International Tables for Crystallography (2006). Vol. A, Section 8.3.5, pp. 736–738.

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	

Table 8.3.5.1. *Sequence of generators for the crystal classes*

The *space-group* generators differ from those listed here by their glide or screw components. The generator 1 is omitted, except for crystal class 1. The subscript of a symbol denotes the characteristic direction of that operation, where necessary. The subscripts z, y, 110, $1\bar{1}0$, $10\bar{1}$ and 111 refer to the directions [001], [010], [110], $[1\bar{1}0]$, $[10\bar{1}]$ and [111], respectively. For mirror reflections *m,* the 'direction of *m*' refers to the normal to the mirror plane. The subscripts may be likewise interpreted as Miller indices of that plane.

Hermann–Mauguin symbol of crystal class	Generators G_i (sequence left to right)
1	1
$\bar{1}$	$\bar{1}$
2	2
m	m
$2/m$	$2, \bar{1}$
222	$2_z, 2_y$
$mm2$	$2_z, m_y$
mmm	$2_z, 2_y, \bar{1}$
4	$2_z, 4$
$\bar{4}$	$2_z, \bar{4}$
$4/m$	$2_z, 4, \bar{1}$
422	$2_z, 4, 2_y$
$4mm$	$2_z, 4, m_y$
$\bar{4}2m$	$2_z, \bar{4}, 2_y$
$\bar{4}m2$	$2_z, \bar{4}, m_y$
$4/mmm$	$2_z, 4, 2_y, \bar{1}$
3	3
$\bar{3}$	$3, \bar{1}$
321	$3, 2_{110}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}$)
312	$3, 2_{1\bar{1}0}$
$3m1$	$3, m_{110}$
(rhombohedral coordinates	$3_{111}, m_{10\bar{1}}$)
$31m$	$3, m_{1\bar{1}0}$
$\bar{3}m1$	$3, 2_{110}, \bar{1}$
(rhombohedral coordinates	$3_{111}, 2_{10\bar{1}}, \bar{1}$)
$\bar{3}1m$	$3, 2_{1\bar{1}0}, \bar{1}$
6	$3, 2_z$
$\bar{6}$	$3, m_z$
$6/m$	$3, 2_z, \bar{1}$
622	$3, 2_z, 2_{110}$
$6mm$	$3, 2_z, m_{110}$
$\bar{6}m2$	$3, m_z, m_{110}$
$\bar{6}2m$	$3, m_z, 2_{110}$
$6/mmm$	$3, 2_z, 2_{110}, \bar{1}$
23	$2_z, 2_y, 3_{111}$
$m\bar{3}$	$2_z, 2_y, 3_{111}, \bar{1}$
432	$2_z, 2_y, 3_{111}, 2_{110}$
$\bar{4}3m$	$2_z, 2_y, 3_{111}, m_{1\bar{1}0}$
$m\bar{3}m$	$2_z, 2_y, 3_{111}, 2_{110}, \bar{1}$

group $m\bar{3}m$ can be described by two generators. Different choices of generators are possible. For the present *Tables*, generators and generating procedures have been chosen such as to make the entries in the blocks *General position* (*cf.* Section 2.2.11) and *Symmetry operations* (*cf.* Section 2.2.9) as transparent as possible. Space groups of the same crystal class are generated in the same way (for sequence chosen, see Table 8.3.5.1), and the aim has been to accentuate important subgroups of space groups as much as possible. Accordingly, a process of generation in the form of a 'composition series' has been adopted, see Ledermann (1976). The generator G_1 is defined as the identity operation, represented by (1) x, y, z. G_2, G_3 and G_4 are the translations with translation vectors **a**, **b** and **c**, respectively. Thus, the coefficients k_2, k_3 and k_4 may have any integral value. If centring translations exist, they are generated by translations G_5 (and G_6 in the case of an F lattice) with translation vectors **d** (and **e**). For a C lattice, for example, **d** is given by $\mathbf{d} = \frac{1}{2}(\mathbf{a} + \mathbf{b})$. The exponents k_5 (and k_6) are restricted to the following values:

Lattice letter A, B, C, I: $k_5 = 0$ or 1.
Lattice letter R (hexagonal axes): $k_5 = 0$, 1 or 2.
Lattice letter F: $k_5 = 0$ or 1; $k_6 = 0$ or 1.

