathcal{G}$ and their lattice extensions are conjugate under the Euclidean normalizer of $\mathcal{G}$, then $\mathcal{G}$ is the common minimal *k*-supergroup of these subgroups $\mathcal{H}_j$. This result is independent of whether the minimal *k*-supergroup $\mathcal{G}$ is isomorphic to the space group $\mathcal{H}$ or not. Therefore, the last paragraph of Section 2.1.7.2 also holds for the non-isomorphic *k*-subgroup pairs of $P2_122$, $P22_12$ and $P222_1$ among the subgroups of $P222$.

Example 2.1.7.1.1

Consider the minimal *k*-supergroups of the space group $P2_12_12$, No. 18. Four entries for 'Additional centring translations' and two for 'Decreased unit cell' are listed in the supergroup data of $\mathcal{H} = P2_12_12$; the missing entry for $\mathbf{c}' = \frac{1}{2}\mathbf{c}$ results in a *k*-supergroup isomorphic to $\mathcal{H}$ and is thus not listed among the supergroup data of $P2_12_12$. The supergroups with 'Additional centring translations' shall be looked at in more detail.

The supergroup $C222$ is obtained directly by adding the *C*-centring to the symmetry operations of $\mathcal{H}$.

Adding the *A*- and *B*-centrings to $\mathcal{H} = P2_12_12$ results in supergroups of the type $C222_1$. For $C222_1$, in the **a** and **b** directions 2 and 2_1 axes alternate, whereas in the **c** direction there are only 2_1 axes. Adding the *A*-centring (0, 1/2, 1/2)+ to $P2_12_12$ results in alternating 2 and 2_1 axes in the directions **b** and **c** but there are only 2_1 axes in the direction of **a**; $A2_122$ is obtained. Adding the *B*-centring (1/2, 0, 1/2)+ to $P2_12_12$ results in alternating 2 and 2_1 axes in the directions **a** and **c** but there are only 2_1 axes in the **b** direction; $B22_12$ is obtained.

These relations can also be derived in another way. Transformation of the relation $P2_122_1 < C222_1$ with its matrix–column pair as listed in the subgroup table of $C222_1$ in Chapter 2.3 results in the relation $P2_12_12 < A2_122$. On the other hand, the relation $P22_12_1 < C222_1$ is transformed by its matrix–column pair to $P2_12_12 < B22_12$.

It is often easy to construct the supergroup from the drawing of the original space group $\mathcal{H}$ in *IT* A by adding the centring vectors or the additional basis vectors. This happens, for example, for the supergroup $I222$, No. 23, where the origin shift by (0, 0, 1/4) is obvious from the comparison of the drawings of $P2_12_12$ and $I222$. This agrees with the data in the subgroup table of $I222$.

The completeness of the data for the minimal *k*-supergroups depends on the completeness of the listed lattice extensions, *i.e.* on the completeness of the listed possible centrings as well as of the possible decreased unit cells of the lattices. These data are well known for the small indices 2, 3 and 4 occurring in these group–subgroup relations.

2.1.7.2. The isomorphic minimal supergroups

It is not necessary to list the isomorphic minimal supergroups, *i.e.* those minimal supergroups $\mathcal{G}$ which belong to the space-group type of $\mathcal{H}$. Therefore, a block 'series of isomorphic minimal supergroups' does not occur among the supergroup data.

The derivation of the isomorphic minimal supergroups $\mathcal{G}$ from the data in the subgroup tables is straightforward. For each index, one looks for the listed isomorphic normal subgroups $\mathcal{H}$ and for the classes of conjugate isomorphic subgroups $\mathcal{H}_q$ in the subgroup table of $\mathcal{G}$. If some of these items are conjugate under the Euclidean normalizer of $\mathcal{G}$, then only one item of this conjugacy class has to be taken into consideration as a representative. For each of these representatives there is one corresponding supergroup of $\mathcal{H}$.

As for the isomorphic maximal subgroups, the indices of the minimal supergroups are p, p^2 or p^3, p prime. However, the large conjugacy classes of isomorphic maximal subgroups always belong to single isomorphic minimal supergroups.

Example 2.1.7.2.1

Consider the p^2 conjugate isomorphic subgroups $\mathcal{H}$ of a space group $P\bar{4}2c$, No. 112, in the series $[p^2]$ $\mathbf{a}' = p\mathbf{a}, \mathbf{b}' = p\mathbf{b}$, prime p fixed. The same supergroup $\mathcal{G}$ belongs to each of these subgroups $\mathcal{H}$. The indices u and v, designating the members of a conjugacy class of subgroups $\mathcal{H}_k < \mathcal{G}$, may have any of their admissible values or may be set to zero. Choosing other values of u and/or v means dealing with the same supergroup $\mathcal{G}$ but transformed by an element of $\mathcal{G}$. Because the parameters u and/or v appear only in the translation parts of the (4×4) symmetry matrices, this may mean a shift of the origin in the description of $\mathcal{G}$. If for practical reasons the origin of $\mathcal{G}$ will be chosen as the origin of $\mathcal{H}_k$, *i.e.* at different points of $\mathcal{G}$ for the different groups $\mathcal{H}_k$, then the (same) group $\mathcal{G}$ is described relative to different origins. These origins are then chosen in different translationally equivalent points of $\mathcal{G}$.

