International Tables for Crystallography (2006). Vol. A1, Section 2.1.6, pp. 53–54.

occurs in the first 'coordinate' of the generators (2) and (3) of $\mathcal{G}$ but not in the generator (5).

The term $2u$ appears in both descriptions. It is introduced in order to adapt the generators to the origin shift u, 0, 0.

In other space groups described in two origin choices, surprisingly, the number of series is different for origin choice 1 and origin choice 2.

Example 2.1.5.5.3.

In the tetragonal space group $I4_1/amd$, No. 141, for origin choice 1 there is *one* series of maximal isomorphic subgroups of index p^2, p prime, with the bases $p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ and origin shifts u, v, 0. For origin choice 2, there are *two* series with the same bases $p\mathbf{a}$, $p\mathbf{b}$, $\mathbf{c}$ but with the different origin shifts u, v, 0 and $\frac{1}{2}+u$, v, 0. What are the reasons for these results?

For origin choice 1, the term $\frac{1}{2}$ appears in the first and second 'coordinates' of all generators (2), (3), (5) and (9) of $\mathcal{G}$. This term $\frac{1}{2}$ is the cause of the translation vectors $(\frac{p}{2}-\frac{1}{2})\mathbf{a}$ and $(\frac{p}{2}-\frac{1}{2})\mathbf{b}$ in the generators of $\mathcal{H}$.

For origin choice 2, fractions $\frac{1}{4}$ and $\frac{3}{4}$ appear in all 'coordinates' of the generator (3) $\bar{y}+\frac{1}{4}, x+\frac{3}{4}, z+\frac{1}{4}$ of $\mathcal{G}$. As a consequence, translational parts with vectors $(\frac{p}{4}+\frac{1}{4})\mathbf{a}$ and $(\frac{3p}{4}-\frac{5}{4})\mathbf{b}$ appear if $p \equiv 3 \pmod 4$. On the other hand, translational parts with vectors $(\frac{p}{4}-\frac{1}{4})\mathbf{a}$, $(\frac{3p}{4}-\frac{3}{4})\mathbf{b}$ are introduced in the generators of $\mathcal{H}$ if $p \equiv 1 \pmod 4$ holds.

Another consequence of the fractions $\frac{1}{4}$ and $\frac{3}{4}$ occurring in the generator (3) of $\mathcal{G}$ is the difference in the origin shifts. They are $\frac{1}{2}+u$, v, 0 for $p \equiv 3 \pmod 4$ and u, v, 0 for $p \equiv 1 \pmod 4$. Thus, the one series in origin choice 1 for odd p is split into two series in origin choice 2 for $p \equiv 3 \pmod 4$ and $p \equiv 1 \pmod 4$.[3]

2.1.6. Minimal supergroups

2.1.6.1. *General description*

In the previous sections, the relation $\mathcal{H} < \mathcal{G}$ was seen from the viewpoint of the group $\mathcal{G}$. In this case, $\mathcal{H}$ was a subgroup of $\mathcal{G}$. However, the same relation may be viewed from the group $\mathcal{H}$. In this case, $\mathcal{G} > \mathcal{H}$ is a *supergroup* of $\mathcal{H}$. As for the subgroups of $\mathcal{G}$, *cf.* Section 1.2.6, different kinds of supergroups of $\mathcal{H}$ may be distinguished. The following definitions are obvious.

Definition 2.1.6.1.1. Let $\mathcal{H} < \mathcal{G}$ be a maximal subgroup of $\mathcal{G}$. Then $\mathcal{G} > \mathcal{H}$ is called a *minimal supergroup* of $\mathcal{H}$. If $\mathcal{H}$ is a *translationengleiche* subgroup of $\mathcal{G}$ then $\mathcal{G}$ is a *translationengleiche supergroup* (*t-supergroup*) of $\mathcal{H}$. If $\mathcal{H}$ is a *klassengleiche* subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a *klassengleiche supergroup* (*k-supergroup*) of $\mathcal{H}$. If $\mathcal{H}$ is an isomorphic subgroup of $\mathcal{G}$, then $\mathcal{G}$ is an *isomorphic supergroup* of $\mathcal{H}$. If $\mathcal{H}$ is a general subgroup of $\mathcal{G}$, then $\mathcal{G}$ is a *general supergroup* of $\mathcal{H}$. □

The search for supergroups of space groups is much more difficult than the search for subgroups. One of the reasons for this difficulty is that the search for subgroups $\mathcal{H} < \mathcal{G}$ is restricted to the elements of the space group $\mathcal{G}$ itself, whereas the search for supergroups $\mathcal{G} > \mathcal{H}$ has to take into account the whole (continuous) group $\mathcal{E}$ of all isometries. For example, there are only a finite number of subgroups $\mathcal{H}$ of any space group $\mathcal{G}$ for any given index i. On the other hand, there may not only be an infinite number of supergroups $\mathcal{G}$ of a space group $\mathcal{H}$ for a finite index i but even an uncountably infinite number of supergroups of $\mathcal{H}$.

Example 2.1.6.1.2.

