GRAU: Enginyeria Matemàtica i Física

Assignatura: FISICA DEL ESTAT SÒLID i SUPERFICIES

(**CRISTAL·LOGRAFIA, SIMETRIA)**

Taules cristal·lografiques

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Els sistemes cristal·lins i les xarxes. Xarxes i grups espacials. (2D)

Table 1.1. *Two-dimensional crystal systems, lattices and space groups*

Crystal system	Point groups compatible with crystal system	Lattices in system	Space groups compatible with lattice
Oblique $a \neq b, \gamma \neq 90°$	1, 2	p (primitive)	p1, p2
Rectangular $a \neq b, \gamma = 90°$	1m, 2mm	p (primitive)	pm, p2mm, pg, p2mg p2gg
		c (centred)	cm, c2mm
Square $a = b, \gamma = 90°$	4, 4mm	p (primitive)	p4, p4mm, p4gm
Hexagonal $a = b, \gamma = 120°$	3, 3m, 6, 6mm	p (primitive)	p3, p31m, p3m1 p6, p6mm

Les 5 cel·les bidimensionals i els elements de simetria de les mateixes

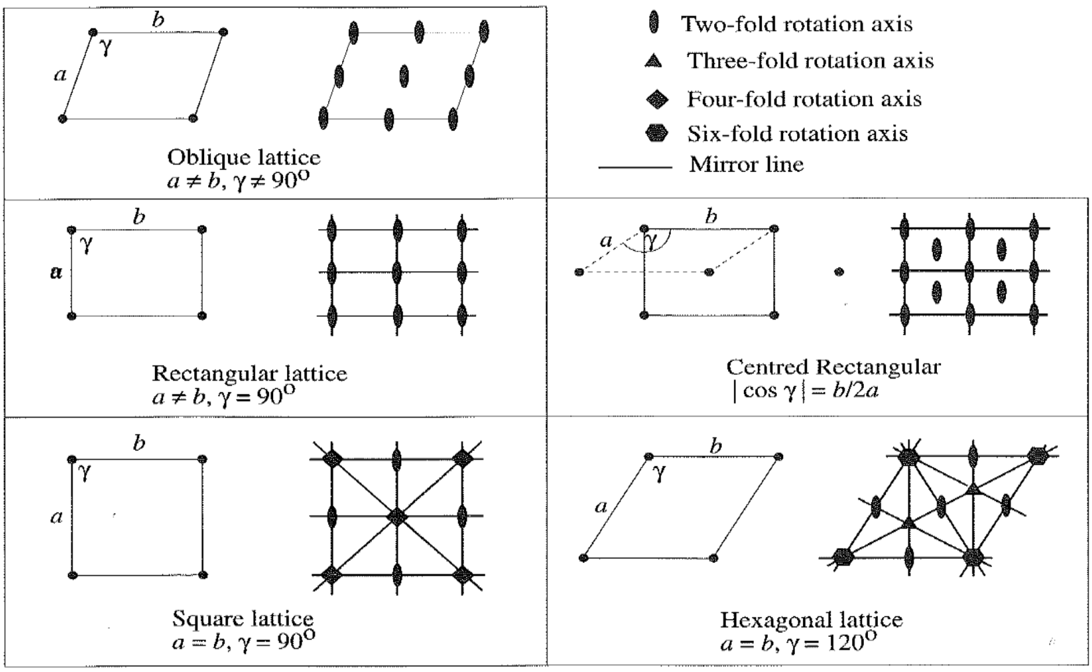


Figure 1.6. The five two-dimensional lattices, and the symmetry of the distribution of lattice points in each. In each case a single unit cell is shown on the left, and the symmetry elements within the cell are shown in the figure on the right.

Els 7 sistemes cristal·lins i les 14 xarxes de BRAVAIS (3-D).

Table 1.2. *The 7 crystal systems and 14 Bravais lattices in 3 dimensions*

Crystal system	Unit cell dimensions	Essential symmetry	Bravais lattices
Triclinic	$a \neq b \neq c$; $\alpha \neq \beta \neq \gamma$	None	P
Monoclinic	$a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	A diad (2-fold) axis	P, C
Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	Three mutually perpendicular diad axes	P, C, I, F
Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	A tetrad (4-fold) axis	P, I
Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$	Four triad (3-fold) axes	P, I, F
Trigonal*	$a = b = c$ $120° > \alpha = \beta = \gamma \neq 90°$	A triad axis	R (rhombohedral)
Hexagonal	$a = b \neq c$ $\alpha = \beta = 90°$, $\gamma = 120°$	A hexad (6-fold) axis	P

* Crystals in the trigonal system may be described by an hexagonal unit cell, even though they do not have a hexad rotation axis.

Les 14 xarxes de BRAVAIS, 1848.

