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2.1. Guide to the subgroup tables and graphs

By Hans Wondratschek and Mois I. Aroyo

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. These items are listed either individually, or as members of (infinite) series, or both. 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* (2002), 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 rule 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. 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 2.1.7.

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. More detailed descriptions are given in the following sections.

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 $\mathcal{G}$. 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 $\mathcal{H}$ 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, 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 been always 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) 24 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 here 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 immediately from the data for the maximal isomorphic subgroups.

For details, see Section 2.1.6.

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 $\mathcal{H}$ 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.

[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'.

2.1.2.5.1. *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 similar 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 $Ia\overline{3}d > I4_1/acd$, 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 standard 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. 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 subgroup data for the two settings of *R*3 shows that the subgroups $P3_2$ (145), $P3_1$ (144) and *P*3 (143) of index 3 appear in the block 'Loss of centring translations' for the hexagonal setting and in the block 'Enlarged unit cell' for the rhombohedral setting.

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.

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*-subgroups 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 2.1.3.2.1 and 2.1.3.2.2.

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.

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

Example 2.1.3.2.1.
$\mathcal{G}$: $C1m1$, 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 2.1.3.2.2.
$\mathcal{G}$: $Fdd2$, 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; $x, y+\frac{1}{2}, z+\frac{1}{2}$; $x+\frac{1}{2}, y, z+\frac{1}{2}$; $x+\frac{1}{2}, y+\frac{1}{2}, z$;
$\bar{x}, \bar{y}, z$; $\bar{x}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$; $\bar{x}+\frac{1}{2}, \bar{y}, z+\frac{1}{2}$; $\bar{x}+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$;

Example 2.1.3.2.3.
$\mathcal{G}$: $P4_2/nmc = P4_2/n\,2_1/m\,2/c$, 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 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 2.1.3.2.4.
$\mathcal{G}$: $P3_112$, 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.

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 $\mathbf{a}, \mathbf{b}, \mathbf{c} = (\boldsymbol{a})^{\rm T}$ be the row of basis vectors of $\mathcal{G}$ and $\mathbf{a}', \mathbf{b}', \mathbf{c}' = (\boldsymbol{a}')^{\rm T}$ the basis of $\mathcal{H}$, then the basis $(\boldsymbol{a}')^{\rm T}$ is expressed in the basis $(\boldsymbol{a})^{\rm T}$ by the system of equations[2]

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

or

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

In matrix notation, this is

$$(\boldsymbol{a}')^{\rm T} = (\boldsymbol{a})^{\rm T}\,\boldsymbol{P}. \qquad (2.1.3.3)$$

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 chosen 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 $(\boldsymbol{Q},\ \boldsymbol{q}) = (\boldsymbol{P}^{-1},\ -\boldsymbol{P}^{-1}\boldsymbol{p})$:

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

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

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

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

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

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

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

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

and

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

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	$\mathbf{c}, \mathbf{b}, -\mathbf{a}-\mathbf{c}$	
[2]	$Pm11$ (6, $P1m1$)	1; 4	$\mathbf{c}, \mathbf{a}, \mathbf{b}$	
[2]	$P112_1$ (4)	1; 2		1/4, 0, 0

This means that the matrices and origin shifts are

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

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

(3) 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 $0 \leq w_j < 1$.

(4) 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.

(5) 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 2.1.3.2.4. 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.

[2] The system of equations (2.1.3.1) is similar but not identical to the system of equations (2.1.3.5), which describes a symmetry operation W by the matrix $\boldsymbol{W}$ and the column $\boldsymbol{w}$. Both $\boldsymbol{W}$ and $\boldsymbol{w}$ are listed as the general position in the space-group tables of *IT* A, *cf.* Part 5 and Chapter 11.2 of *IT* A. The essential difference is 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 $(\boldsymbol{a})^{\rm T}$ 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.

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 representative (4) by the 3_1 screw rotation of $\mathcal{G}$ results in the representative (5) with the column $\boldsymbol{w}_5 = 0, 0, \frac{4}{3}$, which is not exactly the representative (5) but one of its translationally equivalent elements of $\mathcal{G}$ retained in $\mathcal{H}$.

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) $\mathcal{H}_j$ 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 $x, y, z \quad \bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z}$.

