International Tables for Crystallography (2016). Vol. A, Section 1.4.2.5, pp. 56–59.

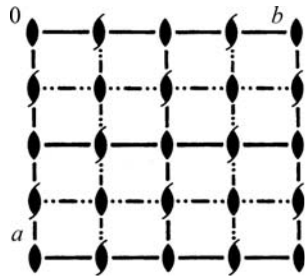

Figure 1.4.2.3
Symmetry-element diagram for space group *Fmm*2 (42) (orthogonal projection along [001]).

in the plane forming the geometric element of W_4. The geometric element of the resulting symmetry operation $\bar{x}, y+\frac{1}{2}, z+\frac{1}{2}$ is still the plane $0, y, z$, but the symmetry operation is now an n glide, *i.e.* a glide reflection with diagonal glide vector.

(ii) $(\frac{1}{2}, 0, \frac{1}{2})$: Analogous to the first centring translation, the composition of W_2 with $t(\frac{1}{2}, 0, \frac{1}{2})$ results in a twofold screw rotation with screw axis $\frac{1}{4}, 0, z$ as geometric element. The roles of the reflections W_3 and W_4 are interchanged, because the translation vector now lies in the plane forming the geometric element of W_3. Therefore, the composition of W_3 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is an n glide with the plane $x, 0, z$ as geometric element, whereas the composition of W_4 with $t(\frac{1}{2}, 0, \frac{1}{2})$ is a c glide with the plane $\frac{1}{4}, y, z$ as geometric element.

(iii) $(\frac{1}{2}, \frac{1}{2}, 0)$: Because this translation vector lies in the plane perpendicular to the rotation axis of W_2, the composition of W_2 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is still a twofold rotation, *i.e.* a symmetry operation of the same type, but the rotation axis is shifted by $\frac{1}{4}, \frac{1}{4}, 0$ in the xy plane to become the axis $\frac{1}{4}, \frac{1}{4}, z$. The composition of W_3 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ results in the symmetry operation $x+\frac{1}{2}, \bar{y}+\frac{1}{2}, z$, which is an a glide with the plane $x, \frac{1}{4}, z$ as geometric element, *i.e.* shifted by $\frac{1}{4}$ along the b axis relative to the geometric element of W_3. Similarly, the composition of W_4 with $t(\frac{1}{2}, \frac{1}{2}, 0)$ is a b glide with the plane $\frac{1}{4}, y, z$ as geometric element.

In this example, all additional symmetry operations are listed in the symmetry-operations block of the space-group tables of *Fmm*2 because they are due to compositions of the coset representatives with centring translations.

The additional symmetry operations can easily be recognized in the symmetry-element diagrams (*cf.* Section 1.4.2.5). Fig. 1.4.2.3 shows the symmetry-element diagram of *Fmm*2 for the projection along the c axis. One sees that twofold rotation axes alternate with twofold screw axes and that mirror planes alternate with 'double' or e-glide planes, *i.e.* glide planes with two glide vectors. For example, the dot–dashed lines at $x = \frac{1}{4}$ and $x = \frac{3}{4}$ in Fig. 1.4.2.3 represent the b and c glides with normal vector along the a axis [for a discussion of e-glide notation, see Sections 1.2.3 and 2.1.2, and de Wolff *et al.*, 1992].

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

8	*g*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{y},x,z$	(4) $y,\bar{x},z$
			(5) $x,\bar{y},z$	(6) $\bar{x},y,z$	(7) $\bar{y},\bar{x},z$	(8) y,x,z

Symmetry operations

(1) 1	(2) 2 $0,0,z$	(3) 4^+ $0,0,z$	(4) 4^- $0,0,z$
(5) m $x,0,z$	(6) m $0,y,z$	(7) m $x,\bar{x},z$	(8) m x,x,z

Figure 1.4.2.4
General-position and symmetry-operations blocks as given in the space-group tables for space group *P*4*mm* (99).

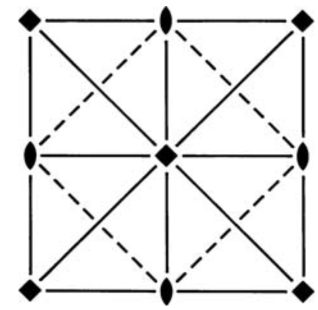

Figure 1.4.2.5
Symmetry-element diagram for space group *P*4*mm* (99) (orthogonal projection along [001]).

