International Tables for Crystallography (2011). Vol. A1, Chapter 2.1, pp. 72–96.

2.1. Guide to the subgroup tables and graphs

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2.1.1. Contents and arrangement of the subgroup tables

In this chapter, the subgroup tables, the subgroup graphs and their general organization are discussed. In the following sections, the different types of data are explained in detail. For every plane group and every space group there is a separate table of maximal subgroups and minimal supergroups. The subgroup data are listed either individually, or as members of (infinite) series, or both. The supergroup data are not as complete as the subgroup data. However, most of them can be obtained by proper evaluation of the subgroup data, as shown in Section 2.1.7. In addition, there are graphs of *translationengleiche* and *klassengleiche* subgroups which contain for each space group all kinds of subgroups, not just the maximal ones.

The presentation of the plane-group and space-group data in the tables of Chapters 2.2 and 2.3 follows the style of the tables of Parts 6 (plane groups) and 7 (space groups) in Vol. A of *International Tables for Crystallography* (2005), henceforth abbreviated as *IT* A. The data comprise:

Headline
Generators selected
General position
I Maximal *translationengleiche* subgroups
II Maximal *klassengleiche* subgroups
I Minimal *translationengleiche* supergroups
II Minimal non-isomorphic *klassengleiche* supergroups.

For the majority of groups, the data can be listed completely on one page. Sometimes two pages are needed. If the data extend less than half a page over one full page and data for a neighbouring space-group table 'overflow' to a similar extent, then the two overflows are displayed on the same page. Such deviations from the standard sequence are indicated on the relevant pages by a remark *Continued on* .... The two overflows are separated by a solid line and are designated by their headlines.

The sequence of the plane groups and space groups $\mathcal{G}$ in this volume follows exactly that of the tables of Part 6 (plane groups) and Part 7 (space groups) in *IT* A. The format of the subgroup tables has also been chosen to resemble that of the tables of *IT* A as far as possible. Graphs for *translationengleiche* and *klassengleiche* subgroups are found in Chapters 2.4 and 2.5. Examples of graphs of subgroups can also be found in Section 10.1.4.3 of *IT* A, but only for subgroups of point groups. The graphs for the space groups are described in Section 2.1.8.

2.1.2. Structure of the subgroup tables

Some basic data in these tables have been repeated from the tables of *IT* A in order to allow the use of the subgroup tables independently of *IT* A. These data and the main features of the tables are described in this section.

2.1.2.1. Headline

The headline contains the specification of the space group for which the maximal subgroups are considered. The headline lists from the outside margin inwards:

(1) The *short (international) Hermann–Mauguin symbol* for the plane group or space group. These symbols will be henceforth referred to as 'HM symbols'. HM symbols are discussed in detail in Chapter 12.2 of *IT* A with a brief summary in Section 2.2.4 of *IT* A.
(2) The plane-group or space-group number as introduced in *International Tables for X-ray Crystallography*, Vol. I (1952). These numbers run from 1 to 17 for the plane groups and from 1 to 230 for the space groups.
(3) The *full (international) Hermann–Mauguin symbol* for the plane or space group, abbreviated 'full HM symbol'. This describes the symmetry in up to three symmetry directions (*Blickrichtungen*) more completely, see Table 12.3.4.1 of *IT* A, which also allows comparison with earlier editions of *International Tables*.
(4) The *Schoenflies symbol* for the space group (there are no Schoenflies symbols for the plane groups). The Schoenflies symbols are primarily point-group symbols; they are extended by superscripts for a unique designation of the space-group types, *cf.* *IT* A, Sections 12.1.2 and 12.2.2.

2.1.2.2. Data from IT A

2.1.2.2.1. Generators selected

As in *IT* A, for each plane group and space group $\mathcal{G}$ a set of symmetry operations is listed under the heading 'Generators selected'. From these group elements, $\mathcal{G}$ can be generated conveniently. The generators in this volume are the same as those in *IT* A. They are explained in Section 2.2.10 of *IT* A and the choice of the generators is explained in Section 8.3.5 of *IT* A.

The generators are listed again in this present volume because many of the subgroups are characterized by their generators. These (often nonconventional) generators of the subgroups can thus be compared with the conventional ones without reference to *IT* A.

2.1.2.2.2. General position

Like the generators, the general position has also been copied from *IT* A, where an explanation can be found in Section 2.2.11. The general position in *IT* A is the first block under the heading 'Positions', characterized by its site symmetry of 1. The elements of the general position have the following meanings:

(1) they are coset representatives of the space group $\mathcal{G}$ with respect to its translation subgroup. The other elements of a coset are obtained from its representative by combination with translations of $\mathcal{G}$;
(2) they form a kind of shorthand notation for the matrix description of the coset representatives of $\mathcal{G}$;
(3) they are the coordinates of those symmetry-equivalent points that are obtained by the application of the coset representatives on a point with the coordinates x, y, z;
(4) their numbers refer to the geometric description of the symmetry operations in the block 'Symmetry operations' of the space-group tables of *IT* A.

Many of the subgroups $\mathcal{H} < \mathcal{G}$ in these tables are characterized by the elements of their general position. These elements are specified by numbers which refer to the corresponding numbers in the general position of $\mathcal{G}$. Other subgroups are listed by the numbers of their generators, which again refer to the corresponding numbers in the general position of $\mathcal{G}$. Therefore, the listing of the general position of $\mathcal{G}$ as well as the listing of the generators of $\mathcal{G}$ is essential for the structure of these tables. For examples, see Sections 2.1.3 and 2.1.4.

2.1.2.3. Specification of the setting

All 17 plane-group types[1] and 230 space-group types are listed and described in *IT* A. However, whereas each plane-group type is represented exactly once, 44 space-group types, *i.e.* nearly 20%, are represented twice. This means that the conventional setting of these 44 space-group types is not uniquely determined and must be specified. The same settings underlie the data of this volume, which follows *IT* A as much as possible.

There are three reasons for listing a space-group type twice:

(1) Each of the 13 monoclinic space-group types is listed twice, with 'unique axis *b*' and 'unique axis *c*', where *b* or *c* is the direction distinguished by symmetry (*monoclinic axis*). The tables of this Part 2 always refer to the conventional cell choice, *i.e.* 'cell choice 1', whereas in *IT* A for each setting three cell choices are shown. In the graphs of Chapters 2.4 and 2.5, the monoclinic space groups are designated by their short HM symbols.

Note on standard monoclinic space-group symbols: In this volume, as in *IT* A, the monoclinic space groups are listed for two settings. Nevertheless, the short symbol for the setting 'unique axis *b*' has always been used as the *standard* (short) HM symbol. It does not carry any information about the setting of the particular description. As in *IT* A, no other short symbols are used for monoclinic space groups and their subgroups in the present volume.

(2) Twenty-four orthorhombic, tetragonal or cubic space-group types are listed with two different origins. In general, the origin is chosen at a point of highest site symmetry ('origin choice 1'); for exceptions see *IT* A, Section 8.3.1. If there are centres of inversion and if by this rule the origin is not at an inversion centre, then the space group is described once more with the origin at a centre of inversion ('origin choice 2').

(3) There are seven trigonal space groups with a rhombohedral lattice. These space groups are described in a hexagonal basis ('hexagonal axes') with a rhombohedrally centred hexagonal lattice as well as in a rhombohedral basis with a primitive lattice ('rhombohedral axes').

If there is a choice of setting for the space group $\mathcal{G}$, the chosen setting is indicated under the HM symbol in the headline. If a subgroup $\mathcal{H} < \mathcal{G}$ belongs to one of these 44 space-group types, its 'conventional setting' must be defined. The rules that are followed in this volume are explained in Section 2.1.2.5.

2.1.2.4. Sequence of the subgroup and supergroup data

As in the subgroup data of *IT* A, the sequence of the maximal subgroups is as follows: subgroups of the same kind are collected in a block. Each block has a heading. Compared with *IT* A, the blocks have been partly reorganized because in this volume *all* maximal isomorphic subgroups are listed, whereas in *IT* A only a few of them are described. In addition, the subgroups are described here in more detail.

The sequence of the subgroups within each block follows the value of the index; subgroups of lowest index are listed first. Subgroups having the same index are listed according to their lattice relations to the lattice of the original group $\mathcal{G}$, *cf.* Section 2.1.4.3. Subgroups with the same lattice relations are listed in decreasing order of space-group number.

Conjugate subgroups have the same index and the same space-group number. They are grouped together and connected by a brace on the left-hand side. Conjugate classes of maximal subgroups and their lengths are therefore easily recognized. In the series of maximal isomorphic subgroups, braces are inapplicable so there the conjugacy classes are stated explicitly.

The block designations are:

(1) In the block **I Maximal *translationengleiche* subgroups**, *all* maximal *translationengleiche* subgroups are listed, see Section 2.1.3. None of them are isomorphic.

(2) Under the heading **II Maximal *klassengleiche* subgroups**, all maximal *klassengleiche* subgroups are listed in up to three separate blocks, each of them marked by a bullet, •. Maximal non-isomorphic subgroups can only occur in the first two blocks, whereas maximal isomorphic subgroups are only found in the last two blocks.

• **Loss of centring translations**. This block is described in Section 2.1.4.2 in more detail.

Subgroups in this block are always non-isomorphic. The block is empty (and is then omitted) for space groups that are designated by an HM symbol starting with the letter *P*.

• **Enlarged unit cell**. In this block, those maximal *klassengleiche* subgroups $\mathcal{H} < \mathcal{G}$ of index 2, 3 and 4 are listed for which the *conventional* unit cell of $\mathcal{H}$ is *larger* than that of $\mathcal{G}$, see Section 2.1.4.3. These subgroups may be non-isomorphic or isomorphic, see Section 2.1.5. Therefore, it may happen that a maximal isomorphic *klassengleiche* subgroup of index 2, 3 or 4 is listed twice: once here explicitly and once implicitly as a member of a series.

• **Series of maximal isomorphic subgroups**. Maximal *klassengleiche* subgroups $\mathcal{H} < \mathcal{G}$ of indices 2, 3 and 4 may be isomorphic while those of index $i > 4$ are always isomorphic to $\mathcal{G}$. The total number of maximal *isomorphic klassengleiche* subgroups is infinite. These infinitely many subgroups cannot be described individually but only by a (small) number of infinite series. In each series, the individual subgroups are characterized by a few integer parameters, see Section 2.1.5.

(3) After the data for the subgroups, the data for the supergroups are listed. The data for minimal non-isomorphic supergroups are split into two main blocks with the headings

I Minimal *translationengleiche* supergroups and
II Minimal non-isomorphic *klassengleiche* supergroups.

(4) The latter block is split into the listings

• **Additional centring translations** and
• **Decreased unit cell**.

(5) Minimal isomorphic supergroups are not listed because they can be read from the data for the maximal isomorphic subgroups.

For details, see Section 2.1.6.

[1] The clumsy terms 'plane-group type' and 'space-group type' are frequently abbreviated by the shorter terms 'plane group' and 'space group' in what follows, as is often done in crystallography. Occasionally, however, it is essential to distinguish the individual group from its 'type of groups'.

2.1.2.5. Special rules for the setting of the subgroups

The multiple listing of 44 space-group types has implications for the subgroup tables. If a subgroup $\mathcal{H} < \mathcal{G}$ belongs to one of these types, its 'conventional setting' must be defined. In many cases there is a natural choice; sometimes, however, such a choice does not exist, and the appropriate conventions have to be stated.

The three reasons for listing a space group twice will be discussed in this section, *cf.* Section 2.1.2.3.

2.1.2.5.1. Monoclinic subgroups

Rules

(*a*) If the monoclinic axis of $\mathcal{H}$ is the *b* or *c* axis of the basis of $\mathcal{G}$, then the setting of $\mathcal{H}$ is also 'unique axis *b*' or 'unique axis *c*'. In particular, if $\mathcal{G}$ is monoclinic, then the settings of $\mathcal{G}$ and $\mathcal{H}$ agree.

(*b*) If the monoclinic axis of $\mathcal{H}$ is neither *b* nor *c* in the basis of $\mathcal{G}$, then for $\mathcal{H}$ the setting 'unique axis *b*' is chosen.

(*c*) The cell choice is always 'cell choice 1' with the symbols *C* and *c* for unique axis *b*, and *A* and *a* for unique axis *c*.

Remarks (see also the following examples):

Rule (*a*) is valid for the many cases where the setting of $\mathcal{H}$ is 'inherited' from $\mathcal{G}$. In particular, this always holds for isomorphic subgroups.

Rule (*b*) is applied if $\mathcal{G}$ is orthorhombic and the monoclinic axis of $\mathcal{H}$ is the *a* axis of $\mathcal{G}$ and if $\mathcal{H}$ is a monoclinic subgroup of a trigonal group. Rule (*b*) is not natural, but specifies a preference for the setting 'unique axis *b*'. This seems to be justified because the setting 'unique axis *b*' is used more frequently in crystallographic papers and the standard short HM symbol is also referred to it.

Rule (*c*) implies a choice of that cell which is most explicitly described in the tables of *IT* A. By this choice, the centring type and the glide vector are fixed to the conventional values of 'cell choice 1'.

The necessary adjustment is performed through a coordinate transformation, *i.e.* by a change of the basis and by an origin shift, see Section 2.1.3.3.

Example 2.1.2.5.1

$\mathcal{G} = P12/m1$, No. 10; unique axis *b*.

II Maximal *klassengleiche* subgroups, Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}$, both subgroups $P12/a1$.

The monoclinic axis *b* is retained but the glide reflection *a* is converted into a glide reflection *c* ($P12/c1$ is the conventional HM symbol for cell choice 1).

[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, all four subgroups $A12/m1$.

The monoclinic axis *b* is retained but the *A* centring is converted into the conventional *C* centring ($C12/m1$ is the conventional HM symbol for cell choice 1).

[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, both subgroups $B12/e1$.

The monoclinic axis *b* is retained. The glide reflection is designated by '*e*' (simultaneous *c*- and *a*-glide reflection in the same plane perpendicular to **b**). The nonconventional *B* centring is converted into the conventional primitive setting *P*, by which the *e*-glide reflection also becomes a *c*-glide reflection.

Example 2.1.2.5.2

$\mathcal{G} = P112/m$, No. 10; unique axis *c*.

II Maximal *klassengleiche* subgroups, Enlarged unit cell

[2] $\mathbf{a}' = 2\mathbf{a}$, both subgroups $P112/a$.

The monoclinic axis *c* and the glide reflection *a* are retained because $P112/a$ is the conventional full HM symbol for unique axis *c*, cell choice 1.

[2] $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, all four subgroups $A112/m$.

The monoclinic axis *c* and the *A* centring are retained because $A112/m$ is the conventional full HM symbol for this setting.

[2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, both subgroups $C112/e$.

The monoclinic axis *c* is retained. The glide reflection is designated by '*e*' (simultaneous *a*- and *b*-glide reflection in the same plane perpendicular to **c**). The nonconventional *C* centring is converted into the conventional primitive setting *P*, by which the *e*-glide reflection also becomes an *a*-glide reflection.

Example 2.1.2.5.3

$\mathcal{G} = Pban$, No. 50; origin choice 1.

I Maximal (monoclinic) ***translationengleiche* subgroups**

[2] $P112/n$: conventional unique axis *c*; nonconventional glide reflection *n*. The monoclinic axis *c* is retained but the glide reflection *n* is adjusted to a glide reflection *a* in order to conform to the conventional symbol $P112/a$ of cell choice 1.

[2] $P12/a1$: conventional unique axis *b*; nonconventional glide reflection *a*. The monoclinic axis *b* is retained but the glide reflection *a* is adjusted to a glide reflection *c* of the conventional symbol $P12/c1$, cell choice 1.

[2] $P2/b11$: nonconventional monoclinic unique axis *a*; nonconventional glide reflection *b*. The monoclinic axis *a* is transformed to the conventional unique axis *b*; the glide reflection *b* is adjusted to the conventional symbol $P12/c1$ of the setting unique axis *b*, cell choice 1.