Space groups $\mathcal{H}_j$ which are conjugate under the Euclidean normalizer of the supergroup $\mathcal{G}$ have the supergroup $\mathcal{G}$ in common if they are complemented by the corresponding conjugate sets of translations. For example, both members of each of the subgroup pairs $P222$ of index [2] in the subgroup table of the space group $P222$, No. 16, for $\mathbf{a}' = 2\mathbf{a}$ or $\mathbf{b}' = 2\mathbf{b}$ or $\mathbf{c}' = 2\mathbf{c}$ have their minimal supergroup $\mathcal{G}$ in common because they are conjugate under the Euclidean normalizer $P(1/2, 1/2, 1/2)mmm$.[6] If for some temperature, pressure and composition of a substance $a = b = c$ holds for the lattice parameters of $P222$, $\mathcal{N}_{\mathcal{E}}(\mathcal{H}) = \mathcal{N}_{\mathcal{A}}(\mathcal{H}) = P(1/2, 1/2, 1/2)m\bar{3}m$, *i.e.* the Euclidean normalizer is equal to the affine normalizer, making the three supergroups $\mathcal{G}$ conjugate in the normalizer. Such relations have little importance in practice if the space group describes the symmetry of a substance. This substance has the crystal symmetry $P222$ independent of the accidentally higher lattice symmetry.

2.1.7.3. *Determination of one minimal t-supergroup by inverting the subgroup data*

A proper *translationengleiche* supergroup $\mathcal{G}$ of a space group $\mathcal{H}$ cannot be isomorphic to $\mathcal{H}$ because it belongs to another crystal class. Therefore, it is not necessary to include the word 'non-isomorphic' in the header.

The minimal *t*-supergroups $\mathcal{G}$ of $\mathcal{H}$ have indices i, $1 < i < 5$; only the conventional HM symbol of the supergroup $\mathcal{G}$ together with the index and the space-group number are listed in the supergroup data of the group $\mathcal{H}$. However, in the subgroup data of $\mathcal{G}$ the subgroups $\mathcal{H}_k$ are explicitly listed with their indices, their (nonconventional and) conventional HM symbols, their space-group numbers, their general positions and their transformation matrices $\boldsymbol{P}$ and columns $\boldsymbol{p}$. Suppose the supergroups $\mathcal{G}_j$ are listed on the line 'I Minimal *translationengleiche* supergroups' of the space group $\mathcal{H}$. In order to determine all supergroups $\mathcal{G}_m > \mathcal{H}$, one takes one of the listed supergroups $\mathcal{G}$, say $\mathcal{G}_1$. In the subgroup table of $\mathcal{G}_1$ one finds a subgroup $\mathcal{H}_1 < \mathcal{G}_1$, isomorphic to $\mathcal{H}$ (at least one must exist, otherwise $\mathcal{G}_1$ would not be listed among the minimal supergroups of $\mathcal{H}$). The transformation $(\boldsymbol{P}_1, \boldsymbol{p}_1)$, listed with the subgroup $\mathcal{H}_1$, transforms the symmetry operations of $\mathcal{H}_1$ from the coordinate system of $\mathcal{G}_1$ to the standard coordinate system of $\mathcal{H}_1$. Such transformations are described by equations (2.1.3.8) and (2.1.3.9) in Section 2.1.3.3. The matrix–column pair $(\boldsymbol{P}_1, \boldsymbol{p}_1)$ also transforms the group $\mathcal{G}_1$ from its standard description to that referred to the coordinate system of $\mathcal{H}_1$. This transformed group $\mathcal{G}'_1$ is one supergroup $\mathcal{G}'_1 > \mathcal{H}_1$ from which one can start to derive other supergroups of this type, if there are any, *cf.* Sections 2.1.7.4 and 2.1.7.5. The same procedure has to be applied to any other maximal *t*-subgroup $\mathcal{H}_k < \mathcal{G}_1$ and to the other listed *t*-supergroups $\mathcal{G} > \mathcal{H}$.

The calculations can be verified by viewing the space-group diagrams of the corresponding space groups in *IT*, Volume A.

Example 2.1.7.3.1

Space group $\mathcal{H}_1 = P222$, No.16. In continuation of Example 2.1.6.2.2, one finds no data for the matrix $\boldsymbol{P}$ and the column $\boldsymbol{p}$ listed in the entry for the subgroup $P222$ in the subgroup tables of $Pmmm$, No. 47, $Pnnn$, No. 48, origin choice 1, $Pban$, No. 50, origin choice 1, $P422$, No. 89, $P4_222$, No. 93, $P\bar{4}2m$, No. 111, and $P23$, No. 195. This means $\boldsymbol{P} = \boldsymbol{I}$ and $\boldsymbol{p} = \boldsymbol{o}$. Thus, $P222$ is a subgroup of these space groups and the standard settings agree, *i.e.* the generators of $\mathcal{G}_1$ can be taken directly from those of $\mathcal{H}_1$, adding the last generator of $\mathcal{G}_1$. This is confirmed by the space-group diagrams. Regarding the tetragonal and cubic supergroups, the lattice restrictions for the space group $\mathcal{H}_1$ have to be obeyed, *cf.* Example 2.1.6.2.2.