Example 2

In a space group of type *P*4*mm* (99), representatives of the space group with respect to the translation subgroup are the powers of a fourfold rotation and reflections with normal vectors along the a and the b axis and along the diagonals [110] and [1$\bar{1}$0] (*cf.* Fig. 1.4.2.4).

In this case, additional symmetry operations occur although there are no centring translations. Consider for example the reflection W_8 with the plane x, x, z as geometric element. Composing this reflection with the translation $t(1, 0, 0)$ gives rise to the symmetry operation represented by $y+1, x, z$. This operation maps a point with coordinates $x+\frac{1}{2}, x, z$ to $x+1, x+\frac{1}{2}, z$ and is thus a glide reflection with the plane $x+\frac{1}{2}, x, z$ as geometric element and $(\frac{1}{2}, \frac{1}{2}, 0)$ as glide vector. In a similar way, composing the other diagonal reflection with translations yields further glide reflections.

These glide reflections are symmetry operations which are not listed in the symmetry-operations block, although they are clearly of a different type to the operations given there. However, in the symmetry-element diagram as shown in Fig. 1.4.2.5, the corresponding symmetry elements are displayed as diagonal dashed lines which alternate with the solid diagonal lines representing the diagonal reflections.

1.4.2.5. Space-group diagrams

In the space-group tables of Chapter 2.3, for each space group there are at least two diagrams displaying the symmetry (there are more diagrams for space groups of low symmetry). The *symmetry-element* diagram displays the location and orientation of the symmetry elements of the space group. The *general-position* diagrams show the arrangement of a set of symmetry-equivalent points of the general position. Because of the periodicity of the arrangements, the presentation of the contents of one unit cell is sufficient. Both types of diagrams are orthogonal projections of the space-group unit cell onto the plane of projection along a basis vector of the conventional crystallographic coordinate system. The symmetry elements of triclinic, monoclinic and orthorhombic groups are shown in three different projections along the basis vectors.

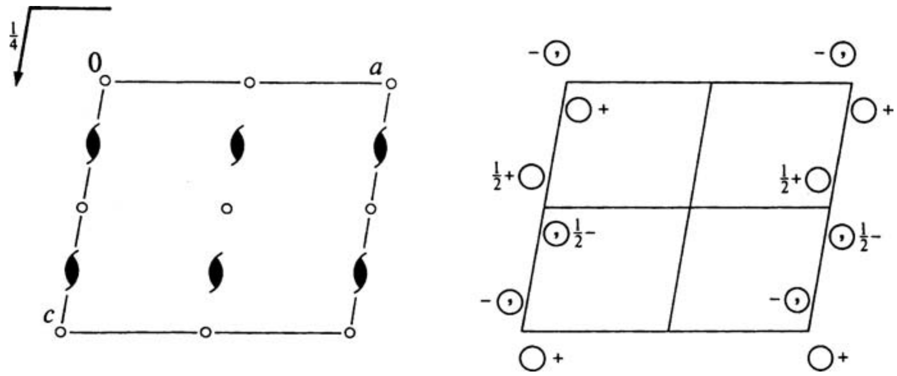

Figure 1.4.2.6
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2_1/c$, No. 14 (unique axis b, cell choice 1).

The thin lines outlining the projection are the traces of the side planes of the unit cell.

Detailed explanations of the diagrams of space groups are found in Section 2.1.3.6. In this section, after a very brief introduction to the diagrams, we will focus mainly on certain important but very often overlooked features of the diagrams.

Symmetry-element diagram

The graphical symbols of the symmetry elements used in the diagrams are explained in Section 2.1.2. The heights along the projection direction above the plane of the diagram are indicated for rotation or screw axes and mirror or glide planes parallel to the projection plane, for rotoinversion axes and inversion centres. The heights (if different from zero) are given as fractions of the shortest translation vector along the projection direction. In Fig. 1.4.2.6 (left) the symmetry elements of $P2_1/c$ (unique axis b, cell choice 1) are represented graphically in a projection of the unit cell along the monoclinic axis **b**. The directions of the basis vectors **c** and **a** can be read directly from the figure. The origin (upper left corner of the unit cell) lies on a centre of inversion indicated by a small open circle. The black lenticular symbols with tails represent the twofold screw axes parallel to **b**. The c-glide plane at height $\frac{1}{4}$ along **b** is shown as a bent arrow with the arrowhead pointing along **c**.

