International Tables for Crystallography (2006). Vol. A1, Section 3.1.3, pp. 430–431.

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:

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

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:

a, **b**, **c**	basis vectors of the starting space group;
O	origin of the starting space group;
a′, **b**′, **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 **a**, −**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 **a**, **b**, **c** in the following ways:

Cyclic exchange: **b c a** or **c a b**.

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

$$\mathbf{b\,a\,\bar{c}} \text{ or } \mathbf{b\,\bar{a}\,c} \text{ or } \mathbf{\bar{b}\,a\,c};$$
$$\mathbf{c\,b\,\bar{a}} \text{ or } \mathbf{c\,\bar{b}\,a} \text{ or } \mathbf{\bar{c}\,b\,a};$$
$$\mathbf{a\,c\,\bar{b}} \text{ or } \mathbf{a\,\bar{c}\,b} \text{ or } \mathbf{\bar{a}\,c\,b}.$$

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 $P2/b\,2_1/c\,2_1/m$), 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:

abc:	$P2/b\,2_1/c\,2_1/m$	$x, \frac{1}{4}, 0$	**abc**:	$P2/b\,2_1/c\,2_1/m$	$x, \frac{1}{4}, 0$
bca:	$P2_1/b\,2_1/m\,2/a$	$\frac{1}{4}, 0, z$	$\mathbf{b\bar{a}c}$:	$P2_1/c\,2/a\,2_1/m$	$\frac{1}{4}, -y, 0$

The notation **b c a** 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.