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Table 1.4.2.4
Linear parts $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ 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^+		4^+
4	$y, \bar{x}$	4^-		4^-
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 $\boldsymbol{R}$ of the Seitz symbols $\{\boldsymbol{R}|\boldsymbol{v}\}$ 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^+		3^+
3	$\bar{x}+y, \bar{x}$	3^-		3^-
4	$\bar{x}, \bar{y}$	2		2
5	$y, \bar{x}+y$	6^-		6^-
6	$x-y, x$	6^+		6^+
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 $\boldsymbol{R}$ 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 $\boldsymbol{R}$ 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 $\boldsymbol{R}$ 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 $\boldsymbol{R}$ symbols in Table 1.4.2.4 corresponds to the numbering scheme of the general-position coordinate doublets of the plane group *p*4*mm*, while those of Table 1.4.2.5 correspond to the general-position sequence of the plane group *p*6*mm*. The same symbols $\boldsymbol{R}$ 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 $(\boldsymbol{W}, \boldsymbol{w})$ of symmetry operations discussed in detail in Chapter 1.2: the translation parts of $\{\boldsymbol{R}|\boldsymbol{v}\}$ and $(\boldsymbol{W}, \boldsymbol{w})$ coincide, while the different (3×3) matrices $\boldsymbol{W}$ are represented by the symbols $\boldsymbol{R}$ 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 $(\boldsymbol{W}, \boldsymbol{w})$ discussed in detail in Chapter 1.2:

(*a*) product of symmetry operations:

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

(*b*) inverse of a symmetry operation:

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

Similarly, the action of a symmetry operation $\{\boldsymbol{R}|\boldsymbol{v}\}$ on the column of point coordinates $\boldsymbol{x}$ is given by $\{\boldsymbol{R}|\boldsymbol{v}\}\boldsymbol{x} = \boldsymbol{R}\boldsymbol{x} + \boldsymbol{v}$ [*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: $\boldsymbol{R}$ 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 $(\boldsymbol{W}, \boldsymbol{w})$ (*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

Table 1.4.2.6

Right coset decomposition of space group $P2_1/c$, No. 14 (unique axis b, cell choice 1) with respect to the normal subgroup of translations $\mathcal{T}$

The numbers u_1, u_2 and u_3 are positive or negative integers.

x	y	z	$\bar{x}$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}$	$\bar{z}$	x	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
$x+1$	y	z	$\bar{x}+1$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}$	$\bar{z}$	$x+1$	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
$x+2$	y	z	$\bar{x}+2$	$y+\frac{1}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}$	$\bar{z}$	$x+2$	$\bar{y}+\frac{1}{2}$	$z+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	$y+1$	z	$\bar{x}$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}+1$	$\bar{z}$	x	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
$x+1$	$y+1$	z	$\bar{x}+1$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}+1$	$\bar{z}$	$x+1$	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
$x+2$	$y+1$	z	$\bar{x}+2$	$y+\frac{3}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}+1$	$\bar{z}$	$x+2$	$\bar{y}+\frac{3}{2}$	$z+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	$y+2$	z	$\bar{x}$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}$	$\bar{y}+2$	$\bar{z}$	x	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
$x+1$	$y+2$	z	$\bar{x}+1$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+1$	$\bar{y}+2$	$\bar{z}$	$x+1$	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
$x+2$	$y+2$	z	$\bar{x}+2$	$y+\frac{5}{2}$	$\bar{z}+\frac{1}{2}$	$\bar{x}+2$	$\bar{y}+2$	$\bar{z}$	$x+2$	$\bar{y}+\frac{5}{2}$	$z+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	y	$z+1$	$\bar{x}$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}$	$\bar{y}$	$\bar{z}+1$	x	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
$x+1$	y	$z+1$	$\bar{x}+1$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+1$	$\bar{y}$	$\bar{z}+1$	$x+1$	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
$x+2$	y	$z+1$	$\bar{x}+2$	$y+\frac{1}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+2$	$\bar{y}$	$\bar{z}+1$	$x+2$	$\bar{y}+\frac{1}{2}$	$z+\frac{3}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
x	$y+1$	$z+1$	$\bar{x}$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}$	$\bar{y}+1$	$\bar{z}+1$	x	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
$x+1$	$y+1$	$z+1$	$\bar{x}+1$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+1$	$\bar{y}+1$	$\bar{z}+1$	$x+1$	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
$x+2$	$y+1$	$z+1$	$\bar{x}+2$	$y+\frac{3}{2}$	$\bar{z}+\frac{3}{2}$	$\bar{x}+2$	$\bar{y}+1$	$\bar{z}+1$	$x+2$	$\bar{y}+\frac{3}{2}$	$z+\frac{3}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	
$x+u_1$	$y+u_2$	$z+u_3$	$\bar{x}+u_1$	$y+u_2+\frac{1}{2}$	$\bar{z}+u_3+\frac{1}{2}$	$\bar{x}+u_1$	$\bar{y}+u_2$	$\bar{z}+u_3$	$x+u_1$	$\bar{y}+u_2+\frac{1}{2}$	$z+u_3+\frac{1}{2}$
	$\vdots$			$\vdots$			$\vdots$			$\vdots$	