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

$\bar{x}, \bar{y}, z + \frac{1}{2}; \quad \bar{x}, y, \bar{z} + \frac{1}{2};$
$\bar{x} + 2, \bar{y}, z + \frac{1}{2}; \quad \bar{x} + 2, y, \bar{z} + \frac{1}{2};$
$\bar{x} + 4, \bar{y}, z + \frac{1}{2}; \quad \bar{x} + 4, y, \bar{z} + \frac{1}{2};$

$\bar{x}, \bar{y}, z + \frac{1}{2}; \quad \bar{x}, y, \bar{z} + \frac{1}{2};$
$\bar{x}, \bar{y} + 2, z + \frac{1}{2}; \quad \bar{x}, y, \bar{z} + \frac{1}{2};$
$\bar{x}, \bar{y} + 4, z + \frac{1}{2}; \quad \bar{x}, y, \bar{z} + \frac{1}{2};$

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 $\mathbf{o}$, $\mathbf{a}$ and $2\mathbf{a}$ for the first triplet of subgroups and $\mathbf{o}$, $\mathbf{b}$ and $2\mathbf{b}$ 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 on the generators are omitted):

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 2$; $p \equiv 3 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	$p > 4$; $p \equiv 1 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

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

$[p]$	$\mathbf{c}' = p\mathbf{c}$		
	$P4_3$ (78)	$p > 4$; $p \equiv 1 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	
	$P4_1$ (76)	$p > 2$; $p \equiv 3 \pmod 4$	$\mathbf{a}, \mathbf{b}, p\mathbf{c}$
		no conjugate subgroups	

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

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

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

2.1.5.2. *Basis transformation*

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

Example 2.1.5.2.1.

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

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

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

Example 2.1.5.2.2.

In space group $P\overline{6}$, 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 $q > 0,\ r > 0,\ p = q^2 + r^2 + qr$ and p 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 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 $\mathcal{G}$, $P\overline{4}2c$, 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 $p\mathbf{a}, p\mathbf{b}, \mathbf{c}$ for the transformation matrix. 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 choice 1 and origin choice 2 and for trigonal space groups with rhombohedral lattices with hexagonal axes and rhombohedral axes.

2.1.5.5.1. *Monoclinic space groups*

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

2.1.5.5.2. *Trigonal space groups with rhombohedral lattice*

In trigonal space groups with rhombohedral lattices, the series with hexagonal axes and with rhombohedral axes appear to be rather different. However, the 'rhombohedral' series are the exact transcript of the 'hexagonal' series by the same transformation formulae as are used for the different monoclinic settings. However, the transformation matrices $\boldsymbol{P}$ 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. Here $(\mathbf{a}_{\rm hex})^{\rm T}$ 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 $p \equiv 3 \pmod 4$. On the other hand, translational parts with vectors $(\frac{p}{4}-\frac{1}{4})\mathbf{a}$, $(\frac{3p}{4}-\frac{3}{4})\mathbf{b}$ are introduced in the generators of $\mathcal{H}$ if $p \equiv 1 \pmod 4$ holds.
Another consequence of the fractions $\frac{1}{4}$ and $\frac{3}{4}$ occurring in the generator (3) of $\mathcal{G}$ is the difference in the origin shifts. They are $\frac{1}{2}+u$, v, 0 for $p \equiv 3 \pmod 4$ and u, v, 0 for $p \equiv 1 \pmod 4$. Thus, the one series in origin choice 1 for odd p is split into two series in origin choice 2 for $p \equiv 3 \pmod 4$ and $p \equiv 1 \pmod 4$).[3]

2.1.6. Minimal supergroups

2.1.6.1. *General description*

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

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

The search for supergroups of space groups is much more difficult than the search for subgroups. One of the reasons for this difficulty is that the search for subgroups $\mathcal{H} < \mathcal{G}$ is restricted to the elements of the space group $\mathcal{G}$ itself, whereas the search for supergroups $\mathcal{G} > \mathcal{H}$ has to take into account the whole (continuous) group $\mathcal{E}$ of all isometries. For example, there are only a finite number of subgroups $\mathcal{H}$ of any space group $\mathcal{G}$ for any given index i. On the other hand, there may not only be an infinite number of supergroups $\mathcal{G}$ of a space group $\mathcal{H}$ for a finite index i but even an uncountably infinite number of supergroups of $\mathcal{H}$.

Example 2.1.6.1.2.
Let $\mathcal{H} = P1$. Then there is an infinite number of *t*-supergroups $P\bar{1}$ of index 2 because there is no restriction for the sites of the centres of inversion and thus of the conventional origin of $P\bar{1}$.