As a consequence, any translation T of $\mathcal{G}$ with translation vector

$$\mathbf{t} = k_2\mathbf{a} + k_3\mathbf{b} + k_4\mathbf{c}(+k_5\mathbf{d} + k_6\mathbf{e})$$

can be obtained as a product

$$\mathsf{T} = (\mathsf{G}_6)^{k_6} * (\mathsf{G}_5)^{k_5} * \mathsf{G}_4^{k_4} * \mathsf{G}_3^{k_3} * \mathsf{G}_2^{k_2} * \mathsf{G}_1,$$

where $k_2, \ldots, k_6$ are integers determined by T. G_6 and G_5 are enclosed between parentheses because they are effective only in centred lattices.

The remaining generators generate those symmetry operations that are not translations. They are chosen in such a way that only terms G_j or G_j^2 occur. For further specific rules, see below.

The process of generating the entries of the space-group tables may be demonstrated by the example of Table 8.3.5.2, where $\mathcal{G}_j$ denotes the group generated by $\mathsf{G}_1, \mathsf{G}_2, \ldots, \mathsf{G}_j$. For $j \geq 5$, the next generator G_{j+1} has always been taken as soon as $\mathsf{G}_j^{k_j} \in \mathcal{G}_{j-1}$, because in this case no new symmetry operation would be generated by $\mathsf{G}_j^{k_j}$. The generating process is terminated when there is no further generator. In the present example, G_7 completes the generation: $\mathcal{G}_7 \equiv P6_122$.

8.3.5.1. *Selected order for non-translational generators*

For the non-translational generators, the following sequence has been adopted:

(*a*) In all centrosymmetric space groups, an inversion (if possible at the origin O) has been selected as the last generator.

(*b*) Rotations precede symmetry operations of the second kind. In crystal classes $\bar{4}2m$–$\bar{4}m2$ and $\bar{6}2m$–$\bar{6}m2$, as an exception, $\bar{4}$ and $\bar{6}$ are generated first in order to take into account the conventional choice of origin in the fixed points of $\bar{4}$ and $\bar{6}$.

(*c*) The non-translational generators of space groups with C, A, B, F, I or R symbols are those of the corresponding space group with a P symbol, if possible. For instance, the generators of $I2_12_12_1$ are those of $P2_12_12_1$ and the generators of *Ibca* are those of *Pbca,* apart from the centring translations.

Exceptions: $I4cm$ and $I4/mcm$ are generated *via* $P4cc$ and $P4/mcc$, because $P4cm$ and $P4/mcm$ do not exist. In space groups with d glides (except $I\bar{4}2d$) and also in $I4_1/a$, the corresponding rotation subgroup has been generated first. The generators of this subgroup are the same as those of the corresponding space group with a lattice symbol P.

Example
$F4_1/d\bar{3}2/m : P4_132 \rightarrow F4_132 \rightarrow F4_1/d\bar{3}2/m.$

(*d*) In some cases, rule (*c*) could not be followed without breaking rule (*a*), *e.g.* in *Cmme.* In such cases, the generators are chosen to correspond to the Hermann–Mauguin symbol as far as possible. For instance, the generators (apart from centring) of *Cmme* and *Imma* are

Table 8.3.5.2. *Example of a space-group generation* $\mathcal{G}$: $P6_122 \equiv D_6^2$ *(No. 178)*

