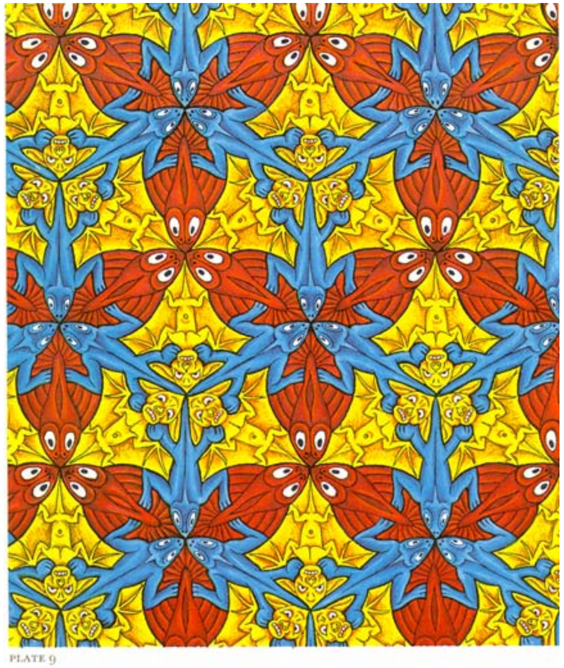
Chapter 7 Space Group



Reading Assignment:

1. W. B-Ott, Crystallography-chapter 9

Contents

Space Group

- 32 point groups- symmetry groups of many molecules
  and of all crystals so long as morphology
  is considered
- space group- symmetry of crystal lattices and
  crystal structures

14 Bravais lattice

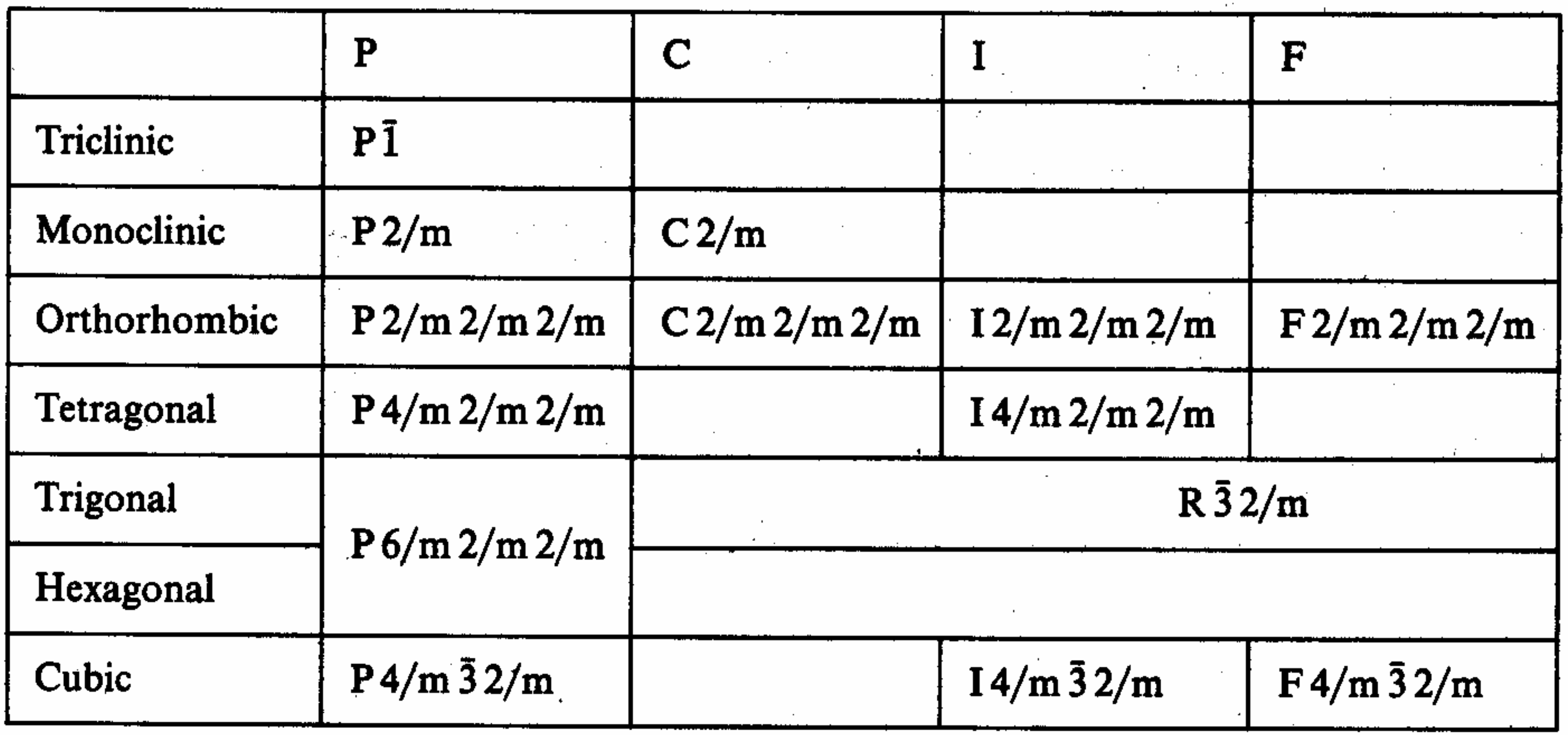
centered lattices- new symmetry operations

reflection + translation

rotation + translation

Space Lattice

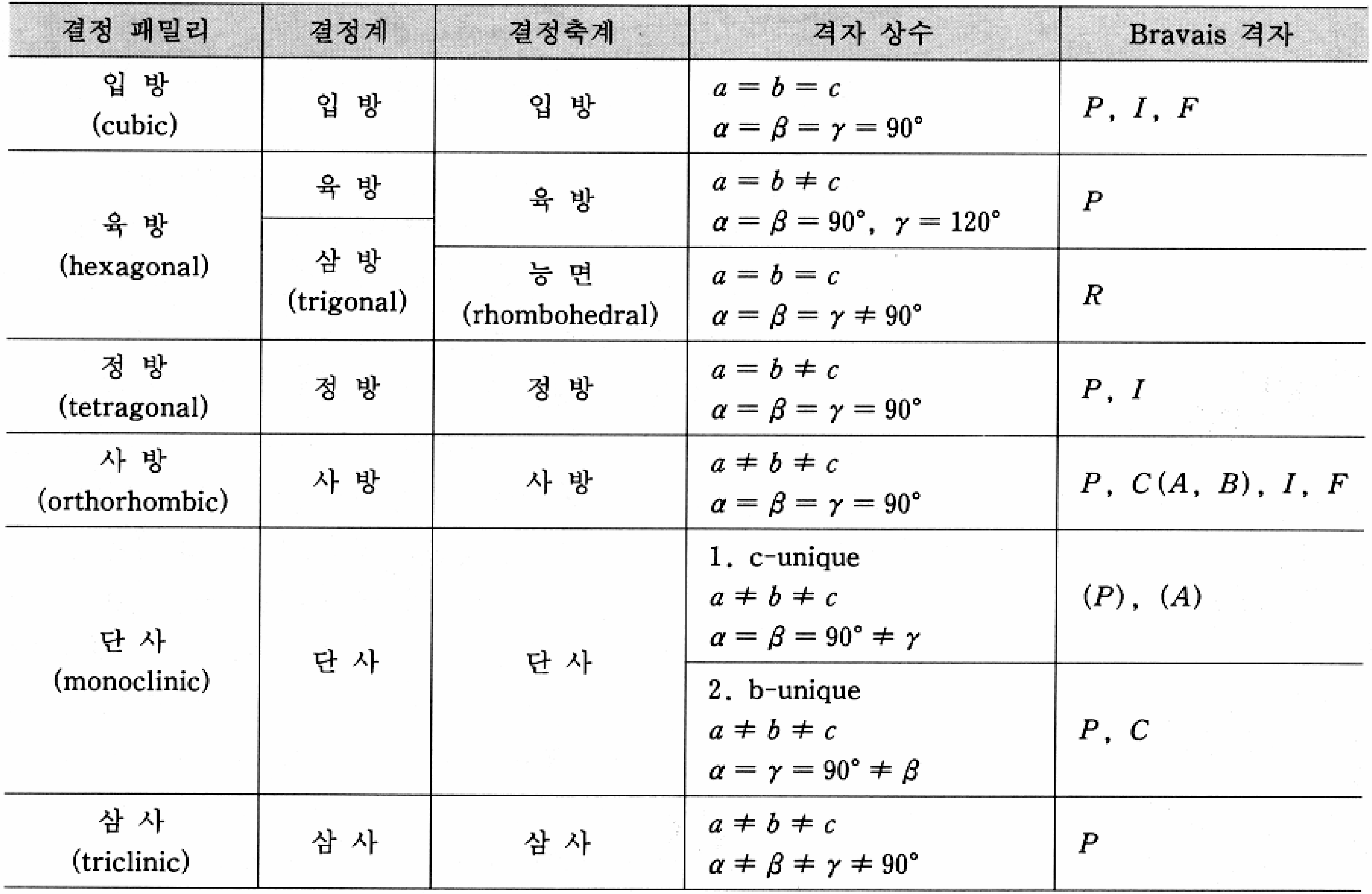
- 14 Bravais lattice



	P	C	I	F
Triclinic	P$\bar{1}$			
Monoclinic	P 2/m	C 2/m		
Orthorhombic	P 2/m 2/m 2/m	C 2/m 2/m 2/m	I 2/m 2/m 2/m	F 2/m 2/m 2/m
Tetragonal	P 4/m 2/m 2/m		I 4/m 2/m 2/m	
Trigonal	P 6/m 2/m 2/m	R $\bar{3}$ 2/m		
Hexagonal				
Cubic	P 4/m $\bar{3}$ 2/m		I 4/m $\bar{3}$ 2/m	F 4/m $\bar{3}$ 2/m

The 14 Bravais lattice represent the 14 and only way in which it is possible to fill space by a three-dimensional periodic array of points.

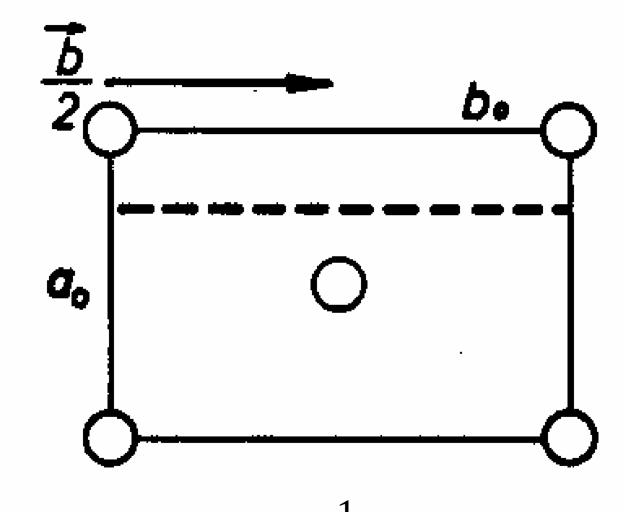
표 1.1 결정계, 결정축계, Bravais 격자



결정 패밀리	결정계	결정축계	격자 상수	Bravais 격자
입 방 (cubic)	입 방	입 방	$a = b = c$ $\alpha = \beta = \gamma = 90°$	P, I, F
육 방 (hexagonal)	육 방	육 방	$a = b \neq c$ $\alpha = \beta = 90°$, $\gamma = 120°$	P
	삼 방 (trigonal)	능 면 (rhombohedral)	$a = b = c$ $\alpha = \beta = \gamma \neq 90°$	R
정 방 (tetragonal)	정 방	정 방	$a = b \neq c$ $\alpha = \beta = \gamma = 90°$	P, I
사 방 (orthorhombic)	사 방	사 방	$a \neq b \neq c$ $\alpha = \beta = \gamma = 90°$	P, $C(A, B)$, I, F
단 사 (monoclinic)	단 사	단 사	1. c-unique $a \neq b \neq c$ $\alpha = \beta = 90° \neq \gamma$	(P), (A)
			2. b-unique $a \neq b \neq c$ $\alpha = \gamma = 90° \neq \beta$	P, C
삼 사 (triclinic)	삼 사	삼 사	$a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90°$	P

New Symmetry Operations

i) orthorhombic C-lattice



reflection at $\frac{1}{4}, y, z$

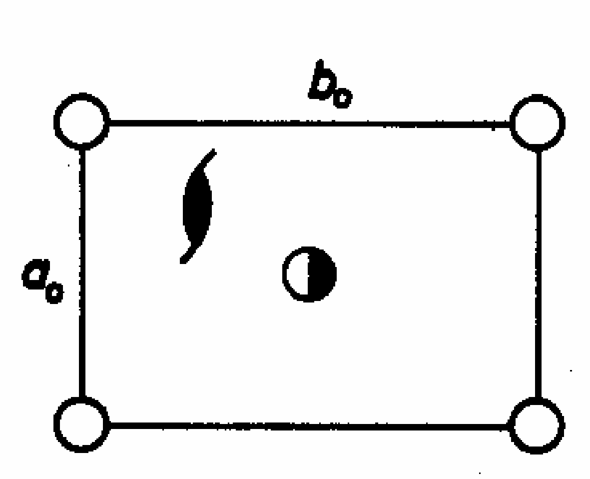
\+ translation $\frac{\vec{b}}{2}$

$0,0,0 \;\rightarrow\; \frac{1}{2},\frac{1}{2},0$

glide reflection

glide plane (b-glide)

ii) orthorhombic I-lattice



rotation about at $\frac{1}{4}, \frac{1}{4}, z$

\+ translation $\frac{\vec{c}}{2}$

$0,0,0 \;\rightarrow\; \frac{1}{2},\frac{1}{2},\frac{1}{2}$

screw rotation

screw axis (2_1-screw)

Compound Symmetry Operation

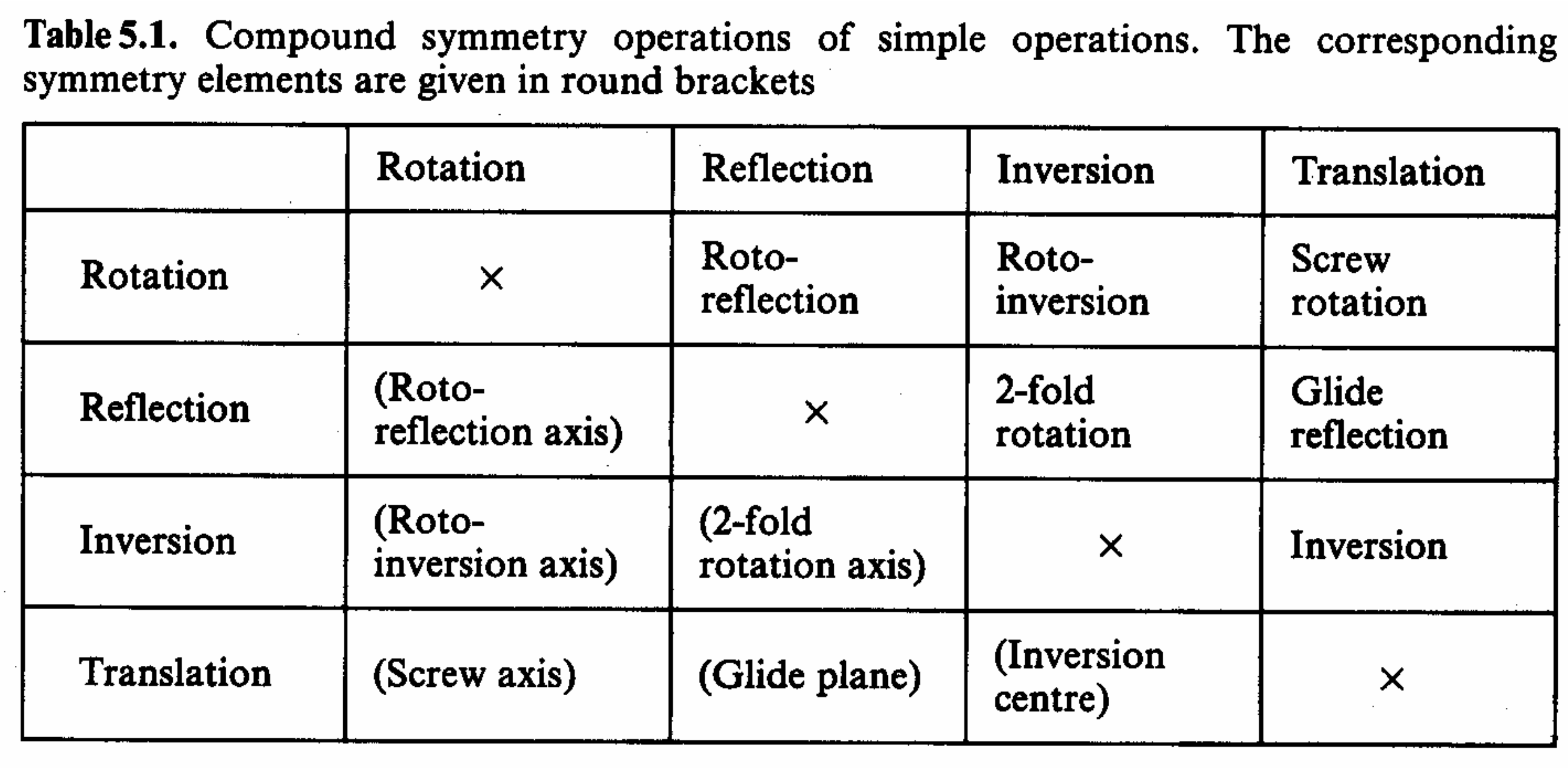


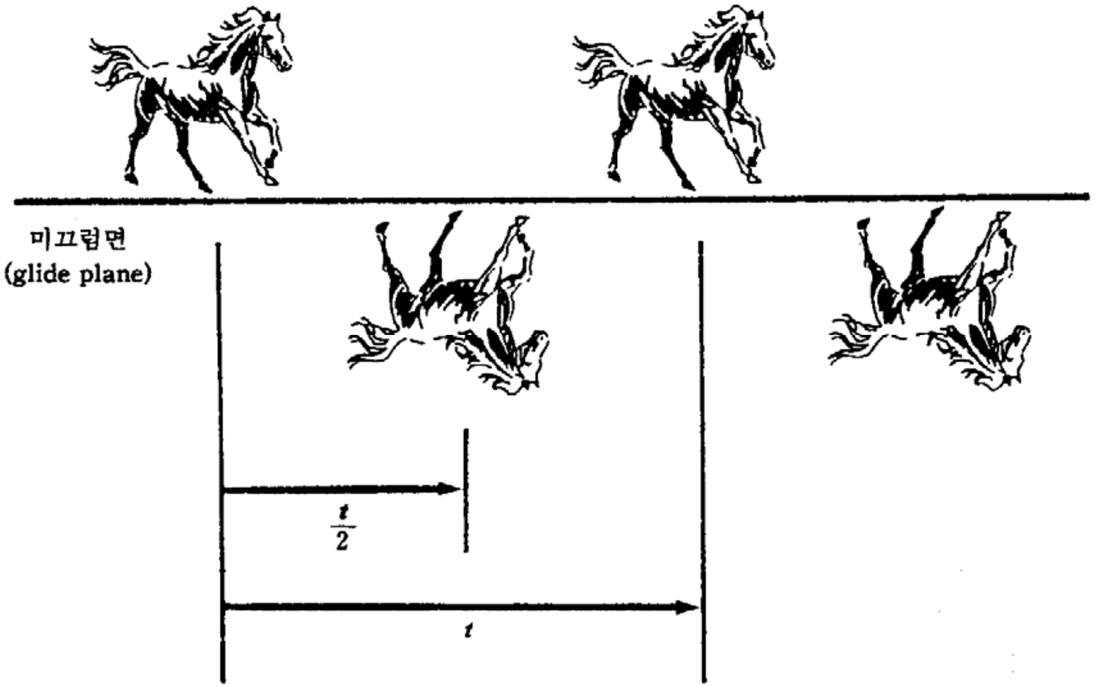
Table 5.1. Compound symmetry operations of simple operations. The corresponding symmetry elements are given in round brackets

	Rotation	Reflection	Inversion	Translation
Rotation	×	Roto-reflection	Roto-inversion	Screw rotation
Reflection	(Roto-reflection axis)	×	2-fold rotation	Glide reflection
Inversion	(Roto-inversion axis)	(2-fold rotation axis)	×	Inversion
Translation	(Screw axis)	(Glide plane)	(Inversion centre)	×

Glide Plane

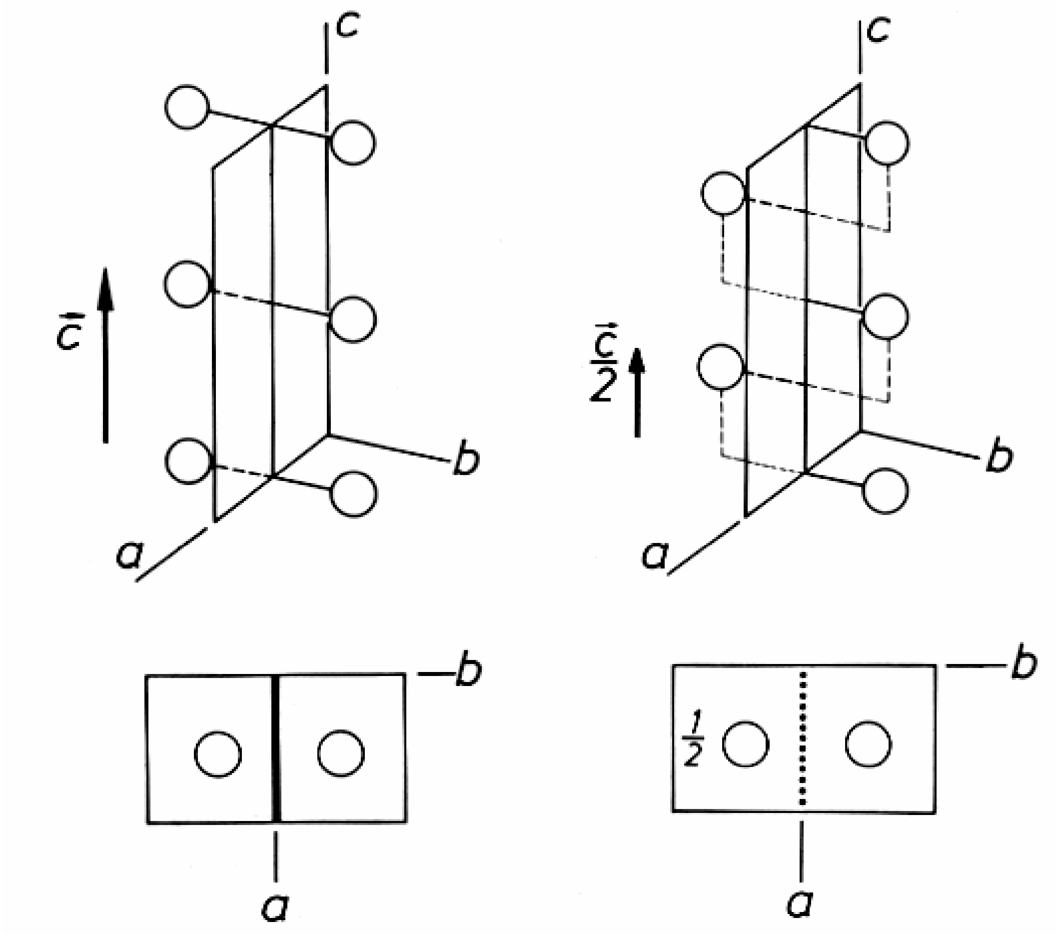
i) reflection

ii) translation by the vector $\vec{g}$ parallel to the plane of glide reflection where $|\vec{g}|$ is called glide component



$\vec{g}$ is one half of a lattice translation parallel to the glide plane $|\vec{g}| = \frac{1}{2}|\vec{t}|$

Mirror Plane vs. Glide Plane



- glide plane can occur in an orientation that is possible for a mirror plane

Glide Plane

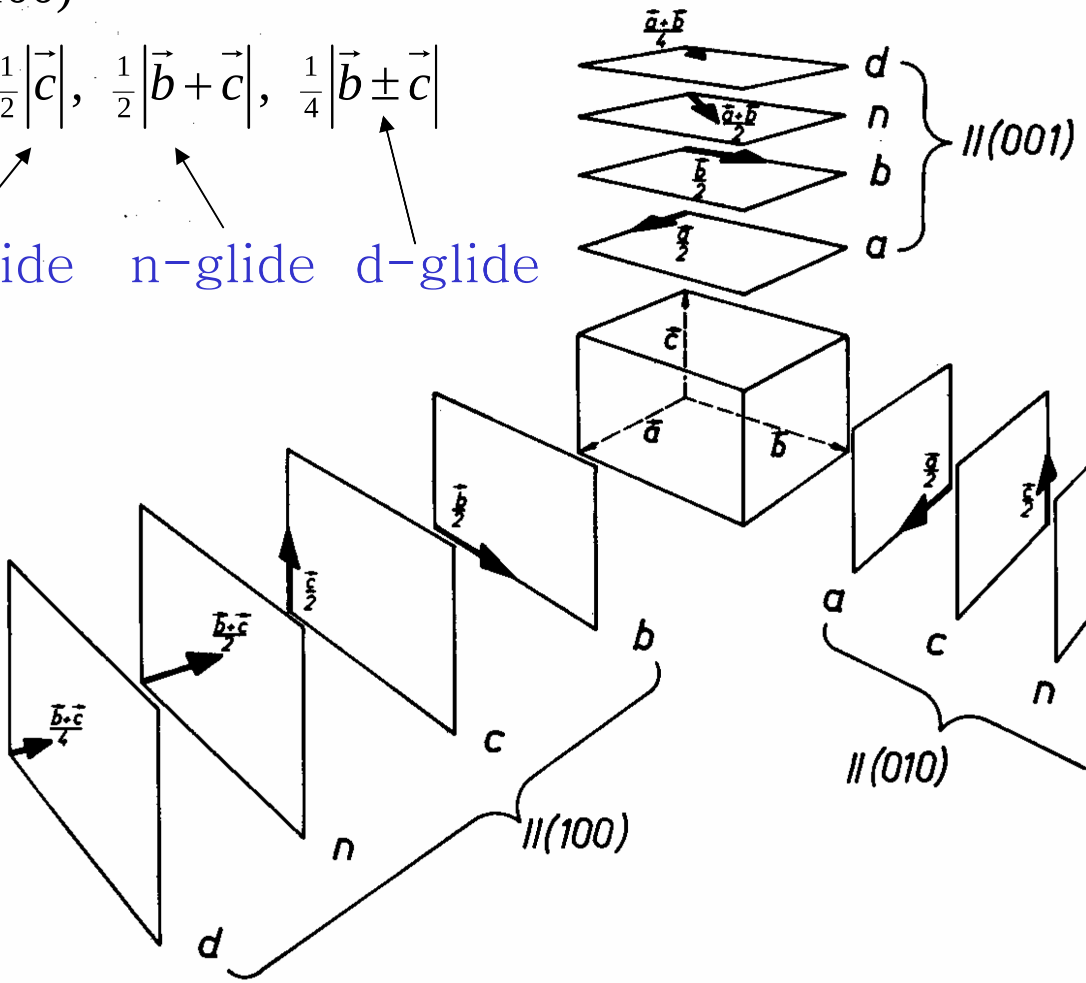
- orthorhombic $P\frac{m}{2}\frac{m}{2}\frac{m}{2}$

(100), (010), (001) possible

glide plane parallel to (100)

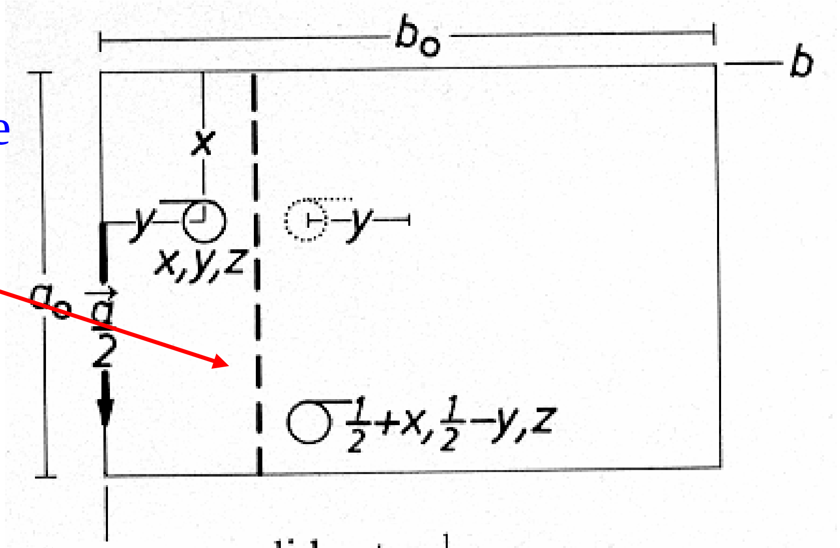
glide component $\frac{1}{2}|\vec{b}|,\ \frac{1}{2}|\vec{c}|,\ \frac{1}{2}|\vec{b}+\vec{c}|,\ \frac{1}{4}|\vec{b}\pm\vec{c}|$

b-glide c-glide n-glide d-glide



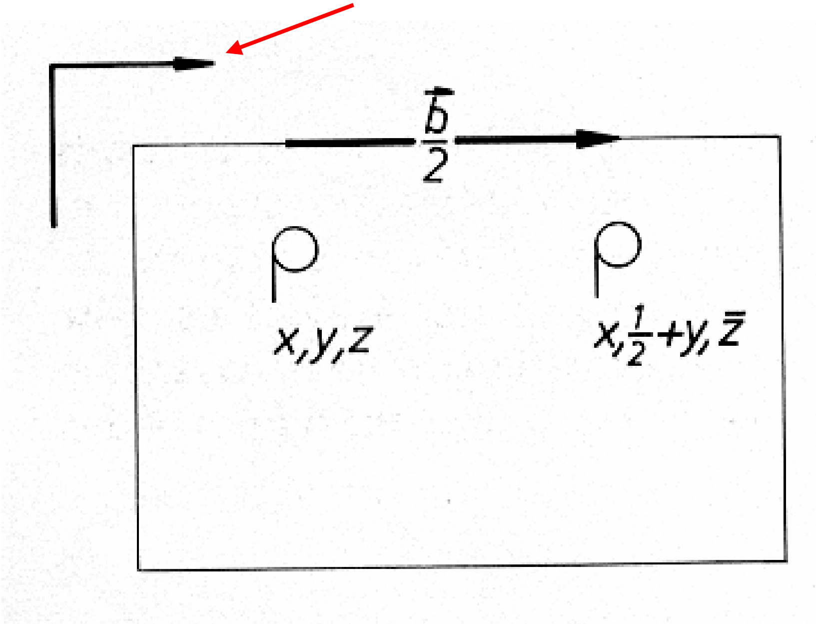
Glide Plane

$\frac{1}{2}$ along the line parallel to the projection plane

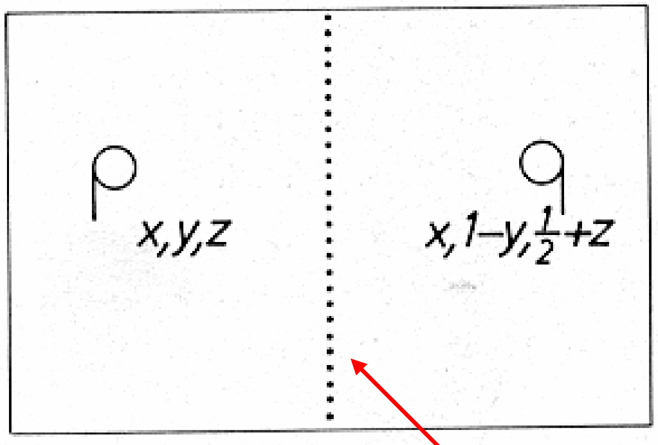


a a-glide at x, $\frac{1}{4}$ z

$\frac{1}{2}$ in the direction of the arrow



b b-glide at x, y, 0



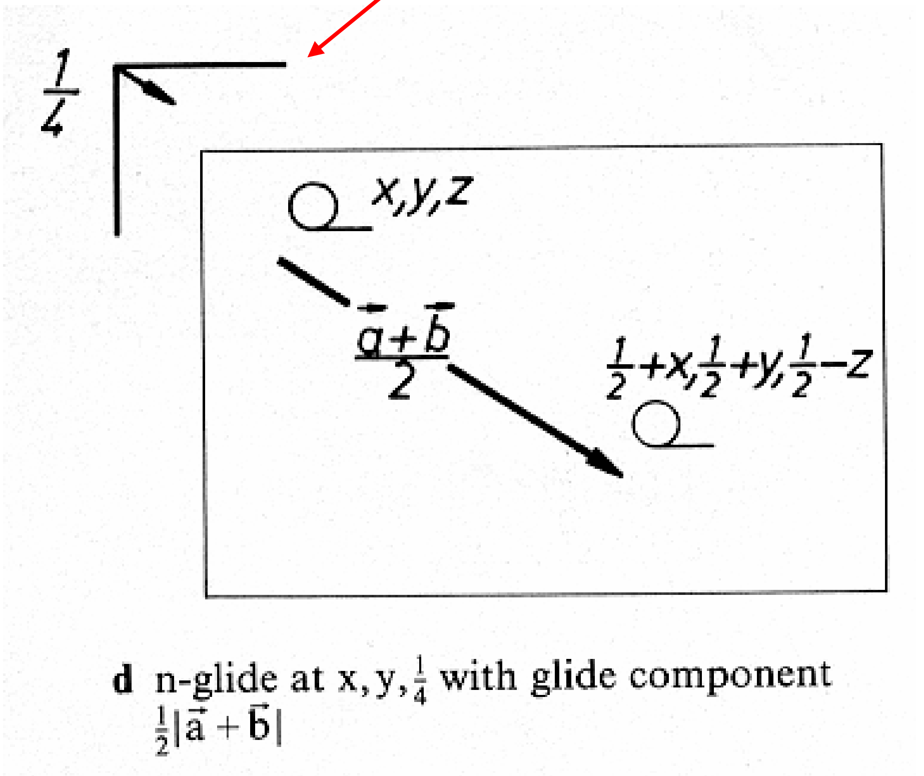
c c-glide at x, $\frac{1}{2}$, z

$\frac{1}{2}$ normal to the projection plane

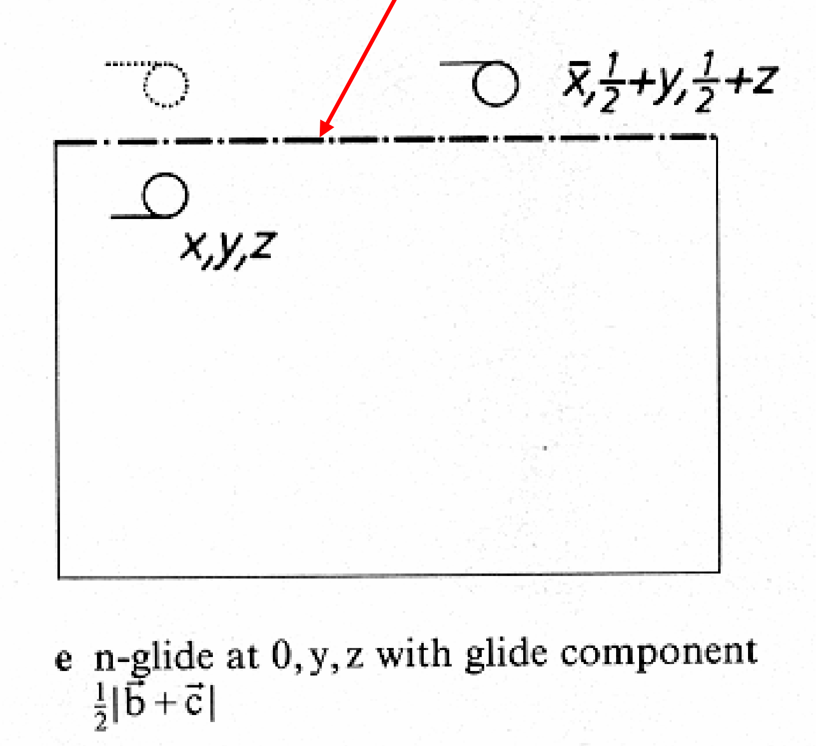
Glide Plane

$\frac{1}{2}$ in the direction of the arrow

$\frac{1}{2}$ along the line parallel to the projection plane combined with $\frac{1}{2}$ normal to the projection plane



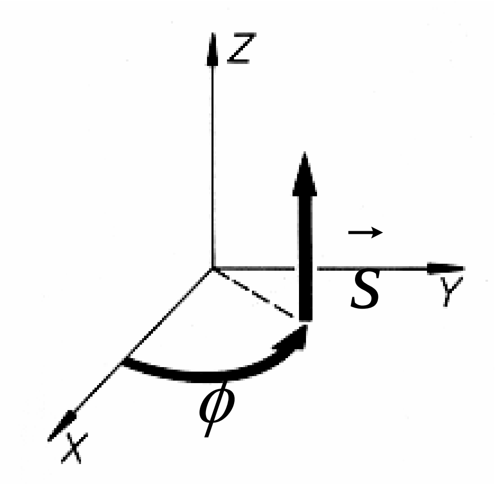
d n-glide at x, y, $\frac{1}{4}$ with glide component $\frac{1}{2}|\vec{a}+\vec{b}|$

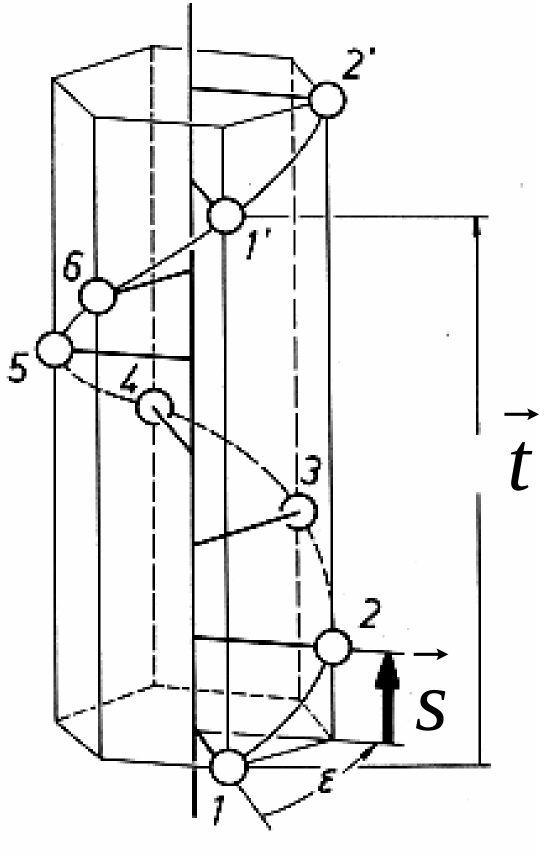


e n-glide at 0, y, z with glide component $\frac{1}{2}|\vec{b}+\vec{c}|$

Screw Axis

- rotation $\phi = \frac{2\pi}{X}$ $(X = 1,2,3,4,6)$
- translation by a vector $\vec{s}$ parallel to the axis where $\left|\vec{s}\right|$ is called the screw component

