3.1. Guide to the tables

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In the tables of Chapter 3.2, all maximal subgroups of the space groups are listed. For all Wyckoff positions of a space group the relations to the Wyckoff positions of the subgroups are given. The Wyckoff positions are always labelled by their multiplicities and their Wyckoff letters, in the same manner as in *International Tables for Crystallography*, Volume A (2002). Reference to Volume A therefore is always necessary, especially when the corresponding coordinate triplets or site symmetries are needed. For general remarks on Wyckoff positions see Chapter 1.3.

3.1.1. Arrangement of the entries

Every space group begins on a new page (with the exception of $P4_3$, $P3_2$, $P6_4$ and $P6_5$, which are listed together with $P4_1$, $P3_1$, $P6_2$ and $P6_1$, respectively). If necessary, continuation occurs on the following page(s), or, in a few correspondingly marked cases, on the preceding page.

The different settings for monoclinic space groups are continued on the same or the following page(s).

3.1.1.1. *Headline*

The headline lists from the outer margin inwards:

(1) The *short Hermann–Mauguin symbol*;
(2) The number of the space group according to Volume A;
(3) The *full Hermann–Mauguin symbol* if it differs from the short symbol;
(4) The *Schoenflies symbol*.

In the case of monoclinic space groups, the headline can have one or two additional entries with the full Hermann–Mauguin symbols for different settings.

3.1.1.2. *Specification of the settings*

Each of the monoclinic space groups is listed several times, namely with unique axis *b* and with unique axis *c*, and, if applicable, with the three cell choices 1, 2 and 3 according to Volume A. Space permitting, the entries for the different settings have been combined on one page or on facing pages, since in most cases the Wyckoff-position relations do not depend on the choice of setting. In the few cases where there is a dependence, arrows ($\Rightarrow$) in the corresponding lines show to which settings they refer. Otherwise, the Wyckoff positions of the subgroups correspond to all of the settings listed on the same page or on facing pages.

The comment 'Space groups of the series of isomorphic subgroups appear in different sequences for cell choices 1, 2 and 3' under a table refers to the infinite series of isomorphic subgroups listed at the bottom of a table of a monoclinic space group. For a given index *p* (*p* = prime number) and enlargement of the basis vectors perpendicular to the monoclinic axis, there are $p + 1$ non-conjugate isomorphic maximal subgroups. Their cells can be calculated by formulae such as '**a**, **b**, $p\mathbf{c}$' and '$p\mathbf{a}$, **b**, $q\mathbf{a} + \mathbf{c}$' with an integer parameter *q* taking any value from $-\frac{1}{2}(p-1)$ to $\frac{1}{2}(p-1)$. The same value of *q* may refer to a different subgroup for cell choices 1, 2 or 3.

Rhombohedral space groups are listed only in the setting with hexagonal axes with a rhombohedrally centred obverse cell [*i.e.*

$\pm(\frac{2}{3}, \frac{1}{3}, \frac{1}{3})$]. However, for cubic space groups, the rhombohedral subgroups are also given with rhombohedral axes.

Settings with different origin choices are taken account of by two separate columns 'Coordinates' with the headings 'origin 1' and 'origin 2'.

3.1.1.3. *List of Wyckoff positions*

Under the column heading 'Wyckoff positions', the complete sequence of the Wyckoff positions of the space group is given by their multiplicities and Wyckoff letters. If necessary, the sequence runs over two or more lines.

3.1.1.4. *Subgroup data*

The subgroups are divided into two sections: **I Maximal** *translationengleiche* **subgroups** and **II Maximal** *klassengleiche* **subgroups**. The latter are further subdivided into three blocks:

Loss of centring translations. This block appears only if the space group has a conventionally centred lattice. The centring has been fully or partly lost in the subgroups listed. The size of the conventional unit cell is not changed.

Enlarged unit cell, non-isomorphic. The *klassengleiche* subgroups listed in this block are non-isomorphic and have conventional unit cells that are enlarged compared with the unit cell of the space group.

Enlarged unit cell, isomorphic. The listing includes the isomorphic subgroups with the smallest possible indices for every kind of cell enlargement. If they exist, index values of 2, 3 and 4 are always given (except for $P\bar{1}$, which is restricted to index 2). If the indices 2, 3 or 4 are not possible, the smallest possible index for the kind of cell enlargement considered is listed. In addition, the infinite series of isomorphic subgroups are given for all possible kinds of cell enlargements. The factor of the cell enlargement corresponds to the index, which is a prime number *p*, a square p^2 of a prime number, or a cube p^3 of a prime number (*cf.* Section 3.1.1.6). If $p > 2$, the specifically listed subgroups with small index values also always belong to the infinite series, so that the corresponding information is given twice in these cases. For $p = 2$ this applies only to certain special cases.