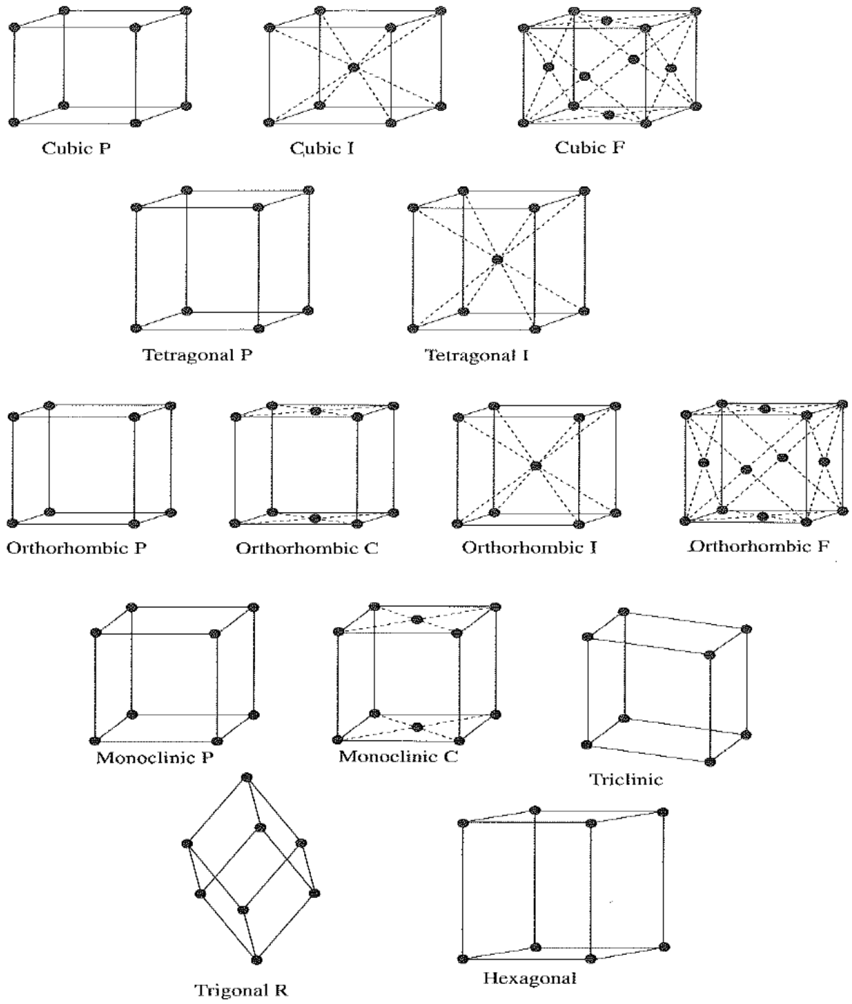


Figure 1.11. The 14 Bravais lattices. All crystalline solids can be described by unit cells which belong to one of these 14 types.

TABLE 2.3.1

Crystallographic Axial and Angular Relationships, and Characteristic Symmetry of the Crystal Systems

Point groups[1]	System	Axial and angular relationships[2]	Axial ratios and angles to be specified for each substance	Characteristic symmetry
$1, \bar{1}$	Triclinic	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$	$a : b : c$ α, β, γ	1-fold (identity or inversion) symmetry only.
$2, m, 2/m$	Monoclinic[3]	1st setting $a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$ 2nd setting $a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	$a : b : c$ γ $a : b : c$ β	2-fold axis (rotation or inversion) in one direction only, this being taken as the z-axis in the first setting and as the y-axis in the second setting.
$222, mm2, mmm$	Orthorhombic	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	$a : b : c$	2-fold axes (rotation or inversion) in three mutually perpendicular directions.
$4, \bar{4}, 4/m, 422, 4mm, \bar{4}2m, 4/mmm$	Tetragonal	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	$c : a$	4-fold axis (rotation or inversion) along the z-axis.
$23, m3, 432, \bar{4}3m, m3m$	Cubic	$a = b = c$ $\alpha = \beta = \gamma = 90°$	None	Four 3-fold axes each inclined at 54° 44′ to the crystallographic axes.
$3, \bar{3}, 32, 3m, \bar{3}m$	Trigonal (may be taken as subdivision of hexagonal)	(Rhombohedral axes) $a = b = c$ $\alpha = \beta = \gamma < 120° \neq 90°$ (Hexagonal axes)[4] $a = b \neq c$ $\alpha = \beta = 90°, \gamma = 120°$	α $c : a$	3-fold axis (rotation or inversion) along [111] using rhombohedral axes, or along the z-direction using hexagonal axes.
$6, \bar{6}, 6/m, 622, 6mm, \bar{6}m2, 6/mmm$	Hexagonal	$a = b \neq c$ [4] $\alpha = \beta = 90°$ $\gamma = 120°$	$c : a$	6-fold axis (rotation or inversion) along the z-axis.

