

## 1.4. SPACE GROUPS AND THEIR DESCRIPTIONS

**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 × 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 × 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:

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

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:

- 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.
- 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