2.1.2.5.2. Subgroups with two origin choices

Altogether, 24 orthorhombic, tetragonal and cubic space groups with inversions are listed twice in *IT* A. There are three kinds of possible ambiguities for such groups with two origin choices:

(*a*) Only the original group $\mathcal{G}$ is listed with two origin choices in *IT* A, $\mathcal{G}(1)$ and $\mathcal{G}(2)$, but the subgroup $\mathcal{H} < \mathcal{G}$ is listed with one origin. Then the matrix parts $\boldsymbol{P}$ for the transformations $(\boldsymbol{P}, \boldsymbol{p}_1)$ and $(\boldsymbol{P}, \boldsymbol{p}_2)$ of the coordinate systems of $\mathcal{G}(1)$ and $\mathcal{G}(2)$ to that of $\mathcal{H}$ are the same but the two columns of origin shift differ, namely $\boldsymbol{p}_1$ from $\mathcal{G}(1)$ to $\mathcal{H}$ and $\boldsymbol{p}_2$ from $\mathcal{G}(2)$ to $\mathcal{H}$. They are related to the shift $\boldsymbol{u}$ between the origins of $\mathcal{G}(1)$ and $\mathcal{G}(2)$. However, the transformations from both settings of the space group $\mathcal{G}$ to the setting of the space group $\mathcal{H}$ are not unique and there is some choice in the transformation matrix and the origin shift.

The transformation has been chosen such that

(i) it transforms the nonconventional description of the space group $\mathcal{H}$ to a conventional one;

(ii) the description of the crystal structure in the subgroup $\mathcal{H}$ is as similar as possible to that in the supergroup $\mathcal{G}$.

If it is not possible to achieve the latter aim, a transformation with simple matrix and column parts has been chosen which fulfils the first condition.

Example 2.1.2.5.4

$\mathcal{G} = Pban$, No. 50, origin choice 1 and origin choice 2.

I Maximal *translationengleiche* subgroups

There are seven maximal *t*-subgroups of *Pban*, No. 50, four of which are orthorhombic, $\mathcal{H} = Pba2$, $Pb2n$, $P2an$ and $P222$, and three of which are monoclinic, $\mathcal{H} = P112/n$, $P12/a1$ and $P2/b11$. In the orthorhombic subgroups, the centres of inversion of $\mathcal{G}$ are lost but at least one kind of twofold axis is retained. Therefore, no origin shift for $\mathcal{H}$ is necessary from the setting 'origin choice 1' of $\mathcal{G}(1)$, where the origin is placed at the intersection of the three twofold axes. For the column part of the transformation $(\boldsymbol{P}, \boldsymbol{p}_1)$, $\boldsymbol{p}_1 = \boldsymbol{o}$ holds. For the monoclinic maximal *t*-subgroups of *Pban* the origin is shifted from the intersection of the three twofold axes in $\mathcal{G}(1)$ to an inversion centre of $\mathcal{H}$.

On the other hand, the origin is situated on an inversion centre for origin choice 2 of $\mathcal{G}(2)$, as is the origin in the conventional description of the three monoclinic maximal *t*-subgroups. For them the origin shift is $\boldsymbol{p}_2 = \boldsymbol{o}$, while there is a nonzero column $\boldsymbol{p}_2$ for the orthorhombic subgroups.

(*b*) Both $\mathcal{G}$ and its subgroup $\mathcal{H} < \mathcal{G}$ are listed with two origins. Then the origin choice of $\mathcal{H}$ is the same as that of $\mathcal{G}$. This rule always applies to isomorphic subgroups as well as in some other cases.

Example 2.1.2.5.5

Maximal *k*-subgroups $\mathcal{H}$ = *Pnnn*, No. 48, of the space group $\mathcal{G}$ = *Pban*, No. 50. There are two such subgroups with the lattice relation $\mathbf{c}' = 2\mathbf{c}$. Both $\mathcal{G}$ and $\mathcal{H}$ are listed with two origins such that the origin choices of $\mathcal{G}$ and $\mathcal{H}$ are either the same or are strongly related.

(*c*) The group $\mathcal{G}$ is listed with one origin but the subgroup $\mathcal{H} < \mathcal{G}$ is listed with two origins. This situation is restricted to maximal *k*-subgroups with the only exception being $Ia\bar{3}d > I4_1/acd$, where there are three conjugate *t*-subgroups of index 3. In all cases the subgroup $\mathcal{H}$ is referred to origin choice 2. This rule is followed in the subgroup tables because it gives a better chance of retaining the origin of $\mathcal{G}$ in $\mathcal{H}$. If there are two origin choices for $\mathcal{H}$, then $\mathcal{H}$ has inversions and these are also elements of the supergroup $\mathcal{G}$. The (unique) origin of $\mathcal{G}$ is placed on one of the inversion centres. For origin choice 2 in $\mathcal{H}$, the origin of $\mathcal{H}$ may agree with that of $\mathcal{G}$, although this is not guaranteed. In addition, origin choice 2 is often preferred in structure determinations.

Example 2.1.2.5.6

Maximal *k*-subgroups of *Pccm*, No. 49. In the block
• Enlarged unit cell, [2] $\mathbf{a}' = 2\mathbf{a}$
one finds two subgroups *Pcna* (50, *Pban*). One of them has the origin of $\mathcal{G}$, the origin of the other subgroup is shifted by $\frac{1}{2}, 0, 0$ and is placed on one of the inversion centres of $\mathcal{G}$ that is removed from the first subgroup. The analogous situation is found in the block [2] $\mathbf{b}' = 2\mathbf{b}$, where the two subgroups of space-group type *Pncb* (50, *Pban*) show the analogous relation. In the next block, [2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, the four subgroups *Ccce* (68) behave similarly.

For $\mathcal{G}$ = *Pmma*, No. 51, the same holds for the two subgroups of the type *Pmmn* (59) in the block [2] $\mathbf{b}' = 2\mathbf{b}$.

On the other hand, for $\mathcal{G}$ = *Immm*, No. 71, in the block 'Loss of centring translations' three subgroups of type *Pmmn* (59) and one of type *Pnnn* (48) are listed. All of them need an origin shift of $\frac{1}{4}, \frac{1}{4}, \frac{1}{4}$ because they have lost the inversion centres of the origin of $\mathcal{G}$.

2.1.2.5.3. Space groups with a rhombohedral lattice

The seven trigonal space groups with a rhombohedral lattice are often called *rhombohedral space groups*. Their HM symbols begin with the lattice letter *R* and they are listed with both hexagonal axes and rhombohedral axes.

Rules

(*a*) A rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is listed in the same setting as $\mathcal{G}$: if $\mathcal{G}$ is referred to hexagonal axes, so is $\mathcal{H}$; if $\mathcal{G}$ is referred to rhombohedral axes, so is $\mathcal{H}$.

(*b*) If $\mathcal{G}$ is a non-rhombohedral trigonal or a cubic space group, then a rhombohedral subgroup $\mathcal{H} < \mathcal{G}$ is always referred to hexagonal axes.

(*c*) A non-rhombohedral subgroup $\mathcal{H}$ of a rhombohedral space group $\mathcal{G}$ is referred to its conventional setting.

Remarks

Rule (*a*) provides a clear definition, in particular for the axes of isomorphic subgroups.

Rule (*b*) has been followed in the subgroup tables because the rhombohedral setting is rarely used in crystallography.

Rule (*c*) implies that monoclinic subgroups of rhombohedral space groups are referred to the setting 'unique axis *b*'.

There is a peculiarity caused by the two settings of the rhombohedral space groups. The rhombohedral lattice appears to be centred in the hexagonal axes setting, whereas it is primitive in the rhombohedral axes setting. Therefore, there are trigonal subgroups of a rhombohedral space group $\mathcal{G}$ which are listed in the block 'Loss of centring translations' for the hexagonal axes setting of $\mathcal{G}$ but are listed in the block 'Enlarged unit cell' when $\mathcal{G}$ is referred to rhombohedral axes. Although unnecessary and not done for other space groups with primitive lattices, the line

• Loss of centring translations none

is listed for the rhombohedral axes setting.

Example 2.1.2.5.7

$\mathcal{G} = R3$, No. 146. Maximal *klassengleiche* subgroups of index 2 and 3. Comparison of the data for the settings 'hexagonal axes' and 'rhombohedral axes'. The data for the general position and the generators are omitted.

HEXAGONAL AXES

	• Loss of centring translations		
[3]	$P3_2$ (145)		0, 1/3, 0
[3]	$P3_1$ (144)		1/3, 1/3, 0
[3]	$P3$ (143)		
	• Enlarged unit cell		
[2]	$\mathbf{a}' = -\mathbf{b}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = 2\mathbf{c}$		
	$R3$ (146)	$-\mathbf{b}, \mathbf{a} + \mathbf{b}, 2\mathbf{c}$	
...			

RHOMBOHEDRAL AXES

	• Loss of centring translations		none
	• Enlarged unit cell		
[2]	$\mathbf{a}' = \mathbf{a} + \mathbf{c}, \mathbf{b}' = \mathbf{a} + \mathbf{b}, \mathbf{c}' = \mathbf{b} + \mathbf{c}$		
	$R3$ (146)	$\mathbf{a} + \mathbf{c}, \mathbf{a} + \mathbf{b}, \mathbf{b} + \mathbf{c}$	
[3]	$\mathbf{a}' = \mathbf{a} - \mathbf{b}, \mathbf{b}' = \mathbf{b} - \mathbf{c}, \mathbf{c}' = \mathbf{a} + \mathbf{b} + \mathbf{c}$		
	$P3_2$ (145)	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$	0, 1/3, −1/3
	$P3_1$ (144)	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$	1/3, 0, −1/3
	$P3$ (143)	$\mathbf{a} - \mathbf{b}, \mathbf{b} - \mathbf{c}, \mathbf{a} + \mathbf{b} + \mathbf{c}$	

The sequence of the blocks has priority over the classification by increasing index. Therefore, in the setting 'hexagonal axes', the subgroups of index 3 precede the subgroup of index 2.
In the tables, the lattice relations are simpler for the setting 'hexagonal axes'.
The complete general position is listed for the maximal k-subgroups of index 3 in the setting 'hexagonal axes'; only the generator is listed for rhombohedral axes.

2.1.3. I Maximal *translationengleiche* subgroups (*t*-subgroups)

2.1.3.1. Introduction

In this block, all maximal t-subgroups $\mathcal{H}$ of the plane groups and the space groups $\mathcal{G}$ are listed individually. Maximal t-sugroups are always non-isomorphic.

For the sequence of the subgroups, see Section 2.1.2.4. There are no lattice relations for t-subgroups because the lattice is retained. Therefore, the sequence is determined only by the rising value of the index and by the decreasing space-group number.

2.1.3.2. A description in close analogy with IT A

The listing is similar to that of *IT* A and presents on one line the following information for each subgroup $\mathcal{H}$:

[i] HMS1 (No., HMS2) sequence matrix shift

Conjugate subgroups are listed together and are connected by a left brace.

The symbols have the following meaning:

[i]	index of $\mathcal{H}$ in $\mathcal{G}$;
HMS1	HM symbol of $\mathcal{H}$ referred to the coordinate system and setting of $\mathcal{G}$. This symbol may be nonconventional;
No.	space-group No. of $\mathcal{H}$;
HMS2	conventional HM symbol of $\mathcal{H}$ if HMS1 is not a conventional HM symbol;
sequence	sequence of numbers; the numbers refer to those coordinate triplets of the general position of $\mathcal{G}$ that are retained in $\mathcal{H}$, *cf. Remarks*; for general position *cf.* Section 2.1.2.2.2;
matrix	matrix part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3;
shift	column part of the transformation to the conventional setting corresponding to HMS2, *cf.* Section 2.1.3.3.

Remarks

In the sequence column for space groups with centred lattices, the abbreviation '(numbers)+' means that the coordinate triplets specified by 'numbers' are to be taken plus those obtained by adding each of the centring translations, see the comments following Examples 2.1.3.2.2 and 2.1.3.2.3.

The symbol HMS2 is omitted if HMS1 is a conventional HM symbol.

The following deviations from the listing of *IT* A are introduced in these tables:

No.: the space-group No. of $\mathcal{H}$ is added.
HMS2: In order to specify the setting clearly, the *full* HM symbol is listed for monoclinic subgroups, not the standard (short) HM symbol as in *IT* A.
matrix, shift: These entries contain information on the transformation of $\mathcal{H}$ from the setting of $\mathcal{G}$ to the standard setting of $\mathcal{H}$. They are explained in Section 2.1.3.3.

In general, the numbers in the list 'Sequence' of $\mathcal{H}$ follow the order of the numbers in the group $\mathcal{G}$, *i.e.* they rise monotonically. Sometimes this sequence is modified because those entries which have the same additional translations are joined together, see, *e.g.* the maximal k-subgroups of $Fm\bar{3}m$ with 'Loss of centring translations'. In addition, in a class of conjugate subgroups, the monotonically rising order may be obeyed only for the first member of the conjugacy class. The order of the other members is then determined by the conjugation of the first member. (In *IT* A the monotonically rising order of the numbers is kept in all conjugate subgroups.)

Example 2.1.3.2.1

$\mathcal{G} = Pm\bar{3}m$, No. 221, tetragonal t-subgroups

I Maximal *translationengleiche* subgroups

{ [3] $P4/m12/m$ (123, $P4/mmm$) 1; 2; 3; 4; 13; 14; 15; 16; ...
{ [3] $P4/m12/m$ (123, $P4/mmm$) 1; 4; 2; 3; 18; 19; 17; 20; ...
{ [3] $P4/m12/m$ (123, $P4/mmm$) 1; 3; 4; 2; 22; 24; 23; 21; ...

Comments:

If $\boldsymbol{W}_1, \boldsymbol{W}_2, \boldsymbol{W}_3, \ldots$ is the order of the first sequence, then the second sequence follows the order $\boldsymbol{C}^{-1}\boldsymbol{W}_1\boldsymbol{C}$, $\boldsymbol{C}^{-1}\boldsymbol{W}_2\boldsymbol{C}$, $\boldsymbol{C}^{-1}\boldsymbol{W}_3\boldsymbol{C}, \ldots$. Here the $\boldsymbol{C}$ means a threefold rotation and is the conjugating element; for the second subgroup $\boldsymbol{C} = (9)\ y, z, x$ of the general position of $Pm\bar{3}m$; for the third subgroup $\boldsymbol{C} = (5)\ z, x, y$. In this example the columns $\boldsymbol{w}$ of the symmetry operations (and thus of the conjugating elements) are the zero columns $\boldsymbol{o}$ and could be omitted.

The description of the subgroups can be explained by the following four examples.

Example 2.1.3.2.2

$\mathcal{G} = C1m1$, No. 8, UNIQUE AXIS b

I Maximal *translationengleiche* subgroups

[2] $C1$ (1, $P1$) 1+

Comments:

HMS1: $C1$ is not a conventional HM symbol. Therefore, the conventional symbol $P1$ is added as HMS2 after the space-group number 1 of $\mathcal{H}$.

sequence: '1+' means $x, y, z;\ x+\frac{1}{2}, y+\frac{1}{2}, z$.

Example 2.1.3.2.3

$\mathcal{G} = Fdd2$, No. 43

I Maximal *translationengleiche* subgroups

...

[2] $F112$ (5, $A112$) (1; 2)+

Comments:

HMS1: $F112$ is not a conventional HM symbol; therefore, the conventional symbol $A112$ is added to the space-group No. 5 as HMS2. The setting unique axis c is inherited from $\mathcal{G}$.

sequence: (1, 2)+ means:

$$x, y, z;\quad x, y+\tfrac{1}{2}, z+\tfrac{1}{2};\quad x+\tfrac{1}{2}, y, z+\tfrac{1}{2};\quad x+\tfrac{1}{2}, y+\tfrac{1}{2}, z;$$
$$\bar{x}, \bar{y}, z;\quad \bar{x}, \bar{y}+\tfrac{1}{2}, z+\tfrac{1}{2};\quad \bar{x}+\tfrac{1}{2}, \bar{y}, z+\tfrac{1}{2};\quad \bar{x}+\tfrac{1}{2}, \bar{y}+\tfrac{1}{2}, z;$$

Example 2.1.3.2.4

$\mathcal{G} = P4_2/nmc = P4_2/n\,2_1/m\,2/c$, No. 137, ORIGIN CHOICE 2

I Maximal *translationengleiche* subgroups

...

