

2. THE SPACE-GROUP TABLES

Table 2.1.1.2

Symbols for the conventional centring types of one-, two- and three-dimensional cells

Symbol	Centring type of cell	Number of lattice points per cell	Coordinates of lattice points within cell
One dimension			
\hbar	Primitive	1	0
Two dimensions			
p	Primitive	1	0, 0
c	Centred	2	0, 0; $\frac{1}{2}, \frac{1}{2}$
$h\ddagger$	Hexagonally centred	3	0, 0; $\frac{2}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}$
Three dimensions			
P	Primitive	1	0, 0, 0
C	C-face centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}, 0$
A	A-face centred	2	0, 0, 0; $0, \frac{1}{2}, \frac{1}{2}$
B	B-face centred	2	0, 0, 0; $\frac{1}{2}, 0, \frac{1}{2}$
I	Body centred	2	0, 0, 0; $\frac{1}{2}, \frac{1}{2}, \frac{1}{2}$
F	All-face centred	4	0, 0, 0; $\frac{1}{2}, \frac{1}{2}, 0$; $0, \frac{1}{2}, \frac{1}{2}$; $0, \frac{1}{2}, \frac{1}{2}$
$R\ddagger$	Rhombohedrally centred (description with 'hexagonal axes')	3	$\left\{ 0, 0, 0; \frac{2}{3}, \frac{1}{3}, \frac{1}{3}; \frac{1}{3}, \frac{2}{3}, \frac{2}{3} \right.$ ('obverse setting')
	Primitive (description with 'rhombohedral axes')	1	$\left. 0, 0, 0; \frac{1}{3}, \frac{2}{3}, \frac{1}{3}; \frac{2}{3}, \frac{1}{3}, \frac{2}{3} \right.$ ('reverse setting')
$H\§$	Hexagonally centred	3	0, 0, 0; $\frac{2}{3}, \frac{1}{3}, 0$; $\frac{1}{3}, \frac{2}{3}, 0$

† The two-dimensional triple hexagonal cell h is an alternative description of the hexagonal plane net, as illustrated in Fig. 1.5.1.8. It is not used for systematic plane-group description in this volume; it is introduced, however, in the sub- and supergroup entries of the plane-group tables of *International Tables for Crystallography*, Vol. A1 (2010), abbreviated as *IT A1*. Plane-group symbols for the h cell are listed in Section 1.5.4. Transformation matrices are contained in Table 1.5.1.1.

‡ In the space-group tables (Chapter 2.3), as well as in *IT* (1935) and *IT* (1952), the seven rhombohedral R space groups are presented with two descriptions, one based on *hexagonal axes* (triple cell), one on *rhombohedral axes* (primitive cell). In the present volume, as well as in *IT* (1952) and *IT A* (2002), the *obverse* setting of the triple hexagonal cell R is used. Note that in *IT* (1935) the *reverse* setting was employed. The two settings are related by a rotation of the hexagonal cell with respect to the rhombohedral lattice around a threefold axis, involving a rotation angle of 60, 180 or 300° (*cf.* Fig. 1.5.1.6). Further details may be found in Section 1.5.4 and Chapter 3.1. Transformation matrices are contained in Table 1.5.1.1.

§ The triple hexagonal cell H is an alternative description of the hexagonal Bravais lattice, as illustrated in Fig. 1.5.1.8. It was used for systematic space-group description in *IT* (1935), but replaced by P in *IT* (1952). It is used in the tables of maximal subgroups and minimal supergroups of the space groups in *IT A1* (2010). Space-group symbols for the H cell are listed in Section 1.5.4. Transformation matrices are contained in Table 1.5.1.1.

conventions based on the lengths of the cell edges) are needed to determine the choice and the labelling of the axes. Reduced bases are treated in Chapter 3.1, orthorhombic settings in Section 2.1.3.6, and monoclinic settings and cell choices in Section 2.1.3.15 (*cf.* Section 1.5.4 for a detailed treatment of alternative settings of space groups).

