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2.1. Guide to the use of the space-group tables

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In this part of the volume, tables and diagrams of crystallographic data for the 17 types of plane groups (Chapter 2.2) and the 230 types of space groups (Chapter 2.3) are presented. With the exception of the data for maximal subgroups and minimal supergroups (which have been transferred to Volume A1), the crystallographic data presented in Chapters 2.2 and 2.3 closely follow those in the fifth (2002) edition of Volume A, hereafter *IT* A (2002). This chapter is a guide to understanding and using these data.

Only a minimum of theory is provided here, as the emphasis is on the practical use of the data. For the theoretical background to these data, the reader is referred to Parts 1 and 3, which also include suitable references. A textbook explaining space-group symmetry and the use of the data in Chapters 2.2 and 2.3 (with exercises) is provided by Hahn & Wondratschek (1994); see also Müller (2013).

Section 2.1.1 displays, with the help of an extensive synoptic table, the classification of the 17 plane groups and 230 space groups. This is followed by an explanation of the characterization of the conventional crystallographic coordinate systems, including the symbols for the centring types of lattices and cells. Section 2.1.2 lists the alphanumeric and graphical symbols for symmetry elements and symmetry operations used throughout this volume. The lists are accompanied by notes and cross-references to related IUCr nomenclature reports. Section 2.1.3 explains in a systematic fashion, with many examples and figures, all the entries and diagrams in the order in which they occur in the plane-group and space-group tables of Chapters 2.2 and 2.3. Detailed treatments are given for the Hermann–Mauguin space-group symbols, the space-group diagrams, the general and special positions, the reflections conditions, monoclinic space groups, and the two crystallographic space groups in one dimension (which are also known as the line groups and are treated in Section 2.1.3.16). Section 2.1.4 discusses the computer generation of the space-group tables in this and earlier editions of the volume.

2.1.1. Conventional descriptions of plane and space groups

By Th. Hahn and A. Looijenga-Vos

2.1.1.1. Classification of space groups

In this volume, the plane groups and space groups are classified according to three criteria:

(i) According to *geometric crystal classes*, *i.e.* according to the crystallographic point group to which a particular space group belongs. There are 10 crystal classes in two dimensions and 32 in three dimensions. They are described and listed in Chapter 3.2 and in column 4 of Table 2.1.1.1. [For arithmetic crystal classes, see Chapter 1.3 and Table 2.1.3.3 in this volume, and Chapter 1.4 of *International Tables for Crystallography*, Vol. C (2004).]

(ii) According to *crystal families*. The term crystal family designates the classification of the 17 plane groups into four categories and of the 230 space groups into *six* categories, as displayed in column 1 of Table 2.1.1.1. Here all 'hexagonal', 'trigonal' and 'rhombohedral' space groups are contained in one family, the hexagonal crystal family. The 'crystal family' thus corresponds to the term 'crystal system', as used frequently in the American and Russian literature.

The crystal families are symbolized by the lower-case letters *a*, *m*, *o*, *t*, *h*, *c*, as listed in column 2 of Table 2.1.1.1. If these letters are combined with the appropriate capital letters for the lattice-centring types (*cf.* Table 2.1.1.2), symbols for the 14 Bravais lattices result. These symbols and their occurrence in the crystal families are shown in column 8 of Table 2.1.1.1; *mS* and *oS* are the standard setting-independent symbols for the centred monoclinic and the one-face-centred orthorhombic Bravais lattices, *cf.* de Wolff *et al.* (1985); symbols between parentheses represent alternative settings of these Bravais lattices.

(iii) According to *crystal systems*. This classification collects the plane groups into four categories and the space groups into *seven* categories. The classifications according to crystal families and crystal systems are the same for two dimensions.

For three dimensions, this applies to the triclinic, monoclinic, orthorhombic, tetragonal and cubic systems. The only complication exists in the hexagonal crystal family, for which several subdivisions into systems have been proposed in the literature. In this volume [as well as in *International Tables for X-ray Crystallography* (1952), hereafter *IT* (1952), and the subsequent editions of *IT*], the space groups of the hexagonal crystal family are grouped into two 'crystal systems' as follows: all space groups belonging to the five crystal classes 3, $\bar{3}$, 32, 3*m* and $\bar{3}m$, *i.e.* having 3, 3_1, 3_2 or $\bar{3}$ as principal axis, form the *trigonal* crystal system, irrespective of whether the Bravais lattice is *hP* or *hR*; all space groups belonging to the seven crystal classes 6, $\bar{6}$, 6/*m*, 622, 6*mm*, $\bar{6}2m$ and 6/*mmm*, *i.e.* having 6, 6_1, 6_2, 6_3, 6_4, 6_5 or $\bar{6}$ as principal axis, form the *hexagonal* crystal system; here the lattice is always *hP* (*cf.* Chapter 1.3). The crystal systems, as defined above, are listed in column 3 of Table 2.1.1.1.