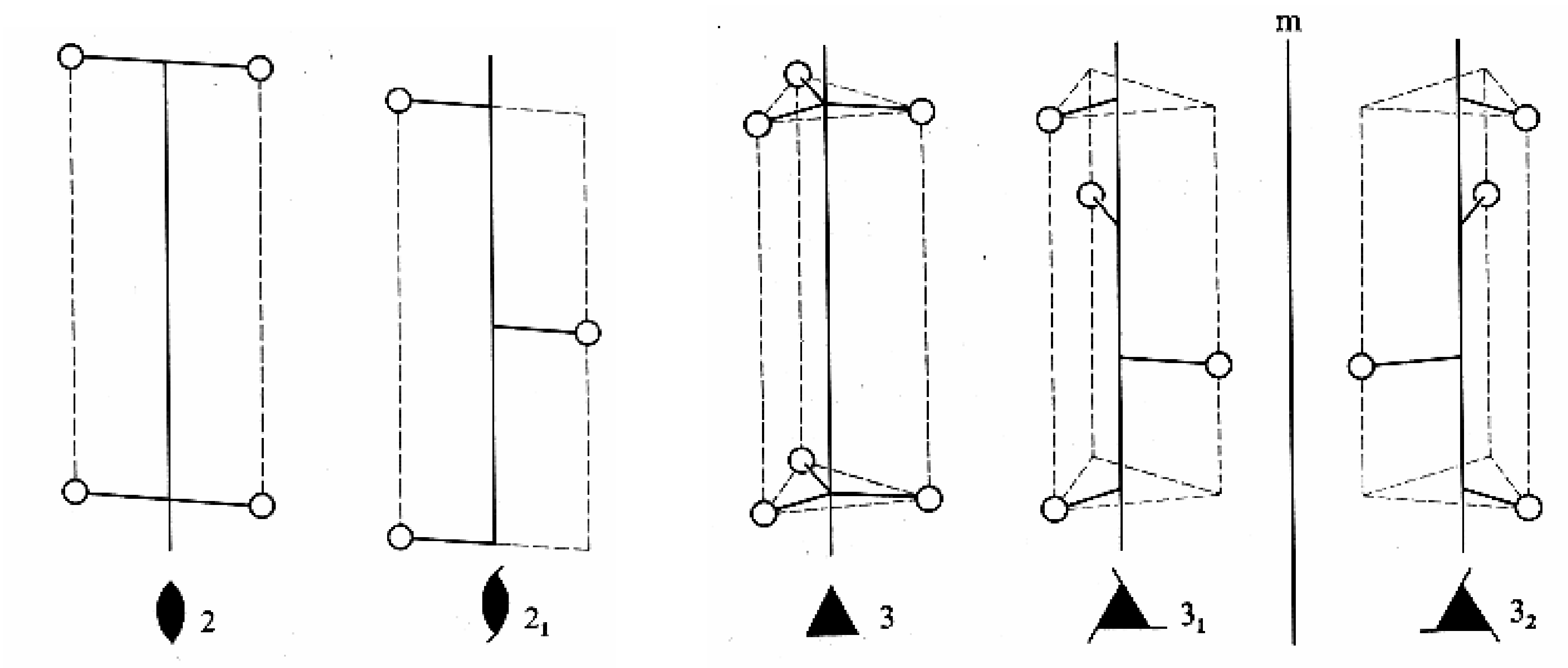




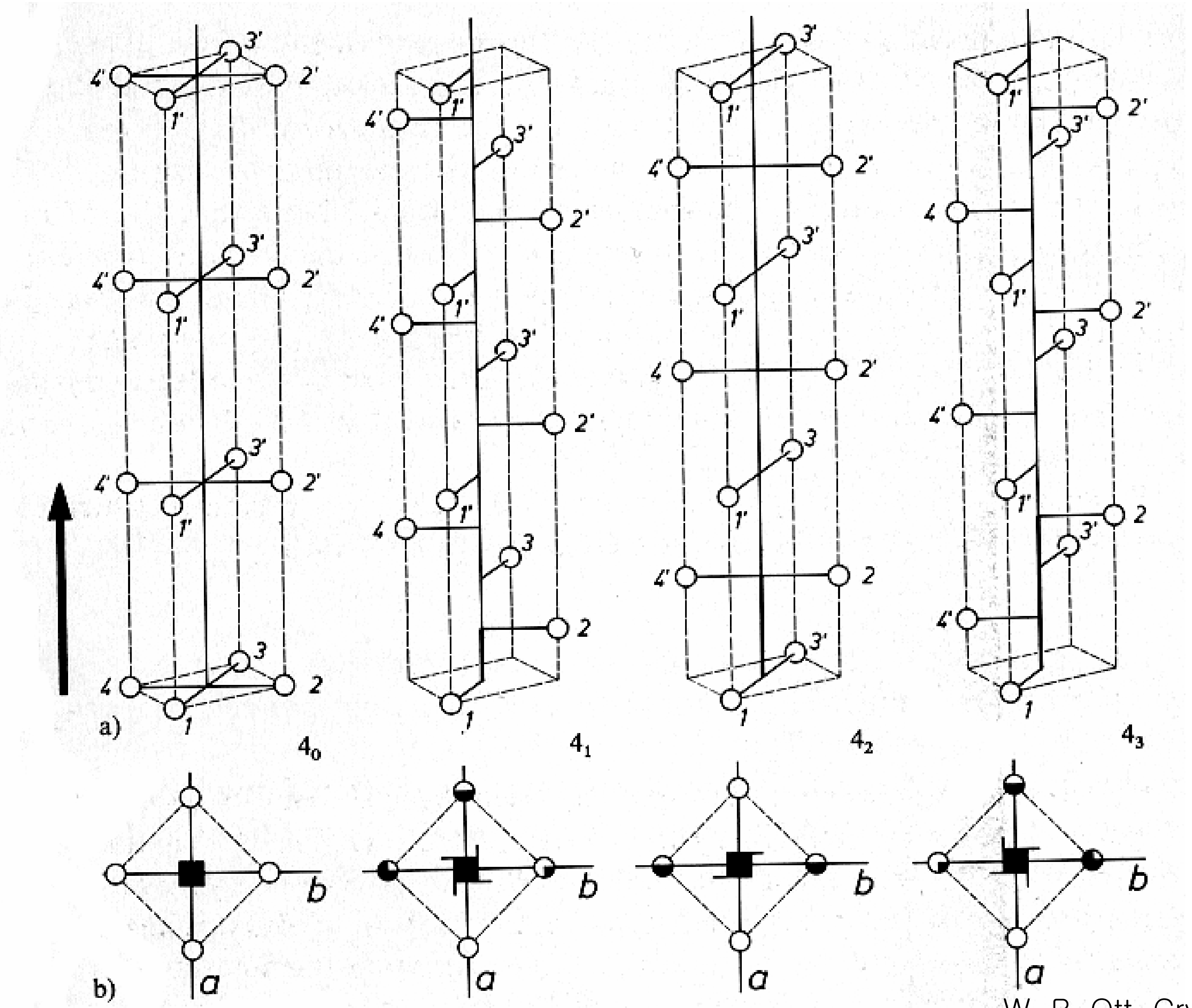
$$\left|\vec{s}\right| = \frac{p}{X}\left|\vec{t}\right| \quad \text{p=0,1,2...,X-1}$$

$$X_p = X_0, X_1, ...X_{X-1}$$

Screw Axis

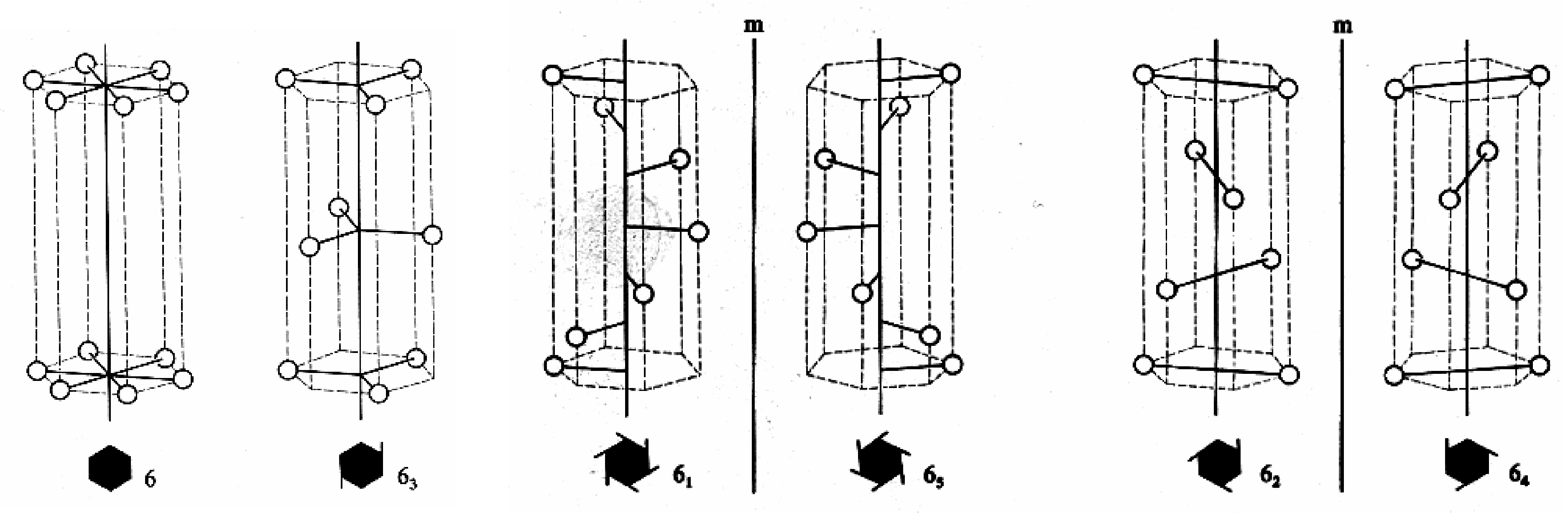


Screw Axis



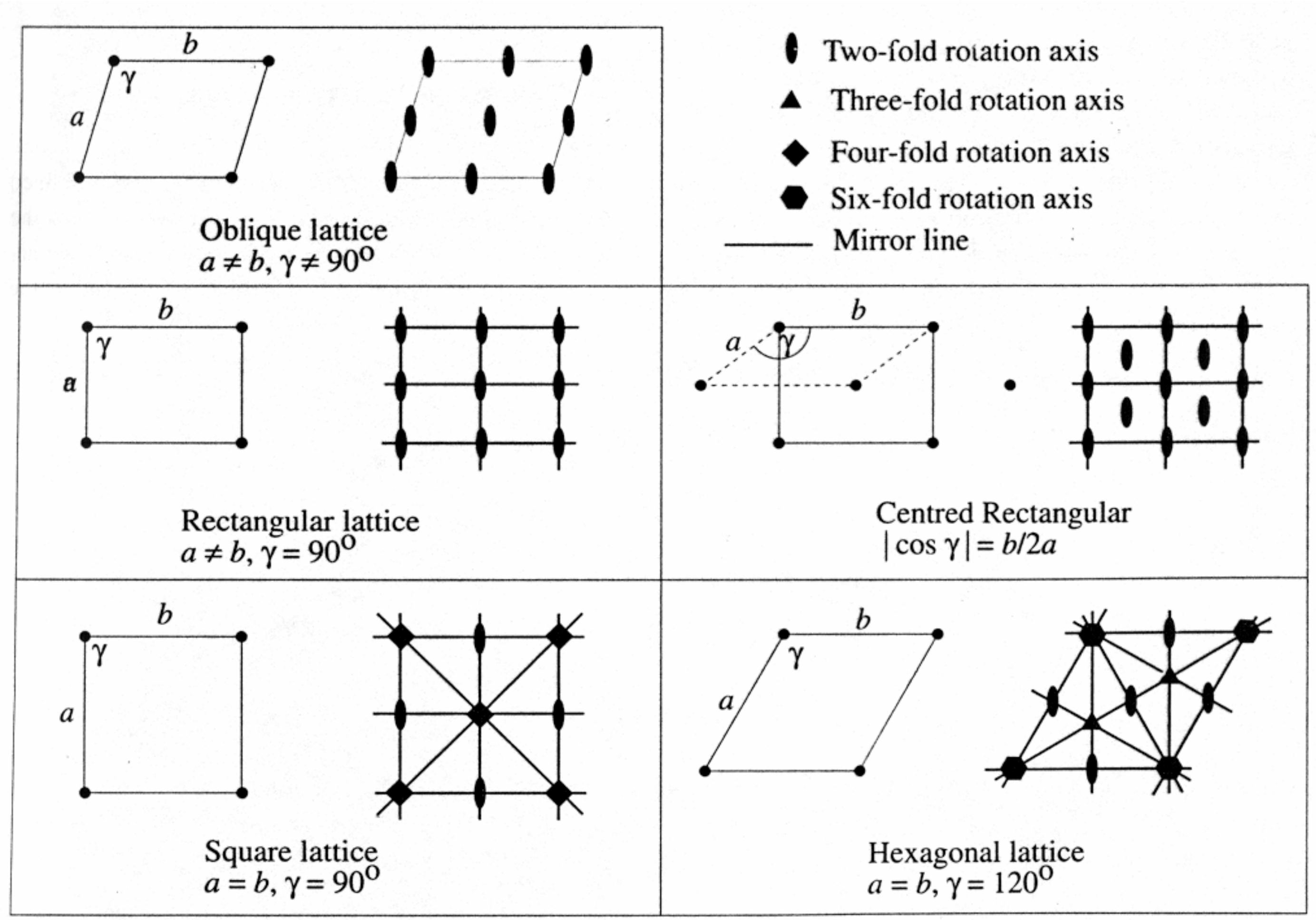
W. B-Ott, Crystallography

Screw Axis



17 Plane Groups

- 5 plane lattices + 10 plane point groups+ glide plane
- criterion: lattice itself must possess at least
  the symmetry of the motif



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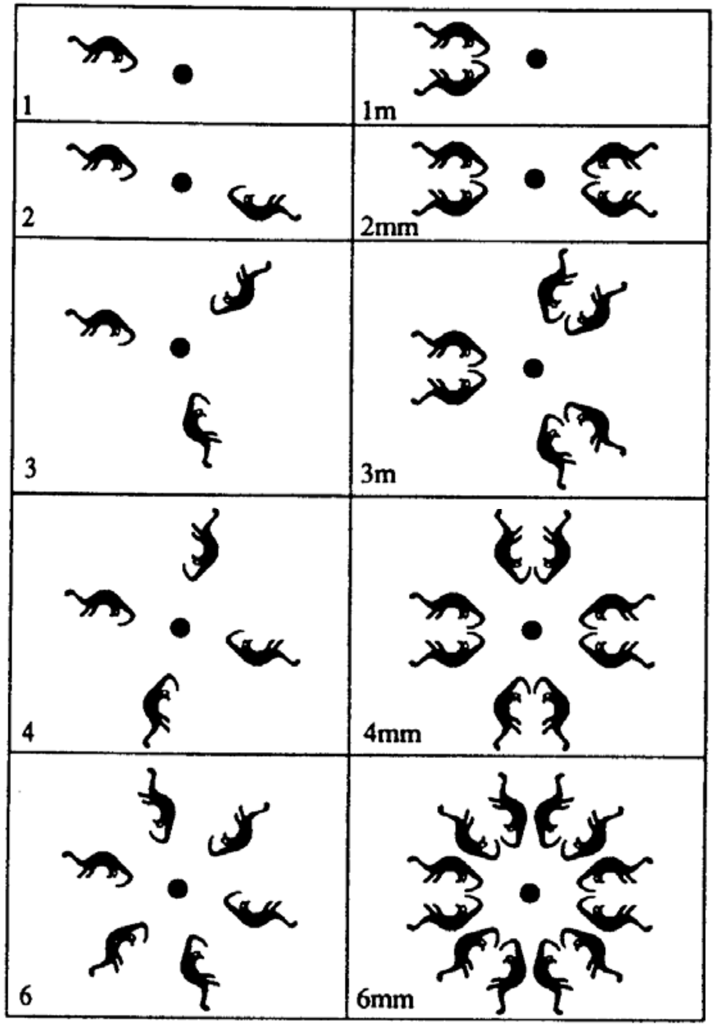
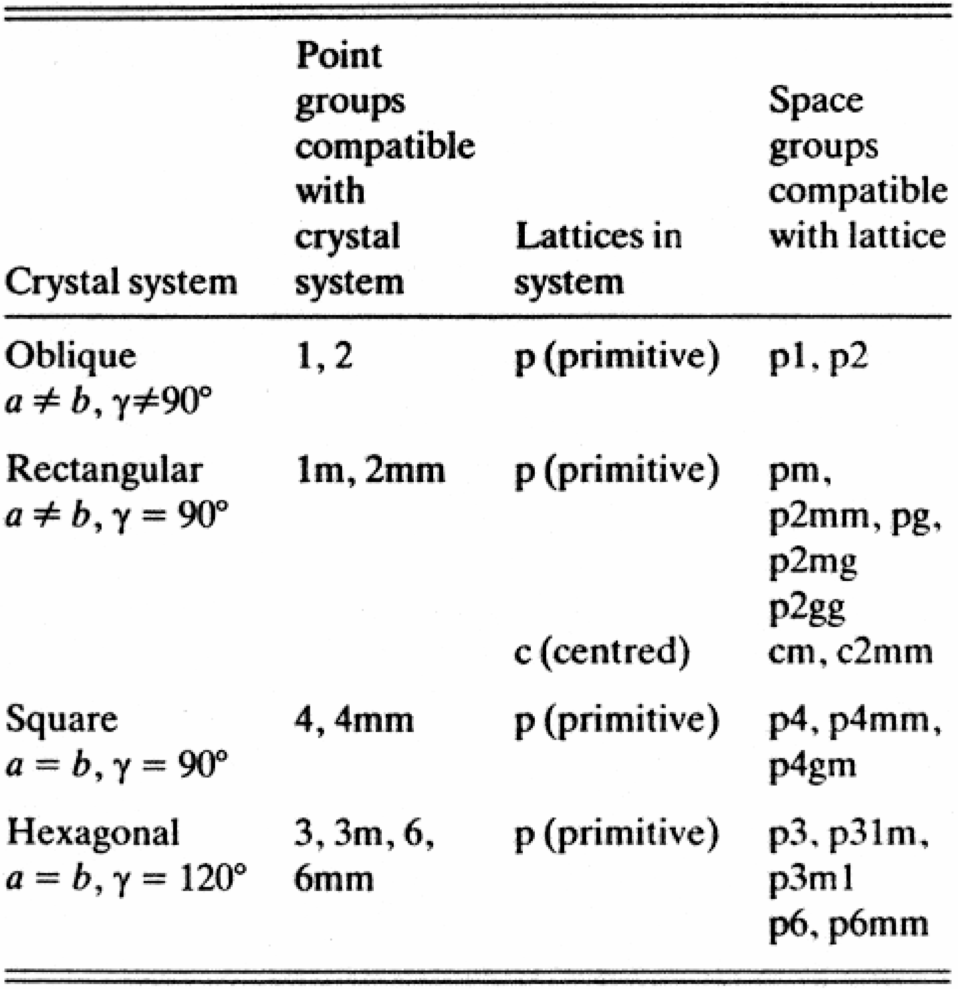
17 Plane Groups





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

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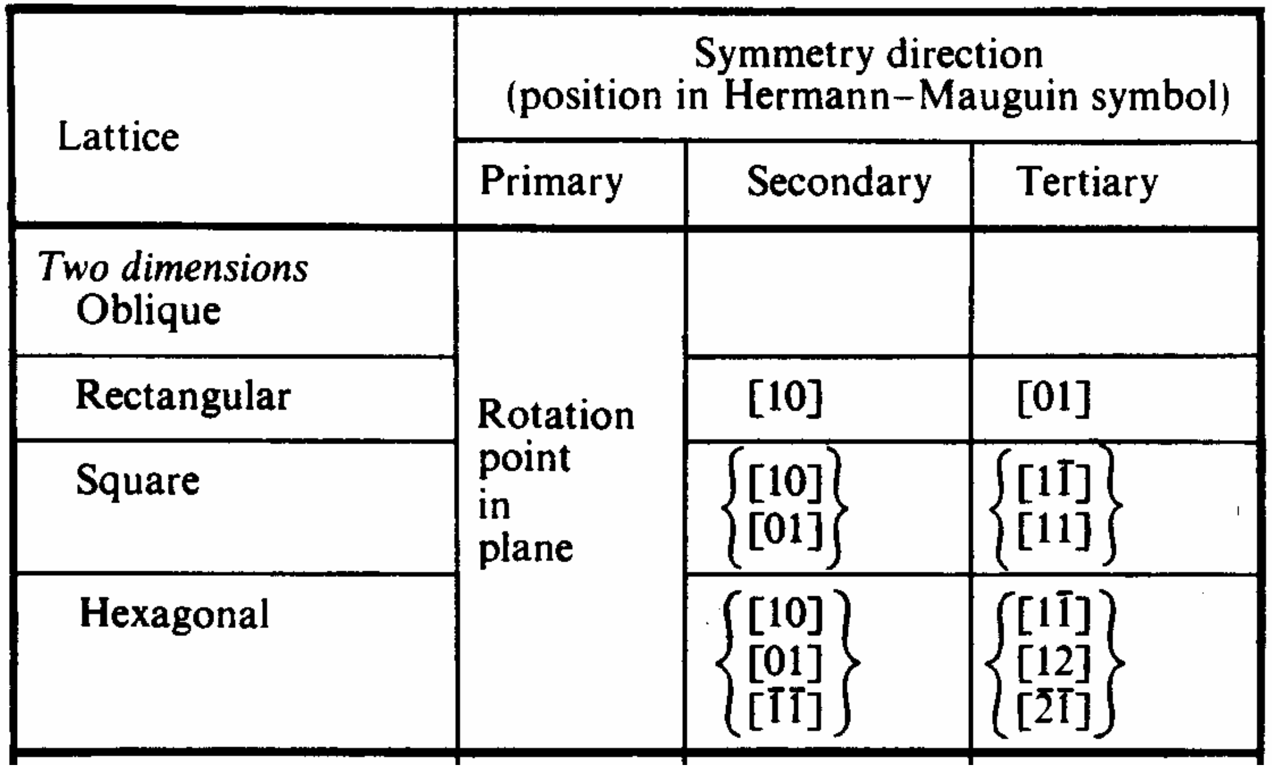
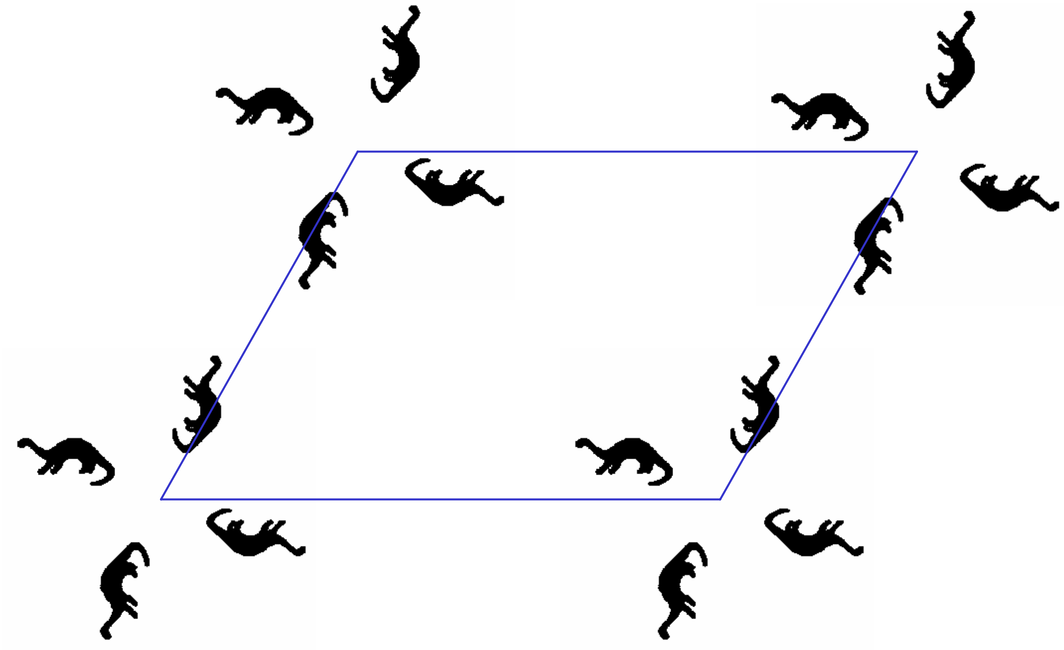
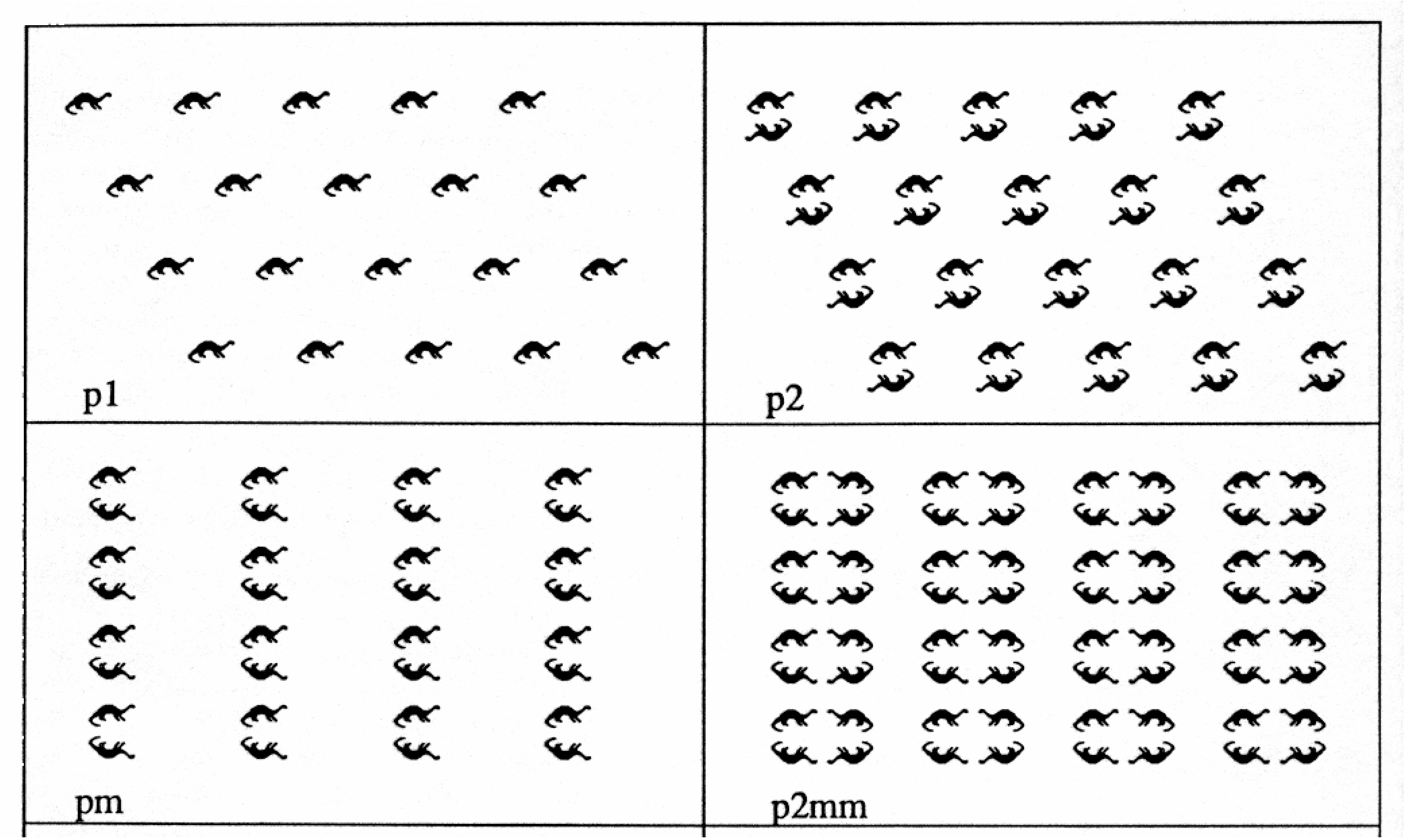


Lattice	Symmetry direction (position in Hermann–Mauguin symbol)		
	Primary	Secondary	Tertiary
Two dimensions Oblique	Rotation point in plane		
Rectangular		[10]	[01]
Square		$\left\{\begin{matrix}[10] \\ {[01]}\end{matrix}\right\}$	$\left\{\begin{matrix}[1\bar{1}] \\ {[11]}\end{matrix}\right\}$
Hexagonal		$\left\{\begin{matrix}[10] \\ {[01]} \\ {[\bar{1}\bar{1}]}\end{matrix}\right\}$	$\left\{\begin{matrix}[1\bar{1}] \\ {[12]} \\ {[\bar{2}\bar{1}]}\end{matrix}\right\}$



17 Plane Groups



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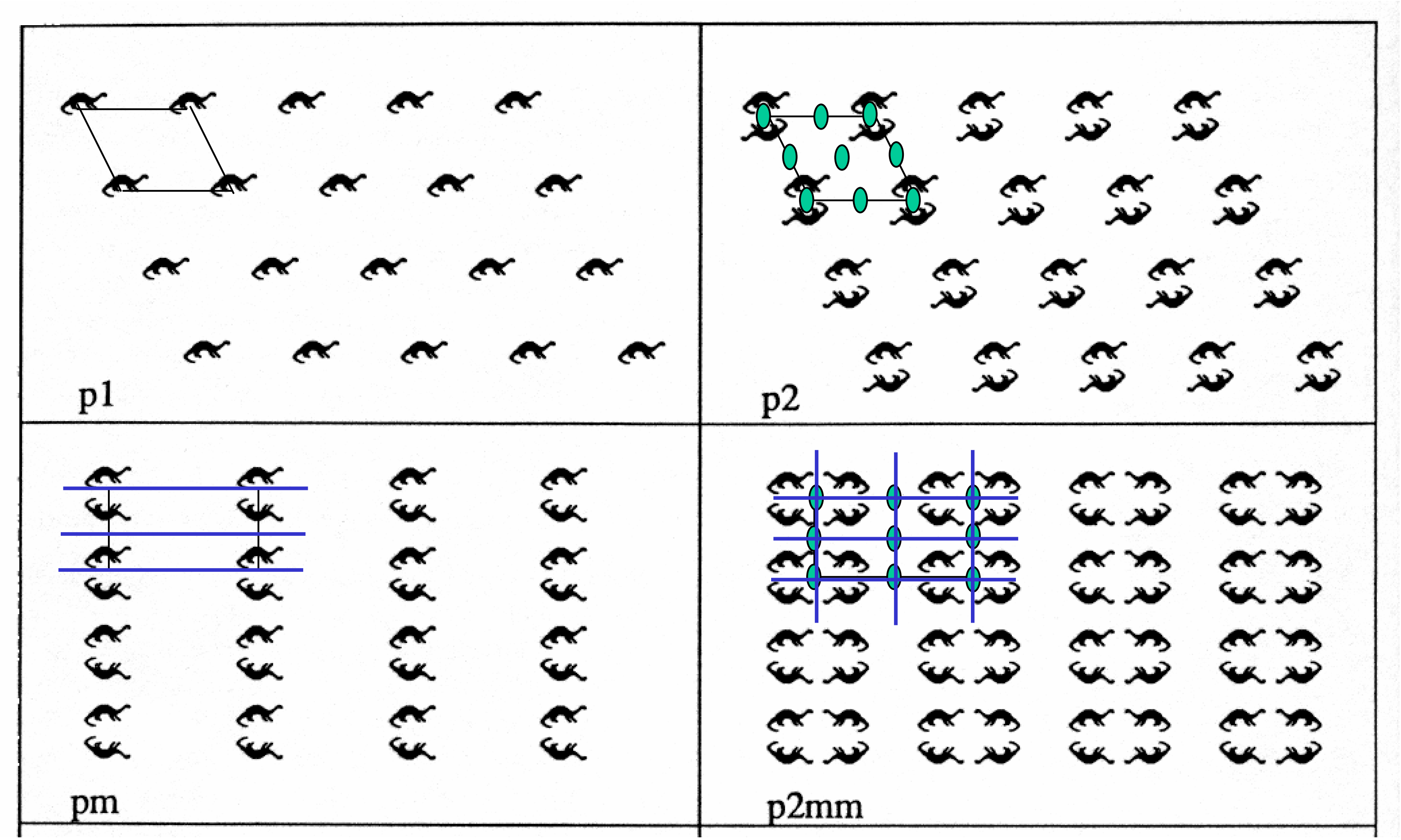

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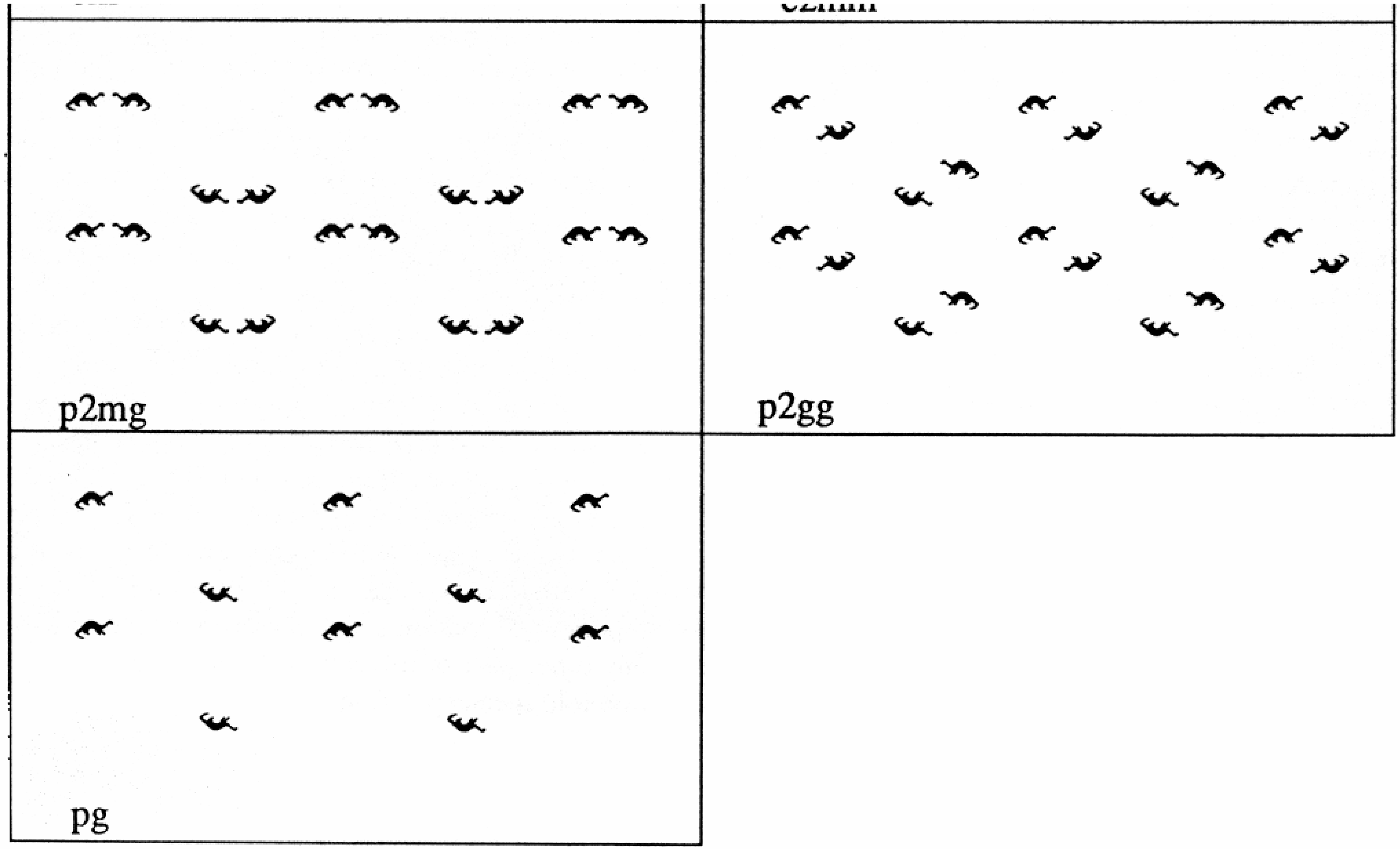

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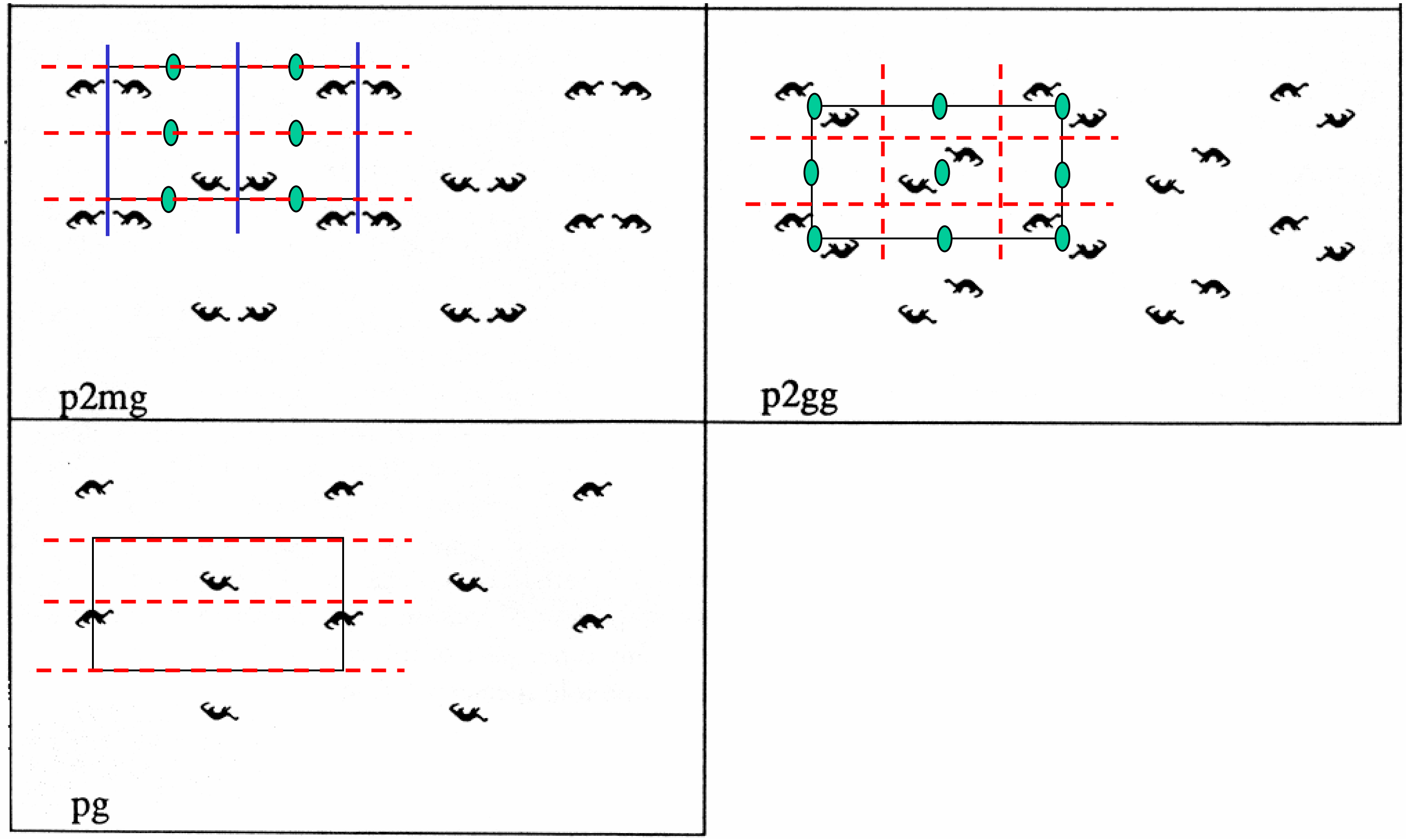

