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2.1. Classification and coordinate systems of space groups

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2.1.1. Introduction

The present volume is a computer-based extension and complete revision of the symmetry tables of the two previous series of *International Tables,* the *Internationale Tabellen zur Bestimmung von Kristallstrukturen* (1935) and the *International Tables for X-ray Crystallography* (1952).*

The main part of the volume consists of tables and diagrams for the 17 types of plane groups (Part 6) and the 230 types of space groups (Part 7). The two types of line groups are treated separately in Section 2.2.17, because of their simplicity. For the history of the *Tables* and a comparison of the various editions, reference is made to the *Preface* of this volume. Attention is drawn to Part 1 where the symbols and terms used in this volume are defined.

The present part forms a *guide* to the entries in the space-group tables with instructions for their practical use. Only a minimum of theory is provided, and the emphasis is on practical aspects. For the theoretical background the reader is referred to Parts 8–15, which include also suitable references. A textbook version of space-group symmetry and the use of these tables (with exercises) is provided by Hahn & Wondratschek (1994).

2.1.2. Space-group classification

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 Part 10 and in column 4 of Table 2.1.2.1. [For arithmetic crystal classes, see Section 8.2.3 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 2.1.2.1. 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 2.1.2.1. If these letters are combined with the appropriate capital letters for the lattice-centring types (*cf.* Chapter 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 2.1.2.1; *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 *IT* (1952), 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.* Section 8.2.8). The crystal systems, as defined above, are listed in column 3 of Table 2.1.2.1.

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 Section 8.2.8, 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 8.2.

2.1.3. 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 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.* Section 8.1.4.

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 2.1.2.1. 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 2.2.2 and 2.2.7), 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 Chapter 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.* Section 8.3.1 and Chapter 9.1 for further details.

In the triclinic, monoclinic and orthorhombic crystal systems, additional conventions (for instance cell reduction or metrical 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 Chapters 9.1 and 9.2, orthorhombic settings in Section 2.2.6.4, and monoclinic settings and cell choices in Section 2.2.16.

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

* Throughout this volume, these editions are abbreviated as *IT* (1935) and *IT* (1952).

Table 2.1.2.1. *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	⫽
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.* $\geq 90°$.

only with a hexagonal coordinate system (primitive cell),* whereas the seven space groups based on the rhombohedral Bravais lattice *hR* are treated in two versions, one referred to 'hexagonal axes' (triple obverse cell) and one to 'rhombohedral axes' (primitive cell); *cf.* Chapter 1.2. In practice, hexagonal axes are preferred because they are easier to visualize.

Note: For convenience, the relations between the cell parameters a, c of the triple hexagonal cell and the cell parameters a', α' of the primitive rhombohedral cell (*cf.* Table 2.1.2.1) are listed:

$$a = a'\sqrt{2}\sqrt{1-\cos\alpha'} = 2a'\sin\frac{\alpha'}{2}$$

$$c = a'\sqrt{3}\sqrt{1+2\cos\alpha'}$$

$$\frac{c}{a} = \sqrt{\frac{3}{2}}\sqrt{\frac{1+2\cos\alpha'}{1-\cos\alpha'}} = \sqrt{\frac{9}{4\sin^2(\alpha'/2)} - 3}$$

$$a' = \tfrac{1}{3}\sqrt{3a^2+c^2}$$

$$\sin\frac{\alpha'}{2} = \frac{3}{2\sqrt{3+(c^2/a^2)}} \text{ or } \cos\alpha' = \frac{(c^2/a^2)-\frac{3}{2}}{(c^2/a^2)+3}.$$

* For a rhombohedral description (*D* cell) of the hexagonal Bravais lattice see Section 4.3.5.3.

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