3.1. Guide to the tables

BY ULRICH MÜLLER

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 '$\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$' and '$p\mathbf{a}$, $\mathbf{b}$, $q\mathbf{a}+\mathbf{c}$' 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 $\mathbf{a}$ are given first, followed by increased $\mathbf{b}$ and $\mathbf{c}$.