In this volume, all space groups within a crystal family are referred to the same kind of conventional coordinate system, with the exception of the hexagonal crystal family in three dimensions. Here, two kinds of coordinate systems are used, the hexagonal and the rhombohedral systems. In accordance with common crystallographic practice, all space groups based on the hexagonal Bravais lattice hP (18 trigonal and 27 hexagonal space groups) are described only with a hexagonal coordinate system (primitive cell), whereas the seven space groups based on the rhombohedral Bravais lattice hR (the so-called 'rhombohedral space groups', *cf.* Section 1.4.1) are treated in two versions, one referred to 'hexagonal axes' (triple obverse cell) and one to 'rhombohedral axes' (primitive cell); *cf.* Table 2.1.1.2. In practice, hexagonal axes are preferred because they are easier to visualize.

Table 2.1.1.2 contains only those conventional centring symbols which occur in the Hermann–Mauguin space-group symbols. There exist, of course, further kinds of centred cells which are unconventional, see for example the synoptic tables of plane (Table 1.5.4.3) and space (Table 1.5.4.4) groups discussed in Chapter 1.5. The centring type of a cell may change with a change of the basis vectors; in particular, a primitive cell may become a centred cell and *vice versa*. Examples of relevant transformation matrices are contained in Table 1.5.1.1.

2.1.2. Symbols of symmetry elements

BY TH. HAHN AND M. I. AROYO

As already introduced in Section 1.2.3, a 'symmetry element' (of a given structure or object) is defined as a concept with two components; it is the combination of a 'geometric element' (that allows the fixed points of a reduced symmetry operation to be located and oriented in space) with the set of symmetry operations having this geometric element in common ('element set'). The element set of a symmetry element is represented by the so-called 'defining operation', which is the simplest symmetry operation from the element set that suffices to identify the geometric element. The alphanumeric and graphical symbols of symmetry elements and the related symmetry operations used throughout the tables of plane (Chapter 2.2) and space groups (Chapter 2.3) are listed in Tables 2.1.2.1 to 2.1.2.7. For detailed discussion of the definition and symbols of symmetry elements, *cf.* Section 1.2.3, de Wolff *et al.* (1989, 1992) and Flack *et al.* (2000).

The alphanumeric symbols shown in Table 2.1.2.1 correspond to those symmetry elements and symmetry operations which occur in the conventional Hermann–Mauguin symbols of point groups and space groups. Further so-called 'additional symmetry elements' are described in Sections 1.4.2.3 and 1.5.4.1, and Tables 1.5.4.3 and 1.5.4.4 show additional symmetry operations that appear in the so-called 'extended Hermann–Mauguin symbols' (*cf.* Section 1.5.4). The symbols of symmetry elements (symmetry operations), except for glide planes (glide reflections), are independent of the choice and the labelling of the basis vectors and of the origin. The symbols of glide planes (glide reflections),

2.1. GUIDE TO THE USE OF THE SPACE-GROUP TABLES

Table 2.1.2.1

Symbols for symmetry elements and for the corresponding symmetry operations in one, two and three dimensions

