

2. THE SPACE-GROUP TABLES

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) }	2		None	2
Twofold screw axis: '2 sub 1'	2 ₁		$\frac{1}{2}$	2 ₁
Threefold rotation axis Threefold rotation point (two dimensions) }	3		None	3
Threefold screw axis: '3 sub 1'	3 ₁		$\frac{1}{3}$	3 ₁
Threefold screw axis: '3 sub 2'	3 ₂		$\frac{2}{3}$	3 ₂
Fourfold rotation axis Fourfold rotation point (two dimensions) }	4		None	4
Fourfold screw axis: '4 sub 1'	4 ₁		$\frac{1}{4}$	4 ₁
Fourfold screw axis: '4 sub 2'	4 ₂		$\frac{1}{2}$	4 ₂
Fourfold screw axis: '4 sub 3'	4 ₃		$\frac{3}{4}$	4 ₃
Sixfold rotation axis Sixfold rotation point (two dimensions) }	6		None	6
Sixfold screw axis: '6 sub 1'	6 ₁		$\frac{1}{6}$	6 ₁
Sixfold screw axis: '6 sub 2'	6 ₂		$\frac{1}{3}$	6 ₂
Sixfold screw axis: '6 sub 3'	6 ₃		$\frac{1}{2}$	6 ₃
Sixfold screw axis: '6 sub 4'	6 ₄		$\frac{2}{3}$	6 ₄
Sixfold screw axis: '6 sub 5'	6 ₅		$\frac{5}{6}$	6 ₅
Centre of symmetry, inversion centre: '1 bar' Reflection point, mirror point (one dimension) }	$\bar{1}$		None	$\bar{1}$
Inversion axis: '3 bar'	$\bar{3}$		None	$\bar{3}, \bar{1}, 3$
Inversion axis: '4 bar'	$\bar{4}$		None	$\bar{4}, 2$
Inversion axis: '6 bar'	$\bar{6}$		None	$\bar{6}, 3$
Twofold rotation axis with centre of symmetry	2/m		None	2, $\bar{1}$
Twofold screw axis with centre of symmetry	2 ₁ /m		$\frac{1}{2}$	2 ₁ , $\bar{1}$
Fourfold rotation axis with centre of symmetry	4/m		None	4, $\bar{4}, \bar{1}$
'4 sub 2' screw axis with centre of symmetry	4 ₂ /m		$\frac{1}{2}$	4 ₂ , $\bar{4}, \bar{1}$
Sixfold rotation axis with centre of symmetry	6/m		None	6, $\bar{6}, \bar{3}, \bar{1}$
'6 sub 3' screw axis with centre of symmetry	6 ₃ /m		$\frac{1}{2}$	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. $\frac{1}{2}$ stands for $h = \frac{1}{2}$ and $\frac{3}{2}$. 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): $\bar{1}: 0, \frac{1}{2}, 4: \frac{1}{4}, \frac{3}{4}$.

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.