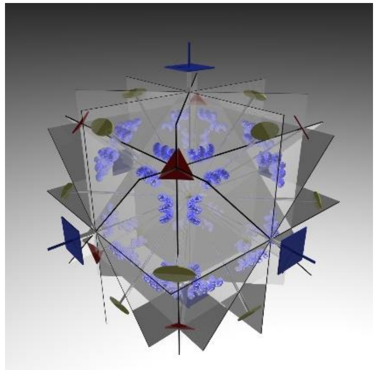
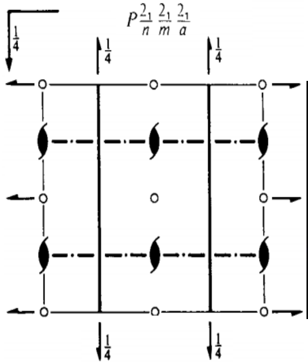
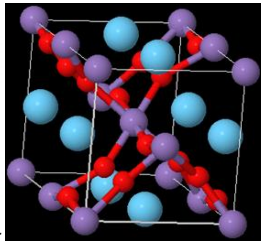
ISOE2019

International School of Oxide Electronics



June 25 – July 5, 2019
Cargèse





CRYSTAL SYMMETRY
Appendix

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1. Point Group Symmetry: *Elementary point symmetries*

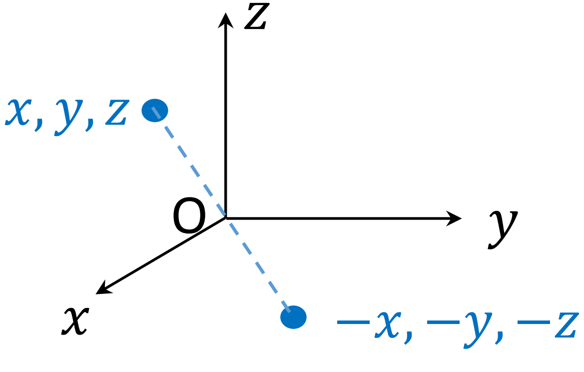
(Complement of Lecture – slide 5)

Point symmetries exist at the macroscopic & atomic scales. They **keep at least one point fixed**: the origin

Inversion (through a point)

→ *centrosymmetric crystal*

$\bar{1}$



$$S_{\bar{1}} = \begin{pmatrix} -1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

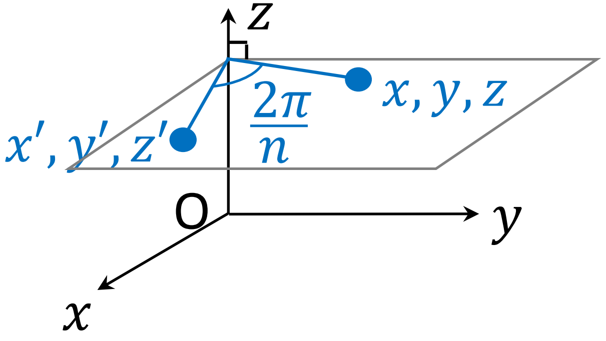
Det = -1

Rotation (around an axis)

Rotation of order n

= rotation by $\frac{2\pi}{n}$

$1, 2, 3, \ldots$



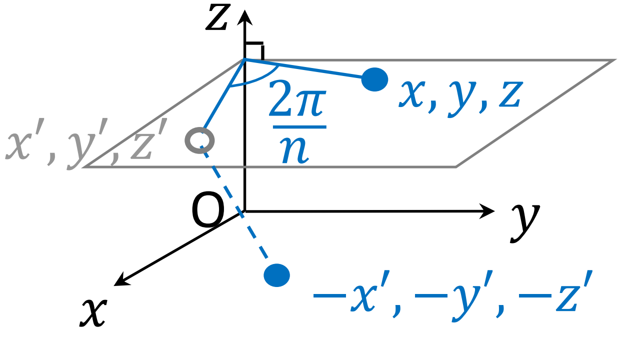
$$S_n = \begin{pmatrix} \cos\phi & -\sin\phi & 0 \\ \sin\phi & \cos\phi & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

Det = +1

Rotoinversion

→ combination of $\bar{1}$ and n

$\bar{1}, \bar{2}, \bar{3}, \ldots$



$$S_{\bar{n}} = \begin{pmatrix} -\cos\phi & \sin\phi & 0 \\ -\sin\phi & -\cos\phi & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

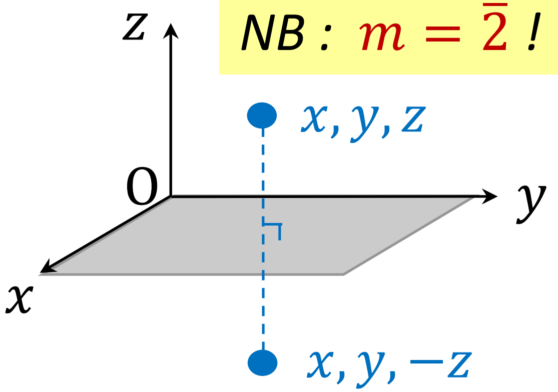
Det = -1

Reflection

(through a mirror plane)

m

NB : $m = \bar{2}$!



$$S_m = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

Det = -1

(Complement of Lecture – slide 5)

The only orders of rotation compatible with the translation symmetry are: 1, 2, 3, 4, 6

Demonstration:

If an axis n going through A exists, there exists another one going trough B such as: $\overrightarrow{AB} = \vec{T}$

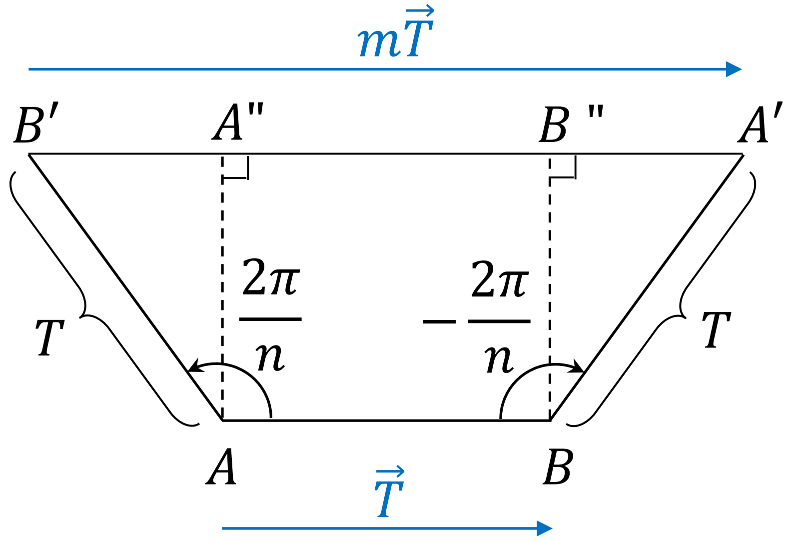
Through $a(n)$ in A: $B \rightarrow B'$
Through $a^{-1}(n)$ in B: $A \rightarrow A'$

A' and B' must be lattice points so that: $\overrightarrow{B'A'} = m\vec{T}$ with m an integer.