Symbol	Symmetry element and its orientation	Defining symmetry operation with glide or screw vector
m	$\left\{ \begin{array}{l} \text{Reflection plane, mirror plane} \\ \text{Reflection line, mirror line (two dimensions)} \\ \text{Reflection point, mirror point (one dimension)} \end{array} \right.$	$\left\{ \begin{array}{l} \text{Reflection through the plane} \\ \text{Reflection through the line} \\ \text{Reflection through the point} \end{array} \right.$
a, b or c	'Axial' glide plane	Glide reflection through the plane, with glide vector
a	$\perp [010]$ or $\perp [001]$	$\frac{1}{2}\mathbf{a}$
b	$\perp [001]$ or $\perp [100]$	$\frac{1}{2}\mathbf{b}$
c †	$\left\{ \begin{array}{l} \perp [100] \text{ or } \perp [010] \\ \perp [1\bar{1}0] \text{ or } \perp [110] \\ \perp [100] \text{ or } \perp [010] \text{ or } \perp [\bar{1}\bar{1}0] \\ \perp [1\bar{1}0] \text{ or } \perp [120] \text{ or } \perp [\bar{2}\bar{1}0] \end{array} \right.$	$\left\{ \begin{array}{l} \frac{1}{2}\mathbf{c} \\ \frac{1}{2}\mathbf{c} \\ \frac{1}{2}\mathbf{c} \end{array} \right.$ } hexagonal coordinate system
e ‡	'Double' glide plane (in centred cells only)	Two glide reflections through <i>one</i> plane, with perpendicular glide vectors
	$\perp [001]$	$\frac{1}{2}\mathbf{a}$ and $\frac{1}{2}\mathbf{b}$
	$\perp [100]$	$\frac{1}{2}\mathbf{b}$ and $\frac{1}{2}\mathbf{c}$
	$\perp [010]$	$\frac{1}{2}\mathbf{a}$ and $\frac{1}{2}\mathbf{c}$
	$\perp [1\bar{1}0]; \perp [110]$	$\frac{1}{2}(\mathbf{a} + \mathbf{b})$ and $\frac{1}{2}\mathbf{c}; \frac{1}{2}(\mathbf{a} - \mathbf{b})$ and $\frac{1}{2}\mathbf{c}$
	$\perp [01\bar{1}]; \perp [011]$	$\frac{1}{2}(\mathbf{b} + \mathbf{c})$ and $\frac{1}{2}\mathbf{a}; \frac{1}{2}(\mathbf{b} - \mathbf{c})$ and $\frac{1}{2}\mathbf{a}$
	$\perp [\bar{1}01]; \perp [101]$	$\frac{1}{2}(\mathbf{a} + \mathbf{c})$ and $\frac{1}{2}\mathbf{b}; \frac{1}{2}(\mathbf{a} - \mathbf{c})$ and $\frac{1}{2}\mathbf{b}$
n	'Diagonal' glide plane	Glide reflection through the plane, with glide vector
	$\perp [001]; \perp [100]; \perp [010]$	$\frac{1}{2}(\mathbf{a} + \mathbf{b}); \frac{1}{2}(\mathbf{b} + \mathbf{c}); \frac{1}{2}(\mathbf{a} + \mathbf{c})$
	$\perp [1\bar{1}0] \text{ or } \perp [01\bar{1}] \text{ or } \perp [\bar{1}01]$	$\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$
	$\perp [110]; \perp [011]; \perp [101]$	$\frac{1}{2}(-\mathbf{a} + \mathbf{b} + \mathbf{c}); \frac{1}{2}(\mathbf{a} - \mathbf{b} + \mathbf{c}); \frac{1}{2}(\mathbf{a} + \mathbf{b} - \mathbf{c})$
d §	'Diamond' glide plane	Glide reflection through the plane, with glide vector
	$\perp [001]; \perp [100]; \perp [010]$	$\frac{1}{4}(\mathbf{a} \pm \mathbf{b}); \frac{1}{4}(\mathbf{b} \pm \mathbf{c}); \frac{1}{4}(\pm \mathbf{a} + \mathbf{c})$
	$\perp [1\bar{1}0]; \perp [01\bar{1}]; \perp [\bar{1}01]$	$\frac{1}{4}(\mathbf{a} + \mathbf{b} \pm \mathbf{c}); \frac{1}{4}(\pm \mathbf{a} + \mathbf{b} + \mathbf{c}); \frac{1}{4}(\mathbf{a} \pm \mathbf{b} + \mathbf{c})$
	$\perp [110]; \perp [011]; \perp [101]$	$\frac{1}{4}(-\mathbf{a} + \mathbf{b} \pm \mathbf{c}); \frac{1}{4}(\pm \mathbf{a} - \mathbf{b} + \mathbf{c}); \frac{1}{4}(\mathbf{a} \pm \mathbf{b} - \mathbf{c})$
g	Glide line (two dimensions)	Glide reflection through the line, with glide vector
	$\perp [01]; \perp [10]$	$\frac{1}{2}\mathbf{a}; \frac{1}{2}\mathbf{b}$
1	None	Identity
	$\left\{ \begin{array}{l} n\text{-fold rotation axis, } n \\ n\text{-fold rotation point, } n \text{ (two dimensions)} \end{array} \right.$	Counter-clockwise rotation of $360/n$ degrees around the axis Counter-clockwise rotation of $360/n$ degrees around the point
2, 3, 4, 6		
$\bar{1}$	Centre of symmetry, inversion centre	Inversion through the point
$\bar{2} = m, \uparrow \bar{3}, \bar{4}, \bar{6}$	Rotoinversion axis, \bar{n} , and inversion point on the axis ††	Counter-clockwise rotation of $360/n$ degrees around the axis, followed by inversion through the point on the axis ††
2_1 $3_1, 3_2$ $4_1, 4_2, 4_3$ $6_1, 6_2, 6_3, 6_4, 6_5$	n -fold screw axis, n_p	Right-handed screw rotation of $360/n$ degrees around the axis, with screw vector (pitch) $(p/n)\mathbf{t}$; here \mathbf{t} is the shortest lattice translation vector parallel to the axis in the direction of the screw

