International Tables for Crystallography (2006). Vol. A1, Chapter 3.1, pp. 428–433.

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 $P\overline{1}$, 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, (**b**, **c**, **a**) or by interchange of **b** with **c** (**a**, $-$**c**, **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 **a**, **b** and **c** of the space group considered. This information is omitted if there is no change of basis vectors.

A formula such as 'q**a** $-$ r**b**, r**a** + q**b**, **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; 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; 0.54, 0.07, 0.10;
0.04, 0.57, 0.10; 0.04, 0.07, 0.60;

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

0.54, 0.57, 0.60; 0.04, 0.57, 0.60;
0.54, 0.07, 0.60; 0.54, 0.57, 0.10.

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

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; 0.02, 0.27, 0.0; 0.02, 0.47, 0.0;
0.02, 0.67, 0.0; 0.02, 0.87, 0.0;
0.22, 0.07, 0.0; 0.22, 0.27, 0.0; 0.22, 0.47, 0.0;
0.22, 0.67, 0.0; 0.22, 0.87, 0.0;
0.42, 0.07, 0.0; 0.42, 0.27, 0.0; 0.42, 0.47, 0.0;
0.42, 0.67, 0.0; 0.42, 0.87, 0.0;
0.62, 0.07, 0.0; 0.62, 0.27, 0.0; 0.62, 0.47, 0.0;
0.62, 0.67, 0.0; 0.62, 0.87, 0.0;
0.82, 0.07, 0.0; 0.82, 0.27, 0.0; 0.82, 0.47, 0.0;
0.82, 0.67, 0.0; 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

[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).

has two choices, the coordinate transformations are given for both choices on separate lines.

3.1.1.6.5. *Wyckoff positions*

The columns under the heading 'Wyckoff positions' contain the Wyckoff symbols of all sites of the subgroups that result therefrom. They are given in the same sequence as in the top line(s). If the symbols at the top run over more than one line, then the symbols for the subgroups take a corresponding number of lines.

When an orbit splits into several independent orbits, the corresponding Wyckoff symbols are separated by semicolons, *i.e.* $1b;4h;4k$. An entry such as $3 \times 8j$ means that a splitting into three orbits takes place, all of which are of the same kind $8j$; they differ in the values of their free parameters.

For the infinite series of isomorphic subgroups general formulae are given. They allow the calculation of the Wyckoff-position relations for any index in a simple manner.

Example 3.1.1.6.4.

The entry $\frac{p(p-1)}{2} \times 24k$ means that for a given prime number p, say $p = 5$, there are $\frac{5(5-1)}{2} = 10$ orbits of the kind $24k$.

In some cases of splittings, there is not enough space to enter all Wyckoff symbols on one line; this requires them to be listed one below the other over two or more lines. Whenever a Wyckoff symbol is followed by a semicolon, another symbol follows.

Example 3.1.1.6.5.

The last subgroup listed for space group $I\bar{4}m2$, No. 119, is $I\bar{4}m2$ with basis vectors $p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$. The entry for the Wyckoff position $2a$ is:

$$\left| \begin{array}{l} 2a; \frac{p-1}{2} \times 8g; \\ \quad \frac{p-1}{2} \times 8i; \\ \frac{(p-1)(p-3)}{8} \times 16j \end{array} \right|$$

If $p = 5$, it shows the splitting of an orbit of position $2a$ into one orbit $2a$, two $(\frac{5-1}{2} = 2)$ orbits $8g$, two orbits $8i$ and one $(\frac{(5-1)(5-3)}{8} = 1)$ orbit $16j$.

Sometimes a Wyckoff label is followed by another Wyckoff label in parentheses together with a footnote marker. In this case, the Wyckoff label in parentheses is to be taken for the cases specified in the footnote.

Example 3.1.1.6.6.

The entry $2c(d^*)$ together with the footnote $^*\, p = 4n-1$ means that the Wyckoff position is $2c$, but it is $2d$ if the index is $p \equiv 3$ modulo 4 (*i.e.* $p = 3, 7, 11, \ldots$).

The Wyckoff positions of an isomorphic subgroup of a space group with two choices for the origin are only identical for the two choices if certain origin shifts are taken into account. Since origin shifts have been avoided as far as possible, in some cases some Wyckoff positions differ for the two origin choices.

Example 3.1.1.6.7.

The isomorphic subgroups of the space group $P4_2/n$, No. 86, with cell enlargements $\mathbf{a}$, $\mathbf{b}$, $p\mathbf{c}$ and $p = 4n-1$ result in identical Wyckoff positions for the two origin choices only if there is no origin shift for choice 1, but an origin shift of $0,0,\frac{1}{2}$ for choice 2. The origin shift for choice 2 has been avoided, but as a consequence some of the Wyckoff labels differ for the two choices. For the Wyckoff position $2a$ of the space group, the entry for these isomorphic subgroups is $2a(b^\dagger);\frac{p-1}{2} \times 4f$. The footnote reads '† origin 2 and $p = 4n-1$'. Therefore, $2a$ is (aside from $4f$) the resulting Wyckoff position for origin choice 1 and any value of p; for origin choice 2 it is also $2a$ if $p = 4n+1$, but it is $2b$ if $p = 4n-1$ (the permitted values for p are $p = 4n \pm 1$).

Warning: *The listed Wyckoff positions of the subgroups apply only to the transformations given in the column 'Coordinates'.* If other cell transformations or origin shifts are used, this may result in an interchange of Wyckoff positions within each Wyckoff set of the subgroup.

3.1.2. Cell transformations

When comparing related crystal structures, unit-cell transformations are troublesome. They result in differing sets of atomic coordinates for corresponding atoms; this can make comparisons more complicated and structural relations may be obscured. Frequently, it is more convenient not to interchange axes and to avoid transformations if possible. The use of a nonconventional setting of a space group may be preferable if this reduces cell transformations. For this reason, in the present tables settings of the subgroups were preferentially chosen in such a way that the directions of the basis vectors of a space group and its subgroup deviate as little as possible. If this results in a nonconventional setting of the subgroup, then the way to transform the basis vectors and coordinates to those of the conventional cell is also given.