[2] $P2/n\ 2_1/m\ 1$ (59, $Pmmn$) 1; 2; 5; 6; 9; 10; 13; 14

Comments:
HMS1: The sequence of the directions in the HM symbol for a tetragonal space group is **c**, **a**, **a** − **b**. From the parts $4_2/n$, $2_1/m$ and $2/c$ of the full HM symbol of $\mathcal{G}$, only $2/n$, $2_1/m$ and 1 remain in $\mathcal{H}$. Therefore, HMS1 is $P2/n\,2_1/m\,1$, and the conventional symbol *Pmmn* is added as HMS2.
No.: The space-group number of $\mathcal{H}$ is 59. The setting origin choice 2 of $\mathcal{H}$ is inherited from $\mathcal{G}$.
sequence: The coordinate triplets of $\mathcal{G}$ retained in $\mathcal{H}$ are: (1) x, y, z; (2) $\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$; (5) $\bar{x}, y+\frac{1}{2}, \bar{z}$; (6) $x+\frac{1}{2}, \bar{y}, \bar{z}$; (9) $\bar{x}, \bar{y}, \bar{z}$; *etc.*

Example 2.1.3.2.5
$\mathcal{G} = P3_112$, No. 151
I Maximal *translationengleiche* subgroups

[2] $P3_111$ (144, $P3_1$)	1; 2; 3			
⎧ [3] $P112$ (5, $C121$)	1; 6	**b**, −2**a** − **b**, **c**		
⎨ [3] $P112$ (5, $C121$)	1; 4	−**a** − **b**, **a** − **b**, **c**	0, 0, 1/3	
⎩ [3] $P112$ (5, $C121$)	1; 5	**a**, **a** + 2**b**, **c**	0, 0, 2/3	

Comments:
brace: The brace on the left-hand side connects the three conjugate monoclinic subgroups.
HMS1: $P112$ is not the conventional HM symbol for unique axis c but the constituent '2' of the nonconventional HM symbol refers to the directions −2**a** − **b**, **a** − **b** and **a** + 2**b**, in the hexagonal basis. According to the rules of Section 2.1.2.5, the standard setting is unique axis b, as expressed by the HM symbol $C121$.
HMS2: Note that the conventional monoclinic cell is centred.
matrix, shift: The entries in the columns 'matrix' and 'shift' are explained in the following Section 2.1.3.3 and evaluated in Example 2.1.3.3.2.

2.1.3.3. Basis transformation and origin shift

Each t-subgroup $\mathcal{H} < \mathcal{G}$ is defined by its representatives, listed under 'sequence' by numbers each of which designates an element of $\mathcal{G}$. These elements form the general position of $\mathcal{H}$. They are taken from the general position of $\mathcal{G}$ and, therefore, are referred to the coordinate system of $\mathcal{G}$. In the general position of $\mathcal{H}$, however, its elements are referred to the coordinate system of $\mathcal{H}$. In order to allow the transfer of the data from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$, the tools for this transformation are provided in the columns 'matrix' and 'shift' of the subgroup tables. The designation of the quantities is that of *IT* A Part 5 and is repeated here for convenience. The transformation described in this section is not restricted to *translationengleiche* subgroups but is applied to *klassengleiche* subgroups as well.

In the following, columns and rows are designated by boldface italic lower-case letters. Point coordinates $\boldsymbol{x}, \boldsymbol{x}'$, translation parts $\boldsymbol{w}, \boldsymbol{w}'$ of the symmetry operations and shifts $\boldsymbol{p}, \boldsymbol{q} = -\boldsymbol{P}^{-1}\boldsymbol{p}$ are represented by columns. The sets of basis vectors $(\mathbf{a}, \mathbf{b}, \mathbf{c}) = (\boldsymbol{a})^{\mathrm{T}}$ and $(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\boldsymbol{a}')^{\mathrm{T}}$ are represented by rows [indicated by $(\ldots)^{\mathrm{T}}$, which means 'transposed']. The quantities with unprimed symbols are referred to the coordinate system of $\mathcal{G}$, those with primes are referred to the coordinate system of $\mathcal{H}$.

The following columns will be used ($\boldsymbol{w}'$ is analogous to $\boldsymbol{w}$):

$$\boldsymbol{w} = \begin{pmatrix} w_1 \\ w_2 \\ w_3 \end{pmatrix};\ \boldsymbol{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix};\ \boldsymbol{x}' = \begin{pmatrix} x' \\ y' \\ z' \end{pmatrix};\ \boldsymbol{p} = \begin{pmatrix} p_1 \\ p_2 \\ p_3 \end{pmatrix};\ \boldsymbol{q} = \begin{pmatrix} q_1 \\ q_2 \\ q_3 \end{pmatrix}.$$

The (3 × 3) matrices $\boldsymbol{W}$ and $\boldsymbol{W}'$ of the symmetry operations, as well as the matrix $\boldsymbol{P}$ for a change of basis and its inverse $\boldsymbol{Q} = \boldsymbol{P}^{-1}$, are designated by boldface italic upper-case letters ($\boldsymbol{W}'$ is analogous to $\boldsymbol{W}$):

$$\boldsymbol{W} = \begin{pmatrix} W_{11} & W_{12} & W_{13} \\ W_{21} & W_{22} & W_{23} \\ W_{31} & W_{32} & W_{33} \end{pmatrix};\ \boldsymbol{P} = \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix};$$

$$\boldsymbol{Q} = \begin{pmatrix} Q_{11} & Q_{12} & Q_{13} \\ Q_{21} & Q_{22} & Q_{23} \\ Q_{31} & Q_{32} & Q_{33} \end{pmatrix}.$$

Let $\mathbf{a}, \mathbf{b}, \mathbf{c} = (\boldsymbol{a})^{\mathrm{T}}$ be the row of basis vectors of $\mathcal{G}$ and $\mathbf{a}', \mathbf{b}', \mathbf{c}' = (\boldsymbol{a}')^{\mathrm{T}}$ the basis of $\mathcal{H}$, then the basis $(\boldsymbol{a}')^{\mathrm{T}}$ is expressed in the basis $(\boldsymbol{a})^{\mathrm{T}}$ by the system of equations

$$\begin{aligned} \mathbf{a}' &= P_{11}\mathbf{a} + P_{21}\mathbf{b} + P_{31}\mathbf{c} \\ \mathbf{b}' &= P_{12}\mathbf{a} + P_{22}\mathbf{b} + P_{32}\mathbf{c} \\ \mathbf{c}' &= P_{13}\mathbf{a} + P_{23}\mathbf{b} + P_{33}\mathbf{c} \end{aligned} \tag{2.1.3.1}$$

or

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}')^{\mathrm{T}} = (\mathbf{a}, \mathbf{b}, \mathbf{c})^{\mathrm{T}} \begin{pmatrix} P_{11} & P_{12} & P_{13} \\ P_{21} & P_{22} & P_{23} \\ P_{31} & P_{32} & P_{33} \end{pmatrix}. \tag{2.1.3.2}$$

In matrix notation, this is

$$(\boldsymbol{a}')^{\mathrm{T}} = (\boldsymbol{a})^{\mathrm{T}}\boldsymbol{P}. \tag{2.1.3.3}$$

The column $\boldsymbol{p}$ of coordinates of the origin O' of $\mathcal{H}$ is referred to the coordinate system of $\mathcal{G}$ and is called the *origin shift*. The matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$ describes the transformation from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$, for details, *cf. IT* A, Part 5. Therefore, $\boldsymbol{P}$ and $\boldsymbol{p}$ are listed in the subgroup tables in the columns 'matrix' and 'shift', *cf.* Section 2.1.3.2. The column 'matrix' is empty if there is no change of basis, *i.e.* if $\boldsymbol{P}$ is the unit matrix $\boldsymbol{I}$. The column 'shift' is empty if there is no origin shift, *i.e.* if $\boldsymbol{p}$ is the column $\boldsymbol{o}$ consisting of zeroes only.

A change of the coordinate system, described by the matrix–column pair $(\boldsymbol{P}, \boldsymbol{p})$, changes the point coordinates from the column $\boldsymbol{x}$ to the column $\boldsymbol{x}'$. The formulae for this change do not contain the pair $(\boldsymbol{P}, \boldsymbol{p})$ itself, but the related pair $(\boldsymbol{Q}, \boldsymbol{q}) = (\boldsymbol{P}^{-1}, -\boldsymbol{P}^{-1}\boldsymbol{p})$:

$$\boldsymbol{x}' = \boldsymbol{Q}\boldsymbol{x} + \boldsymbol{q} = \boldsymbol{P}^{-1}\boldsymbol{x} - \boldsymbol{P}^{-1}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p}). \tag{2.1.3.4}$$

Not only the point coordinates but also the matrix–column pairs for the symmetry operations are changed by a change of the coordinate system. A symmetry operation W is described in the coordinate system of $\mathcal{G}$ by the system of equations[2]

$$\begin{aligned} \tilde{x} &= W_{11}x + W_{12}y + W_{13}z + w_1 \\ \tilde{y} &= W_{21}x + W_{22}y + W_{23}z + w_2 \\ \tilde{z} &= W_{31}x + W_{32}y + W_{33}z + w_3, \end{aligned} \tag{2.1.3.5}$$

or

$$\tilde{\boldsymbol{x}} = \boldsymbol{W}\boldsymbol{x} + \boldsymbol{w} = (\boldsymbol{W}, \boldsymbol{w})\boldsymbol{x}, \tag{2.1.3.6}$$

i.e. by the matrix–column pair $(\boldsymbol{W}, \boldsymbol{w})$. The symmetry operation W will be described in the coordinate system of the subgroup $\mathcal{H}$ by the equation

[2] Please note that in equation (2.1.3.6) the matrix $\boldsymbol{W}$ is multiplied by the column $\boldsymbol{x}$ from the *right-hand* side whereas in equation (2.1.3.3) the matrix $\boldsymbol{P}$ is multiplied by the row $(\boldsymbol{a})^{\mathrm{T}}$ from the *left-hand* side. Therefore, the running index in $\boldsymbol{W}$ is the second one, whereas in $\boldsymbol{P}$ it is the first one.

$$\tilde{\boldsymbol{x}}' = \boldsymbol{W}'\boldsymbol{x}' + \boldsymbol{w}' = (\boldsymbol{W}', \boldsymbol{w}')\boldsymbol{x}', \qquad (2.1.3.7)$$

and thus by the pair $(\boldsymbol{W}', \boldsymbol{w}')$. This pair can be calculated from the pair $(\boldsymbol{W}, \boldsymbol{w})$ by the equations

$$\boldsymbol{W}' = \boldsymbol{Q}\,\boldsymbol{W}\,\boldsymbol{P} = \boldsymbol{P}^{-1}\boldsymbol{W}\boldsymbol{P} \qquad (2.1.3.8)$$

and

$$\boldsymbol{w}' = \boldsymbol{q} + \boldsymbol{Q}\boldsymbol{w} + \boldsymbol{Q}\boldsymbol{W}\boldsymbol{p} = \boldsymbol{P}^{-1}(\boldsymbol{w} + \boldsymbol{W}\boldsymbol{p} - \boldsymbol{p}) = \boldsymbol{P}^{-1}(\boldsymbol{w} + (\boldsymbol{W} - \boldsymbol{I})\boldsymbol{p}). \qquad (2.1.3.9)$$

These equations are rather complicated and unpleasant. They become simple when using augmented matrices and columns. In this case the formulae are reduced formally to normal matrix multiplication [the formalism is simpler but the necessary calculations are not, because the inversion of a (4×4) matrix is tedious if done by hand].

The matrices $\boldsymbol{P}$, $\boldsymbol{Q}$, $\boldsymbol{W}$ and $\boldsymbol{W}'$ may be combined with the corresponding columns $\boldsymbol{p}$, $\boldsymbol{q}$, $\boldsymbol{w}$ and $\boldsymbol{w}'$ to form (4×4) matrices (callled *augmented matrices*):[3]

$$\mathbb{P} = \left(\begin{array}{ccc|c} P_{11} & P_{12} & P_{13} & p_1 \\ P_{21} & P_{22} & P_{23} & p_2 \\ P_{31} & P_{32} & P_{33} & p_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{Q} = \mathbb{P}^{-1} = \left(\begin{array}{ccc|c} Q_{11} & Q_{12} & Q_{13} & q_1 \\ Q_{21} & Q_{22} & Q_{23} & q_2 \\ Q_{31} & Q_{32} & Q_{33} & q_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{W} = \left(\begin{array}{ccc|c} W_{11} & W_{12} & W_{13} & w_1 \\ W_{21} & W_{22} & W_{23} & w_2 \\ W_{31} & W_{32} & W_{33} & w_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right);$$

$$\mathbb{W}' = \left(\begin{array}{ccc|c} W'_{11} & W'_{12} & W'_{13} & w'_1 \\ W'_{21} & W'_{22} & W'_{23} & w'_2 \\ W'_{31} & W'_{32} & W'_{33} & w'_3 \\ \hline 0 & 0 & 0 & 1 \end{array}\right).$$

The coefficients of these augmented matrices are integer, rational or real numbers.

The (3×1) rows $(\boldsymbol{a})^{\rm T}$ and $(\boldsymbol{a}')^{\rm T}$ must be augmented to (4×1) rows by appending some vectors $\mathbf{s}_{\mathcal{G}}$ and $\mathbf{s}'_{\mathcal{H}}$, respectively, as fourth entries in order to enable matrix multiplication with the augmented matrices:

$$(\mathbb{a})^{\rm T} = (\mathbf{a}, \mathbf{b}, \mathbf{c} \mid \mathbf{s}_{\mathcal{G}})^{\rm T} \quad \text{and} \quad (\mathbb{a}')^{\rm T} = (\mathbf{a}', \mathbf{b}', \mathbf{c}' \mid \mathbf{s}'_{\mathcal{H}})^{\rm T}$$

with $\mathbf{s}'_{\mathcal{H}} = \mathbf{p} + \mathbf{s}_{\mathcal{G}}$. As the vector $\mathbf{s}_{\mathcal{G}}$ one can take the zero vector $\mathbf{s}_{\mathcal{G}} = \mathbf{o}$, which results in $\mathbf{s}'_{\mathcal{H}} = \mathbf{p} = p_1\mathbf{a} + p_2\mathbf{b} + p_3\mathbf{c}$, *i.e.*

$$(\mathbb{a})^{\rm T} = (\mathbf{a}, \mathbf{b}, \mathbf{c} \mid \mathbf{o})^{\rm T} \quad \text{and} \quad (\mathbb{a}')^{\rm T} = (\mathbf{a}', \mathbf{b}', \mathbf{c}' \mid \mathbf{p})^{\rm T}.$$

The relation between $(\mathbb{a}')^{\rm T}$ and $(\mathbb{a})^{\rm T}$ is given by equation (2.1.3.10), which replaces equation (2.1.3.3),

$$(\mathbb{a}')^{\rm T} = (\mathbb{a})^{\rm T}\mathbb{P}. \qquad (2.1.3.10)$$

[3] The horizontal and vertical lines in the augmented matrices are useful to facilitate recognition of their coefficients; they have no mathematical meaning.

Analogously, the (3×1) columns $\boldsymbol{x}$ and $\boldsymbol{x}'$ must be augmented to (4×1) columns by a '1' in the fourth row in order to enable matrix multiplication with the augmented matrices:

$$\mathbb{x} = \left(\begin{array}{c} x \\ y \\ z \\ \hline 1 \end{array}\right); \quad \mathbb{x}' = \left(\begin{array}{c} x' \\ y' \\ z' \\ \hline 1 \end{array}\right).$$

The three equations (2.1.3.4), (2.1.3.8) and (2.1.3.9) are replaced by the two equations

$$\mathbb{x}' = \mathbb{Q}\mathbb{x} = \mathbb{P}^{-1}\mathbb{x} \qquad (2.1.3.11)$$

and

$$\mathbb{W}' = \mathbb{Q}\mathbb{W}\mathbb{P} = \mathbb{P}^{-1}\mathbb{W}\mathbb{P}. \qquad (2.1.3.12)$$

Example 2.1.3.3.1

Consider the data listed for the *t*-subgroups of $Pmn2_1$, No. 31:

Index	HM & No.	sequence	matrix	shift
[2]	$P1n1$ (7, $P1c1$)	1; 3	**c**, **b**, −**a** − **c**	
[2]	$Pm11$ (6, $P1m1$)	1; 4	**c**, **a**, **b**	
[2]	$P112_1$ (4)	1; 2		1/4, 0, 0

This means that the transformation matrices and origin shifts are

$$\boldsymbol{P}_1 = \begin{pmatrix} 0 & 0 & \bar{1} \\ 0 & 1 & 0 \\ 1 & 0 & \bar{1} \end{pmatrix}, \boldsymbol{P}_2 = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}, \boldsymbol{P}_3 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

$$\boldsymbol{p}_1 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \ \boldsymbol{p}_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \ \boldsymbol{p}_3 = \begin{pmatrix} \frac{1}{4} \\ 0 \\ 0 \end{pmatrix}.$$

The first subgroup is monoclinic, the symmetry direction is the b axis, which is standard. However, the glide direction $\frac{1}{2}(\mathbf{a} + \mathbf{c})$ is nonconventional. Therefore, the basis of $\mathcal{G}$ is transformed to a basis of the subgroup $\mathcal{H}$ such that the b axis is retained, the glide direction becomes the c' axis and the a' axis is chosen such that the basis is a right-handed one, the angle $\beta' \geq 90°$ and the transformation matrix $\boldsymbol{P}$ is simple. This is done by the chosen matrix $\boldsymbol{P}_1$. The origin shift is the $\boldsymbol{o}$ column.

