International Tables for Crystallography (2006). Vol. A1, Section 2.1.2.5, pp. 43–45.

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.

references