Subgroups listed in nonconventional settings concern orthorhombic and monoclinic space groups. Their transformations to conventional settings frequently only involve an interchange of axes. In the case of tetragonal subgroups, nonconventional settings with C-centred or F-centred cells are not used; this would have caused nonconventional multiplicities of the Wyckoff positions and would have required listings of all positions in these settings. Equally, face-centred monoclinic cells, B-centred monoclinic cells for unique axis b, C-centred monoclinic cells for unique axis c and hexagonal H cells are not used.

Monoclinic space groups allow different descriptions, such as unique axis a, b or c, base- or body-centred cells, and glide vectors in different directions. All settings that are listed in Volume A have been considered to be allowed conventional settings. Whenever a cell transformation can be avoided and the subgroup conforms to any of the settings listed in Volume A (b or c as unique axis; cell choices 1, 2 or 3), then this setting has been chosen. Transformations to other settings are not given in these cases.

3.1.3. Origin shifts

In a group–subgroup relation, an origin shift may be necessary to conform to the conventional origin setting of the subgroup. This causes coordinate changes for equivalent atomic positions and is therefore undesirable for the purpose of comparing related crystal structures. However, in some cases an origin shift can be avoided if the relations between the basis vectors are chosen in a convenient manner. For example, the isomorphic relation of index 27 (for short: $i27$)

$$F4_132 \xrightarrow{i27} F4_132$$

requires an increase of the lattice parameters by a factor of 3. To conform to the conventional setting, the origin must by displaced when the cell of the subgroup is chosen to be $3\mathbf{a}, 3\mathbf{b}, 3\mathbf{c}$. However, no displacement is necessary when the cell of the subgroup is taken to be $3\mathbf{b}, -3\mathbf{a}, 3\mathbf{c}$. Although the x and $-y$ coordinates exchange

places, this may be more convenient, since no values for an origin shift have to be added. For this reason, the latter option is preferred in this case.

Origin shifts can be specified in terms of the coordinate system of the starting space group or of the coordinate system of the subgroup. In Part 2 of this volume, all origin shifts refer to the starting space group. In Part 3, the origin shifts are contained in the column 'Coordinates' as additive fractional numbers. This means that these shifts refer to the *coordinate system of the subgroup*.

When comparing related crystal structures, it is mainly the atomic coordinates which have to be interconverted. Thus the coordinate conversion formulae are needed anyway; they are given in the column 'Coordinates'. When space groups are involved that allow two origin choices, the origin shifts from a group to a subgroup can be different depending on whether origin choice 1 or 2 has been selected. Therefore, all space groups with two origin choices have two columns 'Coordinates', one for each origin choice. The coordinate conversion formulae for a specific subgroup in the two columns only differ in the additive fractional numbers that specify the origin shift. In addition, origin shifts could also have been specified in terms of the coordinate system of the starting space group. This, however, would have been redundant information that would have required an additional column, causing a serious shortage of space.

The origin shifts listed in the column 'Coordinates' can be converted to origin shifts that refer to the coordinate system of the starting space group in the following way:

Take:

$\mathbf{a}, \mathbf{b}, \mathbf{c}$	basis vectors of the starting space group;
O	origin of the starting space group;
$\mathbf{a}', \mathbf{b}', \mathbf{c}'$	basis vectors of the subgroup;
O'	origin of the subgroup;
$x_{o'}, y_{o'}, z_{o'}$	coordinates of O' expressed in the coordinate system of the starting group;
x'_o, y'_o, z'_o	coordinates of O expressed in the coordinate system of the subgroup.

The basis vectors are related according to

$$(\mathbf{a}', \mathbf{b}', \mathbf{c}') = (\mathbf{a}, \mathbf{b}, \mathbf{c})\boldsymbol{P}.$$

$\boldsymbol{P}$ is the 3×3 transformation matrix of the basis change. The origin shift $O \rightarrow O'$ then corresponds to the vector

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\boldsymbol{P} \begin{pmatrix} x'_o \\ y'_o \\ z'_o \end{pmatrix}.$$

Example 3.1.3.1.

In the group–subgroup relation $Fddd \rightarrow C12/c1$, a cell transformation and an origin shift are needed if origin choice 1 has been selected for $Fddd$. In the table for space group $Fddd$, No. 70, the transformation of the basis vectors in the column 'Axes' is given as $\mathbf{a}$, $-\mathbf{b}$, $-\frac{1}{2}(\mathbf{a}+\mathbf{c})$, which means that the transformation matrix is

$$\boldsymbol{P} = \begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix}.$$

In the column 'Coordinates' for origin choice 1, the coordinate transformations are given as x–z, $-y+\frac{1}{8}$, $-2z+\frac{1}{4}$, which implies a coordinate shift of $x'_o = 0$, $y'_o = \frac{1}{8}$ and $z'_o = \frac{1}{4}$ referred to the coordinate system of the subgroup $C12/c1$, No. 15. The origin shift in terms of the starting space group $Fddd$ is

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\begin{pmatrix} 1 & 0 & -\frac{1}{2} \\ 0 & -1 & 0 \\ 0 & 0 & -\frac{1}{2} \end{pmatrix} \begin{pmatrix} 0 \\ \frac{1}{8} \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} \frac{1}{8} \\ \frac{1}{8} \\ \frac{1}{8} \end{pmatrix}.$$

Example 3.1.3.2.

Consider space group *Pnma*, No. 62, and its subgroup $P2_12_12_1$, No. 19. In the table for space group *Pnma*, the coordinate transformation in the column 'Coordinates' is given as $x, y, z + \frac{1}{4}$. Therefore, there is no basis transformation, $\boldsymbol{P} = \boldsymbol{I}$, but there is an origin shift of $x'_o = 0$, $y'_o = 0$, $z'_o = \frac{1}{4}$ expressed in the coordinate system of $P2_12_12_1$. In terms of the coordinate system of *Pnma* this coordinate shift has the opposite sign:

$$\begin{pmatrix} x_{o'} \\ y_{o'} \\ z_{o'} \end{pmatrix} = -\begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ \frac{1}{4} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ -\frac{1}{4} \end{pmatrix}.$$

Note: In Chapter 2.3, the listed origin shifts refer to the starting space group and thus are given in a different way to that in Chapter 3.2. In addition, for a given group–subgroup pair the direction of the origin shift selected in Chapter 2.3 usually differs from the origin shift listed in Chapter 3.2 (often the direction is opposite; see the Appendix).