(1) For explanation of point-group symbols see section 3.1.
(2) The sign $\neq$ implies non-equality by reason of symmetry; accidental equality may, of course, occur.
(3) See Preface to Volume I for explanation of alternative settings.
(4) In drawing the hexagonal axes, it is customary to take three axes, x-, y- and u-, at 120° to each other, and normal to the z-axis.

TABLE 3-1 CRYSTALLOGRAPHIC POINT GROUPS

Crystal system	Schoenflies symbol	Hermann–Mauguin symbol	Order of group	Laue group
Triclinic	C_1	1	1	$\bar{1}$
	C_i	$\bar{1}$	2	
Monoclinic	C_2	2	2	$2/m$
	C_s	m	2	
	C_{2h}	$2/m$	4	
Orthorhombic	D_2	222	4	mmm
	C_{2v}	$mm2$	4	
	D_{2h}	mmm	8	
Tetragonal	C_4	4	4	$4/m$
	S_4	$\bar{4}$	4	
	C_{4h}	$4/m$	8	
	D_4	422	8	$4/mmm$
	C_{4v}	$4mm$	8	
	D_{2d}	$\bar{4}2m$	8	
	D_{4h}	$4/mmm$	16	
Trigonal	C_3	3	3	$\bar{3}$
	C_{3i}	$\bar{3}$	6	
	D_3	32	6	$\bar{3}m$
	C_{3v}	$3m$	6	
	D_{3d}	$\bar{3}m$	12	
Hexagonal	C_6	6	6	$6/m$
	C_{3h}	$\bar{6}$	6	
	C_{6h}	$6/m$	12	
	D_6	622	12	$6/mmm$
	C_{6v}	$6mm$	12	
	D_{3h}	$\bar{6}m2$	12	
	D_{6h}	$6/mmm$	24	
Cubic	T	23	12	$m3$
	T_h	$m3$	24	
	O	432	24	$m3m$
	T_d	$\bar{4}3m$	24	
	O_h	$m3m$	48	

3.3. The 32 Three-dimensional Point Groups

The crystallographic point groups are those groups of symmetry operations which can operate on infinite three-dimensional lattices so as to leave one point unmoved. They are derived by combining the elements of symmetry listed in section 3.1. They may be grouped into systems according to the set of co-ordinate axes to which they are most conveniently referred or, which is the same thing, according to the group of Bravais lattices on which they can operate. This grouping is shown in Table 3.3.1 together with the point-group order adopted in the present volume, which is different from that used in the 1935 *Tables*. The symbol X here stands for the order of the rotation symmetry (a single symmetry operation being rotation through $2\pi/X$ about the axis), and the arrangement across the page is 1, 2, 4, 3, 6, $X3$ (cubic). The close relation between trigonal and hexagonal symmetry makes this more convenient than the direct numerical order would be. The notation is as follows:

Rotation axis X Inversion axis $\bar{X}$

Rotation axis with mirror plane normal to it X/m $\left(\frac{X}{m}\right)$

Rotation axis with diad axis (axes) normal to it $X2$

Rotation axis with mirror plane (planes) parallel to it Xm

Inversion axis with diad axis (axes) normal to it $\bar{X}2$

Inversion axis with mirror plane (planes) parallel to it $\bar{X}m$

Rotation axis with a mirror plane normal to it and mirror planes parallel to it X/mm $\left(\frac{X}{m}m\right)$

TABLE 3.3.1. **Symbols of the 32 Three-dimensional Point Groups**

General symbol	Triclinic	Monoclinic (1st setting)	Tetragonal	Trigonal	Hexagonal	Cubic
X	1	2	4	3	6	23
$\bar{X}$ (of even order)	—	$\bar{2}$ (≡m)	$\bar{4}$	—	$\bar{6}$	—
X plus centre (includes $\bar{X}$ of odd order)	$\bar{1}$	$2/m$	$4/m$	$\bar{3}$	$6/m$	$2/m\,\bar{3}$ ($m3$)
	Monoclinic (2nd setting)	Orthorhombic				
$X2$	2 (≡12)	222	422 {42}	32	622 {62}	432 {43}
Xm	m (≡1m)	$mm2$ {mm}	$4mm$	$3m$	$6mm$	—
$\bar{X}2$ and $\bar{X}m$ (of even order)	—	—	$\bar{4}2m$	—	$\bar{6}m2$	$\bar{4}3m$
$X2$ plus centre, Xm plus centre (includes $\bar{X}m$ of odd order)	$2/m$	$2/m\,2/m\,2/m$ (mmm)	$4/m\,2/m\,2/m$ ($4/mmm$)	$\bar{3}\,2/m$ ($\bar{3}m$)	$6/m\,2/m\,2/m$ ($6/mmm$)	$4/m\,\bar{3}\,2/m$ ($m3m$)

NOTES

1. Although it is convenient to use the concept of centro-symmetry in deriving the above arrangement of the symbols, the centre is not used in systematic symbolism, being replaced by its equivalent inversion axis $\bar{1}$.
2. The symbols given in parentheses, e.g. (mmm), are the short forms of the symbols where these differ from the full symbols.
3. The symbols given in braces, e.g. {42}, are the short symbols used in earlier space-group nomenclature. They are still used where *direction* is unspecified, as in the point symmetry corresponding to the various sets of equivalent positions (section 4.3).
4. The order of the point groups in the following tables (sections 4.3, 4.7 in particular) is that obtained by reading down each column in Table 3.3.1, taking the columns in turn from left to right, the two monoclinic settings being taken together.