† In the rhombohedral space-group symbols $R3c$ (161) and $R\bar{3}c$ (167), the symbol c refers to the description with 'hexagonal axes'; i.e. the glide vector is $\frac{1}{2}\mathbf{c}$, along $[001]$. In the description with 'rhombohedral axes', this glide vector is $\frac{1}{2}(\mathbf{a} + \mathbf{b} + \mathbf{c})$, along $[111]$, i.e. the symbol of the glide plane would be $n: c$. Table 1.5.4.4.

‡ Glide planes 'e' occur in orthorhombic A -, C - and F -centred space groups, tetragonal I -centred and cubic F - and I -centred space groups. The geometric element of an e -glide plane is a plane shared by glide reflections with perpendicular glide vectors, with at least one glide vector along a crystal axis [cf. Section 1.2.3 and de Wolff *et al.* (1992)].

§ Glide planes d occur only in orthorhombic F space groups, in tetragonal I space groups, and in cubic I and F space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a} + \mathbf{b})$ and $\frac{1}{4}(\mathbf{a} - \mathbf{b})$. The second power of a glide reflection d is a centring vector.

¶ Only the symbol m is used in the Hermann–Mauguin symbols, for both point groups and space groups.

†† The inversion point is a centre of symmetry if n is odd.

however, may change with a change of the basis vectors. For this reason, the possible orientations of glide planes and the glide vectors of the corresponding operations are listed explicitly in columns 2 and 3 of Table 2.1.2.1.

In 1992, following a proposal of the Commission on Crystallographic Nomenclature (de Wolff *et al.*, 1992), the International Union of Crystallography introduced the symbol 'e' and graphical symbols for the designation of the so-called 'double' glide planes. The double- or e -glide plane occurs only in centred cells and its geometric element is a plane shared by glide reflections with perpendicular glide vectors related by a centring translation (for details on e -glide planes, cf. Section 1.2.3). The introduction of the symbol e for the designation of double-glide

planes (cf. de Wolff *et al.*, 1992) results in the modification of the Hermann–Mauguin symbols of five orthorhombic groups:

Space group No.	39	41	64	67	68
New symbol:	<i>Aem2</i>	<i>Aea2</i>	<i> Cmce</i>	<i> Cmme</i>	<i> Ccce</i>
Former symbol:	<i> Abm2</i>	<i> Aba2</i>	<i> Cmca</i>	<i> Cmma</i>	<i> Ccca</i>

Since the introduction of its use in *IT A* (2002) the new symbol is the standard one; it is indicated in the headline of these space groups, while the former symbol is given underneath.