The crystallographic symmetry operations are visualized geometrically by the related symmetry elements. Whereas the symmetry element of a symmetry operation is uniquely defined, more than one symmetry operation may belong to the same symmetry element (*cf.* Section 1.2.3). The following examples illustrate some important features of the diagrams related to the fact that the symmetry-element symbols that are displayed visualize all symmetry operations that belong to the element sets of the symmetry elements.

Examples

(1) *Visualization of the twofold screw rotations of* $P2_1/c$ (Fig. 1.4.2.6). The second coset of the decomposition of $P2_1/c$ with respect to its translation subgroup shown in Table 1.4.2.6 is formed by the infinite set of twofold screw rotations represented by the coordinate triplets $\bar{x}+u_1$, $y+\frac{1}{2}+u_2, \bar{z}+\frac{1}{2}+u_3$ (where u_1, u_2, u_3 are integers). To analyse how these symmetry operations are visualized, it is convenient to consider two special cases:

(i) $u_2 = 0$, *i.e.* $\bar{x}+u_1,\ y+\frac{1}{2},\ \bar{z}+\frac{1}{2}+u_3 = \{2_{010}|u_1, \frac{1}{2}, \frac{1}{2}+u_3\}$; these operations correspond to twofold screw rotations around the infinitely many screw axes parallel to the line $0, y, \frac{1}{4}$, *i.e.* around the lines $u_1/2, y, u_3/2+\frac{1}{4}$. The symbols of the symmetry elements (*i.e.* of the twofold screw axes) located in the unit cell at $0, y, \frac{1}{4}$; $0, y, \frac{3}{4}$; $\frac{1}{2}, y, \frac{1}{4}$; $\frac{1}{2}, y, \frac{3}{4}$ (and the translationally equivalent $1, y, \frac{1}{4}$ and $1, y, \frac{3}{4}$) are shown in the symmetry-element diagram (Fig. 1.4.2.6);

(ii) $u_1 = u_3 = 0$, *i.e.* $\bar{x},\ y+\frac{1}{2}+u_2,\ \bar{z}+\frac{1}{2} = \{2_{010}|0, \frac{1}{2}+u_2, \frac{1}{2}\}$; these symmetry operations correspond to screw rotations around the line $0, y, \frac{1}{4}$ with screw components $\frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \ldots, -\frac{1}{2}, -\frac{3}{2}, -\frac{5}{2}, \ldots$, *i.e.* with a screw component $\frac{1}{2}$ to which all lattice translations parallel to the screw axis are added. These operations, infinite in number, share the same geometric element, *i.e.* they form the element set of the same symmetry element, and geometrically they are represented just by one graphical symbol on the symmetry-element diagrams located exactly at $0, y, \frac{1}{4}$.

(iii) The rest of the symmetry operations in the coset, *i.e.* those with the translation parts $\begin{pmatrix} u_1 \\ \frac{1}{2}+u_2 \\ \frac{1}{2}+u_3 \end{pmatrix}$, are combinations of the two special cases above.

(2) *Inversion centres of* $P2_1/c$ (Fig. 1.4.2.6). The element set of an inversion centre consists of only one symmetry operation, *viz.* the inversion through the point located at the centre. In other words, to each inversion centre displayed on a symmetry-element diagram there corresponds one symmetry operation of inversion. The infinitely many inversions $(-\boldsymbol{I}, \boldsymbol{t}) = \bar{x}+u_1, \bar{y}+u_2, \bar{z}+u_3 = \{\bar{1}|u_1, u_2, u_3\}$ of $P2_1/c$ are located at points $u_1/2$, $u_2/2, u_3/2$. Apart from translational equivalence, there are eight centres located in the unit cell: four at $y = 0$, namely at $0, 0, 0$; $\frac{1}{2}, 0, 0$; $0, 0, \frac{1}{2}$; $\frac{1}{2}, 0, \frac{1}{2}$ and four at height $\frac{1}{2}$ of b. It is important to note that only inversion centres at $y = 0$ are indicated on the diagram.

A similar rule is applied to all pairs of symmetry elements of the same type (such as *e.g.* twofold rotation axes, planes *etc.*) whose heights differ by $\frac{1}{2}$ of the shortest lattice direction along the projection direction. For example, the c-glide plane symbol in Fig. 1.4.2.6 with the fraction $\frac{1}{4}$ next to it represents not only the c-glide plane located at height $\frac{1}{4}$ but also the one at height $\frac{3}{4}$.