2

TABLE 3.9.1. [redacted] Symbols of the 32 Crystal Classes

Point groups: International symbol, Short	Point groups: International symbol, Full	Schoenflies symbol	System used in this vo
1	1	C_1	Triclinic
$\bar{1}$	$\bar{1}$	$C_i(S_2)$	
2	2	C_2	Monoclinic
m	m	$C_s(C_{1h})$	
$2/m$	$\frac{2}{m}$	C_{2h}	
222	222	$D_2(V)$	Orthorhombi
$mm2$	$mm2$	C_{2v}	
mmm	$\frac{2}{m}\frac{2}{m}\frac{2}{m}$	$D_{2h}(V_h)$	
4	4	C_4	Tetragonal
$\bar{4}$	$\bar{4}$	S_4	
$4/m$	$\frac{4}{m}$	C_{4h}	
422	422	D_4	
$4mm$	$4mm$	C_{4v}	
$\bar{4}2m$	$\bar{4}2m$	$D_{2d}(V_d)$	
$4/mmm$	$\frac{4}{m}\frac{2}{m}\frac{2}{m}$	D_{4h}	
3	3	C_3	Trigonal
$\bar{3}$	$\bar{3}$	$C_{3i}(S_6)$	
32	32	D_3	
$3m$	$3m$	C_{3v}	
$\bar{3}m$	$\bar{3}\frac{2}{m}$	D_{3d}	
6	6	C_6	Hexagonal
$\bar{6}$	$\bar{6}$	C_{3h}	
$6/m$	$\frac{6}{m}$	C_{6h}	
622	622	D_6	
$6mm$	$6mm$	C_{6v}	
$\bar{6}m2$	$\bar{6}m2$	D_{3h}	
$6/mmm$	$\frac{6}{m}\frac{2}{m}\frac{2}{m}$	D_{6h}	
23	23	T	Cubic
$m3$	$\frac{2}{m}\bar{3}$	T_h	
432	432	O	
$\bar{4}3m$	$\bar{4}3m$	T_d	
$m3m$	$\frac{4}{m}\bar{3}\frac{2}{m}$	O_h	