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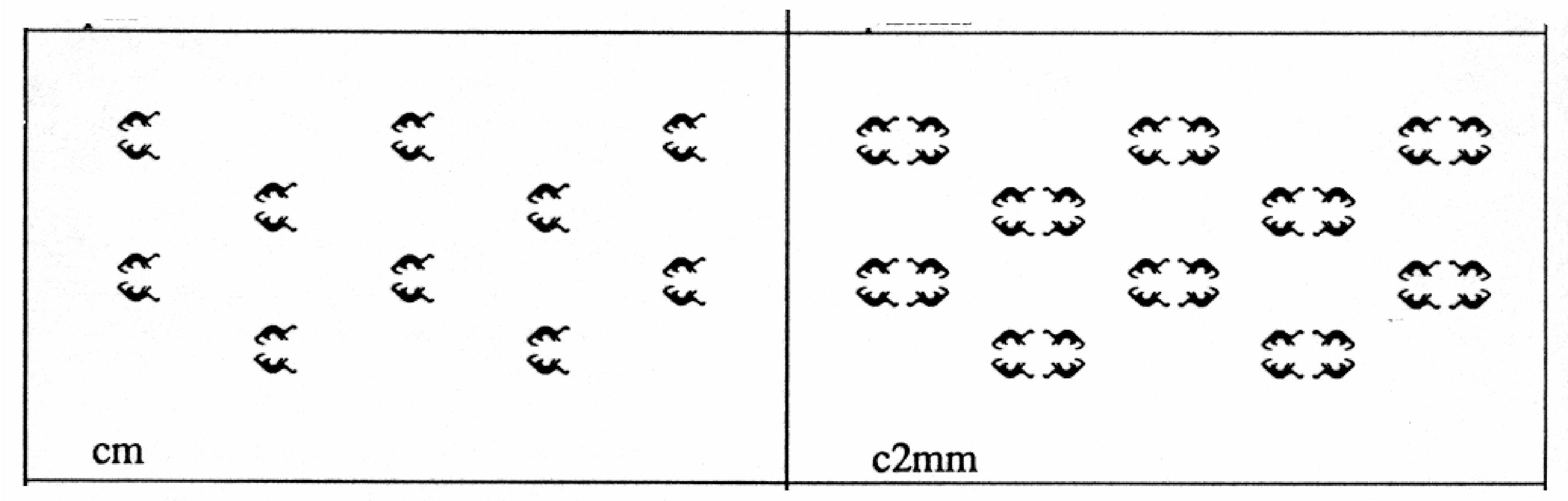

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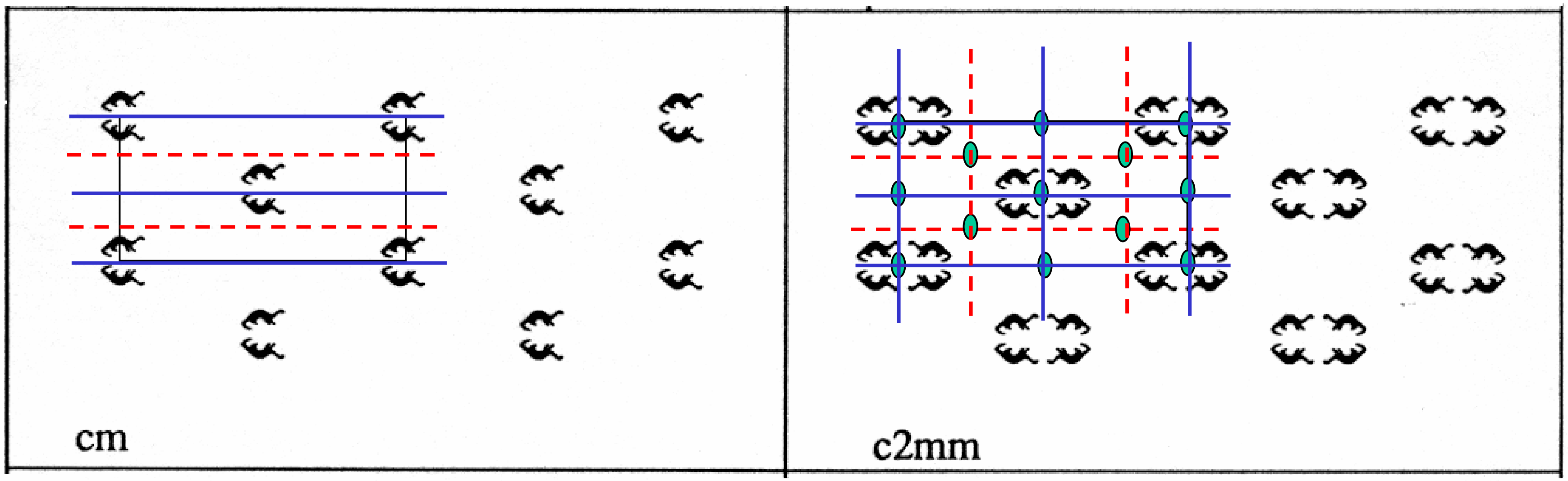

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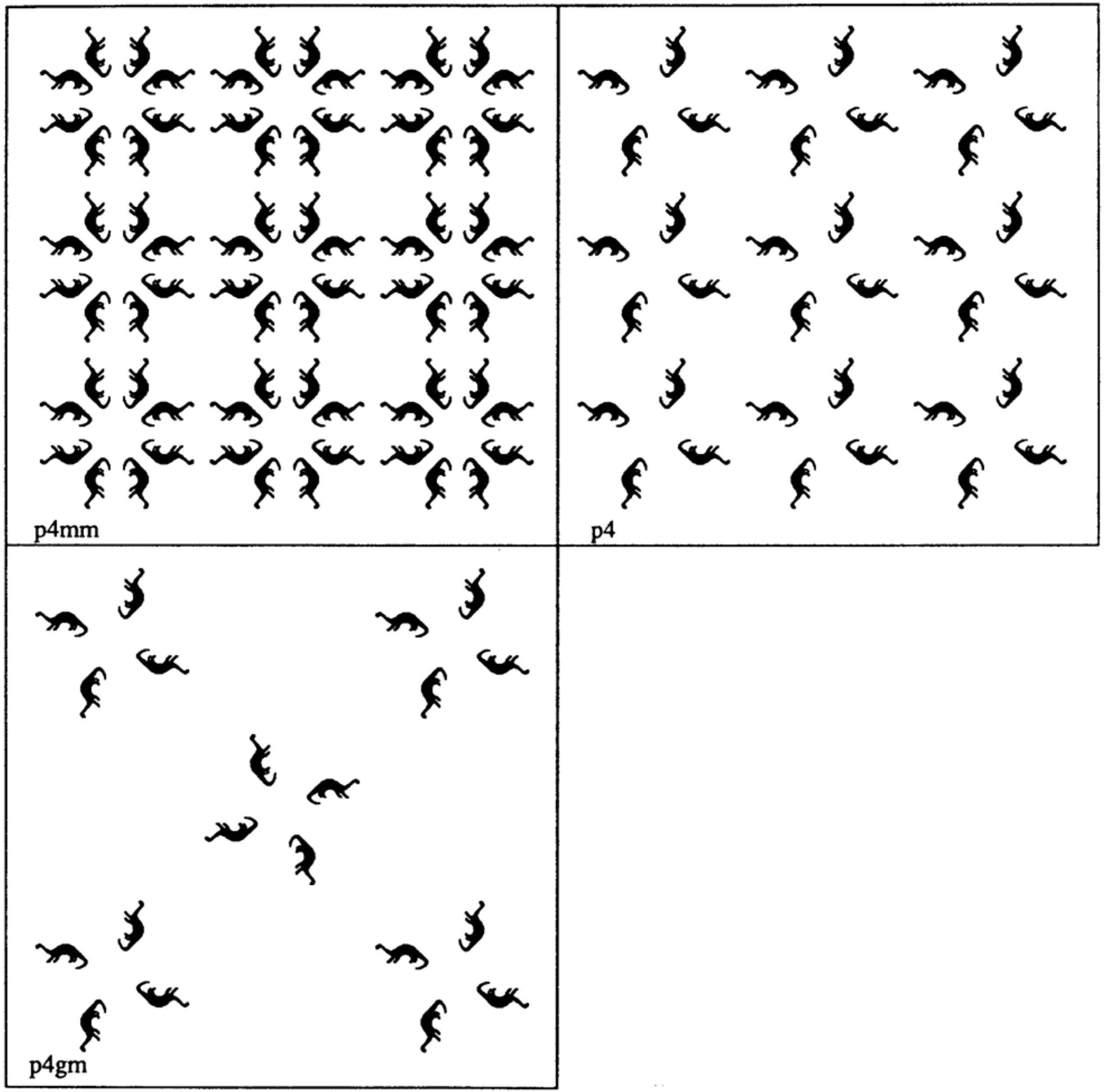

p4mm

p4

p4gm

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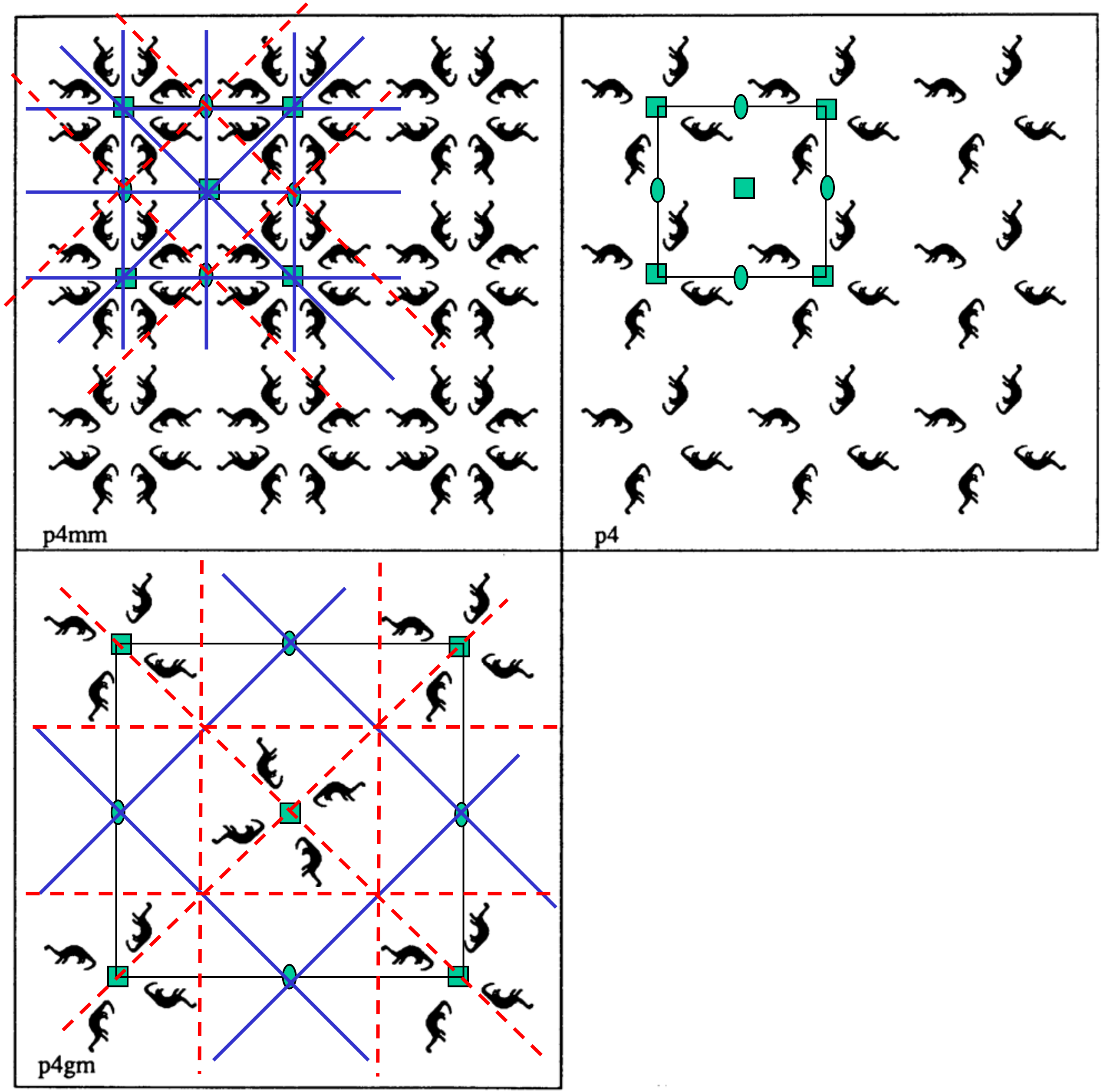
17 Plane Groups



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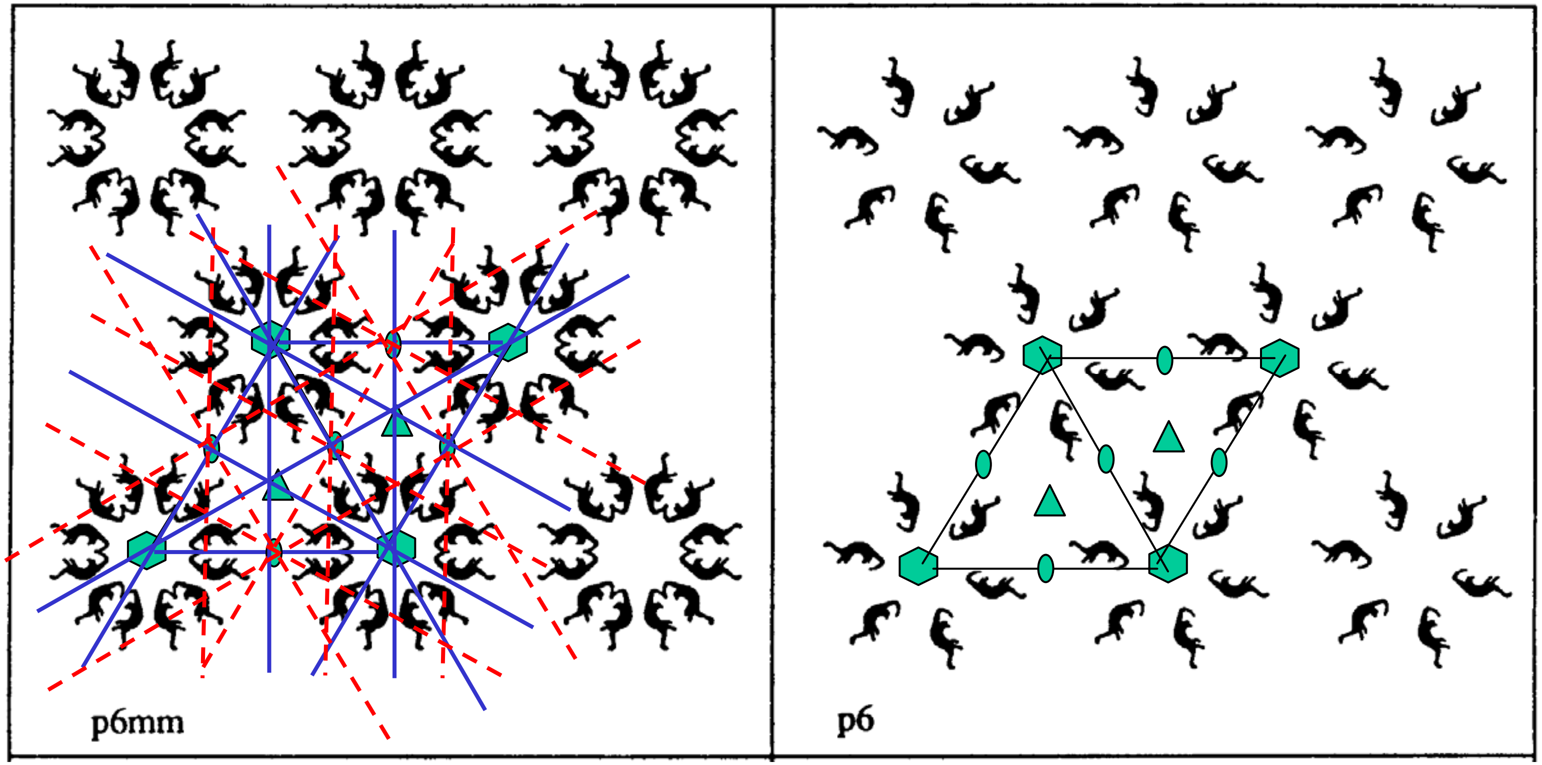

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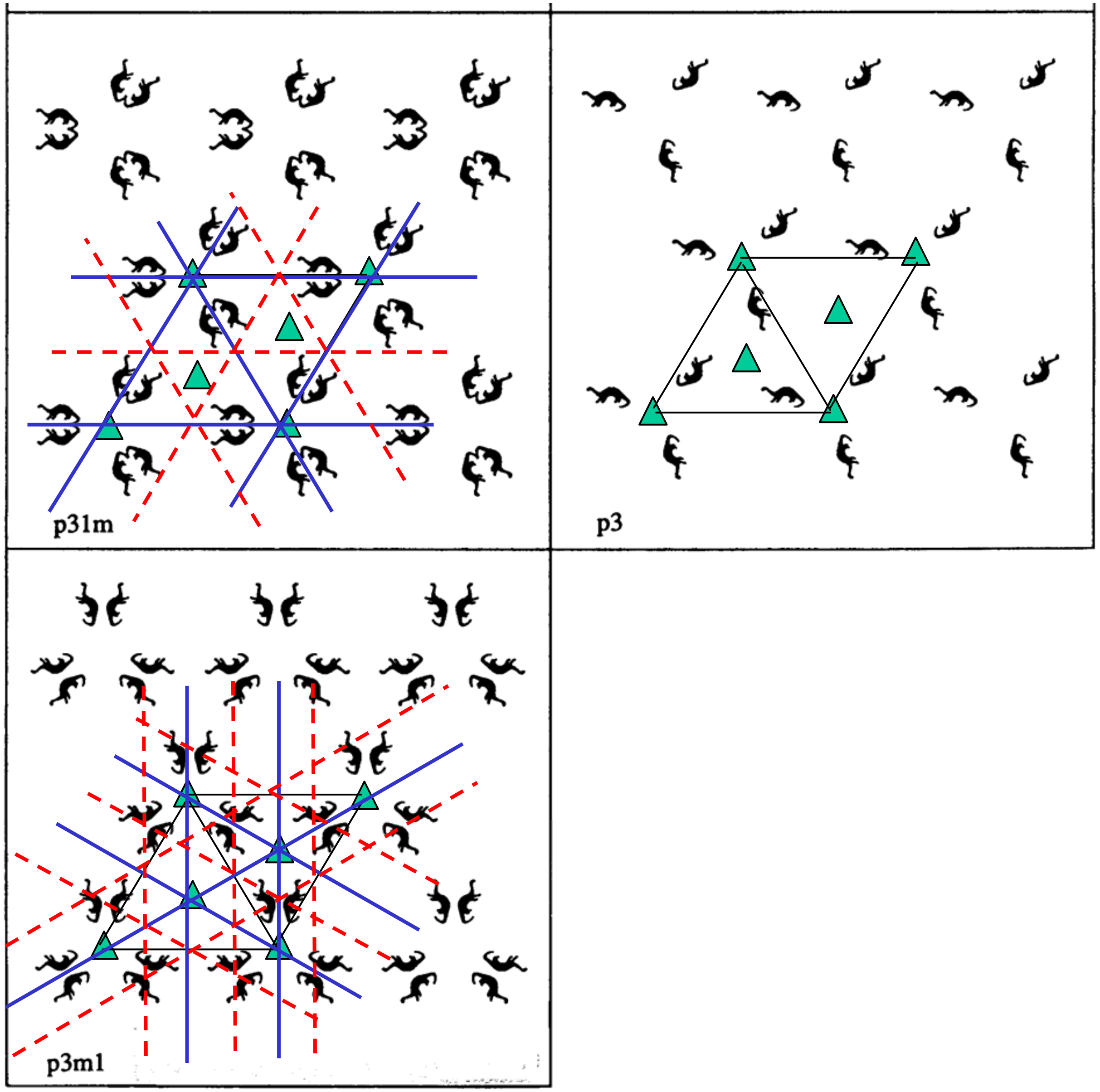

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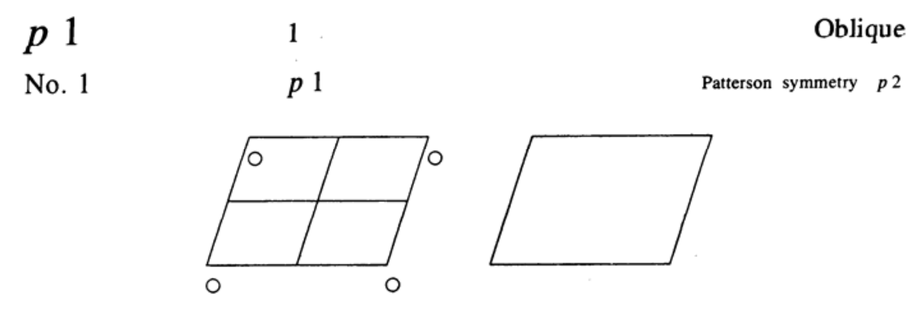
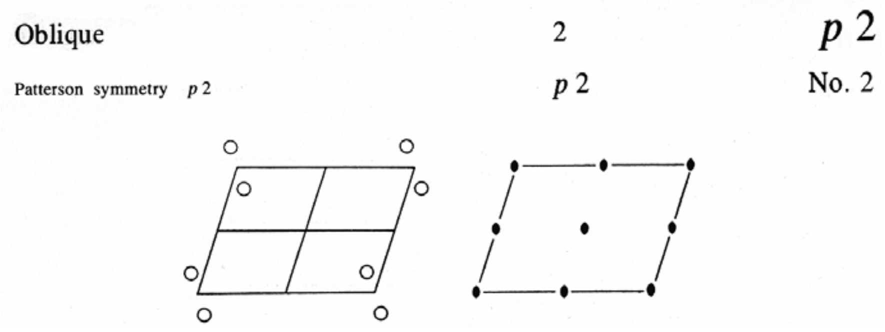
International Tables for X-ray Crystallography



p 1
No. 1

1
p 1

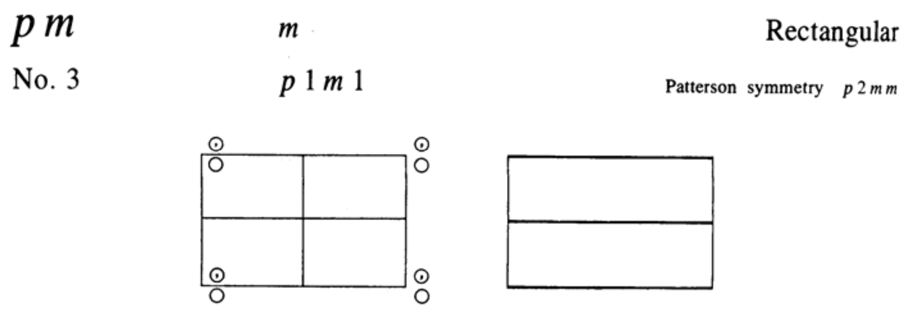
Oblique
Patterson symmetry *p* 2



Oblique
Patterson symmetry *p* 2

2
p 2

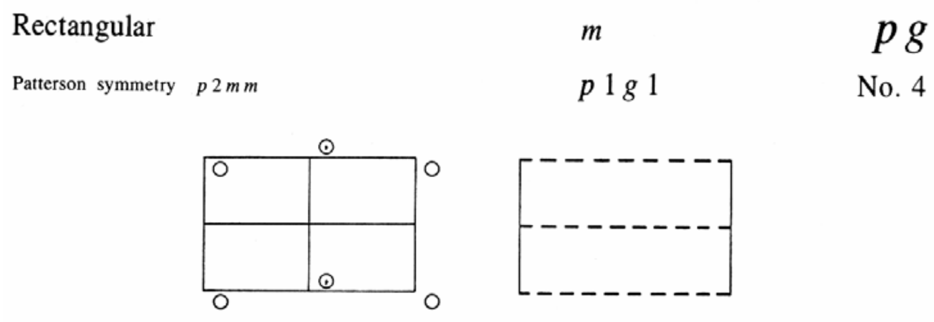
p 2
No. 2



p m
No. 3

m
p 1 *m* 1

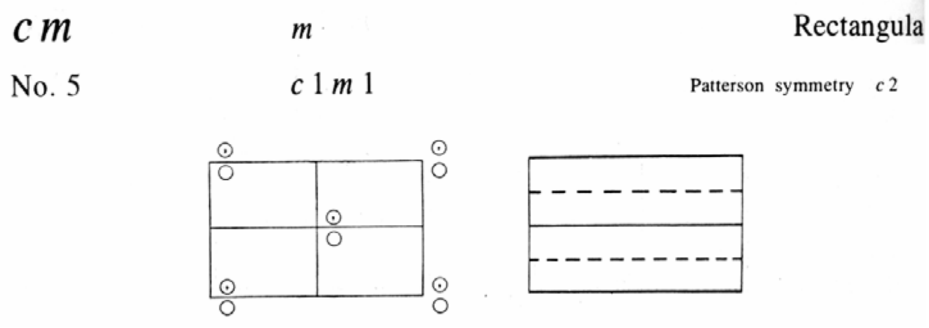
Rectangular
Patterson symmetry *p* 2 *m m*



Rectangular
Patterson symmetry *p* 2 *m m*

m
p 1 *g* 1

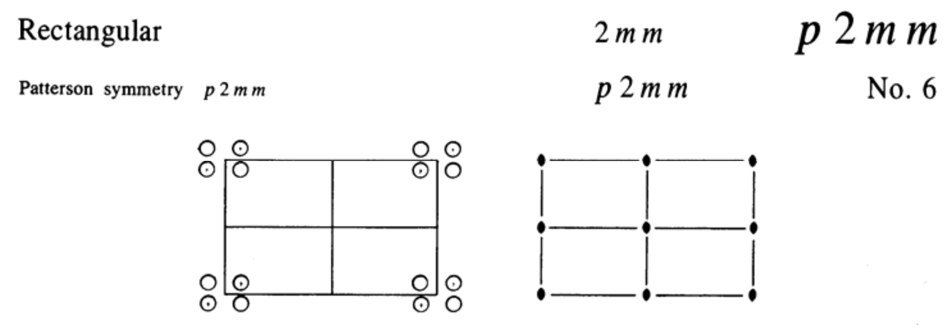
p g
No. 4



c m
No. 5

m
c 1 *m* 1

Rectangula
Patterson symmetry *c* 2



Rectangular
Patterson symmetry *p* 2 *m m*

2 *m m*
p 2 *m m*

p 2 *m m*
No. 6

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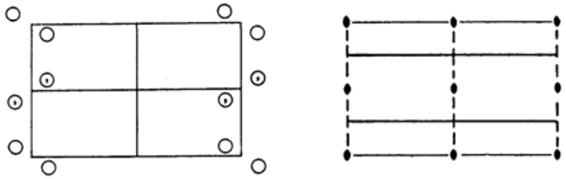
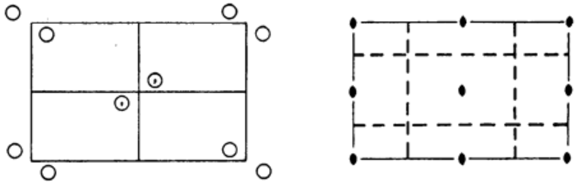
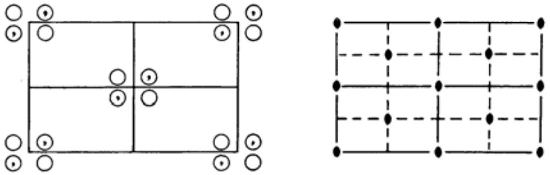
*p*2*mg*
No. 7
2*mm*
*p*2*mg*
Rectangular
Patterson symmetry *p*2*mm*



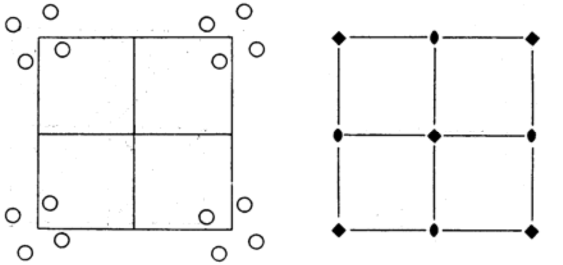
Rectangular
Patterson symmetry *p*2*mm*
2*mm*
*p*2*gg*
*p*2*gg*
No. 8



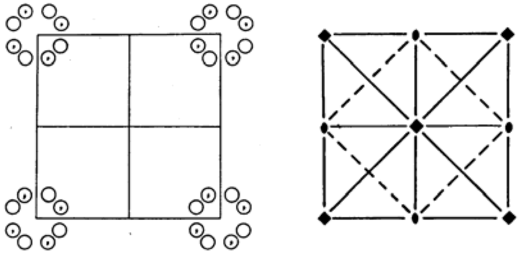
*c*2*mm*
No. 9
2*mm*
*c*2*mm*
Rectangular
Patterson symmetry *c*2*mm*



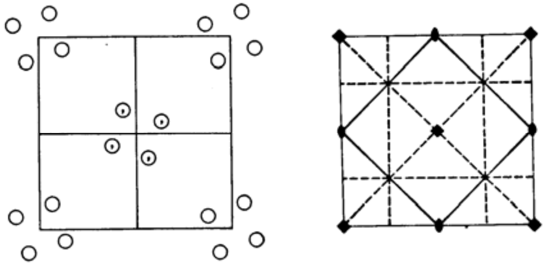
Square
Patterson symmetry *p*4
4
*p*4
p 4
No. 1



*p*4*mm*
No. 11
4*mm*
*p*4*mm*
Square
Patterson symmetry *p*4*mm*



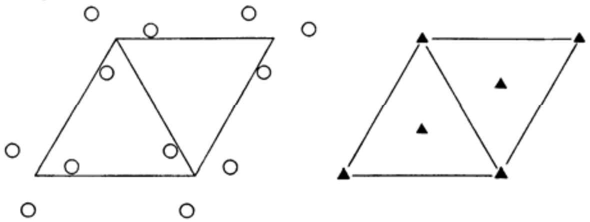
Square
Patterson symmetry *p*4*mm*
4*mm*
*p*4*gm*
*p*4*gm*
No. 12



International Tables for X-ray Crystallography

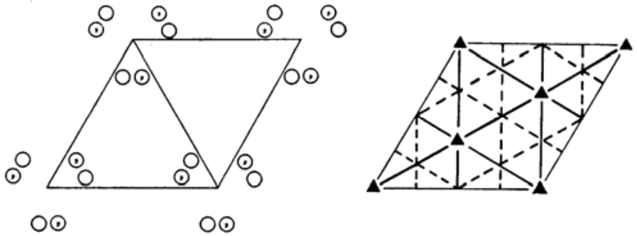
p 3 3 Hexagonal

No. 13 *p* 3 Patterson symmetry *p* 6



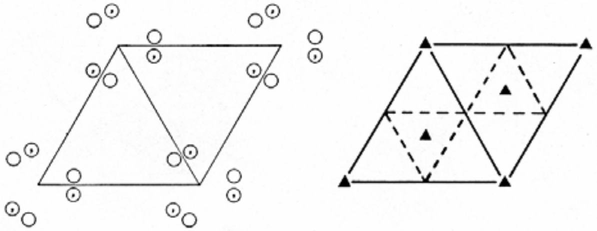
Hexagonal 3 *m* *p* 3 *m* 1

Patterson symmetry *p* 6 *m m* *p* 3 *m* 1 No. 14



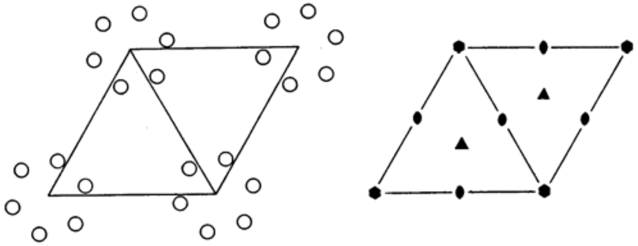
p 3 1 *m* 3 *m* Hexagonal

No. 15 *p* 3 1 *m* Patterson symmetry *p* 6 *m m*



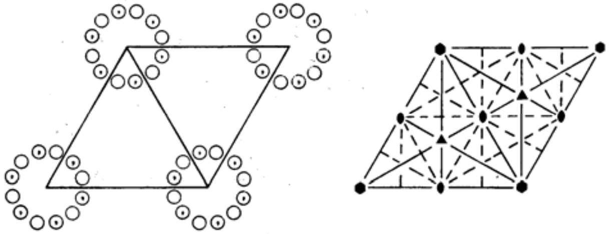
Hexagonal 6 *p* 6

Patterson symmetry *p* 6 *p* 6 No. 16



p 6 *m m* 6 *m m* Hexagonal

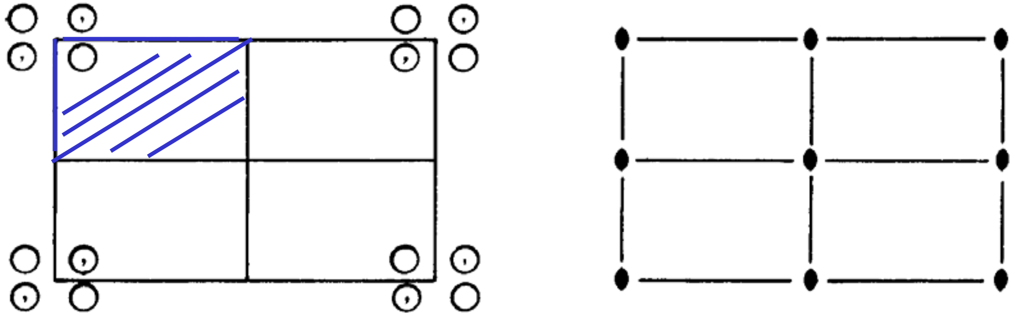
No. 17 *p* 6 *m m* Patterson symmetry *p* 6 *m m*



International Tables for X-ray Crystallography

③ Rectangular ② $2mm$ ① $p\,2mm$

⑥ Patterson symmetry $p\,2mm$ ⑤ $p\,2mm$ ④ No. 6


⑦

Origin at $2mm$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$

Symmetry operations

(1) 1 (2) 2 0,0 (3) m $0,y$ (4) m $x,0$

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

International Tables for X-ray Crystallography

① short international (Hermann–Mauguin) symbol for the plane group
② short international (Hermann–Mauguin) symbol for the point group
③ crystal system
④ sequential number of plane group
⑤ full international (Hermann–Mauguin) symbol for the plane group
⑥ patterson symmetry
⑦ diagram for the symmetry elements and the general position

International Tables for X-ray Crystallography

Generators selected (1); $t(1,0)$; $t(0,1)$; (2); (3)

Positions

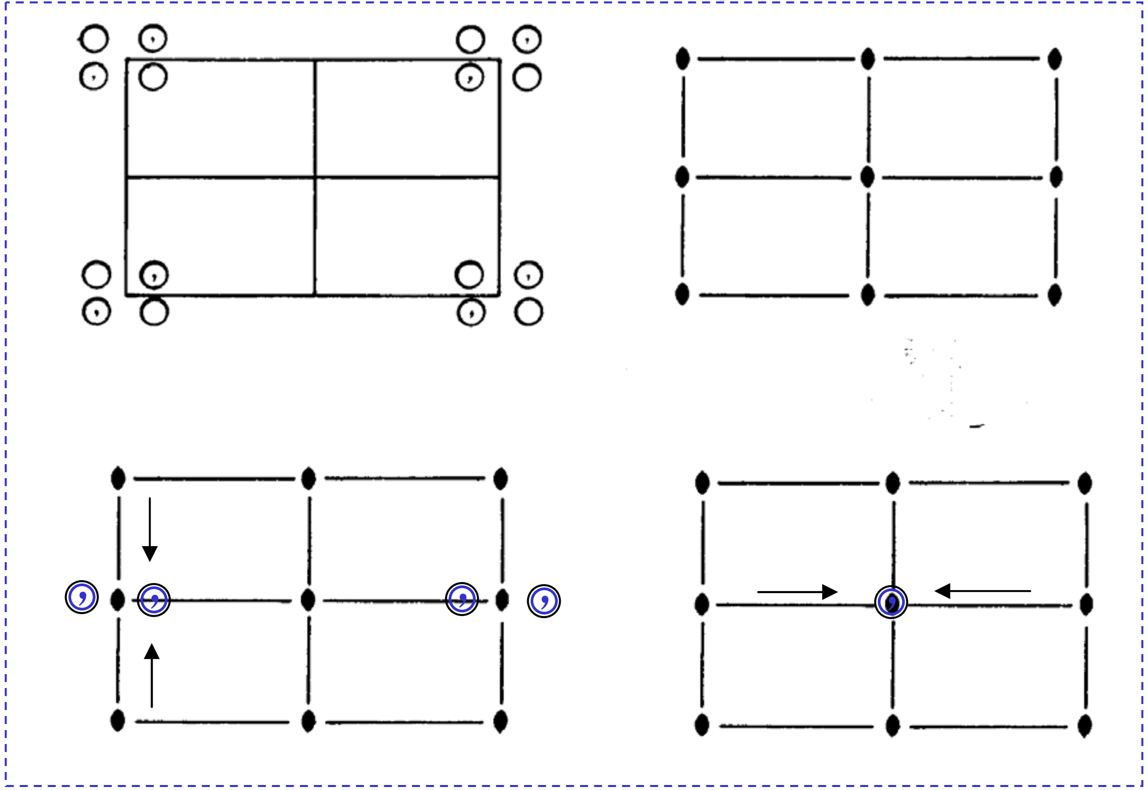
Multiplicity, Wyckoff letter, Site symmetry			Coordinates			
4	i	1	(1) x,y	(2) $\bar{x},\bar{y}$	(3) $\bar{x},y$	(4) $x,\bar{y}$
2	h	$.m.$	$\frac{1}{2},y$	$\frac{1}{2},\bar{y}$		
2	g	$.m.$	$0,y$	$0,\bar{y}$		
2	f	$..m$	$x,\frac{1}{2}$	$\bar{x},\frac{1}{2}$		
2	e	$..m$	$x,0$	$\bar{x},0$		
1	d	$2mm$	$\frac{1}{2},\frac{1}{2}$			
1	c	$2mm$	$\frac{1}{2},0$			
1	b	$2mm$	$0,\frac{1}{2}$			
1	a	$2mm$	$0,0$			

