

1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

Positions		Coordinates						
Multiplicity,	Wyckoff letter,							
Site symmetry		$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$			
16	$e$ 1	(1) $x,y,z$	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$			
<b>Symmetry operations</b>								
For $(0,0,0)+$ set								
(1)	1	(2) 2	$0,0,z$	(3) $m$	$x,0,z$	(4) $m$	$0,y,z$	
For $(0,\frac{1}{2},\frac{1}{2})+$ set								
(1)	$t(0,\frac{1}{2},\frac{1}{2})$	(2) 2	$(0,0,\frac{1}{2})$	$0,\frac{1}{4},z$	(3) $c$	$x,\frac{1}{4},z$	(4) $n(0,\frac{1}{2},\frac{1}{2})$	$0,y,z$
For $(\frac{1}{2},0,\frac{1}{2})+$ set								
(1)	$t(\frac{1}{2},0,\frac{1}{2})$	(2) 2	$(0,0,\frac{1}{2})$	$\frac{1}{4},0,z$	(3) $n(\frac{1}{2},0,\frac{1}{2})$	$x,0,z$	(4) $c$	$\frac{1}{4},y,z$
For $(\frac{1}{2},\frac{1}{2},0)+$ set								
(1)	$t(\frac{1}{2},\frac{1}{2},0)$	(2) 2	$\frac{1}{4},\frac{1}{4},z$	(3) $a$	$x,\frac{1}{4},z$	(4) $b$	$\frac{1}{4},y,z$	

**Figure 1.4.2.2** General-position and symmetry-operations blocks as given in the space-group tables for space group  $Fmm2$  (42). The numbering scheme of the entries in the different symmetry-operations blocks follows that of the general position.

coset representatives of  $P2_1/c$  with respect to its translation subgroup.

For space groups with conventional *centred* cells, there are several (2, 3 or 4) blocks of symmetry operations: one block for each of the translations listed below the subheading ‘Coordinates’. Consider, for example, the four symmetry-operations blocks of the space group  $Fmm2$  (42) reproduced in Fig. 1.4.2.2. They correspond to the four sets of coordinate triplets of the general position obtained by the translations  $t(0, 0, 0)$ ,  $t(0, \frac{1}{2}, \frac{1}{2})$ ,  $t(\frac{1}{2}, 0, \frac{1}{2})$  and  $t(\frac{1}{2}, \frac{1}{2}, 0)$ , cf. Fig. 1.4.2.2. The numbering scheme of the entries in the different symmetry-operations blocks follows that of the general position. For example, the geometric description of entry (4) in the symmetry-operations block under the heading ‘For  $(\frac{1}{2}, \frac{1}{2}, 0)+$  set’ of  $Fmm2$  corresponds to the coordinate triplet  $\bar{x} + \frac{1}{2}, y + \frac{1}{2}, z$ , which is obtained by adding  $t(\frac{1}{2}, \frac{1}{2}, 0)$  to the translation part of the printed coordinate triplet (4)  $\bar{x}, y, z$  (cf. Fig. 1.4.2.2).

**1.4.2.2. Seitz symbols of symmetry operations**

Apart from the notation for the geometric interpretation of the matrix–column representation of symmetry operations ( $\mathbf{W}, \mathbf{w}$ ) discussed in detail in the previous section, there is another notation which has been adopted and is widely used by solid-state physicists and chemists. This is the so-called Seitz notation  $\{\mathbf{R}|\mathbf{v}\}$  introduced by Seitz in a series of papers on the matrix-algebraic development of crystallographic groups (Seitz, 1935).

Seitz symbols  $\{\mathbf{R}|\mathbf{v}\}$  reflect the fact that space-group operations are affine mappings and are essentially shorthand descriptions of the matrix–column representations of the symmetry operations of the space groups. They consist of two parts: a rotation (or linear) part  $\mathbf{R}$  and a translation part  $\mathbf{v}$ . The Seitz symbol is specified between braces and the rotational and the translational parts are separated by a vertical line. The translation parts  $\mathbf{v}$  correspond exactly to the columns  $\mathbf{w}$  of the coordinate triplets of the general-position blocks of the space-group tables. The rotation parts  $\mathbf{R}$  consist of symbols that specify (i) the type and the order of the symmetry operation, and (ii) the orientation of the corresponding symmetry element with respect to the basis. The

orientation is denoted by the direction of the axis for rotations or rotoinversions, or the direction of the normal to reflection planes. (Note that in the latter case this is different from the way the orientation of reflection planes is given in the symmetry-operations block.)