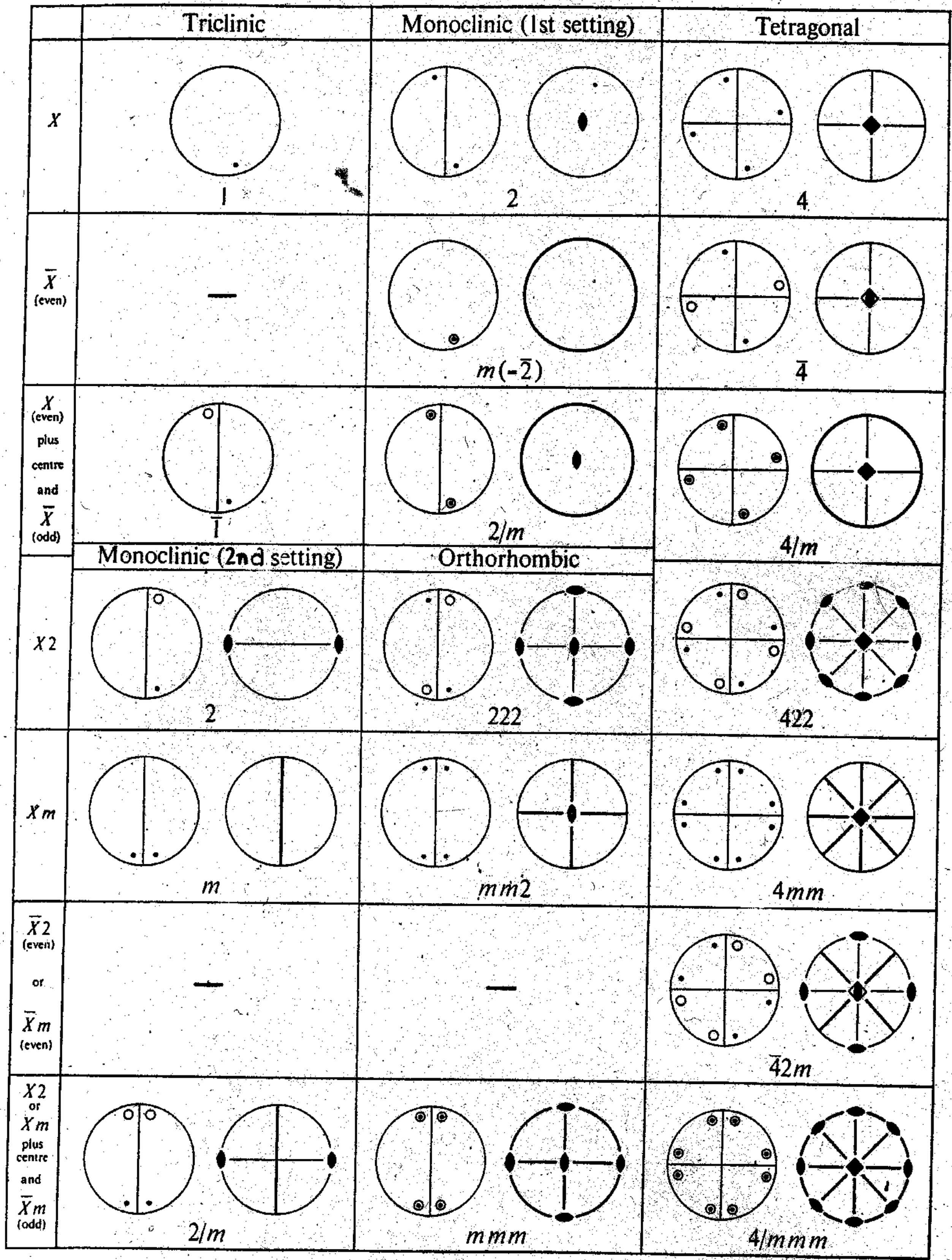
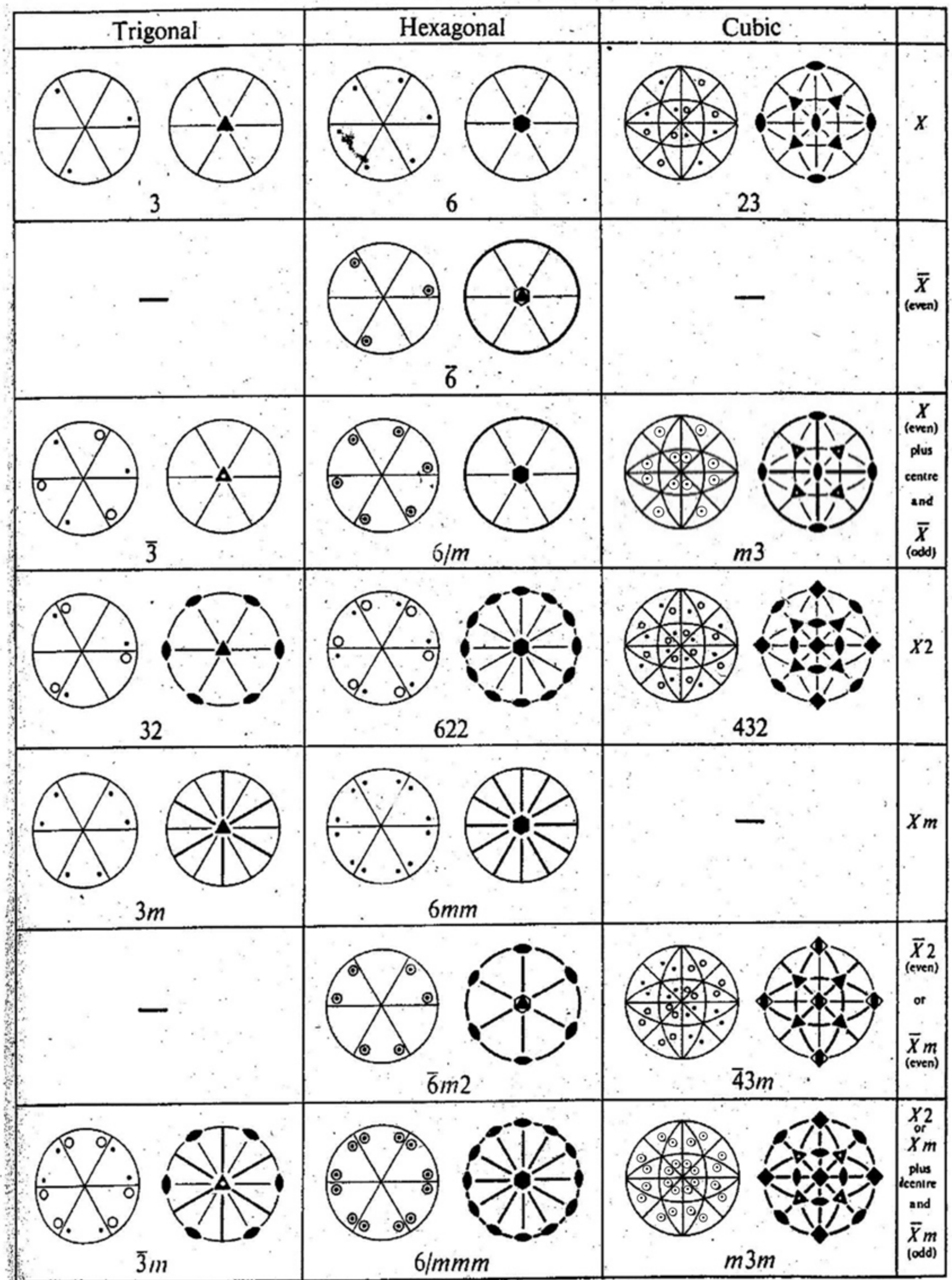


