International Tables for Crystallography (2006). Vol. A1, Section 2.1.7.4, pp. 56–57.

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.

The k-subgroup graphs are trivial for the plane groups $p1$, $p2$, $p4$, $p3$, $p6$ and $p6mm$ because there is only one plane group in its crystal class. The graphs for the crystal classes $4mm$ and $3m$ consist of two plane groups each: $p4mm$ and $p4gm$, $p3m1$ and $p31m$. Nevertheless, the graphs are different: the relation is one-sided for the tetragonal plane-group pair as it is in the space-group pair $P6/m$ (175)–$P6_3/m$ (176) and it is two-sided for the hexagonal plane-group pair as it is in the space-group pair $P\overline{4}$ (81)–$I\overline{4}$ (82). The graph for the three plane groups of the crystal class m corresponds to the space-group graph for the crystal class 2.

Finally, the graph for the four plane groups of crystal class $2mm$ has no direct analogue among the k-subgroup graphs of the space groups. It can be obtained, however, from the graph in Fig. 2.5.1.3 of crystal class $2/m$ by removing the fields of $C2/c$ (15) and $P2_1/m$ (11) with all their connections to the remaining fields. The replacements are then: $C2/m$ (12) by $c2mm$ (9), $P2/m$ (10) by $p2mm$ (6), $P2/c$ (13) by $p2mg$ (7) and $P2_1/c$ (14) by $p2gg$ (8).

2.1.7.5. *Application of the graphs*

If a subgroup is not maximal then there must be a group–subgroup chain $\mathcal{G}$–$\mathcal{H}$ of maximal subgroups with more than two members which connects $\mathcal{G}$ with $\mathcal{H}$. There are three possibilities: $\mathcal{H}$ may be a t-subgroup or a k-subgroup or a general subgroup of $\mathcal{G}$. In the first two cases, the application of the graphs is straightforward because at least one of the graphs will permit one to find the possible chains directly. If $\mathcal{H}$ is a k-subgroup of $\mathcal{G}$, isomorphic subgroups have to be included if necessary. If $\mathcal{H}$ is a general subgroup of $\mathcal{G}$ one has to combine t- and k-subgroup graphs, but the problem is only slightly more complicated. This is because for a general subgroup $\mathcal{H} < \mathcal{G}$, Hermann's theorem 1.2.8.1.2 states the existence of an intermediate group $\mathcal{M}$ with $\mathcal{H} < \mathcal{M} < \mathcal{G}$ and the properties $\mathcal{H} < \mathcal{M}$ is a k-subgroup of $\mathcal{M}$ and $\mathcal{M} < \mathcal{G}$ is a t-subgroup of $\mathcal{G}$.

Thus, however long and complicated the real chain may be, there is also always a chain for which only two graphs are needed: a t-subgroup graph for the relation between $\mathcal{G}$ and $\mathcal{M}$ and a k-subgroup graph for the relation between $\mathcal{M}$ and $\mathcal{H}$.

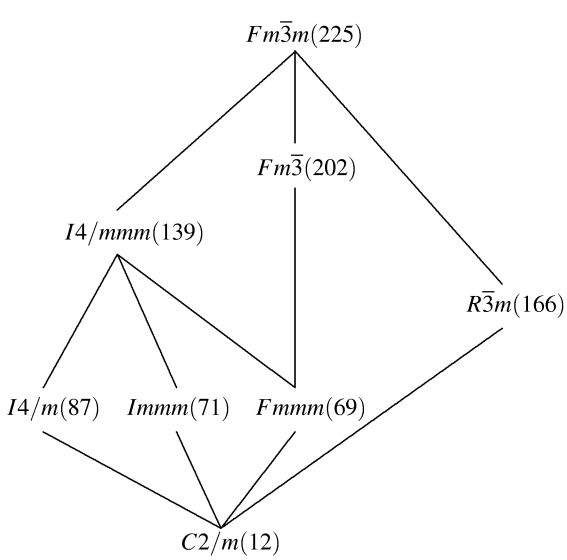

Fig. 2.1.7.1. Contracted graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to those subgroups with index 12 which belong to the space-group type $C2/m$ (12). The graph forms part of the total contracted graph of t-subgroups of $Fm\overline{3}m$ (Fig. 2.4.1.5).