Reflection conditions

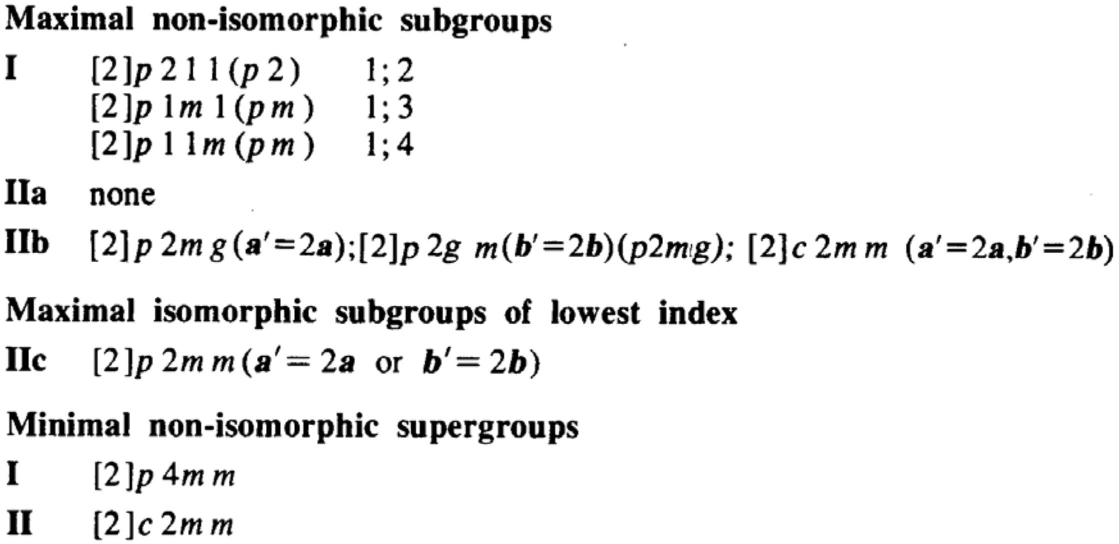
General:

no conditions

Special: no extra conditions



International Tables for X-ray Crystallography



Maximal non-isomorphic subgroups

I [2] *p* 2 1 1 (*p* 2) 1; 2
[2] *p* 1 *m* 1 (*p m*) 1; 3
[2] *p* 1 1 *m* (*p m*) 1; 4

IIa none

IIb [2] *p* 2*m g* ($\mathbf{a}'=2\mathbf{a}$); [2] *p* 2*g m* ($\mathbf{b}'=2\mathbf{b}$) (*p*2*mg*); [2] *c* 2*m m* ($\mathbf{a}'=2\mathbf{a}, \mathbf{b}'=2\mathbf{b}$)

Maximal isomorphic subgroups of lowest index

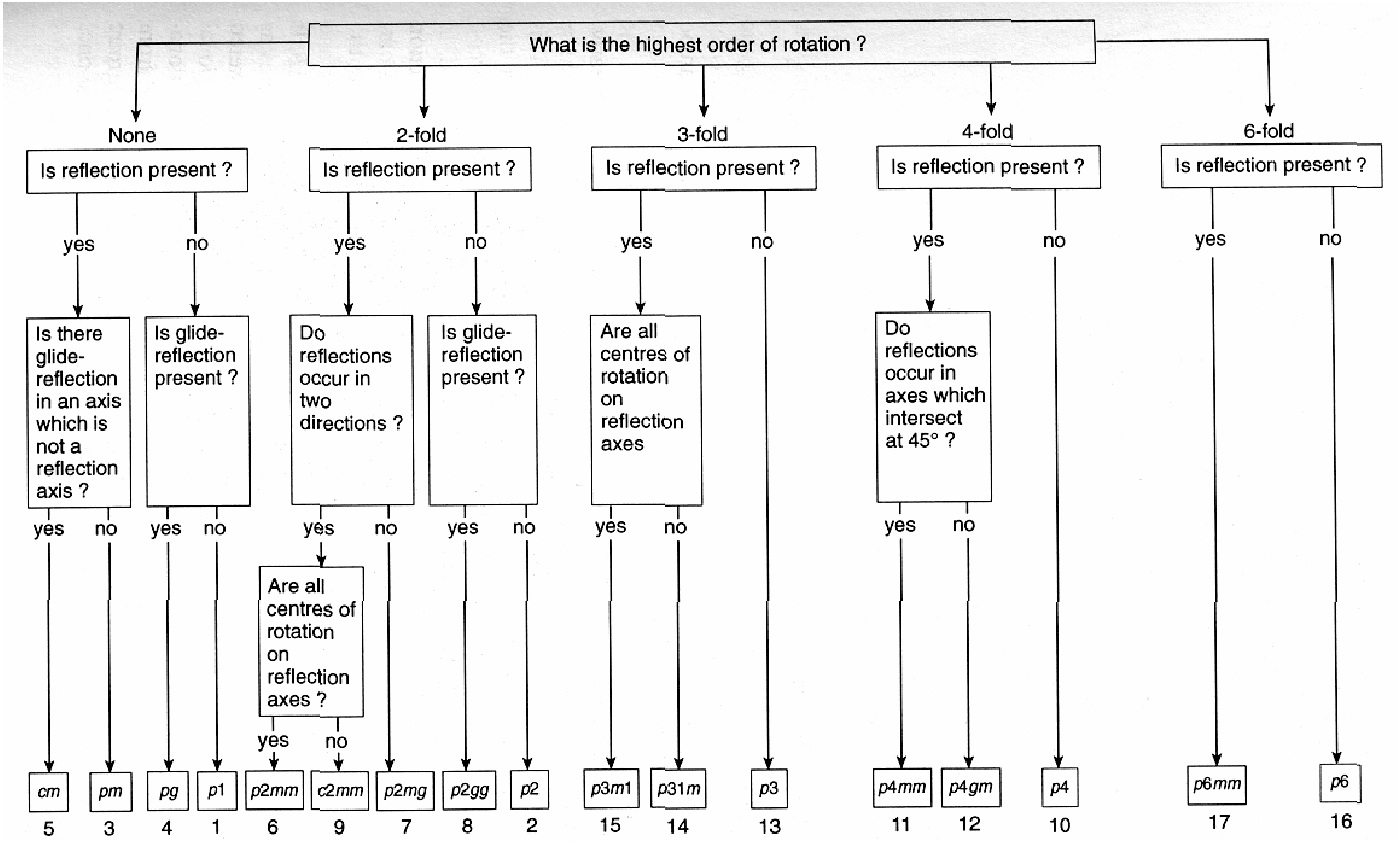
IIc [2] *p* 2*m m* ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{b}'=2\mathbf{b}$)

Minimal non-isomorphic supergroups

I [2] *p* 4*m m*

II [2] *c* 2*m m*

Flow Diagram for Identifying Plane Groups



A. Putnis, Introduction to Mineral Sciences

Example I

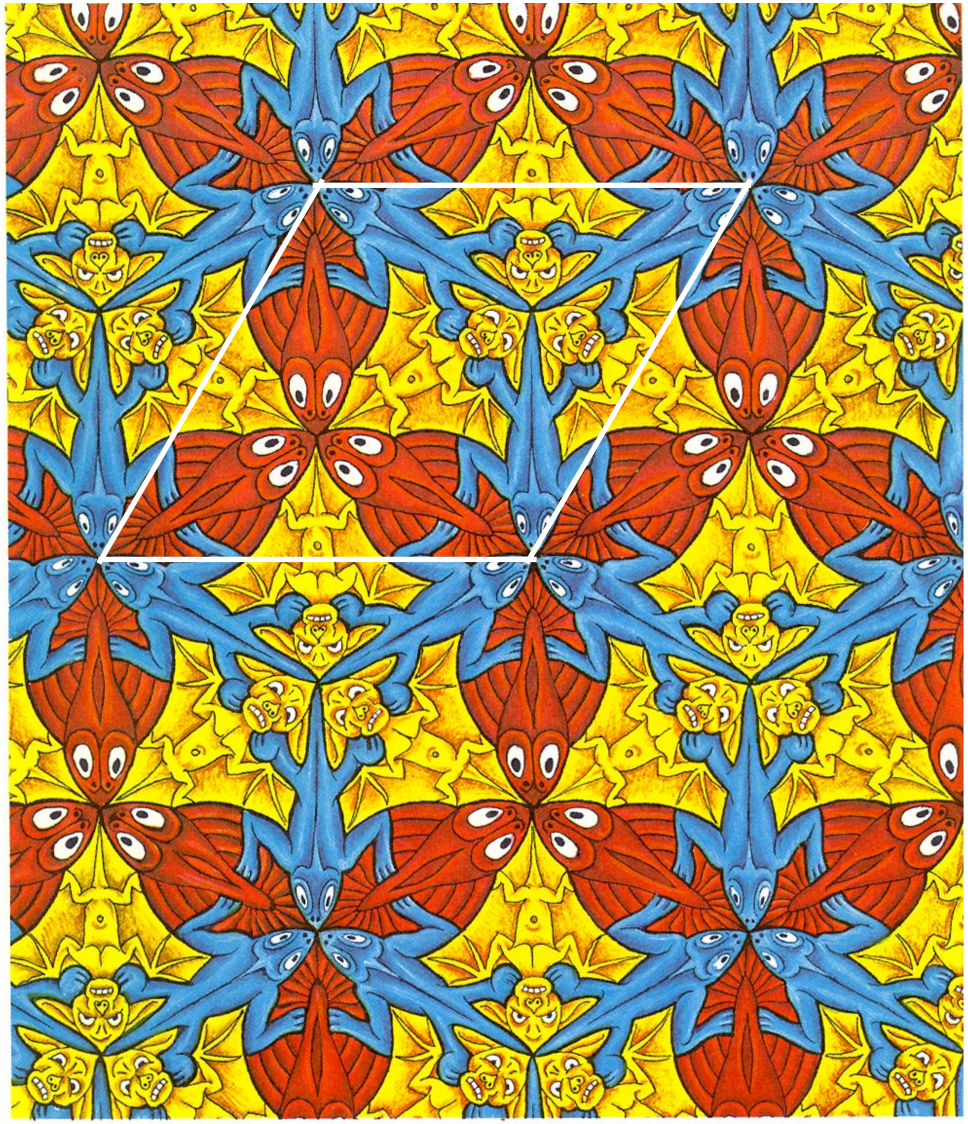
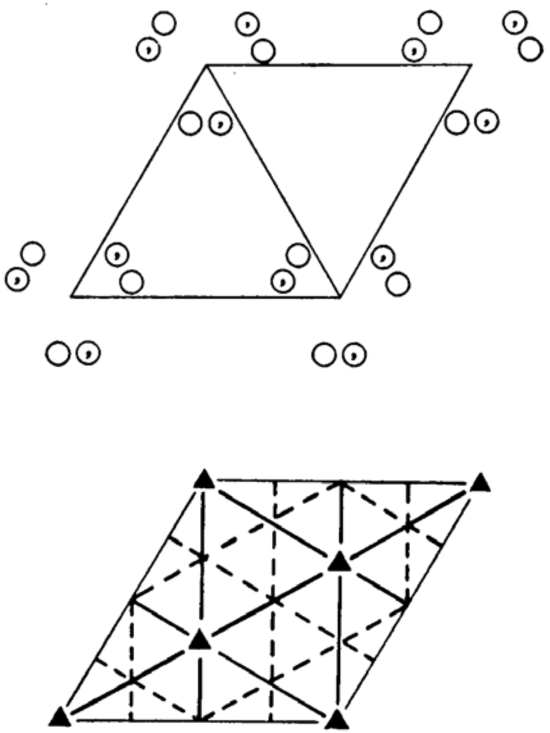
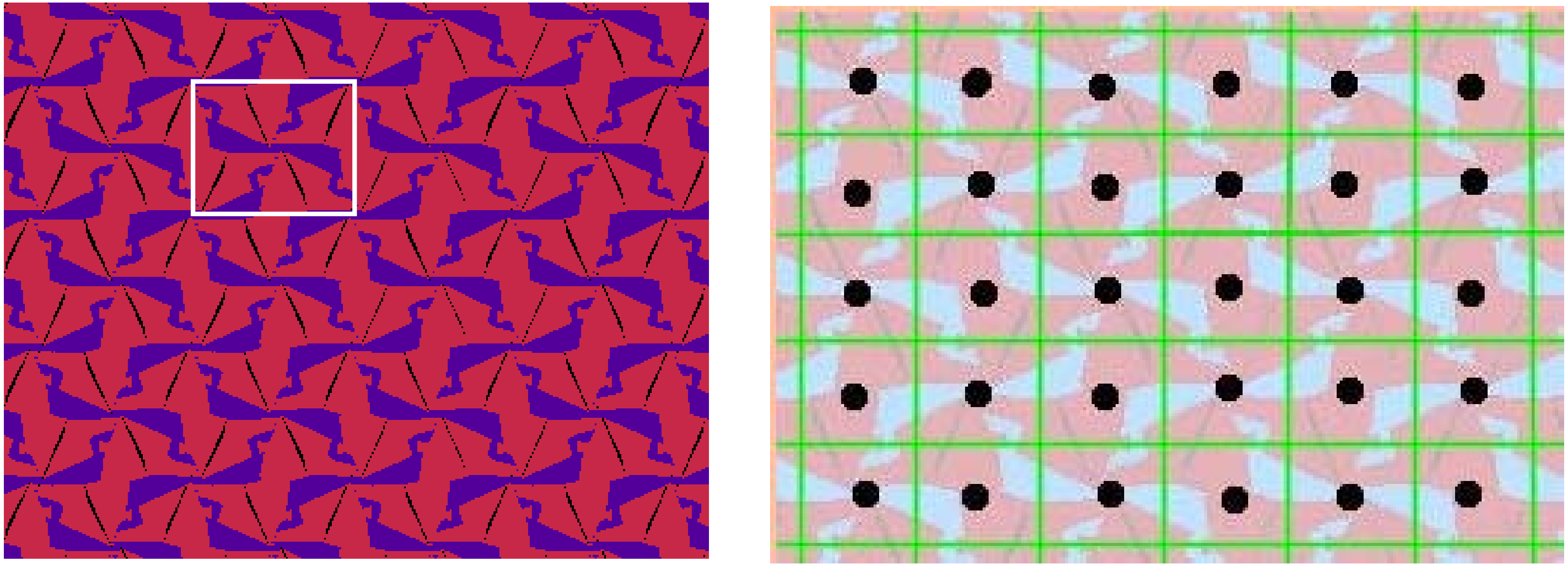


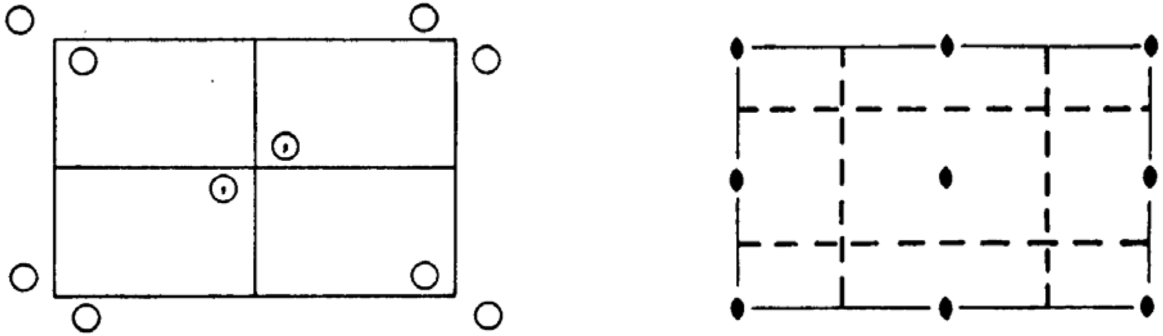
PLATE 9

$P3m1$



Example II





P_{2gg}

http://www.clarku.edu/~djoyce/wallpaper/

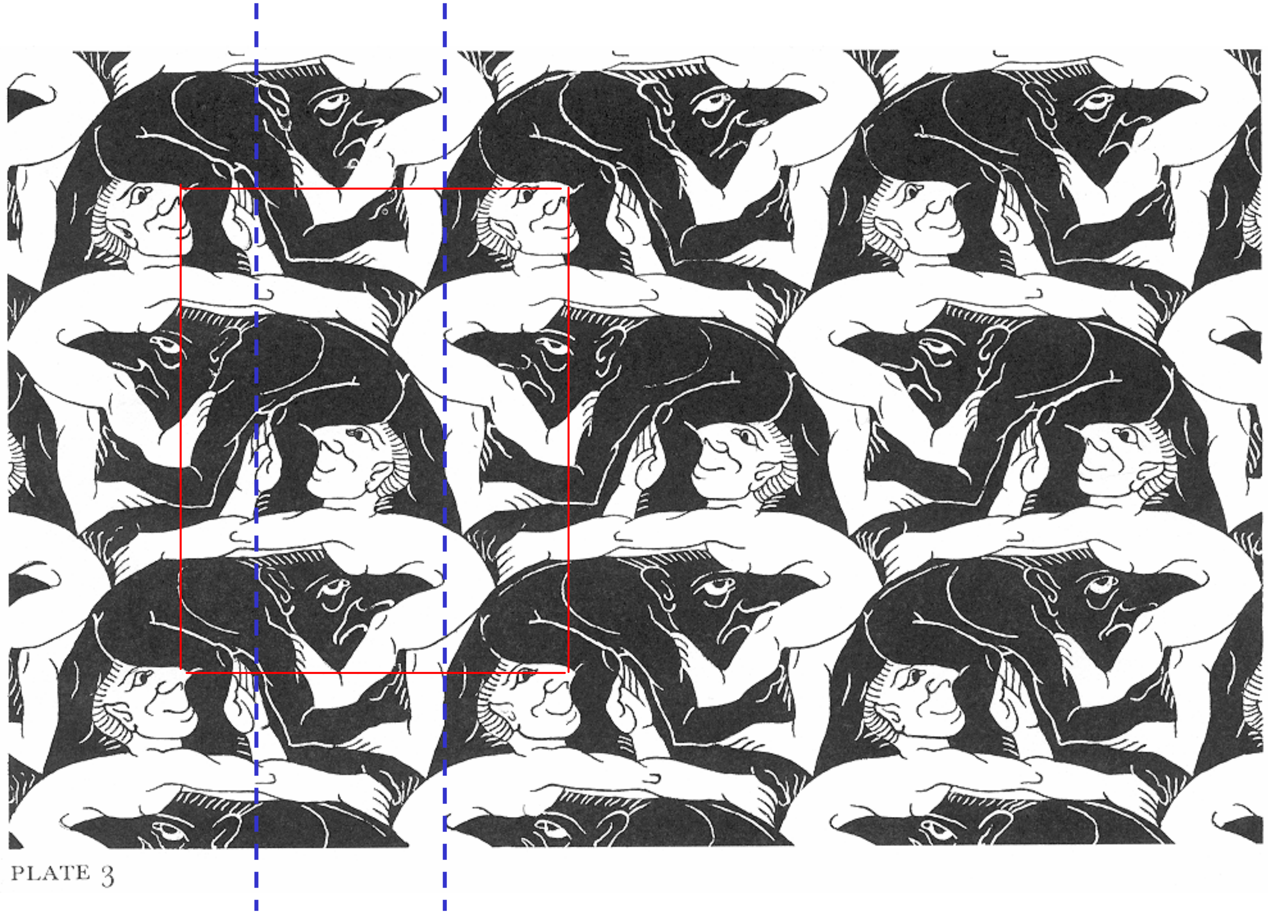


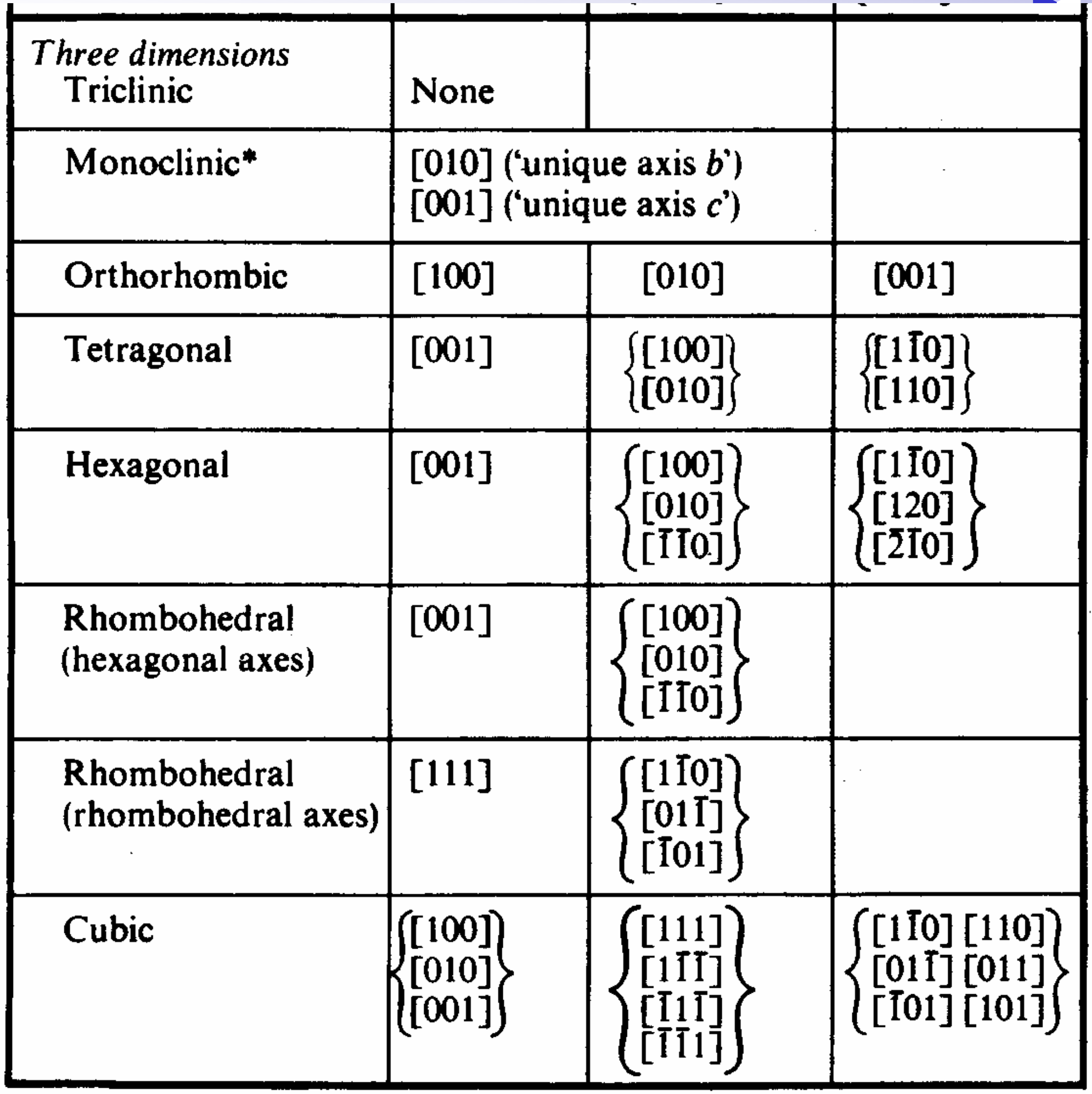
PLATE 3

Pg

Space Groups

-Bravais lattice + point group → 230 space groups
+ screw axis
+ glide plane

- Bravais lattice + point group= 73
- Bravais lattice + screw axis = 41
- Bravais lattice + glide plane = 116



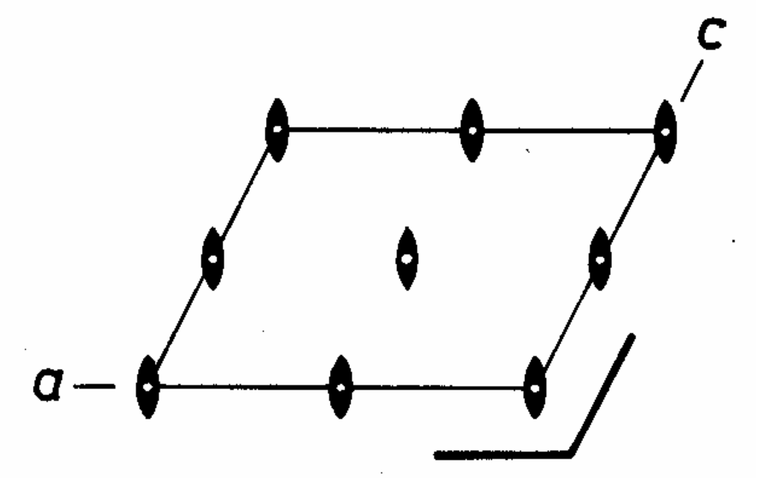
Three dimensions Triclinic	None		
Monoclinic*	[010] ('unique axis *b*') [001] ('unique axis *c*')		
Orthorhombic	[100]	[010]	[001]
Tetragonal	[001]	[100] [010]	$[1\bar{1}0]$ [110]
Hexagonal	[001]	[100] [010] $[\bar{1}\bar{1}0]$	$[1\bar{1}0]$ [120] $[\bar{2}\bar{1}0]$
Rhombohedral (hexagonal axes)	[001]	[100] [010] $[\bar{1}\bar{1}0]$	
Rhombohedral (rhombohedral axes)	[111]	$[1\bar{1}0]$ $[01\bar{1}]$ $[\bar{1}01]$	
Cubic	[100] [010] [001]	[111] $[1\bar{1}\bar{1}]$ $[\bar{1}1\bar{1}]$ $[\bar{1}\bar{1}1]$	$[1\bar{1}0]$ [110] $[01\bar{1}]$ [011] $[\bar{1}01]$ [101]

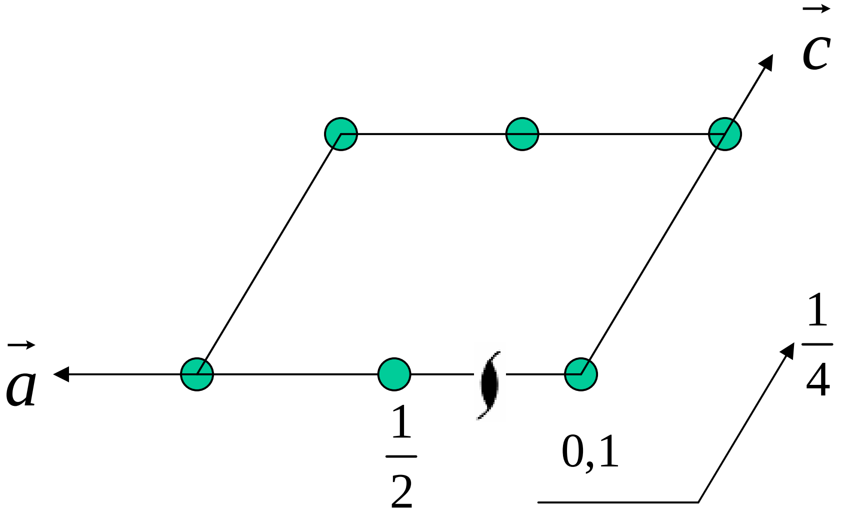
Space Groups-monoclinic

- monoclinic system- highest symmetry

$P\frac{2}{m}$, $C\frac{2}{m}$ (a-glide at x, $\frac{1}{4}, z$, x, $\frac{3}{4}, z$

2_1 screw axis at $\frac{1}{4}, y, 0$, $\frac{1}{4}, y, \frac{1}{2}$, $\frac{3}{4}, y, 0$, $\frac{3}{4}, y, \frac{1}{2}$)

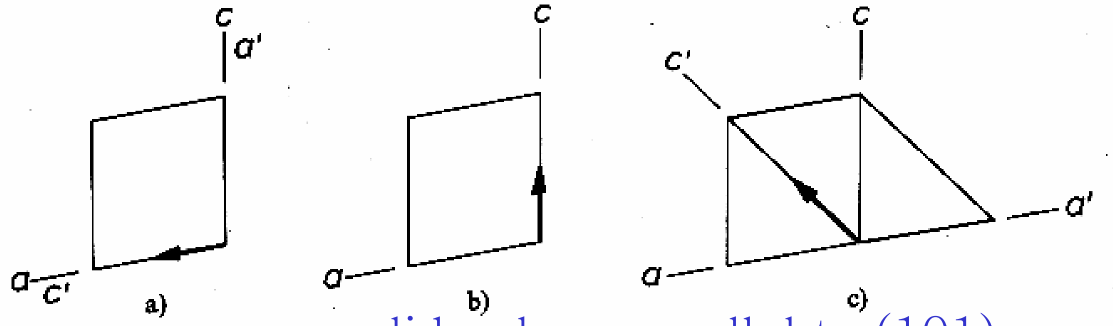




Space Groups-monoclinic

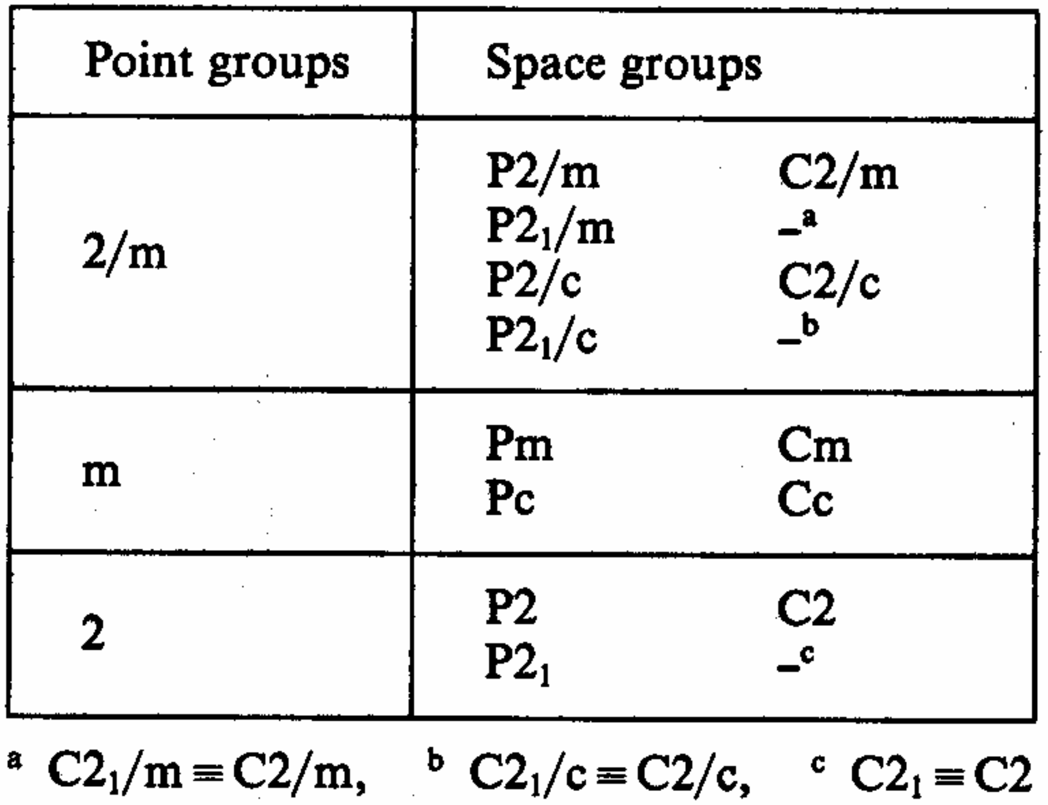
– $\frac{2}{m}$ subgroup 2, m

$2_1 \rightarrow$ 2, c-glide $\rightarrow$ m



glide plane parallel to (101)

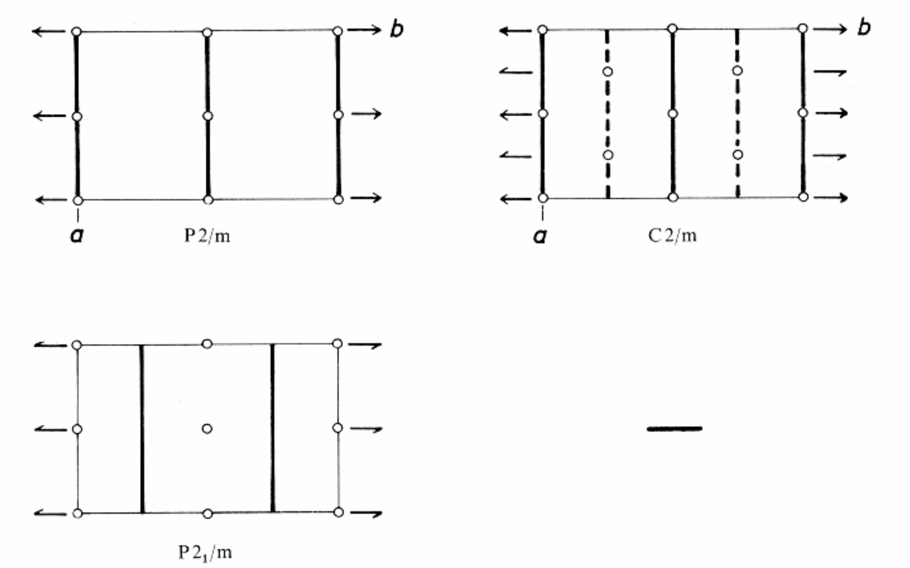
–13 monoclinic space groups

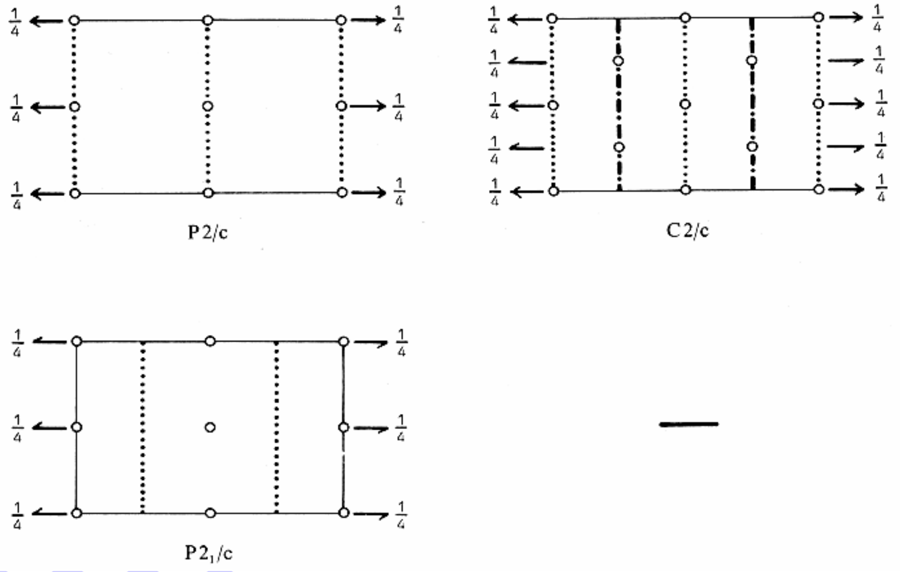


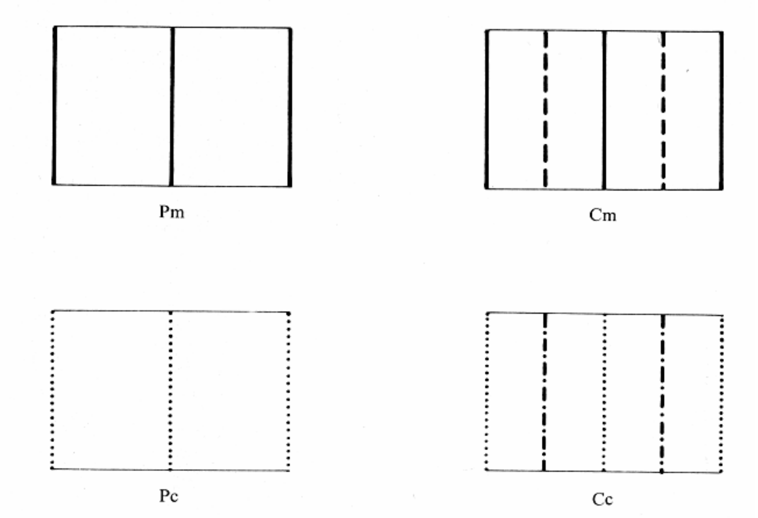
Point groups	Space groups	
2/m	P2/m $P2_1/m$ P2/c $P2_1/c$	C2/m –[a] C2/c –[b]
m	Pm Pc	Cm Cc
2	P2 $P2_1$	C2 –[c]

