Appendix. Differences in the presentation of Parts 2 and 3

By Ulrich Müller and Hans Wondratschek

A1. Comparison of the approaches to subgroups in Parts 2 and 3

The tables in Parts 2 and 3 of this volume deal with two different aspects of the reduction of crystal symmetry. In Part 2, the loss of symmetry is described for the subgroup $\mathcal{H}$ of $\mathcal{G}$ by listing the *general position* of $\mathcal{H}$, *i.e.* a set of representatives of those symmetry operations (group elements) which are retained in $\mathcal{H}$. If there is not enough space to include the full general position, at least a set of generators of $\mathcal{H}$ is listed. Thus, the subject of Part 2 is *symmetry*. In Part 3, the splitting of the point orbits (*Wyckoff positions*) of the space group $\mathcal{G}$ when the symmetry of $\mathcal{G}$ is reduced to that of $\mathcal{H}$ is described. For each Wyckoff position of $\mathcal{G}$ the corresponding Wyckoff positions of $\mathcal{H}$ are listed. Thus, in Part 3 the *implications of symmetry changes for crystal structures* are described.

In both Parts 2 and 3, the data are listed in a way that makes the tables as convenient to use as possible. As the subjects of Parts 2 and 3 are different, the presentation of the data in the two parts differs. In addition, the data in Part 2 are such that they can be used more-or-less independently from Volume A of *International Tables for Crystallography* (2005) (abbreviated as *IT* A). This independence is not possible for the data in Part 3.

In order to facilitate the combined use of the data in the two parts, the differences in the presentation of these data are summarized in this Appendix.

A2. Multiple descriptions of the space groups $\mathcal{G}$ and $\mathcal{H}$

In *IT* A, some space groups are described up to six times:

(i) all monoclinic space groups are referred to unique axis *b* and unique axis *c*; for most of them a further partition is made into cell choice 1, cell choice 2 and cell choice 3;
(ii) twenty-four orthorhombic, tetragonal and cubic space groups are referred to origin choice 1 and origin choice 2;
(iii) seven space groups with rhombohedral lattice are referred to hexagonal axes and rhombohedral axes.

Multiple descriptions of the space group $\mathcal{G}$ are treated differently in Parts 2 and 3 of this volume:

(i) In Part 2, the data for each monoclinic space group $\mathcal{G}$ are listed for unique axis *b* and unique axis *c* on separate pages, but both for cell choice 1 only. In Part 3, the description is more explicit: for each setting unique axis *b* or unique axis *c* with different cell choices in *IT* A, the subgroups are listed for cell choice 1, cell choice 2 and cell choice 3.
(ii) In Part 2, the data for origin choice 1 and origin choice 2 are listed on separate pages. In Part 3, the data for both origin choices are combined on the same page.
(iii) In Part 2, descriptions in both hexagonal axes and rhombohedral axes are given; in Part 3 only a description in hexagonal axes is presented.

Multiple descriptions of the subgroup $\mathcal{H}$ are also sometimes treated differently in the two parts:

(i) The treatment of monoclinic subgroups is broadly the same: if the subgroup is given in a conventional setting (unique axis *b* or unique axis *c*), then this setting is kept. Otherwise, a nonconventional setting is transformed to unique axis *b*. However, in Part 3 the treatment is more explicit and adapted to the practice of crystal-structure description: in some cases several possible choices of axes transformations are listed for the same monoclinic subgroup. It is hoped that one of them corresponds to the cell with the commonly preferred metric values. The different possibilities are indicated by the words 'or' or 'alternative', *e.g.* for the monoclinic subgroup $P112_1/m$, No. 11, of *Cmcm*, No. 63, *cf.* also Section 3.1.6.
(ii) The treatment of two origin choices is the same with one exception: if only $\mathcal{H}$ is listed with two origins in *IT* A, then in Part 2 only the data for origin choice 2 are provided, while in Part 3 the data for both origin choices are listed.
(iii) The treatment of rhombohedral subgroups $\mathcal{H}$ is broadly similar. The subgroup is referred to hexagonal axes with two exceptions:
   (*a*) in Part 2 the setting of the subgroup $\mathcal{H}$ is rhombohedral if the setting of $\mathcal{G}$ is rhombohedral (this does not apply to Part 3);
   (*b*) in Part 3, for the rhombohedral subgroups of cubic space groups both settings are given, whereas in Part 2 only the hexagonal-axes setting is referred to.