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

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

2.1.6.2. *I Minimal translationengleiche supergroups*

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

The supergroups listed on the line **I Minimal *translationengleiche* supergroups** are realized only if the lattice conditions of $\mathcal{H}$ fulfil the lattice conditions for $\mathcal{G}$. For example, if $\mathcal{G} = P422$, No. 89, is a supergroup of $\mathcal{H} = P222$, No. 16, two of the three independent lattice parameters a, b, c of $P222$ must be equal (or in crystallographic practice, approximately equal). These must be a and b if c is the tetragonal axis, b and c if a is the tetragonal axis or c and a if b is the tetragonal axis. In the latter two cases, the setting of $P222$ has to be adapted to the conventional c-axis setting of $P422$. For the cubic supergroup $P23$, No. 195, all three lattice parameters of $P222$ must be (approximately) equal. Such conditions are always to be taken into consideration if the *t*-supergroup belongs to a different crystal family[4] to the original group. Therefore, for $\mathcal{H} = P222$ there is no lattice condition for the supergroup $\mathcal{G} = Pmmm$ because $P222$ and $Pmmm$ belong to the same crystal family.

2.1.6.3. *II Minimal non-isomorphic klassengleiche supergroups*

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

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

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

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

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

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 $Fd\overline{3}c$, No. 228.

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 standard 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'.

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 $F\overline{4}3m$, No. 216, with an empty subblock 'Additional centring translations' but data under the heading 'Decreased unit cell'.

2.1.6.4. *Isomorphic supergroups*

Each space group $\mathcal{G}$ has an infinite number of isomorphic subgroups $\mathcal{H}$ because the number of primes is infinite. For the same reason, each space group $\mathcal{H}$ has an infinite number of isomorphic supergroups $\mathcal{G}$. They are not listed in the tables of this volume because they are implicitly listed among the subgroup data.

2.1.7. The subgroup graphs

2.1.7.1. *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 (2002), Fig. 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. An example is the 'family tree' of Bärnighausen (1980), Fig. 15, now called a *Bärnighausen tree*.

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 2.1.7.3 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 maximal non-isomorphic subgroups $\mathcal{H}$ or minimal non-isomorphic supergroups $\mathcal{S}$ of $\mathcal{G}$. 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 2.1.7.3. Multiple lines may occur in the graphs for *t*-subgroups. They are explained in Section 2.1.7.2. 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 2.1.7.3.

2.1.7.2. *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 (1976), *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 by 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 2.1.7.2.1.

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 2.1.7.2.2. 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 the remark below Example 2.1.7.2.2.

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 2.1.7.2.2. For the sequence and the numbers of the graphs, see the paragraph below Example 2.1.7.2.2.

Example 2.1.7.2.1.

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[5] (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 full 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 2.1.7.2.2.

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 slightly distorted 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. This property makes such graphs particularly useful.

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 $Pm\bar{3}m$.

The *t*-subgroup graphs in Figs. 2.4.1.1 and 2.4.1.5 contain the *t*-subgroups of $Pm\bar{3}m$ (221) and $Fm\bar{3}m$ (225) and their relations. In addition, the *t*-subgroup graph of $Pm\bar{3}m$ includes the *t*-subgroup graphs of *P*432, $P\bar{4}3m$, $Pm\bar{3}$, *P*23, $P4/mmm$, $P\bar{4}2m$, $P\bar{4}m2$, *P*4*mm*, $R\bar{3}m$, *R*3*m etc.*, that of $Fm\bar{3}m$ includes those of *F*432, $F\bar{4}3m$, $Fm\bar{3}$, $I4/mmm$, also $R\bar{3}m$ *etc*. Thus, many other graphs can be extracted from the two basic graphs. 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. 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 2.1.7.2.2 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 $P4_132$ (213), $P4_332$ (212) and $Pa\bar{3}$ (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 space groups of the crystal class $4/mmm$ with lattice symbol *P* and different third and fourth constituents of the HM symbol. They start with $P4/mcc$, No. 124, and end with $P4_2/ncm$, No. 138.
(4) Two (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 $\mathcal{G}$.

2.1.7.3. *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

[5] 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.

determined by the sequence of the point groups in *IT* A, Table 2.1.2.1, fourth column. The graphs of $\overline{4}$, $\overline{3}$ and $6/m$ are nearly trivial, because to these crystal classes only two space-group types belong. The graphs of $mm2$ 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.[6] 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 $mm2$, the connections of $Pmm2$ with $Cmm2$ and with $Amm2$ are displayed by double-headed arrows instead. Furthermore, some arrows in Fig. 2.5.1.5, crystal class $mm2$, 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 2.1.7.3.1.