The linear parts of Seitz symbols are denoted in many different ways in the literature (Litvin & Kopsky, 2011). According to the conventions approved by the Commission of Crystallographic Nomenclature of the International Union of Crystallography (Glazer *et al.*, 2014) the symbol  $\mathbf{R}$  is 1 and  $\bar{1}$  for the identity and the inversion,  $m$  for reflections, the symbols 2, 3, 4 and 6 are used for rotations and  $\bar{3}, \bar{4}$  and  $\bar{6}$  for rotoinversions. For rotations and rotoinversions of order higher than 2, a superscript + or – is used to indicate the sense of the rotation. Subscripts of the symbols  $\mathbf{R}$  denote the characteristic

direction of the operation: for example, the subscripts 100, 010 and  $1\bar{1}0$  refer to the directions [100], [010] and  $[1\bar{1}0]$ , respectively.

*Examples*

(a) Consider the coordinate triplets of the general positions of  $P2_12_12$  (18):

$$(1) x, y, z \quad (2) \bar{x}, \bar{y}, z \quad (3) \bar{x} + \frac{1}{2}, y + \frac{1}{2}, \bar{z} \quad (4) x + \frac{1}{2}, \bar{y} + \frac{1}{2}, \bar{z}$$

The corresponding geometric interpretations of the symmetry operations are given by

$$(1) 1 \quad (2) 2 \quad 0, 0, z \quad (3) 2(0, \frac{1}{2}, 0) \quad \frac{1}{4}, y, 0 \quad (4) 2(\frac{1}{2}, 0, 0) \quad x, \frac{1}{4}, 0$$

In Seitz notation the symmetry operations are denoted by

$$(1) \{1|0\} \quad (2) \{2_{001}|0\} \quad (3) \{2_{010}|\frac{1}{2}, \frac{1}{2}, 0\} \quad (4) \{2_{100}|\frac{1}{2}, \frac{1}{2}, 0\}$$

(b) Similarly, the symmetry operations corresponding to the general-position coordinate triplets of  $P2_1/c$  (14), cf. Fig. 1.4.2.1, in Seitz notation are given as

$$(1) \{1|0\} \quad (2) \{2_{010}|0, \frac{1}{2}, \frac{1}{2}\} \quad (3) \{\bar{1}|0\} \quad (4) \{m_{010}|0, \frac{1}{2}, \frac{1}{2}\}$$

The linear parts  $\mathbf{R}$  of the Seitz symbols of the space-group symmetry operations are shown in Tables 1.4.2.1–1.4.2.3. Each symbol  $\mathbf{R}$  is specified by the shorthand notation of its  $(3 \times 3)$  matrix representation (also known as the *Jones’ faithful representation symbol*, cf. Bradley & Cracknell, 1972), the type of symmetry operation and its orientation as described in the corresponding symmetry-operations block of the space-group tables of this volume. The sequence of  $\mathbf{R}$  symbols in Table 1.4.2.1 corresponds to the numbering scheme of the general-position coordinate triplets of the space groups of the  $m\bar{3}m$  crystal class, while those of Table 1.4.2.2 and Table 1.4.2.3 correspond to the general-position sequences of the space groups of  $6/mmm$  and  $\bar{3}m$  (rhombohedral axes) crystal classes, respectively.

The same symbols  $\mathbf{R}$  can be used for the construction of Seitz symbols for the symmetry operations of subperiodic layer and rod groups (Litvin & Kopsky, 2014), and magnetic groups, or for the designation of the symmetry operations of the point groups of space groups. [One should note that the Seitz symbols applied in

