APPENDIX
Differences in the presentation of Parts 2 and 3

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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* (2002) (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) 24 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, an non-conventional 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 (p. 433).
(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 (p. 45) 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 homogene-