set of matrix–column pairs $\{(\boldsymbol{W}, \boldsymbol{w})\}$. The set $\mathcal{T}_{\mathcal{G}} = \{(\boldsymbol{I}, \boldsymbol{t})\}$ of all translations forms the *translation subgroup* $\mathcal{T}_{\mathcal{G}} \triangleleft \mathcal{G}$, which is a normal subgroup of $\mathcal{G}$ of finite index $[i]$. If $(\boldsymbol{W}, \boldsymbol{w})$ is a fixed symmetry operation, then all the products $\mathcal{T}_{\mathcal{G}}(\boldsymbol{W}, \boldsymbol{w}) = \{(\boldsymbol{I}, \boldsymbol{t})(\boldsymbol{W}, \boldsymbol{w})\} = \{(\boldsymbol{W}, \boldsymbol{w}+\boldsymbol{t})\}$ of translations with $(\boldsymbol{W}, \boldsymbol{w})$ have the same rotation part $\boldsymbol{W}$. Conversely, every symmetry operation W of $\mathcal{G}$ with the same matrix part $\boldsymbol{W}$ is represented in the set $\mathcal{T}_{\mathcal{G}}(\boldsymbol{W}, \boldsymbol{w})$. The infinite set of symmetry operations $\mathcal{T}_{\mathcal{G}}(\boldsymbol{W}, \boldsymbol{w})$ is called a coset of the right coset decomposition of $\mathcal{G}$ with respect to $\mathcal{T}_{\mathcal{G}}$, and $(\boldsymbol{W}, \boldsymbol{w})$ its coset representative. In this way, the symmetry operations of $\mathcal{G}$ can be distributed into a finite set of infinite cosets, the elements of which are obtained by the combination of a coset representative $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ and the infinite set $\mathcal{T}_{\mathcal{G}} = \{(\boldsymbol{I}, \boldsymbol{t})\}$ of translations (*cf.* Section 1.3.3.2):

$$\mathcal{G} = \mathcal{T}_{\mathcal{G}} \cup \mathcal{T}_{\mathcal{G}}(\boldsymbol{W}_2, \boldsymbol{w}_2) \cup \cdots \cup \mathcal{T}_{\mathcal{G}}(\boldsymbol{W}_m, \boldsymbol{w}_m) \cup \cdots \cup \mathcal{T}_{\mathcal{G}}(\boldsymbol{W}_i, \boldsymbol{w}_i), \quad (1.4.2.1)$$

