International Tables for Crystallography (2011). Vol. A1, Section 2.1.6, pp. 84–85.

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 $p = 4n - 1$. 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 $p = 4n + 1$ 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 $p = 4n - 1$ and $u, v, 0$ for $p = 4n + 1$. Thus, the one series in origin choice 1 for odd p is split into two series in origin choice 2 for $p = 4n - 1$ and $p = 4n + 1$.[4]

2.1.6. The data for minimal supergroups

2.1.6.1. Description of the listed data

In the previous sections, the relation $\mathcal{H} < \mathcal{G}$ between space groups 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.

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 $\mathcal{H}$. □

Following from Hermann's theorem, Lemma 1.2.8.1.2, a minimal supergroup of a space group is either a *translationengleiche* supergroup (*t*-supergroup) or a *klassengleiche* supergroup (*k*-supergroup). A proper minimal *t*-supergroup always has an index i, $1 < i < 5$, and is never isomorphic. A minimal *k*-supergroup with index i, $1 < i < 5$, may be isomorphic or non-isomorphic; for indices $i > 4$ a minimal *k*-supergroup can only be an isomorphic *k*-supergroup. The propositions, theorems and their corollaries of Sections 1.4.6 and 1.4.7 for maximal subgroups are correspondingly valid for minimal supergroups.

Subgroups of space groups of finite index are always space groups again. This does not hold for supergroups. For example, the direct product $\mathcal{G}$ of a space group $\mathcal{H}$ with a group of order 2 is not a space group, although $\mathcal{H} < \mathcal{G}$ is a subgroup of index 2 of $\mathcal{G}$. Moreover, supergroups of space groups may be affine groups which are only isomorphic to space groups but not space groups themselves, see Example 2.1.6.2.2. In the following we restrict the considerations to supergroups $\mathcal{G}$ of a space group $\mathcal{H}$ which are themselves space groups. This holds, for example, for the symmetry relations between crystal structures when the symmetries of both structures can be described by space groups. Quasicrystals, incommensurate phases *etc.* are thus excluded. Even under this restriction, supergroups show much more variable behaviour than subgroups do.

One of the reasons for this complication 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 minimal 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, the minimal *translationengleiche* supergroups $\mathcal{G}$ of a space group $\mathcal{H}$ are not listed individually but the type of $\mathcal{G}$ is listed by index, conventional HM symbol and space-group number if $\mathcal{H}$ is listed as a *translationengleiche* subgroup of $\mathcal{G}$ in the subgroup tables. Not listed is the number of supergroups belonging to one entry. Non-isomorphic *klassengleiche* supergroups are listed individually. For them, nonconventional HM symbols are listed in addition; for *klassengleiche* supergroups with 'Decreased unit cell', the lattice relations are added. More details, such as 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.

In this Section 2.1.6, the kind of listing is described explicitly. The data for maximal subgroups $\mathcal{H}$ are complete for all space groups $\mathcal{G}$. Therefore, it is possible to derive:

(1) all minimal *translationengleiche* supergroups $\mathcal{G}$ of $\mathcal{H}$ if the point-group symmetry of $\mathcal{H}$ is at least orthorhombic (*i.e.* neither triclinic nor monoclinic);

(2) all minimal *klassengleiche* supergroups $\mathcal{G}$ for each space group $\mathcal{H}$.

In Section 2.1.7 the procedure is described by which the supergroup data can be obtained from the subgroup data. This procedure is not trivial and care has to be taken to really obtain the full set of supergroups. In Section 2.1.7 one can also find the reasons why this procedure is not applicable when the space group $\mathcal{H}$ belongs to a triclinic or monoclinic point group.

Isomorphic supergroups are not indicated at all because they are implicitly contained in the subgroup data. Their derivation from the subgroup data is discussed in Section 2.1.7.2.

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 the space-group number (in parentheses). The space groups are ordered by ascending space-group number. If this line

[4] 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 $\mathcal{G}$.

is empty, the heading is printed nevertheless and the content is announced by 'none', as in $P6/mmm$, No. 191. Note that the real setting of the supergroup and thus its HM symbol may be nonconventional.

Example 2.1.6.2.1

Let $\mathcal{H} = P2_12_12$, No. 18. Among the entries of the block one finds the space groups of the crystal class *mmm*: [2] *Pbam*, No. 55; [2] *Pccn*, No. 56; [2] *Pbcm*, No. 57; [2] *Pnnm*, No. 58; [2] *Pmmn*, No. 59 and [2] *Pbcn*, No. 60, designated by their standard HM symbols. However, the full HM symbols $P2_1/b2_1/a2/m$, $P2_1/c2_1/c2/n$, $P2/b2_1/c2_1/m$, $P2_1/n2_1/n2/m$, $P2_1/m2_1/m2/n$ and $P2_1/b2/c2_1/n$ reveal that only the four HM symbols *Pbam*, *Pccn*, *Pnnm* and *Pmmn* of these six entries describe supergroups of $P2_12_12$. The symbols $P2/b2_1/c2_1/m$ and $P2_1/b2/c2_1/n$ represent four supergroups of $P2_12_12$, namely $\mathcal{G} = P2_1/b2_1/m2/a$, $P2_1/m2_1/a2/b$, $P2_1/c2_1/n2/b$ and $P2_1/n2_1/c2/a$. This is not obvious but will be derived, as well as the origin shift if necessary, with the procedure described in Examples 2.1.7.3.2 and 2.1.7.4.3.