3.1.1.5. *Sequence of the listed subgroups*

Within each of the aforementioned blocks, the subgroups are listed in the following order. First priority is given to the index, with smallest values first. Subgroups with the same index follow decreasing space-group numbers (according to Volume A). Exception: the *translationengleiche* subgroup of a tetragonal space group listed last is always the one with the axes transformation to a diagonally oriented cell.

Translationengleiche subgroups of cubic space groups are in the order cubic, rhombohedral, tetragonal, orthorhombic.

In the case of the isomorphic subgroups, there is a subdivision according to the kind of cell enlargement. For monoclinic, tetragonal, trigonal and hexagonal space groups, cell enlargements in the direction of the unique axis are given first. For orthorhombic space groups, the isomorphic subgroups with increased **a** are given first, followed by increased **b** and **c**.

The sequence differs somewhat from that in Chapter 2.3 of this volume. In Chapter 2.3, the *klassengleiche* subgroups have been subdivided in more detail according to the different kinds of cell enlargements and the isomorphic subgroups with specific index values have been listed together with the *klassengleiche* subgroups, *i.e.* separately from the infinite series of isomorphic subgroups. A list of the differences in presentation between Chapters 2.3 and 3.2 is given in the Appendix at the end of this volume.

3.1.1.6. *Information for every subgroup*

3.1.1.6.1. *Index*

The entry for every subgroup begins with the index in brackets, for example [2] or [p] or [p^2] (p = prime number).

The index for any of the infinite number of maximal isomorphic subgroups must be either a prime number p, or, in certain cases of tetragonal, trigonal and hexagonal space groups, a square of a prime number p^2; for isomorphic subgroups of cubic space groups the index may only be the cube of a prime number p^3. In many instances only certain prime numbers are allowed (Bertaut & Billiet, 1979; Billiet & Bertaut, 2002; Müller & Brelle, 1995). If restrictions exist, the prime numbers allowed are given under the axes transformations by formulae such as 'p = prime = $3n - 1$'.

3.1.1.6.2. *Subgroup symbol*

The index is followed by the Hermann–Mauguin symbol (short symbol) and the space-group number of the subgroup. If a nonconventional setting has been chosen, then the space-group symbol of the conventional setting is also mentioned in the following line after the symbol $\widehat{=}$.

In some cases of nonconventional settings, the space-group symbol does not show uniquely in which manner it deviates from the conventional setting. For example, the nonconventional setting $P22_12$ of the space group $P222_1$ can result from cyclic exchange of the axes, $(\mathbf{b}, \mathbf{c}, \mathbf{a})$ or by interchange of $\mathbf{b}$ with $\mathbf{c}$ $(\mathbf{a}, -\mathbf{c}, \mathbf{b})$. As a consequence, the relations between the Wyckoff positions can be different. In such cases, cyclic exchange has always been chosen.

3.1.1.6.3. *Basis vectors*

The column 'Axes' shows how the basis vectors of the unit cell of a subgroup result from the basis vectors $\mathbf{a}$, $\mathbf{b}$ and $\mathbf{c}$ of the space group considered. This information is omitted if there is no change of basis vectors.

A formula such as '$q\mathbf{a} - r\mathbf{b}$, $r\mathbf{a} + q\mathbf{b}$, $\mathbf{c}$' together with the restrictions '$p = q^2 + r^2$ = prime = $4n + 1$' and '$q = 2n + 1 \geq 1$; $r = \pm 2n' \neq 0$' means that for a given index p there exist several subgroups with different lattices depending on the values of the integer parameters q (odd) and r (even) within the limits of the restriction. In this example, the prime number p must be $p \equiv 1$ modulo 4 (*i.e.* 5, 13, 17, ...); if it is, say, $p = 13 = 3^2 + (\pm 2)^2$, the values of q and r may be $q = 3$, $r = 2$ and $q = 3$, $r = -2$.[1]

3.1.1.6.4. *Coordinates*

The column 'Coordinates' shows how the atomic coordinates of the subgroups are calculated from the coordinates x, y and z of the starting unit cell. This includes coordinate shifts whenever a shift of the origin is required (*cf.* Section 3.1.3). If the cell of the subgroup is enlarged, the coordinate triplet is followed by a semicolon; then follow fractional numbers in parentheses. This means that in addition to the coordinates given before the semicolon, further coordinates have to be considered; they result from adding the numbers in the parentheses. However, if the subgroup has a centring, the values to be added due to this centring are not mentioned. If no transformation of coordinates is necessary, the entry is omitted.

