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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'.