International Tables for Crystallography (2006). Vol. A, Section 8.3.3.3, pp. 735–736.

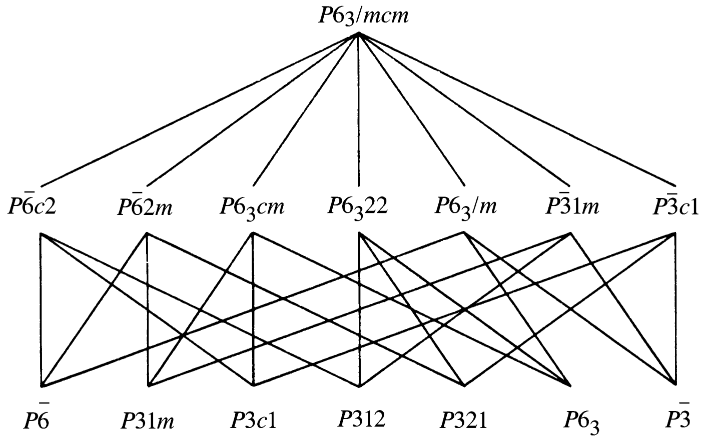

Fig. 8.3.3.1. Space group $P6_3/mcm$ with *t* subgroups of index [2] and [4]. All 21 possible subgroup chains are displayed by lines.

but eliminating all rotations and combinations of rotations with translations. For every space group of space-group type $P2$ such a subgroup $P1$ exists. Thus the relationship exists, in an extended sense, for the two space-group types involved. One can, therefore, list these relationships by means of the symbols of the space-group types.

For every subgroup $\mathcal{H}$ of a space group $\mathcal{G}$, a 'right coset decomposition' of $\mathcal{G}$ relative to $\mathcal{H}$ can be defined as

$$\mathcal{G} = \mathcal{H} + \mathcal{H}\mathsf{G}_2 + \ldots + \mathcal{H}\mathsf{G}_i.$$

The elements $\mathsf{G}_2, \ldots, \mathsf{G}_i$ of $\mathcal{G}$ are such that G_j is contained only in the coset $\mathcal{H}\mathsf{G}_j$. The integer $[i]$, *i.e.* the number of cosets, is called the index of $\mathcal{H}$ in $\mathcal{G}$; *cf.* Section 8.1.6, footnote §.

The index $[i]$ of a subgroup has a geometric significance. It determines the 'dilution' of symmetry operations of $\mathcal{H}$ compared with those of $\mathcal{G}$. This dilution can occur in essentially three different ways:

(i) by reducing the order of the point group, *i.e.* by eliminating all symmetry operations of some kind. The example $P2 \rightarrow P1$ mentioned above is of this type.

(ii) by loss of translations, *i.e.* by 'thinning out' the lattice of translations. For the space group $P121$ mentioned above this may happen in different ways:

(*a*) by suppressing all translations of the kind $(2u+1)\mathbf{a} + v\mathbf{b} + w\mathbf{c}$, u, v, w integral (new basis $\mathbf{a}' = 2\mathbf{a}$, $\mathbf{b}' = \mathbf{b}$, $\mathbf{c}' = \mathbf{c}$), and, hence, by eliminating half of the twofold axes, or

(*b*1) by $\mathbf{b}' = 2\mathbf{b}$, *i.e.* by thinning out the translations parallel to the twofold axes, or

(*b*2) again by $\mathbf{b}' = 2\mathbf{b}$ but replacing the twofold rotation axes by twofold screw axes.

(iii) by combination of (i) and (ii), *e.g.* by reducing the order of the point group *and* by thinning out the lattice of translations.

Subgroups of the first kind (i) are called *translationengleiche* or *t* subgroups* because the set $\mathcal{T}$ of all (pure) translations is retained. In case (ii), the point group $\mathcal{P}$ and thus the crystal class of the space group is unchanged. These subgroups are called *klassengleiche* or *k* subgroups. In the general case (iii), both the translation subgroup $\mathcal{T}$ of $\mathcal{G}$ and the point group $\mathcal{P}$ are changed; the subgroup has lost translations *and* belongs to a crystal class of lower order.

* Hermann (1929) used the term *zellengleich* but this term caused misunderstandings because it was sometimes understood to refer to the conventional unit cell. Not the conservation of the conventional unit cell but rather the retention of *all* translations of the space group is the essential feature of *t* subgroups.

Obviously the third kind (iii) of subgroups is more difficult to survey than kinds (i) and (ii). Fortunately, a theorem of Hermann states that the maximal subgroups of a space group $\mathcal{G}$ are of type (i) or (ii).

