

1.1. Printed symbols for crystallographic items

BY TH. HAHN

1.1.1. Vectors, coefficients and coordinates

Printed symbol	Explanation
a, b, c; or \mathbf{a}_i	Basis vectors of the direct lattice
<i>a, b, c</i>	Lengths of basis vectors, lengths of cell edges
α, β, γ	Interaxial (lattice) angles $\mathbf{b} \wedge \mathbf{c}$, $\mathbf{c} \wedge \mathbf{a}$, $\mathbf{a} \wedge \mathbf{b}$
V	Cell volume of the direct lattice
G	Matrix of the geometrical coefficients (metric tensor) of the direct lattice
g_{ij}	Element of metric matrix (tensor) G
$\mathbf{r};$ or \mathbf{x}	Position vector (of a point or an atom)
<i>r</i>	Length of the position vector \mathbf{r}
$x\mathbf{a}, y\mathbf{b}, z\mathbf{c}$	Components of the position vector \mathbf{r}
$x, y, z;$ or x_i	Coordinates of a point (location of an atom) expressed in units of a, b, c ; coordinates of end point of position vector \mathbf{r} ; coefficients of position vector \mathbf{r}
$\mathbf{x} = \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix}$	Column of point coordinates or vector coefficients
t	Translation vector
<i>t</i>	Length of the translation vector \mathbf{t}
$t_1, t_2, t_3;$ or t_i	Coefficients of translation vector \mathbf{t}
$\mathbf{t} = \begin{pmatrix} t_1 \\ t_2 \\ t_3 \end{pmatrix}$	Column of coefficients of translation vector \mathbf{t}
u	Vector with integral coefficients
$u, v, w;$ or u_i	Integers, coordinates of a (primitive) lattice point; coefficients of vector \mathbf{u}
$\mathbf{u} = \begin{pmatrix} u \\ v \\ w \end{pmatrix} = \begin{pmatrix} u_1 \\ u_2 \\ u_3 \end{pmatrix}$	Column of integral point coordinates or vector coefficients
o	Zero vector
o	Column of zero coefficients
$\mathbf{a}', \mathbf{b}', \mathbf{c}';$ or \mathbf{a}'_i	New basis vectors after a transformation of the coordinate system (basis transformation)
$\mathbf{r}';$ or $\mathbf{x}';$ $x', y', z';$ or x'_i	Position vector and point coordinates after a transformation of the coordinate system (basis transformation)
$\tilde{\mathbf{r}};$ or $\tilde{\mathbf{x}};$ $\tilde{x}, \tilde{y}, \tilde{z};$ or \tilde{x}_i	New position vector and point coordinates after a symmetry operation (motion)

1.1.2. Directions and planes

Printed symbol	Explanation
$[uvw]$	Indices of a lattice direction (zone axis)
$\langle uvw \rangle$	Indices of a set of all symmetrically equivalent lattice directions
(hkl)	Indices of a crystal face, or of a single net plane (Miller indices)
$(hkil)$	Indices of a crystal face, or of a single net plane, for the hexagonal axes $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{c}$ (Bravais–Miller indices)
$\{hkl\}$	Indices of a set of all symmetrically equivalent crystal faces ('crystal form'), or net planes
$\{hkil\}$	Indices of a set of all symmetrically equivalent crystal faces ('crystal form'), or net planes, for the hexagonal axes $\mathbf{a}_1, \mathbf{a}_2, \mathbf{a}_3, \mathbf{c}$
hkl	Indices of the Bragg reflection (Laue indices) from the set of parallel equidistant net planes (hkl)
d_{hkl}	Interplanar distance, or spacing, of neighbouring net planes (hkl)

1.1.3. Reciprocal space

Printed symbol	Explanation
$\mathbf{a}^*, \mathbf{b}^*, \mathbf{c}^*;$ or \mathbf{a}_i^*	Basis vectors of the reciprocal lattice
a^*, b^*, c^*	Lengths of basis vectors of the reciprocal lattice
$\alpha^*, \beta^*, \gamma^*$	Interaxial (lattice) angles of the reciprocal lattice $\mathbf{b}^* \wedge \mathbf{c}^*, \mathbf{c}^* \wedge \mathbf{a}^*, \mathbf{a}^* \wedge \mathbf{b}^*$
$\mathbf{r}^*;$ or \mathbf{h}	Reciprocal-lattice vector
$h, k, l;$ or h_i	Coordinates of a reciprocal-lattice point, expressed in units of a^*, b^*, c^* , coefficients of the reciprocal-lattice vector \mathbf{r}^*
V^*	Cell volume of the reciprocal lattice
\mathbf{G}^*	Matrix of the geometrical coefficients (metric tensor) of the reciprocal lattice

1.1.4. Functions

Printed symbol	Explanation
$\rho(xyz)$	Electron density at the point x, y, z
$P(xyz)$	Patterson function at the point x, y, z
$F(hkl);$ or F	Structure factor (of the unit cell), corresponding to the Bragg reflection hkl
$ F(hkl) ;$ or $ F $	Modulus of the structure factor $F(hkl)$
$\alpha(hkl);$ or α	Phase angle of the structure factor $F(hkl)$