3.1.4. Nonconventional settings of orthorhombic space groups

Orthorhombic space groups can have as many as six different settings, as listed in Chapter 4.3 of Volume A. They result from the interchange of the axes $\mathbf{a}$, $\mathbf{b}$, $\mathbf{c}$ in the following ways:

Cyclic exchange: $\mathbf{bca}$ or $\mathbf{cab}$.

Exchange of two axes, combined with the reversal of the direction of one axis in order to keep a right-handed coordinate system:

$\mathbf{ba\bar{c}}$ or $\mathbf{b\bar{a}c}$ or $\mathbf{\bar{b}ac}$;
$\mathbf{cb\bar{a}}$ or $\mathbf{c\bar{b}a}$ or $\mathbf{\bar{c}ba}$;
$\mathbf{ac\bar{b}}$ or $\mathbf{a\bar{c}b}$ or $\mathbf{\bar{a}cb}$.

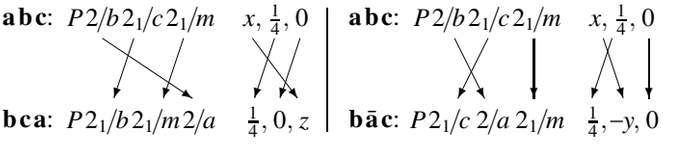
The exchange has two consequences for a Hermann–Mauguin symbol:

(1) the symmetry operations given in the symbol interchange their positions in the symbol;
(2) the labels of the glide directions and of the centrings are interchanged.

In the same way, the sequences and the labels and values of the coordinate triplets have to be interchanged.

Example 3.1.4.1.

Take space group *Pbcm*, No. 57 (full symbol $P2/b2_1/c2_1/m$), and its Wyckoff position $4c$ $(x, \frac{1}{4}, 0)$. The positions in the symbol change as given by the arrows, and simultaneously the labels change:



The notation $\mathbf{bca}$ means: the former b axis is now in the position of the a axis *etc.* or: convert b to a, c to b, and a to c.

The corresponding interchanges of positions and labels for all possible nonconventional settings are listed at the end of the table of each orthorhombic space group. They have to be applied to all subgroups.

Example 3.1.4.2.

Consider the nonconventional setting *Pcam* of *Pbcm*. The entry at the bottom of the page for space group *Pbcm*, No. 57, shows the necessary interchanges for the setting *Pcam*: $a \rightleftarrows b$, $\mathbf{a} \rightleftarrows -\mathbf{b}$, and $x \rightleftarrows -y$.

For the subgroup *Pbna* (last entry in the block of *klassengleiche* non-isomorphic subgroups) this means: *Pbna* has to be replaced by *Pnab*, the axes conversion $2\mathbf{a}, \mathbf{b}, \mathbf{c}$ has to be replaced by $\mathbf{a}, -2\mathbf{b}, \mathbf{c}$ and the coordinate transformation $\frac{1}{2}x + \frac{1}{4}, y, z; +(\frac{1}{2}, 0, 0)$ has to be replaced by $x, -\frac{1}{2}y - \frac{1}{4}, z; +(0, -\frac{1}{2}, 0)$.

Pbna and *Pnab* are nonconventional settings of *Pbcn*, No. 60.

The interchange of the axes does not affect the Wyckoff labels, just the corresponding coordinates.

Example 3.1.4.3.

The Wyckoff position 4*c* $(x, \frac{1}{4}, 0)$ of *Pbcm*, No. 57, retains its label for any of the other settings of this space group. In the setting *Pbma*, this Wyckoff position is still 4*c* and has the coordinates $\frac{1}{4}, 0, z$. In this case, no ambiguity arises because the different settings of space group *Pbcm* all have different Hermann–Mauguin symbols that uniquely show how the axes have to be interchanged (*Pmca*, *Pbma*, *Pcam*, *Pmab* and *Pcmb*).

The interchange of the axes must also be performed for those subgroups that have equivalent directions and where the Hermann–Mauguin symbol does not uniquely show the kind of setting. Otherwise, the wrong Wyckoff positions can result.

Example 3.1.4.4.

Space group *Cmmm*, No. 65, has two *klassengleiche* subgroups of type *Immm*, No. 71, with doubled *c* axis. In the nonconventional setting *Bmmm* of *Cmmm*, the same subgroups *Immm* result from a doubling of the *b* axis. In the conventional setting of *Immm*, the Wyckoff positions 4*e*, 4*g* and 4*i* represent orbits with the coordinates $(x, 0, 0)$, $(0, y, 0)$ and $(0, 0, z)$, respectively. In the space group *Cmmm*, the position 4*k* corresponds to $(0, 0, z)$ and upon transition to either of the subgroups *Immm* it splits to $2 \times 4i$.

If *Bmmm* is obtained from *Cmmm* by cyclic exchange of the axes ($\mathbf{a} \leftarrow \mathbf{b} \leftarrow \mathbf{c} \leftarrow \mathbf{a}$), its Wyckoff position 4*k* obtains the coordinates $(0, y, 0)$. Upon doubling of *b* and transition to *Immm*, 4*k* will split to two orbits with the coordinates $(0, \frac{1}{2}y, 0)$ and $(0, \frac{1}{2}y + \frac{1}{2}, 0)$. These are two orbits 4*i* of *Immm*, but this is only correct if the axes of *Immm* have also been interchanged in the same way. *If the interchange of axes has not been performed in the subgroup Immm in the assumption that in Immm all axes are equivalent anyway, wrong results will be obtained.* That is, *Immm* also has to be used in a nonconventional setting, although this is not apparent from the Hermann–Mauguin symbol. Of course, the Wyckoff symbols can then be relabelled so that they correspond to the conventional listings of Volume A ($4i \rightarrow 4g$ *etc.*). It is recommended that this return to the conventional setting of *Immm* is performed, because using the label 4*i* for $(0, y, 0)$ in *Immm* is likely to cause confusion if the nonconventional setting is not explicitly stressed.