Only an origin shift but no transformation matrix $\boldsymbol{P}$ is listed in the subgroup tables of the supergroups $Pnnn$ origin choice 2, $\boldsymbol{p} = (1/4, 1/4, 1/4)$; $Pccm$, No. 49, $\boldsymbol{p} = (0, 0, 1/4)$; $Pban$ origin choice 2, $\boldsymbol{p} = (1/4, 1/4, 0)$ and $P\bar{4}2c$, No. 112, $\boldsymbol{p} = (0, 0, 1/4)$. Thus, the r matrix parts of the r non-translational generators of $\mathcal{H}_1$, $r = 2$, are retained, $\boldsymbol{W}'_{1r} = \boldsymbol{W}_{1r}$, and equation (2.1.3.9) is reduced to

$$\boldsymbol{w}' = \boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}, \qquad (2.1.7.1)$$

where $(\boldsymbol{W}'_{1r}, \boldsymbol{w}'_{1r})$ are those (two) generators of $\mathcal{G}_j$ which stem from $\mathcal{H}$. The third generator of $\mathcal{G}_1$, the inversion or rotoinversion, has to be transformed correspondingly.

The column parts w'_{1r} of the $r = 2$ generators 2_z and 2_y of the four space groups $Pnnn$ origin choice 2, $Pccm$, $Pban$ origin choice 2 and $P\bar{4}2c$ are then (normalized to values between $0 \le w_r < 1$) the same as those of the group $\mathcal{H}$, *i.e.* they are generators of supergroups of $\mathcal{H}$. The columns of the inversions are

$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix} \text{ and } \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix},$$

respectively. This describes the position of $\bar{1}$ or $\bar{4}$ relative to the origin of the $P222$ framework in the corresponding space-group diagrams of *IT* A. The coordinates of the inversion centre are half the coefficients of the columns. The supergroup $Pnnn$, origin choice 2, is the same as $Pnnn$, origin choice 1; only the setting is different. The space-group diagrams in *IT* A display the agreement of the frameworks of the rotation axes in $\mathcal{H}_1$ and $\mathcal{G}_j$. The supergroup $P\bar{4}2c$ is a space group only if the corresponding lattice relations for $\mathcal{H}_1$ are fulfilled.

Example 2.1.7.3.2

Continued from Example 2.1.6.2.1. For $\mathcal{H}_1 = P2_12_12$, No. 18, and its orthorhombic types of supergroups, the places for the matrix $\boldsymbol{P}$ and the column $\boldsymbol{p}$ under $P2_12_12$ in the subgroup data of $Pbam$, No. 55, and $Pmmn$, No. 59, origin choice 1 are empty. In analogy to the preceding example, $P2_12_12$ is a subgroup of these space groups in the standard setting.

[6] Here we make use of the notation $L(U, V, W)\mathcal{P}_{\mathcal{N}}$ for the HM symbol of the normalizer $\mathcal{N}$. L is the lattice letter, $\mathcal{P}_{\mathcal{N}}$ is the point-group part of the HM symbol of N and U, V, W determine the basis vectors $\mathbf{a}'_i$ of $\mathcal{N}$ referred to the basis vectors $\mathbf{a}_k$ of the lattice of $\mathcal{G}$: $\mathbf{a}' = U\mathbf{a}$, $\mathbf{b}' = V\mathbf{b}$, $\mathbf{c}' = W\mathbf{c}$. Such nomenclature can be used conveniently if the lattice relations are simple, as they are in these examples.

The equation $\boldsymbol{P} = \boldsymbol{I}$ also holds for the subgroup data of *Pccn*, No. 56, *Pnnm*, No. 58, and *Pmmn*, No. 59, origin choice 2, but $\boldsymbol{p} = (1/4, 1/4, 1/4)$, $\boldsymbol{p} = (0, 0, 1/4)$ and $\boldsymbol{p} = (1/4, 1/4, 0)$, respectively. Thus, the reduced equation (2.1.7.1) holds for the generators of $\mathcal{H}_1$ and the inversion.

Again the column parts of the generators 2_z and 2_y of the groups *Pccn*, *Pnnm* and *Pmmn*, origin choice 2, are the same as those of the group $\mathcal{H}_1$, if normalized to values between $0 \leq w_r < 1$, *i.e.* they are generators of supergroups of $\mathcal{H}$. The columns of the inversions are

$$\begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \frac{1}{2} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{2} \end{pmatrix} \text{ and } \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ 0 \end{pmatrix},$$

respectively. As in the previous example, this describes the position of $\overline{1}$ relative to the origin of the $P2_12_12$ framework in the corresponding space-group diagrams of *IT* A. The coordinates of the inversion centre are half the coefficients of the columns. The supergroup *Pmmn*, origin choice 2, is the same as *Pmmn*, origin choice 1; only the setting is different. Again the space-group diagrams in *IT* A display the agreement of the frameworks of rotation and screw rotation axes in $\mathcal{H}_1$ and $\mathcal{G}_j$.

