

2. MAXIMAL SUBGROUPS OF THE PLANE GROUPS AND SPACE GROUPS

- (b) Trigonal space groups with rhombohedral R lattice and hexagonal axes:
 - (i) $\mathbf{a}' = -2\mathbf{b}$, $\mathbf{b}' = 2\mathbf{a} + 2\mathbf{b}$.
- (c) Trigonal space groups with rhombohedral R lattice and rhombohedral axes:
 - (i) $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{b} - \mathbf{c}$, $\mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$,
 - (ii) $\mathbf{a}' = \mathbf{a} - \mathbf{b} + \mathbf{c}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b} - \mathbf{c}$, $\mathbf{c}' = -\mathbf{a} + \mathbf{b} + \mathbf{c}$.
- (6) Hexagonal space groups:
 - (i) $\mathbf{c}' = 3\mathbf{c}$,
 - (ii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$, H -centring,
 - (iii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$.
- (7) Cubic space groups with P lattice:
 - (i) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, I lattice.

2.1.5. Series of maximal isomorphic subgroups

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2.1.5.1. General description

Maximal subgroups of index higher than 4 have index p , p^2 or p^3 , where p is prime, are necessarily isomorphic subgroups and are infinite in number. Only a few of them are listed in *ITA* in the block 'Maximal isomorphic subgroups of lowest index IIC' '. Because of their infinite number, they cannot be listed individually, but are listed in this volume as members of series under the heading 'Series of maximal isomorphic subgroups'. In most of the series, the HM symbol for each isomorphic subgroup $\mathcal{H} < \mathcal{G}$ will be the same as that of \mathcal{G} . However, if \mathcal{G} is an enantiomorphic space group, the HM symbol of \mathcal{H} will be either that of \mathcal{G} or that of its enantiomorphic partner.

Example 2.1.5.1.1

Two of the four series of isomorphic subgroups of the space group $P4_1$, No. 76, are (the data for the generators are omitted):

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	prime $p > 2$; $p = 4n - 1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	prime $p > 4$; $p = 4n + 1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

On the other hand, the corresponding data for $P4_3$, No. 78, are

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	prime $p > 4$; $p = 4n + 1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	prime $p > 2$; $p = 4n - 1$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

Note that in both tables the subgroups of the type $P4_3$, No. 78, are listed first because of the rules on the sequence of the subgroups.

If an isomorphic maximal subgroup of index $i \leq 4$ is a member of a series, then it is listed twice: as a member of its series and individually under the heading 'Enlarged unit cell'.

Most isomorphic subgroups of index 3 are the first members of series but those of index 2 or 4 are rarely so. An example is the space group $P4_2$, No. 77, with isomorphic subgroups of index 2 (not in any series) and 3 (in a series); an exception is found in space group $P4$, No. 75, where the isomorphic subgroup for $\mathbf{c}' = 2\mathbf{c}$ is the first member of the series $[p]\mathbf{c}' = p\mathbf{c}$.

2.1.5.2. Basis transformation

The conventional basis of the unit cell of each isomorphic subgroup in the series has to be defined relative to the basis of the original space group. For this definition the prime p is frequently sufficient as a parameter.

Example 2.1.5.2.1

The isomorphic subgroups of the space group $P4_222$, No. 93, can be described by two series with the bases of their members:

$[p]$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
$[p^2]$	$p\mathbf{a}, p\mathbf{b}, \mathbf{c}$.

In other cases, one or two positive integers, here called q and r , define the series and often the value of the prime p .

Example 2.1.5.2.2

In space group $P\bar{6}$, No. 174, the series $q\mathbf{a} - r\mathbf{b}$, $r\mathbf{a} + (q + r)\mathbf{b}$, \mathbf{c} is listed. The values of q and r have to be chosen such that while $q > 0$, $r > 0$, $p = q^2 + r^2 + qr$ is prime.

Example 2.1.5.2.3

In the space group $P112_1/m$, No. 11, unique axis c , the series $p\mathbf{a}$, $-q\mathbf{a} + \mathbf{b}$, \mathbf{c} is listed. Here p and q are independent and q may take the p values $0 \leq q < p$ for each value of the prime p .

2.1.5.3. Origin shift

Each of the sublattices discussed in Section 2.1.4.3.2 is common to a conjugacy class or belongs to a normal subgroup of a given series. The subgroups in a conjugacy class differ by the positions of their conventional origins relative to the origin of the space group \mathcal{G} . To define the origin of the conventional unit cell of each subgroup in a conjugacy class, one, two or three integers, called u , v or w in these tables, are necessary. For a series of subgroups of index p , p^2 or p^3 there are p , p^2 or p^3 conjugate subgroups, respectively. The positions of their origins are defined by the p or p^2 or p^3 permitted values of u or u, v or u, v, w , respectively.