In the graph in Fig. 2.5.1.1, crystal class 2, a space group $P2$ may be a subgroup of index 2 of a space group $C2$ by 'Loss of 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 occupied twice.

Example 2.1.7.3.2.

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 $P222$ directly to a subgroup of type $C222$ and *vice versa*, the connection from $F222$ directly to $C222$ is one-way. One always has to pass $C222$ on the way from $F222$ to a subgroup of the types $P222$ or $I222$. Thus, the only maximal subgroup of $F222$ among these groups is $C222$. One can go directly from $P222$ to $F222$ but not to $I222$ *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 2.1.7.3.3.

Consider the graph in Fig. 2.5.1.6 for crystal class *mmm*. To the space group *Cmmm* (65) belong maximal non-isomorphic subgroups of the 11 space-group types (from left to right) *Ibam* (72), *Cmcm* (63), *Imma* (74), *Pmmn* (59), *Pbam* (55), *Pban* (50), *Pmma* (51), *Pmna* (53), *Cccm* (66), *Pmmm* (47) and *Immm* (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* (65) to *Pbam* (55). There are among others: the direct connection of index 2, the connection of index 4 over *Ibam* (72), the connection of index 8 over *Imma* (74) and *Pmma* (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 $P3m1$–$P3c1$, $P31m$–$P31c$, $R3m$–$R3c$, $P\overline{3}1m$–$P\overline{3}1c$, $P\overline{3}m1$–$P\overline{3}c1$ and $R\overline{3}m$–$R\overline{3}c$ 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.

2.1.7.4. *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: $p4mm$–$P4mm$, $p6mm$–$P6mm$, $p2mg$–$Pma2$ and $p2gg$–$Pba2$, 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.

[6] 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.

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 $P\overline{4}$ (81)–$I\overline{4}$ (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 $C2/c$ (15) and $P2_1/m$ (11) with all their connections to the remaining fields. The replacements are then: $C2/m$ (12) by *c*2*mm* (9), $P2/m$ (10) by *p*2*mm* (6), $P2/c$ (13) by *p*2*mg* (7) and $P2_1/c$ (14) by *p*2*gg* (8).

2.1.7.5. *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, but the problem is only slightly more complicated. This is because for a general subgroup $\mathcal{H} < \mathcal{G}$, Hermann's theorem 1.2.8.1.2 states the existence of an intermediate group $\mathcal{M}$ with $\mathcal{H} < \mathcal{M} < \mathcal{G}$ and the properties $\mathcal{H} < \mathcal{M}$ is a *k*-subgroup of $\mathcal{M}$ and $\mathcal{M} < \mathcal{G}$ is a *t*-subgroup of $\mathcal{G}$.

Thus, however long and complicated the real chain may be, there is also 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 $\mathcal{H}$.

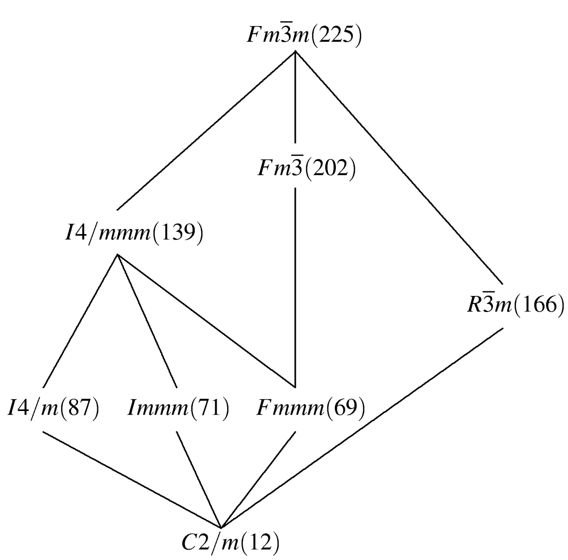

Fig. 2.1.7.1. Contracted graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to those subgroups with index 12 which belong to the space-group type $C2/m$ (12). The graph forms part of the total contracted graph of *t*-subgroups of $Fm\overline{3}m$ (Fig. 2.4.1.5).