Concerning *Pbcm*, No. 57, in its subgroup table one finds the line of $P2_12_12$ with the representatives 1, 2, 3, 4 of the general position and

$$\boldsymbol{I} \neq \boldsymbol{P} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix}; \quad \boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{4} \\ 0 \end{pmatrix}.$$

The representative 1 is described by $(\boldsymbol{W}, \boldsymbol{w}) = (\boldsymbol{I}, \boldsymbol{o})$; it is invariant under the transformation. Using equations (2.1.3.8) and (2.1.3.9) and the above values for $\boldsymbol{P}$ and $\boldsymbol{p}$ for the representatives 2, 3 and 4 of the subgroup $P22_12_1$, these will be transformed to the matrix–column pairs of 2_z, 2_{1y} and 2_{1x} in the standard form of $P2_12_12$. The inversion is transformed to an inversion with the column (1/2, 0, 0), *i.e.* the centre of inversion has the coordinates (1/4, 0, 0). Combining the (screw) rotations with the inversion, one obtains the reflection and the glide reflections, referred to the coordinate system of $P2_12_12$. With the application of the formulae of *IT* A, Chapter 11.2, one finds b_x at $x = 1/4$, m_y at $y = 1/4$ and a_z at $z = 0$. This results in the HM symbol $P\,2_1/b\,2_1/m\,2/a = Pbma$ for this supergroup; see also the diagram in *IT* A.

For *Pbcn*,

$$\boldsymbol{P} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}; \quad \boldsymbol{p} = \begin{pmatrix} 0 \\ \frac{1}{4} \\ \frac{1}{4} \end{pmatrix}.$$

A procedure analogous to that applied for *Pbcm* yields for *Pbcn*, No. 60, the standard setting of $P2_12_12$ and the inversion centre at (1/4, 0, 1/4). Again by combination of the (screw) rotations with the inversion one gets n_x at $x = 0$, c_y at $y = 1/4$ and a_z at $z = 1/4$. The nonconventional HM symbol of this supergroup of $P2_12_12$ is thus *Pnca* or $P\,2_1/n\,2_1/c\,2/a$.

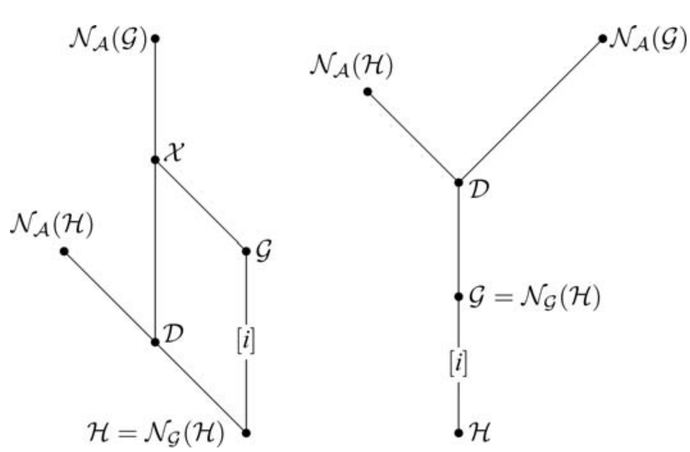

Fig. 2.1.7.1. In the left-hand diagram, there are i conjugate subgroups $\mathcal{H}_k < \mathcal{G}$ of $\mathcal{G}$ if $[i]$ is the index of $\mathcal{H}$ in $\mathcal{G}$; in the right-hand diagram, $\mathcal{H} \triangleleft \mathcal{G}$ is a normal subgroup of $\mathcal{G}$. The group $\mathcal{D} = \mathcal{N}(\mathcal{H}) \cap \mathcal{N}(\mathcal{G})$ is the intersection of the normalizers $\mathcal{N}(\mathcal{H})$ and $\mathcal{N}(\mathcal{G})$. The group $\mathcal{X}$ is the group generated by the groups $\mathcal{D}$ and $\mathcal{G}$.

2.1.7.4. *Derivation of further minimal t-supergroups by using normalizers*

Up to now one minimal *t*-supergroup $\mathcal{G} > \mathcal{H}$ per entry using the tables of maximal subgroups has been found, see Examples 2.1.7.3.1 of $P222$ and 2.1.7.3.2 of $P2_12_12$.

The question arises as to whether this list is complete or whether further *t*-supergroups $\mathcal{G}_j > \mathcal{H}$ exist which belong to the space-group type of $\mathcal{G}$ and are represented by the same entry of the supergroup data. If these supergroups belong to the same space-group type then they are isomorphic and are thus conjugate under the group $\mathcal{A}$ of all affine mappings according to the theorem of Bieberbach. Then there must be an affine mapping $\mathsf{a} \in \mathcal{A}$ such that $\mathsf{a}^{-1}\mathcal{G}\mathsf{a} = \mathcal{G}_j$. To find these mappings, one makes use of the affine normalizers $\mathcal{N}_\mathcal{A}(\mathcal{G})$ and $\mathcal{N}_\mathcal{A}(\mathcal{H})$ and considers their intersection $\mathcal{D} = \mathcal{N}_\mathcal{A}(\mathcal{G}) \cap \mathcal{N}_\mathcal{A}(\mathcal{H})$ (Koch, 1984). One of the two diagrams of Fig. 2.1.7.1 will describe the situation because $\mathcal{G}$ is a minimal supergroup of $\mathcal{H}$. Let $\mathcal{N}_\mathcal{G}(\mathcal{H})$ be the normalizer of the group $\mathcal{H}$ in the group $\mathcal{G}$, *i.e.* the set of all elements of $\mathcal{G}$ which leave $\mathcal{H}$ invariant. Whereas in general $\mathcal{G} \geq \mathcal{N}_\mathcal{G}(\mathcal{H}) \geq \mathcal{H}$ holds, for a minimal supergroup $\mathcal{G}$ either $\mathcal{G} = \mathcal{N}_\mathcal{G}(\mathcal{H})$ (right diagram) or $\mathcal{N}_\mathcal{G}(\mathcal{H}) = \mathcal{H}$ (left diagram) holds.