The graphical symbols of symmetry planes are shown in Tables 2.1.2.2 to 2.1.2.4. Like the alphanumeric symbols, the graphical symbols and their explanations (columns 2 and 3) are indepen-

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Table 2.1.2.2

Graphical symbols of symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)

Description	Graphical symbol	Glide vector(s) of the defining operation(s) of the glide plane (in units of the shortest lattice translation vectors parallel and normal to the projection plane)	Symmetry element represented by the graphical symbol
Reflection plane, mirror plane Reflection line, mirror line (two dimensions) } }		None	<i>m</i>
'Axial' glide plane Glide line (two dimensions) } }		$\frac{1}{2}$ parallel to line in projection plane $\frac{1}{2}$ parallel to line in figure plane	<i>a</i> , <i>b</i> or <i>c</i> <i>g</i>
'Axial' glide plane		$\frac{1}{2}$ normal to projection plane	<i>a</i> , <i>b</i> or <i>c</i>
'Double' glide plane†		Two glide vectors: $\frac{1}{2}$ parallel to line in, and $\frac{1}{2}$ normal to projection plane	<i>e</i>
'Diagonal' glide plane		One glide vector with two components: $\frac{1}{2}$ parallel to line in, and $\frac{1}{2}$ normal to projection plane	<i>n</i>
'Diamond' glide plane‡ (pair of planes)		$\frac{1}{4}$ parallel to line in projection plane, combined with $\frac{1}{4}$ normal to projection plane (arrow indicates direction parallel to the projection plane for which the normal component is positive)	<i>d</i>

† The graphical symbols of the 'e'-glide planes are applied to the diagrams of seven orthorhombic *A*-, *C*- and *F*-centred space groups, five tetragonal *I*-centred space groups, and five cubic *F*- and *I*-centred space groups.

‡ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a} + \mathbf{b})$ and $\frac{1}{4}(\mathbf{a} - \mathbf{b})$. The second power of a glide reflection *d* is a centring vector.

Table 2.1.2.3

Graphical symbols of symmetry planes parallel to the plane of projection

Description	Graphical symbol†	Glide vector(s) of the defining operation(s) of the glide plane (in units of the shortest lattice translation vectors parallel to the projection plane)	Symmetry element represented by the graphical symbol
Reflection plane, mirror plane		None	<i>m</i>
'Axial' glide plane		$\frac{1}{2}$ in the direction of the arrow	<i>a</i> , <i>b</i> or <i>c</i>
'Double' glide plane‡		Two glide vectors: $\frac{1}{2}$ in either of the directions of the two arrows	<i>e</i>
'Diagonal' glide plane		One glide vector with two components $\frac{1}{2}$ in the direction of the arrow	<i>n</i>
'Diamond' glide plane§ (pair of planes)		$\frac{1}{2}$ in the direction of the arrow; the glide vector is always half of a centring vector, i.e. one quarter of a diagonal of the conventional face-centred cell	<i>d</i>

† The symbols are given at the upper left corner of the space-group diagrams. A fraction *h* attached to a symbol indicates two symmetry planes with 'heights' *h* and $h + \frac{1}{2}$ above the plane of projection; *e.g.* $\frac{1}{8}$ stands for $h = \frac{1}{8}$ and $\frac{5}{8}$. No fraction means $h = 0$ and $\frac{1}{2}$ (cf. Section 2.1.3.6).

‡ The graphical symbols of the 'e'-glide planes are applied to the diagrams of seven orthorhombic *A*-, *C*- and *F*-centred space groups, five tetragonal *I*-centred space groups, and five cubic *F*- and *I*-centred space groups.

§ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a} + \mathbf{b})$ and $\frac{1}{4}(\mathbf{a} - \mathbf{b})$. The second power of a glide reflection *d* is a centring vector.

dent of the projection direction and the labelling of the basis vectors. They are, therefore, applicable to any projection diagram of a space group. The alphanumeric symbols of glide planes (column 4), however, may change with a change of the basis vectors. For example, the dash-dotted *n* glide in the hexagonal description becomes an *a*, *b* or *c* glide in the rhombohedral description. In monoclinic space groups, the 'parallel' vector of a

glide plane may be along a lattice translation vector that is inclined to the projection plane.

The 'e'-glide graphical symbols are applied to the diagrams of seven orthorhombic *A*-, *C*- and *F*-centred space groups, five tetragonal *I*-centred space groups, and five cubic *F*- and *I*-centred space groups. The 'double-dotted-dash' symbol for *e* glides 'normal' and 'inclined' to the plane of projection was introduced

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Table 2.1.2.4

Graphical symbols of symmetry planes inclined to the plane of projection (in cubic space groups of classes $\bar{4}3m$ and $m\bar{3}m$ only)

Description	Graphical symbol† for planes normal to		Glide vector(s) (in units of the shortest lattice translation vectors) of the defining operation(s) of the glide plane normal to		Symmetry element represented by the graphical symbol
	[011] and [0 $\bar{1}$ 1]	[101] and [10 $\bar{1}$]	[011] and [0 $\bar{1}$ 1]	[101] and [10 $\bar{1}$]	
Reflection plane, mirror plane			None	None	<i>m</i>
'Axial' glide plane			$\frac{1}{2}$ along [100]	$\frac{1}{2}$ along [010]	<i>a</i> or <i>b</i>
'Axial' glide plane			$\frac{1}{2}$ along [0 $\bar{1}$ 1] or along [011]	$\frac{1}{2}$ along [10 $\bar{1}$] or along [101]	
'Double' glide plane [in space groups $I\bar{4}3m$ (217) and $Im\bar{3}m$ (229) only]			Two glide vectors: $\frac{1}{2}$ along [100] and $\frac{1}{2}$ along [011] or $\frac{1}{2}$ along [0 $\bar{1}$ 1]	Two glide vectors: $\frac{1}{2}$ along [010] and $\frac{1}{2}$ along [101] or $\frac{1}{2}$ along [10 $\bar{1}$]	<i>e</i>
'Diagonal' glide plane			One glide vector: $\frac{1}{2}$ along [1 $\bar{1}$ 1] or along [111]‡	One glide vector: $\frac{1}{2}$ along [1 $\bar{1}$ 1] or along [111]‡	<i>n</i>
'Diamond' glide planes§ (pair of planes)			$\frac{1}{2}$ along [1 $\bar{1}$ 1] or along [111]¶	$\frac{1}{2}$ along [$\bar{1}$ 11] or along [111]	<i>d</i>
			$\frac{1}{2}$ along [$\bar{1}$ 11] or along [$\bar{1}\bar{1}$ 1]¶	$\frac{1}{2}$ along [$\bar{1}\bar{1}$ 1] or along [111]	

† The symbols represent orthographic projections. In the cubic space-group diagrams, complete orthographic projections of the symmetry elements around high-symmetry points, such as 0, 0, 0; $\frac{1}{2}, 0, 0$; $\frac{1}{4}, \frac{1}{4}, 0$, are given as 'inserts'.

‡ In the space groups $F\bar{4}3m$ (216), $Fm\bar{3}m$ (225) and $Fd\bar{3}m$ (227), the shortest lattice translation vectors in the glide directions are $\mathbf{t}(1, \frac{1}{2}, \frac{1}{2})$ or $\mathbf{t}(1, \frac{1}{2}, \frac{1}{2})$ and $\mathbf{t}(\frac{1}{2}, 1, \frac{1}{2})$ or $\mathbf{t}(\frac{1}{2}, 1, \frac{1}{2})$, respectively.