With equations (2.1.3.8) and (2.1.3.9), one obtains for the glide reflection $x, \bar{y}, z - \frac{1}{2}$, which is $x, \bar{y}, z + \frac{1}{2}$ after standardization by $0 \leq w_j < 1$.

For the second monoclinic subgroup, the symmetry direction is the (nonconventional) a axis. The rules of Section 2.1.2.5 require a change to the setting 'unique axis b'. A cyclic permutation of the basis vectors is the simplest way to achieve this. The reflection $\bar{x}, y, z$ is now described by $x, \bar{y}, z$. Again there is no origin shift.

The third monoclinic subgroup is in the conventional setting 'unique axis c', but the origin must be shifted onto the 2_1 screw axis. This is achieved by applying equation (2.1.3.9) with $\boldsymbol{p}_3$, which changes $\bar{x} + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ of $Pmn2_1$ to $\bar{x}, \bar{y}, z + \frac{1}{2}$ of $P112_1$.

Example 2.1.3.3.2

Evaluation of the *t*-subgroup data of the space group $P3_112$, No. 151, started in Example 2.1.3.2.5. The evaluation is now continued with the columns 'sequence', 'matrix' and 'shift'. They are used for the transformation of the elements of $\mathcal{H}$ to their conventional form. Only the monoclinic *t*-subgroups are of interest here because the trigonal subgroup is already in the standard setting.

One takes from the tables of subgroups in Chapter 2.3

Index	HM & No.	sequence	matrix	shift
[3]	$P112$ (5, $C121$)	1; 6	$\mathbf{b}, -2\mathbf{a}-\mathbf{b}, \mathbf{c}$	
[3]	$P112$ (5, $C121$)	1; 4	$-\mathbf{a}-\mathbf{b}, \mathbf{a}-\mathbf{b}, \mathbf{c}$	0, 0, 1/3
[3]	$P112$ (5, $C121$)	1; 5	$\mathbf{a}, \mathbf{a}+2\mathbf{b}, \mathbf{c}$	0, 0, 2/3

Designating the three matrices by $\boldsymbol{P}_6, \boldsymbol{P}_4, \boldsymbol{P}_5$, one obtains

$$\boldsymbol{P}_6 = \begin{pmatrix} 0 & -2 & 0 \\ 1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{P}_4 = \begin{pmatrix} -1 & 1 & 0 \\ -1 & -1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{P}_5 = \begin{pmatrix} 1 & 1 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

with the corresponding inverse matrices

$$\boldsymbol{Q}_6 = \begin{pmatrix} -\frac{1}{2} & 1 & 0 \\ -\frac{1}{2} & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{Q}_4 = \begin{pmatrix} -\frac{1}{2} & -\frac{1}{2} & 0 \\ \frac{1}{2} & -\frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}, \ \boldsymbol{Q}_5 = \begin{pmatrix} 1 & -\frac{1}{2} & 0 \\ 0 & \frac{1}{2} & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

and the origin shifts

$$\boldsymbol{p}_6 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \ \boldsymbol{p}_4 = \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} \end{pmatrix}, \ \boldsymbol{p}_5 = \begin{pmatrix} 0 \\ 0 \\ \frac{2}{3} \end{pmatrix}.$$

For the three new bases this means

$$\mathbf{a}'_6 = \mathbf{b}, \ \mathbf{b}'_6 = -2\mathbf{a}-\mathbf{b}, \ \mathbf{c}'_6 = \mathbf{c}$$
$$\mathbf{a}'_4 = -\mathbf{a}-\mathbf{b}, \ \mathbf{b}'_4 = \mathbf{a}-\mathbf{b}, \ \mathbf{c}'_4 = \mathbf{c} \text{ and}$$
$$\mathbf{a}'_5 = \mathbf{a}, \ \mathbf{b}'_5 = \mathbf{a}+2\mathbf{b}, \ \mathbf{c}'_5 = \mathbf{c}.$$

All these bases span ortho-hexagonal cells with twice the volume of the original hexagonal cell because for the matrices $\det(\boldsymbol{P}_i) = 2$ holds.

In the general position of $\mathcal{G} = P3_112$, No.151, one finds

$$(1)\ x, y, z; \ (4)\ \bar{y}, \bar{x}, \bar{z}+\tfrac{2}{3}; \ (5)\ \bar{x}+y, y, \bar{z}+\tfrac{1}{3}; \ (6)\ x, x-y, \bar{z}.$$

These entries represent the matrix–column pairs ($\boldsymbol{W}$, $\boldsymbol{w}$):

$$(1)\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}; \quad (4)\begin{pmatrix} 0 & \bar{1} & 0 \\ \bar{1} & 0 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{2}{3} \end{pmatrix};$$

$$(5)\begin{pmatrix} \bar{1} & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ \frac{1}{3} \end{pmatrix}; \quad (6)\begin{pmatrix} 1 & 0 & 0 \\ 1 & \bar{1} & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}, \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}.$$

Application of equations (2.1.3.8) on the matrices $\boldsymbol{W}_k$ and (2.1.3.9) on the columns $\boldsymbol{w}_k$ of the matrix–column pairs results in

$$\boldsymbol{W}'_4 = \boldsymbol{W}'_5 = \boldsymbol{W}'_6 = \begin{pmatrix} \bar{1} & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & \bar{1} \end{pmatrix}; \ \boldsymbol{w}'_4 = \boldsymbol{w}'_6 = \boldsymbol{o}; \ \boldsymbol{w}'_5 = \begin{pmatrix} 0 \\ 0 \\ \bar{1} \end{pmatrix}.$$

All translation vectors of $\mathcal{G}$ are retained in the subgroups but the volume of the cells is doubled. Therefore, there must be centring-translation vectors in the new cells. For example, the application of equation (2.1.3.9) with ($\boldsymbol{P}_6$, $\boldsymbol{p}_6$) to the translation of $\mathcal{G}$ with the vector $-\mathbf{a}$, *i.e.* $\boldsymbol{w} = -(1, 0, 0)$, results in the column $\boldsymbol{w}' = (\frac{1}{2}, \frac{1}{2}, 0)$, *i.e.* the centring translation $\frac{1}{2}(\mathbf{a}' + \mathbf{b}')$ of the subgroup. Either by calculation or, more easily, from a small sketch one sees that the vectors $-\mathbf{b}$ for $\boldsymbol{P}_4$, $\mathbf{a}+\mathbf{b}$ for $\boldsymbol{P}_5$ (and $-\mathbf{a}$ for $\boldsymbol{P}_6$) correspond to the cell-centring translation vectors of the subgroup cells.

Comments:

This example reveals that the conjugation of conjugate subgroups does not necessarily imply the conjugation of the representatives of these subgroups in the general positions of *IT* A. The three monoclinic subgroups $C121$ in this example are conjugate in the group $\mathcal{G}$ by the 3_1 screw rotation. Conjugation of the representatives (4) and (6) by the 3_1 screw rotation of $\mathcal{G}$ results in the column $\boldsymbol{w}_5 = 0, 0, \frac{4}{3}$, which is standardized according to the rules of *IT* A to $\boldsymbol{w}_5 = 0, 0, \frac{1}{3}$. Thus, the conjugacy relation is disturbed by the standardization of the representative (5).

2.1.4. II Maximal *klassengleiche* subgroups (*k*-subgroups)

2.1.4.1. *General description*

The listing of the maximal *klassengleiche* subgroups (maximal *k*-subgroups) $\mathcal{H}$ of the space group $\mathcal{G}$ is divided into the following three blocks for practical reasons:

• **Loss of centring translations**. Maximal subgroups $\mathcal{H}$ of this block have the same conventional unit cell as the original space group $\mathcal{G}$. They are always non-isomorphic and have index 2 for plane groups and index 2, 3 or 4 for space groups.

• **Enlarged unit cell**. Under this heading, maximal subgroups of index 2, 3 and 4 are listed for which the *conventional* unit cell has been enlarged. The block contains isomorphic *and* non-isomorphic subgroups with this property.

• **Series of maximal isomorphic subgroups**. In this block *all* maximal isomorphic subgroups of a space group $\mathcal{G}$ are listed in a small number of infinite series of subgroups with no restriction on the index, *cf.* Sections 2.1.2.4 and 2.1.5.

The description of the subgroups is the same within the same block but differs between the blocks. The partition into these blocks differs from the partition in *IT* A, where the three blocks are called 'maximal non-isomorphic subgroups IIa', 'maximal non-isomorphic subgroups IIb' and 'maximal isomorphic subgroups of lowest index IIc'.

The kind of listing in the three blocks of this volume is discussed in Sections 2.1.4.2, 2.1.4.3 and 2.1.5 below.

2.1.4.2. *Loss of centring translations*

Consider a space group $\mathcal{G}$ with a centred lattice, *i.e.* a space group whose HM symbol does not start with the lattice letter P but with one of the letters A, B, C, F, I or R. The block contains those maximal subgroups of $\mathcal{G}$ which have fully or partly lost their centring translations and thus are not *t*-subgroups. The *conventional* unit cell is *not* changed.

Only in space groups with an F-centred lattice can the centring be partially lost, as is seen in the list of the space group $Fmmm$, No. 69. On the other hand, for $F23$, No. 196, the maximal subgroups $P23$, No. 195, or $P2_13$, No. 198, have lost all their centring translations.

For the block 'Loss of centring translations', the listing in this volume is the same as that for *t*-subgroups, *cf.* Section 2.1.3. The centring translations are listed explicitly where applicable, *e.g.* for space group $C2$, No. 5, unique axis b

[2] $P12_11$ (4)   1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$ 1/4, 0, 0.

In this line, the representatives 1; $2 + (\frac{1}{2}, \frac{1}{2}, 0)$ of the general position are x, y, z $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$.

The listing differs from that in *IT* A in only two points:

(1) the full HM symbol is taken as the conventional symbol for monoclinic space groups, whereas in *IT* A the short HM symbol is the conventional one;
(2) the information needed for the transformation of the data from the setting of the space group $\mathcal{G}$ to that of $\mathcal{H}$ is added. In this example, the matrix is the unit matrix and is not listed; the column of origin shift is $\frac{1}{4}, 0, 0$. This transformation is analogous to that of *t*-subgroups and is described in detail in Section 2.1.3.3.

The sequence of the subgroups in this block is one of decreasing space-group number of the subgroups.

2.1.4.3. Enlarged unit cell

Under the heading 'Enlarged unit cell', those maximal *k*-subgroups $\mathcal{H}$ are listed for which the conventional unit cell is enlarged relative to the unit cell of the original space group $\mathcal{G}$. *All* maximal *k*-subgroups with enlarged unit cell of index 2, 3 or 4 of the plane groups and of the space groups are listed *individually*. The listing is restricted to these indices because 4 is the highest index of a maximal *non-isomorphic* subgroup, and the number of these subgroups is finite. Maximal subgroups of higher indices are always isomorphic to $\mathcal{G}$ and their number is infinite.

The description of the subgroups with enlarged unit cell is more detailed than in *IT* A. In the block IIb of *IT* A, different maximal subgroups of the same space-group type with the same lattice relations are represented by the same entry. For example, the eight maximal subgroups of the type *Fmmm*, No. 69, of space group *Pmmm*, No. 47, are represented by one entry in *IT* A.

In the present volume, the description of the maximal subgroups in the block 'Enlarged unit cell' refers to each subgroup individually and contains for each of them a set of space-group generators and the transformation from the setting of the space group $\mathcal{G}$ to the conventional setting of the subgroup $\mathcal{H}$.

Some of the isomorphic subgroups listed in this block may also be found in *IT* A in the block 'Maximal isomorphic subgroups of lowest index IIc'.

Subgroups with the same lattice are collected in small blocks. The heading of each such block consists of the index of the subgroup and the lattice relations of the sublattice relative to the original lattice. Basis vectors that are not mentioned are not changed.

Example 2.1.4.3.1

This example is taken from the table of space group $C222_1$, No. 20.

• **Enlarged unit cell**

[3] $\mathbf{a}' = 3\mathbf{a}$

{ $C222_1$	(20)	$\langle 2; 3\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	
$C222_1$	(20)	$\langle (2; 3) + (2, 0, 0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$1, 0, 0$
$C222_1$	(20)	$\langle (2; 3) + (4, 0, 0)\rangle$	$3\mathbf{a}, \mathbf{b}, \mathbf{c}$	$2, 0, 0$

[3] $\mathbf{b}' = 3\mathbf{b}$

{ $C222_1$	(20)	$\langle 2; 3\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	
$C222_1$	(20)	$\langle 3; 2 + (0, 2, 0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 1, 0$
$C222_1$	(20)	$\langle 3; 2 + (0, 4, 0)\rangle$	$\mathbf{a}, 3\mathbf{b}, \mathbf{c}$	$0, 2, 0$

The entries mean:

Columns 1 and 2: HM symbol and space-group number of the subgroup; *cf.* Section 2.1.3.2.

Column 3: generators, here the pairs

$$\begin{array}{ll} \bar{x}, \bar{y}, z+\frac{1}{2}; & \bar{x}, y, \bar{z}+\frac{1}{2}; \\ \bar{x}+2, \bar{y}, z+\frac{1}{2}; & \bar{x}+2, y, \bar{z}+\frac{1}{2}; \\ \bar{x}+4, \bar{y}, z+\frac{1}{2}; & \bar{x}+4, y, \bar{z}+\frac{1}{2}; \\ & \\ \bar{x}, \bar{y}, z+\frac{1}{2}; & \bar{x}, y, \bar{z}+\frac{1}{2}; \\ \bar{x}, \bar{y}+2, z+\frac{1}{2}; & \bar{x}, y, \bar{z}+\frac{1}{2}; \\ \bar{x}, \bar{y}+4, z+\frac{1}{2}; & \bar{x}, y, \bar{z}+\frac{1}{2}; \end{array}$$

for the six lines listed in the same order.

Column 4: basis vectors of $\mathcal{H}$ referred the basis vectors of $\mathcal{G}$. $3\mathbf{a}, \mathbf{b}, \mathbf{c}$ means $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$; $\mathbf{a}, 3\mathbf{b}, \mathbf{c}$ means $\mathbf{a}' = \mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = \mathbf{c}$.

Column 5: origin shifts, referred to the coordinate system of $\mathcal{G}$. These origin shifts by **o**, **a** and 2**a** for the first triplet of subgroups and **o**, **b** and 2**b** for the second triplet of subgroups are translations of $\mathcal{G}$. The subgroups of each triplet are conjugate, indicated by the left braces.

Often the lattice relations above the data describing the subgroups are the same as the basis vectors in column 4, as in this example. They differ in particular if the sublattice of $\mathcal{H}$ is non-conventionally centred. Examples are the *H*-centred subgroups of trigonal and hexagonal space groups.

The sequence of the subgroups is determined

(1) by the index of the subgroup such that the subgroups of lowest index are given first;
(2) within the same index by the kind of cell enlargement;
(3) within the same cell enlargement by the No. of the subgroup, such that the subgroup of highest space-group number is given first.