Lemma 2.1.7.4.1. Let $\mathcal{G}_1 > \mathcal{H}_1$ be a minimal *t*-supergroup of a space group $\mathcal{H}_1$, let $\mathcal{N}(\mathcal{G}_1)$ and $\mathcal{N}(\mathcal{H}_1)$ be their affine normalizers, and $\mathcal{D} = \mathcal{N}(\mathcal{G}_1) \cap \mathcal{N}(\mathcal{H}_1)$ is the intersection of these normalizers. Then i_n minimal supergroups $\mathcal{G}_j > \mathcal{H}_1$ exist, isomorphic to $\mathcal{G}_1$, where $i_n = |\mathcal{N}(\mathcal{H}_1) : \mathcal{D}|$ is the index of $\mathcal{D}$ in $\mathcal{N}(\mathcal{H}_1)$. If i_n is finite, then the representatives a_m, $m = 1, \ldots, i_n$ of the cosets in the decomposition of $\mathcal{N}(\mathcal{H}_1) : \mathcal{D}$ transform $\mathcal{G}_1$ to $\mathcal{G}_m$. □

The lemma is proven by coset decomposition of $\mathcal{N}(\mathcal{H}_1)$ relative to $\mathcal{D}$.

If $\mathcal{H} < \mathcal{G}$ is a *t*-subgroup, for the translation groups $\mathcal{T}(\mathcal{N}(\mathcal{G}))$ and $\mathcal{T}(\mathcal{N}(\mathcal{H}))$ of the normalizers $\mathcal{T}(\mathcal{N}(\mathcal{G})) \leq \mathcal{T}(\mathcal{N}(\mathcal{H}))$ always holds (Wondratschek & Aroyo, 2001). Therefore, for *t*-supergroups there may be translations of $\mathcal{T}(\mathcal{N}(\mathcal{H}))$ which transform the space group $\mathcal{G} > \mathcal{H}$ into another one, $\mathcal{G}_j > \mathcal{H}$. Transformation of $\mathcal{G}$ and $\mathcal{H}$ by an element of $\mathcal{D}$ will map $\mathcal{G}$ as well as $\mathcal{H}$ onto itself. Transformation of $\mathcal{G}$ and $\mathcal{H}$ by an element $(\boldsymbol{W}, \boldsymbol{w}) \in \mathcal{N}(\mathcal{H})$ but $(\boldsymbol{W}, \boldsymbol{w}) \notin \mathcal{D}$ will map $\mathcal{H}$ onto itself but will map the supergroup $\mathcal{G}$ onto another supergroup $\mathcal{G}_j$.

For applications it is transparent to split the index i_n into the index i_L of the translation lattices and i_P of the point-group parts, $i_n = i_L \times i_P$.

For the application of Lemma 2.1.7.4.1, the kind of the normalizers $\mathcal{N}_\mathcal{A}(\mathcal{H})$ and $\mathcal{N}_\mathcal{A}(\mathcal{G})$ and in particular the index $i_n =$

$i_L \times i_P$ are decisive. The affine normalizers of the plane groups and space groups are listed in the tables of Chapter 15.2 of *IT* A. Their point-group parts are:

(1) infinite groups of integral matrices $\boldsymbol{W}$ with $\det(\boldsymbol{W}) = \pm 1$ for triclinic and monoclinic space groups;
(2) (finite) crystallographic point groups or affine groups isomorphic to crystallographic point groups for orthorhombic, tetragonal, trigonal, hexagonal and cubic space groups.

The translation parts of the normalizers are continuous or partly continuous groups for polar space groups and lattices for non-polar space groups.

The following cases may be distinguished in the use of Lemma 2.1.7.4.1:

(1) Both $\mathcal{H}$ and $\mathcal{G}$ are triclinic: only for the pair $P1$–$P\overline{1}$ can $\mathcal{G}$ be a minimal *translationengleiche* supergroup of $\mathcal{H}$, *cf.* Example 2.1.6.1.2. The point-group index $i_P = 1$, the translation index i_L is uncountably infinite. Such translation indices can be represented by regions of the unit cell for the possible coordinates of the origin, here $0 \le x_0, y_0, z_0 < 1/2$. In any case, continuous ranges of parameters due to infinite indices i_L do not cause difficulties.
(2) $\mathcal{H}$ is triclinic, $\mathcal{G}$ is monoclinic: index $i_P = \infty$. Such relations cannot be treated by the procedure described earlier in this section; monoclinic minimal *t*-supergroups of triclinic space groups are not accessible by the procedure using Lemma 2.1.7.4.1. Other approved procedures are not known to the authors; they are being developed and tested but are not yet available for this edition of *IT* A1.
(3) Both $\mathcal{H}$ and $\mathcal{G}$ are monoclinic: for minimal *t*-supergroups $\mathcal{G}$, inversions $\overline{1}$ have to be added to the symmetry of the space group $\mathcal{H}$. The procedure using Lemma 2.1.7.4.1 needs to be worked out because of the infinity of the linear parts of the normalizers. Another procedure is being tested at the time of writing of this guide. Both methods and their results cannot be presented here.
(4) $\mathcal{H}$ is triclinic or monoclinic, $\mathcal{G}$ is orthorhombic, trigonal or hexagonal: as in (2), $i_P = \infty$ and Lemma 2.1.7.4.1 cannot be applied. No solution can be offered at present.
(5) Both $\mathcal{H}$ and $\mathcal{G}$ are orthorhombic or higher symmetry: the finite index $i_P = q$ allows the application of Lemma 2.1.7.4.1. The index $i_L = r$ may be either finite or $i_L = \infty$, there are either r translationally equivalent supergroups of the same space-group type or an infinite number, described by a continuous region of parameters, *e.g.* of coordinates of the origin.

