

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

Table 2.1.1.1

Crystal families, crystal systems, conventional coordinate systems and Bravais lattices in one, two and three dimensions

Crystal family	Symbol†	Crystal system	Crystallographic point groups‡	No. of space groups	Conventional coordinate system		Bravais lattices†
					Restrictions on cell parameters	Parameters to be determined	
<i>One dimension</i>							
–	–	–	1, $\overline{1}$	2	None	a	$\not\ell$
<i>Two dimensions</i>							
Oblique (monoclinic)	m	Oblique	1, $\overline{2}$	2	None	a, b $\gamma \S$	mp
Rectangular (orthorhombic)	o	Rectangular	$m, \overline{2mm}$	7	$\gamma = 90^\circ$	a, b	op oc
Square (tetragonal)	t	Square	$\overline{4}, \overline{4mm}$	3	$a = b$ $\gamma = 90^\circ$	a	tp
Hexagonal	h	Hexagonal	$3, \overline{6}$ $3m, \overline{6mm}$	5	$a = b$ $\gamma = 120^\circ$	a	hp
<i>Three dimensions</i>							
Triclinic (anorthic)	a	Triclinic	1, $\overline{1}$	2	None	a, b, c α, β, γ	aP
Monoclinic	m	Monoclinic	$2, m, \overline{2/m}$	13	b -unique setting $\alpha = \gamma = 90^\circ$	a, b, c $\beta \S$	mP $mS^\P (mC, mA, mI)$
					c -unique setting $\alpha = \beta = 90^\circ$	a, b, c $\gamma \S$	mP $mS^\P (mA, mB, mI)$
Orthorhombic	o	Orthorhombic	$222, mm2, \overline{mmm}$	59	$\alpha = \beta = \gamma = 90^\circ$	a, b, c	oP $oS^\P (oC, oA, oB)$ oI oF
Tetragonal	t	Tetragonal	$4, \overline{4}, \overline{4/m}$ $422, 4mm, \overline{4}2m,$ $\overline{4}/\overline{mmm}$	68	$a = b$ $\alpha = \beta = \gamma = 90^\circ$	a, c	tP tI
Hexagonal	h	Trigonal	$3, \overline{3}$ $32, 3m, \overline{3}m$	18	$a = b$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	a, c	hP
				7	$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell) $a = b$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$ (hexagonal axes, triple obverse cell)	a, α	hR
		Hexagonal	$6, \overline{6}, \overline{6/m}$ $622, 6mm, \overline{6}2m,$ $\overline{6}/\overline{mmm}$	27	$a = b$ $\alpha = \beta = 90^\circ, \gamma = 120^\circ$	a, c	hP
Cubic	c	Cubic	$23, \overline{m}3$ $432, 43m, \overline{m}3m$	36	$a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	a	cP cI cF

 † The symbols for crystal families (column 2) and Bravais lattices (column 8) were adopted by the International Union of Crystallography in 1985; cf. de Wolff *et al.* (1985).

‡ Symbols surrounded by dashed or full lines indicate Laue groups; full lines indicate Laue groups which are also lattice point symmetries (holohedries).

 § These angles are conventionally taken to be non-acute, *i.e.* $\geq 90^\circ$.

 ¶ For the use of the letter *S* as a new general, setting-independent ‘centring symbol’ for monoclinic and orthorhombic Bravais lattices, see de Wolff *et al.* (1985).

a point of high site symmetry). The choice of such a coordinate system is not mandatory, since in principle a crystal structure can be referred to any coordinate system; cf. Chapters 1.3 and 1.5.

The selection of a crystallographic coordinate system is not unique. Conventionally, a right-handed set of basis vectors is taken such that the symmetry of the plane or space group is displayed best. With this convention, which is followed in the present volume, the specific restrictions imposed on the cell parameters by each crystal family become particularly simple. They are listed in columns 6 and 7 of Table 2.1.1.1. If within these restrictions the smallest cell is chosen, a *conventional* (crystallographic) *basis* results. Together with the selection of an

appropriate *conventional* (crystallographic) *origin* (cf. Sections 2.1.3.2 and 2.1.3.7), such a basis defines a *conventional* (crystallographic) *coordinate system* and a *conventional cell*. The conventional cell of a point lattice or a space group, obtained in this way, turns out to be either *primitive* or to exhibit one of the *centring types* listed in Table 2.1.1.2. The centring type of a conventional cell is transferred to the lattice which is described by this cell; hence, we speak of primitive, face-centred, body-centred *etc.* lattices. Similarly, the cell parameters are often called lattice parameters; cf. Chapters 1.3 and 3.1 for further details.

In the triclinic, monoclinic and orthorhombic crystal systems, additional conventions (for instance cell reduction or metrical