3.1.5. Conjugate subgroups

Conjugate subgroups are different subgroups belonging to the same space-group type (they have the same Hermann–Mauguin symbol) and they have the same unit-cell size and the same shape for the conventional cell. They can be mapped onto one another by a symmetry operation of the starting group, *i.e.* they are symmetry-equivalent in this space group. They can occur only if the index of symmetry reduction is ≥ 3. The relations of the Wyckoff positions of a space group with the Wyckoff positions of any representative of a set of conjugate subgroups are always the same. Therefore, in principle it is sufficient to list the relations for only one representative.

Two kinds of conjugation of maximal subgroups can be distinguished, translational conjugation and orientational conjugation. Non-maximal subgroups can involve both kinds of conjugation, so the situation is more complicated in chains of group–subgroup relations, *cf.* Koch (1984) and Müller (1992). Since the present tables only list maximal subgroups, we will not discuss this here.

3.1.5.1. *Translational conjugation*

Translational conjugation occurs when the group–subgroup relation involves a loss of translational symmetry. This happens when the conventional cell has been enlarged or when centring translations have been lost; this means that the primitive unit cell of the subgroup is larger (by a factor ≥ 3). Translationally conjugate subgroups of a space group are symmetry-equivalent by a translation of the lattice of this space group. This way, isomorphic subgroups of index $p \geq 3$ have p conjugate subgroups (unless the cell enlargement occurs in a direction in which the origin may float). The existence of conjugate subgroups of this kind is not specifically mentioned in the tables. However, they can be recognized by looking in the column 'Coordinates'. If a semicolon appears after the coordinate triplet, followed by values in parentheses to be added, and if, in addition, the index of symmetry reduction is ≥ 3, then conjugate subgroups usually exist. They differ in the locations of their origins by values corresponding to the values given in the parentheses.

Example 3.1.5.1.1.

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

gives the positional coordinates in the subgroup originating from the coordinates of one unit cell of the starting group, namely

$$x, y, \tfrac{1}{3}z; \quad x, y, \tfrac{1}{3}z + \tfrac{1}{3}; \quad x, y, \tfrac{1}{3}z - \tfrac{1}{3}.$$

In addition, this also means that there are three conjugate subgroups. They differ in the locations of their origins referred to the origin of the starting space group by $0,0,0$, $0,0,\frac{1}{3}$ and $0,0,-\frac{1}{3}$, expressed in terms of the coordinate system of the subgroup, which is equivalent to $0,0,0$, $0,0,-1$ and $0,0,1$ in the coordinate system of the starting group.

Primitive subgroups of face-centred cubic space groups have four conjugate subgroups. Because in this case no values have to be added to the coordinates, the existence of conjugate subgroups is expressed by the entry '4 conjugate subgroups'. They differ in their origin locations corresponding to the centring vectors of the face-centred cell.

Cell enlargements do not always produce conjugate subgroups. If the cell is being enlarged in a direction in which the origin may float, *i.e.* is not fixed by symmetry, no conjugate subgroups result. This applies to the following crystal classes:

1, enlargement in any direction;

2, *mm*2, 3, 3*m*, 4, 4*mm*, 6 and 6*mm*, enlargement in the direction of the unique axis;

m, enlargement parallel to the plane of symmetry.

Example 3.1.5.1.2.

The cell enlargement **a**, **b**, 5**c** of space group $Cmc2_1$, No. 36, (crystal class *mm*2) does not produce conjugate subgroups.

If one is unsure whether conjugate subgroups exist, this can be looked up in the tables of Chapter 2.3 of this volume, where all conjugate subgroups are always mentioned and joined by a left brace.

Example 3.1.5.1.3.

For space group $Pm\overline{3}m$, No. 221, two subgroups $Im\overline{3}m$ ($2\mathbf{a}, 2\mathbf{b}, 2\mathbf{c}$) with index 4 are listed. Each of them belongs to a set of four conjugate subgroups which differ in their origin locations $(0,0,0; -1,0,0; 0,-1,0; 0,0,-1$ for the first listed subgroup, referred to the coordinate system of $Pm\overline{3}m$). This can be seen by the coordinate values to be added $(0,0,0; \frac{1}{2},0,0; 0,\frac{1}{2},0; 0,0,\frac{1}{2}$; coordinate system of $Im\overline{3}m$). In Chapter 2.3, all four conjugate subgroups and their origin shifts are listed and joined by a brace.

3.1.5.2. *Orientational conjugation*

In this case, the conjugate subgroups have differently oriented unit cells that are equivalent by a symmetry operation other than a translation of the space group. This occurs in the following cases: orthorhombic subgroups of hexagonal space groups; monoclinic subgroups of trigonal (including rhombohedral) space groups; rhombohedral and tetragonal subgroups of cubic space groups. In these cases, the corresponding cell and coordinate transformations are listed for all conjugate subgroups after the word 'conjugate'. Their Wyckoff symbols, being the same for all conjugate subgroups, are not repeated.

Example 3.1.5.2.1.

The cubic space group $P\overline{4}3m$, No. 215, has three tetragonal conjugate subgroups $P\overline{4}2m$. Their tetragonal *c* axes correspond to the cubic *a*, *b* or *c* axes, respectively. In $P\overline{4}3m$, *a*, *b* and *c* are symmetry-equivalent by the threefold rotation axes.