One can ealisy show that: $\overline{B'A'} = T\left(1 - 2\cos\frac{2\pi}{n}\right)$

so that one must have: $m = 1 - 2\cos\frac{2\pi}{n} \;\; \Rightarrow \;\; -1 \leq m \leq 3$

$m = -1 \;\; \rightarrow \;\; n = 1$
$m = 0 \;\; \rightarrow \;\; n = 6$
$m = 1 \;\; \rightarrow \;\; n = 4$
$m = 2 \;\; \rightarrow \;\; n = 3$
$m = 3 \;\; \rightarrow \;\; n = 2$



(Complement of Lecture – slide 7)

Other notation of the point groups – *Schoenflies symbol*

C_n	cyclic	n-fold rotation axis ($n = 1, 2, 3, 4, 6$)
D_n	dihedral, or two-sided	n-fold rotation axis plus *n* twofold axes $\perp$ to that axis

subscript n : addition of a mirror plane $\perp$ to the *n*-fold axis (C_{nh}, D_{nh})
subscript v : addition of a mirror plane // to the *n*-fold axis (C_{nv}, D_{nv})

S_{2n}	*Spiegel* = mirror	$2n$-fold rotoinversion axis ($2n = 2, 4, 6$)
T	Tetrahedral	symmetry of a tetrahedron with (T_d) or without (T) improper rotations $T_h = T$ with the addition of an inversion
O	Octahedral	symmetry of an octahedron (or cube) with (O_h) or without (O) improper operations

Other notations: $S_2 = C_i$; $S_6 = C_{3i}$; $C_{1h} = Cs$

International notation used for crystallography
Schoenflies notation used for spectroscopy

1. Point Group Symmetry: *Point groups – Schoenflies symbol*

International vs Schoenflies symbols

(table 10.1.2.4. from the International Tables for Crystallography, Volume A)

(Complement of Lecture – slide 7)

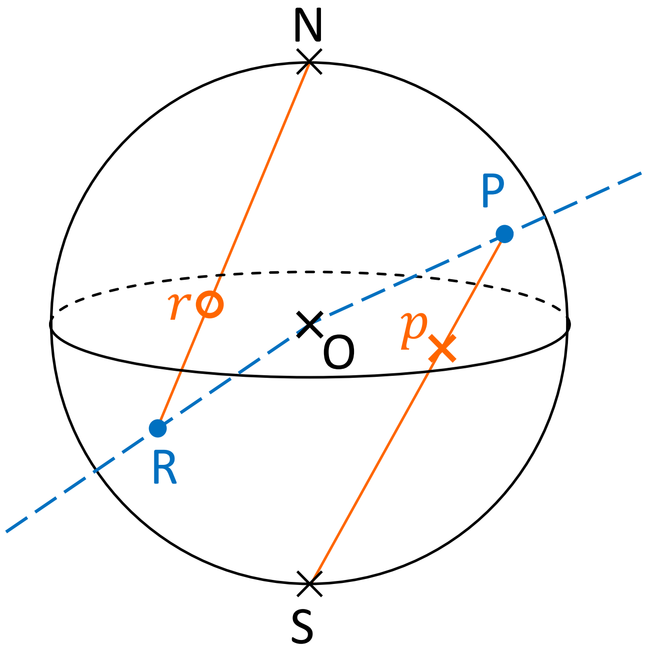
System used in this volume	Point group – International symbol – Short	Point group – International symbol – Full	Schoenflies symbol
Triclinic	1 $\bar{1}$	1 $\bar{1}$	C_1 $C_i(S_2)$
Monoclinic	2 m $2/m$	2 m $\frac{2}{m}$	C_2 $C_s(C_{1h})$ C_{2h}
Orthorhombic	222 $mm2$ mmm	222 $mm2$ $\frac{2}{m}\frac{2}{m}\frac{2}{m}$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

How to represent a point group ?

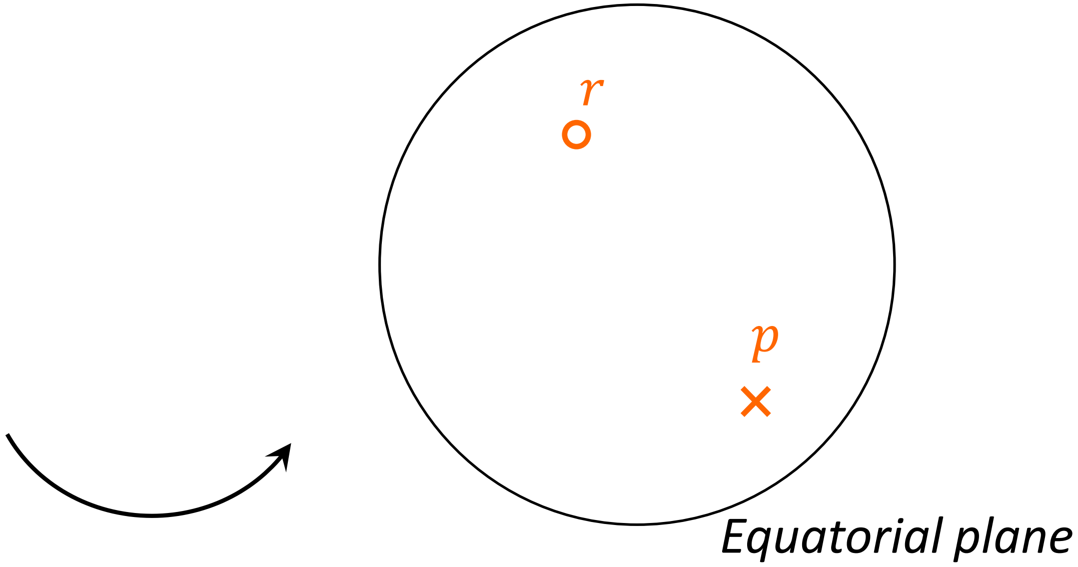
(Complement of Lecture – slide 7)

Stereographic projection:
projection in 2 dimensions of all symmetry elements and all equivalent directions