2.1.4.3.1. Enlarged unit cell, index 2

For sublattices with twice the volume of the unit cell, the sequence of the different cell enlargements is as follows:

(1) Triclinic space groups:
 (i) $\mathbf{a}' = 2\mathbf{a}$,
 (ii) $\mathbf{b}' = 2\mathbf{b}$,
 (iii) $\mathbf{c}' = 2\mathbf{c}$,
 (iv) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
 (v) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
 (vi) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
 (vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.

(2) Monoclinic space groups:
 (*a*) with *P* lattice, unique axis *b*:
  (i) $\mathbf{b}' = 2\mathbf{b}$,
  (ii) $\mathbf{c}' = 2\mathbf{c}$,
  (iii) $\mathbf{a}' = 2\mathbf{a}$,
  (iv) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, *B*-centring,
  (v) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
  (vi) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,
  (vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *F*-centring.
 (*b*) with *P* lattice, unique axis *c*:
  (i) $\mathbf{c}' = 2\mathbf{c}$,
  (ii) $\mathbf{a}' = 2\mathbf{a}$,
  (iii) $\mathbf{b}' = 2\mathbf{b}$,
  (iv) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, *C*-centring,
  (v) $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, *A*-centring,

(vi) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$, B-centring,
(vii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, F-centring.

(*c*) with C lattice, unique axis b: There are three sublattices of index 2 of a monoclinic C lattice. One has lost its centrings such that a P lattice with the same unit cell remains. The subgroups with this sublattice are listed under 'Loss of centring translations'. The block with the other two sublattices consists of $\mathbf{c}' = 2\mathbf{c}$, C-centring and I-centring. The sequence of the subgroups in this block is determined by the space-group number of the subgroup.

(*d*) with A lattice, unique axis c: There are three sublattices of index 2 of a monoclinic A lattice. One has lost its centrings such that a P lattice with the same unit cell remains. The subgroups with this sublattice are listed under 'Loss of centring translations'. The block with the other two sublattices consists of $\mathbf{a}' = 2\mathbf{a}$, A-centring and I-centring. The sequence of the subgroups in this block is determined by the No. of the subgroup.

(3) Orthorhombic space groups:
(*a*) Orthorhombic space groups with P lattice: Same sequence as for triclinic space groups.
(*b*) Orthorhombic space groups with C (or A) lattice: Same sequence as for monoclinic space groups with C (or A) lattice.
(*c*) Orthorhombic space groups with I and F lattice: There are no subgroups of index 2 with enlarged unit cell.

(4) Tetragonal space groups:
(*a*) Tetragonal space groups with P lattice:
(i) $\mathbf{c}' = 2\mathbf{c}$.
(ii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, C-centring. The conventional setting results in a P lattice.
(iii) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, F-centring. The conventional setting results in an I lattice.
(*b*) Tetragonal space groups with I lattice: There are no subgroups of index 2 with enlarged unit cell.

(5) For trigonal and hexagonal space groups, $\mathbf{c}' = 2\mathbf{c}$ holds.
For rhombohedral space groups referred to hexagonal axes, $\mathbf{a}' = -\mathbf{b}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$ or $\mathbf{a}' = \mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a}$, $\mathbf{c}' = 2\mathbf{c}$ holds.
For rhombohedral space groups referred to rhombohedral axes, $\mathbf{a}' = \mathbf{a} + \mathbf{c}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$, $\mathbf{c}' = \mathbf{b} + \mathbf{c}$ or $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, F-centring holds.

(6) Only cubic space groups with a P lattice have subgroups of index 2 with enlarged unit cell. For their lattices the following always holds: $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $\mathbf{c}' = 2\mathbf{c}$, F-centring.

2.1.4.3.2. Enlarged unit cell, index 3 or 4

With a few exceptions for trigonal, hexagonal and cubic space groups, k-subgroups with enlarged unit cells and index 3 or 4 are isomorphic. To each of the listed sublattices belong either one or several conjugacy classes with three or four conjugate subgroups or one or several normal subgroups. Only the sublattices with the numbers (5)(*a*)(v), (5)(*b*)(i), (5)(*c*)(ii), (6)(iii) and (7)(i) have index 4, all others have index 3. The different cell enlargements are listed in the following sequence:

(1) Triclinic space groups:
(i) $\mathbf{a}' = 3\mathbf{a}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$,
(iii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a} + \mathbf{b}$,
(iv) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = \mathbf{a} + \mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = 2\mathbf{a} + \mathbf{c}$,
(vi) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$, $\mathbf{c}' = \mathbf{a} + \mathbf{c}$,
(vii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{c}' = \mathbf{a} + \mathbf{c}$,
(viii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = \mathbf{a} + \mathbf{b}$, $\mathbf{c}' = 2\mathbf{a} + \mathbf{c}$,
(ix) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{c}' = 2\mathbf{a} + \mathbf{c}$,
(x) $\mathbf{b}' = 3\mathbf{b}$,
(xi) $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = \mathbf{b} + \mathbf{c}$,
(xii) $\mathbf{b}' = 3\mathbf{b}$, $\mathbf{c}' = 2\mathbf{b} + \mathbf{c}$,
(xiii) $\mathbf{c}' = 3\mathbf{c}$.

(2) Monoclinic space groups:
(*a*) Space groups $P121$, $P12_11$, $P1m1$, $P12/m1$, $P12_1/m1$ (unique axis b):
(i) $\mathbf{b}' = 3\mathbf{b}$,
(ii) $\mathbf{c}' = 3\mathbf{c}$,
(iii) $\mathbf{a}' = \mathbf{a} - \mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$,
(iv) $\mathbf{a}' = \mathbf{a} - 2\mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a}$.
(*b*) Space groups $P112$, $P112_1$, $P11m$, $P112/m$, $P112_1/m$ (unique axis c):
(i) $\mathbf{c}' = 3\mathbf{c}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$,
(iii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$,
(iv) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -2\mathbf{a} + \mathbf{b}$,
(v) $\mathbf{b}' = 3\mathbf{b}$.
(*c*) Space groups $P1c1$, $P12/c1$, $P12_1/c1$ (unique axis b):
(i) $\mathbf{b}' = 3\mathbf{b}$,
(ii) $\mathbf{c}' = 3\mathbf{c}$,
(iii) $\mathbf{a}' = 3\mathbf{a}$,
(iv) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = -2\mathbf{a} + \mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{c}' = -4\mathbf{a} + \mathbf{c}$.
(*d*) Space groups $P11a$, $P112/a$, $P112_1/a$ (unique axis c):
(i) $\mathbf{c}' = 3\mathbf{c}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$,
(iii) $\mathbf{b}' = 3\mathbf{b}$,
(iv) $\mathbf{a}' = \mathbf{a} - 2\mathbf{b}$, $\mathbf{b}' = 3\mathbf{b}$,
(v) $\mathbf{a}' = \mathbf{a} - 4\mathbf{b}$, $\mathbf{b}' = 3\mathbf{b}$.
(*e*) All space groups with C lattice (unique axis b):
(i) $\mathbf{b}' = 3\mathbf{b}$,
(ii) $\mathbf{c}' = 3\mathbf{c}$,
(iii) $\mathbf{a}' = \mathbf{a} - 2\mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$,
(iv) $\mathbf{a}' = \mathbf{a} - 4\mathbf{c}$, $\mathbf{c}' = 3\mathbf{c}$,
(v) $\mathbf{a}' = 3\mathbf{a}$.
(*f*) All space groups with A lattice (unique axis c):
(i) $\mathbf{c}' = 3\mathbf{c}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$,
(iii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -2\mathbf{a} + \mathbf{b}$,
(iv) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = -4\mathbf{a} + \mathbf{b}$,
(v) $\mathbf{b}' = 3\mathbf{b}$.

(3) Orthorhombic space groups:
(i) $\mathbf{a}' = 3\mathbf{a}$,
(ii) $\mathbf{b}' = 3\mathbf{b}$,
(iii) $\mathbf{c}' = 3\mathbf{c}$.

(4) Tetragonal space groups:
(i) $\mathbf{c}' = 3\mathbf{c}$.

(5) Trigonal space groups:
(*a*) Trigonal space groups with hexagonal P lattice:
(i) $\mathbf{c}' = 3\mathbf{c}$,
(ii) $\mathbf{a}' = 3\mathbf{a}$, $\mathbf{b}' = 3\mathbf{b}$, H-centring,
(iii) $\mathbf{a}' = \mathbf{a} - \mathbf{b}$, $\mathbf{b}' = \mathbf{a} + 2\mathbf{b}$, $\mathbf{c}' = 3\mathbf{c}$, R lattice,
(iv) $\mathbf{a}' = 2\mathbf{a} + \mathbf{b}$, $\mathbf{b}' = -\mathbf{a} + \mathbf{b}$, $\mathbf{c}' = 3\mathbf{c}$, R lattice,
(v) $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$.

(*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

By Y. Billiet

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 *IT* A 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 $p > 2$; $p = 4n - 1$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
	$P4_1$ (76)	prime $p > 4$; $p = 4n + 1$ no conjugate subgroups	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$

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

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

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 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 $\boldsymbol{P}$ and $\boldsymbol{P}^{-1}$ 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.* $\mathbf{a}'_{\rm hex} = \mathbf{a}_{\rm hex}$, $\mathbf{b}'_{\rm hex} = \mathbf{b}_{\rm hex}$, $\mathbf{c}'_{\rm hex} = p\,\mathbf{c}_{\rm hex}$, and the origin shift $0, 0, u$. We discuss the basis transformation first. It can be written

$$(\mathbf{a}'_{\rm hex})^{\rm T} = (\mathbf{a}_{\rm hex})^{\rm T}\boldsymbol{X} \qquad (2.1.5.1)$$

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

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

With rhombohedral axes, equation (2.1.5.1) would be written

$$(\mathbf{a}'_{\rm rh})^{\rm T} = (\mathbf{a}_{\rm rh})^{\rm T}\boldsymbol{Y}, \qquad (2.1.5.2)$$

with the matrix $\boldsymbol{Y}$ to be determined.

The transformation from hexagonal to rhombohedral axes is described by

$$(\mathbf{a}_{\rm rh})^{\rm T} = (\mathbf{a}_{\rm hex})^{\rm T}\boldsymbol{P}^{-1}, \qquad (2.1.5.3)$$

where the matrices

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

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

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

From equation (2.1.5.4) it follows that

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

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

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

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

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

The column of the origin shift $\boldsymbol{u}_{\rm hex} = 0, 0, u$ in hexagonal axes must be transformed by $\boldsymbol{u}_{\rm rh} = \boldsymbol{P}\boldsymbol{u}_{\rm hex}$. The result is the column $\boldsymbol{u}_{\rm rh} = u,\ u,\ u$ 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 $(\frac{3p}{4}-\frac{5}{4})\mathbf{b}$ 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 $\mathcal{H}$. □

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 $\mathcal{H}=P1$. 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, 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. 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 the space-group number (in parentheses). The space groups are ordered by ascending space-group number. If this line

[4] 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 $\mathcal{G}$.

is empty, the heading is printed nevertheless and the content is announced by 'none', as in $P6/mmm$, No. 191. Note that the real setting of the supergroup and thus its HM symbol may be nonconventional.

Example 2.1.6.2.1

Let $\mathcal{H} = P2_12_12$, No. 18. Among the entries of the block one finds the space groups of the crystal class *mmm*: [2] *Pbam*, No. 55; [2] *Pccn*, No. 56; [2] *Pbcm*, No. 57; [2] *Pnnm*, No. 58; [2] *Pmmn*, No. 59 and [2] *Pbcn*, No. 60, designated by their standard HM symbols. However, the full HM symbols $P2_1/b\,2_1/a\,2/m$, $P2_1/c\,2_1/c\,2/n$, $P2/b\,2_1/c\,2_1/m$, $P2_1/n\,2_1/n\,2/m$, $P2_1/m\,2_1/m\,2/n$ and $P2_1/b\,2/c\,2_1/n$ reveal that only the four HM symbols *Pbam*, *Pccn*, *Pnnm* and *Pmmn* of these six entries describe supergroups of $P2_12_12$. The symbols $P2/b\,2_1/c\,2_1/m$ and $P2_1/b\,2/c\,2_1/n$ represent four supergroups of $P2_12_12$, namely $\mathcal{G} = P2_1/b\,2_1/m\,2/a$, $P2_1/m\,2_1/a\,2/b$, $P2_1/c\,2_1/n\,2/b$ and $P2_1/n\,2_1/c\,2/a$. This is not obvious but will be derived, as well as the origin shift if necessary, with the procedure described in Examples 2.1.7.3.2 and 2.1.7.4.3.

The supergroups listed in this block represent space groups only if the lattice conditions of $\mathcal{H}$ fulfil the lattice conditions for $\mathcal{G}$. This is not a problem if group $\mathcal{H}$ and supergroup $\mathcal{G}$ belong to the same crystal family,[5] *cf.* Example 2.1.6.2.1. Otherwise the lattice parameters of $\mathcal{H}$ have to be checked correspondingly, as in Example 2.1.6.2.2.

Example 2.1.6.2.2

Space group $\mathcal{H} = P222$, No. 16. For the minimal supergroups $\mathcal{G} = Pmmm$, No. 47, *Pnnn*, No. 48, *Pccm*, No. 49, and *Pban*, No. 50, there is no lattice condition because *P*222 and all these supergroups belong to the same orthorhombic crystal family and thus are space groups. If, however, a space group of the types $\mathcal{G} = P422$, No. 89, $P4_222$, No. 93, $P\bar{4}2m$, No. 111, or $P\bar{4}2c$, No. 112, is considered as a supergroup of $\mathcal{H} = P222$, two of the three independent lattice parameters *a*, *b*, *c* of *P*222 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 *P*222 has to be transformed to the *c*-axis setting of *P*422. For the cubic supergroup *P*23, No. 195, all three lattice parameters of *P*222 must be (approximately) equal. If they are not, elements of $\mathcal{G}$ are not isometries and $\mathcal{G}$ is an affine group which is only isomorphic to a space group.

The lattice conditions are useful in the search for supergroups $\mathcal{G} > \mathcal{H}$ which are space groups, *i.e.* form the symmetry of crystal structures. Whereas a subgroup $\mathcal{H} < \mathcal{G}$ does not become noticeable in the lattice parameters of a space group $\mathcal{G}$, a space group $\mathcal{G} > \mathcal{H}$ of another crystal family must be indicated by the lattice parameters of the space group $\mathcal{H}$. Thus it may be an important advantage if the conditions of temperature, pressure or composition allow the start of the search for possible phase transitions of the low-symmetry phase.

As mentioned already, the number of the minimal *t*-supergroups cannot be taken or concluded from the subgroup tables. It is different in the different cases of Example 2.1.6.2.2 above. The space group *P*222 has one minimal supergroup of the type *Pmmm* and one of *Pnnn*; there are three minimal supergroups of type *Pccm*, namely *Pccm*, *Pmaa* and *Pbmb*, as well as three minimal supergroups of type *Pban*, *viz*. *Pban*, *Pncb* and *Pcna*. There are six minimal supergroups of the type *P*422 and four minimal supergroups of the type *P*23; they are space groups if the lattice conditions are fulfilled. The number of different supergroups will be calculated in Examples 2.1.7.3.1 and 2.1.7.4.2 by the procedure described in Section 2.1.7.4.

[5] For the term 'crystal family' see Section 1.2.5.2 or, for more details, *IT* A, Section 8.2.7.

2.1.6.3. II Minimal non-isomorphic klassengleiche supergroups

If $\mathcal{G}$ is a *k*-supergroup of $\mathcal{H}$, $\mathcal{G}$ and $\mathcal{H}$ always belong to the same crystal family and there are no lattice restrictions for $\mathcal{H}$.

As mentioned above, in the tables of this volume only non-isomorphic minimal *k*-supergroups are listed among the supergroup data; no isomorphic minimal supergroups are given. 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 empty subblock is then designated by 'none'; in the other subblock the supergroups are listed. The kind of listing depends on the subblock. Examples may be found in the tables of *P*222, No. 16, and $Fd\bar{3}c$, No. 228.

As discussed in Section 2.1.7.1, there is exactly one supergroup for each of the non-isomorphic *k*-supergroup entries of $\mathcal{H}$, although often not in the conventional setting. A transformation of the general-position representatives or of the generators to the conventional setting may be necessary to obtain the standard HM symbol of $\mathcal{G}$ in the same way as in Examples 2.1.7.3.1 and 2.1.7.3.2, which refer to *translationengleiche* supergroups.