[a] $C2_1/m \equiv C2/m$, [b] $C2_1/c \equiv C2/c$, [c] $C2_1 \equiv C2$

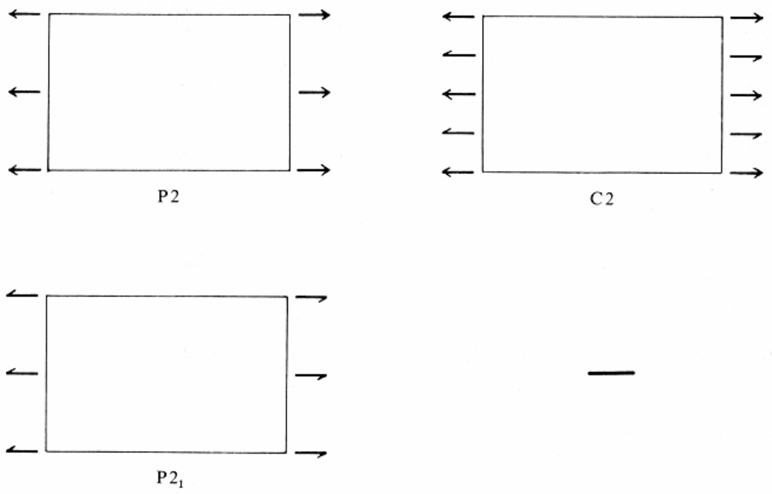
Space Groups-monoclinic



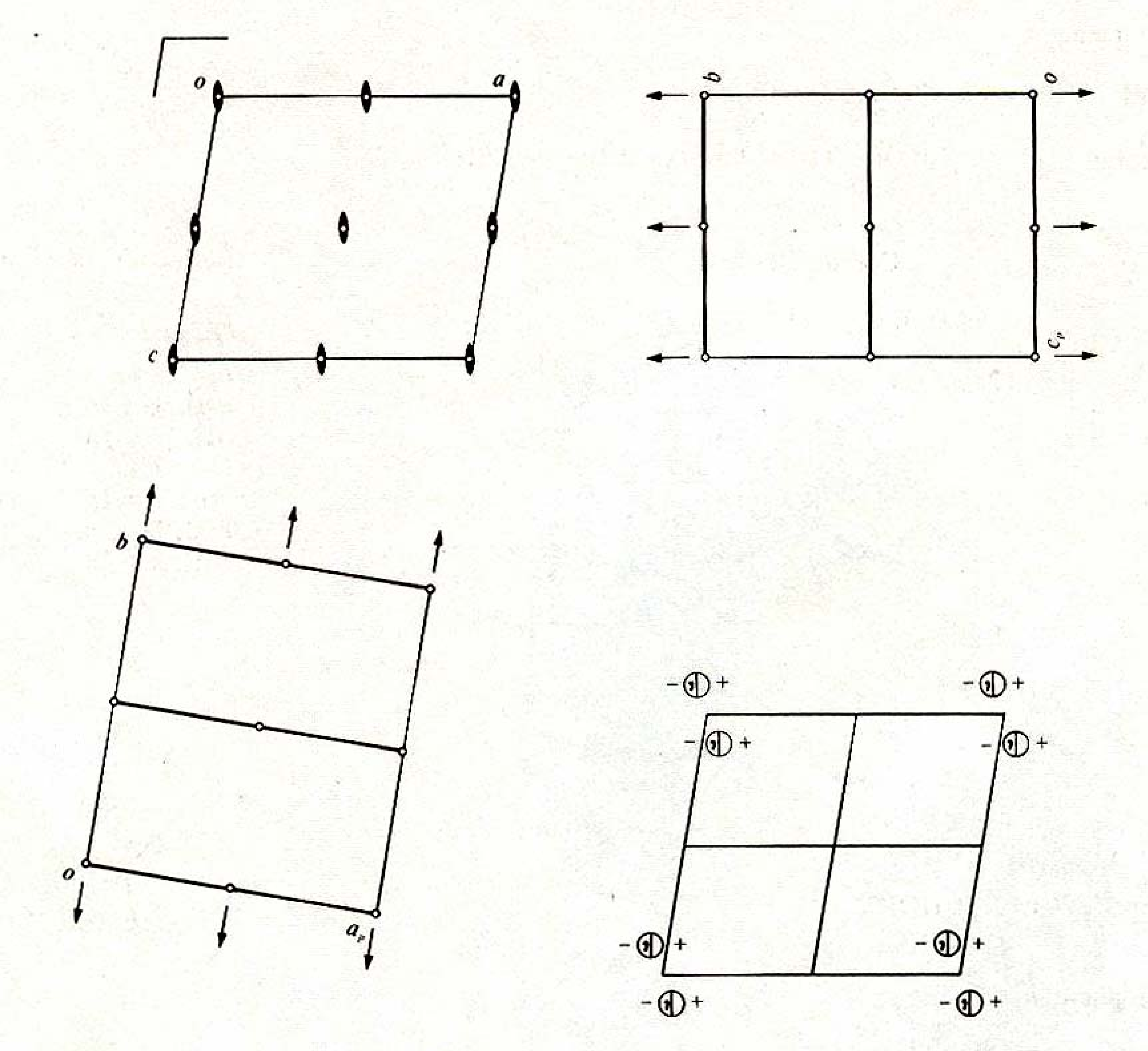




b Space groups of point group m

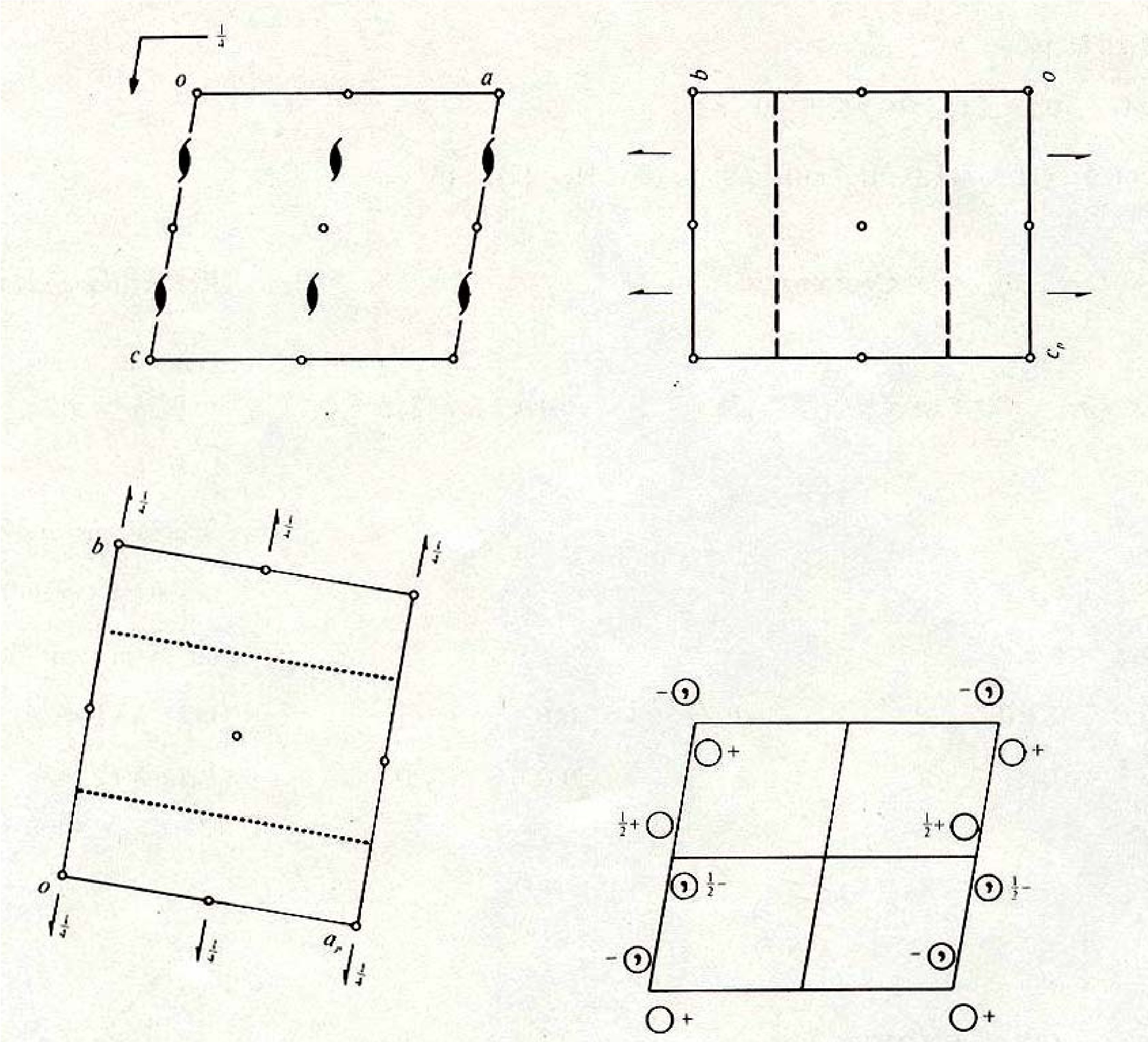


$P\frac{2}{m}$



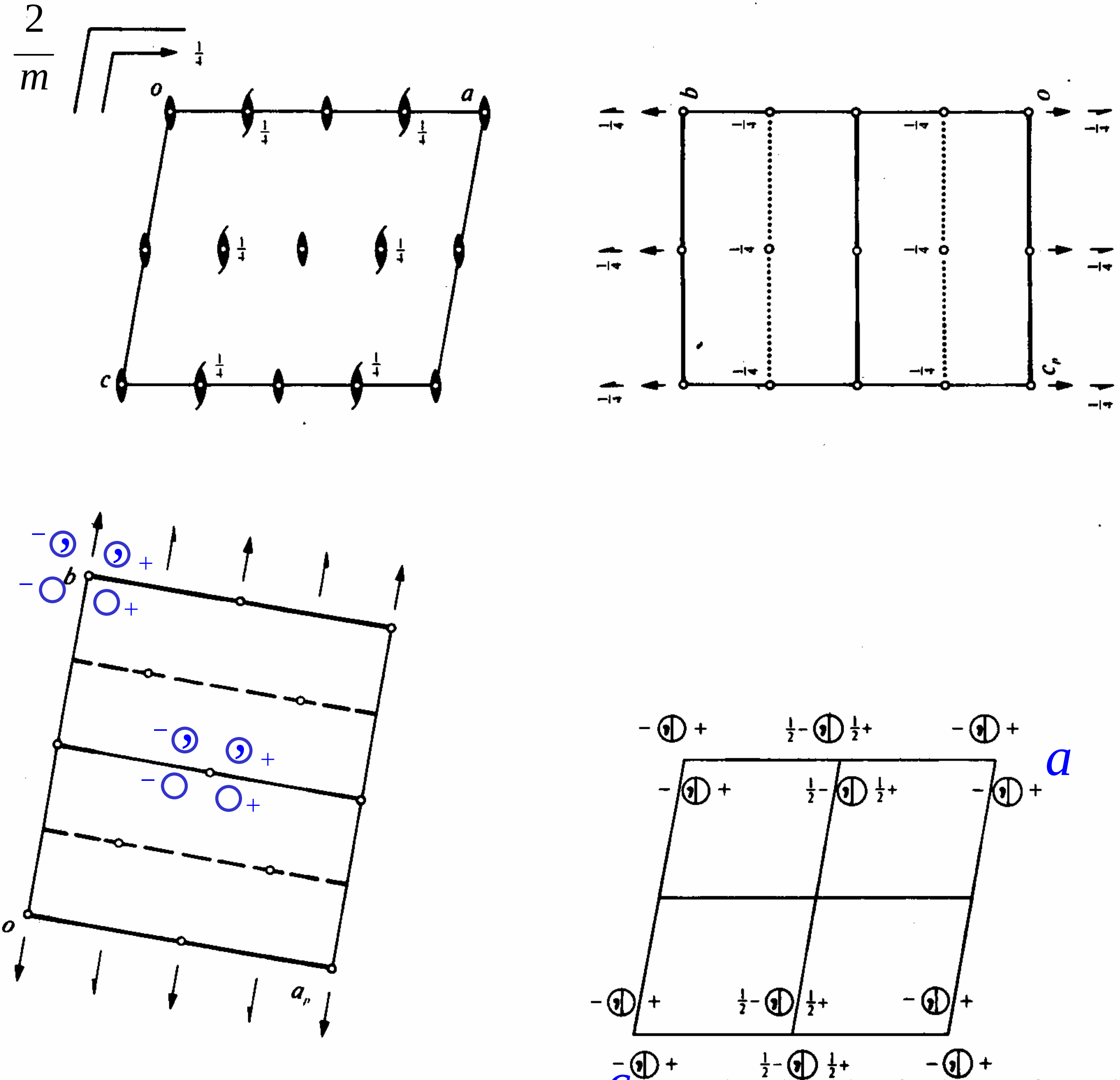
International Tables for X-ray Crystallography

$P\frac{2_1}{c}$

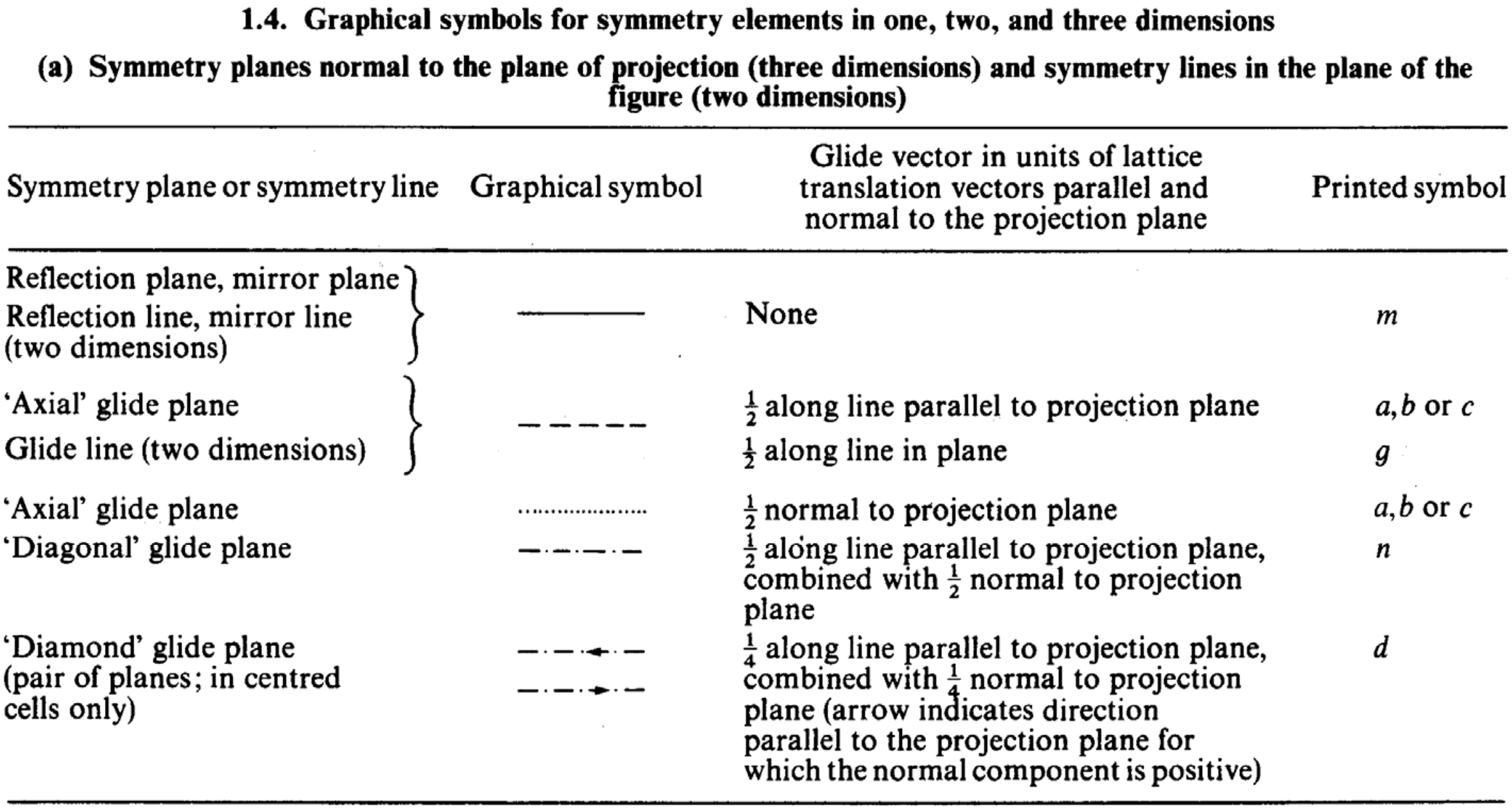


International Tables for X-ray Crystallography

$C\frac{2}{m}$



International Tables for X-ray Crystallography



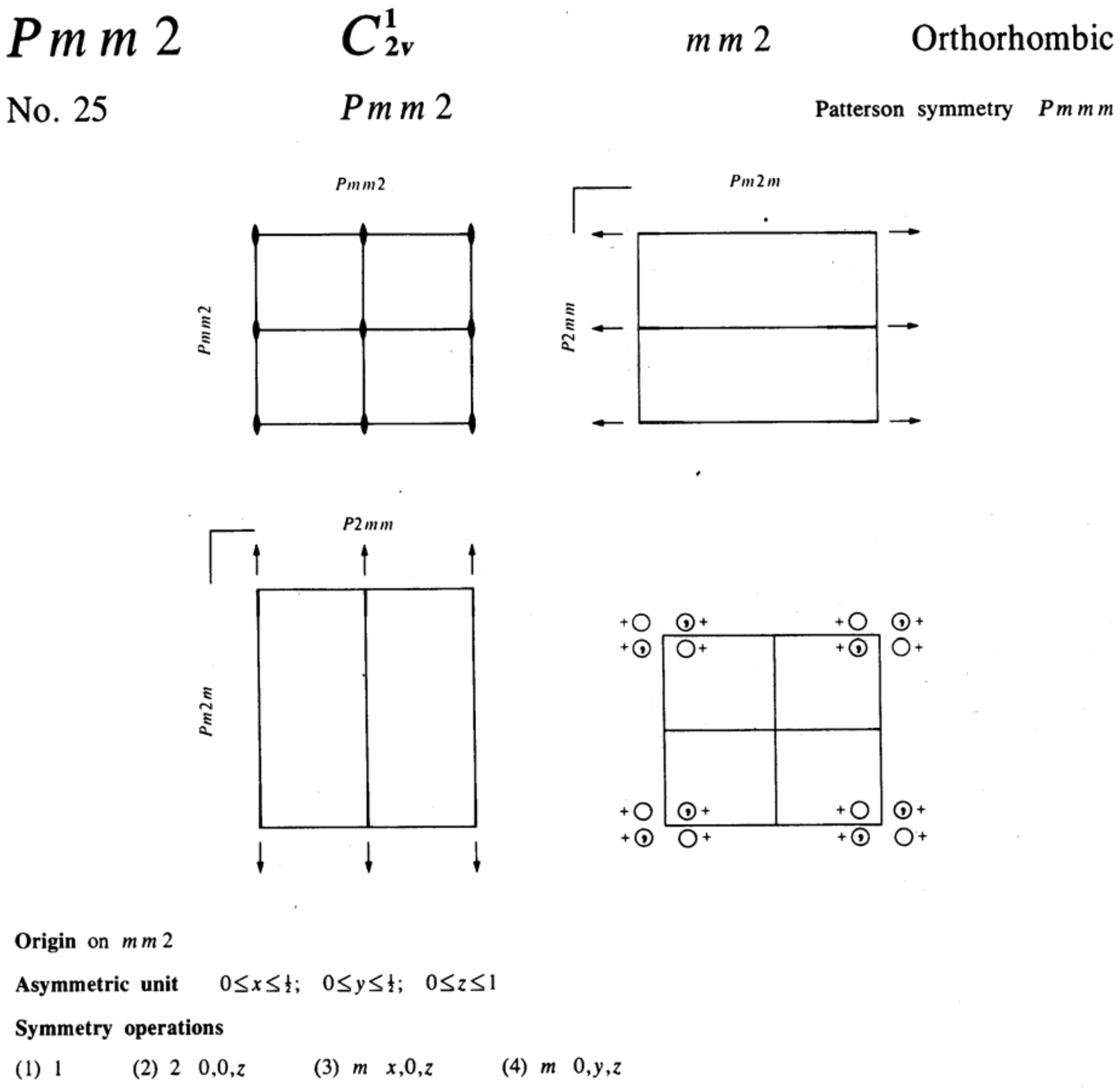
1.4. Graphical symbols for symmetry elements in one, two, and three dimensions

(a) Symmetry planes normal to the plane of projection (three dimensions) and symmetry lines in the plane of the figure (two dimensions)

Symmetry plane or symmetry line	Graphical symbol	Glide vector in units of lattice translation vectors parallel and normal to the projection plane	Printed symbol
Reflection plane, mirror plane Reflection line, mirror line (two dimensions)	———	None	m
'Axial' glide plane	– – – – –	$\frac{1}{2}$ along line parallel to projection plane	a, b or c
Glide line (two dimensions)		$\frac{1}{2}$ along line in plane	g
'Axial' glide plane	…………	$\frac{1}{2}$ normal to projection plane	a, b or c
'Diagonal' glide plane	—·—·—	$\frac{1}{2}$ along line parallel to projection plane, combined with $\frac{1}{2}$ normal to projection plane	n
'Diamond' glide plane (pair of planes; in centred cells only)	—·—◀·— —·—▶·—	$\frac{1}{4}$ along line parallel to projection plane, combined with $\frac{1}{4}$ normal to projection plane (arrow indicates direction parallel to the projection plane for which the normal component is positive)	d

International Tables for X-ray Crystallography

Space Groups-Pmm2



$Pmm2$ C_{2v}^{1} $mm2$ Orthorhombic

No. 25 $Pmm2$ Patterson symmetry $Pmmm$

Origin on $mm2$

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le 1$

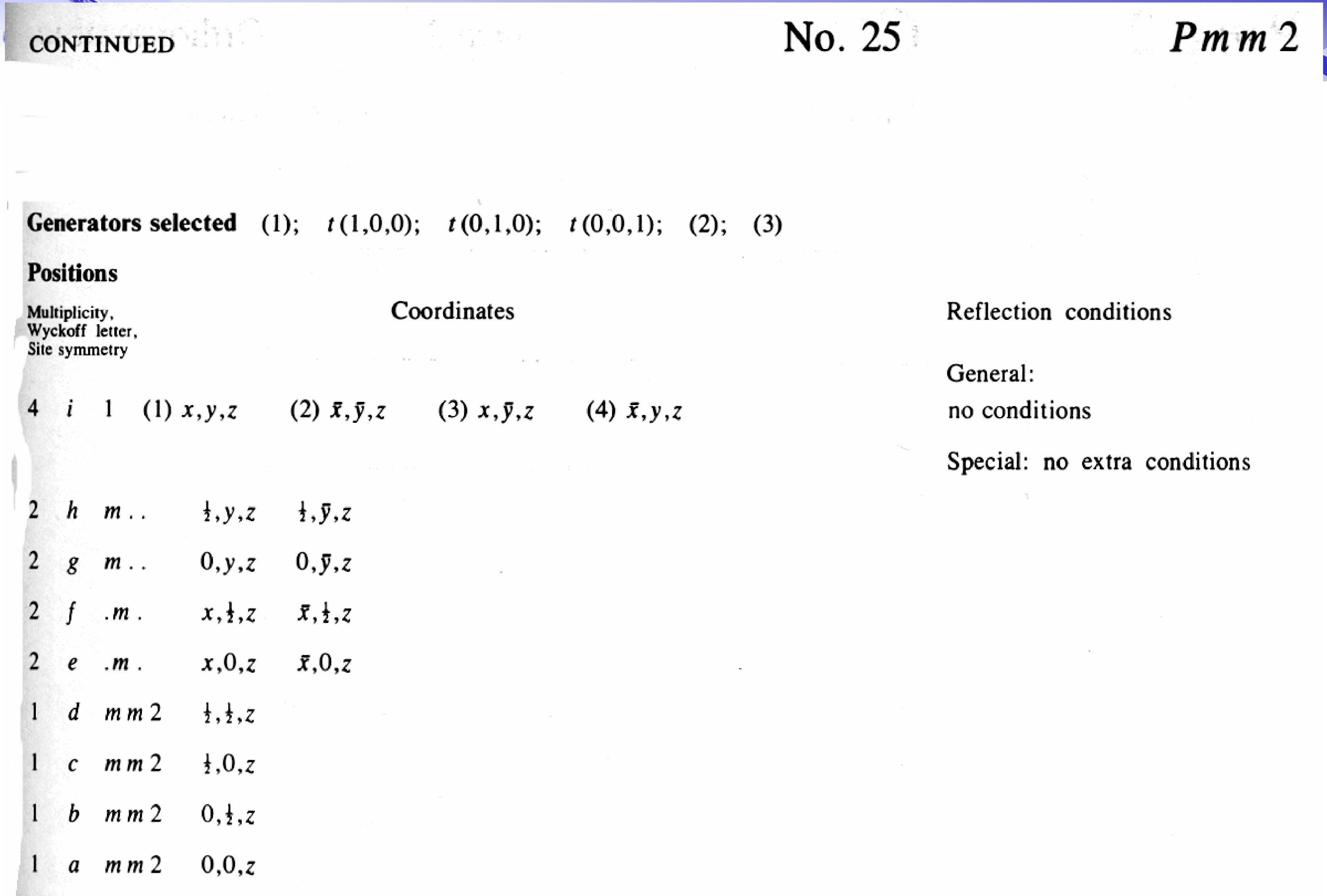
Symmetry operations

(1) 1 (2) 2 0,0,z (3) m x,0,z (4) m 0,y,z

short space group symbol
Schoenflies symbol
point group
crystal system
number of space group
full space group symbol

projection of symmetry elements
projection of general position

International Tables for X-ray Crystallography



CONTINUED No. 25 $Pmm2$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
4	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	no conditions
							Special: no extra conditions
2	*h*	m . .	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$			
2	*g*	m . .	$0,y,z$	$0,\bar{y},z$			
2	*f*	. m .	$x,\frac{1}{2},z$	$\bar{x},\frac{1}{2},z$			
2	*e*	. m .	$x,0,z$	$\bar{x},0,z$			
1	*d*	$m\,m\,2$	$\frac{1}{2},\frac{1}{2},z$				
1	*c*	$m\,m\,2$	$\frac{1}{2},0,z$				
1	*b*	$m\,m\,2$	$0,\frac{1}{2},z$				
1	*a*	$m\,m\,2$	$0,0,z$				

Space Groups-Pmm2

- origin

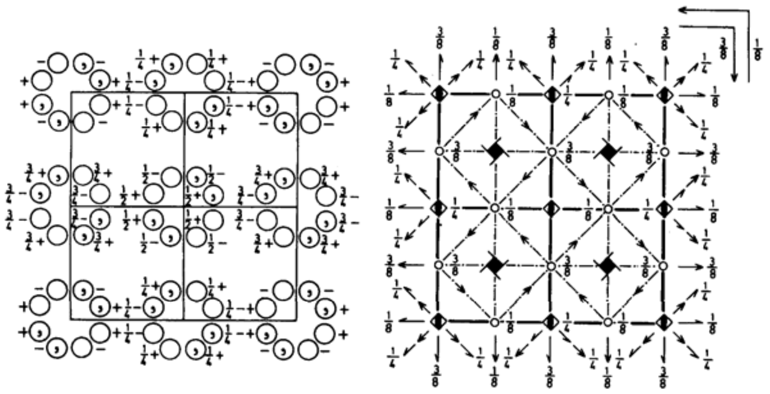
(i) all centrosymmetric space groups are described with an inversion centers as origin.
a second description is given if a space group contains points of high site symmetry that do not coincide with a center of symmetry

(ii) for non-centrosymmetric space groups, the origin is at a point of highest site symmetry.
if no site symmetry is higher than 1, the origin is placed on a screw axis or a glide plane, or at the intersection of several such symmetry elements

$I\,4_1/a\,m\,d$ D_{4h}^{19} $4/m\,m\,m$ Tetragonal

No. 141 $I\,4_1/a\,2/m\,2/d$ Patterson symmetry $I\,4/m\,m\,m$

ORIGIN CHOICE 1

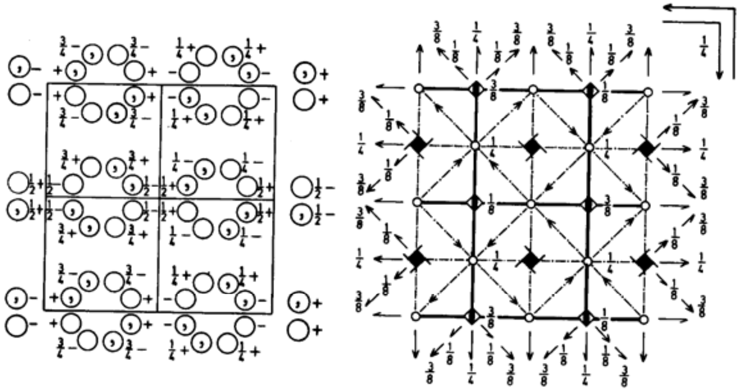


Origin at $\bar{4}m\,2$, at $0, \frac{1}{4}, -\frac{1}{8}$ from centre $(2/m)$

$I\,4_1/a\,m\,d$ D_{4h}^{19} $4/m\,m\,m$ Tetragonal

No. 141 $I\,4_1/a\,2/m\,2/d$ Patterson symmetry $I\,4/m\,m\,m$

ORIGIN CHOICE 2

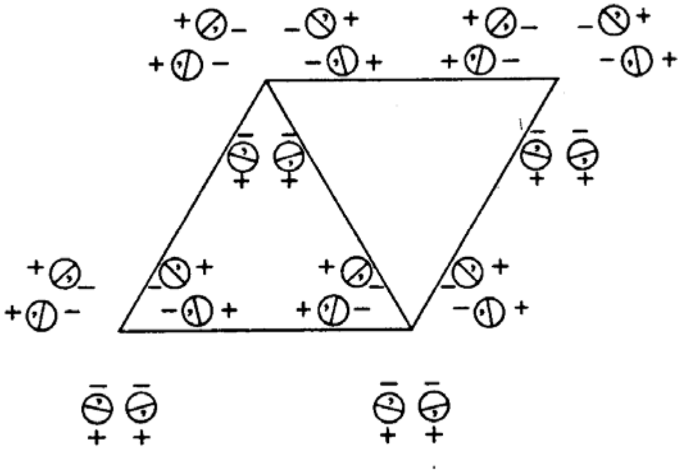


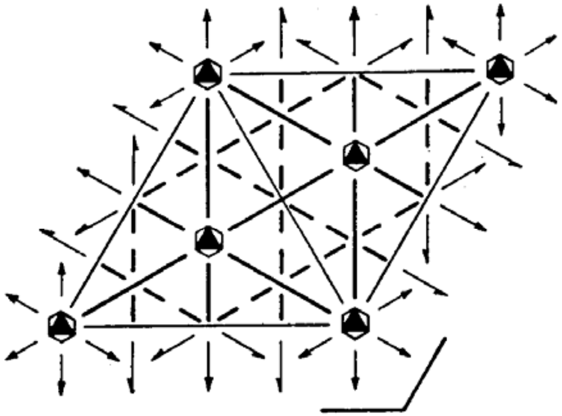
Origin at centre $(2/m)$ at $b\,(2/m\,,2_1/n)\,d$, at $0, -\frac{1}{4}, \frac{1}{8}$ from $\bar{4}m\,2$

International Tables for X-ray Crystallography

$P\bar{6}m2$ D_{3h}^1 $\bar{6}m2$ Hexagonal

No. 187 $P\bar{6}m2$ Patterson symmetry $P6/mmm$



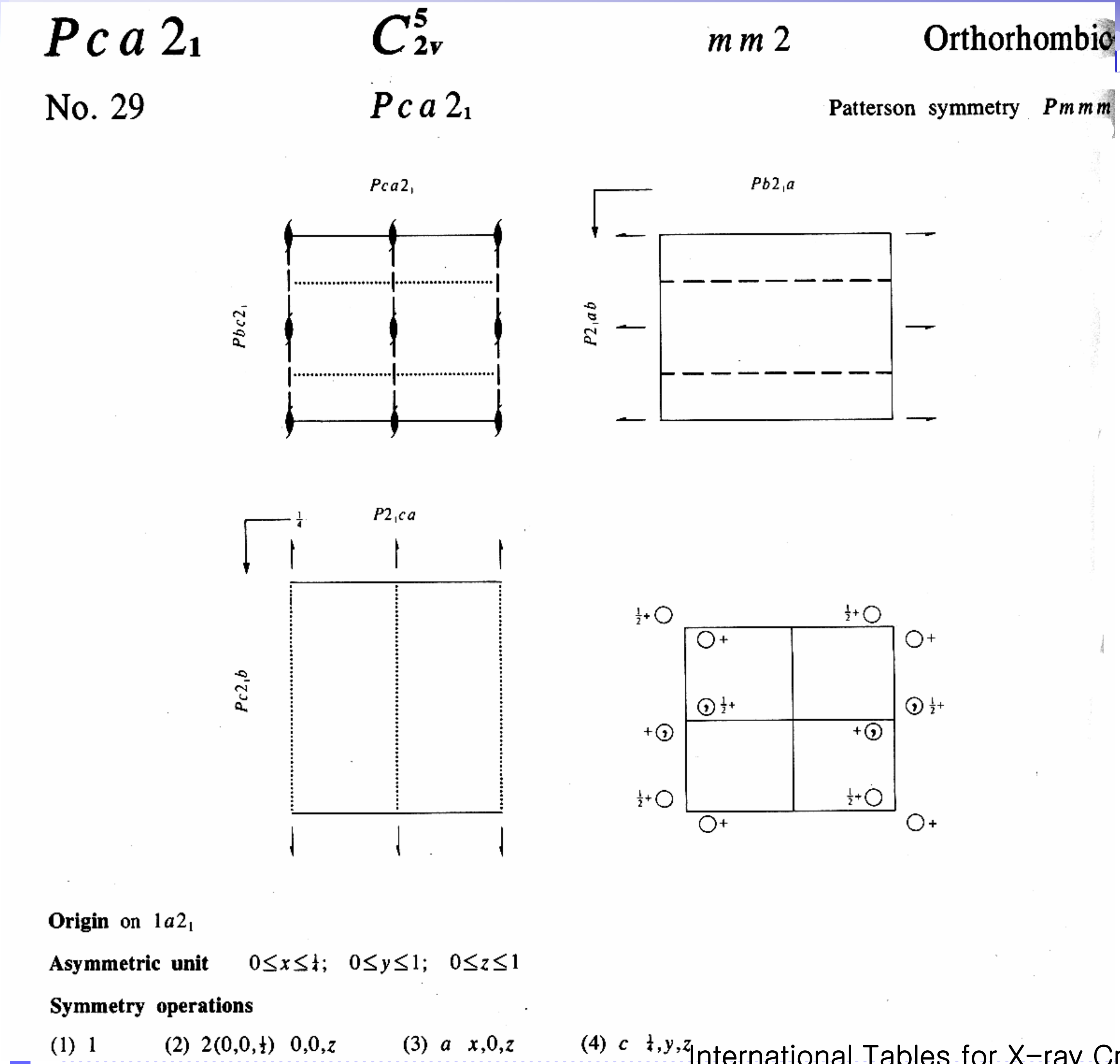


Origin at $\bar{6}m2$

Asymmetric unit $0 \leq x \leq \frac{2}{3}$; $0 \leq y \leq \frac{2}{3}$; $0 \leq z \leq \frac{1}{2}$; $x \leq 2y$; $y \leq \min(1-x, 2x)$

Vertices $0,0,0$ $\frac{2}{3},\frac{1}{3},0$ $\frac{1}{3},\frac{2}{3},0$
$0,0,\frac{1}{2}$ $\frac{2}{3},\frac{1}{3},\frac{1}{2}$ $\frac{1}{3},\frac{2}{3},\frac{1}{2}$

International Tables for X-ray Crystallography



$Pca2_1$ C^5_{2v} $mm2$ Orthorhombic

No. 29 $Pca2_1$ Patterson symmetry $Pmmm$

Origin on $1a2_1$

Asymmetric unit $0 \le x \le \frac{1}{4}$; $0 \le y \le 1$; $0 \le z \le 1$

Symmetry operations

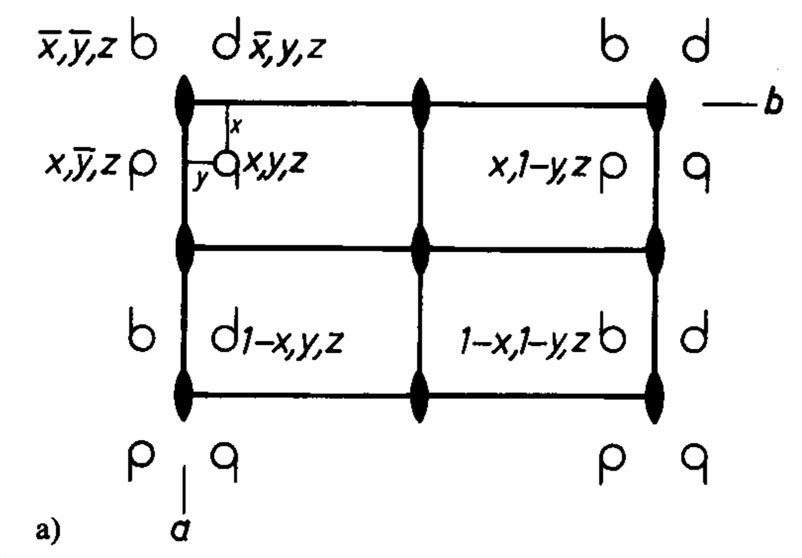
(1) 1 (2) $2(0,0,\frac{1}{2})$ $0,0,z$ (3) a $x,0,z$ (4) c $\frac{1}{4},y,z$

International Tables for X-ray Crystallography

Space Groups-Pmm2

- Pmm2- for a point x, y, z (general point) symmetry element generates $\bar{x}, y, z;\ x, \bar{y}, z;\ \bar{x}, \bar{y}, z$

  $x, y, z;\ \bar{x}, y, z;\ x, \bar{y}, z;\ \bar{x}, \bar{y}, z$ are equivalent (multiplicity of 4)
- The number of equivalent points in the unit cell is called its multiplicity.
- A general position is a set of equivalent points with point symmetry (site symmetry) 1.



Space Groups-Pmm2

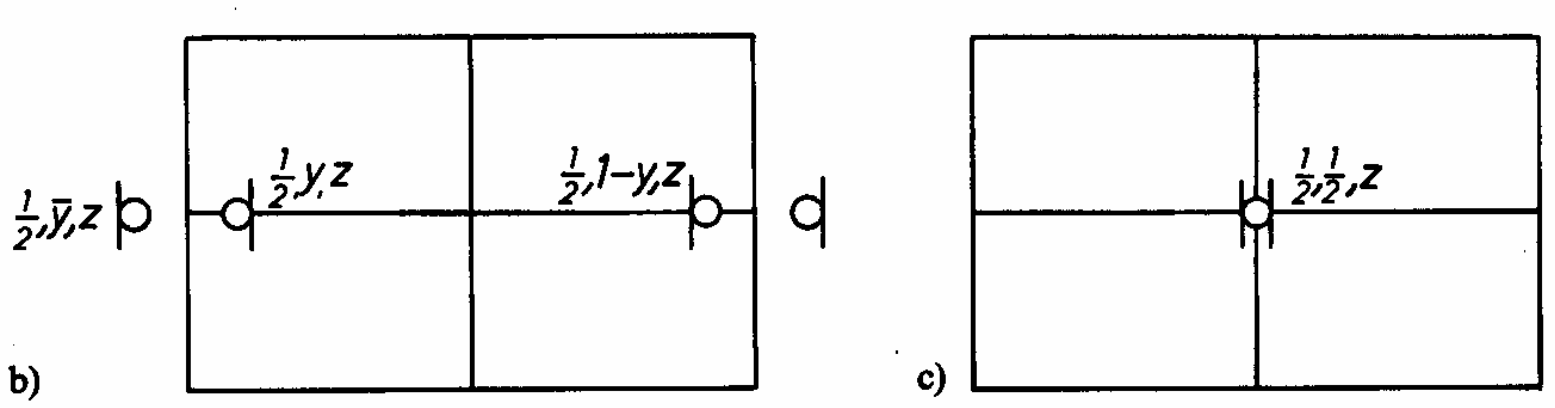
- move a point x, y, z on to mirror plane at $\frac{1}{2}, y, z$

  x, y, z and $1 - x, y, z$ coalesce to $\frac{1}{2}, y, z$

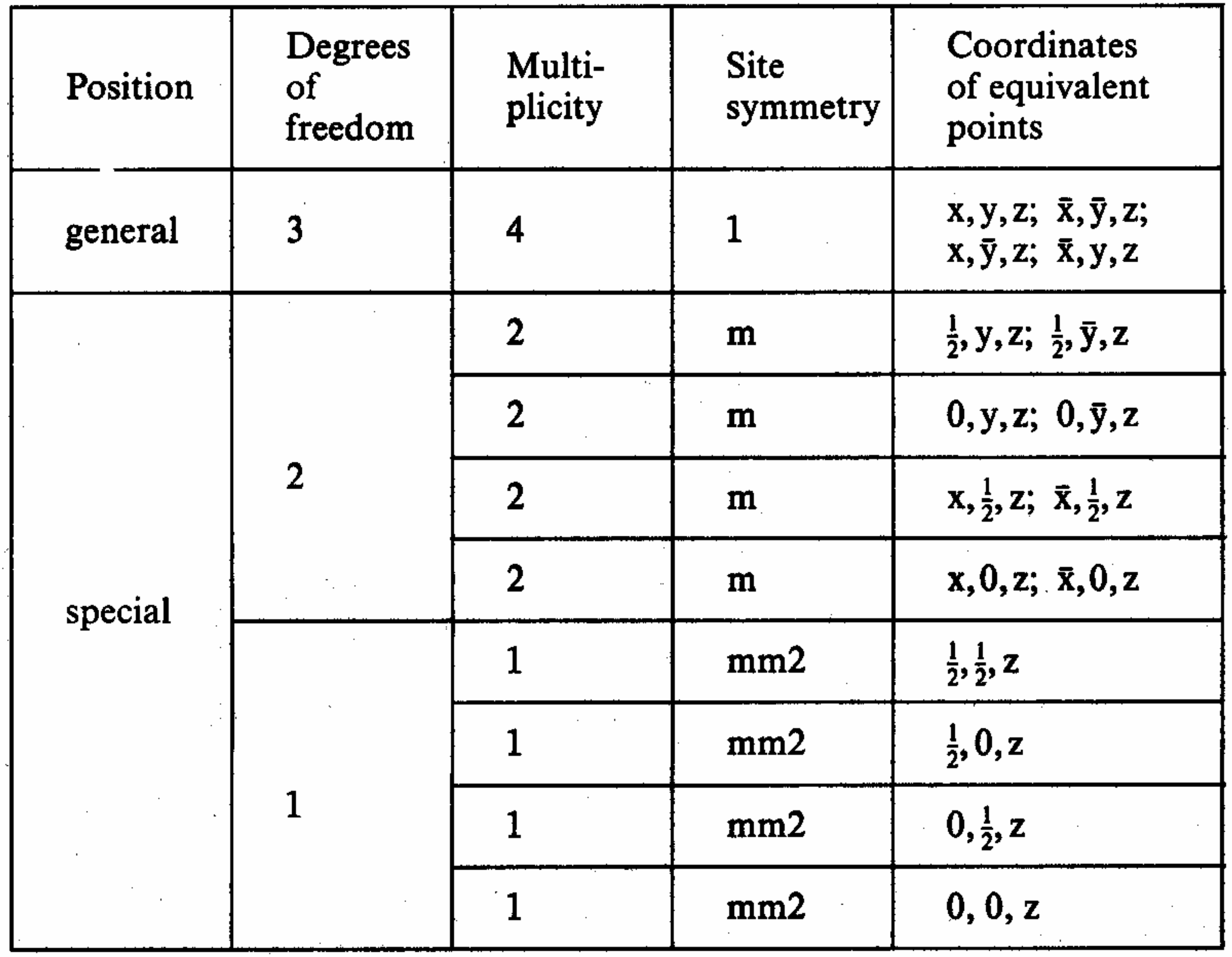
  $x, 1 - y, z$ and $1 - x, 1 - y, z$ coalesce to $\frac{1}{2}, 1 - y, z$

  multiplicity of 2

  as long as the point remains on the mirror plane, its multiplicity is unchanged- degree of freedom 2
- A special position is a set of equivalent points with point symmetry (site symmetry) higher than 1.