A3. The transformation matrix and the origin shift

When starting from a space group $\mathcal{G}$ and proceeding to one of its subgroups $\mathcal{H} < \mathcal{G}$, the symmetry operations and the point coordinates are primarily referred to the coordinate system of $\mathcal{G}$. This coordinate system consists of a coordinate basis of three linearly independent basis vectors and an origin. In general, the conventional coordinate system of $\mathcal{H}$ will not be identical to that of $\mathcal{G}$ but the transition from the coordinate system of $\mathcal{G}$ to that of $\mathcal{H}$ may involve a change of the basis and an origin shift. This transition or coordinate transformation is not uniquely determined but may be chosen within certain limits. The optimal choice will be the coordinate transformation that is the most convenient and easy for the user to work with.

For the following, it is assumed that the original crystal structure and its space group $\mathcal{G}$ and symmetry operations are referred to a conventional coordinate system, because the data in the tables of this volume and in *IT* A are listed under this condition. Otherwise, a coordinate transformation to a conventional coordinate system has to precede the use of most of the data. The coordinate transformation itself is described by the matrix $\boldsymbol{P}$ of the coefficients of the basis vectors of the new basis referred to the old basis and by a column $\boldsymbol{p}$ which consists of the coordinates of the new origin referred to the old coordinate system, *cf.* Section 2.1.3 or, more explicitly, *IT* A, Part 5. The matrix $\boldsymbol{P}$ is presented in Parts 2 and 3 by listing the new basis vectors as linear combinations of the old ones, *e.g.* $(\mathbf{a}' =)\ \mathbf{a} - \mathbf{b}$, $(\mathbf{b}' =)\ \mathbf{a} + \mathbf{b}$, $(\mathbf{c}' =)\ \mathbf{c}$. The column $\boldsymbol{p}$ is presented in Part 2 by listing the coefficients of the shift vector, *e.g.* 0, 1/2, 1/4. For Part 3, the representatives of the Wyckoff positions are taken as

triplets of point coordinates. The transformation behaviour of coordinates is different from that of the symmetry operations, *viz* $\boldsymbol{x}' = \boldsymbol{P}^{-1}(\boldsymbol{x} - \boldsymbol{p})$, where $\boldsymbol{x}$ and $\boldsymbol{x}'$ are the coordinate columns of the points of the crystal structure in the old and in the new coordinate systems.

The criteria for selecting the coordinate transformations are different in Parts 2 and 3. In Part 2, emphasis is placed on homogeneity by using similar transformation matrices in similar situations. In Part 3, the preferred transformation is that which avoids an origin shift, *i.e.* for which the resulting shift vector is the **o** vector.

Example

In the relation

$$I4_1/amd\ (141) \rightarrow Fddd\ (70)$$

the axes must be transformed, either by $\mathbf{a} - \mathbf{b}$, $\mathbf{a} + \mathbf{b}$, $\mathbf{c}$ or by $\mathbf{a} + \mathbf{b}$, $-\mathbf{a} + \mathbf{b}$, $\mathbf{c}$. If origin choice 1 is selected for both space groups, then the first of these transformations requires an origin shift of $0, \frac{1}{2}, \frac{1}{4}$ (referred to the coordinate system of $I4_1/amd$). The first transformation is used in Part 2 because in all such relations the new basis of $\mathcal{H}$ is rotated against the old basis of $\mathcal{G}$ by a clockwise rotation of 45° and the necessary origin shift is then accepted. No origin shift is needed for the second transformation and, therefore, it has been used in Part 3; this can be seen in the transformation of the coordinates:

$$(x' =) \tfrac{1}{2}(x + y),\ (y' =) \tfrac{1}{2}(-x + y),\ (z' =)\ z.$$

Another difference between Parts 2 and 3 concerns the origin shifts chosen and their presentation. The common point of view is to make the origin shift positive unless special conditions lead to a preference for negative coefficients. However, the shift vector **s** of Part 3 is calculated by $\mathbf{s} = -\boldsymbol{P}^{-1}\mathbf{p}$ from the shift vector **p** of Part 2, so the two vectors usually have opposite directions. Therefore, very often a positive shift vector in Part 2 corresponds to a negative shift vector in Part 3 and *vice versa*. This is not obvious at first glance, because in Part 2 the vector **p** is listed, whereas in Part 3 the shift vector is given as part of the coordinate transformations.

