

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	<ul style="list-style-type: none"> Reflection plane, mirror plane Reflection line, mirror line (two dimensions) Reflection point, mirror point (one dimension) 	<ul style="list-style-type: none"> Reflection through the plane Reflection through the line Reflection through the point
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 †	<ul style="list-style-type: none"> $\perp [100]$ or $\perp [010]$ $\perp [1\bar{1}0]$ or $\perp [110]$ $\perp [100]$ or $\perp [010]$ or $\perp [\bar{1}\bar{1}0]$ $\perp [1\bar{1}0]$ or $\perp [120]$ or $\perp [2\bar{1}0]$ 	<ul style="list-style-type: none"> $\frac{1}{2}\mathbf{c}$ $\frac{1}{2}\mathbf{c}$ $\frac{1}{2}\mathbf{c}$
e ‡	'Double' glide plane (in centred cells only)	Two glide reflections through one 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
	$\perp [001]$; $\perp [100]$; $\perp [010]$	$\frac{1}{2}(\mathbf{a} + \mathbf{b})$; $\frac{1}{2}(\mathbf{b} + \mathbf{c})$; $\frac{1}{2}(\mathbf{a} + \mathbf{c})$
	$\perp [1\bar{1}0]$ or $\perp [01\bar{1}]$ 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
	n -fold rotation axis, n	Counter-clockwise rotation of $360/n$ degrees around the axis
2, 3, 4, 6	n -fold rotation point, n (two dimensions)	Counter-clockwise rotation of $360/n$ degrees around the point
$\bar{1}$	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:	$Aem2$	$Aea2$	$Cmce$	$Cmme$	$Ccce$
Former symbol:	$Abm2$	$Aba2$	$Cmca$	$Cmma$	$Ccca$

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-