Theorem of Hermann (1929). A maximal subgroup of a space group $\mathcal{G}$ is either a *t* subgroup or a *k* subgroup of $\mathcal{G}$.

According to this theorem, subgroups of kind (iii) can never occur among the maximal subgroups. They can, however, be derived by a stepwise process of linking maximal subgroups of types (i) and (ii), as has been shown by the chains discussed above.

8.3.3.1. *Translationengleiche or t subgroups of a space group*

The 'point group' $\mathcal{P}$ of a given space group $\mathcal{G}$ is a finite group. Hence, the number of subgroups and consequently the number of maximal subgroups of $\mathcal{P}$ is finite. There exist, therefore, only a finite number of maximal *t* subgroups of $\mathcal{G}$. *All* maximal *t* subgroups of every space group $\mathcal{G}$ are listed in the space-group tables of this volume; *cf.* Section 2.2.15. The possible *t* subgroups were first listed by Hermann (1935); corrections have been reported by Ascher *et al.* (1969).

8.3.3.2. *Klassengleiche or k subgroups of a space group*

Every space group $\mathcal{G}$ has an infinite number of maximal *k* subgroups. For dimensions 1, 2 and 3, however, it can be shown that the number of maximal *k* subgroups is finite, if subgroups belonging to the same affine space-group type as $\mathcal{G}$ are excluded. The number of maximal subgroups of $\mathcal{G}$ belonging to the same affine space-group type as $\mathcal{G}$ is always infinite. These subgroups are called *maximal isomorphic subgroups*. In Part 13 isomorphic subgroups are treated in detail. In the space-group tables, only data on the isomorphic subgroups of lowest index are listed. The way in which the isomorphic and non-isomorphic *k* subgroups are listed in the space-group tables is described in Section 2.2.15.

Remark: Enantiomorphic space groups have an infinite number of maximal isomorphic subgroups of the same type *and* an infinite number of maximal isomorphic subgroups of the enantiomorphic type.

Example

All *k* subgroups $\mathcal{G}'$ of a given space group $\mathcal{G} \equiv P3_1$, with basis vectors $\mathbf{a}' = \mathbf{a}, \mathbf{b}' = \mathbf{b}, \mathbf{c}' = p\mathbf{c}, p$ being any prime number except 3, are maximal isomorphic subgroups. They belong to space-group type $P3_1$ if $p = 3r+1, r$ any integer. They belong to the enantiomorphic space-group type $P3_2$ if $p = 3r+2$.

Even though in the space-group tables some kinds of maximal subgroups are listed completely whereas others are listed only partly, it must be emphasized that in principle there is no difference in importance between *t*, non-isomorphic *k* and isomorphic *k* subgroups. Roughly speaking, a group–subgroup relation is 'strong' if the index $[i]$ of the subgroup is low. All maximal *t* and maximal non-isomorphic *k* subgroups have indices less than four in E^2 and five in E^3, index four already being rather exceptional. Maximal isomorphic *k* subgroups of arbitrarily high index exist for every space group.

8.3.3.3. *Supergroups*

Sometimes a space group $\mathcal{H}$ is known and the possible space groups $\mathcal{G}$, of which $\mathcal{H}$ is a subgroup, are of interest.

Definition: A space group $\mathcal{R}$ is called a *minimal supergroup* of a space group $\mathcal{G}$ if $\mathcal{G}$ is a maximal subgroup of $\mathcal{R}$.

Examples

In Fig. 8.3.3.1, the space group $P6_3/mcm$ is a minimal supergroup of $P\bar{6}c2, \ldots, P\bar{3}c1$; $P\bar{6}c2$ is a minimal supergroup of $P\bar{6}, P3c1$ and $P312$; *etc.*

If $\mathcal{G}$ is a maximal *t* subgroup of $\mathcal{R}$ then $\mathcal{R}$ is a minimal *t* supergroup of $\mathcal{G}$. If $\mathcal{G}$ is a maximal *k* subgroup of $\mathcal{R}$ then $\mathcal{R}$ is a minimal *k* supergroup of $\mathcal{G}$. Finally, if $\mathcal{G}$ is a maximal isomorphic subgroup of $\mathcal{R}$, then $\mathcal{R}$ is a minimal isomorphic supergroup of $\mathcal{G}$. Data on minimal *t* and minimal non-isomorphic *k* supergroups are listed in the space-group tables; *cf.* Section 2.2.15. Data on minimal isomorphic supergroups are not listed because they can be derived easily from the corresponding subgroup relations.