    One has to take care to select from these supergroups those which are space groups and those which are affine groups isomorphic to space groups (Koch, 1984).

The application of Lemma 2.1.7.4.1 will be described by three examples. Example 2.1.7.4.2 is the continuation of Example 2.1.7.3.1, Example 2.1.7.4.3 is the continuation of Example 2.1.7.3.2 and Example 2.1.7.4.4 deals with the minimal *t*-supergroups of space group $\mathcal{H} = Pmm2$, No. 25.

Example 2.1.7.4.2

Application of the normalizers to the minimal *t*-supergroups of $\mathcal{H} = P222$, No. 16; continuation of Example 2.1.7.3.1.

The affine normalizer $\mathcal{N}_{\mathcal{A}}(P222) = P(1/2, 1/2, 1/2)m\overline{3}m$, *cf.* *IT* A, Table 15.2.1.3. [In the header of this table, only the words *Euclidean normalizer* are found. It is mentioned in Section 15.2.2, *Affine normalizers of plane and space groups*, that the type of affine normalizers corresponds to the type of the highest-symmetry Euclidean normalizers belonging to that space (plane)-group type.] The affine normalizers of the supergroups *Pmmm*, No. 47, and *Pnnn*, No. 48, are the same as that of *P*222. The index $i_n = 1 = 1 \times 1$, there is only one supergroup with the same origin (origin choice 1 for *Pnnn*) of each of these types.

The affine normalizers of $\mathcal{G} = Pccm$, No. 49, and $\mathcal{G} = Pban$, No. 50, are $\mathcal{N}_{\mathcal{A}}(\mathcal{G}) = P(1/2, 1/2, 1/2)4/mmm = \mathcal{D}$ such that the index $i_n = 3 = 1 \times 3$. Coset decomposition of $\mathcal{N}_{\mathcal{A}}(P222)$ relative to $\mathcal{D}$ reveals the coset representatives 3_{111} and 3^{-1}_{111} so that from *Pccm* (origin shift $0, 0, 1/4$) the space groups (in unconventional HM symbols) *Pmaa* and *Pbmb* are generated with the origin shifts $1/4, 0, 0$ and $0, 1/4, 0$; from *Pban* (no origin shift for origin choice 1) one obtains *Pncb* and *Pcna* with no origin shifts. To all these orthorhombic supergroups there are no translationally equivalent supergroups.

The tetragonal supergroups *P*422, No. 89, $P4_222$, No. 93, $P\overline{4}2m$, No. 111, and $P\overline{4}2c$, No. 112, are space groups if one of the conditions $a = b$ or $b = c$ or $c = a$ holds for the lattice parameters, with the tetragonal axes perpendicular to the tetragonal plane. Otherwise the tetragonal supergroups are affine groups which are only isomorphic to space groups. They all have affine normalizer $C(1, 1, 1/2)4/mmm$, such that the index $i_n = 6 = 2 \times 3$. The supergroups *P*422 form three pairs; one pair with its tetragonal axes parallel to **c** and with the origins either coinciding with that of *P*222 or shifted by $\frac{1}{2}\mathbf{a}$ (or equivalently by $\frac{1}{2}\mathbf{b}$). The other two pairs point with their tetragonal axes parallel to **a** and to **b**, with one origin at the origin of *P*222 and the other origin shifted by $\frac{1}{2}\mathbf{b}$ (or equivalently **c**) and $\frac{1}{2}\mathbf{a}$ (or equivalently **c**). The same holds for the six supergroups of type $P4_222$ and for the six supergroups of type $P\overline{4}2m$. The six supergroups of type $P\overline{4}2c$ again form three pairs with their tetragonal axes along **c** or **a** or **b** but their origins are shifted against that of *P*222 by 1/4 along the tetragonal axes because of the entry $\boldsymbol{p} = 0, 0, 1/4$ in the subgroup table of $P\overline{4}2c$, see also Example 2.1.7.3.1.

For the supergroups with the symbol *P*23, No. 195, which is a space group if $a = b = c$, the affine normalizer is $\mathcal{N}_{\mathcal{A}}(P23) = I(1, 1, 1)m\overline{3}m$ with point-group index $i_P = 1$ but translation index $i_L = 4$. Thus, there are four such (translationally equivalent) supergroups with their origins at $0, 0, 0$; $1/2, 0, 0$; $0, 1/2, 0$; and $0, 0, 1/2$.