1st step: Spherical projection



2nd step: Stereographic projection

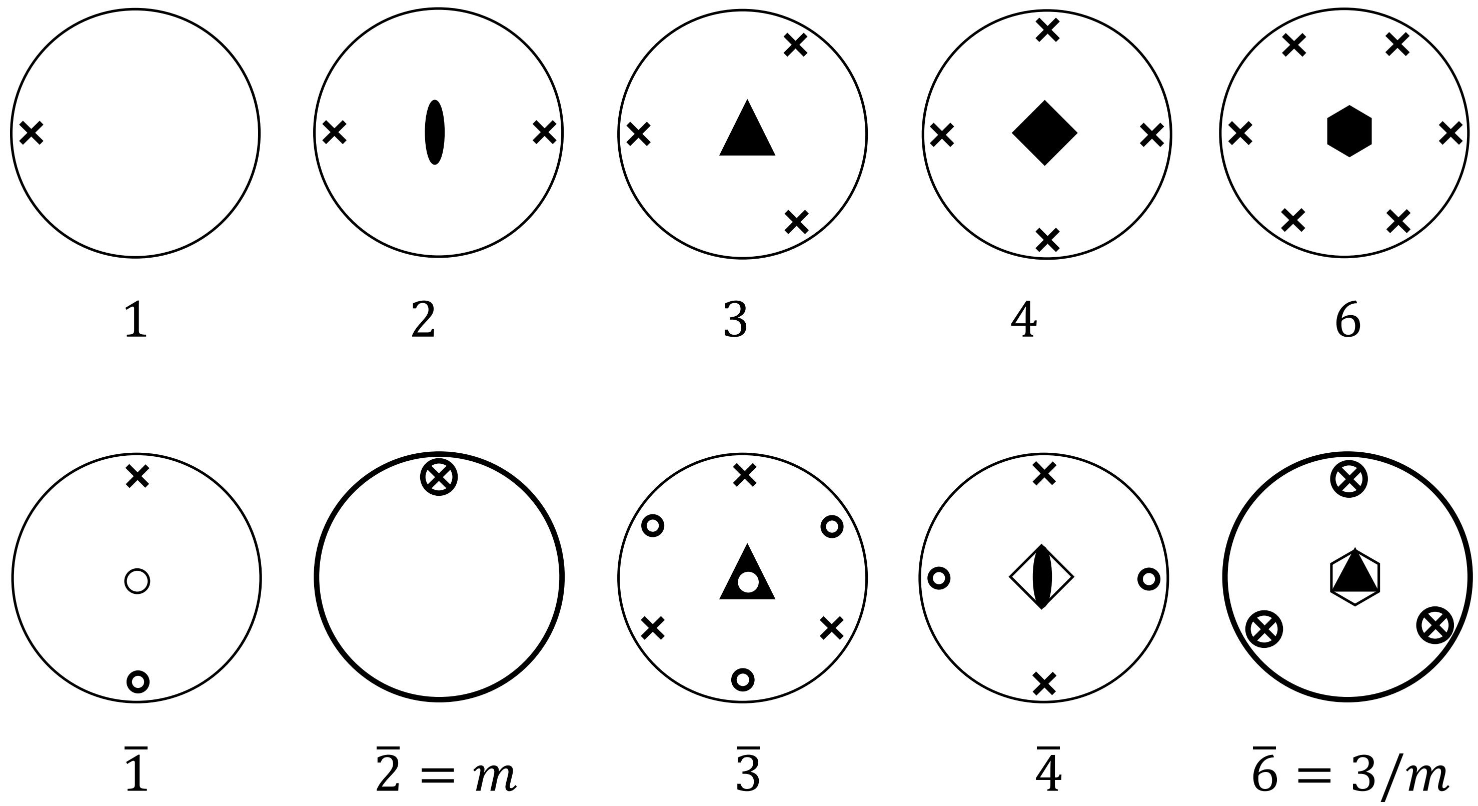


P $\in$ north hemisphere
R $\in$ south hemisphere

PS $\cap$ equatorial plane $\Rightarrow p$ (cross)
RN $\cap$ equatorial plane $\Rightarrow r$ (circle)

(Complement of Lecture – slide 7)

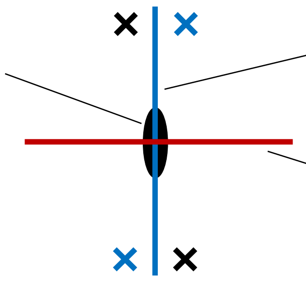
Stereographic projection for the 10 elementary point symmetries:



(Complement of Lecture – slide 7)

Starting from an axis 2 and a mirror plane passing through this axis …

Primary direction: 2



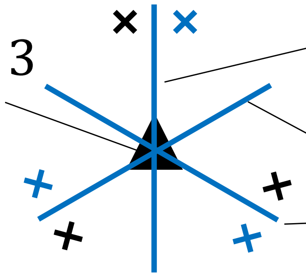
Secundary direction: m

Point group: $2mm$

m along a direction
not equivalent to the two others
$\Rightarrow$ tertiary direction

Starting from an axis 3 and a mirror plane passing through this axis …

Primary direction: 3



Secundary direction: m

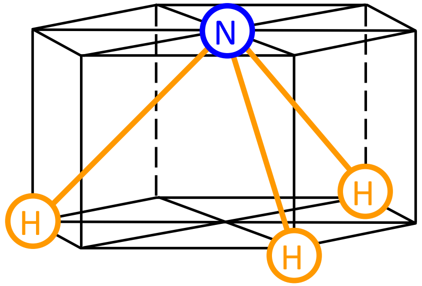
Point group: $3m$

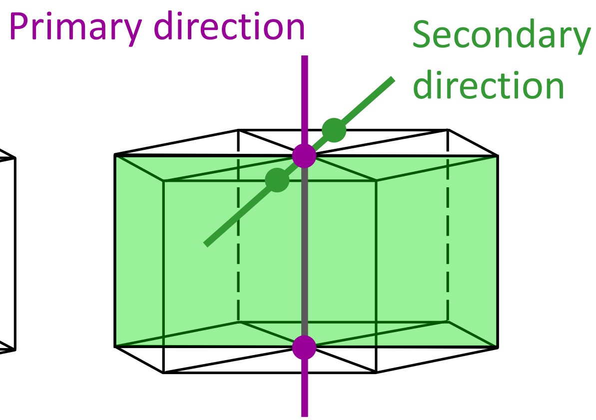
m along two additional directions
both equivalent to the secondary direction
$\Rightarrow$ no tertiary direction

Examples: point groups of molecules

(Complement of Lecture – slide 8)

