ity 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 $0, 1/2, 1/4$ (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 $1/4, 1/4, 0$ of Part 2 has the opposite direction to that of Part 3, where it is indicated as part of the transformation '$x+\frac{1}{4}, y+\frac{1}{4}, z(+0)$'. 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, an 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	Subgroup entry in Part 3
Space group $P222$, No. 16	$A222$ (21, $C222$)	$A222$ (21) $\widehat{=}\, C222$
Space group $I4_122$, No. 98	$I2_112$ (22, $F222$)	$F222$ (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 (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.