Differences in the Presentation of Parts 2 and 3

If the setting of a subgroup is nonconventional, in Part 2, as in IT A, an nonconventional Hermann–Mauguin symbol is listed referred to the basis of \( G \), 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 \( \equiv \) and the symbol of the conventional setting.

**Examples.**

<table>
<thead>
<tr>
<th>Subgroup entry</th>
<th>in Part 2</th>
<th>in Part 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Space group P222, No. 16</td>
<td>A222 (21, C222)</td>
<td>A222 (21) ( \equiv ) C222</td>
</tr>
<tr>
<td>Space group I4122, No. 98</td>
<td>I212 (22, F222)</td>
<td>F222 (22)</td>
</tr>
</tbody>
</table>

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.

**A4. Nonconventional settings**

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 \( s = -P \cdot p \) 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 Ccmm, No. 66, in the block ‘Loss of centring translations’. The origin shift 1/4, 1/4, 0 of Part 2 has the opposite direction to that of Part 3, where it is indicated as part of the transformation ‘\( x + \frac{1}{2}, y + \frac{1}{2}, z + 0 \)’.

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 \( 2a \rightarrow 2d \) and \( 2b \rightarrow 2c \) 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 \( 2a \rightarrow 2c \) and \( 2b \rightarrow 2d \).

**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 \( H \) to that of \( G \), 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 (p. 433). 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.