NH_3

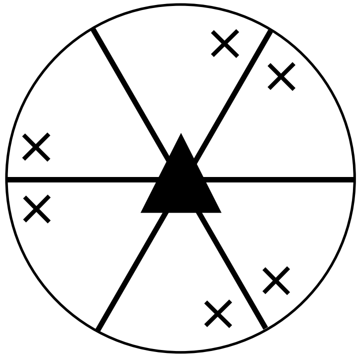




Axis 3
3 equivalent mirrors

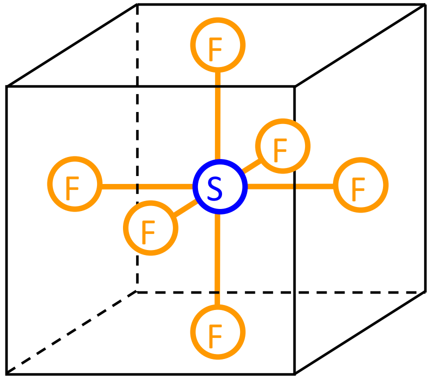
⇓

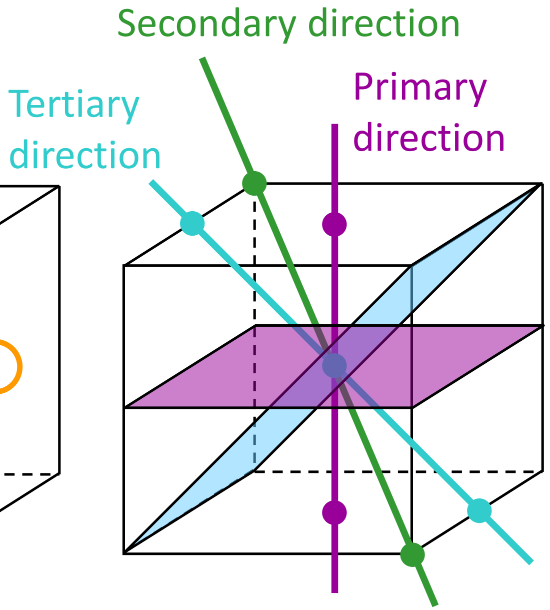
Point group: $3m$



$3m$

SF_6

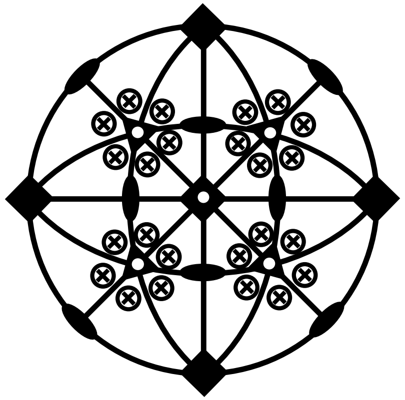




axis 4 and mirrors
Axis $\bar{3}$
axis 2 and mirror

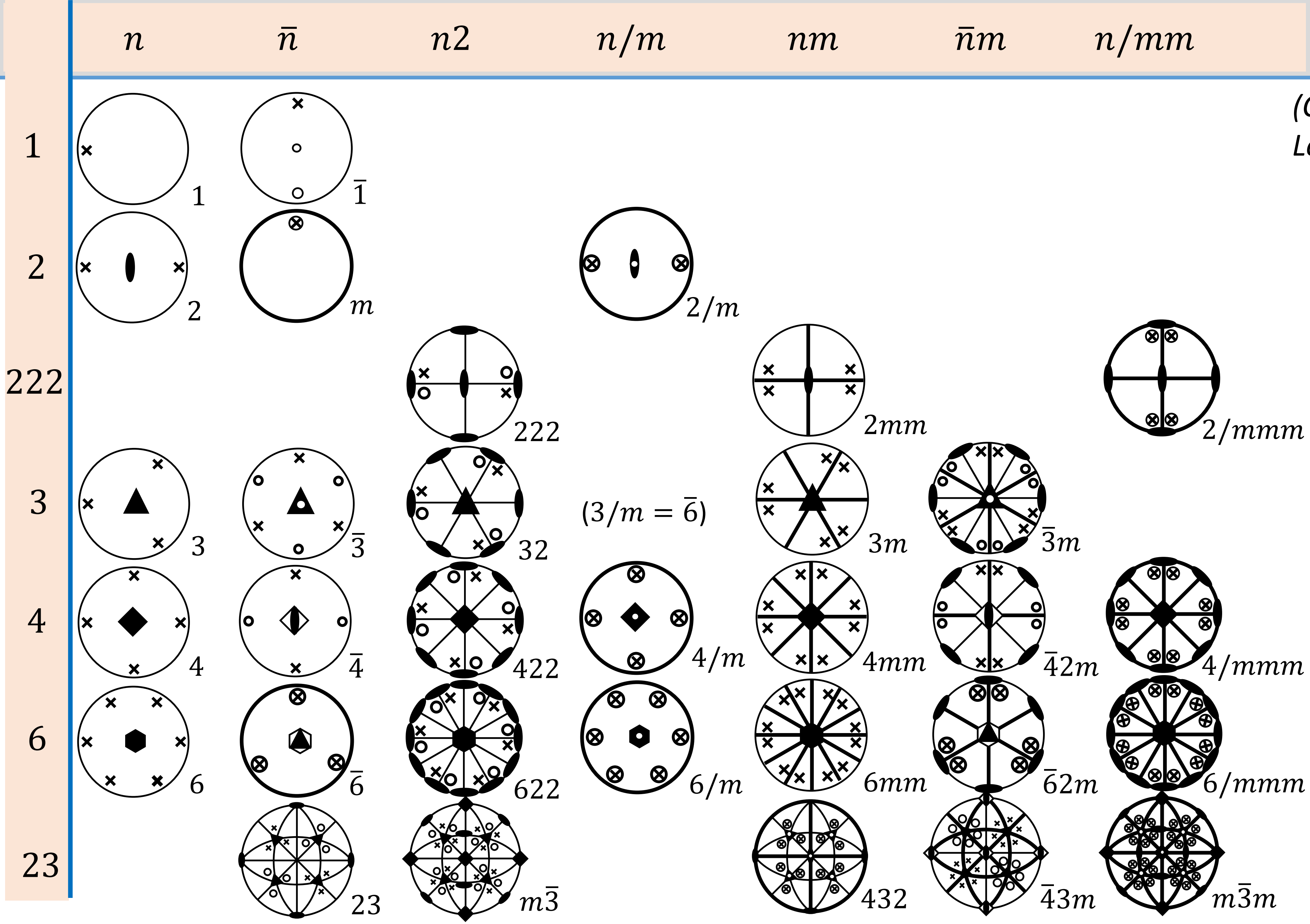
⇓

Point group: $\frac{4}{m}\bar{3}\frac{2}{m}$



$m\bar{3}m$

(Complement of Lecture – slide 9)

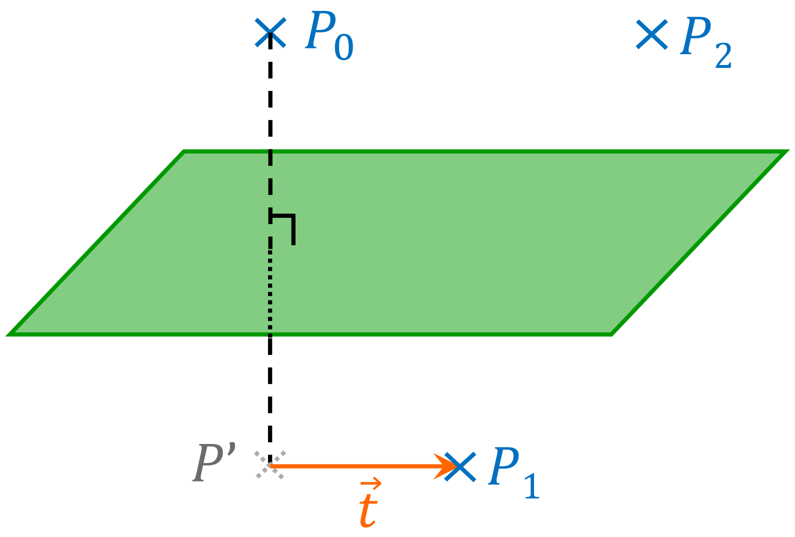


- Glide plane

(Complement of Lecture – slide 29)

Combination of a reflection (through a plane) and a fractional translation $\vec{t}$ ∥ plane

↑ *acting inside the unit cell*



Example: **glide plane** $a \perp \vec{c}$ at $z = \frac{1}{4}$

$a \times a \rightarrow$ lattice translation

$$P_0P_2 = \vec{a} \rightarrow \boxed{\vec{t} = \frac{\vec{a}}{2}}$$

Seitz notation: $\{\alpha|\vec{t}_\alpha\} = \{m_z|\frac{1}{2}, 0, \frac{1}{2}\}$

4 × 4 matrix: $\begin{pmatrix} 1 & 0 & 0 & 1/2 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & -1 & 1/2 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

α: point symmetry

$\vec{t}_\alpha$: translation embedding the glide translation + the position of α

3. Space group symmetry: *Short vs full symbols*

(Complement of Lecture – Slide 33)

Short international symbols

The short symbol form leaves out symmetry elements that are implicitly present.
Example: the orthorhombic space group $Pbca$ implicitly has three 2_1 screw axes due to the presence of the three mutually-perpendicular glide planes. These 2_1 axes are omitted from the short symbol, but retained in the full symbol.