# 1. INTRODUCTION TO SPACE-GROUP SYMMETRY

**Table 1.4.2.1**

Linear parts  $R$  of the Seitz symbols  $\{R|\nu\}$  for space-group symmetry operations of cubic, tetragonal, orthorhombic, monoclinic and triclinic crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix-column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	$x, y, z$	1		1
2	$\bar{x}, \bar{y}, z$	2	0, 0, z	$2_{001}$
3	$\bar{x}, y, \bar{z}$	2	0, y, 0	$2_{010}$
4	$x, \bar{y}, \bar{z}$	2	x, 0, 0	$2_{100}$
5	$z, x, y$	$3^+$	x, x, x	$3_{111}^+$
6	$z, \bar{x}, \bar{y}$	$3^+$	$\bar{x}, x, \bar{x}$	$3_{1\bar{1}\bar{1}}^+$
7	$\bar{z}, \bar{x}, y$	$3^+$	x, $\bar{x}, \bar{x}$	$3_{\bar{1}\bar{1}1}^+$
8	$\bar{z}, x, \bar{y}$	$3^+$	$\bar{x}, \bar{x}, x$	$3_{\bar{1}1\bar{1}}^+$
9	$y, z, x$	$3^-$	x, x, x	$3_{111}^-$
10	$\bar{y}, z, \bar{x}$	$3^-$	x, $\bar{x}, \bar{x}$	$3_{1\bar{1}\bar{1}}^-$
11	$y, \bar{z}, \bar{x}$	$3^-$	$\bar{x}, \bar{x}, x$	$3_{\bar{1}\bar{1}1}^-$
12	$\bar{y}, \bar{z}, x$	$3^-$	$\bar{x}, x, \bar{x}$	$3_{\bar{1}1\bar{1}}^-$
13	$y, x, \bar{z}$	2	x, x, 0	$2_{110}$
14	$\bar{y}, \bar{x}, \bar{z}$	2	x, $\bar{x}, 0$	$2_{\bar{1}\bar{1}0}$
15	$y, \bar{x}, z$	$4^-$	0, 0, z	$4_{001}^-$
16	$\bar{y}, x, z$	$4^+$	0, 0, z	$4_{001}^+$
17	$x, z, \bar{y}$	$4^-$	x, 0, 0	$4_{100}^-$
18	$\bar{x}, z, y$	2	0, y, y	$2_{011}$
19	$\bar{x}, \bar{z}, \bar{y}$	2	0, y, $\bar{y}$	$2_{01\bar{1}}$
20	$x, \bar{z}, y$	$4^+$	x, 0, 0	$4_{100}^+$
21	$z, y, \bar{x}$	$4^+$	0, y, 0	$4_{010}^+$
22	$z, \bar{y}, x$	2	x, 0, x	$2_{101}$
23	$\bar{z}, y, x$	$4^-$	0, y, 0	$4_{010}^-$
24	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
25	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
26	$x, y, \bar{z}$	$m$	x, y, 0	$m_{001}$
27	$x, \bar{y}, z$	$m$	x, 0, z	$m_{010}$
28	$\bar{x}, y, z$	$m$	0, y, z	$m_{100}$
29	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^+$	x, x, x	$\bar{3}_{111}^+$
30	$\bar{z}, x, y$	$\bar{3}^+$	$\bar{x}, x, \bar{x}$	$\bar{3}_{1\bar{1}\bar{1}}^+$
31	$z, x, \bar{y}$	$\bar{3}^+$	x, $\bar{x}, \bar{x}$	$\bar{3}_{\bar{1}\bar{1}1}^+$
32	$z, \bar{x}, y$	$\bar{3}^+$	$\bar{x}, \bar{x}, x$	$\bar{3}_{\bar{1}1\bar{1}}^+$
33	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^-$	x, x, x	$\bar{3}_{111}^-$
34	$y, \bar{z}, x$	$\bar{3}^-$	x, $\bar{x}, \bar{x}$	$\bar{3}_{1\bar{1}\bar{1}}^-$
35	$\bar{y}, z, x$	$\bar{3}^-$	$\bar{x}, \bar{x}, x$	$\bar{3}_{\bar{1}\bar{1}1}^-$
36	$y, z, \bar{x}$	$\bar{3}^-$	$\bar{x}, x, \bar{x}$	$\bar{3}_{\bar{1}1\bar{1}}^-$
37	$\bar{y}, \bar{x}, z$	$m$	x, $\bar{x}, z$	$m_{110}$
38	$y, x, z$	$m$	x, x, z	$m_{1\bar{1}0}$
39	$\bar{y}, x, \bar{z}$	$\bar{4}^-$	0, 0, z	$\bar{4}_{001}^-$
40	$y, \bar{x}, \bar{z}$	$\bar{4}^+$	0, 0, z	$\bar{4}_{001}^+$
41	$\bar{x}, \bar{z}, y$	$\bar{4}^-$	x, 0, 0	$\bar{4}_{100}^-$
42	$x, \bar{z}, \bar{y}$	$m$	x, y, $\bar{y}$	$m_{011}$
43	$x, z, y$	$m$	x, y, y	$m_{01\bar{1}}$
44	$\bar{x}, z, \bar{y}$	$\bar{4}^+$	x, 0, 0	$\bar{4}_{100}^+$
45	$\bar{z}, \bar{y}, x$	$\bar{4}^+$	0, y, 0	$\bar{4}_{010}^+$
46	$\bar{z}, y, \bar{x}$	$m$	$\bar{x}, y, x$	$m_{101}$
47	$z, \bar{y}, \bar{x}$	$\bar{4}^-$	0, y, 0	$\bar{4}_{010}^-$
48	$z, y, x$	$m$	x, y, x	$m_{10\bar{1}}$