(3) *Glide reflections visualized by mirror planes*. As discussed in Section 1.2.3, the element set of a mirror or glide plane consists of a defining operation and all its coplanar equivalents (*cf.* Table 1.2.3.1). The corresponding symmetry element is a mirror plane if among the infinite set of the coplanar glide reflections there is one with zero glide vector. Thus, the symmetry element is a mirror plane and

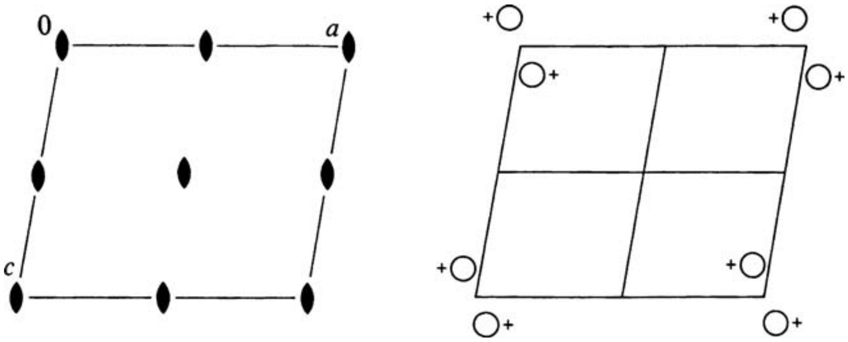

Figure 1.4.2.7
Symmetry-element diagram (left) and general-position diagram (right) for the space group $P2$, No. 3 (unique axis b, cell choice 1).

the graphical symbol for a mirror plane is used for its representation on the symmetry-element diagrams of the space groups. For example, the mirror plane $0, y, z$ shown on the symmetry-element diagram of $Fmm2$ (42), *cf.* Fig. 1.4.2.3, represents all glide reflections of the element set of the defining operation $0, y, z$ [symmetry operation (4) of the general-position $(0, 0, 0)+$ set, *cf.* Fig. 1.4.2.2], including the n-glide reflection $\bar{x}, y + \frac{1}{2}, z + \frac{1}{2}$ [entry (4) of the general-position $(0, \frac{1}{2}, \frac{1}{2})+$ set]. In a similar way, the graphical symbols of the mirror planes $x, 0, z$ also represent the n-glide reflections $x + \frac{1}{2}, \bar{y}, z + \frac{1}{2}$ [entry (3) of the general-position $(\frac{1}{2}, 0, \frac{1}{2})+$ set] of $Fmm2$.

General-position diagram

The graphical presentations of the space-group symmetries provided by the general-position diagrams consist of a set of general-position points which are symmetry equivalent under the symmetry operations of the space group. Starting with a point in the upper left corner of the unit cell, indicated by an open circle with a sign '+', all the displayed points inside and near the unit cell are images of the starting point under some symmetry operation of the space group. Because of the one-to-one correspondence between the image points and the symmetry operations, the number of general-position points in the unit cell (excluding the points that are equivalent by integer translations) equals the multiplicity of the general position. The coordinates of the points in the projection plane can be read directly from the diagram. For all systems except cubic, only one parameter is necessary to describe the height along the projection direction. For example, if the height of the starting point above the projection plane is indicated by a '+' sign, then signs '+', '−' or their combinations with fractions (*e.g.* $\frac{1}{2}+$, $\frac{1}{2}-$ *etc.*) are used to specify the heights of the image points. A circle divided by a vertical line represents two points with different coordinates along the projection direction but identical coordinates in the projection plane. A comma ',' in the circle indicates an image point obtained by a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ of the second kind [*i.e.* with $\det(\boldsymbol{W}) = -1$, *cf.* Section 1.2.2].

Example

The general-position diagram of $P2_1/c$ (unique axis b, cell choice 1) is shown in Fig. 1.4.2.6 (right). The open circles indicate the location of the four symmetry-equivalent points of the space group within the unit cell along with additional eight translation-equivalent points to complete the presentation. The circles with a comma inside indicate the image points generated by operations of the second kind – inversions and glide planes in the present case. The fractions and signs close to the circles indicate their heights in units of b of the symmetry-equivalent points along the monoclinic axis. For example, $\frac{1}{2}-$ is a shorthand notation for $\frac{1}{2} - y$.