Space Groups-Pmm2



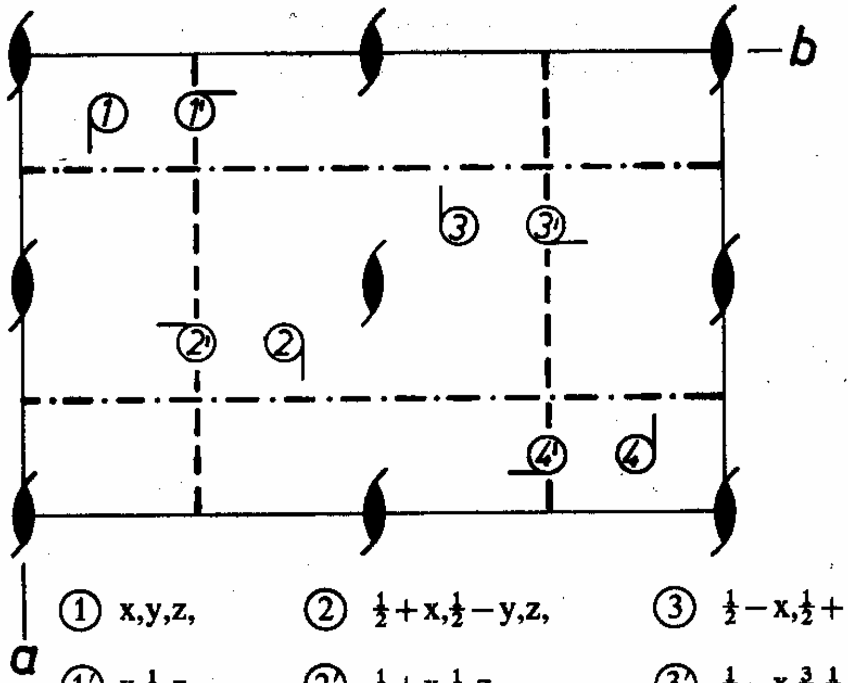
Position	Degrees of freedom	Multi-plicity	Site symmetry	Coordinates of equivalent points
general	3	4	1	$x,y,z;\ \bar{x},\bar{y},z;$ $x,\bar{y},z;\ \bar{x},y,z$
special	2	2	m	$\frac{1}{2},y,z;\ \frac{1}{2},\bar{y},z$
		2	m	$0,y,z;\ 0,\bar{y},z$
		2	m	$x,\frac{1}{2},z;\ \bar{x},\frac{1}{2},z$
		2	m	$x,0,z;\ \bar{x},0,z$
	1	1	mm2	$\frac{1}{2},\frac{1}{2},z$
		1	mm2	$\frac{1}{2},0,z$
		1	mm2	$0,\frac{1}{2},z$
		1	mm2	$0,0,z$

Space Groups-multiplicity

- screw axis and glide plane do not alter the multiplicity of a point

-Pna2_1: orthorhombic

n-glide normal to a-axis
a-glide normal to b-axis
2_1 screw axis along c-axis



① $x, y, z,$
② $\frac{1}{2}+x, \frac{1}{2}-y, z,$
③ $\frac{1}{2}-x, \frac{1}{2}+y, \frac{1}{2}+z,$
④ $1-x, 1-y, \frac{1}{2}+z$
①' $x, \frac{1}{4}, z,$
②' $\frac{1}{2}+x, \frac{1}{4}, z,$
③' $\frac{1}{2}-x, \frac{3}{4}, \frac{1}{2}+z,$
④' $1-x, \frac{3}{4}, \frac{1}{2}+z$

no special position

Space Groups-asymmetric unit

-The asymmetric unit of a space group is the smallest part of the unit cell from which the whole cell may be filled by the operation of all the symmetry operations. It volume is given by:

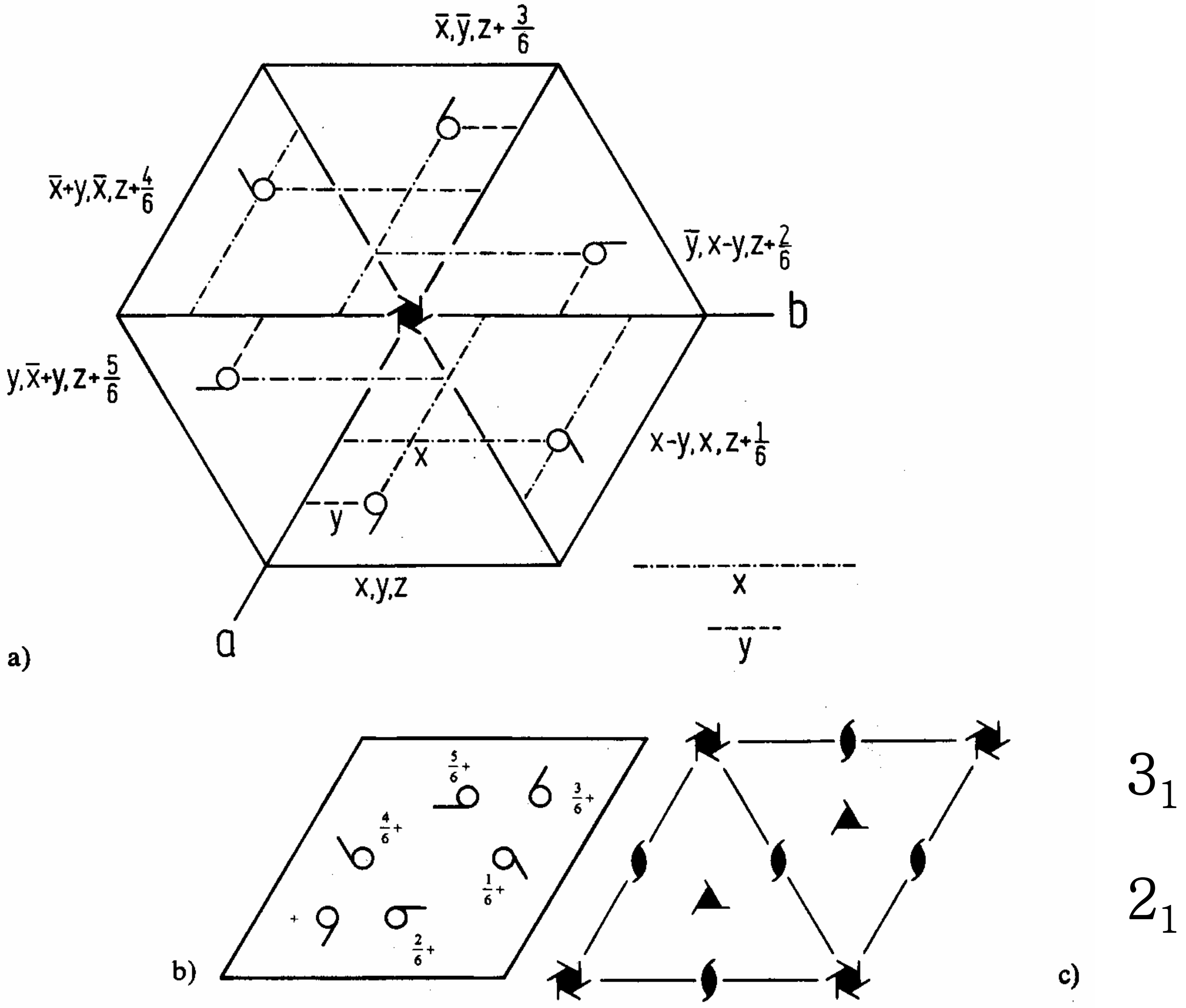
$$V_{\text{asymm.unit}} = \frac{V_{\text{unit cell}}}{\text{multiplicity of general position}}$$

ex) Pmm2- multiplicity of 4, vol. of asymm=1/4 unit cell

$$0 \leq x \leq \tfrac{1}{2},\ 0 \leq y \leq \tfrac{1}{2},\ 0 \leq z \leq 1$$

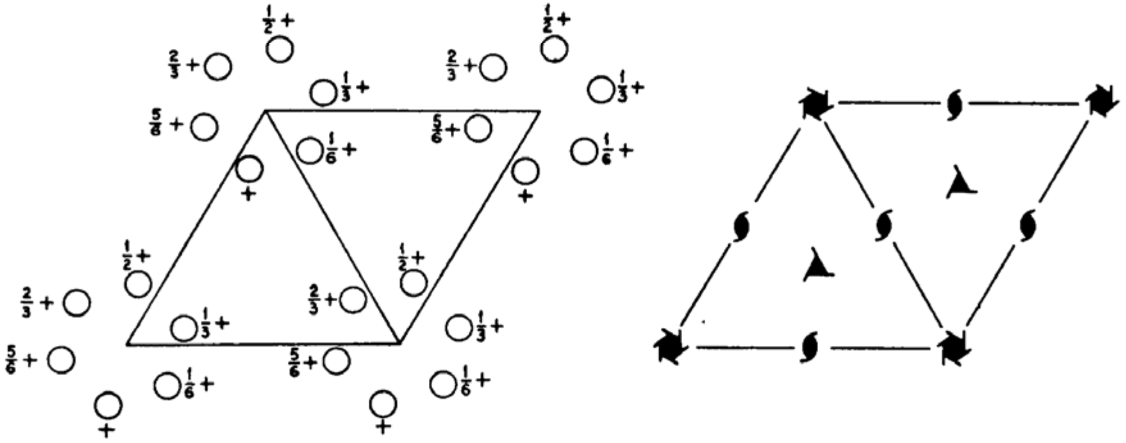
-An asymmetric unit contains all the information necessary for the complete descript of a crystal structure.

Space Groups-P6_1



$P\,6_1$ C_6^2 6 Hexagonal

No. 169 $P\,6_1$ Patterson symmetry $P\,6/m$



Origin on 6_1

Asymmetric unit $0\leq x\leq 1;\ \ 0\leq y\leq 1;\ \ 0\leq z\leq \frac{1}{6}$

Vertices	0,0,0	1,0,0	1,1,0	0,1,0
	0,0,$\frac{1}{6}$	1,0,$\frac{1}{6}$	1,1,$\frac{1}{6}$	0,1,$\frac{1}{6}$

Symmetry operations

(1) 1
(2) $3^{+}(0,0,\frac{1}{3})$ $0,0,z$
(3) $3^{-}(0,0,\frac{2}{3})$ $0,0,z$
(4) $2(0,0,\frac{1}{2})$ $0,0,z$
(5) $6^{-}(0,0,\frac{5}{6})$ $0,0,z$
(6) $6^{+}(0,0,\frac{1}{6})$ $0,0,z$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (4)

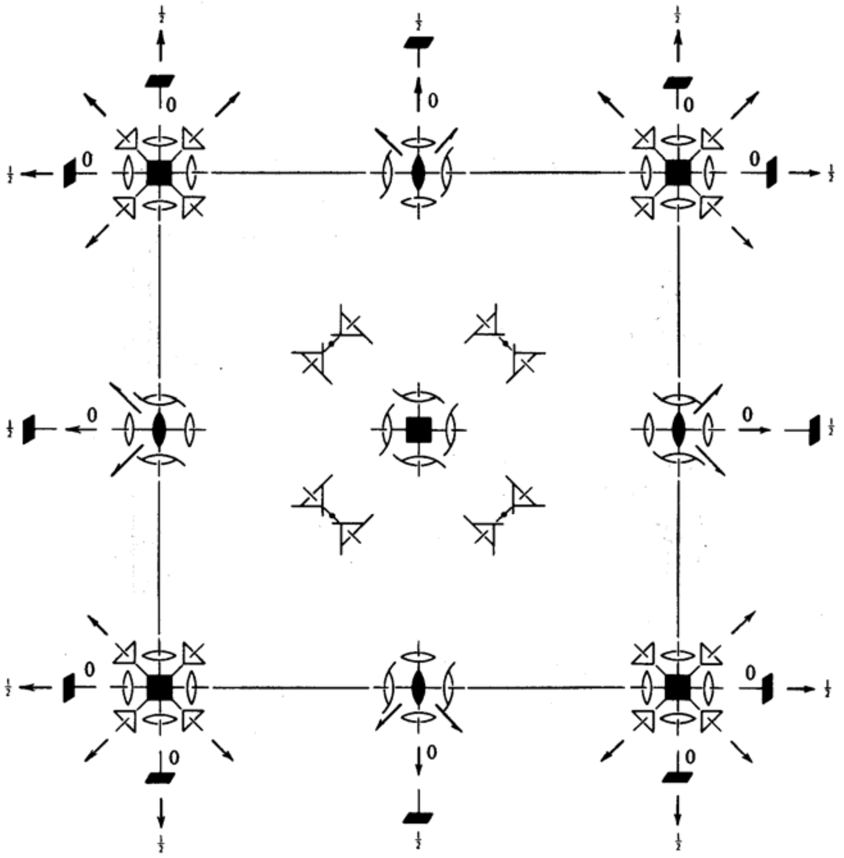
Positions

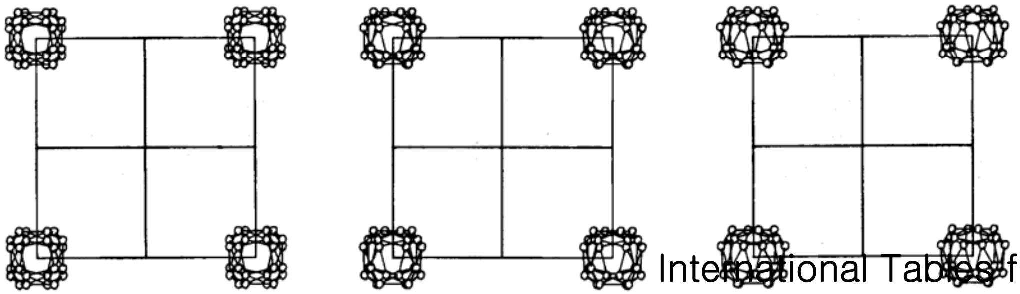
Multiplicity, Wyckoff letter, Site symmetry	Coordinates			Reflection conditions
				General:
6 *a* 1	(1) x,y,z	(2) $\bar{y},x-y,z+\frac{1}{3}$	(3) $\bar{x}+y,\bar{x},z+\frac{2}{3}$	$000l$: $l=6n$
	(4) $\bar{x},\bar{y},z+\frac{1}{2}$	(5) $y,\bar{x}+y,z+\frac{5}{6}$	(6) $x-y,x,z+\frac{1}{6}$	

International Tables for X-ray Crystallography

P 4 3 2 O^1 432 **Cubic**

No. 207 P 4 3 2 Patterson symmetry $Pm\bar{3}m$

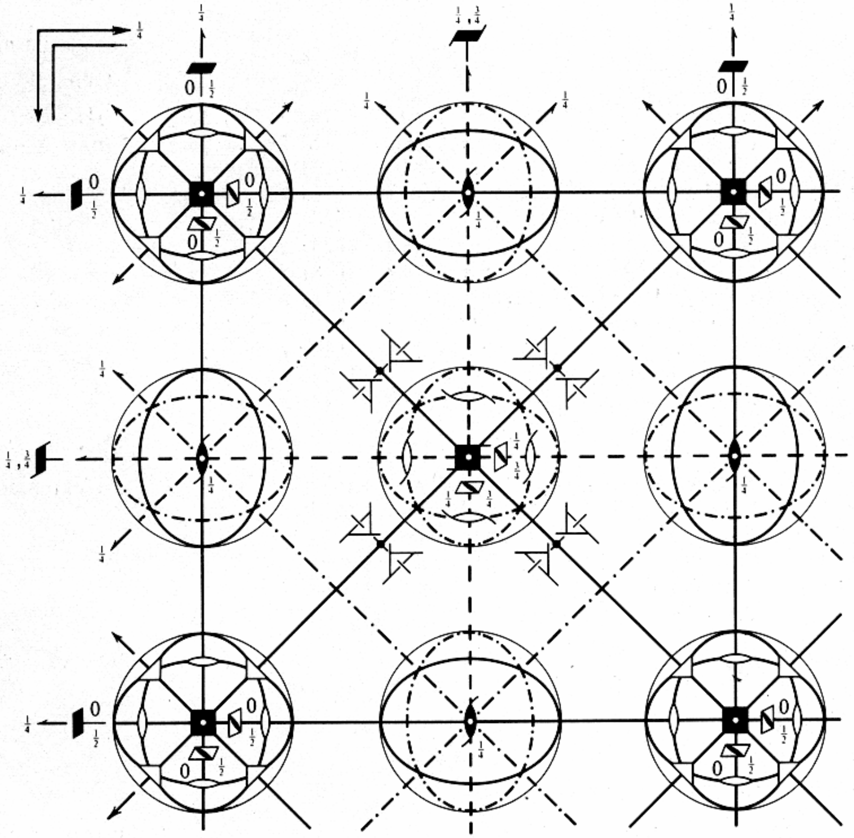




International Tables for X-ray Crystallography

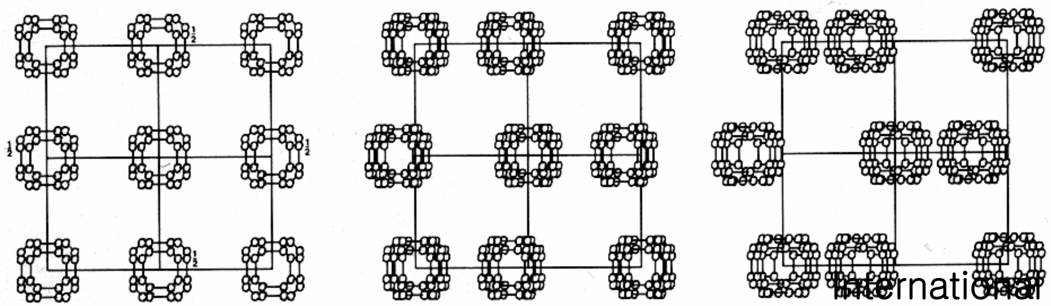
$Fm\bar{3}m$ O_h^5 $m\bar{3}m$ Cubic

No. 225 $F4/m\,\bar{3}\,2/m$ Patterson symmetry $Fm\bar{3}m$

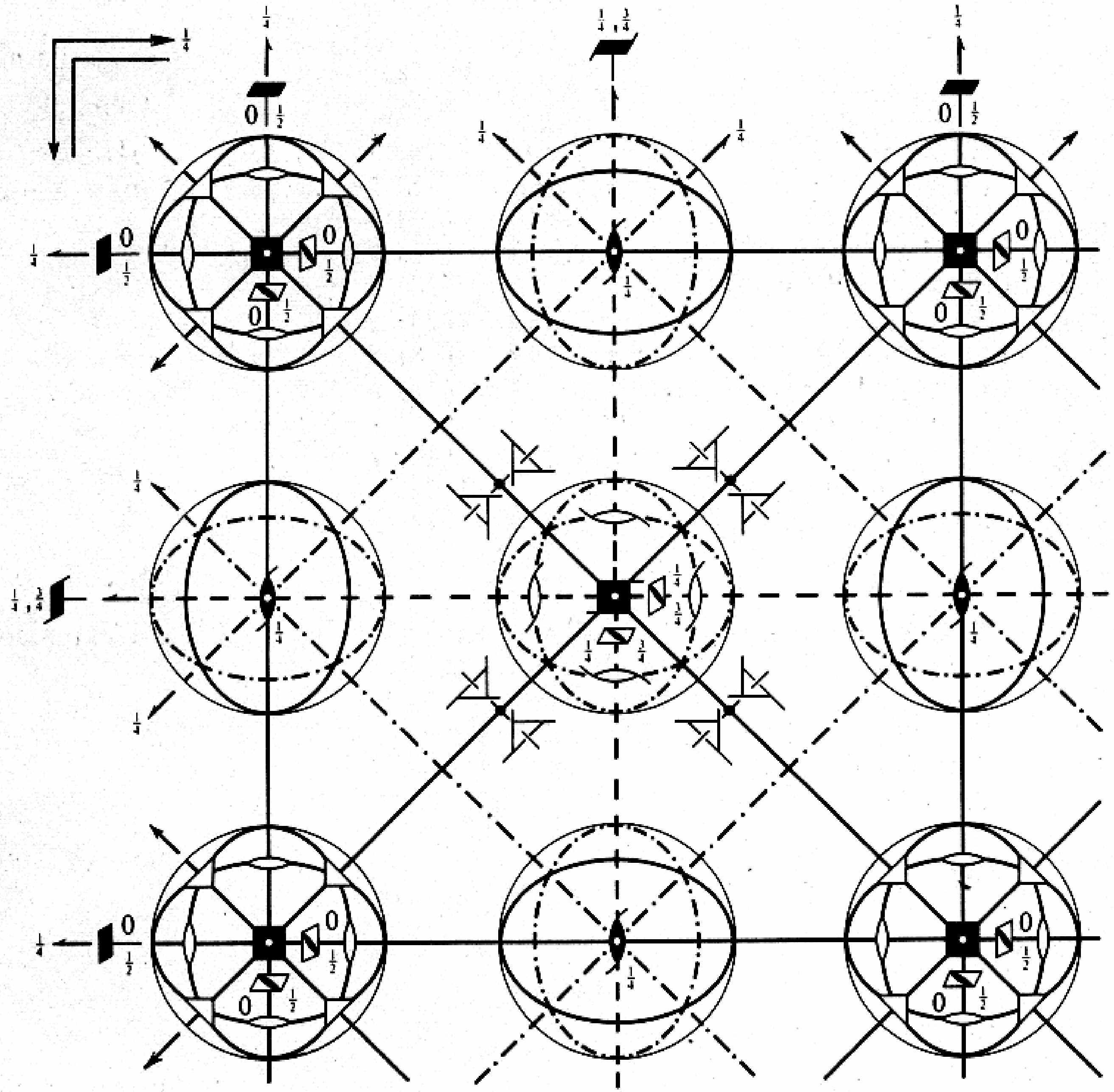


Upper left quadrant only

orthographic
representation

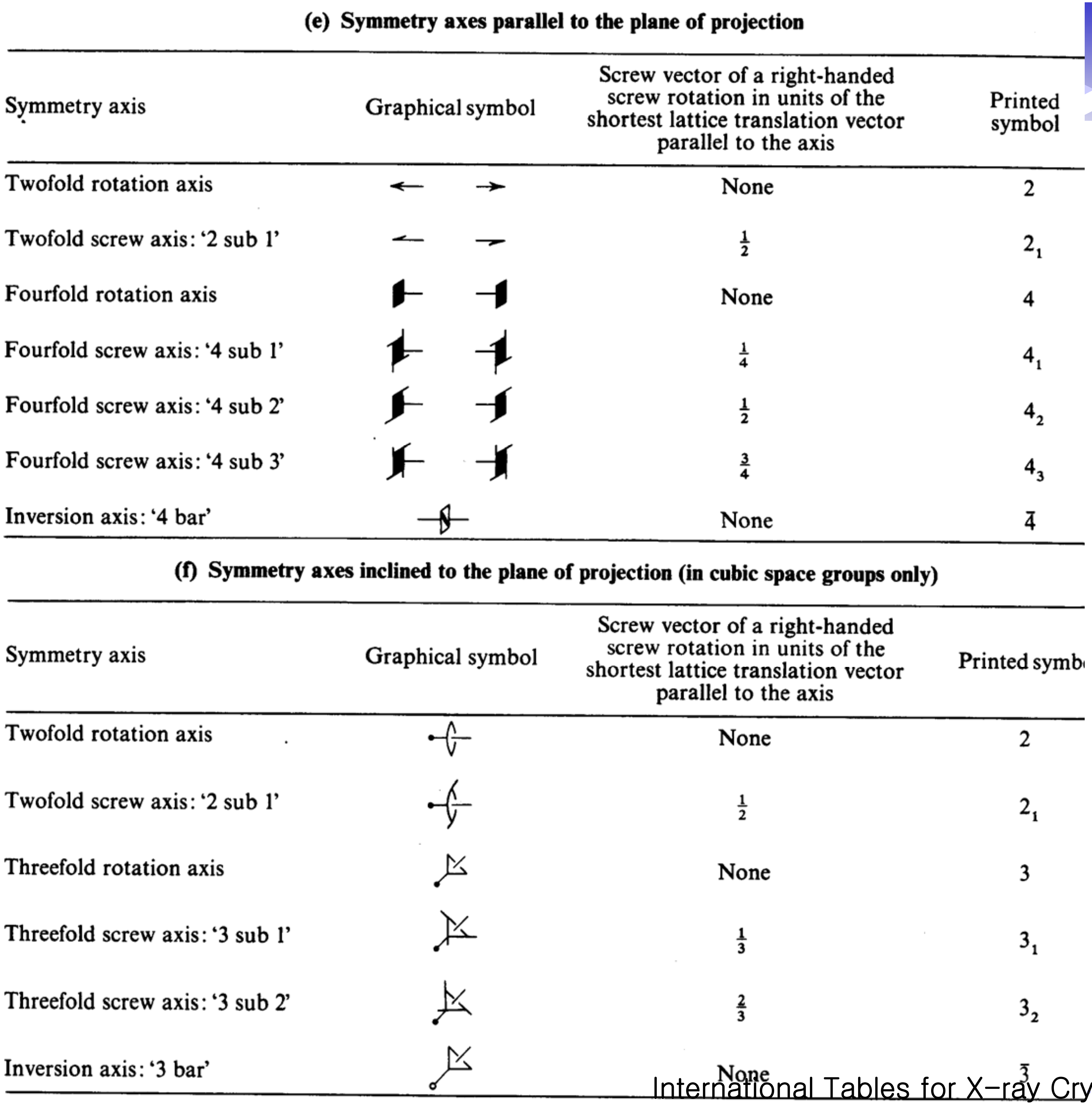


International Tables for X-ray Crystallography



Upper left quadrant only

International Tables for X-ray Crystallography



(e) Symmetry axes parallel to the plane of projection

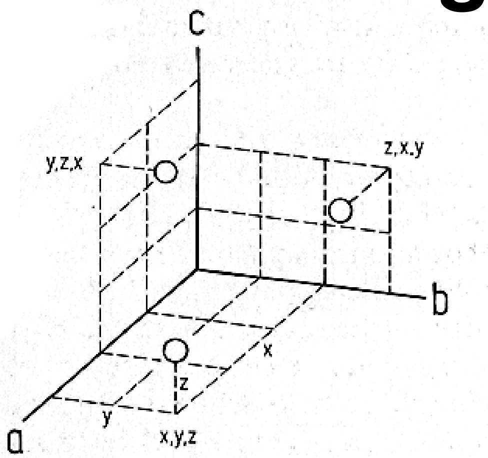
Symmetry axis	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symbol
Twofold rotation axis		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Fourfold rotation axis		None	4
Fourfold screw axis: '4 sub 1'		$\frac{1}{4}$	4_1
Fourfold screw axis: '4 sub 2'		$\frac{1}{2}$	4_2
Fourfold screw axis: '4 sub 3'		$\frac{3}{4}$	4_3
Inversion axis: '4 bar'		None	$\bar{4}$

(f) Symmetry axes inclined to the plane of projection (in cubic space groups only)

Symmetry axis	Graphical symbol	Screw vector of a right-handed screw rotation in units of the shortest lattice translation vector parallel to the axis	Printed symb
Twofold rotation axis		None	2
Twofold screw axis: '2 sub 1'		$\frac{1}{2}$	2_1
Threefold rotation axis		None	3
Threefold screw axis: '3 sub 1'		$\frac{1}{3}$	3_1
Threefold screw axis: '3 sub 2'		$\frac{2}{3}$	3_2
Inversion axis: '3 bar'		None	$\bar{3}$

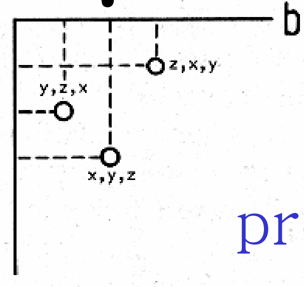
International Tables for X-ray Crystallography

48-fold general position



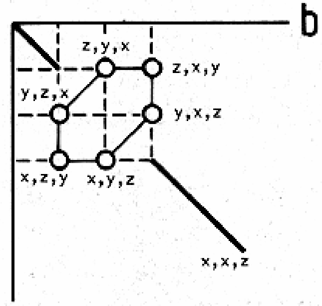
a)

3-fold rotation



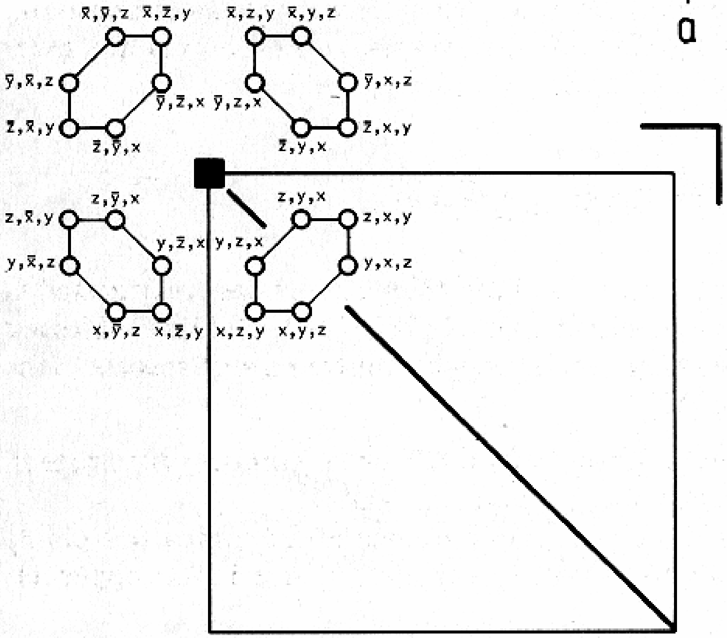
projection on x,y,0

b)



c)

mirror plane at x,x,z

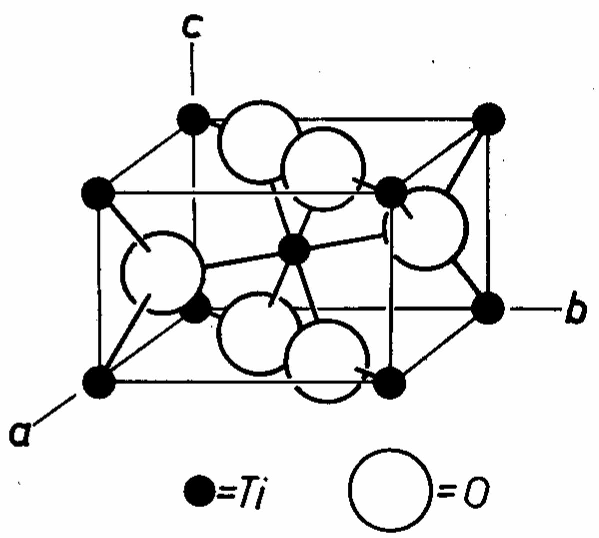


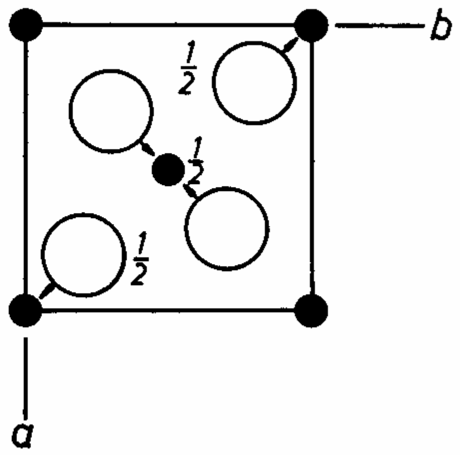
d)

4-fold rotation at 0,0,z

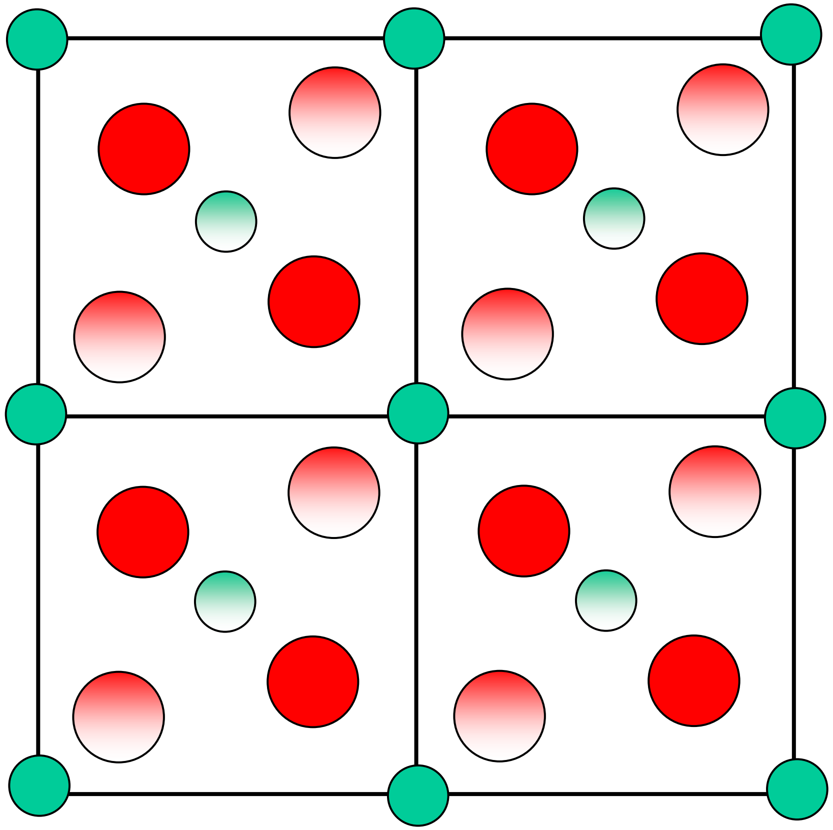
Rutile, TiO_2

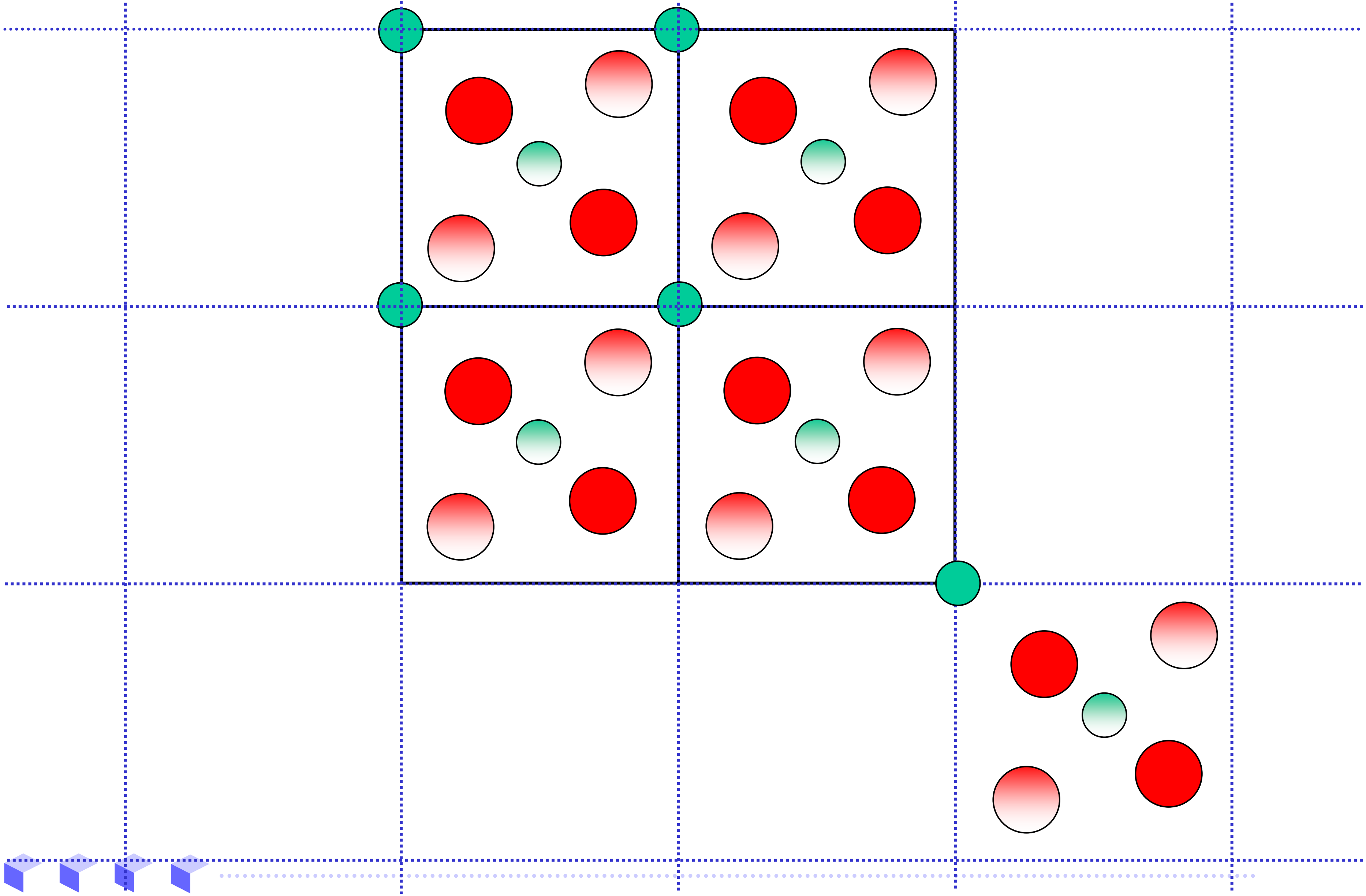
A		B			
Lattice	Basis	Space group	Positions of the atoms		
tetragonal P	Ti: 0,0,0 $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	P 4_2/mnm	a	Ti: 0,0,0 $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	
$a_0 = 4.59$ Å $c_0 = 2.96$ Å	O: 0.3, 0.3, 0 0.8, 0.2, $\frac{1}{2}$ 0.2, 0.8, $\frac{1}{2}$ 0.7, 0.7, 0	$a_0 = 4.59$ Å $c_0 = 2.96$ Å	f	O: x,x,0 $\frac{1}{2}+x, \frac{1}{2}-x, \frac{1}{2}$ $\frac{1}{2}-x, \frac{1}{2}+x, \frac{1}{2}$ $\bar{x}, \bar{x}, 0$	x = 0.3