**Table 1.4.2.2**

Linear parts  $R$  of the Seitz symbols  $\{R|\nu\}$  for space-group symmetry operations of hexagonal and trigonal crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix-column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	$x, y, z$	1		1
2	$\bar{y}, x - y, z$	$3^+$	0, 0, z	$3_{001}^+$
3	$\bar{x} + y, \bar{x}, z$	$3^-$	0, 0, z	$3_{001}^-$
4	$\bar{x}, \bar{y}, z$	2	0, 0, z	$2_{001}$
5	$y, \bar{x} + y, z$	$6^-$	0, 0, z	$6_{001}^-$
6	$x - y, x, z$	$6^+$	0, 0, z	$6_{001}^+$
7	$y, x, \bar{z}$	2	x, x, 0	$2_{110}$
8	$x - y, \bar{y}, \bar{z}$	2	x, 0, 0	$2_{100}$
9	$\bar{x}, \bar{x} + y, \bar{z}$	2	0, y, 0	$2_{010}$
10	$\bar{y}, \bar{x}, \bar{z}$	2	x, $\bar{x}, 0$	$2_{\bar{1}\bar{1}0}$
11	$\bar{x} + y, y, \bar{z}$	2	x, 2x, 0	$2_{120}$
12	$x, x - y, \bar{z}$	2	2x, x, 0	$2_{210}$
13	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
14	$y, \bar{x} + y, \bar{z}$	$\bar{3}^+$	0, 0, z	$\bar{3}_{001}^+$
15	$x - y, x, \bar{z}$	$\bar{3}^-$	0, 0, z	$\bar{3}_{001}^-$
16	$x, y, \bar{z}$	$m$	x, y, 0	$m_{001}$
17	$\bar{y}, x - y, \bar{z}$	$\bar{6}^-$	0, 0, z	$\bar{6}_{001}^-$
18	$\bar{x} + y, \bar{x}, \bar{z}$	$\bar{6}^+$	0, 0, z	$\bar{6}_{001}^+$
19	$\bar{y}, \bar{x}, z$	$m$	x, $\bar{x}, z$	$m_{110}$
20	$\bar{x} + y, y, z$	$m$	x, 2x, z	$m_{100}$
21	$x, x - y, z$	$m$	2x, x, z	$m_{010}$
22	$y, x, z$	$m$	x, x, z	$m_{1\bar{1}0}$
23	$x - y, \bar{y}, z$	$m$	x, 0, z	$m_{120}$
24	$\bar{x}, \bar{x} + y, z$	$m$	0, y, z	$m_{210}$

**Table 1.4.2.3**

Linear parts  $R$  of the Seitz symbols  $\{R|\nu\}$  for symmetry operations of rhombohedral space groups (rhombohedral-axes setting)

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix-column presentation, the type of symmetry operation and its characteristic direction.