3.1.6. Monoclinic and triclinic subgroups

Aside from the two choices for the unique axis and the three possible cell choices given in Volume A, the unit cell of a monoclinic space group allows many more settings that can be interconverted by transformations such as $\mathbf{a} \pm q\mathbf{c}, \mathbf{b}, \mathbf{c}$ with an integer value for *q* (Sayari & Billiet, 1977). The most commonly chosen cell is the one with the shortest basis vectors **a** and **c** and a non-acute angle β. For triclinic space groups the 'reduced' cell is preferred, which depends on the metric values of the lattice (Billiet & Rolley Le Coz, 1980).

Some relations always require a cell transformation, for example rhombohedral to monoclinic relations. A group–subgroup relation in which the subgroup is monoclinic or triclinic can always be chosen together with a cell transformation that produces one of the cells mentioned. The transformation to be chosen depends on the cell metrics of the starting space group. For general tables we therefore cannot specify *a priori* the kind of cell transformation that will be needed.

The settings listed for monoclinic and triclinic subgroups were chosen in such a way that axes transformations are avoided or kept to a minimum. Depending on the cell metrics, this may result in cells that do not have the shortest possible basis vectors. Unfortunately, transformation of a monoclinic or triclinic cell setting to another one may cause an interchange of Wyckoff labels (within the Wyckoff sets). Frequently, several possible cell settings of the same monoclinic subgroup have been listed; the entry for the subgroup then is followed by the word 'or' or 'alternative', plus another entry.

Example 3.1.6.1.

Space group *Cmcm*, No. 63, has the subgroup $P112_1/m$, No. 11. It requires a cell transformation which is given as $\mathbf{a}, \frac{1}{2}(-\mathbf{a}+\mathbf{b}), \mathbf{c}$. The following two lines list two other possible cell transformations for the *same* subgroup after the words 'or': $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \mathbf{b}, \mathbf{c}$ and $\frac{1}{2}(\mathbf{a}-\mathbf{b}), \frac{1}{2}(\mathbf{a}+\mathbf{b}), \mathbf{c}$. These three options cause different relations for the Wyckoff positions 4*b* and 8*d* of *Cmcm*.

Caution should also be exerted when different cell choices of monoclinic cells are involved. Monoclinic subgroups may refer to any of the three cell choices listed in Volume A. As long as these cell choices are used as listed in Volume A, no problems should arise. However, interconversions from one setting to another and especially nonconventional settings require special attention.

Example 3.1.6.2.

The common setting of space group No. 15 is $C12/c1$, which means unique axis *b* and cell choice 1; the glide plane *c* is located at $y = 0$ (and $y = \frac{1}{2}$). By interchanging the axes **b** and $-\mathbf{c}$, $C12/c1$ becomes $B112/b$ with the *b* glide plane at $z = 0$. This was the setting listed in *International Tables for X-ray Crystallography* (1952, 1965, 1969) for unique axis *c*. However, since the 1983 edition of Volume A, $B112/b$ does not correspond to one of the listed cell choices. Instead, they are now $A112/a$ (cell choice 1) or $B112/n$ (cell choice 2) or $I112/b$ (cell choice 3). Note that for all three cell choices the glide plane mentioned in the symbol is at $z = 0$. $B112/n$ also has a glide plane in the **b** direction, but unlike $B112/b$ it is at $z = \frac{1}{4}$. $B112/n$ and $B112/b$ can be set up with the same unit-cell dimensions, but with origins shifted by $\frac{1}{4}, 0, \frac{1}{4}$. The full Hermann–Mauguin symbol always shows uniquely which is the setting.

References

Aroyo, M. I. & Perez-Mato, J. M. (1998). *Symmetry-mode analysis of displacive phase transitions using International Tables for Crystallography. Acta Cryst.* A**54**, 19–30.

Ascher, E. (1966). *Role of particular maximal subgroups in continuous phase transitions. Phys. Lett.* **20**, 352–354.

Ascher, E. (1967). *Symmetry changes in continuous transitions. A simplified theory applied to V_3Si. Chem. Phys. Lett.* **1**, 69–72.

Ascher, E. (1968). *Lattices of equi-translation subgroups of the space groups*. Geneva: Battelle Institute.

Ascher, E., Gramlich, V. & Wondratschek, H. (1969). *Corrections to the sections 'Untergruppen' of the space groups in Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935) Vol. I. Acta Cryst.* B**25**, 2154–2156.

Astbury, W. T. & Yardley, K. (1924). *Tabulated data for the examination of the 230 space-groups by homogeneous X-rays. Philos. Trans. R. Soc. London*, **224**, 221–257.

Barlow, W. (1894). *Über die geometrischen Eigenschaften homogener starrer Strukturen. Z. Kristallogr. Mineral.* **23**, 1–63.

Bärnighausen, H. (1975). *Group–subgroup relations between space groups as an ordering principle in crystal chemistry: the "family tree" of perovskite-like structures. Acta Cryst.* A**31**, part S3, S3, 01.1-9.

Bärnighausen, H. (1980). *Group–subgroup relations between space groups: a useful tool in crystal chemistry. MATCH Comm. Math. Chem.* **9**, 139–175.

Baur, W. H. (1994). *Rutile type derivatives. Z. Kristallogr.* **209**, 143–150.

Baur, W. H. & Kassner, D. (1992). *The perils of Cc: comparing the frequencies of falsely assigned space groups with their general population. Acta Cryst.* B**48**, 356–369.

Baur, W. H. & McLarnan, T. J. (1982). *Observed wurtzite derivatives and related tetrahedral structures. J. Solid State Chem.* **42**, 300–321.

Bertaut, E. F. & Billiet, Y. (1979). *On equivalent subgroups and supergroups of the space groups. Acta Cryst.* A**35**, 733–745.

Billiet, Y. (1973). *Les sous-groupes isosymboliques des groupes spatiaux. Bull. Soc. Fr. Minéral. Cristallogr.* **96**, 327–334.

Billiet, Y. (1980). *The subgroups of finite index of the space groups: determination via conventional coordinate systems. MATCH Comm. Math. Chem.* **9**, 127–190.

Billiet, Y. & Bertaut, E. F. (2002). *Isomorphic subgroups of space groups. International Tables for Crystallography*, Vol. A, *Space-group symmetry*, edited by Th. Hahn, Part 13. Dordrecht: Kluwer Academic Publishers.

