

2. MAXIMAL SUBGROUPS OF THE PLANE GROUPS AND SPACE GROUPS

2.1.5.4. Generators

The generators of the p (or p^2 or p^3) conjugate isomorphic subgroups \mathcal{H} are obtained from those of \mathcal{G} by adding translational components. These components are determined by the parameters p (or q and r , if relevant) and u (and v and w , if relevant).

Example 2.1.5.4.1.

Space group $P2_13$, No. 198.

In the series defined by the lattice relations $p\mathbf{a}$, $p\mathbf{b}$, $p\mathbf{c}$ and the origin shift u , v , w there exist exactly p^3 conjugate subgroups for each value of p . The generators of each subgroup are defined by the parameter p and the triplet u , v , w in combination with the generators (2), (3) and (5) of \mathcal{G} . Consider the subgroup characterized by the basis $7\mathbf{a}$, $7\mathbf{b}$, $7\mathbf{c}$ and by the origin shift $u = 3$, $v = 4$, $w = 6$. One obtains from the generator (2) $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ of \mathcal{G} the corresponding generator of \mathcal{H} by adding the translation vector $(\frac{p}{2} - \frac{1}{2} + 2u)\mathbf{a} + 2v\mathbf{b} + (\frac{p}{2} - \frac{1}{2})\mathbf{c}$ to the translation vector $\frac{1}{2}\mathbf{a} + \frac{1}{2}\mathbf{c}$ of the generator (2) of \mathcal{G} and obtains $\frac{19}{2}\mathbf{a} + 8\mathbf{b} + \frac{7}{2}\mathbf{c}$, so that this generator of \mathcal{H} is written $\bar{x} + \frac{19}{2}, \bar{y} + 8, z + \frac{7}{2}$.

2.1.5.5. Special series

For most space groups, there is only one description of their series of the isomorphic subgroups. However, if a space group is described twice in *IT A*, then there are also two different descriptions of these series. This happens for monoclinic space groups with the settings unique axis b and unique axis c , for some orthorhombic, tetragonal and cubic space groups with origin choice 1 and origin choice 2 and for trigonal space groups with rhombohedral lattices with hexagonal axes and rhombohedral axes.

2.1.5.5.1. Monoclinic space groups

In the monoclinic space groups, the series in the listings ‘unique axis b ’ and ‘unique axis c ’ are closely related by a simple cyclic permutation of the axes a , b and c , see *IT A*, Section 2.2.16.

2.1.5.5.2. Trigonal space groups with rhombohedral lattice

In trigonal space groups with rhombohedral lattices, the series with hexagonal axes and with rhombohedral axes appear to be rather different. However, the ‘rhombohedral’ series are the exact transcript of the ‘hexagonal’ series by the same transformation formulae as are used for the different monoclinic settings. However, the transformation matrices \mathbf{P} and \mathbf{P}^{-1} in Part 5 of *IT A* are more complicated in this case.

Example 2.1.5.5.1.

Space group $R\bar{3}$, No. 148. The second series is described with hexagonal axes by the basis transformation \mathbf{a} , \mathbf{b} , $p\mathbf{c}$, i.e. $\mathbf{a}'_{\text{hex}} = \mathbf{a}_{\text{hex}}$, $\mathbf{b}'_{\text{hex}} = \mathbf{b}_{\text{hex}}$, $\mathbf{c}'_{\text{hex}} = p\mathbf{c}_{\text{hex}}$, and the origin shift $0, 0, u$. We discuss the basis transformation first. It can be written

$$(\mathbf{a}'_{\text{hex}})^T = (\mathbf{a}_{\text{hex}})^T \mathbf{X} \quad (2.1.5.1)$$

in analogy to Part 5, *IT A*. Here $(\mathbf{a}_{\text{hex}})^T$ is the row of basis vectors of the conventional hexagonal basis. The matrix \mathbf{X} is defined by

$$\mathbf{X} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & p \end{pmatrix}.$$

With rhombohedral axes, equation (2.1.5.1) would be written

$$(\mathbf{a}'_{\text{rh}})^T = (\mathbf{a}_{\text{rh}})^T \mathbf{Y}, \quad (2.1.5.2)$$

with the matrix \mathbf{Y} to be determined.