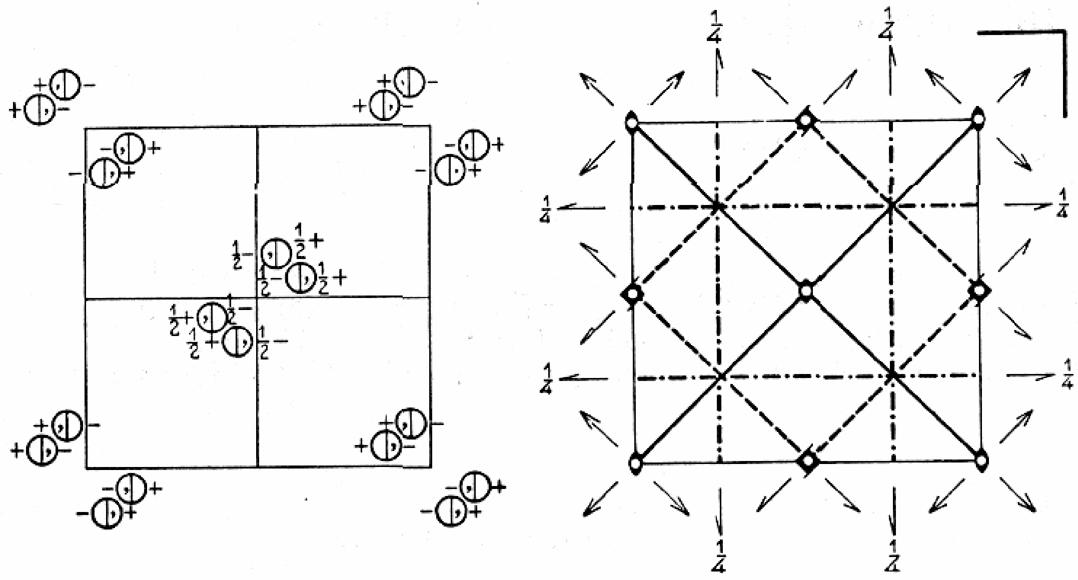
Rutile, TiO_2





$P\,4_2/m\,n\,m$ $\quad$ D_{4h}^{14} $\quad$ $4/m\,m\,m$ $\quad$ Tetragonal

No. 136 $\quad$ $P\,4_2/m\,2_1/n\,2/m$ $\quad$ Patterson symmetry $P\,4/m\,m\,m$



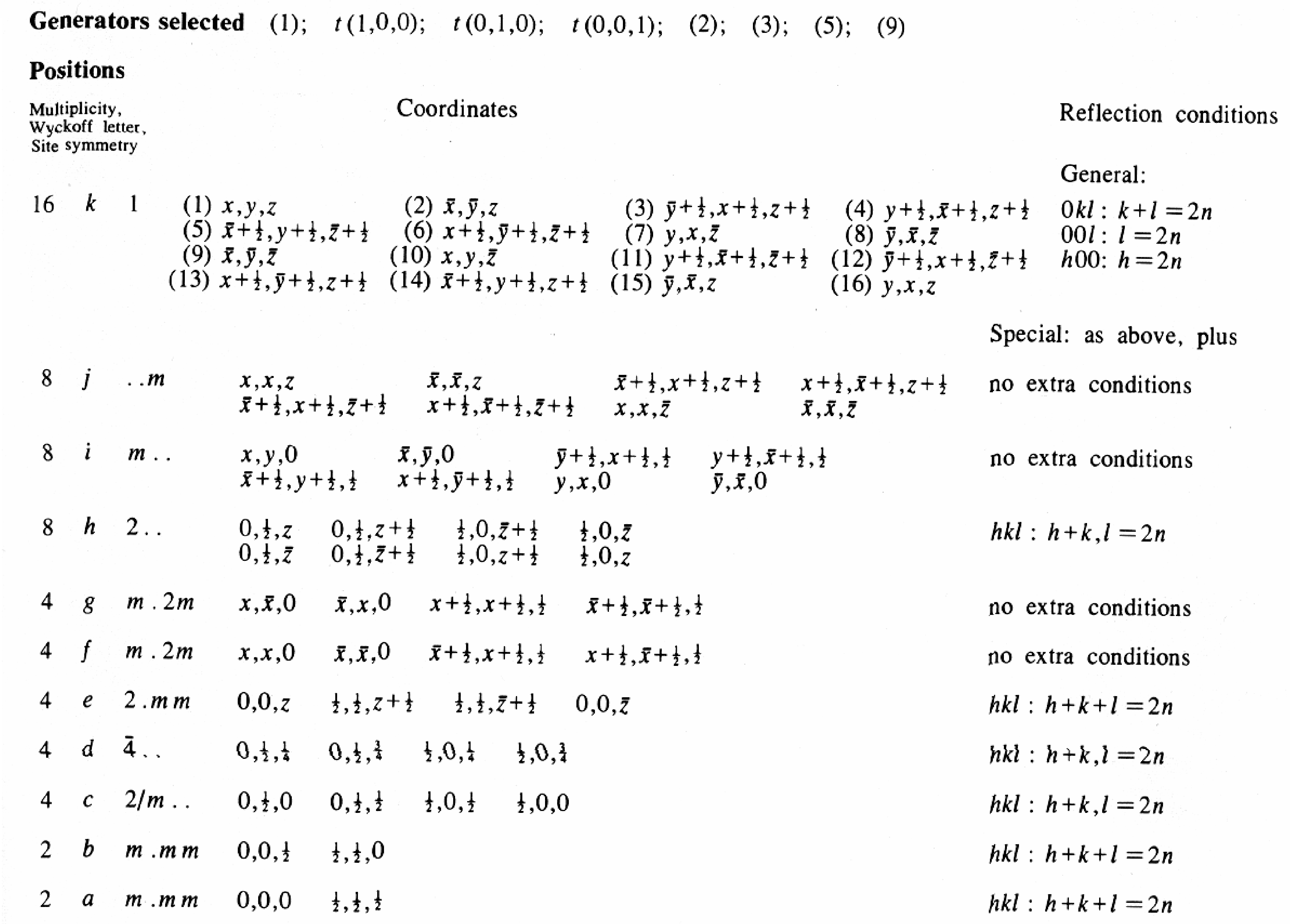
Origin at centre $(m\,m\,m)$ at $2/m\,1\,2/m$

Asymmetric unit $\quad 0\leq x\leq\frac{1}{2};\quad 0\leq y\leq\frac{1}{2};\quad 0\leq z\leq\frac{1}{2};\quad x\leq y$

Symmetry operations

(1) 1	(2) $2\quad 0,0,z$	(3) $4^+(0,0,\frac{1}{2})\quad 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\quad \frac{1}{2},0,z$
(5) $2(0,\frac{1}{2},0)\quad \frac{1}{4},y,\frac{1}{4}$	(6) $2(\frac{1}{2},0,0)\quad x,\frac{1}{4},\frac{1}{4}$	(7) $2\quad x,x,0$	(8) $2\quad x,\bar{x},0$
(9) $\bar{1}\quad 0,0,0$	(10) $m\quad x,y,0$	(11) $\bar{4}^+\quad \frac{1}{2},0,z;\ \frac{1}{2},0,\frac{1}{4}$	(12) $\bar{4}^-\quad 0,\frac{1}{2},z;\ 0,\frac{1}{2},\frac{1}{4}$
(13) $n(\frac{1}{2},0,\frac{1}{2})\quad x,\frac{1}{4},z$	(14) $n(0,\frac{1}{2},\frac{1}{2})\quad \frac{1}{4},y,z$	(15) $m\quad x,\bar{x},z$	(16) $m\quad x,x,z$

International Tables for X-ray Crystallography



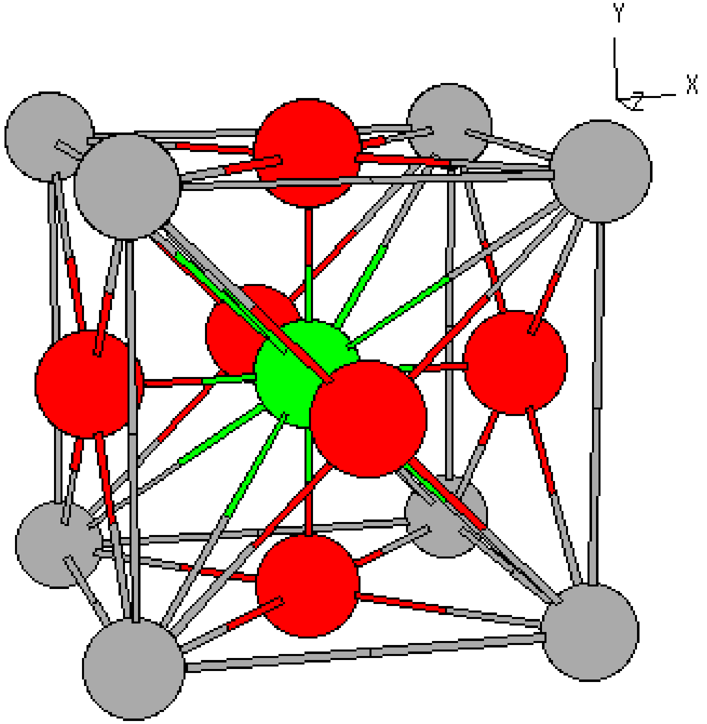
Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (9)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates	Reflection conditions
				General:
16	k	1	(1) x,y,z (2) $\bar{x},\bar{y},z$ (3) $\bar{y}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ (4) $y+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ (5) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}+\frac{1}{2}$ (6) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (7) $y,x,\bar{z}$ (8) $\bar{y},\bar{x},\bar{z}$ (9) $\bar{x},\bar{y},\bar{z}$ (10) $x,y,\bar{z}$ (11) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (12) $\bar{y}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ (13) $x+\frac{1}{2},\bar{y}+\frac{1}{2},z+\frac{1}{2}$ (14) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$ (15) $\bar{y},\bar{x},z$ (16) y,x,z	$0kl$: $k+l=2n$ $00l$: $l=2n$ $h00$: $h=2n$
				Special: as above, plus
8	j	$..m$	x,x,z $\bar{x},\bar{x},z$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},z+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},z+\frac{1}{2}$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}+\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}+\frac{1}{2}$ $x,x,\bar{z}$ $\bar{x},\bar{x},\bar{z}$	no extra conditions
8	i	$m..$	$x,y,0$ $\bar{x},\bar{y},0$ $\bar{y}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $y+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},y+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\bar{y}+\frac{1}{2},\frac{1}{2}$ $y,x,0$ $\bar{y},\bar{x},0$	no extra conditions
8	h	$2..$	$0,\frac{1}{2},z$ $0,\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,\bar{z}$ $0,\frac{1}{2},\bar{z}$ $0,\frac{1}{2},\bar{z}+\frac{1}{2}$ $\frac{1}{2},0,z+\frac{1}{2}$ $\frac{1}{2},0,z$	hkl : $h+k,l=2n$
4	g	$m.2m$	$x,\bar{x},0$ $\bar{x},x,0$ $x+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $\bar{x}+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	f	$m.2m$	$x,x,0$ $\bar{x},\bar{x},0$ $\bar{x}+\frac{1}{2},x+\frac{1}{2},\frac{1}{2}$ $x+\frac{1}{2},\bar{x}+\frac{1}{2},\frac{1}{2}$	no extra conditions
4	e	$2.mm$	$0,0,z$ $\frac{1}{2},\frac{1}{2},z+\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},\bar{z}+\frac{1}{2}$ $0,0,\bar{z}$	hkl : $h+k+l=2n$
4	d	$\bar{4}..$	$0,\frac{1}{2},\frac{1}{4}$ $0,\frac{1}{2},\frac{3}{4}$ $\frac{1}{2},0,\frac{1}{4}$ $\frac{1}{2},0,\frac{3}{4}$	hkl : $h+k,l=2n$
4	c	$2/m..$	$0,\frac{1}{2},0$ $0,\frac{1}{2},\frac{1}{2}$ $\frac{1}{2},0,\frac{1}{2}$ $\frac{1}{2},0,0$	hkl : $h+k,l=2n$
2	b	$m.mm$	$0,0,\frac{1}{2}$ $\frac{1}{2},\frac{1}{2},0$	hkl : $h+k+l=2n$
2	a	$m.mm$	$0,0,0$ $\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+k+l=2n$

International Tables for X-ray Crystallography

Perovskite, $CaTiO_3$



- Ca-corner
  O- face centered
  Ti- body centered
- high temperature- cubic
  Pm3m (No.221)

$$Ca: \ 1a, \ m\bar{3}m, \ \ 0,0,0$$

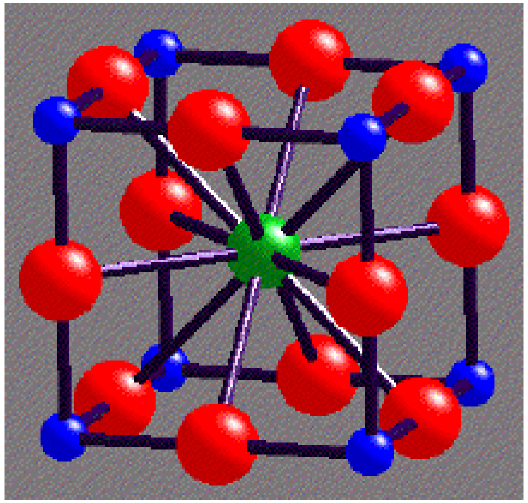
$$Ti: \ 1b, \ m\bar{3}m, \ \ \frac{1}{2},\frac{1}{2},\frac{1}{2}$$

$$O: \ 3c, \ 4/mmm, \ \ 0,\frac{1}{2},\frac{1}{2} \quad \frac{1}{2},0,\frac{1}{2} \quad \frac{1}{2},\frac{1}{2},0$$

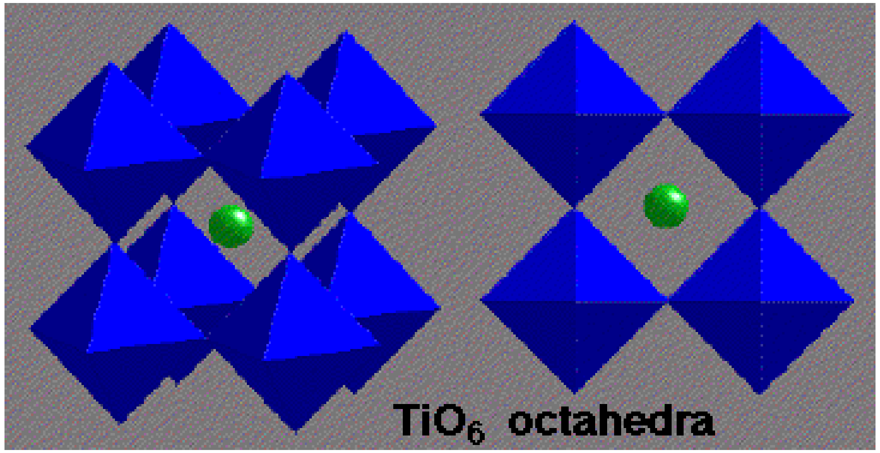
- Ti- 6O
  O- 4Ca+ 2Ti
  Ca- 12O

Perovskite
$CaTiO_3$

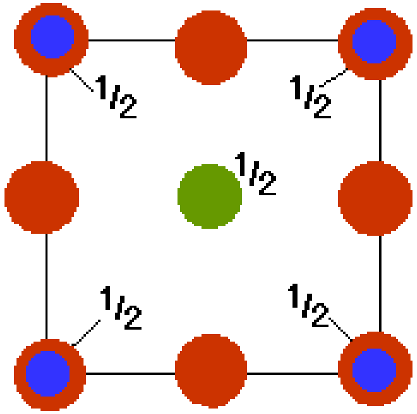
● Ca ● Ti ● O

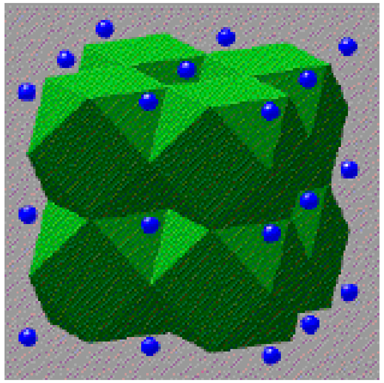


A-Cell

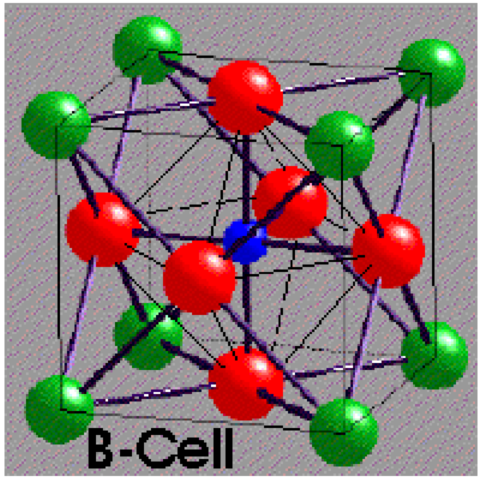


TiO_6 octahedra

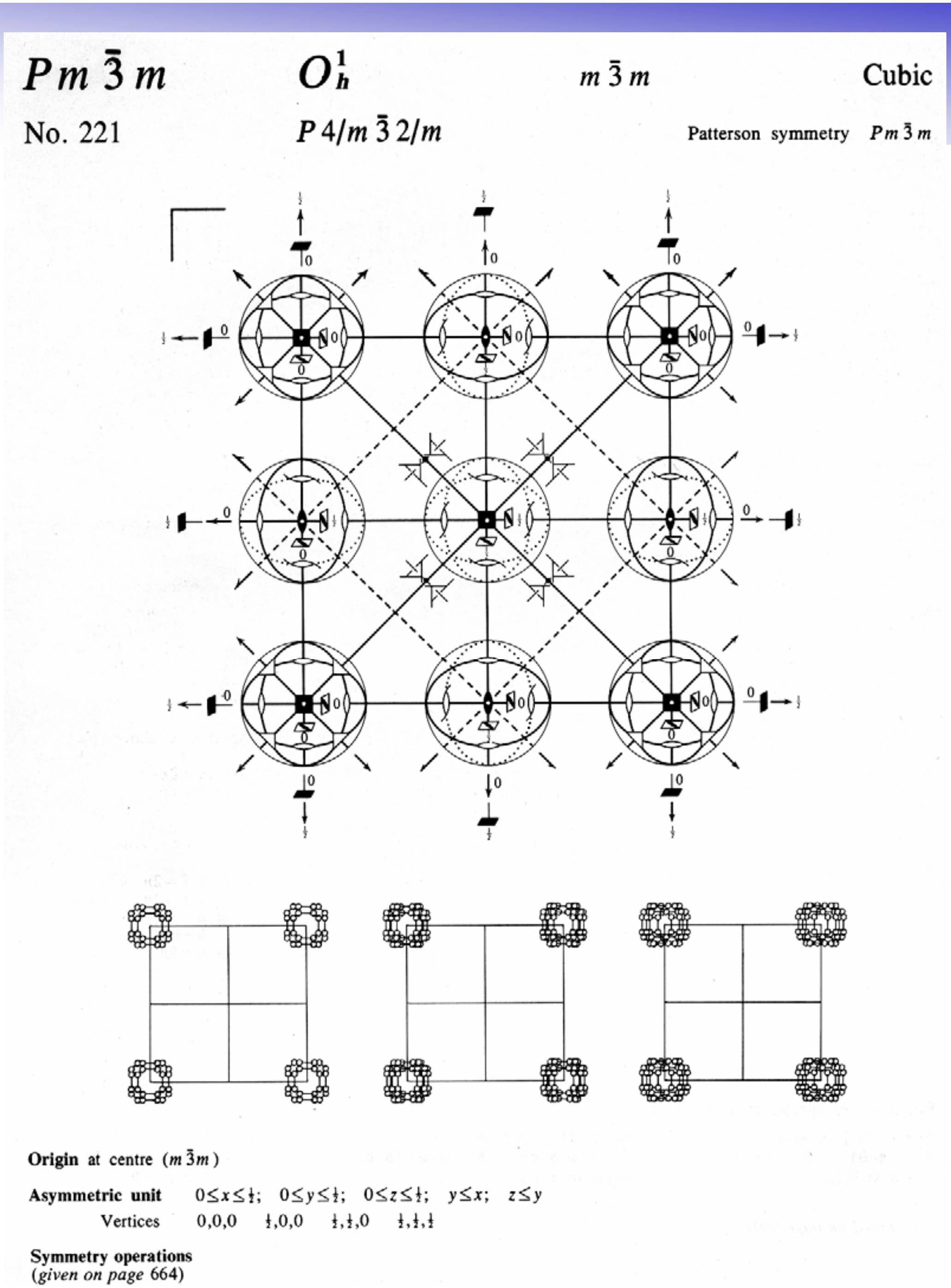




CaO_{12} cuboctahedra



B-Cell



$Pm\bar{3}m$ O_h^1 $m\bar{3}m$ Cubic

No. 221 $P4/m\,\bar{3}\,2/m$ Patterson symmetry $Pm\bar{3}m$

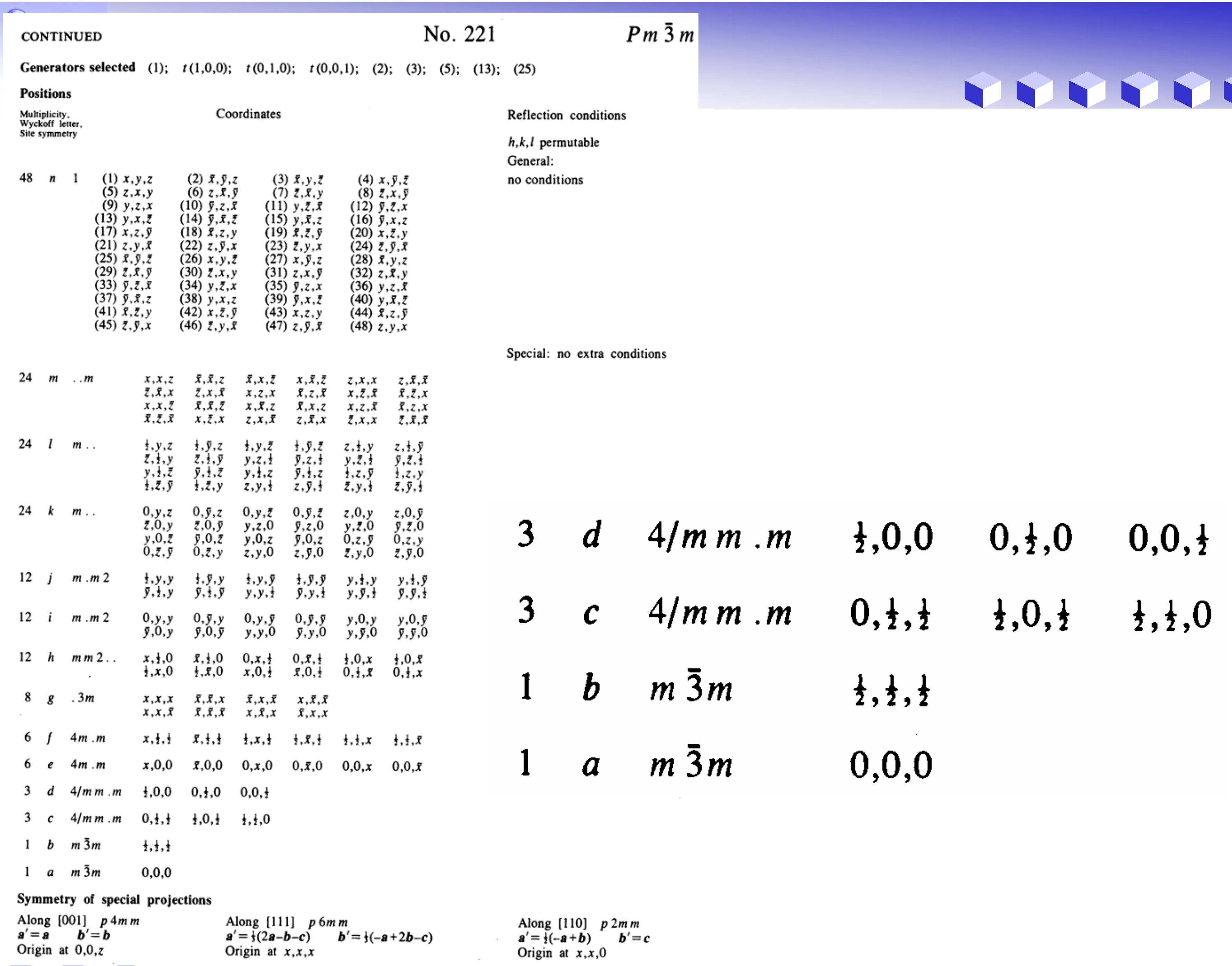
Origin at centre ($m\bar{3}m$)

Asymmetric unit $0 \le x \le \frac{1}{2}$; $0 \le y \le \frac{1}{2}$; $0 \le z \le \frac{1}{2}$; $y \le x$; $z \le y$

Vertices 0,0,0 ½,0,0 ½,½,0 ½,½,½

Symmetry operations
(*given on page* 664)

International Tables for X-ray Crystallography



CONTINUED No. 221 $Pm\bar{3}m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; (2); (3); (5); (13); (25)

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates					
48	n	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$		
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$		
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$		
			(13) $y,x,\bar{z}$	(14) $\bar{y},\bar{x},\bar{z}$	(15) $y,\bar{x},z$	(16) $\bar{y},x,z$		
			(17) $x,z,\bar{y}$	(18) $\bar{x},z,y$	(19) $\bar{x},\bar{z},\bar{y}$	(20) $x,\bar{z},y$		
			(21) $z,y,\bar{x}$	(22) $z,\bar{y},x$	(23) $\bar{z},y,x$	(24) $\bar{z},\bar{y},\bar{x}$		
			(25) $\bar{x},\bar{y},\bar{z}$	(26) $x,y,\bar{z}$	(27) $x,\bar{y},z$	(28) $\bar{x},y,z$		
			(29) $\bar{z},\bar{x},\bar{y}$	(30) $\bar{z},x,y$	(31) $z,x,\bar{y}$	(32) $z,\bar{x},y$		
			(33) $\bar{y},\bar{z},\bar{x}$	(34) $y,\bar{z},x$	(35) $\bar{y},z,x$	(36) $y,z,\bar{x}$		
			(37) $\bar{y},\bar{x},z$	(38) y,x,z	(39) $\bar{y},x,\bar{z}$	(40) $y,\bar{x},\bar{z}$		
			(41) $\bar{x},\bar{z},y$	(42) $x,\bar{z},\bar{y}$	(43) x,z,y	(44) $\bar{x},z,\bar{y}$		
			(45) $\bar{z},\bar{y},x$	(46) $\bar{z},y,\bar{x}$	(47) $z,\bar{y},\bar{x}$	(48) z,y,x		
24	m	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
			$x,x,\bar{z}$	$\bar{x},\bar{x},\bar{z}$	$x,\bar{x},z$	$\bar{x},x,z$	$x,z,\bar{x}$	$\bar{x},z,x$
			$\bar{x},\bar{z},\bar{x}$	$x,\bar{z},x$	$z,x,\bar{x}$	$z,\bar{x},x$	$\bar{z},x,x$	$\bar{z},\bar{x},\bar{x}$
24	l	$m..$	$\frac{1}{2},y,z$	$\frac{1}{2},\bar{y},z$	$\frac{1}{2},y,\bar{z}$	$\frac{1}{2},\bar{y},\bar{z}$	$z,\frac{1}{2},y$	$z,\frac{1}{2},\bar{y}$
			$\bar{z},\frac{1}{2},y$	$\bar{z},\frac{1}{2},\bar{y}$	$y,z,\frac{1}{2}$	$\bar{y},z,\frac{1}{2}$	$y,\bar{z},\frac{1}{2}$	$\bar{y},\bar{z},\frac{1}{2}$
			$y,\frac{1}{2},\bar{z}$	$\bar{y},\frac{1}{2},\bar{z}$	$y,\frac{1}{2},z$	$\bar{y},\frac{1}{2},z$	$\frac{1}{2},z,\bar{y}$	$\frac{1}{2},z,y$
			$\frac{1}{2},\bar{z},\bar{y}$	$\frac{1}{2},\bar{z},y$	$z,y,\frac{1}{2}$	$z,\bar{y},\frac{1}{2}$	$\bar{z},y,\frac{1}{2}$	$\bar{z},\bar{y},\frac{1}{2}$
24	k	$m..$	$0,y,z$	$0,\bar{y},z$	$0,y,\bar{z}$	$0,\bar{y},\bar{z}$	$z,0,y$	$z,0,\bar{y}$
			$\bar{z},0,y$	$\bar{z},0,\bar{y}$	$y,z,0$	$\bar{y},z,0$	$y,\bar{z},0$	$\bar{y},\bar{z},0$
			$y,0,\bar{z}$	$\bar{y},0,\bar{z}$	$y,0,z$	$\bar{y},0,z$	$0,z,\bar{y}$	$0,z,y$
			$0,\bar{z},\bar{y}$	$0,\bar{z},y$	$z,y,0$	$z,\bar{y},0$	$\bar{z},y,0$	$\bar{z},\bar{y},0$
12	j	$m.m2$	$\frac{1}{2},y,y$	$\frac{1}{2},\bar{y},y$	$\frac{1}{2},y,\bar{y}$	$\frac{1}{2},\bar{y},\bar{y}$	$y,\frac{1}{2},y$	$y,\frac{1}{2},\bar{y}$
			$\bar{y},\frac{1}{2},y$	$\bar{y},\frac{1}{2},\bar{y}$	$y,y,\frac{1}{2}$	$\bar{y},y,\frac{1}{2}$	$y,\bar{y},\frac{1}{2}$	$\bar{y},\bar{y},\frac{1}{2}$
12	i	$m.m2$	$0,y,y$	$0,\bar{y},y$	$0,y,\bar{y}$	$0,\bar{y},\bar{y}$	$y,0,y$	$y,0,\bar{y}$
			$\bar{y},0,y$	$\bar{y},0,\bar{y}$	$y,y,0$	$\bar{y},y,0$	$y,\bar{y},0$	$\bar{y},\bar{y},0$
12	h	$mm2..$	$x,\frac{1}{2},0$	$\bar{x},\frac{1}{2},0$	$0,x,\frac{1}{2}$	$0,\bar{x},\frac{1}{2}$	$\frac{1}{2},0,x$	$\frac{1}{2},0,\bar{x}$
			$\frac{1}{2},x,0$	$\frac{1}{2},\bar{x},0$	$x,0,\frac{1}{2}$	$\bar{x},0,\frac{1}{2}$	$0,\frac{1}{2},\bar{x}$	$0,\frac{1}{2},x$
8	g	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
			$x,x,\bar{x}$	$\bar{x},\bar{x},\bar{x}$	$x,\bar{x},x$	$\bar{x},x,x$		
6	f	$4m.m$	$x,\frac{1}{2},\frac{1}{2}$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},x,\frac{1}{2}$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},x$	$\frac{1}{2},\frac{1}{2},\bar{x}$
6	e	$4m.m$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
3	d	$4/mm.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$			
3	c	$4/mm.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
1	a	$m\bar{3}m$	$0,0,0$					

Reflection conditions

h,k,l permutable

General:

no conditions

Special: no extra conditions

Symmetry of special projections

Along [001] $p4mm$
$\mathbf{a}'=\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

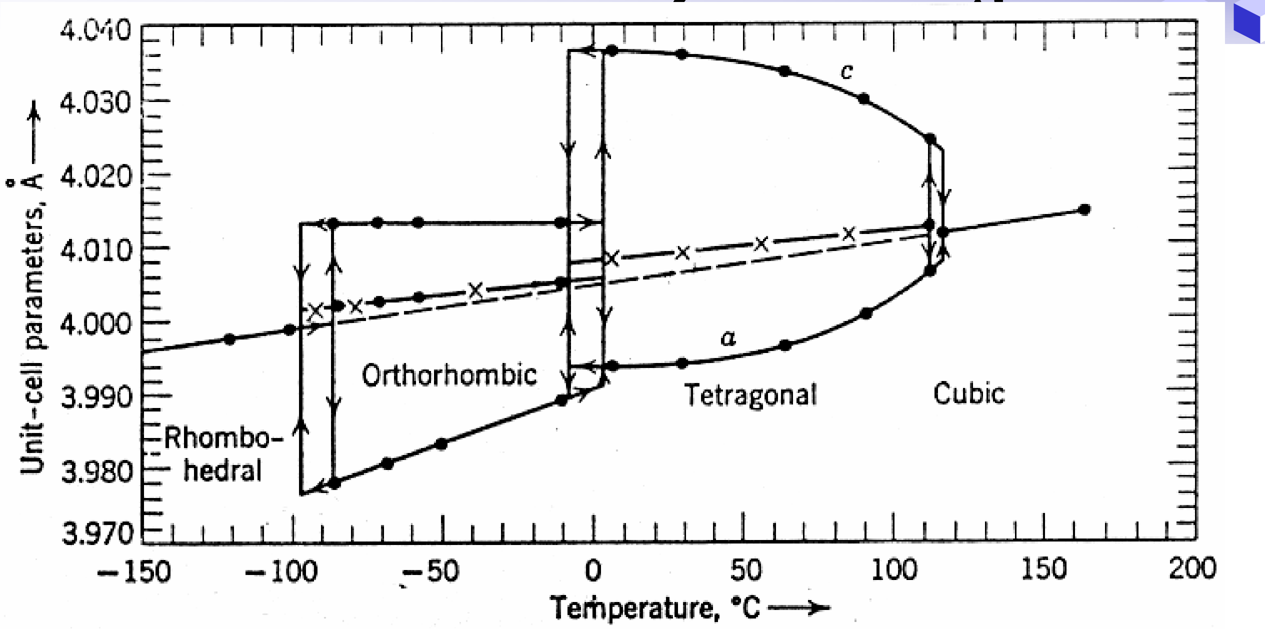
Along [111] $p6mm$
$\mathbf{a}'=\frac{1}{3}(2\mathbf{a}-\mathbf{b}-\mathbf{c})$ $\mathbf{b}'=\frac{1}{3}(-\mathbf{a}+2\mathbf{b}-\mathbf{c})$
Origin at x,x,x

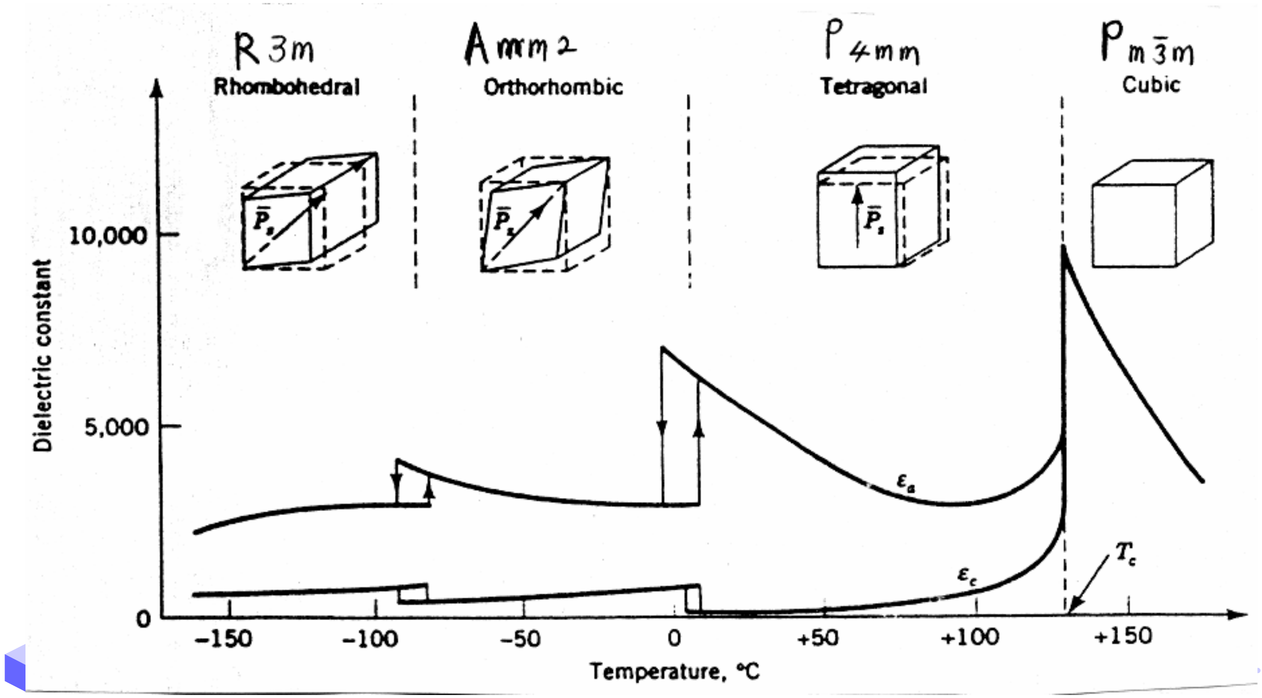
Along [110] $p2mm$
$\mathbf{a}'=\frac{1}{2}(-\mathbf{a}+\mathbf{b})$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,x,0$

3	d	$4/mm.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$
3	c	$4/mm.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
1	a	$m\bar{3}m$	$0,0,0$		