Under the heading 'Additional centring translations', the supergroups are listed by their indices and either by their nonconventional HM symbols, with the space-group numbers and the conventional HM symbols in parentheses, or by their conventional HM symbols and only their space-group numbers in parentheses. Examples are provided by space group *Pbca*, No. 61, with both subblocks non-empty and by space group *P*222, No. 16, with supergroups only under the heading 'Additional centring translations'.

Not only the HM symbols but also the centrings themselves may be nonconventional. In this volume, the nonconventional centrings tetragonal *c* ($c4gm$ as a supergroup of $p4gm$) and *h* ($h31m$ as a supergroup of $p31m$) are used for HM symbols of plane groups, tetragonal *C* ($C\bar{4}m2$ as a supergroup of $P\bar{4}m2$), $R_{\rm rev}$ 'reverse', different from the conventional $R_{\rm obv}$ 'obverse' ($R_{\rm rev}3$ as supergroup of *P*3), and *H* (*H*312 as supergroup of *P*312) are used for HM symbols of space groups.

Under the heading 'Decreased unit cell' each supergroup is listed by its index and by its lattice relations, where the basis vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{c}'$ refer to the supergroup $\mathcal{G}$ and the basis vectors **a**, **b** and **c** to the original group $\mathcal{H}$. After these data are listed either the nonconventional HM symbol, followed by the space-group number and the conventional HM symbol in parentheses, or the conventional HM symbol with the space-group number in parentheses. Examples are provided again by space group *Pbca*, No. 61, with both subblocks occupied and space group $F\bar{4}3m$, No. 216, with an empty subblock 'Additional centring translations' but data under the heading 'Decreased unit cell'.

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 $0 \leq w_r < 1$) 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 $0 \le w_r < 1$, *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 $P\,2_1/n\,2_1/c\,2/a$.

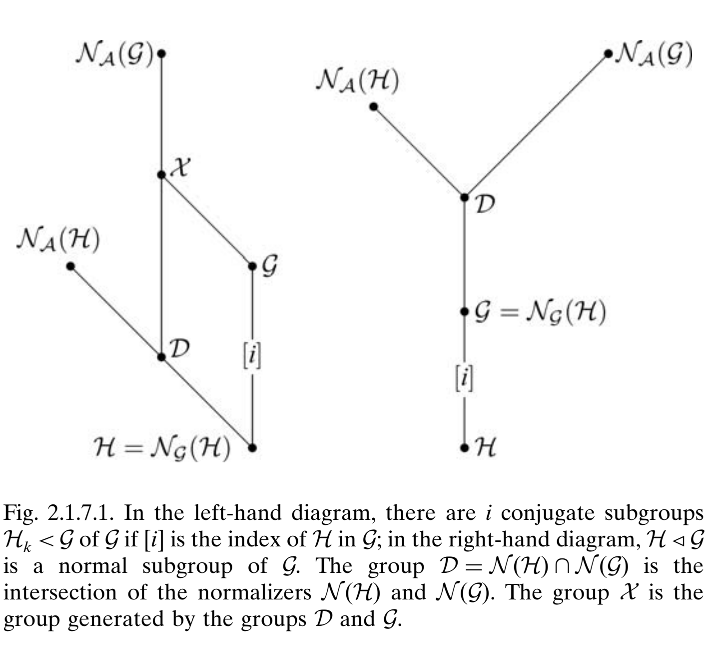

Fig. 2.1.7.1. In the left-hand diagram, there are i conjugate subgroups $\mathcal{H}_k < \mathcal{G}$ of $\mathcal{G}$ if $[i]$ is the index of $\mathcal{H}$ in $\mathcal{G}$; in the right-hand diagram, $\mathcal{H} \triangleleft \mathcal{G}$ is a normal subgroup of $\mathcal{G}$. The group $\mathcal{D} = \mathcal{N}(\mathcal{H}) \cap \mathcal{N}(\mathcal{G})$ 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 *P*222 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 $a \in \mathcal{A}$ such that $a^{-1}\mathcal{G}a = \mathcal{G}_j$. 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 $\mathcal{G} \ge \mathcal{N}_\mathcal{G}(\mathcal{H}) \ge \mathcal{H}$ 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 $\mathcal{T}(\mathcal{N}(\mathcal{G})) \le \mathcal{T}(\mathcal{N}(\mathcal{H}))$ 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 $P1$–$P\bar{1}$ 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 $\bar{1}$ 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 $\mathcal{N}_{\mathcal{A}}(P222) = P(1/2, 1/2, 1/2)m\bar{3}m$, *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, $P\bar{4}2m$, No. 111, and $P\bar{4}2c$, 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 $P\bar{4}2m$. The six supergroups of type $P\bar{4}2c$ 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 $P\bar{4}2c$, 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 $\mathcal{N}_{\mathcal{A}}(P23) = I(1, 1, 1)m\bar{3}m$ 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 relation between the space-group types, keeping in mind the difference between space groups and space-group types, *cf.* Section 1.2.5.3.

The space groups in the graphs are denoted by the standard HM symbols and the space-group numbers. In each graph, each space-group type is displayed at most once. Such graphs are called *contracted graphs* here. Without this contraction, the more complex graphs would be much too large for the page size of this volume.

The symbol of a space group $\mathcal{G}$ is connected by uninterrupted straight lines with the symbols of all its maximal non-isomorphic subgroups or minimal non-isomorphic supergroups. In general, the *maximal subgroups* of $\mathcal{G}$ are drawn on a *lower level* than $\mathcal{G}$; in the same way, the *minimal supergroups* of $\mathcal{G}$ are mostly drawn on a *higher level* than $\mathcal{G}$. For exceptions see Section 2.1.8.3. Multiple lines may occur in the graphs for *t*-subgroups. They are explained in Section 2.1.8.2. No indices are attached to the lines. They can be taken from the corresponding subgroup tables of Chapter 2.3, and are also provided by the general formulae of Section 1.2.8. For the *k*-subgroup graphs, they are further specified at the end of Section 2.1.8.3.

2.1.8.2. *Graphs for translationengleiche subgroups*

Let $\mathcal{G}$ be a space group and $\mathcal{T}(\mathcal{G})$ the normal subgroup of all its translations. Owing to the isomorphism between the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ and the point group $\mathcal{P}_{\mathcal{G}}$, see Section 1.2.5.4, according to the first isomorphism theorem, Ledermann & Weir (1996), *t*-subgroup graphs are the same (up to the symbols) as the corresponding graphs between point groups. However, in this volume, the graphs are not complete but are contracted, displaying each space-group type at most once. This contraction may cause the graphs to look different from the point-group graphs and also different for different space groups of the same point group, *cf.* Example 2.1.8.2.1.

One can indicate the connections between a space group $\mathcal{G}$ and its maximal subgroups in different ways. In the contracted *t*-subgroup graphs one line is drawn for each conjugacy class of maximal subgroups of $\mathcal{G}$. Thus, a line represents the connection to an individual subgroup only if this is a normal maximal subgroup of $\mathcal{G}$, otherwise it represents the connection to more than one subgroup. The conjugacy relations are not necessarily transferable to non-maximal subgroups, *cf.* Example 2.1.8.2.2. On the other hand, multiple lines are possible, see the examples. Although it is not in general possible to reconstruct the complete graph from the contracted one, the content of information of such a graph is higher than that of a graph which is drawn with simple lines only.

The graph for the space group at its top also contains the contracted graphs for all subgroups which occur in it, see Example 2.1.8.2.3.

Owing to lack of space for the large graphs, in all graphs of *t*-subgroups the group *P*1, No. 1, and its connections have been omitted. Therefore, to obtain the full graph one has to supplement the graphs by *P*1 at the bottom and to connect *P*1 by one line to each of the symbols that have no connection downwards.

Within the same graph, symbols on the same level indicate subgroups of the same index relative to the group at the top. The distance between the levels indicates the size of the index. For a more detailed discussion, see Example 2.1.8.2.2. For the sequence and the numbers of the graphs, see the paragraph after Example 2.1.8.2.2.

Example 2.1.8.2.1

Compare the *t*-subgroup graphs in Figs. 2.4.4.2, 2.4.4.3 and 2.4.4.8 of *Pnna*, No. 52, *Pmna*, No. 53, and *Cmce*, No. 64, respectively. The *complete* (uncontracted) *graphs* would have the shape of the graph of the point group *mmm* with *mmm* at the top (first level), seven point groups[7] (222, *mm*2, *m*2*m*, 2*mm*, $112/m$, $12/m1$ and $2/m11$) in the second level, seven point groups (112, 121, 211, 11*m*, 1*m*1, *m*11 and $\bar{1}$) in the third level and the point group 1 at the bottom (fourth level). The group *mmm* is connected to each of the seven subgroups at the second level by one line. Each of the groups of the second level is connected with three groups of the third level by one line. All seven groups of the third level are connected by one line each with the point group 1 at the bottom.

The *contracted graph* of the point group *mmm* would have *mmm* at the top, three point-group types (222, *mm*2 and $2/m$) at the second level and three point-group types (2, *m* and $\bar{1}$) at the third level. The point group 1 at the bottom would not be displayed (no fourth level). Single lines would connect *mmm* with 222, *mm*2 with 2, $2/m$ with 2, $2/m$ with *m* and $2/m$ with $\bar{1}$; a double line would connect *mm*2 with *m*; triple lines would connect *mmm* with *mm*2, *mmm* with $2/m$ and 222 with 2.

The number of fields in a contracted *t*-subgroup graph is between the numbers of fields in the complete and in the contracted point-group graphs. The graph in Fig. 2.4.4.2 of *Pnna*, No. 52, has six space-group types at the second level and four space-group types at the third level. For the graph in Fig. 2.4.4.3 of *Pmna*, No. 53, these numbers are seven and five and for the graph in Fig. 2.4.4.8 of *Cmce*, No. 64 (formerly *Cmca*), the numbers are seven and six. However, in all these graphs the number of connections is always seven from top to the second level and three from each field of the second level downwards to the ground level, independent of the amount of contraction and of the local multiplicity of lines.

Example 2.1.8.2.2

Compare the *t*-subgroup graphs shown in Fig. 2.4.1.1 for $Pm\bar{3}m$, No. 221, and Fig. 2.4.1.5, $Fm\bar{3}m$, No. 225. These graphs are contracted from the point-group graph $m\bar{3}m$. There are altogether nine levels (without the lowest level of *P*1). The indices relative to the top space groups $Pm\bar{3}m$ and $Fm\bar{3}m$ are 1, 2, 3, 4, 6, 8, 12, 16 and 24, corresponding to the point-group orders 48, 24, 16, 12, 8, 6, 4, 3 and 2, respectively. The height of the levels in the graphs reflects the index; the distances between the levels are proportional to the logarithms of the indices but are slightly distorted here in order to adapt to the density of the lines.

From the top space-group symbol there are five lines to the symbols of maximal subgroups: The three symbols at the level of index 2 are those of cubic normal subgroups, the one (tetragonal) symbol at the level of index 3 represents a conjugacy class of three, the symbol $R\bar{3}m$, No. 166, at the level of index 4 represents a conjugacy class of four subgroups.

The graphs differ in the levels of the indices 12 and 24 (orthorhombic, monoclinic and triclinic subgroups) by the number of symbols (nine and seven for index 12, five and three for index 24). The number of lines between neighbouring connected levels depends only on the number and kind of symbols in the upper level.

[7] The HM symbols used here are nonconventional. They display the setting of the point group and follow the rules of *IT* A, Section 2.2.4.

However, for non-maximal subgroups the conjugacy relations may not hold. For example, in Fig. 2.4.1.1, the space group *P*222 has three normal maximal subgroups of type *P*2 and is thus connected to its symbol by a triple line, although these subgroups are conjugate subgroups of the non-minimal supergroup $Pm\bar{3}m$.

Example 2.1.8.2.3

The *t*-subgroup graphs in Figs. 2.4.1.1 and 2.4.1.5 contain the *t*-subgroups of the summits $Pm\bar{3}m$ and $Fm\bar{3}m$ and their relations. In addition, the *t*-subgroup graph of $Pm\bar{3}m$ includes the *t*-subgroup graphs of the cubic summits *P*432, $P\bar{4}3m$, $Pm\bar{3}$ and *P*23, those of the tetragonal summits $P4/mmm$, $P\bar{4}2m$, $P\bar{4}m2$, $P4mm$, *P*422, $P4/m$, $P\bar{4}$ and *P*4, those of the rhombohedral summits $R\bar{3}m$, $R3m$, *R*32, $R\bar{3}$ and *R*3 *etc.*, as well as the *t*-subgroup graphs of several orthorhombic and monoclinic summits. The graph of the summit $Fm\bar{3}m$ includes analogously the graphs of the cubic summits *F*432, $F\bar{4}3m$, $Fm\bar{3}$ and *F*23, of the tetragonal summits $I4/mmm$, $I\bar{4}m2$ *etc.*, also the graphs of rhombohedral summits $R\bar{3}m$ *etc.* Thus, many other graphs are included in the two basic graphs and can be extracted from them. The same holds for the other graphs displayed in Figs. 2.4.1.2 to 2.4.4.8: each of them includes the contracted graphs of all its subgroups as summits. For this reason one does not need 229 or 218 different graphs to cover all *t*-subgroup graphs of the 229 space-group types but only 37 (*P*1 can be excluded as trivial).

The preceding Example 2.1.8.2.3 suggests that one should choose the graphs in such a way that their number can be kept small. It is natural to display the 'big' graphs first and later those smaller graphs that are still missing. This procedure is behind the sequence of the *t*-subgroup graphs in this volume.

(1) The ten graphs of $Pm\bar{3}m$, No. 221, to $Ia\bar{3}d$, No. 230, form the first set of graphs in Figs. 2.4.1.1 to 2.4.1.10.
(2) There are a few cubic space groups left which do not appear in the first set. They are covered by the graphs of $P4_132$, No. 213, $P4_332$, No. 212, and $Pa\bar{3}$, No. 205. These graphs have large parts in common so that they can be united in Fig. 2.4.1.11.
(3) No cubic space group is left now, but only eight tetragonal space groups of crystal class $4/mmm$ have appeared up to now. Among them are all graphs for $4/mmm$ space groups with an *I* lattice which are contained in Figs. 2.4.1.5 to 2.4.1.8 of the *F*-centred cubic space groups. The next 12 graphs, Figs. 2.4.2.1 to 2.4.2.12, are those for the missing space groups of the crystal class $4/mmm$ with lattice symbol *P*. They start with $P4/mcc$, No. 124, and end with $P4_2/ncm$, No. 138.
(4) Four (enantiomorphic) tetragonal space-group types are left which are compiled in Fig. 2.4.2.13.
(5) The next set is formed by the four graphs in Figs. 2.4.3.1 to 2.4.3.4 of the hexagonal space groups $P6/mmm$, No. 191, to $P6_3/mmc$, No. 194. The hexagonal and trigonal enantiomorphic space groups do not appear in these graphs. They are combined in Fig. 2.4.3.5, the last one of hexagonal origin.
(6) Several orthorhombic space groups are still left. They are treated in the eight graphs in Figs. 2.4.4.1 to 2.4.4.8, from *Pmma*, No. 51, to *Cmce*, No. 64 (formerly *Cmca*).
(7) For each space group, the contracted graph of all its *t*-subgroups is provided in at least one of these 37 graphs.

For the index of a maximal *t*-subgroup, Lemma 1.2.8.2.3 is repeated: the index of a maximal non-isomorphic subgroup $\mathcal{H}$ is always 2 for oblique, rectangular and square plane groups and for triclinic, monoclinic, orthorhombic and tetragonal space groups $\mathcal{G}$. The index is 2 or 3 for hexagonal plane groups and for trigonal and hexagonal space groups $\mathcal{G}$. The index is 2, 3 or 4 for cubic space groups $\mathcal{G}$.

