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 (4*i* → 4*g* *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.