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