Symmetry
Point group
Bravais lattice
Space group

Ott Chapter 6, 7, 8, 9 (9.2, 9.6, 9.7 제외, Fig 9.4 포함), 10

Sherwood & Cooper Chapter 3.1 ~ 3.8

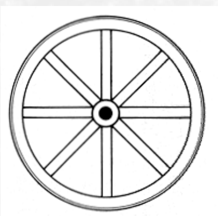
Hammond Chapter 2.1 ~ 2.5; 3.1 ~ 3.3; 4.1 ~ 4.7; 5.1 ~ 5.6; 12.5.1 ~ 12.5.2

Krawitz Chapter 1.1 ~ 1.8; 2.1 ~ 2.4

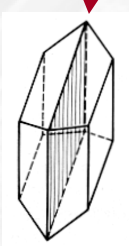
Symmetry

- All repetition operations are called symmetry operations.
  - ✓ Symmetry consists of the repetition of a pattern by the application of specific rules.
- When a symmetry operation has a locus, that is a point, or a line, or a plane that is left unchanged by the operation, this locus is referred to as the symmetry element.

Symmetry operation	Geometrical representation	Symmetry element
Rotation	Axis (line)	Rotation axis
Inversion	Point (center)	Inversion center (center of symmetry)
Reflection	Plane	Mirror plane
Translation	vector	Translation vector

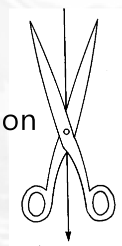


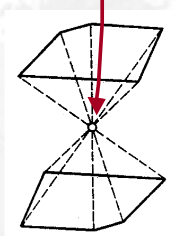
rotation



reflection

rotation





inversion

Symmetry operation, symmetry elements

(1) Translation

(2) Rotation; **1 2 3 4 6**

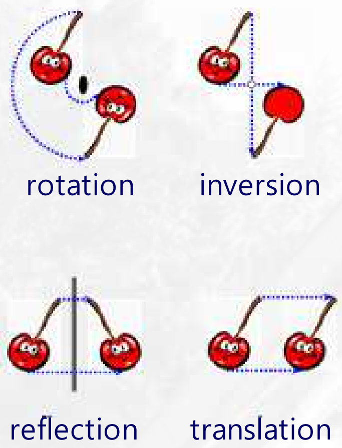
(3) Reflection; **m** (= $\bar{2}$)

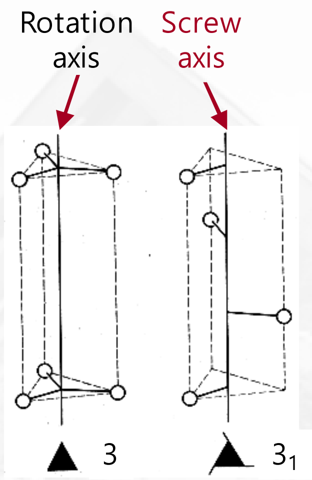
(4) Inversion (center of symmetry) (= $\bar{1}$)

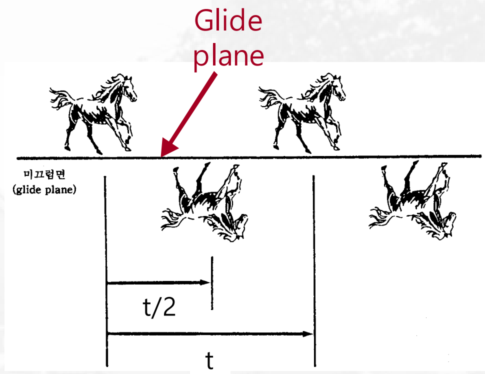
(5) Rotation-inversion; $\bar{1}$ (=center of symmetry), $\bar{2}$ (= mirror), $\bar{3}$, $\bar{4}$, $\bar{6}$

(6) Screw axis; rotation + translation **2_1, 3_1, 3_2, 4_1, 4_2, 4_3, 6_1,---, 6_5**