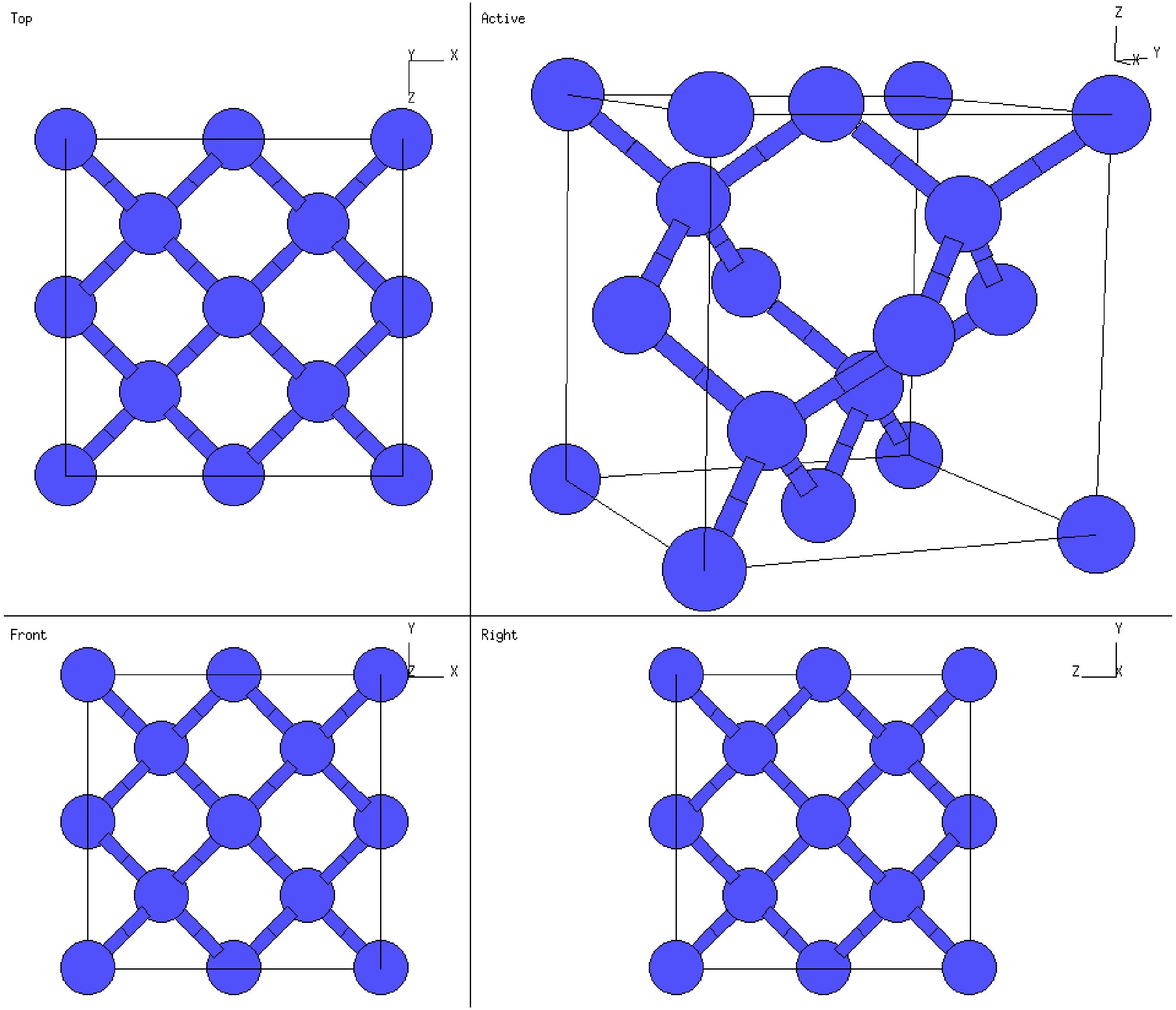
International Tables for X-ray Crystallography

Perovskite, $BaTiO_3$





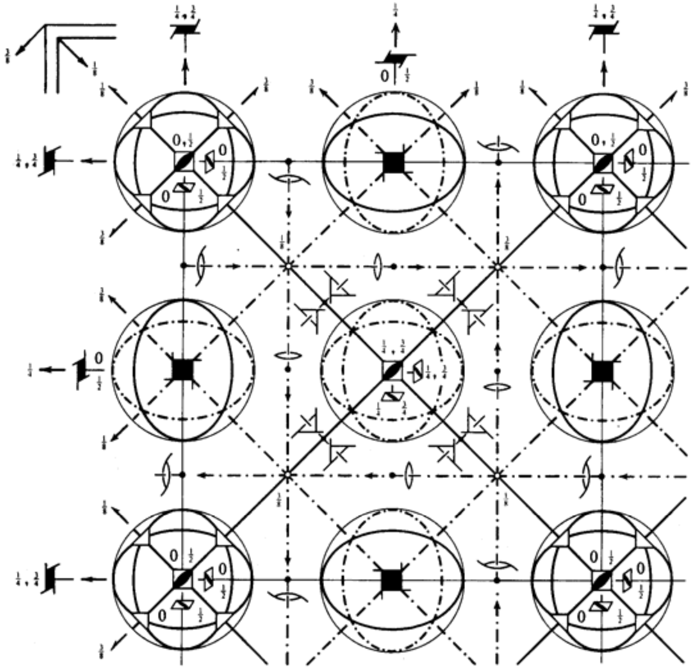
Diamond, C $F\frac{4_1}{d}\bar{3}\frac{2}{m}$ (No.227)



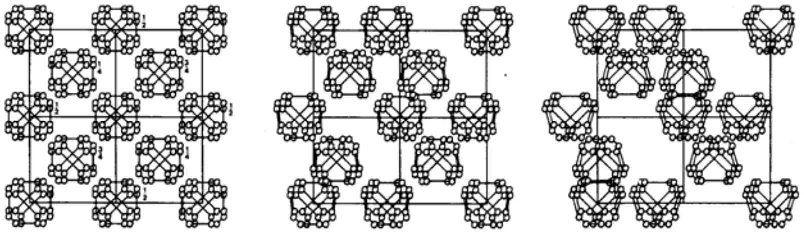
$Fd\bar{3}m$ O_h^7 $m\bar{3}m$ Cubic

No. 227 $F4_1/d\bar{3}2/m$ Patterson symmetry $Fm\bar{3}m$

ORIGIN CHOICE 1



Upper left quadrant only



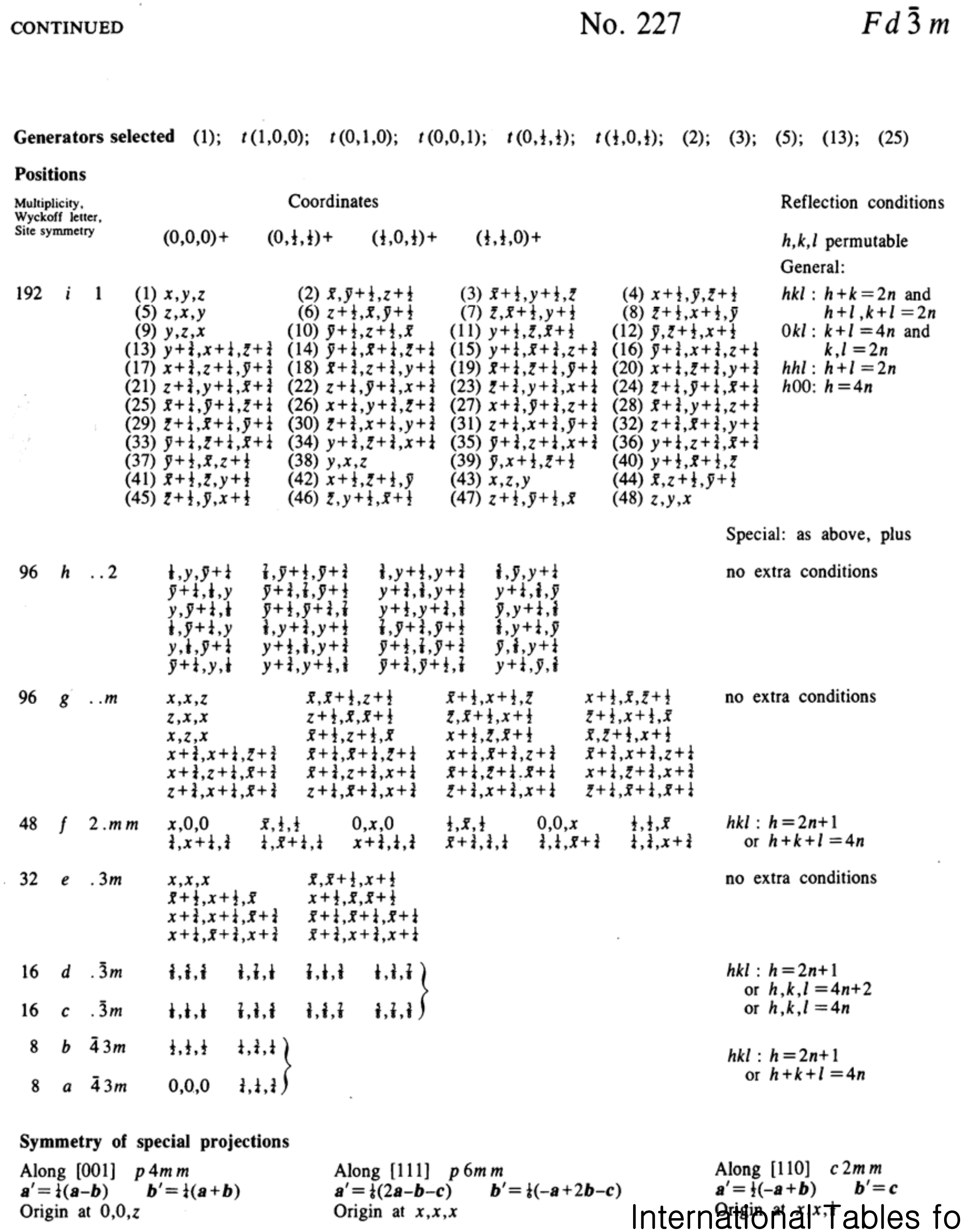
Origin at $\bar{4}3m$, at $-\frac{1}{8},-\frac{1}{8},-\frac{1}{8}$ from centre ($\bar{3}m$)

Asymmetric unit $0\leq x\leq\frac{1}{2}$; $0\leq y\leq\frac{1}{8}$; $-\frac{1}{8}\leq z\leq\frac{1}{8}$; $y\leq\min(\frac{1}{2}-x,x)$; $-y\leq z\leq y$

Vertices $0,0,0$ $\frac{1}{2},0,0$ $\frac{3}{8},\frac{1}{8},\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},\frac{1}{8}$ $\frac{3}{8},\frac{1}{8},-\frac{1}{8}$ $\frac{1}{8},\frac{1}{8},-\frac{1}{8}$

Symmetry operations
(*given on page* 689)

International Tables for X-ray Crystallography



CONTINUED No. 227 $Fd\bar{3}m$

Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13); (25)

Positions

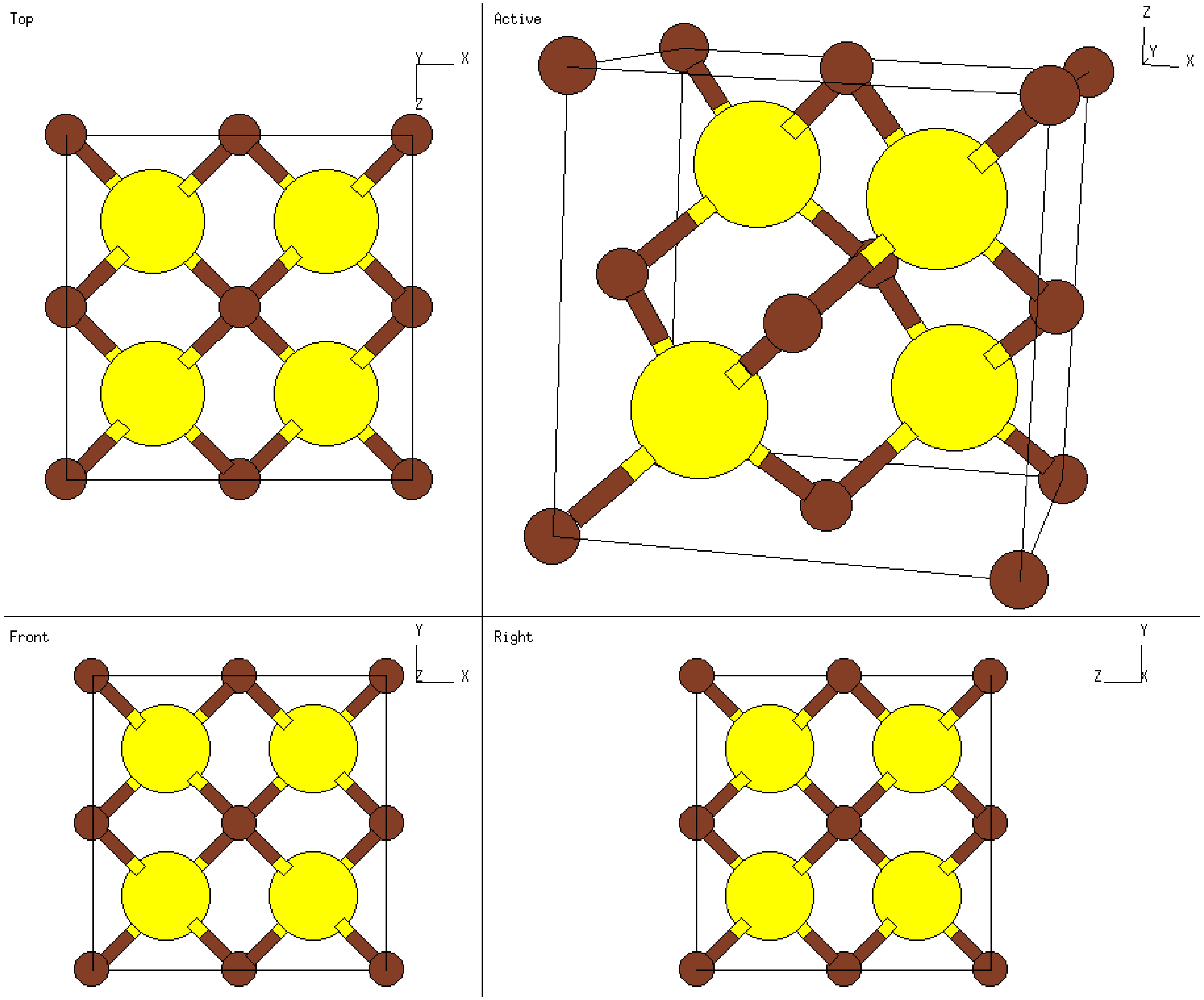
Multiplicity, Wyckoff letter, Site symmetry	Coordinates						Reflection conditions
	$(0,0,0)+$	$(0,\frac{1}{2},\frac{1}{2})+$	$(\frac{1}{2},0,\frac{1}{2})+$	$(\frac{1}{2},\frac{1}{2},0)+$			*h,k,l* permutable General:
192 *i* 1	(1) x,y,z	(2) $\bar{x},\bar{y}+\frac{1}{2},z+\frac{1}{2}$	(3) $\bar{x}+\frac{1}{2},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y},\bar{z}+\frac{1}{2}$			$hkl: h+k=2n$ and
	(5) z,x,y	(6) $z+\frac{1}{2},\bar{x},\bar{y}+\frac{1}{2}$	(7) $\bar{z},\bar{x}+\frac{1}{2},y+\frac{1}{2}$	(8) $\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{y}$			$h+l, k+l=2n$
	(9) y,z,x	(10) $\bar{y}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	(11) $y+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	(12) $\bar{y},\bar{z}+\frac{1}{2},x+\frac{1}{2}$			$0kl: k+l=4n$ and
	(13) $y+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	(14) $\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(15) $y+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	(16) $\bar{y}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$			$k,l=2n$
	(17) $x+\frac{3}{4},z+\frac{1}{4},\bar{y}+\frac{3}{4}$	(18) $\bar{x}+\frac{3}{4},z+\frac{3}{4},y+\frac{1}{4}$	(19) $\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(20) $x+\frac{1}{4},\bar{z}+\frac{3}{4},y+\frac{3}{4}$			$hhl: h+l=2n$
	(21) $z+\frac{3}{4},y+\frac{1}{4},\bar{x}+\frac{3}{4}$	(22) $z+\frac{1}{4},\bar{y}+\frac{3}{4},x+\frac{3}{4}$	(23) $\bar{z}+\frac{3}{4},y+\frac{3}{4},x+\frac{1}{4}$	(24) $\bar{z}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{x}+\frac{1}{4}$			$h00: h=4n$
	(25) $\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4}$	(26) $x+\frac{1}{4},y+\frac{3}{4},\bar{z}+\frac{3}{4}$	(27) $x+\frac{3}{4},\bar{y}+\frac{3}{4},z+\frac{1}{4}$	(28) $\bar{x}+\frac{3}{4},y+\frac{1}{4},z+\frac{3}{4}$			
	(29) $\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{y}+\frac{1}{4}$	(30) $\bar{z}+\frac{3}{4},x+\frac{1}{4},y+\frac{3}{4}$	(31) $z+\frac{1}{4},x+\frac{3}{4},\bar{y}+\frac{3}{4}$	(32) $z+\frac{3}{4},\bar{x}+\frac{3}{4},y+\frac{1}{4}$			
	(33) $\bar{y}+\frac{1}{4},\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4}$	(34) $y+\frac{3}{4},\bar{z}+\frac{3}{4},x+\frac{1}{4}$	(35) $\bar{y}+\frac{3}{4},z+\frac{1}{4},x+\frac{3}{4}$	(36) $y+\frac{1}{4},z+\frac{3}{4},\bar{x}+\frac{3}{4}$			
	(37) $\bar{y}+\frac{1}{2},\bar{x},z+\frac{1}{2}$	(38) y,x,z	(39) $\bar{y},x+\frac{1}{2},\bar{z}+\frac{1}{2}$	(40) $y+\frac{1}{2},\bar{x}+\frac{1}{2},\bar{z}$			
	(41) $\bar{x}+\frac{1}{2},\bar{z},y+\frac{1}{2}$	(42) $x+\frac{1}{2},\bar{z}+\frac{1}{2},\bar{y}$	(43) x,z,y	(44) $\bar{x},z+\frac{1}{2},\bar{y}+\frac{1}{2}$			
	(45) $\bar{z}+\frac{1}{2},\bar{y},x+\frac{1}{2}$	(46) $\bar{z},y+\frac{1}{2},\bar{x}+\frac{1}{2}$	(47) $z+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{x}$	(48) z,y,x			
							Special: as above, plus
96 *h* ..2	$\frac{1}{8},y,\bar{y}+\frac{1}{4}$	$\frac{7}{8},\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4}$	$\frac{3}{8},y+\frac{1}{2},y+\frac{3}{4}$	$\frac{5}{8},\bar{y},y+\frac{1}{4}$			no extra conditions
	$\bar{y}+\frac{1}{4},\frac{1}{8},y$	$\bar{y}+\frac{3}{4},\frac{7}{8},\bar{y}+\frac{1}{2}$	$y+\frac{3}{4},\frac{3}{8},y+\frac{1}{2}$	$y+\frac{1}{4},\frac{5}{8},\bar{y}$			
	$y,\bar{y}+\frac{1}{4},\frac{1}{8}$	$\bar{y}+\frac{1}{2},\bar{y}+\frac{3}{4},\frac{7}{8}$	$y+\frac{1}{2},y+\frac{3}{4},\frac{3}{8}$	$\bar{y},y+\frac{1}{4},\frac{5}{8}$			
	$\frac{1}{8},\bar{y}+\frac{1}{4},y$	$\frac{3}{8},y+\frac{3}{4},y+\frac{1}{2}$	$\frac{7}{8},\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2}$	$\frac{5}{8},y+\frac{1}{4},\bar{y}$			
	$y,\frac{1}{8},\bar{y}+\frac{1}{4}$	$y+\frac{1}{2},\frac{3}{8},y+\frac{3}{4}$	$\bar{y}+\frac{1}{2},\frac{7}{8},\bar{y}+\frac{3}{4}$	$\bar{y},\frac{5}{8},y+\frac{1}{4}$			
	$\bar{y}+\frac{1}{4},y,\frac{1}{8}$	$y+\frac{3}{4},y+\frac{1}{2},\frac{3}{8}$	$\bar{y}+\frac{3}{4},\bar{y}+\frac{1}{2},\frac{7}{8}$	$y+\frac{1}{4},\bar{y},\frac{5}{8}$			
96 *g* ..*m*	x,x,z	$\bar{x},\bar{x}+\frac{1}{2},z+\frac{1}{2}$	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{z}$	$x+\frac{1}{2},\bar{x},\bar{z}+\frac{1}{2}$			no extra conditions
	z,x,x	$z+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$	$\bar{z},\bar{x}+\frac{1}{2},x+\frac{1}{2}$	$\bar{z}+\frac{1}{2},x+\frac{1}{2},\bar{x}$			
	x,z,x	$\bar{x}+\frac{1}{2},z+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{z},\bar{x}+\frac{1}{2}$	$\bar{x},\bar{z}+\frac{1}{2},x+\frac{1}{2}$			
	$x+\frac{3}{4},x+\frac{1}{4},\bar{z}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}$	$x+\frac{1}{4},\bar{x}+\frac{3}{4},z+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},z+\frac{1}{4}$			
	$x+\frac{3}{4},z+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{3}{4},z+\frac{3}{4},x+\frac{1}{4}$	$\bar{x}+\frac{1}{4},\bar{z}+\frac{1}{4}.\bar{x}+\frac{1}{4}$	$x+\frac{1}{4},\bar{z}+\frac{3}{4},x+\frac{3}{4}$			
	$z+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$z+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{z}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$	$\bar{z}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$			
48 *f* 2.*mm*	$x,0,0$	$\bar{x},\frac{1}{2},\frac{1}{2}$	$0,x,0$	$\frac{1}{2},\bar{x},\frac{1}{2}$	$0,0,x$	$\frac{1}{2},\frac{1}{2},\bar{x}$	$hkl: h=2n+1$
	$\frac{3}{4},x+\frac{1}{4},\frac{3}{4}$	$\frac{1}{4},\bar{x}+\frac{1}{4},\frac{1}{4}$	$x+\frac{3}{4},\frac{1}{4},\frac{3}{4}$	$\bar{x}+\frac{3}{4},\frac{3}{4},\frac{1}{4}$	$\frac{3}{4},\frac{1}{4},\bar{x}+\frac{3}{4}$	$\frac{1}{4},\frac{3}{4},x+\frac{3}{4}$	or $h+k+l=4n$
32 *e* .3*m*	x,x,x	$\bar{x},\bar{x}+\frac{1}{2},x+\frac{1}{2}$					no extra conditions
	$\bar{x}+\frac{1}{2},x+\frac{1}{2},\bar{x}$	$x+\frac{1}{2},\bar{x},\bar{x}+\frac{1}{2}$					
	$x+\frac{3}{4},x+\frac{1}{4},\bar{x}+\frac{3}{4}$	$\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4},\bar{x}+\frac{1}{4}$					
	$x+\frac{1}{4},\bar{x}+\frac{3}{4},x+\frac{3}{4}$	$\bar{x}+\frac{3}{4},x+\frac{3}{4},x+\frac{1}{4}$					
16 *d* .$\bar{3}m$	$\frac{5}{8},\frac{5}{8},\frac{5}{8}$	$\frac{3}{8},\frac{7}{8},\frac{1}{8}$	$\frac{7}{8},\frac{1}{8},\frac{3}{8}$	$\frac{1}{8},\frac{3}{8},\frac{7}{8}$			$hkl: h=2n+1$ or $h,k,l=4n+2$ or $h,k,l=4n$
16 *c* .$\bar{3}m$	$\frac{1}{8},\frac{1}{8},\frac{1}{8}$	$\frac{7}{8},\frac{3}{8},\frac{5}{8}$	$\frac{3}{8},\frac{5}{8},\frac{7}{8}$	$\frac{5}{8},\frac{7}{8},\frac{3}{8}$			
8 *b* $\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	$\frac{1}{4},\frac{3}{4},\frac{1}{4}$					$hkl: h=2n+1$ or $h+k+l=4n$
8 *a* $\bar{4}3m$	$0,0,0$	$\frac{3}{4},\frac{1}{4},\frac{3}{4}$					

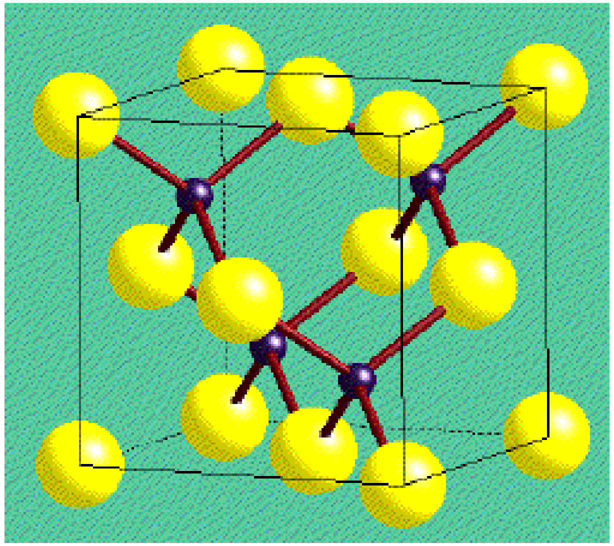
Symmetry of special projections

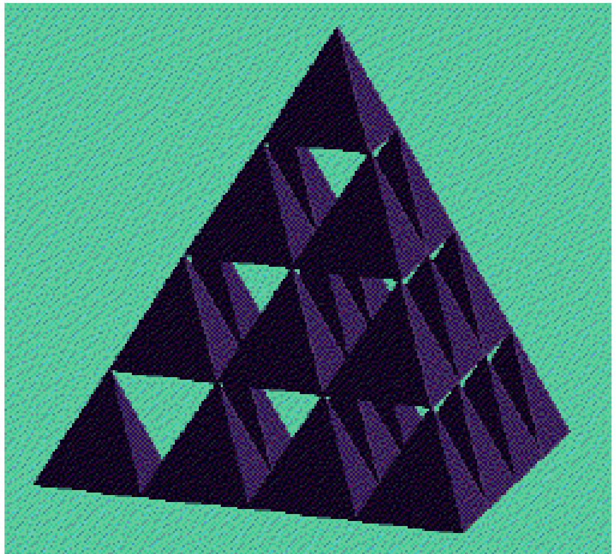
Along [001] $p4mm$	Along [111] $p6mm$	Along [110] $c2mm$
$\boldsymbol{a}'=\frac{1}{2}(\boldsymbol{a}-\boldsymbol{b})$ $\boldsymbol{b}'=\frac{1}{2}(\boldsymbol{a}+\boldsymbol{b})$	$\boldsymbol{a}'=\frac{1}{3}(2\boldsymbol{a}-\boldsymbol{b}-\boldsymbol{c})$ $\boldsymbol{b}'=\frac{1}{3}(-\boldsymbol{a}+2\boldsymbol{b}-\boldsymbol{c})$	$\boldsymbol{a}'=\frac{1}{2}(-\boldsymbol{a}+\boldsymbol{b})$ $\boldsymbol{b}'=\boldsymbol{c}$
Origin at $0,0,z$	Origin at x,x,x	Origin at $x,x,\frac{1}{8}$

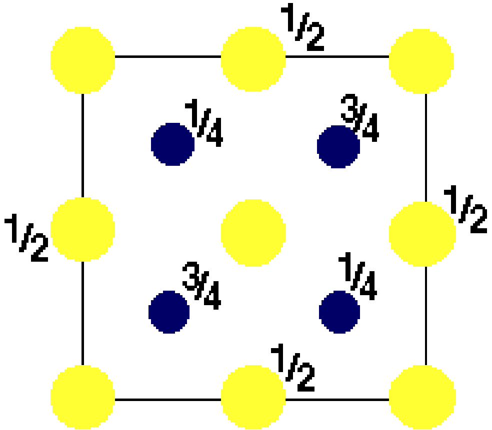
International Tables for X-ray Crystallography

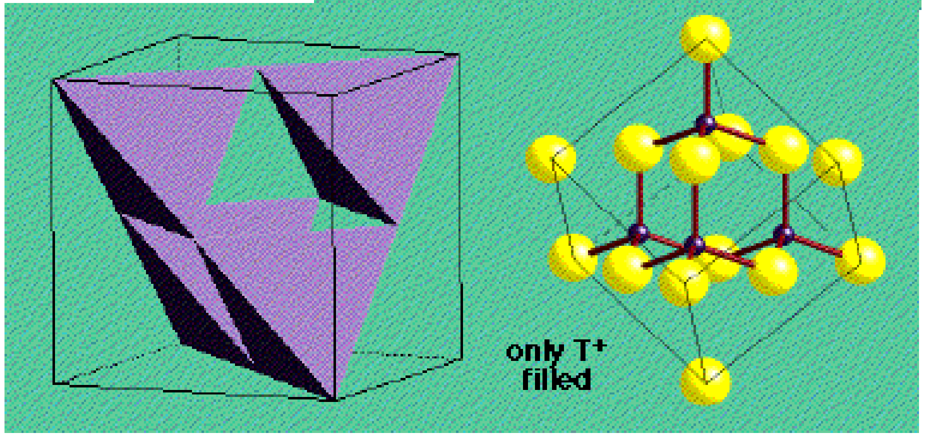
Zinc Blende, ZnS








1/2
1/4
3/4
1/2
1/2
3/4
1/4
1/2


only T+ filled

Zinc Blende, ZnS

-diamond derivative structure
-Zn and S replace the C atoms
-Zn cubic close packing
 S ½ tetrahedral site
-Zn and S cubic close packing displaced by $\frac{1}{4},\frac{1}{4},\frac{1}{4}$
-Space group

$$F\bar{4}3m \text{ (No.216)}$$

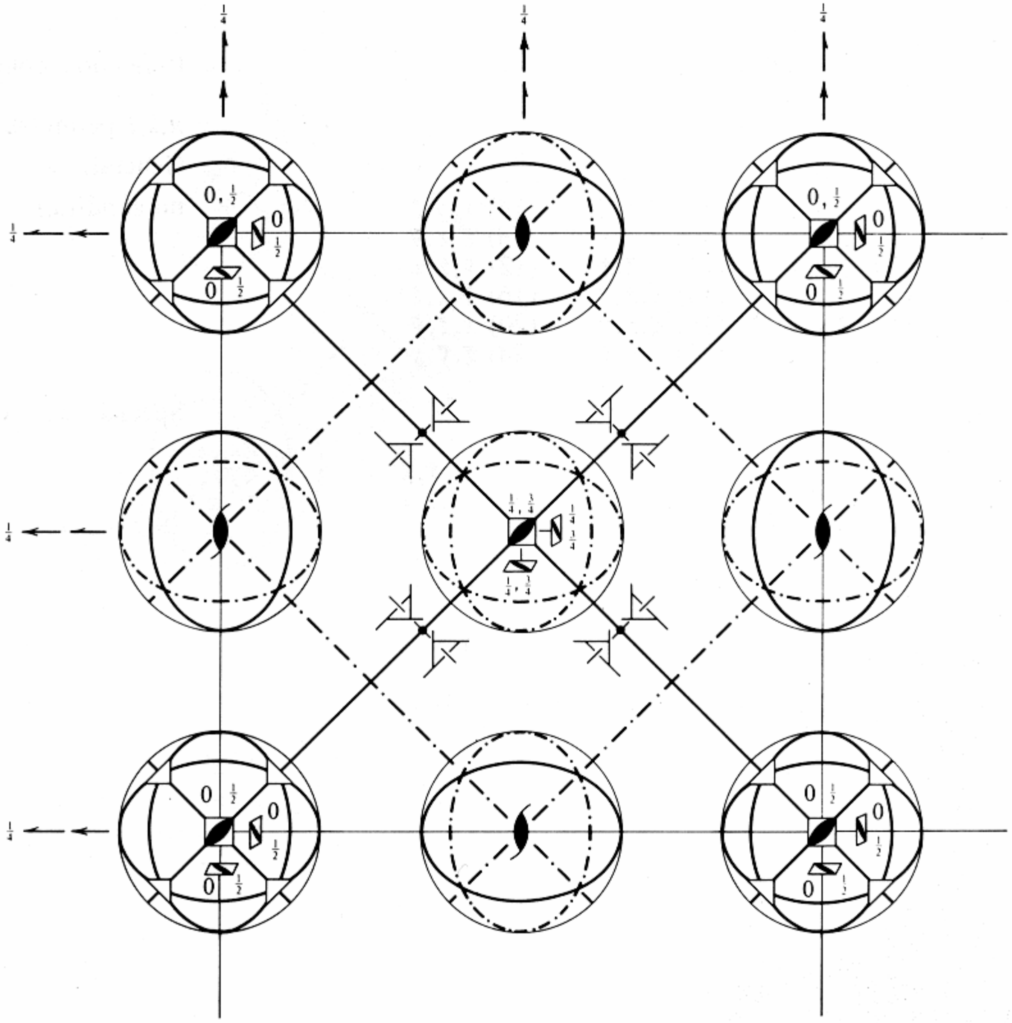
$$\text{Zn: 4a, } \bar{4}3m, \ 0,0,0$$

$$\text{Zn: 4c, } \bar{4}3m, \ \frac{1}{4},\frac{1}{4},\frac{1}{4}$$

Zinc Blende, ZnS

$F\bar{4}3m$ T_d^2 $\bar{4}3m$ Cubic

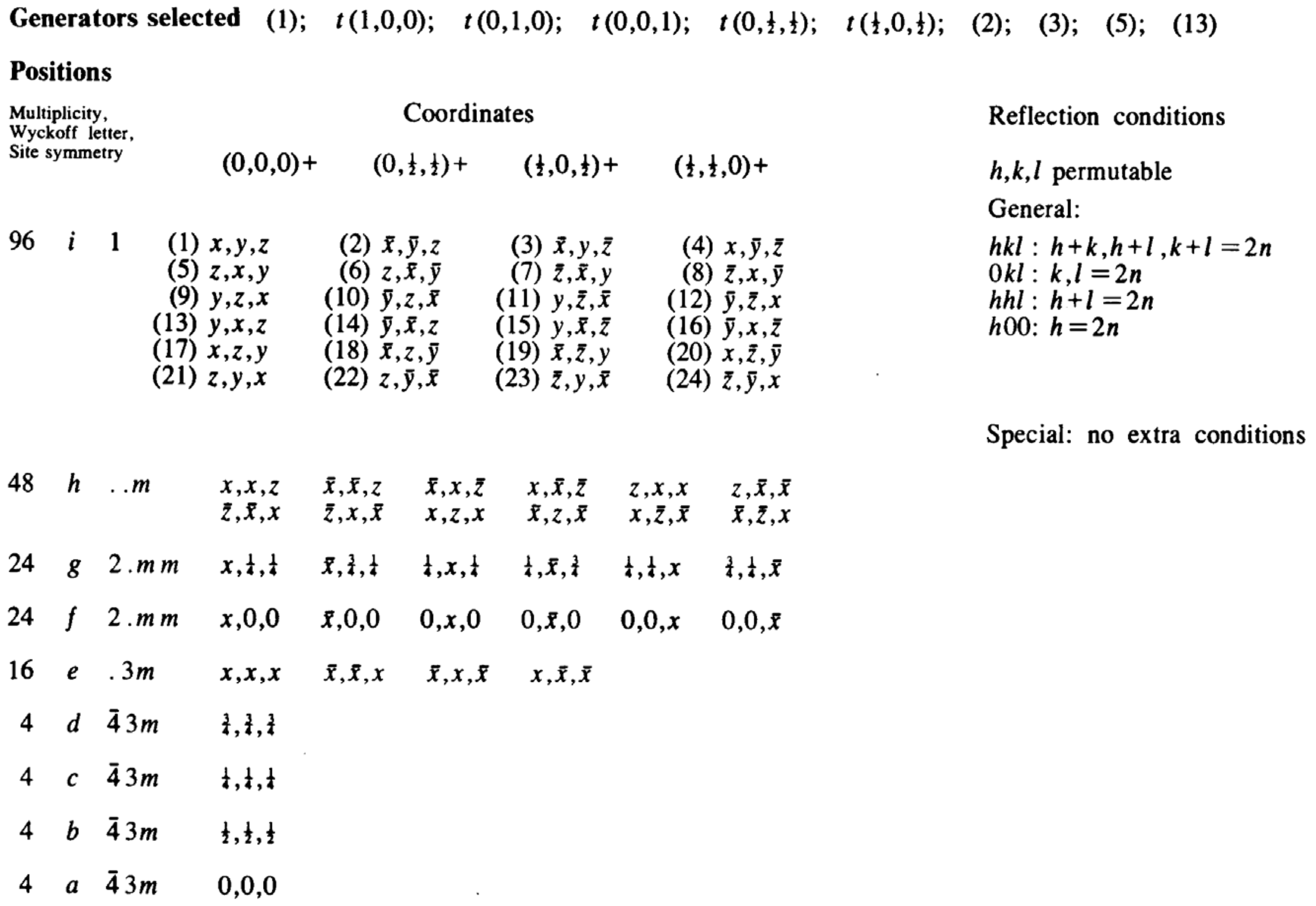
No. 216 $F\bar{4}3m$ Patterson symmetry $Fm\bar{3}m$



Upper left quadrant only

International Tables for X-ray Crystallography

Zinc Blende, ZnS



Generators selected (1); $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$; $t(0,\frac{1}{2},\frac{1}{2})$; $t(\frac{1}{2},0,\frac{1}{2})$; (2); (3); (5); (13)

Positions

Multiplicity,
Wyckoff letter,
Site symmetry

Coordinates

$(0,0,0)+$ $(0,\frac{1}{2},\frac{1}{2})+$ $(\frac{1}{2},0,\frac{1}{2})+$ $(\frac{1}{2},\frac{1}{2},0)+$

96	*i*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $\bar{x},y,\bar{z}$	(4) $x,\bar{y},\bar{z}$		
			(5) z,x,y	(6) $z,\bar{x},\bar{y}$	(7) $\bar{z},\bar{x},y$	(8) $\bar{z},x,\bar{y}$		
			(9) y,z,x	(10) $\bar{y},z,\bar{x}$	(11) $y,\bar{z},\bar{x}$	(12) $\bar{y},\bar{z},x$		
			(13) y,x,z	(14) $\bar{y},\bar{x},z$	(15) $y,\bar{x},\bar{z}$	(16) $\bar{y},x,\bar{z}$		
			(17) x,z,y	(18) $\bar{x},z,\bar{y}$	(19) $\bar{x},\bar{z},y$	(20) $x,\bar{z},\bar{y}$		
			(21) z,y,x	(22) $z,\bar{y},\bar{x}$	(23) $\bar{z},y,\bar{x}$	(24) $\bar{z},\bar{y},x$		
48	*h*	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,\bar{z}$	$x,\bar{x},\bar{z}$	z,x,x	$z,\bar{x},\bar{x}$
			$\bar{z},\bar{x},x$	$\bar{z},x,\bar{x}$	x,z,x	$\bar{x},z,\bar{x}$	$x,\bar{z},\bar{x}$	$\bar{x},\bar{z},x$
24	*g*	$2.mm$	$x,\frac{1}{4},\frac{1}{4}$	$\bar{x},\frac{3}{4},\frac{1}{4}$	$\frac{1}{4},x,\frac{1}{4}$	$\frac{1}{4},\bar{x},\frac{3}{4}$	$\frac{1}{4},\frac{1}{4},x$	$\frac{3}{4},\frac{1}{4},\bar{x}$
24	*f*	$2.mm$	$x,0,0$	$\bar{x},0,0$	$0,x,0$	$0,\bar{x},0$	$0,0,x$	$0,0,\bar{x}$
16	*e*	$.3m$	x,x,x	$\bar{x},\bar{x},x$	$\bar{x},x,\bar{x}$	$x,\bar{x},\bar{x}$		
4	*d*	$\bar{4}3m$	$\frac{3}{4},\frac{3}{4},\frac{3}{4}$					
4	*c*	$\bar{4}3m$	$\frac{1}{4},\frac{1}{4},\frac{1}{4}$					
4	*b*	$\bar{4}3m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$					
4	*a*	$\bar{4}3m$	$0,0,0$					

Reflection conditions

h,k,l permutable

General:

hkl : $h+k, h+l, k+l = 2n$
$0kl$: $k,l = 2n$
hhl : $h+l = 2n$
$h00$: $h = 2n$

Special: no extra conditions