Notes:

(1) The close relation between the symmetry-element and the general-position diagrams is obvious. For example, the points shown on the general-position diagram are images of a general-position point under the action of the space-group symmetry operations displayed by the corresponding symmetry elements on the symmetry-element diagram. With

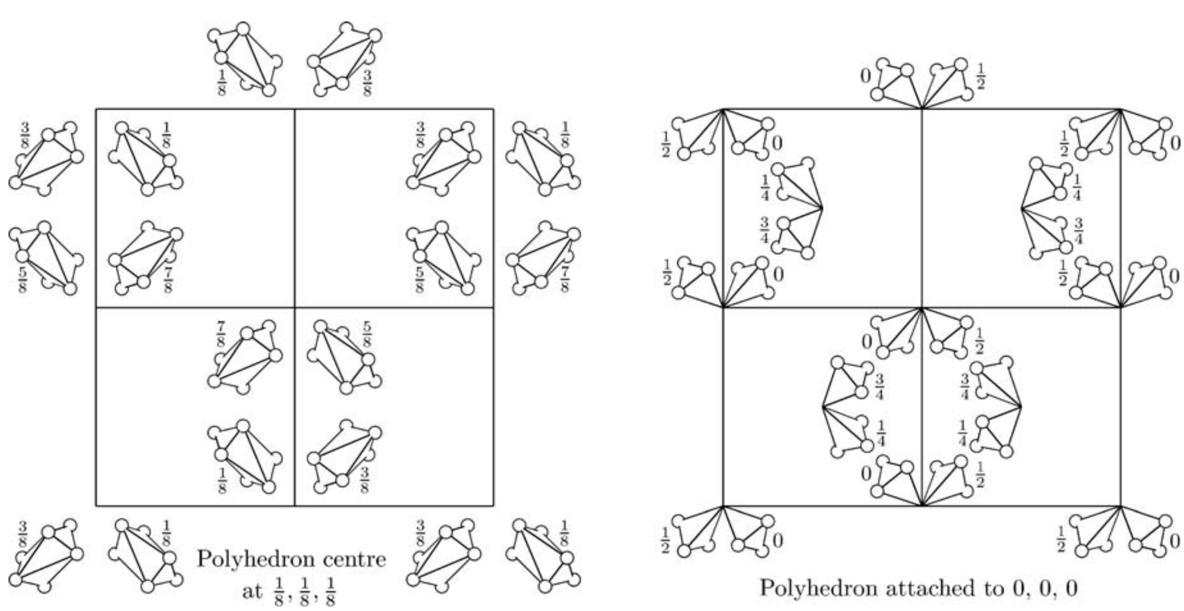

Figure 1.4.2.8
General-position diagrams for the space group $I4_132$ (214). Left: polyhedra (twisted trigonal antiprisms) with centres at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points (site-symmetry group .32). Right: polyhedra (sphenoids) attached to 0, 0, 0 and its equivalent points (site-symmetry group .3.).

some practice each of the diagrams can be generated from the other. In a number of texts, the two diagrams are considered as completely equivalent descriptions of the same space group. This statement is true for most of the space groups. However, there are a number of space groups for which the point configuration displayed on the general-position diagram has higher symmetry than the generating space group (Suescun & Nespolo, 2012; Müller, 2012). For example, consider the diagrams of the space group $P2$, No. 3 (unique axis b, cell choice 1) shown in Fig. 1.4.2.7. It is easy to recognise that, apart from the twofold rotations, the point configuration shown in the general-position diagram is symmetric with respect to a reflection through a plane containing the general-position points, and as a result the space group of the general-position configuration is of $P2/m$ type, and not of $P2$. There are a number of space groups for which the general-position diagram displays higher space-group symmetry, for example: $P1$, $P2_1$, $P4mm$, $P6$ *etc.* The analysis of the eigensymmetry groups of the general-position orbits results in a systematic procedure for the determination of such space groups: the general-position diagrams do not reflect the space-group symmetry correctly if the general-position orbits are *non-characteristic*, *i.e.* their eigensymmetry groups are supergroups of the space groups. (An introduction to terms like eigensymmetry groups, characteristic and non-characteristic orbits, and further discussion of space groups with non-characteristic general-position orbits are given in Section 1.4.4.4.)