Example 2.1.7.4.3

Application of the normalizers to the *t*-supergroups of $\mathcal{H} = P2_12_12$, No. 18.

The normalizer $\mathcal{N}(P2_12_12) = P(1/2, 1/2, 1/2)4/mmm$ is the same as those for the minimal *t*-supergroups *Pbam*, No. 55, *Pccn*, No. 56, *Pnnm*, No. 58, and *Pmmn*, No. 59. There is one supergroup for each of these types with the origin shifts $0, 0, 0$; $1/4, 1/4, 1/4$; $0, 0, 1/4$; and $0, 0, 0$ (origin choice 1), respectively, according to the $\boldsymbol{p}$ values listed in the subgroup tables of the supergroups. This can also be concluded from the space-group diagrams of *IT* A.

The listed HM symbols *Pbcm*, No. 57, and *Pbcn*, No. 60, do not refer to supergroups of $P2_12_12$, but *Pbma* and *Pnca* do. This can be seen either from the full HM symbols, *cf.* Example 2.1.6.2.1, or by applying the $(\boldsymbol{P}, \boldsymbol{p})$ data of the supergroups for the subgroup $P2_12_12$, from which the origin shifts may also be taken, *cf.* Example 2.1.7.3.2. Both supergroups have normalizer $\mathcal{N}_{\mathcal{A}} = P(1/2, 1/2, 1/2)mmm$ with index $i_n = 2 = 1 \times 2$. There are two supergroups of each type, the second one, *Pmab* and *Pcnb*, generated from that already listed by the fourfold rotation in the normalizer of $P2_12_12$.

The tetragonal supergroups (they are space groups if for their lattice parameters the equation $a = b$ holds) $P42_12$, No. 90, $P4_22_12$, No. 94, $P\bar{4}2_1m$, No. 113, and $P\bar{4}2_1c$, No. 114, all have normalizer $C(1,1,1/2)4/mmm$, such that the index $i_n = 2 = 2 \times 1$. There are two translationally equivalent supergroups in each case, one with origin at 0, 0, 0; 0, 0, 1/4; 0, 0, 0; and 0, 0, 1/4, respectively, the other shifted against the first one by the translation $t(1/2, 0, 0)$ or (equivalently) by $t(0, 1/2, 0)$.

The procedure just described works fine if the symmetry of the group $\mathcal{H}$ is higher than triclinic or monoclinic. The following example shows that an infinite lattice index is acceptable.

Example 2.1.7.4.4

Application of the normalizers to the *t*-supergroups of $\mathcal{H} = Pmm2$, No. 25.

The affine normalizer is $\mathcal{N}_{\mathcal{A}}(Pmm2) = P(1/2, 1/2, \varepsilon)4/mmm$.

The list of *t*-supergroups of *Pmm*2 starts with *Pmmm*, No. 47. The affine normalizer $\mathcal{N}_{\mathcal{A}}(Pmmm) = P(1/2, 1/2, 1/2)m\bar{3}m$; its point group $m\bar{3}m$ is a supergroup of the point group $4/mmm$ of $\mathcal{N}_{\mathcal{A}}(Pmm2)$ such that the intersection of the point groups is $4/mmm$ and $i_P = 1$. The index $i_L = \infty$, leading to a continuous sequence of supergroups with origins at $0, 0, z_0$; $0 \le z_0 < 1/2$.

The *t*-supergroup *Pmma*, No. 51, follows. $\mathcal{N}_{\mathcal{A}}(Pmma) = P(1/2, 1/2, 1/2)Pmmm$ such that $\mathcal{D} = P(1/2, 1/2, 1/2)Pmmm$ with $i_P = 2$ and $i_L = \infty$. There is a continuous set of supergroups *Pmma*. Because of the origin shift $\boldsymbol{p} = 1/4, 0, 0$ for *Pmm*2 in the subgroup table of *Pmma*, the origins of these supergroups are placed at $1/4, 0, z_0$ with $0 \le z_0 < 1/2$. Because $i_P = 2$, there is a second set of supergroups, rotated by 90° relative to the first set, such that its (unconventional) HM symbol is *Pmmb* and its origins are placed at $0, 1/4, z_0$, $0 \le z_0 < 1/2$.

The normalizer $\mathcal{N}_{\mathcal{A}} = P(1/2, 1/2, 1/2)4/mmm$ of the last orthorhombic *t*-supergroup *Pmmn*, No. 59, has the same point-group part as that of *Pmm*2 and its translation part differs only in $z = 1/2$ instead of $z = \varepsilon$. There are no transformation data for *Pmm*2 in the subgroup table of *Pmmn*, origin choice 1. There is one set of supergroups *Pmmn* with the origins at $0, 0, z_0$ for $0 \le z_0 < 1/2$.

The tetragonal minimal supergroups *P*4*mm*, No. 99, $P4_2mc$, No. 105, and $P\bar{4}m2$, No. 115, are space groups if $a = b$ holds for the lattice parameters of *Pmm*2. The affine and Euclidean normalizers of tetragonal space groups are the same.