	Coordinates	Symmetry operations
G_1	(1) x, y, z;	Identity I
G_2	$t(100)$	These are the generating translations.
G_3	$t(010)$	$\mathcal{G}_4$ is the group $\mathcal{T}$ of all translations
G_4	$t(001)$	of $P6_122$
G_5	(2) $\bar{y}, x-y, z+\frac{1}{3}$;	Threefold screw rotation
G_5^2	(3) $\bar{x}+y, \bar{x}, z+\frac{2}{3}$;	Threefold screw rotation
$G_5^3 = t(001)$:	Now the space group $\mathcal{G}_5 \equiv P3_1$ has been generated	
G_6	(4) $\bar{x}, \bar{y}, z+\frac{1}{2}$;	Twofold screw rotation
$G_6 * G_5$	(5) $y, \bar{x}+y, z+\frac{5}{6}$;	Sixfold screw rotation
$G_6 * G_5^2$	$x-y, x, z+\frac{7}{6} \sim$ (6) $x-y, x, z+\frac{1}{6}$;	Sixfold screw rotation
$G_6^2 = t(001)$:	Now the space group $\mathcal{G}_6 \equiv P6_1$ has been generated	
G_7	(7) $y, x, \bar{z}+\frac{1}{3}$;	Twofold rotation, direction of axis [110]
$G_7 * G_5$	(8) $x-y, \bar{y}, \bar{z}$;	Twofold rotation, axis [100]
$G_7 * G_5^2$	$\bar{x}, \bar{x}+y, \bar{z}-\frac{1}{3} \sim$ (9) $\bar{x}, \bar{x}+y, \bar{z}+\frac{2}{3}$;	Twofold rotation, axis [010]
$G_7 * G_6$	$\bar{y}, \bar{x}, \bar{z}-\frac{1}{6} \sim$ (10) $\bar{y}, \bar{x}, \bar{z}+\frac{5}{6}$;	Twofold rotation, axis [$\bar{1}$10]
$G_7 * G_6 * G_5$	$\bar{x}+y, y, \bar{z}-\frac{1}{2} \sim$ (11) $\bar{x}+y, y, \bar{z}+\frac{1}{2}$;	Twofold rotation, axis [120]
$G_7 * G_6 * G_5^2$	$x, x-y, \bar{z}-\frac{5}{6} \sim$ (12) $x, x-y, \bar{z}+\frac{1}{6}$;	Twofold rotation, axis [210]
$G_7^2 = I$	$\mathcal{G}_7 \sim P6_122$	

those of *Pmmb,* which is a non-standard setting of *Pmma.* (Combination of the generators of *Pmma* with the *C*- or *I*-centring translation results in non-standard settings of *Cmme* and *Imma.*)

For the space groups with lattice symbol *P*, the generation procedure has given the same triplets (except for their sequence) as in *IT* (1952). In non-*P* space groups, the triplets listed sometimes differ from those of *IT* (1952) by a centring translation.

8.3.6. Normalizers of space groups

The concept of normalizers, well known to mathematicians since the nineteenth century, is finding more and more applications in crystallography. Normalizers play an important role in the general theory of space groups of *n*-dimensional space. By the so-called Zassenhaus algorithm, one can determine the space-group types of *n*-dimensional space, provided the arithmetic crystal classes and for each arithmetic crystal class a representative integral $(n \times n)$-matrix group are known. The crucial step is then to determine for these matrix groups their normalizers in GL(*n*, *Z*). This was done for $n = 4$ by Brown *et al.* (1978) in the derivation of the 4894 space-group types. Now, the program package *Carat* solves this problem and was used, among others, for the enumeration of the 28 927 922 affine space-group types for six-dimensional space, see Table 8.1.1.1.

Crystallographers have been applying normalizers in their *practical* work for some time without realizing this fact, and only in the last decades have they become aware of the importance of normalizers. Normalizers first seem to have been derived visually, see Hirshfeld (1968). A derivation of the normalizers of the space groups using matrix methods is found in a paper by Boisen *et al.* (1990).