Example 2.1.5.3.1

The space group \mathcal{G} , $P\bar{4}2c$, No. 112, has two series of maximal isomorphic subgroups \mathcal{H} . For one of them the lattice relations are $[p^2]\mathbf{a}' = p\mathbf{a}$, $\mathbf{b}' = p\mathbf{b}$, listed as $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$. The index is p^2 . For each value of p there exist exactly p^2 conjugate subgroups with origins in the points $u, v, 0$, where the parameters u and v run independently: $0 \leq u < p$ and $0 \leq v < p$.

In another type of series there is exactly one (normal) subgroup \mathcal{H} for each index p ; the location of its origin is always chosen at the origin $0, 0, 0$ of \mathcal{G} and is thus not indicated as an origin shift.

Example 2.1.5.3.2

Consider the space group $Pca2_1$, No. 29. Only one subgroup exists for each value of p in the series $\mathbf{a}, \mathbf{b}, p\mathbf{c}$. This is indicated in the tables by the statement 'no conjugate subgroups'.

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

2.1. GUIDE TO THE SUBGROUP TABLES AND GRAPHS

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 choices 1 and 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*. $(\mathbf{a}_{\text{hex}})^T$ 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 2.1.5.3

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 $p = 4n - 1$. 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 $p = 4n + 1$ 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 $p = 4n - 1$ and u , v , 0 for $p = 4n + 1$. Thus, the one series in origin choice 1 for odd p is split into two series in origin choice 2 for $p = 4n - 1$ and $p = 4n + 1$.⁴

2.1.6. The data for minimal supergroups

2.1.6.1. Description of the listed data

In the previous sections, the relation $\mathcal{H} < \mathcal{G}$ between space groups 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.

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

Following from Hermann’s theorem, Lemma 1.2.8.1.2, a minimal supergroup of a space group is either a *translationengleiche* supergroup (*t-supergroup*) or a *klassengleiche* supergroup (*k-supergroup*). A proper minimal *t-supergroup* always has an index i , $1 < i < 5$, and is never isomorphic. A minimal *k-supergroup* with index i , $1 < i < 5$, may be isomorphic or non-isomorphic; for indices $i > 4$ a minimal *k-supergroup* can only be an isomorphic *k-supergroup*. The propositions, theorems and their corollaries of Sections 1.4.6 and 1.4.7 for maximal subgroups are correspondingly valid for minimal supergroups.

Subgroups of space groups of finite index are always space groups again. This does not hold for supergroups. For example, the direct product \mathcal{G} of a space group \mathcal{H} with a group of order 2 is not a space group, although $\mathcal{H} < \mathcal{G}$ is a subgroup of index 2 of \mathcal{G} . Moreover, supergroups of space groups may be affine groups which are only isomorphic to space groups but not space groups

themselves, see Example 2.1.6.2.2. In the following we restrict the considerations to supergroups \mathcal{G} of a space group \mathcal{H} which are themselves space groups. This holds, for example, for the symmetry relations between crystal structures when the symmetries of both structures can be described by space groups. Quasicrystals, incommensurate phases *etc.* are thus excluded. Even under this restriction, supergroups show much more variable behaviour than subgroups do.

One of the reasons for this complication 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 minimal supergroups of \mathcal{H} .

Example 2.1.6.1.2

Let $\mathcal{H} = P\bar{1}$. 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, the minimal *translationengleiche* supergroups \mathcal{G} of a space group \mathcal{H} are not listed individually but the type of \mathcal{G} is listed by index, conventional HM symbol and space-group number if \mathcal{H} is listed as a *translationengleiche* subgroup of \mathcal{G} in the subgroup tables. Not listed is the number of supergroups belonging to one entry. Non-isomorphic *klassengleiche* supergroups are listed individually. For them, nonconventional HM symbols are listed in addition; for *klassengleiche* supergroups with ‘Decreased unit cell’, the lattice relations are added. More details, such as 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.

In this Section 2.1.6, the kind of listing is described explicitly. The data for maximal subgroups \mathcal{H} are complete for all space groups \mathcal{G} . Therefore, it is possible to derive:

- (1) all minimal *translationengleiche* supergroups \mathcal{G} of \mathcal{H} if the point-group symmetry of \mathcal{H} is at least orthorhombic (*i.e.* neither triclinic nor monoclinic);
- (2) all minimal *klassengleiche* supergroups \mathcal{G} for each space group \mathcal{H} .

In Section 2.1.7 the procedure is described by which the supergroup data can be obtained from the subgroup data. This procedure is not trivial and care has to be taken to really obtain the full set of supergroups. In Section 2.1.7 one can also find the reasons why this procedure is not applicable when the space group \mathcal{H} belongs to a triclinic or monoclinic point group.

Isomorphic supergroups are not indicated at all because they are implicitly contained in the subgroup data. Their derivation from the subgroup data is discussed in Section 2.1.7.2.

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

2.1.6.2. 1 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 the space-group number (in parentheses). The space groups are ordered by ascending space-group number. If this line

⁴F. 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} .