Example

Consider *Pccn*, No. 56, as a subgroup of *Cccm*, No. 66, in the block 'Loss of centring translations'. The origin shift $\frac{1}{4}, \frac{1}{4}, 0$ of Part 2 has the opposite direction to that of Part 3, where it is indicated as part of the transformation '$x + \frac{1}{4}, y + \frac{1}{4}, z(+0)$'. The components $\frac{1}{4}, \frac{1}{4}, 0$ of this transformation correspond to a vector $\mathbf{p} = (-\frac{1}{4}, -\frac{1}{4}, 0)$, which is the opposite of the vector **p** of Part 2.

Since the Wyckoff letters of the positions in *IT* A may depend not only on the chosen basis but also on the chosen origin, a difference in the origin shift may induce a difference in the relations between the Wyckoff positions.

Example

Consider $P4_2/m$, No. 84, as a *translationengleiche* subgroup of $P4_2/mnm$, No. 136. The coordinate transformation $x + \frac{1}{2}, y, z$ of Part 3 results in the relations $2a \longrightarrow 2d$ and $2b \longrightarrow 2c$ of the Wyckoff positions. The origin shift 0, 1/2, 0 of Part 2 (which corresponds to a coordinate transformation $x, -\frac{1}{2} + y, z$) results in the relations $2a \longrightarrow 2c$ and $2b \longrightarrow 2d$.

A4. Nonconventional settings

If the setting of a subgroup is nonconventional, in Part 2, as in *IT* A, a nonconventional Hermann–Mauguin symbol is listed referred to the basis of $\mathcal{G}$, followed by the space-group number and the conventional symbol in parentheses. In Part 3, nonconventional settings are given only by Hermann–Mauguin symbols that correspond to the conventions of the crystal system followed on the next line by $\widehat{=}$ and the symbol of the conventional setting.

Examples

	Subgroup entry	
	in Part 2	in Part 3
Space group *P*222, No. 16	*A*222 (21, *C*222)	*A*222 (21) $\widehat{=}$ *C*222
Space group $I4_122$, No. 98	$I2_112$ (22, *F*222)	*F*222 (22)

In Part 3, unlike Part 2, no use is made of centred triclinic cells, *F*- and *R*-centred monoclinic cells, *C*- and *F*-centred tetragonal cells and *H*-centred hexagonal cells.

A5. The sequence of the subgroups

The sequence of the subgroups follows the same principles in both parts. The *translationengleiche* subgroups are listed first, the *klassengleiche* subgroups follow. The subgroups are distributed into blocks; within the same block the index generally determines the sequence (lower index precedes higher index). For the same index, the space-group number determines the sequence (higher space-group number precedes lower space-group number). A difference in the sequence is caused by two special rules that apply to Part 3:

(i) The sequence of the *translationengleiche* subgroups of cubic space groups does not follow the index value, but is in the order cubic, rhombohedral, tetragonal, orthorhombic.

(ii) The last *translationengleiche* subgroup of a tetragonal space group is always the one with the diagonally oriented cell, irrespective of its space-group number.

The sequence of the listings of the *klassengleiche* subgroups differs more often, because the partition of the subgroups into blocks in Part 2 is different from and finer than that in Part 3. The blocks in Part 2 are determined by the relation of the lattice of $\mathcal{H}$ to that of $\mathcal{G}$, *i.e.* by the different kinds of cell enlargement, and the index and space-group numbers are decisive for the sequence within these (small) blocks only.

The isomorphic subgroups are placed differently in Parts 2 and 3. Those with index values of 2, 3 and 4 are listed in Part 2 together with the other *klassengleiche* subgroups; they may also be contained in the infinite series of isomorphic subgroups that follow. In Part 3, all isomorphic subgroups are listed in a separate block.

A6. Conjugate subgroups

Conjugate subgroups are listed in Part 3 only in the case of orientational conjugation, *cf.* Section 3.1.5.2. They are marked by the word 'conjugate'. In Part 2, all conjugate subgroups of index 3 and 4 are listed individually and are joined by a left brace. In the series of maximal isomorphic subgroups, the conjugacy relations are given by statements.

References

International Tables for Crystallography (2005). Vol. A, *Space-Group Symmetry*, edited by Th. Hahn, 5th ed. Heidelberg: Springer.