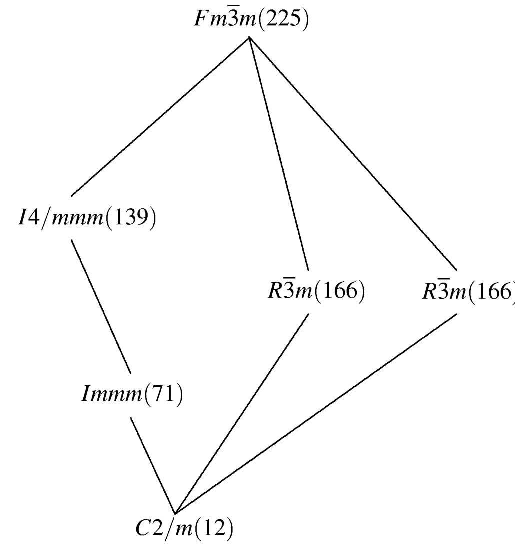

Fig. 2.1.7.2. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one representative of those six $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the $\langle 110\rangle$ directions of $Fm\overline{3}m$.

There is, however, a severe shortcoming to using contracted graphs for the analysis of group–subgroup relations, and great care has to be taken in such investigations. All subgroups $\mathcal{H}_j$ with the same space-group type are represented by the same field of the graph, but these different non-maximal subgroups may permit different routes to a common original (super)group.

Example 2.1.7.5.1.

An example for *translationengleiche* subgroups is provided by the group–subgroup chain $Fm\overline{3}m$ (225)–$C2/m$ (12) of index 12. The contracted graph may be drawn by the program *Subgroupgraph* from the Bilbao Crystallographic Server, http://www.cryst.ehu.es/. It is shown in Fig. 2.1.7.1; each field represents all occurring subgroups of a space-group type: $I4/mmm$ (139) represents three subgroups, $R\overline{3}m$ (166) represents four subgroups, … and $C2/m$ (12) represents nine subgroups belonging to two conjugacy classes. Fig. 2.1.7.1 is part of the contracted total graph of the *translationengleiche* subgroups of the space group $Fm\overline{3}m$, which is displayed in Fig.

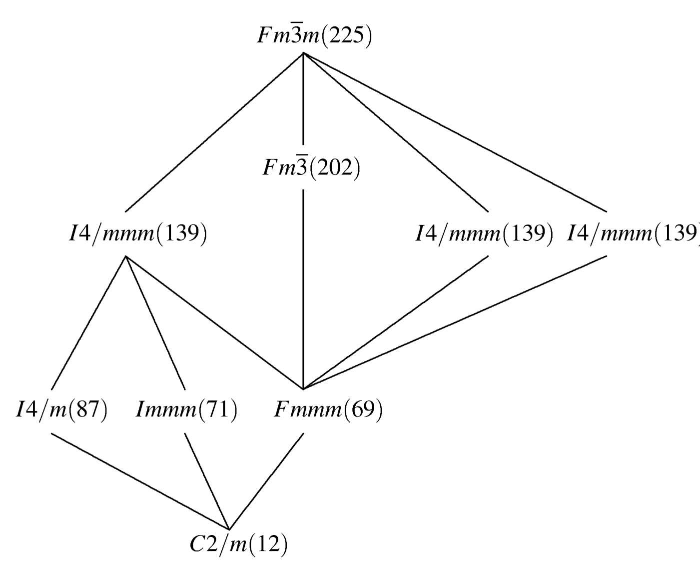

Fig. 2.1.7.3. Complete graph of the group–subgroup chains from $Fm\overline{3}m$ (225) to one representative of those three $C2/m$ (12) subgroups with index 12 whose monoclinic axes are along the $\langle 001\rangle$ directions of $Fm\overline{3}m$.