Let $\mathcal{H} = P1$. Then there is an infinite number of t-supergroups $P\bar{1}$ of index 2 because there is no restriction for the sites of the centres of inversion and thus of the conventional origin of $P\bar{1}$.

In the tables of this volume, a supergroup $\mathcal{G}$ of a space group $\mathcal{H}$ is listed by its type if $\mathcal{H}$ is listed as a subgroup of $\mathcal{G}$. The entry contains at least the index of $\mathcal{H}$ in $\mathcal{G}$, the conventional HM symbol of $\mathcal{G}$ and its space-group number. Additional data may be given for *klassengleiche* supergroups. More details, *e.g.* the representatives of the general position or the generators as well as the transformation matrix and the origin shift, would only duplicate the subgroup data. The number of supergroups belonging to one entry can neither be concluded from the subgroup data nor is it listed among the supergroup data.

Like the subgroup data, the supergroup data are also partitioned into blocks.

2.1.6.2. *I Minimal translationengleiche supergroups*

For each space group $\mathcal{H}$, under this heading are listed those space-group types $\mathcal{G}$ for which $\mathcal{H}$ appears as an entry under the heading **I Maximal *translationengleiche* subgroups**. The listing consists of the index in brackets [...], the conventional HM symbol and (in parentheses) the space-group number (...). The space groups are ordered by ascending space-group number. If this line is empty, the heading is printed nevertheless and the content is announced by 'none', as in $P6/mmm$, No. 191.

The supergroups listed on the line **I Minimal *translationengleiche* supergroups** are realized only if the lattice conditions of $\mathcal{H}$ fulfil the lattice conditions for $\mathcal{G}$. For example, if $\mathcal{G} = P422$, No. 89, is a supergroup of $\mathcal{H} = P222$, No. 16, two of the three independent lattice parameters a, b, c of $P222$ must be equal (or in crystallographic practice, approximately equal). These must be a and b if c is the tetragonal axis, b and c if a is the tetragonal axis or c and a if b is the tetragonal axis. In the latter two cases, the setting of $P222$ has to be adapted to the conventional c-axis setting of $P422$. For the cubic supergroup $P23$, No. 195, all three lattice parameters of $P222$ must be (approximately) equal. Such conditions are always to be taken into consideration if the t-supergroup belongs to a different crystal family[4] to the original group. Therefore, for $\mathcal{H} = P222$ there is no lattice condition for the supergroup $\mathcal{G} = Pmmm$ because $P222$ and $Pmmm$ belong to the same crystal family.

2.1.6.3. *II Minimal non-isomorphic klassengleiche supergroups*

Klassengleiche supergroups $\mathcal{G} > \mathcal{H}$ always belong to the crystal family of $\mathcal{H}$. Therefore, there are no restrictions for the lattice parameters of $\mathcal{H}$.

The block **II Minimal non-isomorphic *klassengleiche* supergroups** is divided into two subblocks with the headings **Additional centring translations** and **Decreased unit cell**. If both subblocks are empty, only the heading of the block is listed, stating 'none' for the content of the block, as in $P6/mmm$, No. 191.

If at least one of the subblocks is non-empty, then the heading of the block and the headings of both subblocks are listed. An

[3] F. Gähler (private communication) has shown that such a splitting can be avoided if one allows the prime p to enter the formulae for the origin shifts. In these tables we have not made use of this possibility in order to keep the origin shifts in the same form for all space groups $\mathcal{G}$.

[4] For the term 'crystal family' *cf.* Section 1.2.5.2, or, for more details, *IT* A, Section 8.2.7.

empty subblock is then designated by 'none'; in the other subblock the supergroups are listed. The kind of listing depends on the subblock. Examples may be found in the tables of *P*222, No. 16, and $Fd\bar{3}c$, No. 228.

Under the heading 'Additional centring translations', the supergroups are listed by their indices and either by their nonconventional HM symbols, with the space-group numbers and the standard HM symbols in parentheses, or by their conventional HM symbols and only their space-group numbers in parentheses. Examples are provided by space group *Pbca*, No. 61, with both subblocks non-empty and by space group *P*222, No. 16, with supergroups only under the heading 'Additional centring translations'.

Under the heading 'Decreased unit cell' each supergroup is listed by its index and by its lattice relations, where the basis vectors $\mathbf{a}'$, $\mathbf{b}'$ and $\mathbf{c}'$ refer to the supergroup $\mathcal{G}$ and the basis vectors **a**, **b** and **c** to the original group $\mathcal{H}$. After these data are listed either the nonconventional HM symbol, followed by the space-group number and the conventional HM symbol in parentheses, or the conventional HM symbol with the space-group number in parentheses. Examples are provided again by space group *Pbca*, No. 61, with both subblocks occupied and space group $F\bar{4}3m$, No. 216, with an empty subblock 'Additional centring translations' but data under the heading 'Decreased unit cell'.

2.1.6.4. *Isomorphic supergroups*

Each space group $\mathcal{G}$ has an infinite number of isomorphic subgroups $\mathcal{H}$ because the number of primes is infinite. For the same reason, each space group $\mathcal{H}$ has an infinite number of isomorphic supergroups $\mathcal{G}$. They are not listed in the tables of this volume because they are implicitly listed among the subgroup data.