Billiet, Y. & Rolley Le Coz, M. (1980). *Le groupe P*1 *et ses subgroupes. II. Tables des sous-groupes. Acta Cryst.* A**36**, 242–248.

Billiet, Y. & Sayari, A. (1984). *Les sous-groupes isomorphes d'un group d'espace de type p*4*. I. Détermination univoque. Acta Cryst.* A**40**, 624–631.

Billiet, Y., Sayari, A. & Zarrouk, H. (1978). *L'association des familles de Wyckoff dans les changements de repère conventionnel des groupes spatiaux et les passages aux sous-groupes spatiaux. Acta Cryst.* A**34**, 811–819.

Biltz, W. (1934). *Raumchemie der festen Stoffe.* Leipzig: L. Voss.

Birman, J. L. (1966*a*). *Full group and subgroup methods in crystal physics. Phys. Rev.* **150**, 771–782.

Birman, J. L. (1966*b*). *Simplified theory of symmetry change in second–order phase transitions: application to V_3Si. Phys. Rev. Lett.* **17**, 1216–1219.

Bock, O. & Müller, U. (2002*a*). *Symmetrieverwandtschaften bei Varianten des Perowskit-Typs. Acta Cryst.* B**58**, 594–606.

Bock, O. & Müller, U. (2002*b*). *Symmetrieverwandtschaften bei Varianten des ReO_3-Typs. Z. Anorg. Allg. Chem.* **628**, 987–992.

Boyle, L. L. & Lawrenson, J. E. (1973). *The origin dependence of the Wyckoff site description of a crystal structure. Acta Cryst.* A**29**, 353–357.

Bravais, A. (1850). *Mémoire sur les systèmes formés par les points distribués régulièrement sur un plan ou dans l'espace. J. Ecole Polytech.* **19**, 1–128. (English: Memoir 1, Crystallographic Society of America, 1949.)

Brown, H., Bülow, R., Neubüser, J., Wondratschek, H. & Zassenhaus, H. (1978). *Crystallographic groups of four-dimensional space*. New York: John Wiley & Sons.

Buerger, M. J. (1947). *Derivative crystal structures. J. Chem. Phys.* **15**, 1–16.

Buerger, M. J. (1951). *Phase transformations in solids*, ch. 6. New York: Wiley.

Burckhardt, J. J. (1988). *Die Symmetrie der Kristalle.* Basel: Birkhäuser.

Byström, A., Hök, B. & Mason, B. (1941). *The crystal structure of zinc metaantimonate and similar compounds. Ark. Kemi Mineral. Geol.* **15B**, 1–8.

Chapuis, G. C. (1992). *Symmetry relationships between crystal structures and their practical applications. Modern perspectives in inorganic chemistry*, edited by E. Parthé, pp. 1–16. Dordrecht: Kluwer Academic Publishers.

Cracknell, A. P. (1975). *Group theory in solid state physics.* New York: Taylor and Francis Ltd. and Pergamon.

Deonarine, S. & Birman, J. L. (1983). *Group–subgroup phase transitions, Hermann's space group decomposition theorem, and chain subduction criterion in crystals. Phys. Rev. B*, **27**, 4261–4273.

Eick, B., Gähler, F. & Nickel, W. (1997). *Computing maximal subgroups and Wyckoff positions of space groups. Acta Cryst.* A**53**, 467–474.

Eick, B., Gähler, F. & Nickel, W. (2001). *The 'Cryst' Package*. Version 4.1. http://www.itap.physik.uni-stuttgart.de/~gaehler/gap/packages.html.

Fedorov, E. (1891). *Symmetry of regular systems and figures*. *Zap. Mineral. Obshch. (2)*, **28**, 1–46. (In Russian.) (English: *Symmetry of crystals*, American Crystallographic Association, 1971.)

Finken, H., Neubüser, J. & Plesken, W. (1980). *Space groups and groups of prime power order II. Arch. Math.* **35**, 203–209.

Fischer, W. & Koch, E. (1983). *On the equivalence of point configurations due to Euclidean normalizers (Cheshire groups) of space groups. Acta Cryst.* A**39**, 907–915.

Flack, H. D., Wondratschek, H., Hahn, Th. & Abrahams, S. C. (2000). *Symmetry elements in space groups and point groups. Addenda to two IUCr reports on the nomenclature of symmetry. Acta Cryst.* A**56**, 96–98.

Goldschmidt, V. M. (1926). *Untersuchungen über den Bau und Eigenschaften von Krystallen. Skr. Nor. Vidensk. Akad. Oslo Mat.-Nat. Kl.* 1926 No. 2 and 1927 No. 8.

Haag, F. (1887). *Die regulären Krystallkörper. Programm des Königlichen Gymnasiums in Rottweil zum Schlusse des Schuljahres 1886–1887.*

Hahn, Th. & Wondratschek, H. (1994). *Symmetry of crystals. Introduction to International Tables for Crystallography, Vol. A*. Sofia: Heron Press.

Heesch, H. (1930). *Zur systematischen Strukturtheorie. II. Z. Kristallogr.* **72**, 177–201.

Hermann, C. (1929). *Zur systematischen Strukturtheorie. IV. Untergruppen. Z. Kristallogr.* **69**, 533–555.

International Tables for Crystallography (1983). Vol. A, *Space-group symmetry*, edited by Th. Hahn, 1st ed. Dordrecht: Kluwer Academic Publishers. (Abbreviated *IT* A.)

International Tables for Crystallography (2002). Vol. A, *Space-group symmetry*, edited by Th. Hahn, 5th ed. Dordrecht: Kluwer Academic Publishers. (Abbreviated *IT* A.)

International Tables for Crystallography (2002). Vol. E, *Subperiodic groups*, edited by V. Kopský & D. B. Litvin. Dordrecht: Kluwer Academic Publishers.