(7) Glide plane; reflection + translation, **a, b, c, n, d**







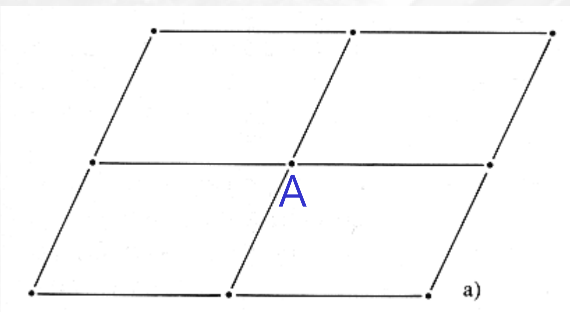
Ott Chap 10
Pecharsky Chap 2, 3

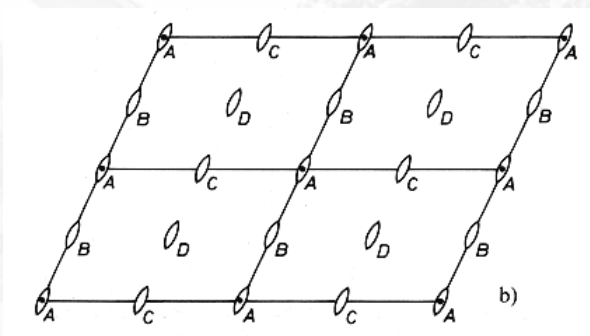
Rotation Axis

- general plane lattice
- 180° rotation about the central lattice point A → coincidence

  → 2-fold rotation axis; symbol 2, ⬮ (normal to plane of paper), → (parallel to plane of paper)

Order (multiplicity) of the rotation axis $n = \frac{360^o}{\phi} = \frac{2\pi}{\phi}$



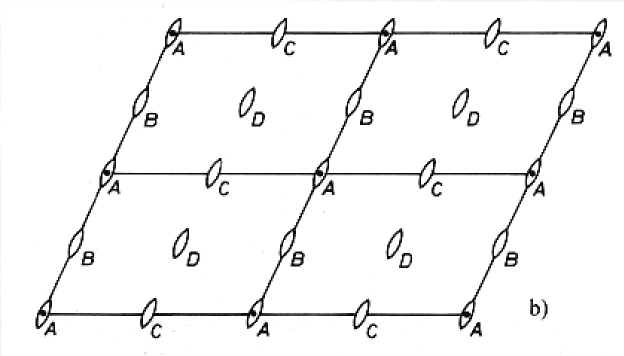


Ott Chap 6

Equivalent vs. Identical

- Two objects are EQUIVALENT
  - ✓ When they can be brought into coincidence by application of a symmetry operation.
- Two objects are IDENTICAL
  - ✓ When no symmetry operation except lattice translation is involved.
  - ✓ equivalent by translation

- All A's are equivalent to one another
- A is not equivalent to B

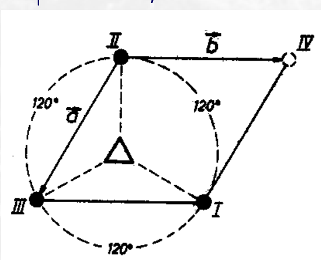


Rotation Axis

- n-fold axis $n = \frac{360^o}{\phi} = \frac{2\pi}{\phi}$ ϕ: minimum angle required to reach a position indistinguishable from the starting point
- Axis with n > 2 will have at least 2 other points lying in a plane ⊥ to it.
  - ✓ 3 non-colinear points define a plane. → must be a lattice plane. (translational periodicity)