§ Glide planes *d* occur only in orthorhombic *F* space groups, in tetragonal *I* space groups, and in cubic *I* and *F* space groups. They always occur in pairs with alternating glide vectors, for instance $\frac{1}{4}(\mathbf{a} + \mathbf{b})$ and $\frac{1}{4}(\mathbf{a} - \mathbf{b})$. The second power of a glide reflection *d* is a centring vector.

¶ The glide vector is half of a centring vector, i.e. one quarter of the diagonal of the conventional body-centred cell in space groups $I\bar{4}3d$ (220) and $Ia\bar{3}d$ (230).

in 1992 (de Wolff *et al.*, 1992), while the 'double-arrowed' graphical symbol for *e*-glide planes oriented 'parallel' to the projection plane had already been used in *IT* (1935) and *IT* (1952).

The graphical symbols of symmetry axes and their descriptions are shown in Tables 2.1.2.5–2.1.2.7. The screw vectors of the defining operations of screw axes are given in units of the shortest lattice translation vectors parallel to the axes. The symbols in the last column of the tables indicate the symmetry elements that are represented by the graphical symbols in the symmetry-element diagrams of the space groups. Two main cases may be distinguished:

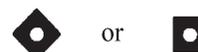
- (i) graphical symbols of symmetry elements that in the space-group diagrams represent just one symmetry element. Thus, the graphical symbol of a fourfold rotation axis or an inversion centre represent the symmetry element 4 or $\bar{1}$. Similarly, the graphical symbols of symmetry planes (Tables 2.1.2.2–2.1.2.4) represent just one symmetry element (namely, mirror or glide plane) in the space-group diagrams;

- (ii) graphical symbols of symmetry elements that in the space-group diagrams represent more than one symmetry element. For example, the graphical symbol described in Table 2.1.2.5 as 'Inversion axis: 3 bar' ($\bar{3}$),



represents in the diagrams the three different symmetry elements $\bar{3}$, 3, $\bar{1}$.

The last six entries of Table 2.1.2.5 are combinations of symbols of symmetry axes with that of a centre of inversion. When displayed on the space-group diagrams, the combined graphical symbols represent more than one symmetry element. For example, the symbol for a fourfold rotation axis with a centre of inversion ($4/m$),



represents the symmetry elements $\bar{4}$, 4 and $\bar{1}$.

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Table 2.1.2.5

Graphical symbols of symmetry axes normal to the plane of projection and symmetry points in the plane of the figure

Description	Alphanumeric symbol	Graphical symbol†	Screw vector of the defining operation of the screw axis (in units of the shortest lattice translation vector parallel to the axis)	Symmetry elements represented by the graphical symbol
Twofold rotation axis Twofold rotation point (two dimensions) } Twofold screw axis: '2 sub 1'	2 2 ₁		None $\frac{1}{2}$	2 2 ₁
Threefold rotation axis Threefold rotation point (two dimensions) } Threefold screw axis: '3 sub 1' Threefold screw axis: '3 sub 2'	3 3 ₁ 3 ₂		None $\frac{1}{3}$ $\frac{2}{3}$	3 3 ₁ 3 ₂
Fourfold rotation axis Fourfold rotation point (two dimensions) } Fourfold screw axis: '4 sub 1' Fourfold screw axis: '4 sub 2' Fourfold screw axis: '4 sub 3'	4 4 ₁ 4 ₂ 4 ₃		None $\frac{1}{4}$ $\frac{1}{2}$ $\frac{3}{4}$	4 4 ₁ 4 ₂ 4 ₃
Sixfold rotation axis Sixfold rotation point (two dimensions) } Sixfold screw axis: '6 sub 1' Sixfold screw axis: '6 sub 2' Sixfold screw axis: '6 sub 3' Sixfold screw axis: '6 sub 4' Sixfold screw axis: '6 sub 5'	6 6 ₁ 6 ₂ 6 ₃ 6 ₄ 6 ₅		None $\frac{1}{6}$ $\frac{1}{3}$ $\frac{1}{2}$ $\frac{2}{3}$ $\frac{5}{6}$	6 6 ₁ 6 ₂ 6 ₃ 6 ₄ 6 ₅
Centre of symmetry, inversion centre: '1 bar' Reflection point, mirror point (one dimension) } Inversion axis: '3 bar' Inversion axis: '4 bar' Inversion axis: '6 bar'	$\bar{1}$ $\bar{3}$ $\bar{4}$ $\bar{6}$		None None None None	$\bar{1}$ $\bar{3}, \bar{1}, 3$ $\bar{4}, 2$ $\bar{6}, 3$
Twofold rotation axis with centre of symmetry Twofold screw axis with centre of symmetry Fourfold rotation axis with centre of symmetry '4 sub 2' screw axis with centre of symmetry Sixfold rotation axis with centre of symmetry '6 sub 3' screw axis with centre of symmetry	$2/m$ $2_1/m$ $4/m$ $4_2/m$ $6/m$ $6_3/m$		None $\frac{1}{2}$ None $\frac{1}{2}$ None $\frac{1}{2}$	$2, \bar{1}$ $2_1, \bar{1}$ $4, \bar{4}, \bar{1}$ $4_2, \bar{4}, \bar{1}$ $6, \bar{6}, \bar{3}, \bar{1}$ $6_3, \bar{6}, \bar{3}, \bar{1}$