For the practical application of normalizers in crystallographic problems, see Part 15, which also contains detailed lists of normalizers of the point groups and space groups, as well as of space groups with special metrics. In this section, a short elementary introduction to normalizers will be presented.

In Section 8.1.6, the elements of a space group $\mathcal{G}$ have been divided into classes with respect to the subgroup $\mathcal{T}$ of all translations of $\mathcal{G}$; these classes have been called *cosets.* 'Coset decomposition' can be performed for any pair 'group $\mathcal{G}$ and subgroup $\mathcal{H}$'. The subgroup $\mathcal{H}$ is called *normal* if the decomposition of $\mathcal{G}$ into right and left cosets results in the same cosets.

The decomposition of the elements of a group $\mathcal{G}$ into 'conjugacy classes' is equally important in crystallography. These classes are defined as follows:

Definition: The elements A and B of a group $\mathcal{G}$ are said to be *conjugate in* $\mathcal{G}$, if there exists an element $G \in \mathcal{G}$ such that $B = G^{-1}AG$.

Example

The symmetry group 4*mm* of a square consists of the symmetry operations 1, 2, 4, 4^{-1}, m_x, m_y, m_d and $m_{d'}$, see Fig. 8.3.6.1. Vertex 1 is left invariant by 1 and $m_{d'}$, vertex 2 by 1 and m_d. The operations m_d and $m_{d'}$ are conjugate, because $m_{d'} = 4^{-1}m_d4$ holds, as are m_x and m_y ($m_y = 4^{-1}m_x4$), or 4 and 4^{-1} ($4^{-1} = m_x^{-1}4m_x$). The operations 1 and 2 have no conjugates.

As proved in mathematical textbooks, *e.g.* Ledermann (1976), conjugacy indeed subdivides a group into classes of elements. The unit element 1 always forms a conjugacy class for itself, as does any element that commutes with every other element of the group. For finite groups, the number of elements in a conjugacy class is a factor of the group order. In infinite groups, such as space groups, conjugacy classes may contain an infinite number of elements.

Conjugacy can be transferred from elements to groups. Let $\mathcal{H}$ be a subgroup of $\mathcal{G}$. Then another subgroup $\mathcal{H}'$ of $\mathcal{G}$ is said to be *conjugate to* $\mathcal{H}$ in $\mathcal{G}$, if there exists an element $G \in \mathcal{G}$, such that $\mathcal{H}' = G^{-1}\mathcal{H}G$. In this way, the set of all subgroups $\mathcal{H}_i$ of a group $\mathcal{G}$ is divided into *classes of conjugate subgroups* or *conjugacy classes of subgroups.* Conjugacy classes may contain different numbers of subgroups but, for finite groups, the number of subgroups in each class is always a factor of the order of the group. Conjugacy classes which contain only one subgroup are of special interest; they are called *normal subgroups.* There are always two trivial normal subgroups of a group $\mathcal{G}$: the group $\mathcal{G}$ itself and the group $\mathcal{I}$ consisting of the unit element 1 only. For space groups, the group $\mathcal{T}$ of all translations of the group always forms a normal subgroup of $\mathcal{G}$.

In the above-mentioned example of the square, the subgroups $\{1, m_x\}$ and $\{1, m_y\}$ as well as $\{1, m_d\}$ and $\{1, m_{d'}\}$ each form conjugate pairs, whereas the subgroups $\{1, 2, 4, 4^{-1}\}$, $\{1, 2, m_x, m_y\}$, $\{1, 2, m_d, m_{d'}\}$ and $\{1, 2\}$ are normal subgroups.

The characterization of normal subgroups, $\mathcal{H}$ must obey the condition $\mathcal{H} = G^{-1}\mathcal{H}G$ for all elements $G \in \mathcal{G}$, is identical with the one used in Section 8.1.6. This relation can also be expressed as

references