2.1.8.3. Graphs for klassengleiche subgroups

There are 29 graphs for *klassengleiche* or *k*-subgroups, one for each crystal class with the exception of the crystal classes 1, $\bar{1}$ and $\bar{6}$ with only one space-group type each: *P*1, No. 1, $P\bar{1}$, No. 2, and $P\bar{6}$, No. 174, respectively. The sequence of the graphs is determined by the sequence of the point groups in *IT* A, Table 2.1.2.1, fourth column. The graphs of $\bar{4}$, $\bar{3}$ and $6/m$ are nearly trivial, because to these crystal classes only two space-group types belong. The graphs of *mm*2 with 22, of *mmm* with 28 and of $4/mmm$ with 20 space-group types are the most complicated ones.

Isomorphic subgroups are special cases of *k*-subgroups. With the exception of both partners of the enantiomorphic space-group types, isomorphic subgroups are not displayed in the graphs. The explicit display of the isomorphic subgroups would add an infinite number of lines from each field for a space group back to this field, or at least one line (*e.g.* a circle) implicitly representing the infinite number of isomorphic subgroups, see the tables of maximal subgroups of Chapter 2.3.[8] Such a line would have to be attached to every space-group symbol. Thus, there would be no more information.

Nevertheless, connections between isomorphic space groups are included indirectly if the group–subgroup chain encloses a space group of another type. In this case, a space group $\mathcal{X}$ may be a subgroup of a space group $\mathcal{Y}$ and $\mathcal{Y}'$ a subgroup of $\mathcal{X}$, where $\mathcal{Y}$ and $\mathcal{Y}'$ belong to the same space-group type. The subgroup chain is then $\mathcal{Y} - \mathcal{X} - \mathcal{Y}'$. The two space groups $\mathcal{Y}$ and $\mathcal{Y}'$ are not identical but isomorphic. Whereas in general the label for the subgroup is positioned at a lower level than that for the original space group, for such relations the symbols for $\mathcal{X}$ and $\mathcal{Y}$ can only be drawn on the same level, connected by horizontal lines. If this happens at the top of a graph, the top level is occupied by more than one symbol (the number of symbols in the top level is the same as the number of symmorphic space-group types of the crystal class).

Horizontal lines are drawn as left or right arrows depending on the kind of relation. The arrow is always directed from the supergroup to the subgroup. If the relation is two-sided, as is always the case for enantiomorphic space-group types, then the relation is displayed by a pair of horizontal lines, one of them formed by a right and the other by a left arrow. In the graph in Fig. 2.5.1.5 for crystal class *mm*2, the connections of *Pmm*2 with *Cmm*2 and with *Amm*2 are displayed by double-headed arrows instead. Furthermore, some arrows in Fig. 2.5.1.5, crystal class *mm*2, and Fig. 2.5.1.6, *mmm*, are dashed or dotted in order to better distinguish the different lines and to increase clarity.

The different kinds of relations are demonstrated in the following examples.

Example 2.1.8.3.1

In the graph in Fig. 2.5.1.1, crystal class 2, a space group *P*2 may be a subgroup of index 2 of a space group *C*2 by 'Loss of

[8] One could contemplate adding one line for each series of maximal isomorphic subgroups. However, the number of series depends on the rules that define the distribution of the isomorphic subgroups into the series and is thus not constant.

centring translations'. On the other hand, subgroups of $P2$ in the block 'Enlarged unit cell', $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $C2$ (3) belong to the type $C2$, see the tables of maximal subgroups in Chapter 2.3. Therefore, both symbols are drawn at the same level and are connected by a pair of arrows pointing in opposite directions. Thus, the top level is occupied twice. In the graph in Fig. 2.5.1.2 of crystal class *m*, both the top level and the bottom level are each occupied by the symbols of two space-group types.

Example 2.1.8.3.2

There are four symbols at the top level of the graph in Fig. 2.5.1.4, crystal class 222. Their relations are rather complicated. Whereas one can go (by index 2) from *P*222 directly to a subgroup of type *C*222 and *vice versa*, the connection from *F*222 directly to *C*222 is one-way. One always has to pass *C*222 on the way from *F*222 to a subgroup of the types *P*222 or *I*222. Thus, the only maximal subgroup of *F*222 among these groups is *C*222. One can go directly from *P*222 to *F*222 but not to *I*222 *etc*.

Because of the horizontal connecting arrows, it is clear that there cannot be much correspondence between the level in the graphs and the subgroup index. However, in no graph is a subgroup positioned at a higher level than the supergroup.

Example 2.1.8.3.3

Consider the graph in Fig. 2.5.1.6 for crystal class *mmm*. To the space group *Cmmm*, No. 65, belong maximal non-isomorphic subgroups of the 11 space-group types (from left to right) *Ibam*, No. 72, *Cmcm*, No. 63, *Imma*, No. 74, *Pmmn*, No. 59, *Pbam*, No. 55, *Pban*, No. 50, *Pmma*, No. 51, *Pmna*, No. 53, *Cccm*, No. 66, *Pmmm*, No. 47, and *Immm*, No. 71. Although all of them have index 2, their symbols are positioned at very different levels of the graph.

The table for the subgroups of *Cmmm* in Chapter 2.3 lists 22 non-isomorphic *k*-subgroups of index 2, because some of the space-group types mentioned above are represented by two or four different subgroups. This multiplicity cannot be displayed by multiple lines because the density of the lines in some of the *k*-subgroup graphs does not permit this kind of presentation, *e.g.* for *mmm*. The multiplicity may be taken from the subgroup tables in Chapter 2.3, where each non-isomorphic subgroup is listed individually.

Consider the connections from *Cmmm*, No. 65, to *Pbam*, No. 55. There are among others: the direct connection of index 2, the connection of index 4 over *Ibam*, No. 72, the connection of index 8 over *Imma*, No. 74, and *Pmma*, No. 51. Thus, starting from the same space group of type *Cmmm* one arrives at different space groups of the type *Pbam* with different unit cells but all belonging to the same space-group type and thus represented by the same field of the graph.

The index of a *k*-subgroup is restricted by Lemma 1.2.8.2.3 and by additional conditions. For the following statements one has to note that enantiomorphic space groups are isomorphic.

(1) A non-isomorphic maximal *k*-subgroup of an oblique, rectangular or tetragonal plane group or of a triclinic, monoclinic, orthorhombic or tetragonal space group always has index 2.
(2) In general, a non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a trigonal space group $\mathcal{G}$ has index 3. Exceptions are the pairs $P3m1$–$P3c1$, $P31m$–$P31c$, $R3m$–$R3c$, $P\bar{3}1m$–$P\bar{3}1c$, $P\bar{3}m1$–$P\bar{3}c1$ and $R\bar{3}m$–$R\bar{3}c$ with space-group Nos. between 156 and 167. They have index 2.
(3) A non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a hexagonal space group has index 2 or 3.
(4) A non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a cubic space group $\mathcal{G}$ has either index 2 or index 4. The index is 2 if $\mathcal{G}$ has an *I* lattice and $\mathcal{H}$ a *P* lattice or if $\mathcal{G}$ has a *P* lattice and $\mathcal{H}$ an *F* lattice. The index is 4 if $\mathcal{G}$ has an *F* lattice and $\mathcal{H}$ a *P* lattice or if $\mathcal{G}$ has a *P* lattice and $\mathcal{H}$ an *I* lattice.

2.1.8.4. Graphs for plane groups

There are no graphs for plane groups in this volume. The four graphs for *t*-subgroups of plane groups are apart from the symbols the same as those for the corresponding space groups: *p*4*mm*–*P*4*mm*, *p*6*mm*–*P*6*mm*, *p*2*mg*–*Pma*2 and *p*2*gg*–*Pba*2, where the graphs for the space groups are included in the *t*-subgroup graphs in Figs. 2.4.1.1, 2.4.3.1, 2.4.2.1 and 2.4.2.3, respectively.

The *k*-subgroup graphs are trivial for the plane groups *p*1, *p*2, *p*4, *p*3, *p*6 and *p*6*mm* because there is only one plane group in its crystal class. The graphs for the crystal classes 4*mm* and 3*m* consist of two plane groups each: *p*4*mm* and *p*4*gm*, *p*3*m*1 and *p*31*m*. Nevertheless, the graphs are different: the relation is one-sided for the tetragonal plane-group pair as it is in the space-group pair $P6/m$ (175)–$P6_3/m$ (176) and it is two-sided for the hexagonal plane-group pair as it is in the space-group pair $P\bar{4}$ (81)–$I\bar{4}$ (82). The graph for the three plane groups of the crystal class *m* corresponds to the space-group graph for the crystal class 2.

Finally, the graph for the four plane groups of crystal class 2*mm* has no direct analogue among the *k*-subgroup graphs of the space groups. It can be obtained, however, from the graph in Fig. 2.5.1.3 of crystal class $2/m$ by removing the fields of $C2/c$, No. 15, and $P2_1/m$, No. 11, with all their connections to the remaining fields. The replacements are then: $C2/m$, No. 12, by *c*2*mm*, No. 9, $P2/m$, No. 10, by *p*2*mm*, No. 6, $P2/c$, No. 13, by *p*2*mg*, No. 7, and $P2_1/c$, No. 14, by *p*2*gg*, No. 8.

2.1.8.5. Application of the graphs

If a subgroup is not maximal then there must be a group–subgroup chain $\mathcal{G}$–$\mathcal{H}$ of maximal subgroups with more than two members which connects $\mathcal{G}$ with $\mathcal{H}$. There are three possibilities: $\mathcal{H}$ may be a *t*-subgroup or a *k*-subgroup or a general subgroup of $\mathcal{G}$. In the first two cases, the application of the graphs is straightforward because at least one of the graphs will permit one to find the possible chains directly. If $\mathcal{H}$ is a *k*-subgroup of $\mathcal{G}$, isomorphic subgroups have to be included if necessary. If $\mathcal{H}$ is a general subgroup of $\mathcal{G}$ one has to combine *t*- and *k*-subgroup graphs.

There is, however, a severe shortcoming to using contracted graphs for the analysis of group–subgroup relations, and great care has to be taken in such investigations. All subgroups $\mathcal{H}_j$ with the same space-group type are represented by the same field of the graph, but these different non-maximal subgroups may permit different routes to a common original (super)group.

Example 2.1.8.5.1

An example for *translationengleiche* subgroups is provided by the group–subgroup chain $Fm\bar{3}m$ (225)–$C2/m$ (12) of index 12. The contracted graph may be drawn by the program *Subgroupgraph* from the Bilbao Crystallographic Server, http://www.cryst.ehu.es/. It is shown in Fig. 2.1.8.1; each field represents all occurring subgroups of a space-group type: $I4/mmm$, No. 139, represents three subgroups, $R\overline{3}m$, No. 166, represents four subgroups, ... and $C2/m$, No. 12, represents nine subgroups belonging to two conjugacy classes. Fig. 2.1.8.1 is part of the contracted total graph of the *translationengleiche* subgroups of the space group $Fm\overline{3}m$, which is displayed in Fig. 2.4.1.5. With *Subgroupgraph* one can also obtain the *complete graph* between $Fm\overline{3}m$ and the set of all nine subgroups of the type $C2/m$. It is too large to be reproduced here.

More instructive are the complete graphs for different single subgroups of the type $C2/m$ of $Fm\overline{3}m$. They can also be obtained with the program *Subgroupgraph* with the exception of the direction indices. In Fig. 2.1.8.2 such a 'complete' graph is displayed for one of the six subgroups of type $C2/m$ of index 12 whose monoclinic axes point in the $\langle 110\rangle$ directions of $Fm\overline{3}m$. Similarly, in Fig. 2.1.8.3 the complete graph is drawn for one of the three subgroups of $C2/m$ of index 12 whose monoclinic axes point in the $\langle 001\rangle$ directions of $Fm\overline{3}m$. It differs markedly from the contracted graph and from the first complete graph. It is easily seen that it may be very misleading to use the contracted graph or the wrong individual complete graph instead of the right individual complete graph.

In a contracted graph, no basis transformations and origin shifts can be included because they are often ambiguous. In the complete graphs the basis transformations and origin shifts should be listed if these graphs display structural information and not just group–subgroup relations. The group–subgroup relations do not depend on the coordinate systems relative to which the groups are described. On the other hand, the coordinate system is decisive for the coordinates of the atoms of the crystal structures displayed and connected in a Bärnighausen tree. Therefore, for the description of structural relations in a Bärnighausen tree knowledge of the transformations (matrix and column) is essential and great care has to be taken to list them correctly, see Chapter 1.6 and Example 2.1.8.5.4. If one wants to list the transformations in subgroup graphs, one can use the transformations which are presented in the subgroup tables.

The use of the graphs of Chapters 2.4 and 2.5 is advantageous if general subgroups, in particular those of higher indices, are sought. As stated by Hermann's theorem, Lemma 1.2.8.1.2, a Hermann group $\mathcal{M}$ always exists and it is uniquely determined for any specific group–subgroup pair $\mathcal{G} > \mathcal{H}$. If the subgroup relation is general, the group $\mathcal{M}$ divides the chain $\mathcal{G} > \mathcal{H}$ into two subchains, the chain between the *translationengleiche* space groups $\mathcal{G} > \mathcal{M}$ and that between the *klassengleiche* space groups $\mathcal{M} > \mathcal{H}$. Thus, however long and complicated the real chain may be, there is always a chain for which only two graphs are needed: a *t*-subgroup graph for the relation between $\mathcal{G}$ and $\mathcal{M}$ and a *k*-subgroup graph for the relation between $\mathcal{M}$ and $\mathcal{H}$.

For a given pair of space-group types $\mathcal{G} > \mathcal{H}$ and a given index $[i]$, however, there could exist several Hermann groups of different space-group types. The graphs of this volume are very helpful in their determination. The index $[i]$ is the product of the index $[i_P]$, which is the ratio of the crystal class orders of $\mathcal{G}$ and $\mathcal{H}$, and the index $[i_L]$ of the lattice reduction from $\mathcal{G}$ to $\mathcal{H}$, $[i] = [i_P] \cdot [i_L]$. The graphs of *t*-subgroups (Chapter 2.4) are used to find the types of subgroups $\mathcal{Z}$ of $\mathcal{G}$ with index $[i_P]$, belonging to the crystal class of $\mathcal{H}$. From the *k*-graphs (Chapter 2.5) it can be seen whether $\mathcal{Z}$ can be a supergroup of $\mathcal{H}$ with index $[i_L]$ and thus a possible Hermann group $\mathcal{M}$. The following two examples

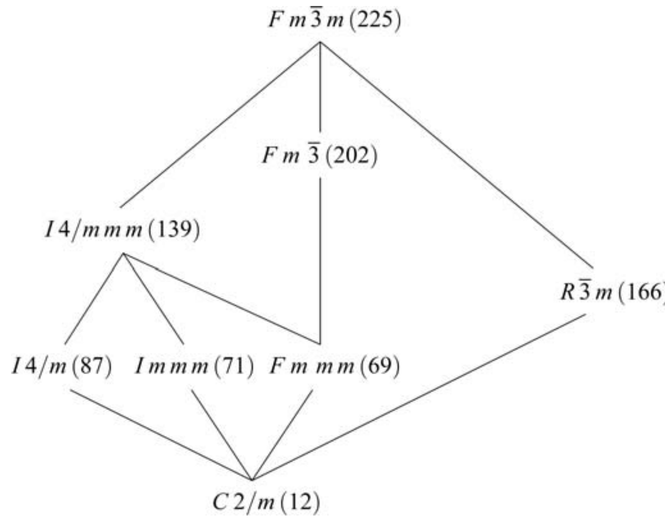

Fig. 2.1.8.1. Contracted graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one of those subgroups with index 12 which belong to the space-group type $C2/m$ (12). The graph forms part of the total contracted graph of *t*-subgroups of $Fm\overline{3}m$ (Fig. 2.4.1.5).

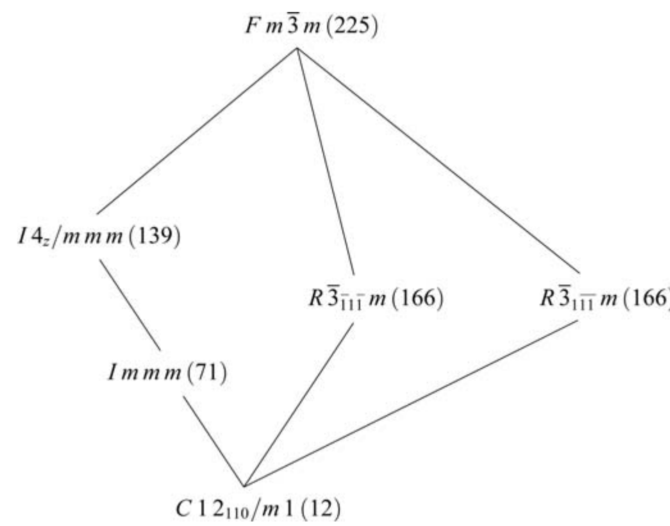

Fig. 2.1.8.2. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one representative belonging to those six $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the $\langle 110\rangle$ directions of $Fm\overline{3}m$. The direction symbols given as subscripts refer to the basis of $Fm\overline{3}m$.

