International Tables for Crystallography (2006). Vol. A1, Section 2.1.7.3, pp. 55–56.

Example 2.1.7.2.1.

Compare the *t*-subgroup graphs in Figs. 2.4.4.2, 2.4.4.3 and 2.4.4.8 of *Pnna*, No. 52, *Pmna*, No. 53, and *Cmce*, No. 64, respectively. The *complete* (uncontracted) *graphs* would have the shape of the graph of the point group *mmm* with *mmm* at the top (first level), seven point groups[5] (222, *mm*2, *m*2*m*, 2*mm*, $112/m$, $12/m1$ and $2/m11$) in the second level, seven point groups (112, 121, 211, 11*m*, 1*m*1, *m*11 and $\overline{1}$) in the third level and the point group 1 at the bottom (fourth level). The group *mmm* is connected to each of the seven subgroups at the second level by one line. Each of the groups of the second level is connected with three groups of the third level by one line. All seven groups of the third level are connected by one line each with the point group 1 at the bottom.

The *contracted graph* of the point group *mmm* would have *mmm* at the top, three point-group types (222, *mm*2 and $2/m$) at the second level and three point-group types (2, *m* and $\overline{1}$) at the third level. The point group 1 at the bottom would not be displayed (no fourth level). Single lines would connect *mmm* with 222, *mm*2 with 2, $2/m$ with 2, $2/m$ with *m* and $2/m$ with $\overline{1}$; a double line would connect *mm*2 with *m*; triple lines would connect *mmm* with *mm*2, *mmm* with $2/m$ and 222 with 2.

The number of fields in a contracted *t*-subgroup graph is between the numbers of fields in the full and in the contracted point-group graphs. The graph in Fig. 2.4.4.2 of *Pnna*, No. 52, has six space-group types at the second level and four space-group types at the third level. For the graph in Fig. 2.4.4.3 of *Pmna*, No. 53, these numbers are seven and five and for the graph in Fig. 2.4.4.8 of *Cmce*, No. 64 (formerly *Cmca*), the numbers are seven and six. However, in all these graphs the number of connections is always seven from top to the second level and three from each field of the second level downwards to the ground level, independent of the amount of contraction and of the local multiplicity of lines.

Example 2.1.7.2.2.

Compare the *t*-subgroup graphs shown in Fig. 2.4.1.1 for $Pm\overline{3}m$, No. 221, and Fig. 2.4.1.5, $Fm\overline{3}m$, No. 225. These graphs are contracted from the point-group graph $m\overline{3}m$. There are altogether nine levels (without the lowest level of *P*1). The indices relative to the top space groups $Pm\overline{3}m$ and $Fm\overline{3}m$ are 1, 2, 3, 4, 6, 8, 12, 16 and 24, corresponding to the point-group orders 48, 24, 16, 12, 8, 6, 4, 3 and 2, respectively. The height of the levels in the graphs reflects the index; the distances between the levels are slightly distorted in order to adapt to the density of the lines. From the top space-group symbol there are five lines to the symbols of maximal subgroups: The three symbols at the level of index 2 are those of cubic normal subgroups, the one (tetragonal) symbol at the level of index 3 represents a conjugacy class of three, the symbol $R\overline{3}m$, No. 166, at the level of index 4 represents a conjugacy class of four subgroups.

The graphs differ in the levels of the indices 12 and 24 (orthorhombic, monoclinic and triclinic subgroups) by the number of symbols (nine and seven for index 12, five and three for index 24). The number of lines between neighbouring connected levels depends only on the number and kind of symbols in the upper level. This property makes such graphs particularly useful.

However, for non-maximal subgroups the conjugacy relations may not hold. For example, in Fig. 2.4.1.1, the space group *P*222 has three normal maximal subgroups of type *P*2 and is thus connected to its symbol by a triple line, although these subgroups are conjugate subgroups of the non-minimal supergroup $Pm\overline{3}m$.