(2) The graphical presentation of the general-position points of cubic groups is more difficult: three different parameters are required to specify the height of the points along the projection direction. To make the presentation clearer, the general-position points are grouped around points of higher site symmetry and represented in the form of polyhedra. For most of the space groups the initial general point is taken as 0.048, 0.12, 0.089, and the polyhedra are centred at 0, 0, 0 (and its equivalent points). Additional general-position diagrams are shown for space groups with special sites different from 0, 0, 0 that have site-symmetry groups of equal or higher order. Consider, for example, the two general-position diagrams of the space group $I4_132$ (214) shown in Fig. 1.4.2.8. The polyhedra of the left-hand diagram are centred at special points of highest site-symmetry, namely, at $\frac{1}{8}, \frac{1}{8}, \frac{1}{8}$ and its equivalent points in the unit cell. The site-symmetry groups are of the type 32 leading to polyhedra in the form of *twisted trigonal antiprisms* (*cf.* Table 3.2.3.2). The polyhedra (sphenoids) of the right-hand diagram are attached to the origin 0, 0, 0 and its equivalent points in the unit cell, site-symmetry group of the type 3. The fractions attached to the polyhedra indicate the heights of the high-symmetry points along the projection direction (*cf.* Section 2.1.3.6 for further explanations of the diagrams).

Table 1.4.3.1
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 generators are represented by the corresponding Seitz symbols (*cf.* Tables 1.4.2.1–1.4.2.3). Following the conventions, the subscript of a symbol denotes the characteristic direction of that operation, where necessary. For example, the subscripts 001, 010, 110 *etc.* refer to the directions [001], [010], [110] *etc.* For mirror reflections m, the 'direction of m' refers to the normal of the mirror 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	$2_{001}, 2_{010}$
$mm2$	$2_{001}, m_{010}$
mmm	$2_{001}, 2_{010}, \bar{1}$
4	$2_{001}, 4^+_{001}$
$\bar{4}$	$2_{001}, \bar{4}^+_{001}$
$4/m$	$2_{001}, 4^+_{001}, \bar{1}$
422	$2_{001}, 4^+_{001}, 2_{010}$
$4mm$	$2_{001}, 4^+_{001}, m_{010}$
$\bar{4}2m$	$2_{001}, \bar{4}^+_{001}, 2_{010}$
$\bar{4}m2$	$2_{001}, \bar{4}^+_{001}, m_{010}$
$4/mmm$	$2_{001}, 4^+_{001}, 2_{010}, \bar{1}$
3	3^+_{001}
(rhombohedral coordinates	3^+_{111})
$\bar{3}$	$3^+_{001}, \bar{1}$
(rhombohedral coordinates	$3^+_{111}, \bar{1}$
321	$3^+_{001}, 2_{110}$
(rhombohedral coordinates	$3^+_{111}, 2_{\bar{1}01}$)
312	$3^+_{001}, 2_{1\bar{1}0}$
$3m1$	$3^+_{001}, m_{110}$
(rhombohedral coordinates	$3^+_{111}, m_{\bar{1}01}$)
$31m$	$3^+_{001}, m_{1\bar{1}0}$
$\bar{3}m1$	$3^+_{001}, 2_{110}, \bar{1}$
(rhombohedral coordinates	$3^+_{111}, 2_{\bar{1}01}, \bar{1}$)
$\bar{3}1m$	$3^+_{001}, 2_{1\bar{1}0}, \bar{1}$
6	$3^+_{001}, 2_{001}$
$\bar{6}$	$3^+_{001}, m_{001}$
$6/m$	$3^+_{001}, 2_{001}, \bar{1}$
622	$3^+_{001}, 2_{001}, 2_{110}$
$6mm$	$3^+_{001}, 2_{001}, m_{110}$
$\bar{6}m2$	$3^+_{001}, m_{001}, m_{110}$
$\bar{6}2m$	$3^+_{001}, m_{001}, 2_{110}$
$6/mmm$	$3^+_{001}, 2_{001}, 2_{110}, \bar{1}$
23	$2_{001}, 2_{010}, 3^+_{111}$
$m\bar{3}$	$2_{001}, 2_{010}, 3^+_{111}, \bar{1}$
432	$2_{001}, 2_{010}, 3^+_{111}, 2_{110}$
$\bar{4}3m$	$2_{001}, 2_{010}, 3^+_{111}, m_{1\bar{1}0}$
$m\bar{3}m$	$2_{001}, 2_{010}, 3^+_{111}, 2_{110}, \bar{1}$

1.4.3. Generation of space groups

By H. Wondratschek

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 a finite 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,

$$W = g_h^{k_h} \cdot g_{h-1}^{k_{h-1}} \cdot \ldots \cdot g_p^{k_p} \cdot \ldots \cdot g_3^{k_3} \cdot g_2^{k_2} \cdot g_1,$$

where the powers k_j are positive or negative integers (including zero). The description of a group by means of generators has the advantage of compactness. For instance, the 48 symmetry operations in point group $m\bar{3}m$ can be described by two