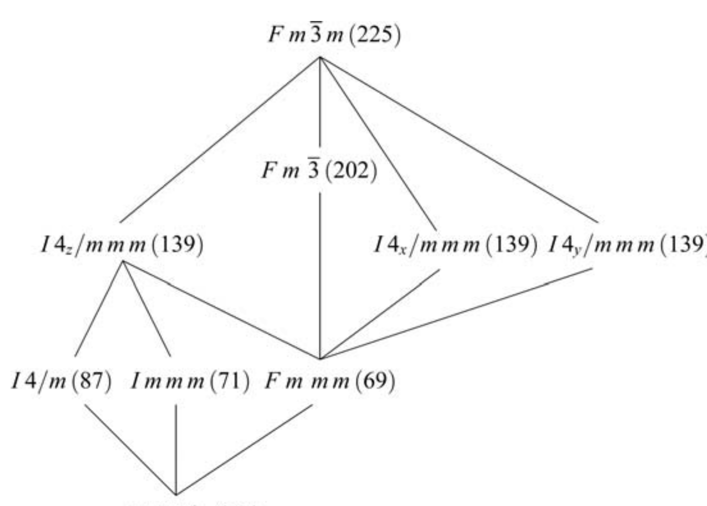

Fig. 2.1.8.3. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to $A112/m$, which is one representative of those three $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the $\langle 001\rangle$ directions of $Fm\overline{3}m$.

illustrate this two-step procedure for the determination of the space-group types of Hermann groups.

Example 2.1.8.5.2

Consider a pair of the space-group types $Pm\bar{3}m > P2_1/m$ with index $[i] = 24$. The factorization of the index $[i]$ into $[i_P] = 12$ and $[i_L] = 2$ follows from the crystal classes of $\mathcal{G}$ and $\mathcal{H}$. From the graph of *t*-subgroups of $Pm\bar{3}m$ (Fig. 2.4.1.1) one finds that there are two space-group types, namely $P2/m$ and $C2/m$, of the relevant crystal class ($2/m$) and index $[i_P] = 12$. Checking the graph (Fig. 2.5.1.3) of the *k*-subgroups of the space groups of the crystal class $2/m$ confirms that space groups of both space-group types $P2/m$ and $C2/m$ have (maximal) $P2_1/m$ subgroups, *i.e.* space groups of both space-group types are Hermann groups for the pair $Pm\bar{3}m > P2_1/m$ of index $[i] = 24$, depending on the individual space group $P2_1/m$.

Example 2.1.8.5.3

The determination of the space-group types of the Hermann groups for the pair $Im\bar{3}m$ (No. 229) > $Cmcm$ (No. 63) of index $[i] = 12$ follows the same procedure as in the previous example. The index $[i] = 12$ is factorized into $[i_P] = 6$ and $[i_L] = 2$ taking into account the orders of the point groups of $\mathcal{G}$ and $\mathcal{H}$. The graph of *t*-subgroups of $Im\bar{3}m$ (Fig. 2.4.1.9) shows that the subgroups of the space-group types $Fmmm$ and $Immm$ are candidates for Hermann groups. Reference to the graph of *k*-subgroups of the crystal class mmm (Fig. 2.5.1.6) indicates that $Immm$ has no maximal subgroups of $Cmcm$ type, *i.e.* only space groups of $Fmmm$ type can be Hermann groups for the pair $Im\bar{3}m > Cmcm$ of index $[i] = 12$.

Apart from the chains $\mathcal{G} \geq \mathcal{M} \geq \mathcal{H}$ that can be found by the above considerations, other chains may exist. In some relatively simple cases, the graphs of this volume may be helpful to find such chains. However, one has to take into account that the tabulated graphs are contracted ones. In particular this means that they contain nothing about the numbers of subgroups of a certain kind and on their relations, for example conjugacy relations.

The following practical example may display the situation. It is based on the combination of the graphs of Chapters 2.4 and 2.5 with the subgroup tables of Chapters 2.2 and 2.3.

Example 2.1.8.5.4

Let $\mathcal{G}$ be a space group of type $Pm\bar{3}m$, No. 221. What are its subgroups $\mathcal{H}_i$ of type $I4/mcm$, No. 140, and index 6?

As the order of the crystal class is reduced from cubic (48) to tetragonal (16) by index 3, the reduction of the translation subgroup must have index 2. To find the Hermann group $\mathcal{M}$, we look in the subgroup table of $Pm\bar{3}m$ for tetragonal *t*-subgroups and find one class of three conjugate maximal *t*-subgroups of crystal class $4/mmm$: $P4/mmm$, No. 123. By each of the three conjugate subgroups one of the axes **a**, **b** or **c** is distinguished. As this distinguished direction is kept in the other steps, one can take one of the conjugates as the representative and can continue with the consideration of only this representative. For the representative direction we choose the **c** axis, because this is the standard setting of $P4/mmm$. The relations of the other conjugates can then be obtained by replacing **c** by **a** or **b**.

The coordinate systems of $Pm\bar{3}m$ and $P4/mmm$ are the same, but $\mathbf{c} \neq \mathbf{a}, \mathbf{b}$ is possible for $P4/mmm$. In the subgroup table of $P4/mmm$ one looks for subgroups of type $I4/mcm$ and index 2 and finds four non-conjugate subgroups with the same basis but different origin shifts. There can be no other subgroups of type $I4/mcm$ because $P4/mmm$ is the only possible Hermann group $\mathcal{M}$. Are there other chains from $Pm\bar{3}m$ to the subgroups $I4/mcm$?

Such a new chain of subgroups must have two steps. The first one leads from $Pm\bar{3}m$ to a *k*-subgroup. In the graph for *k*-subgroups of $Pm\bar{3}m$ one finds two subgroups of index 2, namely $Fm\bar{3}m$ and $Fm\bar{3}c$. One finds from the corresponding graphs of *t*-subgroups or from the subgroup tables that only $Fm\bar{3}c$ has subgroups of space-group type $I4/mcm$. The subgroup tables of $Pm\bar{3}m$ and $Fm\bar{3}c$ show that there are two non-conjugate subgroups of type $Fm\bar{3}c$ which each have one conjugacy class of three subgroups of type $I4/mcm$. For the preferred direction **c** only one of the conjugate subgroups is relevant. Therefore, there are two subgroups $I4/mcm$ of index 2 belonging to chains passing $Fm\bar{3}c$. It follows that two of the four subgroups obtained from Hermann's group are also subgroups of $Fm\bar{3}c$ and two are not.

The two common subgroups are found by comparing their origin shifts from $Pm\bar{3}m$, which must be the same for both ways. The use of (4×4) matrices is convenient. The relevant equations for the bases and origin shifts are:

$$\mathbb{P}_1 = \left(\begin{array}{ccc|c} 2 & 0 & 0 & 0 \\ 0 & 2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \cdot \left(\begin{array}{ccc|c} \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{4} \\ -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) = \left(\begin{array}{ccc|c} 1 & 1 & 0 & \frac{1}{2} \\ -1 & 1 & 0 & \frac{1}{2} \\ 0 & 0 & 2 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

leading to an origin shift of $(\frac{1}{2}, \frac{1}{2}, 0)$ and

$$\mathbb{P}_2 = \left(\begin{array}{ccc|c} 2 & 0 & 0 & \frac{1}{2} \\ 0 & 2 & 0 & \frac{1}{2} \\ 0 & 0 & 2 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right) \cdot \left(\begin{array}{ccc|c} \frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{4} \\ -\frac{1}{2} & \frac{1}{2} & 0 & \frac{1}{4} \\ 0 & 0 & 1 & 0 \\ \hline 0 & 0 & 0 & 1 \end{array}\right) = \left(\begin{array}{ccc|c} 1 & 1 & 0 & 1 \\ -1 & 1 & 0 & 1 \\ 0 & 0 & 2 & \frac{1}{2} \\ \hline 0 & 0 & 0 & 1 \end{array}\right),$$

leading to an origin shift of $(1, 1, \frac{1}{2})$, which is equivalent to $(0, 0, \frac{1}{2})$ because an integer origin shift means only the choice of another conventional origin.

The result is Fig. 2.1.8.4, which is a complete graph, *i.e.* each field of the graph represents exactly one space group. The names of the substances belonging to the different subgroups show that the occurrence of such unexpected relations is not unrealistic. The crystal structures of $KCuF_3$ and *LT*-$SrTiO_3$ both belong to the space-group type $I4/mcm$. They can be derived by different distortions from the same ideal perovskite ABX_3 structure, space group $Pm\bar{3}m$ (Figs. 2.1.8.4 and 2.1.8.5). The subgroup realized by *LT*-$SrTiO_3$ is not a subgroup of $Fm\bar{3}c$. The other subgroup, which is realized by $KCuF_3$, is a subgroup of $Fm\bar{3}c$. This cannot be concluded from the contracted graphs, but can be seen from the combination of the graphs with the tables or from the complete graph (Billiet, 1981; Koch, 1984; Wondratschek & Aroyo, 2001).

The remaining two subgroups do not form symmetries of distorted perovskites. The listed orbits of the Wyckoff positions, 4*a*, 4*b*, 4*c*, 4*d* and 8*e*, are all *extraordinary orbits*, *i.e.* they have more translations than the lattice of $I4/mcm$, see Engel *et al.* (1984). In *Strukturbericht* 1 (1931) the possible space groups for the cubic perovskites are listed on p. 301; there are five possible space groups from $P23$ to $Pm\bar{3}m$. The latter space-group symbol is framed and is considered to be the *true*

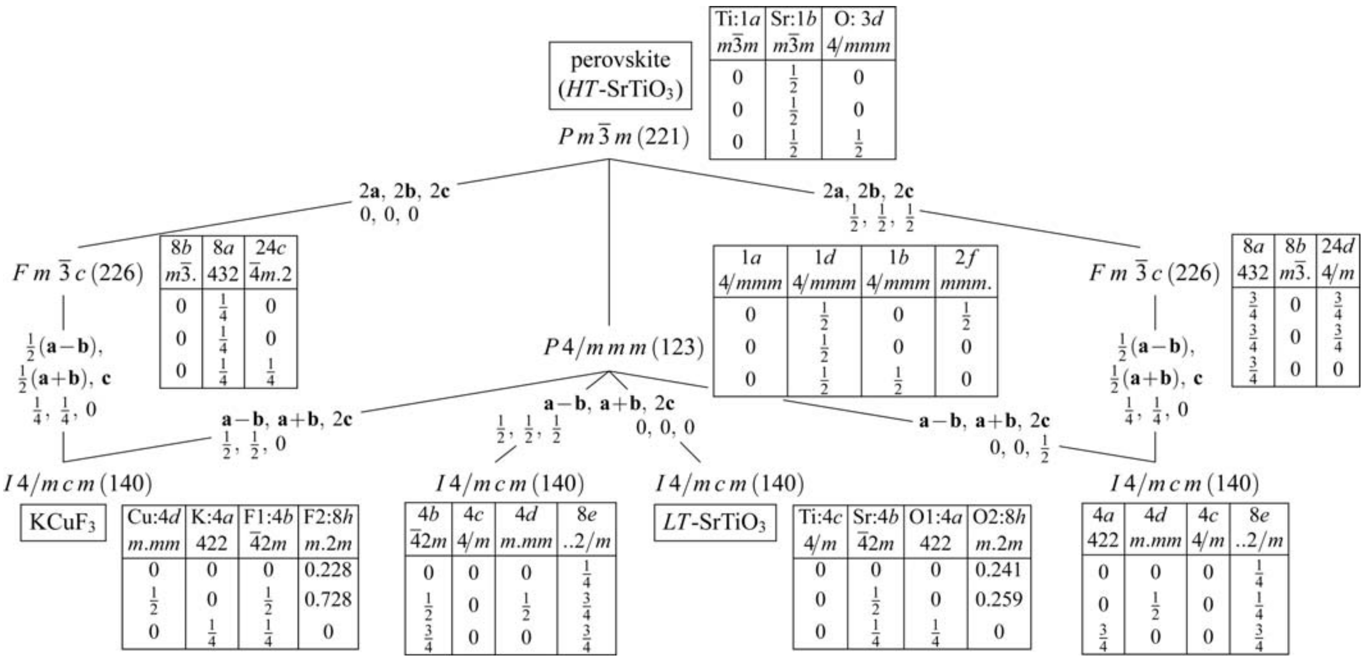

Fig. 2.1.8.4. Complete graph of the group–subgroup chains from perovskite, $Pm\overline{3}m$, here high-temperature $SrTiO_3$, to the four subgroups of type *I*4/*mcm* with their tetragonal axes in the **c** direction. Two of them correspond to $KCuF_3$ and low-temperature $SrTiO_3$. The transformations and origin shifts given in the connecting lines specify the basis vectors and origins of the maximal subgroups in terms of the bases of the preceding space groups (Bärnighausen tree as explained in Section 1.6.3).

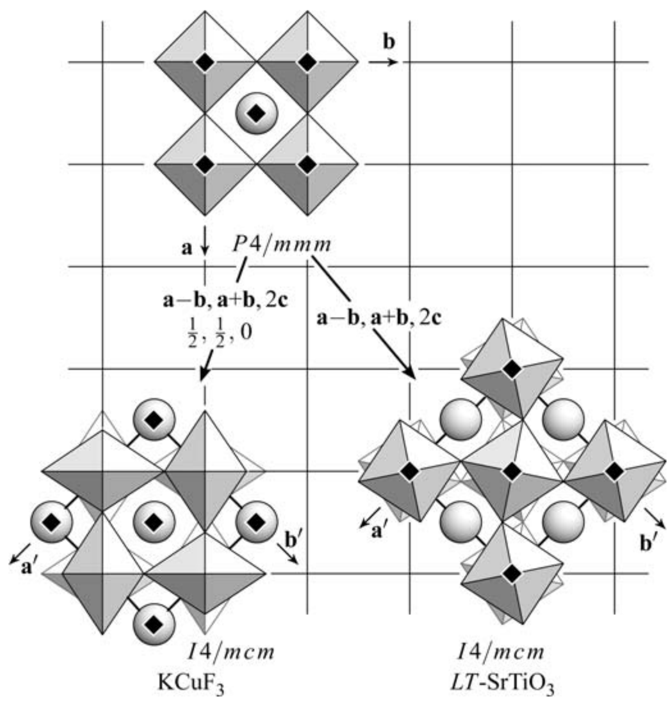

Fig. 2.1.8.5. Two different subgroups of *P*4/*mmm*, both of type *I*4/*mcm*, correspond to two kinds of distortions of the coordination octahedra of the perovskite structure. The difference is due to the origin shift by $\frac{1}{2}, \frac{1}{2}, 0$ on the left side, resulting in a different selection of the fourfold rotation axes that are retained in the subgroups.

symmetry of cubic perovskites. The other space groups are *t*-subgroups of $Pm\overline{3}m$. They would be taken if for some reason the site symmetries of the orbits would contradict the site symmetries of $Pm\overline{3}m$. Similarly, the true symmetry of these tetragonal perovskite derivatives would be *P*4/*mmm* with the original (only tetragonally distorted) lattice and not *I*4/*mcm*.[9] For the two (empty) subgroups *I*4/*mcm* a distorted variant of the perovskite structure does not exist. Other special positions or the general position of the original cubic space group have to be occupied if the space group *I*4/*mcm* shall be realized. This example shows clearly the difference between the subgroup graphs of group theory and the Bärnighausen trees of crystal chemistry.

[9] The restriction to *t*-subgroups in the space-group tables of *Strukturbericht* 1 is probably a consequence of the fact that only these subgroups of space groups were known in 1931. No tetragonal perovskites are described in that volume. In the later volumes, *Strukturbericht* 2 *ff.*, the listing of the space-group tables has been discontinued.

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