Derivation of the full symbol from the short symbol

Example: $Pbcn$ (orthorhombic)

3 glide planes at 90° from each other → 2-fold axes (2 or 2_1) along their intersections

Glide planes $b \perp \vec{a}$ ($\vec{t} = \frac{\vec{b}}{2}$) and $c \perp \vec{b}$ ($\vec{t} = \frac{\vec{c}}{2}$) $\Rightarrow$ 2-fold axis $\parallel \vec{c}$ with $\vec{t} = \frac{\vec{c}}{2}$ $\Rightarrow$ $2_1 \parallel \vec{c}$

Glide planes $c \perp \vec{b}$ ($\vec{t} = \frac{\vec{c}}{2}$) and $n \perp \vec{c}$ ($\vec{t} = \frac{\vec{a}+\vec{b}}{2}$) $\Rightarrow$ 2-fold axis $\parallel \vec{a}$ with $\vec{t} = \frac{\vec{a}}{2}$ $\Rightarrow$ $2_1 \parallel \vec{a}$

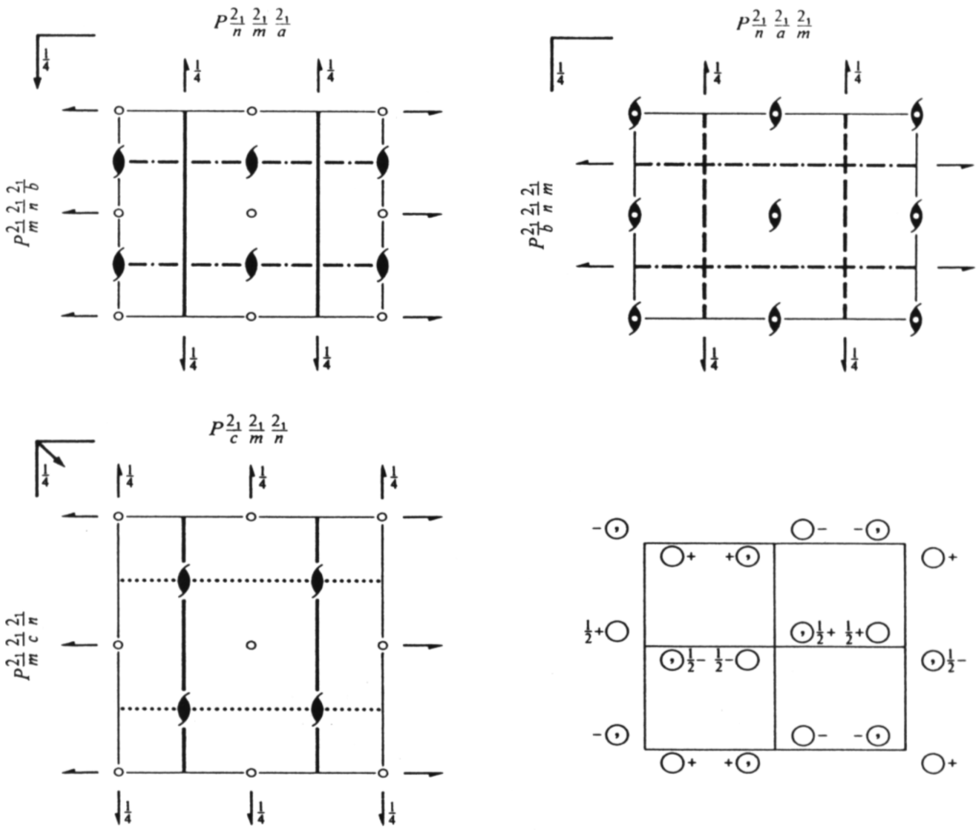
Glide planes $n \perp \vec{c}$ ($\vec{t} = \frac{\vec{a}+\vec{b}}{2}$) and $b \perp \vec{a}$ ($\vec{t} = \frac{\vec{b}}{2}$) $\Rightarrow$ 2-fold axis $\parallel \vec{b}$ with $\vec{t} = \vec{b} \equiv \vec{0}$ $\Rightarrow$ $2 \parallel \vec{b}$

Conclusion: short symbol $Pbcn$ → full symbol $P\frac{2_1}{b}\frac{2}{c}\frac{2_1}{n}$

3. Space group symmetry: *Space group Pnma – ITC, volume A*

(Complement of Lecture – Slides 34-36)

$Pnma$	D_{2h}^{16}	mmm	Orthorhombic
No. 62	$P\,2_1/n\,2_1/m\,2_1/a$		Patterson symmetry $Pmmm$



Origin at $\bar{1}$ on $1\,2_1\,1$

Asymmetric unit $0 \le x \le \frac{1}{2};\quad 0 \le y \le \frac{1}{4};\quad 0 \le z \le 1$

Symmetry operations

(1) 1	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)\ \ 0,y,0$	(4) $2(\frac{1}{2},0,0)\ \ x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}\ \ 0,0,0$	(6) $a\ \ x,y,\frac{1}{4}$	(7) $m\ \ x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,z$

3. Space group symmetry: *Space group Pnma – ITC, volume A*

Bravais lattice

❶ $Pnma$ ❸ D_{2h}^{16} ❺ mmm ❻ Orthorhombic

❷ No. 62 ❹ $P\,2_1/n\,2_1/m\,2_1/a$ Patterson symmetry $Pmmm$

❶	$Pnma$	international symbol of the space group (reduced Hermann-Mauguin symbol)
❷	No. 62	space group number
❸	D_{2h}^{16}	Schoenflies symbol of the space group
❹	$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$	complete Hermann-Mauguin symbol

❺ mmm point group (pure orientation symmetry) obtained from the space group by suppressing all translation operations

glide mirror → reflection plane

screw axis → rotation axis

❻ orthorhombic crystal system → Bravais lattice : orthorhombic primitive

3. Space group symmetry: *Space group $Pnma$ – ITC, volume A*

Space group: $Pnma$ (short international symbol)

Orthorhombic lattice ($a \neq b \neq c$; $\alpha = \beta = \gamma = 90°$)

$P \rightarrow$ primitive

$n \rightarrow$ glide mirror $n \perp$ [100] : glide translation $\frac{\vec{b}+\vec{c}}{2}$

$m \rightarrow$ reflection plane $\perp$ [010]

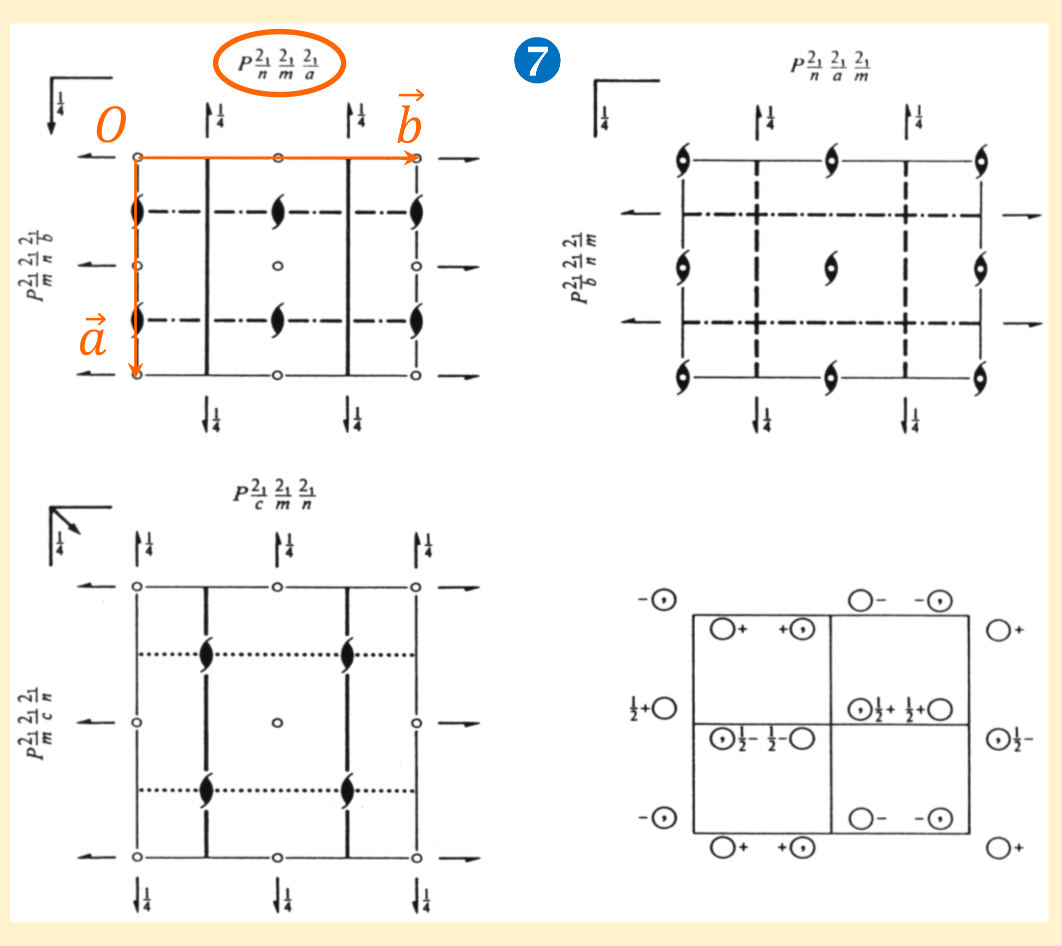
$a \rightarrow$ glide mirror $a \perp$ [001] : glide translation $\frac{\vec{a}}{2}$