IT A description				Seitz symbol
No.	Coordinate triplet	Type	Orientation	
1	$x, y, z$	1		1
2	$z, x, y$	$3^+$	x, x, x	$3_{111}^+$
3	$y, z, x$	$3^-$	x, x, x	$3_{111}^-$
4	$\bar{z}, \bar{y}, \bar{x}$	2	$\bar{x}, 0, x$	$2_{\bar{1}01}$
5	$\bar{y}, \bar{x}, \bar{z}$	2	x, $\bar{x}, 0$	$2_{\bar{1}\bar{1}0}$
6	$\bar{x}, \bar{z}, \bar{y}$	2	0, y, $\bar{y}$	$2_{01\bar{1}}$
7	$\bar{x}, \bar{y}, \bar{z}$	$\bar{1}$		$\bar{1}$
8	$\bar{z}, \bar{x}, \bar{y}$	$\bar{3}^+$	x, x, x	$\bar{3}_{111}^+$
9	$\bar{y}, \bar{z}, \bar{x}$	$\bar{3}^-$	x, x, x	$\bar{3}_{111}^-$
10	$z, y, x$	$m$	x, y, x	$m_{101}$
11	$y, x, z$	$m$	x, x, z	$m_{1\bar{1}0}$
12	$x, z, y$	$m$	x, y, y	$m_{01\bar{1}}$

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**Table 1.4.2.4**

Linear parts  $\mathbf{R}$  of the Seitz symbols  $\{\mathbf{R}|\mathbf{v}\}$  for plane-group symmetry operations of oblique, rectangular and square crystal systems

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction (if applicable).

IT A description				Seitz symbol
No.	Coordinate doublet	Type	Orientation	
1	$x, y$	1		1
2	$\bar{x}, \bar{y}$	2		2
3	$\bar{y}, x$	4 <sup>+</sup>		4 <sup>+</sup>
4	$y, \bar{x}$	4 <sup>−</sup>		4 <sup>−</sup>
5	$\bar{x}, y$	$m$	0, $y$	$m_{10}$
6	$x, \bar{y}$	$m$	$x, 0$	$m_{01}$
7	$y, x$	$m$	$x, x$	$m_{1\bar{1}}$
8	$\bar{y}, \bar{x}$	$m$	$x, \bar{x}$	$m_{11}$

**Table 1.4.2.5**

Linear parts  $\mathbf{R}$  of the Seitz symbols  $\{\mathbf{R}|\mathbf{v}\}$  for plane-group symmetry operations of the hexagonal crystal system

Each symmetry operation is specified by the shorthand description of the rotation part of its matrix–column presentation, the type of symmetry operation and its characteristic direction (if applicable).

IT A description				Seitz symbol
No.	Coordinate doublet	Type	Orientation	
1	$x, y$	1		1
2	$\bar{y}, x - y$	3 <sup>+</sup>		3 <sup>+</sup>
3	$\bar{x} + y, \bar{x}$	3 <sup>−</sup>		3 <sup>−</sup>
4	$\bar{x}, \bar{y}$	2		2
5	$y, \bar{x} + y$	6 <sup>−</sup>		6 <sup>−</sup>
6	$x - y, x$	6 <sup>+</sup>		6 <sup>+</sup>
7	$\bar{y}, \bar{x}$	$m$	$x, \bar{x}$	$m_{11}$
8	$\bar{x} + y, y$	$m$	$x, 2x$	$m_{10}$
9	$x, x - y$	$m$	$2x, x$	$m_{01}$
10	$y, x$	$m$	$x, x$	$m_{1\bar{1}}$
11	$x - y, \bar{y}$	$m$	$x, 0$	$m_{12}$
12	$\bar{x}, \bar{x} + y$	$m$	0, $y$	$m_{21}$

the first and second editions of *IT E* and in the IUCr e-book on magnetic groups (Litvin, 2012) differ from the standard symbols adopted by the Commission of Crystallographic Nomenclature.]

The Seitz symbols for plane groups are constructed following similar rules to those for space groups. The rotation part  $\mathbf{R}$  is 1 for the identity,  $m$  for reflections, and 2, 3, 4 and 6 are used for rotations. The orientation of a reflection line is specified by a subscript indicating the direction of its ‘normal’. Obviously, the direction indicators are of no relevance for the rotation points. The linear parts  $\mathbf{R}$  of the Seitz symbols of the plane-group symmetry operations are shown in Tables 1.4.2.4 and 1.4.2.5. Each symbol  $\mathbf{R}$  is specified by the shorthand notation of its  $(2 \times 2)$  matrix representation, the type of symmetry operation and, if applicable, its orientation as described in the corresponding symmetry-operations block of the plane-group tables of this volume. The sequence of  $\mathbf{R}$  symbols in Table 1.4.2.4 corresponds to the numbering scheme of the general-position coordinate doublets of the plane group  $p4mm$ , while those of Table 1.4.2.5 correspond to the general-position sequence of the plane group  $p6mm$ . The same symbols  $\mathbf{R}$  can be used for the construction of

Seitz symbols for the symmetry operations of subperiodic frieze groups (Litvin & Kopsky, 2014).