The transformation from hexagonal to rhombohedral axes is described by

$$(\mathbf{a}_{\text{rh}})^T = (\mathbf{a}_{\text{hex}})^T \mathbf{P}^{-1}, \quad (2.1.5.3)$$

where the matrices

$$\mathbf{P}^{-1} = \begin{pmatrix} \frac{2}{3} & -\frac{1}{3} & -\frac{1}{3} \\ \frac{1}{3} & \frac{1}{3} & -\frac{2}{3} \\ \frac{1}{3} & \frac{1}{3} & \frac{1}{3} \end{pmatrix} \text{ and } \mathbf{P} = \begin{pmatrix} 1 & 0 & 1 \\ \bar{1} & 1 & 1 \\ 0 & \bar{1} & 1 \end{pmatrix}$$

are listed in *IT A*, Table 5.1.3.1, see also Figs. 5.1.3.6 (a) and (c) in *IT A*.

Applying equations (2.1.5.3), (2.1.5.1) and (2.1.5.2), one gets

$$(\mathbf{a}'_{\text{rh}})^T = (\mathbf{a}'_{\text{hex}})^T \mathbf{P}^{-1} = (\mathbf{a}_{\text{hex}})^T \mathbf{X} \mathbf{P}^{-1} = (\mathbf{a}_{\text{rh}})^T \mathbf{Y} = (\mathbf{a}_{\text{hex}})^T \mathbf{P}^{-1} \mathbf{Y}. \quad (2.1.5.4)$$

From equation (2.1.5.4) it follows that

$$\mathbf{X} \mathbf{P}^{-1} = \mathbf{P}^{-1} \mathbf{Y} \text{ or } \mathbf{Y} = \mathbf{P} \mathbf{X} \mathbf{P}^{-1}. \quad (2.1.5.5)$$

One obtains \mathbf{Y} from equation (2.1.5.5) by matrix multiplication,

$$\mathbf{Y} = \begin{pmatrix} \frac{p+2}{3} & \frac{p-1}{3} & \frac{p-1}{3} \\ \frac{p-1}{3} & \frac{p+2}{3} & \frac{p-1}{3} \\ \frac{p-1}{3} & \frac{p-1}{3} & \frac{p+2}{3} \end{pmatrix},$$

and from \mathbf{Y} for the bases of the subgroups with rhombohedral axes

$$\begin{aligned} \mathbf{a}'_{\text{rh}} &= \frac{1}{3}[(p+2)\mathbf{a}_{\text{rh}} + (p-1)\mathbf{b}_{\text{rh}} + (p-1)\mathbf{c}_{\text{rh}}], \\ \mathbf{b}'_{\text{rh}} &= \frac{1}{3}[(p-1)\mathbf{a}_{\text{rh}} + (p+2)\mathbf{b}_{\text{rh}} + (p-1)\mathbf{c}_{\text{rh}}], \\ \mathbf{c}'_{\text{rh}} &= \frac{1}{3}[(p-1)\mathbf{a}_{\text{rh}} + (p-1)\mathbf{b}_{\text{rh}} + (p+2)\mathbf{c}_{\text{rh}}]. \end{aligned}$$

The column of the origin shift $\mathbf{u}_{\text{hex}} = 0, 0, u$ in hexagonal axes must be transformed by $\mathbf{u}_{\text{rh}} = \mathbf{P} \mathbf{u}_{\text{hex}}$. The result is the column $\mathbf{u}_{\text{rh}} = u, u, u$ in rhombohedral axes.

2.1.5.5.3. Space groups with two origin choices

Space groups with two origin choices are always described in the same basis, but origin 1 is shifted relative to origin 2 by the shift vector \mathbf{s} . For most space groups with two origins, the appearance of the two series related by the origin shift is similar; there are only differences in the generators.

Example 2.1.5.5.2.

Consider the space group $Pnnn$, No. 48, in both origin choices and the corresponding series defined by $p\mathbf{a}$, \mathbf{b} , \mathbf{c} and $u, 0, 0$. In origin choice 1, the generator (5) of \mathcal{G} is described by the ‘coordinates’ $\bar{x} + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z} + \frac{1}{2}$. The translation part $(\frac{p}{2} - \frac{1}{2})\mathbf{a}$ of the third generator of \mathcal{H} stems from the term $\frac{1}{2}$ in the first ‘coordinate’ of the generator (5) of \mathcal{G} . Because $(\frac{p}{2} - \frac{1}{2})\mathbf{a}$ must be a translation vector of \mathcal{G} , p is odd. Such a translation part is not found in the generators (2) and (3) of \mathcal{H} because the term $\frac{1}{2}$ does not appear in the ‘coordinates’ of the corresponding generators of \mathcal{G} .