$P\frac{2_1}{n}\frac{2_1}{m}\frac{2_1}{a}$ The complete Hermann-Mauguin symbol shows that the presence of mirrors n, m, and a implies the presence of screw axes 2_1 along the crystallographic directions (a, b and c-axes).

Point group : mmm

By suppression of the translations :

$n \rightarrow m$
$m \rightarrow m$
$a \rightarrow m$



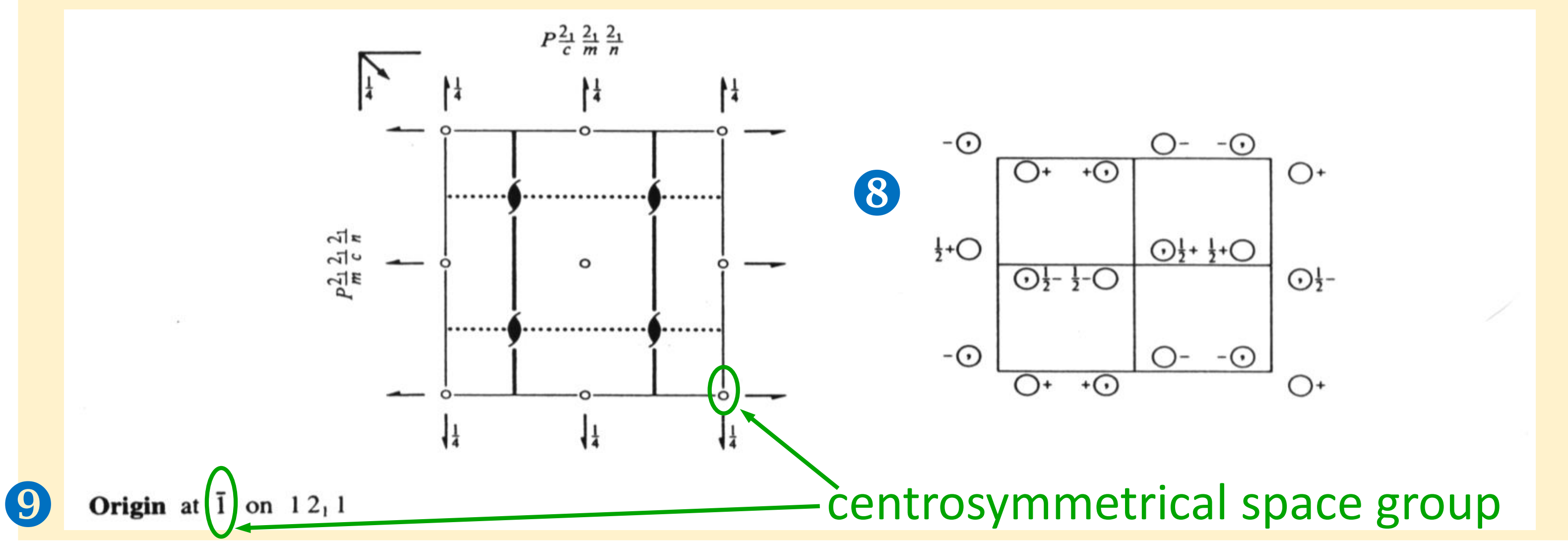
❼ Diagram of the symmetry elements

● Projection in (a, b) plane of the unit cell:

- $\vec{a}$-axis points downwards,
  $\vec{b}$-axis to the right in the page,
  $\vec{c}$-axis points upwards from the page.
- origin of the cell at the upper left corner.

● All symmetry planes and symmetry axes are indicated in the diagram (nature and position). For planes and axes $\perp$ to $\vec{c}$-axis, their height, if not zero, is indicated next to their graphical symbol.

● The upper left diagram corresponds to the $Pnma$ setting ; the 2 others, as well as them three if looking at them from the left (by turning the paper from 90°), correspond to other settings of the $Pnma$ space group (when permuting the a, b and c axes).



❽ Diagram of the equivalent positions

- Projection of the unit cell for the $Pnma$ setting.
- Equivalent general positions (circles) inside and next to the cell.
- Height of the atoms: the symbol '+' means a distance '$+z$' , '-' means '$-z$',

'½+' means 'z + ½', '½-' means ' $-z$ + ½'

❾ Origin Position chosen in previous diagrams for the origin of the unit cell:

$\bar{1}$ on 1 2_1 1 $\rightarrow$ on the inversion center located on a screw axis $2_1 \parallel \vec{b}$

⑩ **Symmetry operations**

(1) 1	(2) $2(0,0,\frac{1}{2})$ $\frac{1}{4},0,z$	(3) $2(0,\frac{1}{2},0)$ $0,y,0$	(4) $2(\frac{1}{2},0,0)$ $x,\frac{1}{4},\frac{1}{4}$
(5) $\bar{1}$ $0,0,0$	(6) a $x,y,\frac{1}{4}$	(7) m $x,\frac{1}{4},z$	(8) $n(0,\frac{1}{2},\frac{1}{2})$ $\frac{1}{4},y,z$

⑩ Symmetry operations

(Number) - nature - position for all symmetry operations of the space group (except translations of the lattice), each of them generating one atom.