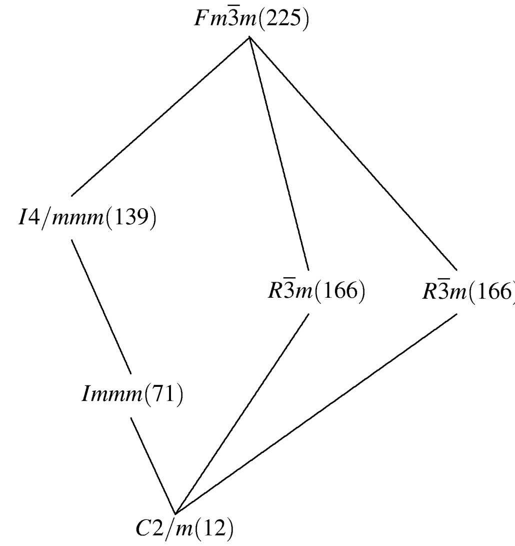

Fig. 2.1.7.2. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one representative of those six $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the ⟨110⟩ directions of $Fm\overline{3}m$.

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 2.1.7.5.1.

An example for *translationengleiche* subgroups is provided by the group–subgroup chain $Fm\overline{3}m$ (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. 2.1.7.1; each field represents all occurring subgroups of a space-group type: $I4/mmm$ (139) represents three subgroups, $R\overline{3}m$ (166) represents four subgroups, … and $C2/m$ (12) represents nine subgroups belonging to two conjugacy classes. Fig. 2.1.7.1 is part of the contracted total graph of the *translationengleiche* subgroups of the space group $Fm\overline{3}m$, which is displayed in Fig.

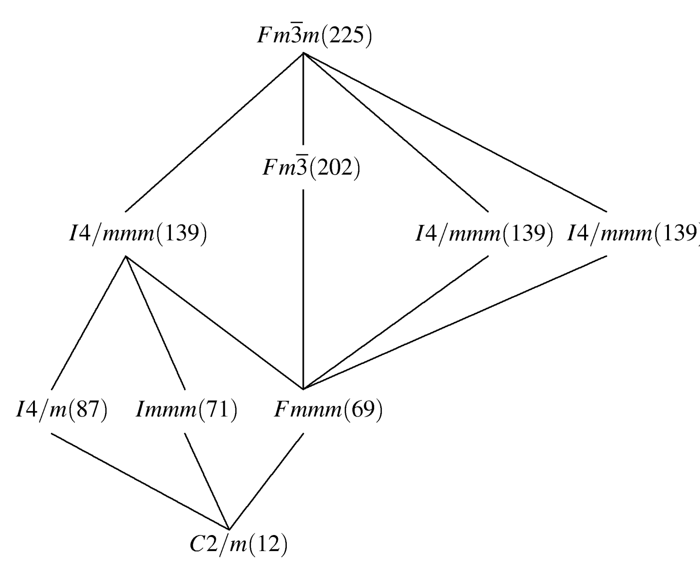

Fig. 2.1.7.3. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one representative of those three $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the ⟨001⟩ directions of $Fm\overline{3}m$.

2.4.1.5. With *Subgroupgraph* one can also obtain the *complete graph* between $Fm\bar{3}m$ 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 $Fm\bar{3}m$. They can be obtained with the program *Symmodes* from the same server as above. In Fig. 2.1.7.2 such a 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 $Fm\bar{3}m$. Similarly, in Fig. 2.1.7.3 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 $Fm\bar{3}m$. 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.

The following example deals with general subgroups.

Example 2.1.7.5.2.

The crystal structures of $SrTiO_3$ and $KCuF_3$ both belong to the space-group type $I4/mcm$, No. 140. They can be derived by different distortions from the same ideal perovskite ABX_3 structure with the space group $Pm\bar{3}m$, No. 221. Common to both chains is Hermann's group $\mathcal{M}$ of space group $P4/mmm$, No. 123, and the unit cell of ABX_3. This is the only intermediate group for $SrTiO_3$. For the pair ABX_3–$KCuF_3$, on the other hand, there exists another chain with an intermediate space group of type $Fm\bar{3}c$, No. 226. The combination of the graph in Fig. 2.4.1.1 for *t*-subgroups with the graph in Fig. 2.5.2.7 for *k*-subgroups is thus possible for both crystal–chemical relations. The combination of the graph in Fig. 2.5.5.5 for *k*-subgroups with the graph in Fig. 2.4.1.6 for *t*-subgroups is, however, only meaningful for the chain ABX_3–$KCuF_3$. This cannot be concluded from the contracted graphs but can be seen from the complete graph, as displayed in Fig. 1 of Wondratschek & Aroyo (2001).

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