

2.1. GUIDE TO THE SUBGROUP TABLES AND GRAPHS

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 types¹ 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.

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'.

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.