Fig. 3.3.1. Stereograms of poles of general equivalent directions, and symmetry

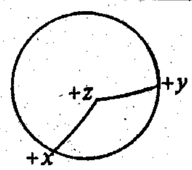
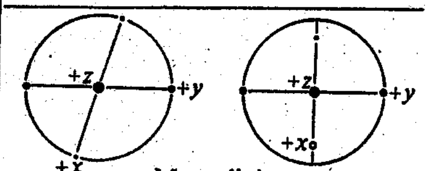
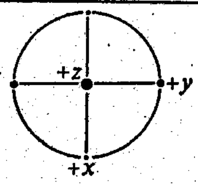
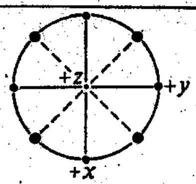
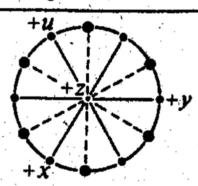
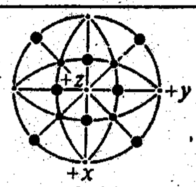


elements of each of the 32 point groups (z-axis normal to the paper in all drawings)

5

TABLE 3.3.2

Order of Positions in the Symbols of the Three-dimensional Point Groups as applied to Lattices

System and point groups	Position in point-group symbol			Stereographic representation (• Poles of directions for primary position • secondary ditto • tertiary ditto)
	Primary	Secondary	Tertiary	
Triclinic 1, $\bar{1}$	Only one symbol which denotes all directions in the crystal.			 Triclinic
Monoclinic 2, *m*, 2/*m*	The symbol gives the nature of the unique diad axis[1] (rotation and/or inversion). 1st setting: *z*-axis unique[2] 2nd setting: *y*-axis unique			 Monoclinic 1st setting 2nd setting
Orthorhombic 222, *mm*2, *mmm*	Diad (rotation and/or inversion) along *x*-axis	Diad (rotation and/or inversion) along *y*-axis	Diad (rotation and/or inversion) along *z*-axis	 Orthorhombic
Tetragonal 4, $\bar{4}$, 4/*m*; 422, 4*mm*, $\bar{4}$2*m*, 4/*mmm*	Tetrad (rotation and/or inversion) along *z*-axis	Diads (rotation and/or inversion) along *x*- and *y*-axes	Diads (rotation and/or inversion) along [110] and [$1\bar{1}0$] axes	 Tetragonal
Trigonal and hexagonal[3] 3, $\bar{3}$; 32, 3*m*, $\bar{3}$*m*; 6, $\bar{6}$, 6/*m*; 622, 6*mm*, $\bar{6}$*m*2, 6/*mmm*	Triad or hexad (rotation and/or inversion) along *z*-axis	Diads (rotation and/or inversion) along *x*-, *y*- and *u*-axes	Diads (rotation and/or inversion) normal to *x*-, *y*-, *u*-axes in the plane (0001)	 Trigonal and hexagonal
Cubic 23, *m*3; 432, $\bar{4}$3*m*, *m*3*m*	Diads or tetrads (rotation and/or inversion) along ⟨100⟩ axes	Triads (rotation and/or inversion) along ⟨111⟩ axes	Diads (rotation and/or inversion) along ⟨110⟩ axes	 Cubic

(1) The monoclinic symmetries are a diad rotation axis and/or a mirror plane normal to that axis. The latter is equivalent to a diad inversion axis along the normal to the plane.

(2) See Preface to Volume I. The 2nd setting is usual for crystallographic work.

(3) Both on hexagonal axes. If referred to rhombohedral axes, the unique axis is [111] and the diads (rotation and/or inversion) are along the three ⟨$1\bar{1}0$⟩ and the three ⟨$11\bar{2}$⟩ directions, respectively.