The situation is inverted in the description for origin choice 2. The translation term $(\frac{p}{2} - \frac{1}{2})\mathbf{a}$ appears in the first and second generator of \mathcal{H} and not in the third one because the term $\frac{1}{2}$

occurs in the first ‘coordinate’ of the generators (2) and (3) of \mathcal{G} but not in the generator (5).

The term $2u$ appears in both descriptions. It is introduced in order to adapt the generators to the origin shift $u, 0, 0$.

In other space groups described in two origin choices, surprisingly, the number of series is different for origin choice 1 and origin choice 2.

Example 2.1.5.5.3.

In the tetragonal space group $I4_1/amd$, No. 141, for origin choice 1 there is *one* series of maximal isomorphic subgroups of index p^2 , p prime, with the bases $p\mathbf{a}$, $p\mathbf{b}$, \mathbf{c} and origin shifts $u, v, 0$. For origin choice 2, there are *two* series with the same bases $p\mathbf{a}$, $p\mathbf{b}$, \mathbf{c} but with the different origin shifts $u, v, 0$ and $\frac{1}{2} + u, v, 0$. What are the reasons for these results?

For origin choice 1, the term $\frac{1}{2}$ appears in the first and second ‘coordinates’ of all generators (2), (3), (5) and (9) of \mathcal{G} . This term $\frac{1}{2}$ is the cause of the translation vectors $(\frac{p}{2} - \frac{1}{2})\mathbf{a}$ and $(\frac{p}{2} - \frac{1}{2})\mathbf{b}$ in the generators of \mathcal{H} .

For origin choice 2, fractions $\frac{1}{4}$ and $\frac{3}{4}$ appear in all ‘coordinates’ of the generator (3) $\bar{y} + \frac{1}{4}, x + \frac{3}{4}, z + \frac{1}{4}$ of \mathcal{G} . As a consequence, translational parts with vectors $(\frac{p}{4} + \frac{1}{4})\mathbf{a}$ and $(\frac{3p}{4} - \frac{3}{4})\mathbf{b}$ appear if $p \equiv 3 \pmod{4}$. On the other hand, translational parts with vectors $(\frac{p}{4} - \frac{1}{4})\mathbf{a}$, $(\frac{3p}{4} - \frac{3}{4})\mathbf{b}$ are introduced in the generators of \mathcal{H} if $p \equiv 1 \pmod{4}$ holds.

Another consequence of the fractions $\frac{1}{4}$ and $\frac{3}{4}$ occurring in the generator (3) of \mathcal{G} is the difference in the origin shifts. They are $\frac{1}{2} + u, v, 0$ for $p \equiv 3 \pmod{4}$ and $u, v, 0$ for $p \equiv 1 \pmod{4}$. Thus, the one series in origin choice 1 for odd p is split into two series in origin choice 2 for $p \equiv 3 \pmod{4}$ and $p \equiv 1 \pmod{4}$.³

2.1.6. Minimal supergroups

2.1.6.1. General description

In the previous sections, the relation $\mathcal{H} < \mathcal{G}$ was seen from the viewpoint of the group \mathcal{G} . In this case, \mathcal{H} was a subgroup of \mathcal{G} . However, the same relation may be viewed from the group \mathcal{H} . In this case, $\mathcal{G} > \mathcal{H}$ is a *supergroup* of \mathcal{H} . As for the subgroups of \mathcal{G} , cf. Section 1.2.6, different kinds of supergroups of \mathcal{H} may be distinguished. The following definitions are obvious.

Definition 2.1.6.1.1. Let $\mathcal{H} < \mathcal{G}$ be a maximal subgroup of \mathcal{G} . Then $\mathcal{G} > \mathcal{H}$ is called a *minimal supergroup* of \mathcal{H} . If \mathcal{H} is a *translationengleiche* subgroup of \mathcal{G} then \mathcal{G} is a *translationengleiche supergroup* (*t-supergroup*) of \mathcal{H} . If \mathcal{H} is a *klassengleiche* subgroup of \mathcal{G} , then \mathcal{G} is a *klassengleiche supergroup* (*k-supergroup*) of \mathcal{H} . If \mathcal{H} is an isomorphic subgroup of \mathcal{G} , then \mathcal{G} is an *isomorphic supergroup* of \mathcal{H} . If \mathcal{H} is a general subgroup of \mathcal{G} , then \mathcal{G} is a *general supergroup* of \mathcal{H} . \square