Example 3.1.1.6.1.

The entry

$$\tfrac{1}{3}x + \tfrac{1}{4}, y + \tfrac{1}{4}, z; \pm(\tfrac{1}{3}, 0, 0)$$

means: starting from the coordinates of, say, 0.63, 0.12, 0.0, sites with the following coordinates result in the subgroup:

$$0.46, 0.37, 0.0; \quad 0.793333, 0.37, 0.0;$$
$$0.1266667, 0.37, 0.0.$$

Example 3.1.1.6.2.

The entry of an *I*-centred subgroup

$$\tfrac{1}{2}x, \tfrac{1}{2}y, \tfrac{1}{2}z; +(\tfrac{1}{2}, 0, 0); +(0, \tfrac{1}{2}, 0); +(0, 0, \tfrac{1}{2})$$

means: starting from the coordinates of, say, 0.08, 0.14, 0.20, sites with the following coordinates result in the subgroup:

$$0.04, 0.07, 0.10; \quad 0.54, 0.07, 0.10;$$
$$0.04, 0.57, 0.10; \quad 0.04, 0.07, 0.60;$$

in addition, there are all coordinates with $+(\tfrac{1}{2}, \tfrac{1}{2}, \tfrac{1}{2})$ due to the *I*-centring:

$$0.54, 0.57, 0.60; \quad 0.04, 0.57, 0.60;$$
$$0.54, 0.07, 0.60; \quad 0.54, 0.57, 0.10.$$

For the infinite series of isomorphic subgroups, coordinate formulae are, for example, in the form $x, y, \tfrac{1}{p}z; +(0, 0, \tfrac{u}{p})$ with $u = 1, \ldots, p - 1$. Then there are p coordinate values running from $x, y, \tfrac{1}{p}z$ to $x, y, \tfrac{1}{p}z + \tfrac{p-1}{p}$.

Example 3.1.1.6.3.

For a subgroup with index $p^2 = 25$ ($p = 5$) the entry

$$\tfrac{1}{p}x, \tfrac{1}{p}y, z; +(\tfrac{u}{p}, \tfrac{v}{p}, 0); u, v = 1, \ldots, p - 1$$

means: starting from the coordinates of, say, 0.10, 0.35, 0.0, sites with the following coordinates result in the subgroup:

$$0.02, 0.07, 0.0; \quad 0.02, 0.27, 0.0; \quad 0.02, 0.47, 0.0;$$
$$0.02, 0.67, 0.0; \quad 0.02, 0.87, 0.0;$$
$$0.22, 0.07, 0.0; \quad 0.22, 0.27, 0.0; \quad 0.22, 0.47, 0.0;$$
$$0.22, 0.67, 0.0; \quad 0.22, 0.87, 0.0;$$
$$0.42, 0.07, 0.0; \quad 0.42, 0.27, 0.0; \quad 0.42, 0.47, 0.0;$$
$$0.42, 0.67, 0.0; \quad 0.42, 0.87, 0.0;$$
$$0.62, 0.07, 0.0; \quad 0.62, 0.27, 0.0; \quad 0.62, 0.47, 0.0;$$
$$0.62, 0.67, 0.0; \quad 0.62, 0.87, 0.0;$$
$$0.82, 0.07, 0.0; \quad 0.82, 0.27, 0.0; \quad 0.82, 0.47, 0.0;$$
$$0.82, 0.67, 0.0; \quad 0.82, 0.87, 0.0.$$

If Volume A allows two choices for the origin, coordinate transformations for both are listed in separate columns with the headings 'origin 1' and 'origin 2'. If two origin choices are allowed for both the group as well as the subgroup, then it is understood that the origin choices of the group and the subgroup are the same (either origin choice 1 for both groups or origin choice 2 for both). If the space group has only one origin choice, but the subgroup

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[1] If the sum of two square numbers is a prime number p, then it is $p = 2$ or $p = 4n + 1$, and every prime number of this type can be expressed as such a sum. Index number restrictions of this kind occur among isomorphic subgroups of certain tetragonal space groups. A similar relation occurring among trigonal and hexagonal space groups concerns prime numbers $p = q^2 - qr + r^2$; $p = 3$ or $p = 6n + 1$ always holds for integer q, r and every prime number $p = 6n + 1$ can be expressed by such a sum. For details, see Müller & Brelle (1995).

references