International Tables for Crystallography (2016). Vol. A, Figure 1.4.2.2, p. 51.

Positions

Multiplicity, Wyckoff letter, Site symmetry	Coordinates			
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$
16 *e* 1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$

Symmetry operations

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 *Fmm*2 (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 *Fmm*2 (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 *Fmm*2 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 $(\boldsymbol{W}, \boldsymbol{w})$ 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 $\{\boldsymbol{R}|\boldsymbol{v}\}$ introduced by Seitz in a series of papers on the matrix-algebraic development of crystallographic groups (Seitz, 1935).

Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ 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 $\boldsymbol{R}$ and a translation part $\boldsymbol{v}$. The Seitz symbol is specified between braces and the rotational and the translational parts are separated by a vertical line. The translation parts $\boldsymbol{v}$ correspond exactly to the columns $\boldsymbol{w}$ of the coordinate triplets of the general-position blocks of the space-group tables. The rotation parts $\boldsymbol{R}$ 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 $\boldsymbol{R}$ 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 $\boldsymbol{R}$ 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 (2) $\bar{x}, \bar{y}, z$ (3) $\bar{x}+\frac{1}{2}, y+\frac{1}{2}, \bar{z}$ (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 (2) 2 $0, 0, z$ (3) $2(0,\frac{1}{2},0)$ $\frac{1}{4}, y, 0$ (4) $2(\frac{1}{2},0,0)$ $x, \frac{1}{4}, 0$

In Seitz notation the symmetry operations are denoted by

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

The linear parts $\boldsymbol{R}$ of the Seitz symbols of the space-group symmetry operations are shown in Tables 1.4.2.1–1.4.2.3. Each symbol $\boldsymbol{R}$ is specified by the shorthand notation of its (3×3) 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 $\boldsymbol{R}$ 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 $\boldsymbol{R}$ 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