6

14 XARXES DE BRAVAIS
XARXES TRIDIMENSIONALS

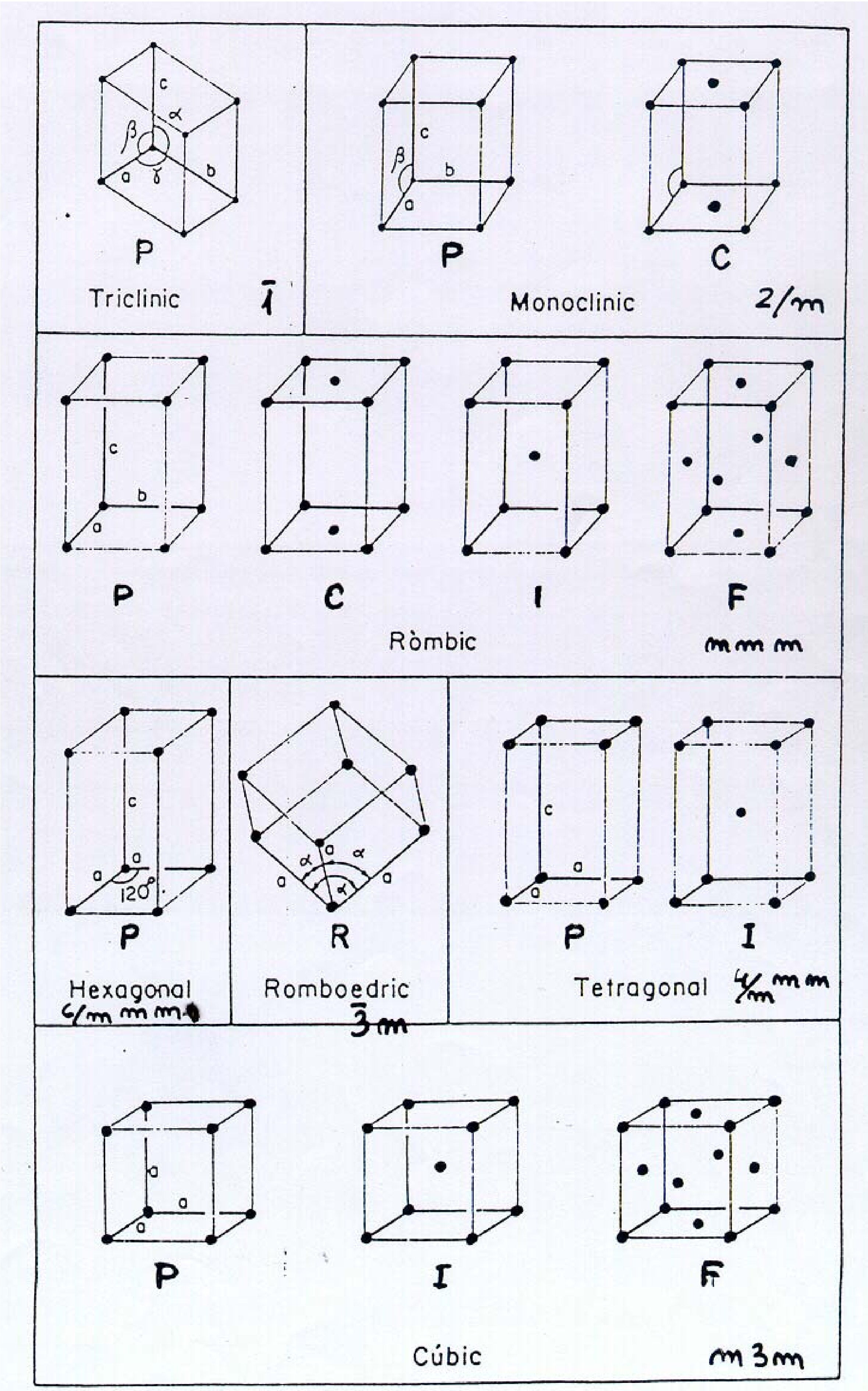
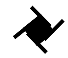
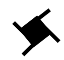
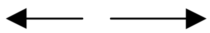
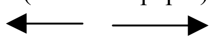


TABLE 4.1.6. **Symbols of Symmetry Planes**

Symbol	Symmetry plane	Graphical symbol: Normal to plane of projection	Graphical symbol: Parallel to plane of projection	Nature of glide translation
m	Reflection plane (mirror)			None (NOTE. If the plane is at $z=\frac{1}{4}$ this is shown by printing $\frac{1}{4}$ beside the symbol.)
a, b	Axial glide plane			$a/2$ along [100] or $b/2$ along [010]; or along $\langle 100 \rangle$.
c	Axial glide plane		None	$c/2$ along z-axis; or $(a+b+c)/2$ along [111] on rhombohedral axes.
n	Diagonal glide plane (net)			$(a+b)/2$ or $(b+c)/2$ or $(c+a)/2$; or $(a+b+c)/2$ (tetragonal and cubic).
d	"Diamond" glide plane			$(a \pm b)/4$ or $(b \pm c)/4$ or $(c \pm a)/4$; or $(a \pm b \pm c)/4$ (tetragonal and cubic). See note below.