where $(\boldsymbol{W}_1, \boldsymbol{w}_1) = (\boldsymbol{I}, \boldsymbol{o})$ is omitted. Obviously, the coset representatives $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ of the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ represent in a clear and compact way the infinite number of symmetry operations of the space group $\mathcal{G}$. Each coset in the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ is characterized by its linear part $\boldsymbol{W}_j$ and its entries differ only by lattice translations. The translations $(\boldsymbol{I}, \boldsymbol{t}) \in \mathcal{T}_{\mathcal{G}}$ form the first coset with the identity $(\boldsymbol{I}, \boldsymbol{o})$ as a coset representative. The symmetry operations with rotation part $\boldsymbol{W}_2$ form the second coset *etc*. The number of cosets equals the number of different matrices $\boldsymbol{W}_j$ of the symmetry operations of the space group. This number $[i]$ is always finite and is equal to the order of the point group $\mathcal{P}_{\mathcal{G}}$ of the space group (*cf.* Section 1.3.3.2).

For each space group, a set of coset representatives $\{(\boldsymbol{W}_j, \boldsymbol{w}_j), 1 \le j \le [i]\}$ of the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ is listed under the general-position block of the space-group tables. In general, any element of a coset may be chosen as a coset representative. For convenience, the representatives listed in the space-group tables are always chosen such that the components $w_{j,k}$, $k = 1, 2, 3$, of the translation parts $\boldsymbol{w}_j$ fulfil $0 \le w_{j,k} < 1$ (by subtracting integers). To save space, each matrix–column pair $(\boldsymbol{W}_j, \boldsymbol{w}_j)$ is represented by the corresponding *coordinate triplet* (*cf.* Section 1.2.2.3 for the shorthand notation of matrix–column pairs).

Example

The right coset decomposition of $P2_1/c$, No. 14 (unique axis b, cell choice 1) with respect to its translation subgroup is shown in Table 1.4.2.6. All possible symmetry operations of $P2_1/c$ are distributed into four cosets:

The first column represents the infinitely many translations $t = (\boldsymbol{I}, \boldsymbol{t}) = x + u_1, y + u_2, z + u_3 = \{1|u_1, u_2, u_3\}$ of the translation subgroup $\mathcal{T}$ of $P2_1/c$. The numbers u_1, u_2 and u_3 are positive or negative integers. The identity operation $(\boldsymbol{I}, \boldsymbol{o})$ is usually chosen as a coset representative.

The third coset of the decomposition $(\mathcal{G} : \mathcal{T}_{\mathcal{G}})$ represents the infinite set of 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 the space group $P2_1/c$ with inversion centres located at $u_1/2, u_2/2, u_3/2$ (*cf.* Section 1.2.2.4 for the determination of the location of the inversion centres). The inversion in the origin, *i.e.* $\bar{x}, \bar{y}, \bar{z} = \{\bar{1}|0\}$, is taken as a coset representative.

The coset representative of the second coset is the twofold screw rotation $\{2_{010}|0, \frac{1}{2}, \frac{1}{2}\}$ around the line $0, y, \frac{1}{4}$, followed by its infinite combinations with all lattice translations: $\bar{x} + u_1, y + \frac{1}{2} + u_2, \bar{z} + \frac{1}{2} + u_3 = \{2_{010}|u_1, \frac{1}{2} + u_2, \frac{1}{2} + u_3\}$. These are twofold screw rotations around the lines $u_1/2, y, u_3/2 + \frac{1}{4}$ with screw components $\begin{pmatrix} 0 \\ \frac{1}{2} + u_2 \\ 0 \end{pmatrix}$.

The symmetry operations of the fourth column represented by $x + u_1, \;\bar{y} + \frac{1}{2} + u_2, \;z + \frac{1}{2} + u_3 = \{m_{010}|u_1, \frac{1}{2} + u_2, \frac{1}{2} + u_3\}$ correspond to glide reflections with glide components $\begin{pmatrix} u_1 \\ 0 \\ \frac{1}{2} + u_3 \end{pmatrix}$ through the (infinite) set of glide planes at $x, \frac{1}{4}, z$;

$x, \frac{3}{4}, z$; $x, \frac{5}{4}, z$; $\ldots$; $x, (2u_2+1)/4, z$. As usual, the symmetry operation with $u_1 = u_2 = u_3 = 0$, *i.e.* $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$ = $\{m_{010}|0, \frac{1}{2}, \frac{1}{2}\}$, is taken as a coset representative of the coset of glide reflections.