† Notes on the 'heights' h of symmetry points $\bar{1}, \bar{3}, \bar{4}$ and $\bar{6}$:

- (1) Centres of symmetry $\bar{1}$ and $\bar{3}$, as well as inversion points $\bar{4}$ and $\bar{6}$ on $\bar{4}$ and $\bar{6}$ axes parallel to $[001]$, occur in pairs at 'heights' h and $h + \frac{1}{2}$. In the space-group diagrams, only one fraction h is given, e.g. $\frac{1}{4}$ stands for $h = \frac{1}{4}$ and $\frac{3}{4}$. No fraction means $h = 0$ and $\frac{1}{2}$. In *cubic* space groups, however, because of their complexity, *both* fractions are given for vertical $\bar{4}$ axes, including $h = 0$ and $\frac{1}{2}$.
- (2) Symmetries $4/m$ and $6/m$ contain vertical $\bar{4}$ and $\bar{6}$ axes; their $\bar{4}$ and $\bar{6}$ inversion points coincide with the centres of symmetry. This is not indicated in the space-group diagrams.
- (3) Symmetries $4_2/m$ and $6_3/m$ also contain vertical $\bar{4}$ and $\bar{6}$ axes, but their $\bar{4}$ and $\bar{6}$ inversion points alternate with the centres of symmetry; i.e. $\bar{1}$ points at h and $h + \frac{1}{2}$ interleave with $\bar{4}$ or $\bar{6}$ points at $h + \frac{1}{4}$ and $h + \frac{3}{4}$. In the tetragonal and hexagonal space-group diagrams, only *one* fraction for $\bar{1}$ and one for $\bar{4}$ or $\bar{6}$ is given. In the cubic diagrams, *all four* fractions are listed for $4_2/m$; e.g. $Pm\bar{3}n$ (223): $\bar{1}: 0, \frac{1}{2}, \frac{1}{4}, \frac{3}{4}$.

The meaning of a graphical symbol on the space-group diagrams is often confused with the set of symmetry elements that constitute the site-symmetry group associated with the symmetry element displayed. As an example, consider the rotoinversion axis $\bar{6}$ (described as 'Inversion axis: 6 bar' in Table 2.1.2.5). The

site-symmetry group $\bar{6}$ can be decomposed into three symmetry elements: $\bar{6}, 3$ and m (cf. de Wolff *et al.*, 1989). However, the graphical symbol of $\bar{6}$ in the diagrams represents the two symmetry elements $\bar{6}$ and 3 , as the symmetry element ' m ' (that 'belongs' to $\bar{6}$) is represented by a separate graphical symbol.