The search for supergroups of space groups is much more difficult than the search for subgroups. One of the reasons for this difficulty is that the search for subgroups $\mathcal{H} < \mathcal{G}$ is restricted to the elements of the space group \mathcal{G} itself, whereas the search for supergroups $\mathcal{G} > \mathcal{H}$ has to take into account the whole (continuous) group \mathcal{E} of all isometries. For example, there are only a finite number of subgroups \mathcal{H} of any space group \mathcal{G} for any given

index i . On the other hand, there may not only be an infinite number of supergroups \mathcal{G} of a space group \mathcal{H} for a finite index i but even an uncountably infinite number of supergroups of \mathcal{H} .

Example 2.1.6.1.2.

Let $\mathcal{H} = P1$. Then there is an infinite number of t -supergroups $P\bar{1}$ of index 2 because there is no restriction for the sites of the centres of inversion and thus of the conventional origin of $P\bar{1}$.

In the tables of this volume, a supergroup \mathcal{G} of a space group \mathcal{H} is listed by its type if \mathcal{H} is listed as a subgroup of \mathcal{G} . The entry contains at least the index of \mathcal{H} in \mathcal{G} , the conventional HM symbol of \mathcal{G} and its space-group number. Additional data may be given for *klassengleiche* supergroups. More details, e.g. the representatives of the general position or the generators as well as the transformation matrix and the origin shift, would only duplicate the subgroup data. The number of supergroups belonging to one entry can neither be concluded from the subgroup data nor is it listed among the supergroup data.

Like the subgroup data, the supergroup data are also partitioned into blocks.

2.1.6.2. I Minimal translationengleiche supergroups

For each space group \mathcal{H} , under this heading are listed those space-group types \mathcal{G} for which \mathcal{H} appears as an entry under the heading **I Maximal translationengleiche subgroups**. The listing consists of the index in brackets [...], the conventional HM symbol and (in parentheses) the space-group number (...). The space groups are ordered by ascending space-group number. If this line is empty, the heading is printed nevertheless and the content is announced by ‘none’, as in $P6/mmm$, No. 191.

The supergroups listed on the line **I Minimal translationengleiche supergroups** are realized only if the lattice conditions of \mathcal{H} fulfil the lattice conditions for \mathcal{G} . For example, if $\mathcal{G} = P422$, No. 89, is a supergroup of $\mathcal{H} = P222$, No. 16, two of the three independent lattice parameters a, b, c of $P222$ must be equal (or in crystallographic practice, approximately equal). These must be a and b if c is the tetragonal axis, b and c if a is the tetragonal axis or c and a if b is the tetragonal axis. In the latter two cases, the setting of $P222$ has to be adapted to the conventional c -axis setting of $P422$. For the cubic supergroup $P23$, No. 195, all three lattice parameters of $P222$ must be (approximately) equal. Such conditions are always to be taken into consideration if the t -supergroup belongs to a different crystal family⁴ to the original group. Therefore, for $\mathcal{H} = P222$ there is no lattice condition for the supergroup $\mathcal{G} = Pmmm$ because $P222$ and $Pmmm$ belong to the same crystal family.

2.1.6.3. II Minimal non-isomorphic klassengleiche supergroups

Klassengleiche supergroups $\mathcal{G} > \mathcal{H}$ always belong to the crystal family of \mathcal{H} . Therefore, there are no restrictions for the lattice parameters of \mathcal{H} .

The block **II Minimal non-isomorphic klassengleiche supergroups** is divided into two subblocks with the headings **Additional centring translations** and **Decreased unit cell**. If both subblocks are empty, only the heading of the block is listed, stating ‘none’ for the content of the block, as in $P6/mmm$, No. 191.

If at least one of the subblocks is non-empty, then the heading of the block and the headings of both subblocks are listed. An

³ F. Gähler (private communication) has shown that such a splitting can be avoided if one allows the prime p to enter the formulae for the origin shifts. In these tables we have not made use of this possibility in order to keep the origin shifts in the same form for all space groups \mathcal{G} .

⁴ For the term ‘crystal family’ cf. Section 1.2.5.2, or, for more details, *IT A*, Section 8.2.7.