A different subdivision of the hexagonal crystal family is in use, mainly in the French literature. It consists of grouping all space groups based on the hexagonal Bravais lattice *hP* (lattice point symmetry 6/*mmm*) into the 'hexagonal' system and all space groups based on the rhombohedral Bravais lattice *hR* (lattice point symmetry $\bar{3}m$) into the 'rhombohedral' system. In Chapter 1.3, these systems are called 'lattice systems'. They were called 'Bravais systems' in earlier editions of this volume.

The theoretical background for the classification of space groups is provided in Chapter 1.3.

2.1.1.2. Conventional coordinate systems and cells

A plane group or space group usually is described by means of a *crystallographic coordinate system*, consisting of a *crystallographic basis* (basis vectors are lattice vectors) and a *crystallographic origin* (origin at a centre of symmetry or at

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	
One dimension							
–	–	–	1, $\boxed{m}$	2	None	a	$\not\!p$
Two dimensions							
Oblique (monoclinic)	m	Oblique	1, $\boxed{2}$	2	None	a, b γ§	mp
Rectangular (orthorhombic)	o	Rectangular	m, $\boxed{2mm}$	7	$\gamma = 90°$	a, b	op oc
Square (tetragonal)	t	Square	$\boxed{4}$, $\boxed{4mm}$	3	$a = b$ $\gamma = 90°$	a	tp
Hexagonal	h	Hexagonal	3, $\boxed{6}$ $3m$, $\boxed{6mm}$	5	$a = b$ $\gamma = 120°$	a	hp
Three dimensions							
Triclinic (anorthic)	a	Triclinic	1, $\boxed{\bar{1}}$	2	None	a, b, c α, β, γ	aP
Monoclinic	m	Monoclinic	$2, m$, $\boxed{2/m}$	13	b-unique setting $\alpha = \gamma = 90°$	a, b, c β §	mP mS¶ (mC, mA, mI)
					c-unique setting $\alpha = \beta = 90°$	a, b, c γ §	mP mS¶ (mA, mB, mI)
Orthorhombic	o	Orthorhombic	222, $mm2$, $\boxed{mmm}$	59	$\alpha = \beta = \gamma = 90°$	a, b, c	oP oS¶ (oC, oA, oB) oI oF
Tetragonal	t	Tetragonal	$4, \bar{4}$, $\boxed{4/m}$ $422, 4mm, \bar{4}2m$, $\boxed{4/mmm}$	68	$a = b$ $\alpha = \beta = \gamma = 90°$	a, c	tP tI
Hexagonal	h	Trigonal	3, $\boxed{\bar{3}}$ $32, 3m$, $\boxed{\bar{3}m}$	18	$a = b$ $\alpha = \beta = 90°$, $\gamma = 120°$	a, c	hP
				7	$a = b = c$ $\alpha = \beta = \gamma$ (rhombohedral axes, primitive cell) $a = b$ $\alpha = \beta = 90°, \gamma = 120°$ (hexagonal axes, triple obverse cell)	a, α	hR
		Hexagonal	$6, \bar{6}$, $\boxed{6/m}$ $622, \bar{6}mm, \bar{6}2m$, $\boxed{6/mmm}$	27	$a = b$ $\alpha = \beta = 90°, \gamma = 120°$	a, c	hP
Cubic	c	Cubic	23, $\boxed{m\bar{3}}$ $432, \bar{4}3m$, $\boxed{m\bar{3}m}$	36	$a = b = c$ $\alpha = \beta = \gamma = 90°$	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.* $\geq 90°$.
¶ 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

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			
p	Primitive	1	0
Two dimensions			
p	Primitive	1	0, 0
c	Centred	2	0, 0; $\frac{1}{2}, \frac{1}{2}$
h†	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, $\frac{1}{2}, \frac{1}{2}$, $\frac{1}{2}$, 0, $\frac{1}{2}$
R‡	Rhombohedrally centred (description with 'hexagonal axes')	3	0, 0, 0; $\frac{2}{3}, \frac{1}{3}, \frac{1}{3}$; $\frac{1}{3}, \frac{2}{3}, \frac{2}{3}$ ('obverse setting') 0, 0, 0; $\frac{1}{3}, \frac{2}{3}, \frac{1}{3}$; $\frac{2}{3}, \frac{1}{3}, \frac{2}{3}$ ('reverse setting')
	Primitive (description with 'rhombohedral axes')	1	0, 0, 0
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

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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),