The normalizers $C(1, 1, \varepsilon)4/mmm$ of *P*4*mm* and $P4_2mc$ differ from $\mathcal{N}_{\mathcal{A}}(Pmm2)$ only in the translation part such that $i_P = 1$ and $i_L = 2$ and the additional translations of $\mathcal{N}_{\mathcal{A}}(Pmm2)$ relative to $\mathcal{D}$ may be represented by $t(1/2, 0, 0)$. There are two supergroups each: *P*4*mm* and $P4_2mc$, with their origins at 0, 0, 0 and 1/2, 0, 0 of *Pmm*2.

Finally, the normalizer $\mathcal{N}(P\bar{4}m2) = C(1, 1, 1/2)P4/mmm$ and there are two continuous sets of supergroups $P\bar{4}m2$ with their origins at $0, 0, z_0$ and $1/2, 0, z_0$; $0 \le z_0 < 1/2$.

2.1.7.5. Derivation of the remaining minimal t-supergroups

By the procedure discussed in Section 2.1.7.4, from a supergroup $\mathcal{G} > \mathcal{H}$ other supergroups $\mathcal{G}_j > \mathcal{H}$ could be found which are isomorphic to $\mathcal{G}$ with the same index. The question arises as to whether there exist further minimal supergroups $\mathcal{G}_q > \mathcal{H}$ isomorphic to $\mathcal{G}$ and of the same index which can not be obtained by consideration of the normalizers.

Suppose $\mathcal{G}_s > \mathcal{H}$ is such a supergroup. According to the theorem of Bieberbach for space groups, isomorphism and affine equivalence result in the same classification of the space groups, *cf.* Section 8.2.2 of *IT* A. Therefore, there exists an affine mapping $\mathsf{a}_s \in \mathcal{A}$ in the group $\mathcal{A}$ of all affine mappings which transforms $\mathcal{G}$ onto the space group $\mathcal{G}_s = \mathsf{a}_s^{-1}\,\mathcal{G}\,\mathsf{a}_s$ and does not belong to $\mathcal{N}_{\mathcal{A}}(\mathcal{H})$, $\mathsf{a}_s \notin \mathcal{N}_{\mathcal{A}}(\mathcal{H})$. Let $\mathcal{H}_s = \mathsf{a}_s\,\mathcal{H}\,\mathsf{a}_s^{-1}$ be obtained from $\mathcal{H}$ by the inverse of the transformation which transforms $\mathcal{G}$ to $\mathcal{G}_s$. Then the group $\mathcal{H}_s$ is a subgroup of $\mathcal{G}$ if and only if $\mathcal{H}$ is a subgroup of $\mathcal{G}_s$. Therefore, if the space group $\mathcal{G}$ has a subgroup $\mathcal{H}_s < \mathcal{G}$ in addition to $\mathcal{H} < \mathcal{G}$, then the space group $\mathcal{H}$ has an additional supergroup $\mathcal{G}_s > \mathcal{H}$ which can be found using the transformation of $\mathcal{H}$ to $\mathcal{H}_s$. This transformation is effective only if it does not belong to the normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$, otherwise it would transform the space group $\mathcal{G}$ onto itself. Therefore, only those subgroups $\mathcal{H}_s < \mathcal{G}$ have to be taken into consideration which are not conjugate to $\mathcal{H}$ under the normalizer $\mathcal{N}_{\mathcal{A}}(\mathcal{G})$.

An example of the application of this procedure is given in Section 1.7.1 and Example 1.7.3.2.2. It refers to minimal *k*-supergroups; an example for minimal *t*-subgroups is not known to the authors.

In Sections 2.1.7.4 and 2.1.7.5 only minimal *t*-supergroups are dealt with. The same considerations can be applied to minimal *k*-supergroups with corresponding results. It was not necessary to mention the minimal *k*-supergroups here, as because of the more detailed data in the tables of this volume, the simpler procedure of Sections 2.1.7.1 and 2.1.7.2 could be used to determine the minimal *k*-supergroups.

2.1.8. The subgroup graphs

2.1.8.1. General remarks

The group–subgroup relations between the space groups may also be described by graphs. This way is chosen in Chapters 2.4 and 2.5. Graphs for the group–subgroup relations between crystallographic point groups have been published, for example, in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and in *IT* A (2005), Figs. 10.1.3.2 and 10.1.4.3. Three kinds of graphs for subgroups of space groups have been constructed and can be found in the literature:

(1) Graphs for *t*-subgroups, such as the graphs of Ascher (1968).
(2) Graphs for *k*-subgroups, such as the graphs for cubic space groups of Neubüser & Wondratschek (1966).
(3) Mixed graphs, combining *t*- and *k*-subgroups. These are used, for example, when relations between existing or suspected crystal structures are to be displayed. Examples are the 'family trees' after Bärnighausen (1980), as shown in Chapter 1.6, now called *Bärnighausen trees*.

A complete collection of graphs of the first two kinds is presented in this volume: in Chapter 2.4 those displaying the *translationengleiche* or *t*-subgroup relations and in Chapter 2.5 those for the *klassengleiche* or *k*-subgroup relations. Neither type of graph is restricted to maximal subgroups but both contain *t*- or *k*-subgroups of higher indices, with the exception of isomorphic subgroups, *cf.* Section 2.1.8.3 below.

The group–subgroup relations are direct relations between the space groups themselves, not between their types. However, each such relation is valid for a pair of space groups, one from each of the types, and for each space group of a given type there exists a corresponding relation. In this sense, one can speak of a

references