International Tables for X-ray Crystallography (1952, 1965, 1969). Vol. I, *Symmetry groups*, edited by N. F. M. Henry & K. Lonsdale. Birmingham: Kynoch Press.

Internationale Tabellen zur Bestimmung von Kristallstrukturen (1935). 1. Bd. Edited by C. Hermann. Berlin: Borntraeger. (In German, English and French.) (Abbreviated *IT* 35.)

Izyumov, Y. A. & Syromyatnikov, V. N. (1990). *Phase transitions and crystal symmetry.* Dordrecht: Kluwer Academic Publishers.

Janovec, V. (1976). *A symmetry approach to domain structures. Ferroelectrics*, **12**, 43–53.

Janovec, V. & Přívratská, J. (2003). *Domain structures*. *International tables for crystallography*, Vol. D, edited by A. Authier, *Physical properties of crystals*, ch. 3.4. Dordrecht: Kluwer Academic Publishers.

Koch, E. (1984). *The implications of normalizers on group–subgroup relations between space groups. Acta Cryst.* A**40**, 593–600.

Koch, E. & Fischer, W. (1975). *Automorphismengruppen von Raumgruppen und die Zuordnung von Punktlagen zu Konfigurationslagen. Acta Cryst.* A**31**, 88–95.

Koch, E. & Fischer, W. (1985). *Lattice complexes and limiting complexes versus orbit types and non-characteristic orbits: a comparative discussion. Acta Cryst.* A**41**, 421–426.

Koch, E., Fischer, W. & Müller, U. (2002). *Normalizers of space groups and their use in crystallography*. *International tables for crystallography*, Vol. A, *Space-group symmetry*, edited by Th. Hahn, Part 15. Dordrecht: Kluwer Academic Publishers.

Kroumova, E., Aroyo, M. I. & Pérez-Mato, J. M. (2002). *Prediction of new displacive ferroelectrics through systematic pseudosymmetry search. Results for materials with Pba*2 *and Pmc*2_1 *symmetry. Acta Cryst.* B**58**, 921–933.

Kroumova, E., Perez-Mato, J. M. & Aroyo, M. I. (1998). *WYCKSPLIT. Computer program for the determination of the relations of Wyckoff positions for a group–subgroup pair. J. Appl. Cryst.* **31**, 646. Accessible at: http:// www.cryst.ehu.es/cryst/wpsplit.html.

Lamport, L. (1994). *A document preparation system.* 2nd ed. Reading, MA: Addison-Wesley.

Landau, L. D. (1937). *Theory of phase transitions*. *Zh. Eksp. Teoret. Fiz.* **7**, pp. 19–32, 627–636. (In Russian.) (German: *Phys. Z. Sowjetunion*, **11**, pp. 20–47, 545–555.)

Landau, L. D. & Lifshitz, E. M. (1980). *Statistical physics*, Part 1, 3rd ed., pp. 459–471. London: Pergamon. (Russian: *Statisticheskaya Fizika,* chast 1. Moskva: Nauka, 1976; German: *Lehrbuch der theoretischen Physik*, 6. Aufl., Bd. 5, Teil 1, S. 436–447. Berlin: Akademie-Verlag, 1984).

Lawrenson, J. E. (1972). *Theoretical studies in crystallography.* Dissertation, University of Kent at Canterbury.

Ledermann, W. (1976). *Introduction to group theory*. London: Longman. (German: *Einführung in die Gruppentheorie*, Braunschweig: Vieweg, 1977.)

Levanyuk, A. P. & Sannikov, D. G. (1971). *Phenomenological theory of dielectric anomalies in ferroelectric materials with several phase transitions at temperatures close together. Sov. Phys. JETP*, **11**, 600–604.

McLarnan, T. J. (1981*a*). *Mathematical tools for counting polytypes. Z. Kristallogr.* **155**, 227–245.

McLarnan, T. J. (1981*b*). *The numbers of polytypes in close packings and related structures. Z. Kristallogr.* **155**, 269–291.

McLarnan, T. J. (1981*c*). *The combinatorics of cation-deficient close-packed structures. J. Solid State Chem.* **26**, 235–244.

Marsh, R. E., Kapon, M., Hu, S. & Herbstein, F. H. (2002). *Some 60 new space-group corrections. Acta Cryst.* B**58**, 62–77.

Megaw, H. D. (1973). *Crystal structures: A working approach*. Philadelphia: Saunders.

Meyer, A. (1981). *Symmmetriebeziehungen zwischen Kristallstrukturen des Formeltyps* AX_2, ABX_4 *und* AB_2X_6 *sowie deren Ordnungs- und Leerstellenvarianten.* Dissertation, Universität Karlsruhe.

Müller, U. (1978). *Strukturmöglichkeiten für Pentahalogenide mit Doppeloktaeder-Molekülen* $(MX_5)_2$ *bei dichtester Packung der Halogenatome. Acta Cryst.* A**34**, 256–267.

Müller, U. (1980). *Strukturverwandtschaften unter den* EPh_4^+*- Salzen. Acta Cryst.* B**36**, 1075–1081.

Müller, U. (1981). MX_4*-Ketten aus kantenverknüpften Oktaedern: mögliche Kettenkonfigurationen und mögliche Kristallstrukturen. Acta Cryst.* B**37**, 532–545.

Müller, U. (1986). MX_5*-Ketten aus eckenverknüpften Oktaedern. Mögliche Kettenkonfigurationen und mögliche Kristallstrukturen bei dichtester Packung der X-atome. Acta Cryst.* B**42**, 557–564.

Müller, U. (1992). *Berechnung der Anzahl möglicher Strukturtypen für Verbindungen mit dichtest gepackter Anionenteilstruktur. I. Das Rechenverfahren. Acta Cryst.* B**48**, 172–178.

Müller, U. (1993). *Inorganic structural chemistry*, pp. 233–246. Chichester, New York: Wiley. (German: *Anorganische Strukturchemie*, 3. Aufl., 1996, S. 296–309. Stuttgart: Teubner.)