Examples :

- (2): operation number 2
  $2\left(0\ 0\ \frac{1}{2}\right)$: combination of a diad rotation (order 2) and
  a glide translation $\vec{c}/2 \rightarrow$ screw axis 2_1 // $\vec{c}$-axis
  $\frac{1}{4}, 0, z$: axis ∥ $\vec{c}$, at $x = 1/4$ and $y = 0$
- (6): operation number 6
  a: glide mirror of type a (glide translation $\vec{a}/2$)
  $x, y, \frac{1}{4}$: plane ∥ $(\vec{a}, \vec{b})$ and thus $\perp z$, at $z = 1/4$

3. Space group symmetry: *Space group $Pnma$ – ITC, volume A*

CONTINUED — No. 62 — $Pnma$

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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$	$0kl$: $k+l=2n$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$hk0$: $h=2n$
							$h00$: $h=2n$
							$0k0$: $k=2n$
							$00l$: $l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+l,k=2n$

Symmetry of special projections

Along [001] $p2gm$
$\mathbf{a}'=\frac{1}{2}\mathbf{a}$ $\mathbf{b}'=\mathbf{b}$
Origin at $0,0,z$

Along [100] $c2mm$
$\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}$
Origin at $x,\frac{1}{4},\frac{1}{4}$

Along [010] $p2gg$
$\mathbf{a}'=\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$
Origin at $0,y,0$

Maximal non-isomorphic subgroups

I
- [2]$P2_12_12_1$ 1; 2; 3; 4
- [2]$P112_1/a$ ($P2_1/c$) 1; 2; 5; 6
- [2]$P12_1/m1$ ($P2_1/m$) 1; 3; 5; 7
- [2]$P2_1/n11$ ($P2_1/c$) 1; 4; 5; 8
- [2]$Pnm2_1$ ($Pmn2_1$) 1; 2; 7; 8
- [2]$Pn2_1a$ ($Pna2_1$) 1; 3; 6; 8
- [2]$P2_1ma$ ($Pmc2_1$) 1; 4; 6; 7

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [3]$Pnma$ ($\mathbf{a}'=3\mathbf{a}$); [3]$Pnma$ ($\mathbf{b}'=3\mathbf{b}$); [3]$Pnma$ ($\mathbf{c}'=3\mathbf{c}$)

Minimal non-isomorphic supergroups

I none

II [2]$Amma$($Cmcm$); [2]$Bbmm$($Cmcm$); [2]$Ccmb$($Cmca$); [2]$Imma$; [2]$Pnmm$ ($2\mathbf{a}'=\mathbf{a}$)($Pmmn$); [2]$Pcma$ ($2\mathbf{b}'=\mathbf{b}$)($Pbam$); [2]$Pbma$ ($2\mathbf{c}'=\mathbf{c}$)($Pbcm$)

3. Space group symmetry: *Space group $Pnma$ – ITC, volume A*

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

Positions

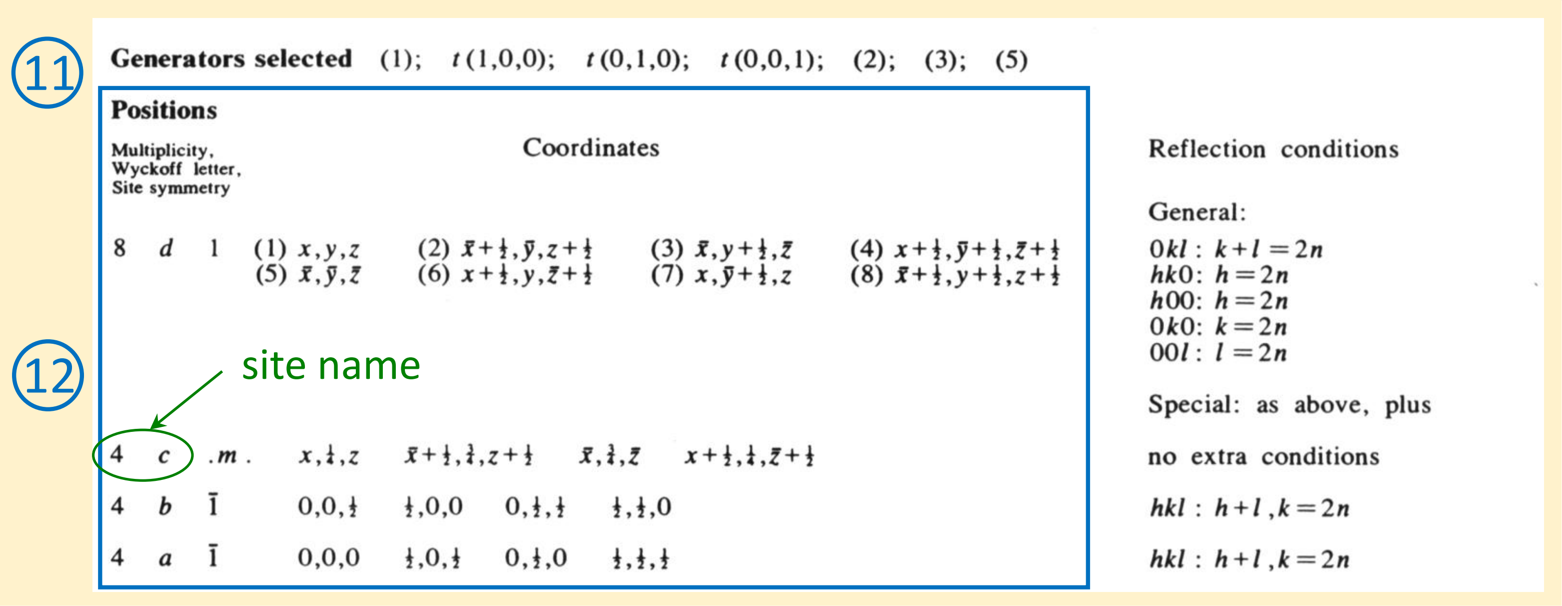
Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$ $hk0$: $h=2n$ $h00$: $h=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl : $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl : $h+l,k=2n$

(11) Generators selected

= set of symmetry operations generating the SG (arbitrary choice)

- (1); (2); (3); (5): numbers of the 4 symmetries selected from the previous list
- $t(1,0,0)$; $t(0,1,0)$; $t(0,0,1)$: translations of the lattice

3. Space group symmetry: *Space group Pnma – ITC, volume A*



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

Positions

Multiplicity, Wyckoff letter, Site symmetry			Coordinates				Reflection conditions
							General:
8	d	1	(1) x,y,z (5) $\bar{x},\bar{y},\bar{z}$	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$ (6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$ (7) $x,\bar{y}+\frac{1}{2},z$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$ (8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$	$0kl$: $k+l=2n$; $hk0$: $h=2n$; $h00$: $h=2n$; $0k0$: $k=2n$; $00l$: $l=2n$
							Special: as above, plus
4	c	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$	no extra conditions
4	b	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$	hkl: $h+l,k=2n$
4	a	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$	hkl: $h+l,k=2n$

(12) Equivalent positions and point symmetry: Wyckoff sites

List of the different sites from the most general (*i.e* less symemtrical) to the less general (*i.e.* most symmetrical: special position) given in 4 columns:

1- Multiplicity of the site = number of equivalent positions for the site
$\rightarrow$ decreases as the symmetry increases

2- Wyckoff letter: all sites are denoted by a letter, a, b, … in the reversed order (from the most symmetrical to the less one)

3- Site symmetry: symbol for the symmetry of the position of the site

4- Coordinates of all equivalent positions for the site

3. Space group symmetry: *Space group Pnma – ITC, volume A*

General position

Wyckoff site 8*d*

8	*d*	1	(1) x,y,z	(2) $\bar{x}+\frac{1}{2},\bar{y},z+\frac{1}{2}$	(3) $\bar{x},y+\frac{1}{2},\bar{z}$	(4) $x+\frac{1}{2},\bar{y}+\frac{1}{2},\bar{z}+\frac{1}{2}$
			(5) $\bar{x},\bar{y},\bar{z}$	(6) $x+\frac{1}{2},y,\bar{z}+\frac{1}{2}$	(7) $x,\bar{y}+\frac{1}{2},z$	(8) $\bar{x}+\frac{1}{2},y+\frac{1}{2},z+\frac{1}{2}$

8 general equivalent positions generated by the 8 symmetries of the space group
$\rightarrow$ their number corresponds to the one of the symmetry operation acting
on the starting general position x, y, z (placed on a 1 axis).