The complete data on maximal subgroups of plane and space groups are listed in Volume A1 of *International Tables for Crystallography* (2004). For each space group, all maximal subgroups of index [2], [3] and [4] are listed individually. The infinitely many maximal isomorphic subgroups are listed as members of a few (infinite) series. The main parameter in these series is the index p, p^2 or p^3, where p runs through the infinite number of primes.

8.3.4. Sequence of space-group types

The sequence of space-group entries in the space-group tables follows that introduced by Schoenflies (1891) and is thus established historically. Within each geometric crystal class, Schoenflies has numbered the space-group types in an obscure way. As early as 1919, Niggli (1919) considered this Schoenflies sequence to be unsatisfactory and suggested that another sequence might be more appropriate. Fedorov (1891) used a different sequence in order to distinguish between symmorphic, hemisymmorphic and asymmorphic space groups.

The basis of the Schoenflies symbols and thus of the Schoenflies listing is the geometric crystal class. For the present *Tables*, a sequence might have been preferred in which, in addition, space-group types belonging to the same arithmetic crystal class were grouped together. It was decided, however, that the long-established sequence in the earlier editions of *International Tables* should not be changed.

In Table 8.3.4.1, those geometric crystal classes are listed in which the Schoenflies sequence separates space groups belonging to the same arithmetic crystal class. The space groups are rearranged in such a way that space groups of the same arithmetic crystal class are grouped together. The arithmetic crystal classes are separated by broken lines, the geometric crystal classes by full lines. In all cases not listed in Table 8.3.4.1, the Schoenflies sequence, as used in these *Tables,* does not break up arithmetic crystal classes. Nevertheless, some rearrangement would be desirable in other arithmetic crystal classes too. For example, the symmorphic space group should always be the first entry of each arithmetic crystal class.

8.3.5. Space-group generators

In group theory, a *set of generators of a group* is a set of group elements such that each group element may be obtained as an ordered product of the generators. For space groups of one, two and three dimensions, generators may always be chosen and ordered in such a way that each symmetry operation W can be written as the product of powers of *h* generators G_j $(j = 1, 2, \ldots, h)$. Thus,

$$\mathsf{W} = \mathsf{G}_h^{k_h} * \mathsf{G}_{h-1}^{k_{h-1}} * \ldots * \mathsf{G}_3^{k_3} * \mathsf{G}_2^{k_2} * \mathsf{G}_1,$$

where the powers k_j are positive or negative integers (including zero).

Description of a group by means of generators has the advantage of compactness. For instance, the 48 symmetry operations in point

Table 8.3.4.1. *Listing of space-group types according to their geometric and arithmetic crystal classes*

No.	Hermann–Mauguin symbol	Schoenflies symbol	Geometric crystal class
10	$P2/m$	C_{2h}^1	$2/m$
11	$P2_1/m$	C_{2h}^2	
13	$P2/c$	C_{2h}^4	
14	$P2_1/c$	C_{2h}^5	
12	$C2/m$	C_{2h}^3	
15	$C2/c$	C_{2h}^6	
149	$P312$	D_3^1	32
151	$P3_112$	D_3^3	
153	$P3_212$	D_3^5	
150	$P321$	D_3^2	
152	$P3_121$	D_3^4	
154	$P3_221$	D_3^6	
155	$R32$	D_3^7	
156	$P3m1$	C_{3v}^1	$3m$
158	$P3c1$	C_{3v}^3	
157	$P31m$	C_{3v}^2	
159	$P31c$	C_{3v}^4	
160	$R3m$	C_{3v}^5	
161	$R3c$	C_{3v}^6	
195	$P23$	T^1	23
198	$P2_13$	T^4	
196	$F23$	T^2	
197	$I23$	T^3	
199	$I2_13$	T^5	
200	$Pm\bar{3}$	T_h^1	$m\bar{3}$
201	$Pn\bar{3}$	T_h^2	
205	$Pa\bar{3}$	T_h^6	
202	$Fm\bar{3}$	T_h^3	
203	$Fd\bar{3}$	T_h^4	
204	$Im\bar{3}$	T_h^5	
206	$Ia\bar{3}$	T_h^7	
207	$P432$	O^1	432
208	$P4_232$	O^2	
213	$P4_132$	O^7	
212	$P4_332$	O^6	
209	$F432$	O^3	
210	$F4_132$	O^4	
211	$I432$	O^5	
214	$I4_132$	O^8	
215	$P\bar{4}3m$	T_d^1	$\bar{4}3m$
218	$P\bar{4}3n$	T_d^4	
216	$F\bar{4}3m$	T_d^2	
219	$F\bar{4}3c$	T_d^5	
217	$I\bar{4}3m$	T_d^3	
220	$I\bar{4}3d$	T_d^6	

references