The coordinate triplets of the general-position block of $P2_1/c$ (unique axis b, cell choice 1) (*cf.* Fig. 1.4.2.1) correspond to the coset representatives of the decomposition of the group listed in the first line of Table 1.4.2.6.

When the space group is referred to a primitive basis (which is always done for '*P*' space groups), each coordinate triplet of the general-position block corresponds to one coset of $(\mathcal{G} : \mathcal{T}_\mathcal{G})$, *i.e.* the *multiplicity* of the general position and the number of cosets is the same. If, however, the space group is referred to a centred cell, then the complete set of general-position coordinate triplets is obtained by the combinations of the listed coordinate triplets with the centring translations. In this way, the total number of coordinate triplets per conventional unit cell, *i.e.* the multiplicity of the general position, is given by the product $[i] \times [p]$, where $[i]$ is the index of $\mathcal{T}_\mathcal{G}$ in $\mathcal{G}$ and $[p]$ is the index of the group of integer translations in the group $\mathcal{T}_\mathcal{G}$ of all (integer and centring) translations.

Example

The listing of the general position for the space–group type *Fmm*2 (42) of the space-group tables is reproduced in Fig. 1.4.2.2. The four entries, numbered (1) to (4), are to be taken as they are printed [indicated by (0, 0, 0)+]. The additional 12 more entries are obtained by adding the centring translations $(0, \frac{1}{2}, \frac{1}{2})$, $(\frac{1}{2}, 0, \frac{1}{2})$, $(\frac{1}{2}, \frac{1}{2}, 0)$ to the translation parts of the printed entries [indicated by $(0, \frac{1}{2}, \frac{1}{2})+$, $(\frac{1}{2}, 0, \frac{1}{2})+$ and $(\frac{1}{2}, \frac{1}{2}, 0)+$, respectively]. Altogether there are 16 entries, which is announced by the multiplicity of the general position, *i.e.* by the first number in the row. (The additional information specified on the left of the general-position block, namely the Wyckoff letter and the site symmetry, will be dealt with in Section 1.4.4.)

1.4.2.4. Additional symmetry operations and symmetry elements

The symmetry operations of a space group are conveniently partitioned into the cosets with respect to the translation subgroup. All operations which belong to the same coset have the same linear part and, if a single operation from a coset is given, all other operations in this coset are obtained by composition with a translation. However, not all symmetry operations in a coset with respect to the translation subgroup are operations of the same type and, furthermore, they may belong to element sets of different symmetry elements. In general, one can distinguish the following cases:

(i) The composition $W' = tW$ of a symmetry operation W with a translation t is an operation of the same type as W, with the same or a different type of symmetry element.

(ii) The composition $W' = tW$ is an operation of a different type to W with the same or a different type of symmetry element.

In order to distinguish the different cases, a closer analysis of the type of a symmetry operation and its symmetry element is required. These types, however, might be obscured by two obstacles:

(1) The origin in the chosen coordinate system might not lie on the geometric element of the symmetry operation. For example, the symmetry operation represented by the coordinate triplet $\bar{x}+1, \bar{y}+1, \bar{z}$ (*cf.* Section 1.4.2.3) is in fact an inversion through the point $1/2, 1/2, 0$ and thus of the same type as the inversion $\{\bar{1}|0\}$ through the origin.