Special positions

4	*c*	$.m.$	$x,\frac{1}{4},z$	$\bar{x}+\frac{1}{2},\frac{3}{4},z+\frac{1}{2}$	$\bar{x},\frac{3}{4},\bar{z}$	$x+\frac{1}{2},\frac{1}{4},\bar{z}+\frac{1}{2}$
4	*b*	$\bar{1}$	$0,0,\frac{1}{2}$	$\frac{1}{2},0,0$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
4	*a*	$\bar{1}$	$0,0,0$	$\frac{1}{2},0,\frac{1}{2}$	$0,\frac{1}{2},0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$

Wyckoff site 4*c*

special equivalent positions generated by the 8 symmetries of the
space group from an atom sitting in the special position $.m.$
$\rightarrow$ on the m plane $\perp \vec{b}$-axis $\rightarrow$ $y = 1/4 \rightarrow$ their number is twice smaller
(1) = (7), (2) = (8), (3) = (5), (4) = (6)

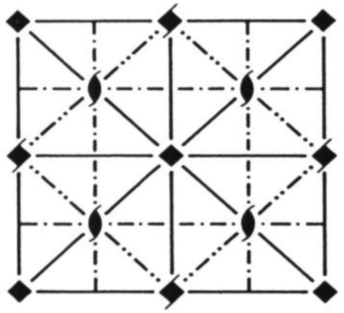
Wyckoff sites 4*b* and 4*a*

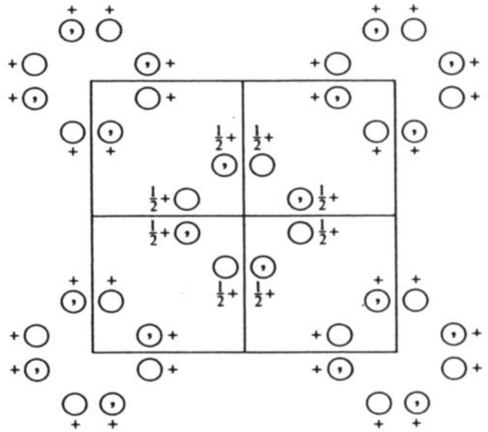
4 special equivalent positions starting from an atom sitting on $\bar{1}$:
0, 0, ½ ($4b$) or 0, 0, 0 ($4a$) → The number is also divided by 2

3. Space group symmetry: *Space group $I4mm$ – ITC, volume A*

$I\,4\,m\,m$ $\quad$ C_{4v}^{9} $\quad$ $4\,m\,m$ $\quad$ Tetragonal

No. 107 $\quad$ $I\,4\,m\,m$ $\quad$ Patterson symmetry $I\,4/m\,m\,m$





Origin on $4mm$

Asymmetric unit $\quad 0\le x\le \frac{1}{2};\ \ 0\le y\le \frac{1}{2};\ \ 0\le z\le \frac{1}{4};\ \ x\le y$

Symmetry operations

For (0,0,0)+ set

(1) 1	(2) $2\ \ 0,0,z$	(3) $4^{+}\ \ 0,0,z$	(4) $4^{-}\ \ 0,0,z$
(5) $m\ \ x,0,z$	(6) $m\ \ 0,y,z$	(7) $m\ \ x,\bar{x},z$	(8) $m\ \ x,x,z$

For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})$+ set

(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^{+}(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^{-}(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,z$	(7) $c\ \ x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,z$

Bravais lattice: body centered (I) tetragonal

Axis $4 \parallel \vec{c}$; mirrors $m \perp a$ and b; mirrors $\perp [110]$ and $[1\bar{1}0]$

Symmetry operations

I lattice — Tetrad rotation

For $(0,0,0)+$ set			
(1) 1	(2) $2\ \ 0,0,z$	(3) $4^+\ \ 0,0,z$	(4) $4^-\ \ 0,0,z$
(5) $m\ \ x,0,z$	(6) $m\ \ 0,y,z$	(7) $m\ \ x,\bar{x},z$	(8) $m\ \ x,x,z$
For $(\frac{1}{2},\frac{1}{2},\frac{1}{2})+$ set			
(1) $t(\frac{1}{2},\frac{1}{2},\frac{1}{2})$	(2) $2(0,0,\frac{1}{2})\ \ \frac{1}{4},\frac{1}{4},z$	(3) $4^+(0,0,\frac{1}{2})\ \ 0,\frac{1}{2},z$	(4) $4^-(0,0,\frac{1}{2})\ \ \frac{1}{2},0,z$
(5) $n(\frac{1}{2},0,\frac{1}{2})\ \ x,\frac{1}{4},z$	(6) $n(0,\frac{1}{2},\frac{1}{2})\ \ \frac{1}{4},y,z$	(7) $c\ \ x+\frac{1}{2},\bar{x},z$	(8) $n(\frac{1}{2},\frac{1}{2},\frac{1}{2})\ \ x,x,z$

- The symmetry operations are given :
  - for an atom in x, y, z : $(0,0,0)^+$ set
  - and for an atom in $x+½, y+½, z+½$ (due to the I lattice): $\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)^+$ set

- The symmetry operations are given in such a manner that they generate only 1 atom
  - $\rightarrow$ the tetrad axis, starting from an atom in x, y, z, generates 3 other atoms and is thus split into 3 parts

$(0,0,0)^+$ set: 8 symmetry operations

(2) 2	$0,0,z$	rotation of order 4 applied twice $\rightarrow$ rotation 2
(3) 4^+	$0,0,z$	rotation of order 4 applied once in positive way (4^+)
(4) 4^-	$0,0,z$	rotation of order 4 applied three times in positive way *i.e.* applied once in negative way (4^-)

$\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)^+$ set: due to the I lattice, number of symmetry operations multiplied by 2
$\rightarrow$ 8 additional symmetry operations with a glide translation

3. Space group symmetry: *Space group $I4mm$ – ITC, volume A*

CONTINUED | No. 107 | $I\,4\,m\,m$

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

I lattice

Positions

Multiplicity, Wyckoff letter, Site symmetry — Coordinates — Reflection conditions

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

			Coordinates				Reflection conditions
16	e	1	(1) x,y,z (5) $x,\bar{y},z$	(2) $\bar{x},\bar{y},z$ (6) $\bar{x},y,z$	(3) $\bar{y},x,z$ (7) $\bar{y},\bar{x},z$	(4) $y,\bar{x},z$ (8) y,x,z	General: $hkl: h+k+l=2n$; $hk0: h+k=2n$; $0kl: k+l=2n$; $hhl: l=2n$; $00l: l=2n$; $h00: h=2n$
							Special: as above, plus
8	d	$.m.$	$x,0,z$	$\bar{x},0,z$	$0,x,z$	$0,\bar{x},z$	no extra conditions
8	c	$..m$	x,x,z	$\bar{x},\bar{x},z$	$\bar{x},x,z$	$x,\bar{x},z$	no extra conditions
4	b	$2mm.$	$0,\frac{1}{2},z$	$\frac{1}{2},0,z$			$hkl: l=2n$
2	a	$4mm$	$0,0,z$				no extra conditions

In addition to the $(1,0,0)$, $(0,1,0)$ and $(0,0,1)$ translations of the lattice, one must add the translation $\left(\frac{1}{2},\frac{1}{2},\frac{1}{2}\right)$ accounting for its I type.

Only one half of coordinates are given, one must add $\frac{1}{2},\frac{1}{2},\frac{1}{2}$ to each of them to obtain all equivalent positions (Example: site 16*e* $\rightarrow$ 16 general equivalent positions, from which only 8 are given).