NOTE. In the "diamond" glide plane the glide translation is half of the resultant of the two possible axial glide translations. The arrows in the first diagram show the direction of the horizontal component of the translation when the z-component is positive. In the second diagram the arrow shows the actual direction of the glide translation; there is always another diamond-glide reflection plane parallel to the first with a height difference of $\frac{1}{4}$ and with the arrow pointing along the other diagonal of the cell face.

TABLE 4.1.7
Symbols of Symmetry Axes

Symbol	Symmetry axis	Graphical symbol	Nature of right-handed screw translation the axis	Symbol	Symmetry axis	Graphical symbol	Nature of right-handed screw translation the axis
1	Rotation monad	None	None	4	Rotation tetrad		None
I	Inversion monad	°	None	4_1	Screw tetrads		$c/4$
2	Rotation diad	 (normal to paper)	None	4_2			$2c/4$
				4_3			$3c/4$
		 (parallel to paper)		$\bar{4}$	Inversion tetrad		None
2_1	Screw diad	 (normal to paper)  (parallel to paper)	$c/2$	6	Rotation hexad		None
		Normal to paper		6_1	Screw hexads		$c/6$
				6_2			$2c/6$
3	Rotation triad		None	6_3			$3c/6$
				6_4			$4c/6$
3_1	Screw triads		$c/3$	6_5			$5c/6$
3_2			$2c/3$				
$\bar{3}$	Inversion triad		None	$\bar{6}$	Inversion hexad		None

EXTINCIONES SISTEMATICAS

Class of reflection	Condition for nonextinction (n = an integer)	Interpretation of extinction		Symbol of symmetry element
hkl	$h+k+l=2n$	Body-centered lattice		I
	$h+k=2n$	C-centered lattice		C
	$h+l=2n$	B-centered lattice		B
	$k+l=2n$	A-centered lattice		A
	$\left\{\begin{matrix} h+k=2n \\ h+l=2n \\ k+l=2n \end{matrix}\right\}$ ⇔ h, k, l, all even or all odd	Face-centered lattice		F
	$-h+k+l=3n$	Rhombohedral lattice indexed on hexagonal reference system		R
	$h+k+l=3n$	Hexagonal lattice indexed on rhombohedral reference system		H
$0kl$	$k=2n$	(100) glide plane, component	$\frac{b}{2}$	$b(P,B,C)$
	$l=2n$		$\frac{c}{2}$	$c(P,C,I)$
	$k+l=2n$		$\frac{b}{2}+\frac{c}{2}$	$n(P)$
	$k+l=4n$		$\frac{b}{4}+\frac{c}{4}$	$d(F)$
$h0l$	$h=2n$	(010) glide plane, component	$\frac{a}{2}$	$a(P,A,I)$
	$l=2n$		$\frac{c}{2}$	$c(P,A,C)$
	$h+l=2n$		$\frac{a}{2}+\frac{c}{2}$	$n(P)$
	$h+l=4n$		$\frac{a}{4}+\frac{c}{4}$	$d(F)$. (B)
$hk0$	$h=2n$	(001) glide plane, component	$\frac{a}{2}$	$a(P,B,I)$
	$k=2n$		$\frac{b}{2}$	$b(P,A,B)$
	$h+k=2n$		$\frac{a}{2}+\frac{b}{2}$	$n(P)$
	$h+k=4n$		$\frac{a}{4}+\frac{b}{4}$	$d(F)$

Class of reflection	Condition for nonextinction (n = an integer)	Interpretation of extinction	Symbol of symmetry element
hhl	$l = 2n$	(110) glide plane, component $\frac{c}{2}$	$c(P, C, F)$
	$h = 2n$	$\frac{a}{2} + \frac{b}{2}$	$b(C)$
	$h + l = 2n$	$\frac{a}{4} + \frac{b}{4} + \frac{c}{4}$	$n(C)$
	$2h + l = 4n$	$\frac{a}{2} + \frac{b}{4} + \frac{c}{4}$	$d(I)$
$h00$	$h = 2n$	[100] screw axis, component $\frac{a}{2}$	$2_1, 4_2$
	$h = 4n$	$\frac{a}{4}$	$4_1, 4_3$
$0k0$	$k = 2n$	[010] screw axis, component $\frac{b}{2}$	$2_1, 4_2$
	$k = 4n$	$\frac{b}{4}$	$4_1, 4_3$
$00l$	$l = 2n$	[001] screw axis, component $\frac{c}{2}$	$2_1, 4_2, 6_3$
	$l = 3n$	$\frac{c}{3}$	$3_1, 3_2, 6_2, 6_4$
	$l = 4n$	$\frac{c}{4}$	$4_1, 4_3$
	$l = 6n$	$\frac{c}{6}$	$6_1, 6_5$
$hh0$	$h = 2n$	[110] screw axis, component $\frac{a}{2} + \frac{b}{2}$	2_1

† From M. J. Buerger, *X-ray crystallography* (John Wiley & Sons, Inc., New York, 1942).