The supergroups listed in this block represent space groups only if the lattice conditions of $\mathcal{H}$ fulfil the lattice conditions for $\mathcal{G}$. This is not a problem if group $\mathcal{H}$ and supergroup $\mathcal{G}$ belong to the same crystal family,[5] *cf.* Example 2.1.6.2.1. Otherwise the lattice parameters of $\mathcal{H}$ have to be checked correspondingly, as in Example 2.1.6.2.2.

Example 2.1.6.2.2

Space group $\mathcal{H} = P222$, No. 16. For the minimal supergroups $\mathcal{G} = Pmmm$, No. 47, *Pnnn*, No. 48, *Pccm*, No. 49, and *Pban*, No. 50, there is no lattice condition because *P*222 and all these supergroups belong to the same orthorhombic crystal family and thus are space groups. If, however, a space group of the types $\mathcal{G} = P422$, No. 89, $P4_222$, No. 93, $P\bar{4}2m$, No. 111, or $P\bar{4}2c$, No. 112, is considered as a supergroup of $\mathcal{H} = P222$, two of the three independent lattice parameters *a*, *b*, *c* of *P*222 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 *P*222 has to be transformed to the *c*-axis setting of *P*422. For the cubic supergroup *P*23, No. 195, all three lattice parameters of *P*222 must be (approximately) equal. If they are not, elements of $\mathcal{G}$ are not isometries and $\mathcal{G}$ is an affine group which is only isomorphic to a space group.

The lattice conditions are useful in the search for supergroups $\mathcal{G} > \mathcal{H}$ which are space groups, *i.e.* form the symmetry of crystal structures. Whereas a subgroup $\mathcal{H} < \mathcal{G}$ does not become noticeable in the lattice parameters of a space group $\mathcal{G}$, a space group $\mathcal{G} > \mathcal{H}$ of another crystal family must be indicated by the lattice parameters of the space group $\mathcal{H}$. Thus it may be an important advantage if the conditions of temperature, pressure or composition allow the start of the search for possible phase transitions of the low-symmetry phase.

As mentioned already, the number of the minimal *t*-supergroups cannot be taken or concluded from the subgroup tables. It is different in the different cases of Example 2.1.6.2.2 above. The space group *P*222 has one minimal supergroup of the type *Pmmm* and one of *Pnnn*; there are three minimal supergroups of type *Pccm*, namely *Pccm*, *Pmaa* and *Pbmb*, as well as three minimal supergroups of type *Pban*, *viz*. *Pban*, *Pncb* and *Pcna*. There are six minimal supergroups of the type *P*422 and four minimal supergroups of the type *P*23; they are space groups if the lattice conditions are fulfilled. The number of different supergroups will be calculated in Examples 2.1.7.3.1 and 2.1.7.4.2 by the procedure described in Section 2.1.7.4.

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

2.1.6.3. II Minimal non-isomorphic klassengleiche supergroups

If $\mathcal{G}$ is a *k*-supergroup of $\mathcal{H}$, $\mathcal{G}$ and $\mathcal{H}$ always belong to the same crystal family and there are no lattice restrictions for $\mathcal{H}$.

As mentioned above, in the tables of this volume only non-isomorphic minimal *k*-supergroups are listed among the supergroup data; no isomorphic minimal supergroups are given. 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 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.

As discussed in Section 2.1.7.1, there is exactly one supergroup for each of the non-isomorphic *k*-supergroup entries of $\mathcal{H}$, although often not in the conventional setting. A transformation of the general-position representatives or of the generators to the conventional setting may be necessary to obtain the standard HM symbol of $\mathcal{G}$ in the same way as in Examples 2.1.7.3.1 and 2.1.7.3.2, which refer to *translationengleiche* supergroups.

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 conventional 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'.

Not only the HM symbols but also the centrings themselves may be nonconventional. In this volume, the nonconventional centrings tetragonal *c* (*c*4*gm* as a supergroup of *p*4*gm*) and *h* (*h*31*m* as a supergroup of *p*31*m*) are used for HM symbols of plane groups, tetragonal *C* ($C\bar{4}m2$ as a supergroup of $P\bar{4}m2$), $R_{\rm rev}$ 'reverse', different from the conventional $R_{\rm obv}$ 'obverse' ($R_{\rm rev}3$ as supergroup of *P*3), and *H* (*H*312 as supergroup of *P*312) are used for HM symbols of space groups.

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'.

references