The *t*-subgroup graphs in Figs. 2.4.1.1 and 2.4.1.5 contain the *t*-subgroups of $Pm\overline{3}m$ (221) and $Fm\overline{3}m$ (225) and their relations. In addition, the *t*-subgroup graph of $Pm\overline{3}m$ includes the *t*-subgroup graphs of *P*432, $P\overline{4}3m$, $Pm\overline{3}$, *P*23, $P4/mmm$, $P\overline{4}2m$, $P\overline{4}m2$, *P*4*mm*, $R\overline{3}m$, *R*3*m* *etc.*, that of $Fm\overline{3}m$ includes those of *F*432, $F\overline{4}3m$, $Fm\overline{3}$, $I4/mmm$, also $R\overline{3}m$ *etc*. Thus, many other graphs can be extracted from the two basic graphs. The same holds for the other graphs displayed in Figs. 2.4.1.2 to 2.4.4.8: each of them includes the contracted graphs of all its subgroups. For this reason one does not need 229 or 218 different graphs to cover all *t*-subgroup graphs of the 229 space-group types but only 37 (*P*1 can be excluded as trivial).

The preceding Example 2.1.7.2.2 suggests that one should choose the graphs in such a way that their number can be kept small. It is natural to display the 'big' graphs first and later those smaller graphs that are still missing. This procedure is behind the sequence of the *t*-subgroup graphs in this volume.

(1) The ten graphs of $Pm\overline{3}m$, No. 221, to $Ia\overline{3}d$, No. 230, form the first set of graphs in Figs. 2.4.1.1 to 2.4.1.10.
(2) There are a few cubic space groups left which do not appear in the first set. They are covered by the graphs of $P4_132$ (213), $P4_332$ (212) and $Pa\overline{3}$ (205). These graphs have large parts in common so that they can be united in Fig. 2.4.1.11.
(3) No cubic space group is left now, but only eight tetragonal space groups of crystal class $4/mmm$ have appeared up to now. Among them are all graphs for $4/mmm$ space groups with an *I* lattice which are contained in Figs. 2.4.1.5 to 2.4.1.8 of the *F*-centred cubic space groups. The next 12 graphs, Figs. 2.4.2.1 to 2.4.2.12, are those for the space groups of the crystal class $4/mmm$ with lattice symbol *P* and different third and fourth constituents of the HM symbol. They start with $P4/mcc$, No. 124, and end with $P4_2/ncm$, No. 138.
(4) Two (enantiomorphic) tetragonal space-group types are left which are compiled in Fig. 2.4.2.13.
(5) The next set is formed by the four graphs in Figs. 2.4.3.1 to 2.4.3.4 of the hexagonal space groups $P6/mmm$, No. 191, to $P6_3/mmc$, No. 194. The hexagonal and trigonal enantiomorphic space groups do not appear in these graphs. They are combined in Fig. 2.4.3.5, the last one of hexagonal origin.
(6) Several orthorhombic space groups are still left. They are treated in the eight graphs in Figs. 2.4.4.1 to 2.4.4.8, from *Pmma*, No. 51, to *Cmce*, No. 64 (formerly *Cmca*).
(7) For each space group, the contracted graph of all its *t*-subgroups is provided in at least one of these 37 graphs.

For the index of a maximal *t*-subgroup, Lemma 1.2.8.2.3 is repeated: the index of a maximal non-isomorphic subgroup $\mathcal{H}$ is always 2 for oblique, rectangular and square plane groups and for triclinic, monoclinic, orthorhombic and tetragonal space groups $\mathcal{G}$. The index is 2 or 3 for hexagonal plane groups and for trigonal and hexagonal space groups $\mathcal{G}$. The index is 2, 3 or 4 for cubic space groups $\mathcal{G}$.