Müller, U. (1998). *Strukturverwandtschaften zwischen trigonalen Verbindungen mit hexagonal-dichtester Anionenteilstruktur und besetzten Oktaederlücken. Z. Anorg. Allg. Chem.* **624**, 529–532.

Müller, U. (2002). *Kristallpackungen mit linear koordinierten Atomen. Z. Anorg. Allg. Chem.* **628**, 1269–1278.

Müller, U. (2003). *Die Zahl der Substitutions- und Leerstellenvarianten des NaCl-Typs bei verdoppelter Elementarzelle* (**a**, **b**, 2**c**). *Z. Anorg. Allg. Chem.* **629**, 487–492.

Müller, U. & Brelle, A. (1995). *Über isomorphe Untergruppen von Raumgruppen der Kristallklassen* 4, $\bar{4}$, $4/m$, 3, $\bar{3}$, 6, $\bar{6}$ *und* $6/m$. *Acta Cryst.* A**51**, 300–304.

Nespolo, M. & Ferraris, G. (2004). *Applied geminography – symmetry analysis of twinned crystals and definition of twinning by reticular polyholohedry. Acta Cryst.* A**60**, 89–95.

Neubüser, J. & Wondratschek, H. (1966). *Untergruppen der Raumgruppen. Krist. Tech.* **1**, 529–543.

Niggli, P. (1919). *Geometrische Kristallographie des Diskontinuums*. Leipzig: Gebrüder Borntraeger. Reprint (1973) Wiesbaden: Dr M. Saendig.

Nolze, G. (1996). *POWDER CELL. Computer program for the calculation of X-ray powder diagrams.* Bundesanstalt für Materialforschung, Berlin.

Pauling, L. (1928). *The coordination theory of the structure of ionic compounds. Probleme der modernen Physik* (Sommerfeld-Festschrift), p. 11. Leipzig: S. Hirzel.

Pauling, L. (1929). *The principles determining the structures of complex ionic crystals. J. Am. Chem. Soc.* **51**, 1010–1026.

Plesken, W. & Schulz, T. (2000). *Counting crystallographic groups in low dimensions. Exp. Math.* **9**, 407–411.

Pöttgen, R. & Hoffmann, R.-D. (2001). AlB_2*-related intermetallic compounds – a comprehensive view based on a group–subgroup scheme. Z. Kristallogr.* **216**, 127–145.

Salje, E. K. H. (1990). *Phase transitions in ferroelastic and co-elastic crystals.* Cambridge University Press.

Sayari, A. (1976). *Contribution à l'étude des groupes d'espace bidimensionnels, dérivation des sous-groupes et des surstructures.* Thesis, University of Tunis, Tunisia.

Sayari, A. & Billiet, Y. (1977). *Subgroups and changes of standard settings of triclinic and monoclinic space groups. Acta Cryst.* A**33**, 985–986.

Schoenflies, A. M. (1891). *Krystallsysteme und Krystallstruktur.* Leipzig: Teubner. Reprint 1984: Springer.

Sohncke, L. (1879). *Entwickelung einer Theorie der Krystallstruktur.* Leipzig: Teubner.

Sowa, H. (2001). *On the transition from the wurtzite to the NaCl type. Acta Cryst.* A**57**, 176–182.

Stokes, H. T. & Hatch, D. M. (1988). *Isotropy subgroups of the 230 crystallographic space groups.* Singapore: World Scientific.

Stokes, H. T. & Hatch, D. M. (2002). *Procedure for obtaining microscopic mechanisms of reconstructive phase transitions in crystalline solids. Phys. Rev. B*, **65**, 144114–144123.

Strukturbericht 1913–1928 (1931). Edited by P. P. Ewald & C. Hermann. Leipzig: Akademische Verlagsgesellschaft. Continued by *Structure Reports*.

Tendeloo, G. van & Amelinckx, S. (1974). *Group-theoretical considerations concerning domain formation in ordered alloys. Acta Cryst.* A**30**, 431–440.

The *GAP* Group (2002). *GAP – Groups, Algorithms and Programming*. Version 4.3. http://www.gap-system.org.

Tolédano, J.-C., Janovec, V., Kopský, V., Scott, J.-F. & Boček, P. (2003). *Structural phase transitions*. *International tables for crystallography*, Vol. D, *Physical properties of crystals*, edited by A. Authier, ch. 3.1. Dordrecht: Kluwer Academic Publishers.

Tolédano, J.-C. & Tolédano, P. (1987). *The Landau theory of phase transitions.* Singapore: World Scientific.

Wiener, C. (1863). *Grundzüge der Weltordnung. I. Atomlehre*, p. 82. Leipzig: Heidelberg.

Wondratschek, H. (1976). *Extraordinary orbits of space groups. Theoretical considerations. Z. Kristallogr.* **143**, 460– 470.

Wondratschek, H. (1980). *Crystallographic orbits, lattice complexes, and orbit types. MATCH Comm. Math. Chem.* **9**, 121–125.

Wondratschek, H. (1993). *Splitting of Wyckoff positions (orbits). Mineral. Petrol.* **48**, 87–96.

Wondratschek, H. (2002). *Special topics on space groups. International tables for crystallography*, Vol. A, *Space-group symmetry*, edited by Th. Hahn, Part 8. Dordrecht: Kluwer Academic Publishers.

Wondratschek, H. & Aroyo, M. I. (2001). *The application of Hermann's group $\mathcal{M}$ in group–subgroup relations between space groups. Acta Cryst.* A**57**, 311–320.

Wondratschek, H. & Jeitschko, W. (1976). *Twin domains and antiphase domains. Acta Cryst.* A**32**, 664–666.

Wondratschek, H., Müller, U., Aroyo, M. I. & Sens, I. (1995). *Splitting of Wyckoff positions (orbits). II. Group–subgroup chains of index 6. Z. Kristallogr.* **210**, 567–573.

Wyckoff, R. W. G. (1922). *The analytical expression of the results of the theory of space groups*. Washington: Carnegie Institution.

Wyckoff, R. W. G. (1965). *Crystal structures*, 2nd ed., Vol. 3, pp. 361–362. New York: Interscience.