As illustrated in the examples above, zero translations are normally specified by a single zero in the Seitz symbols, but in cases where it is unclear whether the symbol refers to a space- or a plane-group symmetry operation, an explicit indication of the components of the translation vector is recommended.

From the description given above, it is clear that Seitz symbols can be considered as shorthand modifications of the matrix–column presentation  $(\mathbf{W}, \mathbf{w})$  of symmetry operations discussed in detail in Chapter 1.2: the translation parts of  $\{\mathbf{R}|\mathbf{v}\}$  and  $(\mathbf{W}, \mathbf{w})$  coincide, while the different  $(3 \times 3)$  matrices  $\mathbf{W}$  are represented by the symbols  $\mathbf{R}$  shown in Tables 1.4.2.1–1.4.2.3. As a result, the expressions for the product and the inverse of symmetry operations in Seitz notation are rather similar to those of the matrix–column pairs  $(\mathbf{W}, \mathbf{w})$  discussed in detail in Chapter 1.2:

(a) product of symmetry operations:

$$\{\mathbf{R}_1|\mathbf{v}_1\}\{\mathbf{R}_2|\mathbf{v}_2\} = \{\mathbf{R}_1\mathbf{R}_2|\mathbf{R}_1\mathbf{v}_2 + \mathbf{v}_1\};$$

(b) inverse of a symmetry operation:

$$\{\mathbf{R}|\mathbf{v}\}^{-1} = \{\mathbf{R}^{-1}|\mathbf{v} - \mathbf{R}^{-1}\mathbf{v}\}.$$

Similarly, the action of a symmetry operation  $\{\mathbf{R}|\mathbf{v}\}$  on the column of point coordinates  $\mathbf{x}$  is given by  $\{\mathbf{R}|\mathbf{v}\}\mathbf{x} = \mathbf{R}\mathbf{x} + \mathbf{v}$  [cf. Chapter 1.2, equation (1.2.2.4)].

The rotation parts of the Seitz symbols partly resemble the geometric-description symbols of symmetry operations described in Section 1.4.2.1 and listed in the symmetry-operation blocks of the space-group tables of this volume:  $\mathbf{R}$  contains the information on the type and order of the symmetry operation, and its characteristic direction. The Seitz symbols do not *directly* indicate the location of the symmetry operation, nor its glide or screw component, if any.

### 1.4.2.3. Symmetry operations and the general position

The classifications of space groups introduced in Chapter 1.3 allow one to reduce the practically unlimited number of possible space groups to a finite number of space-group types. However, each individual space-group type still consists of an infinite number of symmetry operations generated by the set of all translations of the space group. A practical way to represent the symmetry operations of space groups is based on the coset decomposition of a space group with respect to its translation subgroup, which was introduced and discussed in Section 1.3.3.2. For our further considerations, it is important to note that the listings of the general position in the space-group tables can be interpreted in two ways:

- (i) Each of the numbered entries lists the coordinate triplets of an image point of a starting point with coordinates  $x, y, z$  under a symmetry operation of the space group. This feature of the general position will be discussed in detail in Section 1.4.4.
- (ii) Each of the numbered entries of the general position lists a symmetry operation of the space group by the shorthand notation of its matrix–column pair  $(\mathbf{W}, \mathbf{w})$  (cf. Section 1.2.2.1). This fact is not as obvious as the more ‘crystallographic’ aspect described under (i), but its importance becomes evident from the following discussion, where it is shown how to extract the full analytical symmetry information of space groups from the general-position data in the space-group tables of Chapter 2.3.

With reference to a conventional coordinate system, the set of symmetry operations  $\{W\}$  of a space group  $\mathcal{G}$  is described by the