2.1.7.3. *Graphs for klassengleiche subgroups*

There are 29 graphs for *klassengleiche* or *k*-subgroups, one for each crystal class with the exception of the crystal classes 1, $\overline{1}$ and $\overline{6}$ with only one space-group type each: *P*1, No. 1, $P\overline{1}$, No. 2, and $P\overline{6}$, No. 174, respectively. The sequence of the graphs is

[5] The HM symbols used here are nonconventional. They display the setting of the point group and follow the rules of *IT* A, Section 2.2.4.

determined by the sequence of the point groups in *IT* A, Table 2.1.2.1, fourth column. The graphs of $\overline{4}$, $\overline{3}$ and $6/m$ are nearly trivial, because to these crystal classes only two space-group types belong. The graphs of $mm2$ with 22, of mmm with 28 and of $4/mmm$ with 20 space-group types are the most complicated ones.

Isomorphic subgroups are special cases of *k*-subgroups. With the exception of both partners of the enantiomorphic space-group types, isomorphic subgroups are not displayed in the graphs. The explicit display of the isomorphic subgroups would add an infinite number of lines from each field for a space group back to this field, or at least one line (*e.g.* a circle) implicitly representing the infinite number of isomorphic subgroups, see the tables of maximal subgroups of Chapter 2.3.[6] Such a line would have to be attached to every space-group symbol. Thus, there would be no more information.

Nevertheless, connections between isomorphic space groups are included indirectly if the group–subgroup chain encloses a space group of another type. In this case, a space group $\mathcal{X}$ may be a subgroup of a space group $\mathcal{Y}$ and $\mathcal{Y}'$ a subgroup of $\mathcal{X}$, where $\mathcal{Y}$ and $\mathcal{Y}'$ belong to the same space-group type. The subgroup chain is then $\mathcal{Y} - \mathcal{X} - \mathcal{Y}'$. The two space groups $\mathcal{Y}$ and $\mathcal{Y}'$ are not identical but isomorphic. Whereas in general the label for the subgroup is positioned at a lower level than that for the original space group, for such relations the symbols for $\mathcal{X}$ and $\mathcal{Y}$ can only be drawn on the same level, connected by horizontal lines. If this happens at the top of a graph, the top level is occupied by more than one symbol (the number of symbols in the top level is the same as the number of symmorphic space-group types of the crystal class).

Horizontal lines are drawn as left or right arrows depending on the kind of relation. The arrow is always directed from the supergroup to the subgroup. If the relation is two-sided, as is always the case for enantiomorphic space-group types, then the relation is displayed by a pair of horizontal lines, one of them formed by a right and the other by a left arrow. In the graph in Fig. 2.5.1.5 for crystal class $mm2$, the connections of $Pmm2$ with $Cmm2$ and with $Amm2$ are displayed by double-headed arrows instead. Furthermore, some arrows in Fig. 2.5.1.5, crystal class $mm2$, and Fig. 2.5.1.6, mmm, are dashed or dotted in order to better distinguish the different lines and to increase clarity.

The different kinds of relations are demonstrated in the following examples.

Example 2.1.7.3.1.

In the graph in Fig. 2.5.1.1, crystal class 2, a space group $P2$ may be a subgroup of index 2 of a space group $C2$ by 'Loss of centring translations'. On the other hand, subgroups of $P2$ in the block 'Enlarged unit cell', $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = 2\mathbf{b}$, $C2$ (3) belong to the type $C2$, see the tables of maximal subgroups in Chapter 2.3. Therefore, both symbols are drawn at the same level and are connected by a pair of arrows pointing in opposite directions. Thus, the top level is occupied twice. In the graph in Fig. 2.5.1.2 of crystal class m, both the top level and the bottom level are occupied twice.

Example 2.1.7.3.2.

There are four symbols at the top level of the graph in Fig. 2.5.1.4, crystal class 222. Their relations are rather complicated. Whereas one can go (by index 2) from $P222$ directly to a subgroup of type $C222$ and *vice versa*, the connection from $F222$ directly to $C222$ is one-way. One always has to pass $C222$ on the way from $F222$ to a subgroup of the types $P222$ or $I222$. Thus, the only maximal subgroup of $F222$ among these groups is $C222$. One can go directly from $P222$ to $F222$ but not to $I222$ *etc*.