2.1.7. The subgroup graphs

2.1.7.1. *General remarks*

The group–subgroup relations between the space groups may also be described by graphs. This way is chosen in Chapters 2.4 and 2.5. Graphs for the group–subgroup relations between crystallographic point groups have been published, for example, in *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and in *IT* A (2002), Fig. 10.1.4.3. Three kinds of graphs for subgroups of space groups have been constructed and can be found in the literature:

(1) Graphs for *t*-subgroups, such as the graphs of Ascher (1968).
(2) Graphs for *k*-subgroups, such as the graphs for cubic space groups of Neubüser & Wondratschek (1966).
(3) Mixed graphs, combining *t*- and *k*-subgroups. These are used, for example, when relations between existing or suspected crystal structures are to be displayed. An example is the 'family tree' of Bärnighausen (1980), Fig. 15, now called a *Bärnighausen tree*.

A complete collection of graphs of the first two kinds is presented in this volume: in Chapter 2.4 those displaying the *translationengleiche* or *t*-subgroup relations and in Chapter 2.5 those for the *klassengleiche* or *k*-subgroup relations. Neither type of graph is restricted to maximal subgroups but both contain *t*- or *k*-subgroups of higher indices, with the exception of isomorphic subgroups, *cf.* Section 2.1.7.3 below.

The group–subgroup relations are direct relations between the space groups themselves, not between their types. However, each such relation is valid for a pair of space groups, one from each of the types, and for each space group of a given type there exists a corresponding relation. In this sense, one can speak of a relation between the space-group types, keeping in mind the difference between space groups and space-group types, *cf.* Section 1.2.5.3.

The space groups in the graphs are denoted by the standard HM symbols and the space-group numbers. In each graph, each space-group type is displayed at most once. Such graphs are called *contracted graphs* here. Without this contraction, the more complex graphs would be much too large for the page size of this volume.

The symbol of a space group $\mathcal{G}$ is connected by uninterrupted straight lines with the symbols of all maximal non-isomorphic subgroups $\mathcal{H}$ or minimal non-isomorphic supergroups $\mathcal{S}$ of $\mathcal{G}$. In general, the *maximal subgroups* of $\mathcal{G}$ are drawn on a *lower level* than $\mathcal{G}$; in the same way, the *minimal supergroups* of $\mathcal{G}$ are mostly drawn on a *higher level* than $\mathcal{G}$. For exceptions see Section 2.1.7.3. Multiple lines may occur in the graphs for *t*-subgroups. They are explained in Section 2.1.7.2. No indices are attached to the lines. They can be taken from the corresponding subgroup tables of Chapter 2.3, and are also provided by the general formulae of Section 1.2.8. For the *k*-subgroup graphs, they are further specified at the end of Section 2.1.7.3.

2.1.7.2. *Graphs for translationengleiche subgroups*

Let $\mathcal{G}$ be a space group and $\mathcal{T}(\mathcal{G})$ the normal subgroup of all its translations. Owing to the isomorphism between the factor group $\mathcal{G}/\mathcal{T}(\mathcal{G})$ and the point group $\mathcal{P}_{\mathcal{G}}$, see Section 1.2.5.4, according to the first isomorphism theorem, Ledermann (1976), *t*-subgroup graphs are the same (up to the symbols) as the corresponding graphs between point groups. However, in this volume, the graphs are not complete but are contracted by displaying each space-group type at most once. This contraction may cause the graphs to look different from the point-group graphs and also different for different space groups of the same point group, *cf.* Example 2.1.7.2.1.

One can indicate the connections between a space group $\mathcal{G}$ and its maximal subgroups in different ways. In the contracted *t*-subgroup graphs one line is drawn for each conjugacy class of maximal subgroups of $\mathcal{G}$. Thus, a line represents the connection to an individual subgroup only if this is a normal maximal subgroup of $\mathcal{G}$, otherwise it represents the connection to more than one subgroup. The conjugacy relations are not necessarily transferable to non-maximal subgroups, *cf.* Example 2.1.7.2.2. On the other hand, multiple lines are possible, see the examples. Although it is not in general possible to reconstruct the complete graph from the contracted one, the content of information of such a graph is higher than that of a graph which is drawn with simple lines only.

The graph for the space group at its top also contains the contracted graphs for all subgroups which occur in it, see the remark below Example 2.1.7.2.2.

Owing to lack of space for the large graphs, in all graphs of *t*-subgroups the group *P*1, No. 1, and its connections have been omitted. Therefore, to obtain the full graph one has to supplement the graphs by *P*1 at the bottom and to connect *P*1 by one line to each of the symbols that have no connection downwards.

Within the same graph, symbols on the same level indicate subgroups of the same index relative to the group at the top. The distance between the levels indicates the size of the index. For a more detailed discussion, see Example 2.1.7.2.2. For the sequence and the numbers of the graphs, see the paragraph below Example 2.1.7.2.2.

references