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2.1. Guide to the subgroup tables and graphs

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2.1.1. Contents and arrangement of the subgroup tables

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

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

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

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

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

2.1.2. Structure of the subgroup tables

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

2.1.2.1. Headline

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

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

2.1.2.2. Data from IT A

2.1.2.2.1. Generators selected

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

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

2.1.2.2.2. General position

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

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

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

2.1.2.3. Specification of the setting

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

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

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

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

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

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

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

2.1.2.4. Sequence of the subgroup and supergroup data

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

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

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

The block designations are:

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

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

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

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

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

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

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

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

(4) The latter block is split into the listings

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

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

For details, see Section 2.1.6.

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

2.1.2.5. Special rules for the setting of the subgroups

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

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

2.1.2.5.1. Monoclinic subgroups

Rules

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

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

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

Remarks (see also the following examples):

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

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

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

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

Example 2.1.2.5.1

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

II Maximal *klassengleiche* subgroups, Enlarged unit cell

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

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

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

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

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

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

Example 2.1.2.5.2

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

II Maximal *klassengleiche* subgroups, Enlarged unit cell

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

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

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

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

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

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

Example 2.1.2.5.3

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

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

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

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

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

2.1.2.5.2. Subgroups with two origin choices

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

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

The transformation has been chosen such that

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

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

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

Example 2.1.2.5.4

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

I Maximal *translationengleiche* subgroups

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

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

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

Example 2.1.2.5.5

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

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

Example 2.1.2.5.6

Maximal *k*-subgroups of *Pccm*, No. 49. In the block

• **Enlarged unit cell**, [2] $\mathbf{a}' = 2\mathbf{a}$

one finds two subgroups *Pcna* (50, *Pban*). One of them has the origin of $\mathcal{G}$, the origin of the other subgroup is shifted by $\frac{1}{2}, 0, 0$ and is placed on one of the inversion centres of $\mathcal{G}$ that is removed from the first subgroup. The analogous situation is found in the block [2] $\mathbf{b}' = 2\mathbf{b}$, where the two subgroups of space-group type *Pncb* (50, *Pban*) show the analogous relation. In the next block, [2] $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, the four subgroups *Ccce* (68) behave similarly.

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

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

2.1.2.5.3. Space groups with a rhombohedral lattice

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

Rules

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

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

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

Remarks

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

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

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

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

• **Loss of centring translations** none

is listed for the rhombohedral axes setting.

Example 2.1.2.5.7

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

HEXAGONAL AXES

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

RHOMBOHEDRAL AXES

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

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

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

2.1.3.1. Introduction

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

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

2.1.3.2. A description in close analogy with IT A

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

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

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

The symbols have the following meaning:

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

Remarks

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

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

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

No.: the space-group No. of $\mathcal{H}$ is added.
HMS2: In order to specify the setting clearly, the *full* HM symbol is listed for monoclinic subgroups, not the standard (short) HM symbol as in *IT* A.

matrix, shift: These entries contain information on the transformation of $\mathcal{H}$ from the setting of $\mathcal{G}$ to the standard setting of $\mathcal{H}$. They are explained in Section 2.1.3.3.

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

Example 2.1.3.2.1

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

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$$\left\{\begin{array}{ll}[3]\ P4/m12/m\ (123,\ P4/mmm) & 1;\ 2;\ 3;\ 4;\ 13;\ 14;\ 15;\ 16;\ \ldots\\ [3]\ P4/m12/m\ (123,\ P4/mmm) & 1;\ 4;\ 2;\ 3;\ 18;\ 19;\ 17;\ 20;\ \ldots\\ [3]\ P4/m12/m\ (123,\ P4/mmm) & 1;\ 3;\ 4;\ 2;\ 22;\ 24;\ 23;\ 21;\ \ldots\end{array}\right.$$

Comments:

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

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

Example 2.1.3.2.2

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

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

Comments:

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

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

Example 2.1.3.2.3

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

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. . .

[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:

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

Example 2.1.3.2.4

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

I Maximal *translationengleiche* subgroups

. . .

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

references