Because of the horizontal connecting arrows, it is clear that there cannot be much correspondence between the level in the graphs and the subgroup index. However, in no graph is a subgroup positioned at a higher level than the supergroup.

Example 2.1.7.3.3.

Consider the graph in Fig. 2.5.1.6 for crystal class mmm. To the space group $Cmmm$ (65) belong maximal non-isomorphic subgroups of the 11 space-group types (from left to right) $Ibam$ (72), $Cmcm$ (63), $Imma$ (74), $Pmmn$ (59), $Pbam$ (55), $Pban$ (50), $Pmma$ (51), $Pmna$ (53), $Cccm$ (66), $Pmmm$ (47) and $Immm$ (71). Although all of them have index 2, their symbols are positioned at very different levels of the graph.

The table for the subgroups of $Cmmm$ in Chapter 2.3 lists 22 non-isomorphic *k*-subgroups of index 2, because some of the space-group types mentioned above are represented by two or four different subgroups. This multiplicity cannot be displayed by multiple lines because the density of the lines in some of the *k*-subgroup graphs does not permit this kind of presentation, *e.g.* for mmm. The multiplicity may be taken from the subgroup tables in Chapter 2.3, where each non-isomorphic subgroup is listed individually.

Consider the connections from $Cmmm$ (65) to $Pbam$ (55). There are among others: the direct connection of index 2, the connection of index 4 over $Ibam$ (72), the connection of index 8 over $Imma$ (74) and $Pmma$ (51). Thus, starting from the same space group of type $Cmmm$ one arrives at different space groups of the type $Pbam$ with different unit cells but all belonging to the same space-group type and thus represented by the same field of the graph.

The index of a *k*-subgroup is restricted by Lemma 1.2.8.2.3 and by additional conditions. For the following statements one has to note that enantiomorphic space groups are isomorphic.

(1) A non-isomorphic maximal *k*-subgroup of an oblique, rectangular or tetragonal plane group or of a triclinic, monoclinic, orthorhombic or tetragonal space group always has index 2.
(2) In general, a non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a trigonal space group $\mathcal{G}$ has index 3. Exceptions are the pairs $P3m1$–$P3c1$, $P31m$–$P31c$, $R3m$–$R3c$, $P\overline{3}1m$–$P\overline{3}1c$, $P\overline{3}m1$–$P\overline{3}c1$ and $R\overline{3}m$–$R\overline{3}c$ with space-group Nos. between 156 and 167. They have index 2.
(3) A non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a hexagonal space group has index 2 or 3.
(4) A non-isomorphic maximal *k*-subgroup $\mathcal{H}$ of a cubic space group $\mathcal{G}$ has either index 2 or index 4. The index is 2 if $\mathcal{G}$ has an I lattice and $\mathcal{H}$ a P lattice or if $\mathcal{G}$ has a P lattice and $\mathcal{H}$ an F lattice. The index is 4 if $\mathcal{G}$ has an F lattice and $\mathcal{H}$ a P lattice or if $\mathcal{G}$ has a P lattice and $\mathcal{H}$ an I lattice.

2.1.7.4. *Graphs for plane groups*

There are no graphs for plane groups in this volume. The four graphs for *t*-subgroups of plane groups are apart from the symbols the same as those for the corresponding space groups: $p4mm$–$P4mm$, $p6mm$–$P6mm$, $p2mg$–$Pma2$ and $p2gg$–$Pba2$, where the graphs for the space groups are included in the *t*-subgroup graphs in Figs. 2.4.1.1, 2.4.3.1, 2.4.2.1 and 2.4.2.3, respectively.

[6] One could contemplate adding one line for each series of maximal isomorphic subgroups. However, the number of series depends on the rules that define the distribution of the isomorphic subgroups into the series and is thus not constant.

references