(2) The screw or glide part might not be reduced to a vector within the unit cell. For example, the symmetry operation $\bar{x}, \bar{y}, z+1$, which is a twofold screw rotation 2 (0, 0, 1) 0, 0, z along the c axis, is the composition of the twofold rotation $\bar{x}, \bar{y}, z$ with the lattice translation $t(0, 0, 1)$ along the screw axis. Although the two operations $\bar{x}, \bar{y}, z$ and $\bar{x}, \bar{y}, z+1$ are of different types, they are coaxial equivalents and belong to the element set of the same symmetry element (*cf.* Section 1.2.3).

These issues can be overcome by decomposing the translation part $\boldsymbol{w}$ of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ into an intrinsic translation part $\boldsymbol{w}_g$ which is fixed by the linear part $\boldsymbol{W}$ of W and thus parallel to the geometric element of W, and a location part $\boldsymbol{w}_l$, which is perpendicular to the intrinsic translation part. Note that the subspace of vectors fixed by $\boldsymbol{W}$ and the subspace perpendicular to this space of fixed vectors are complementary subspaces, *i.e.* their dimensions add up to 3, therefore this decomposition is always possible.

The procedure for determining the intrinsic translation part of a symmetry operation is described in Section 1.2.2.4, and is based on the fact that the kth power of a symmetry operation $W = (\boldsymbol{W}, \boldsymbol{w})$ with linear part $\boldsymbol{W}$ of order k must be a pure translation, *i.e.* $W^k = (\boldsymbol{I}, \boldsymbol{t})$ for some lattice translation $\boldsymbol{t}$. The *intrinsic translation part* of W is then defined as $\boldsymbol{w}_g = \frac{1}{k}\boldsymbol{t}$.

The difference $\boldsymbol{w}_l = \boldsymbol{w} - \boldsymbol{w}_g$ is perpendicular to $\boldsymbol{w}_g$ and it is called the *location part* of $\boldsymbol{w}$. This terminology is justified by the fact that the location part can be reduced to $\boldsymbol{o}$ by an origin shift, *i.e.* the location part indicates whether the origin of the chosen coordinate system lies on the geometric element of W.

The transformation of point coordinates and matrix–column pairs under an origin shift is explained in detail in Sections 1.5.1.3 and 1.5.2.3, and the complete procedure for determining the additional symmetry operations will be discussed in the context of the synoptic tables in Section 1.5.4. In this section we will restrict ourselves to a detailed discussion of two examples which illustrate typical phenomena.

Example 1

Consider a space group of type *Fmm*2 (42). The information on the general position and on the symmetry operations given in the space-group tables are reproduced in Fig. 1.4.2.2. From this information one deduces that coset representatives with respect to the translation subgroup are the identity element $W_1 = x, y, z$, a rotation $W_2 = \bar{x}, \bar{y}, z$ with the c axis as geometric element, a reflection $W_3 = x, \bar{y}, z$ with the plane $x, 0, z$ as geometric element and a reflection $W_4 = \bar{x}, y, z$ with the plane $0, y, z$ as geometric element (with the indices following the numbering in the table).

Composing these coset representatives with the centring translations $t(0, \frac{1}{2}, \frac{1}{2})$, $t(\frac{1}{2}, 0, \frac{1}{2})$ and $t(\frac{1}{2}, \frac{1}{2}, 0)$ gives rise to elements in the same cosets, but with different types of symmetry operations and symmetry elements in several cases.

(i) $(0, \frac{1}{2}, \frac{1}{2})$: The composition of the rotation W_2 with $t(0, \frac{1}{2}, \frac{1}{2})$ results in the symmetry operation $\bar{x}, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$, which is a twofold screw rotation with screw axis $0, \frac{1}{4}, z$. This means that both the type of the symmetry operation and the location of the geometric element are changed. Composing the reflection W_3 with $t(0, \frac{1}{2}, \frac{1}{2})$ gives the symmetry operation $x, \bar{y}+\frac{1}{2}, z+\frac{1}{2}$, which is a c 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. In the composition of W_4 with $t(0, \frac{1}{2}, \frac{1}{2})$, the translation lies