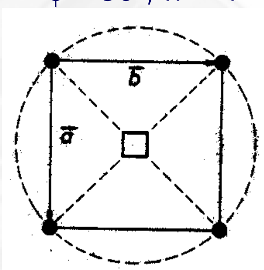
3-fold axis ▲

ϕ = 120°, n = 3



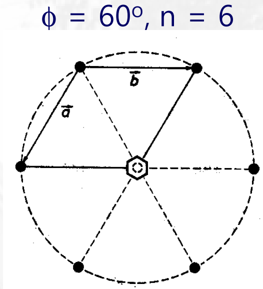
4-fold axis ■

ϕ = 90°, n = 4



6-fold axis ⬢

ϕ = 60°, n = 6



- In space lattices and consequently in crystals, only 1-, 2-, 3-, 4-, and 6-fold rotation axes can occur.

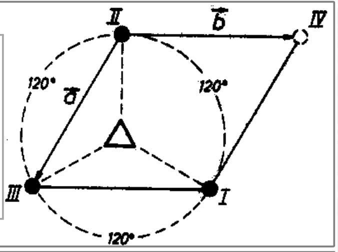
Why there is no 5-fold rotation axis?

- The points generated by rotation axis must fulfil the **conditions for being a lattice plane** --- parallel lattice lines should have the same translation period (all the lattice points should have identical surroundings).

3-fold rotation axis

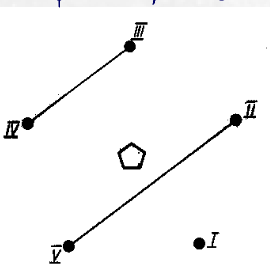
- Lattice translation moves I → IV
- 4 points produce a unit mesh of a lattice plane

→ 3 fold axes are compatible with space lattice



No 5-fold rotation axis in space lattice

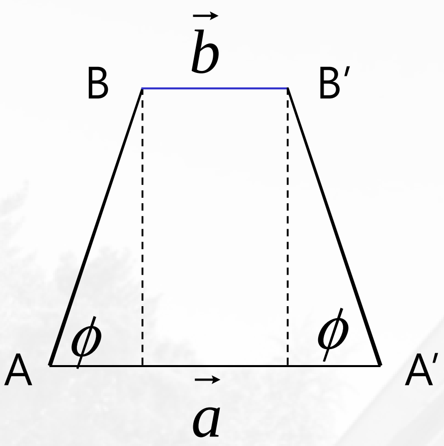
ϕ= 72°, n=5



- II-V and III-IV parallel but not equal or integral ratio
  → no 5-fold axes in space lattice
- This structure does not have translational symmetry in 3-dimensions
  → do not have finite unit cell → quasicrystal
  - ✓ Quasi – because there is no translational symmetry
  - ✓ Crystal – because they produce discrete, crystal-like diffraction patterns
- It is impossible to completely fill the area in 2-dimensions with pentagons without creating gaps

Rotation axis > why 1, 2, 3, 4 and 6 only ?

- limitation of ϕ set by **translation periodicity**



$$\vec{b} = m\vec{a}$$ where m is an integer

$$ma = a - 2a\cos\phi$$

$$m = 1 - 2\cos\phi$$

$$\cos\phi = \frac{1-m}{2}$$

m	cos ϕ	ϕ	n
-1	1	2π	**1**
0	½	$\pi/3$	**6**
1	0	$\pi/2$	**4**
2	- ½	$2\pi/3$	**3**
3	-1	π	**2**

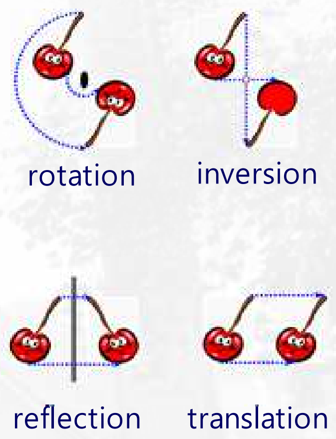
1, 2, 3, 4, 6

See Sherwood & Cooper page 78

Symmetry operation vs Symmetry element, Proper vs Improper

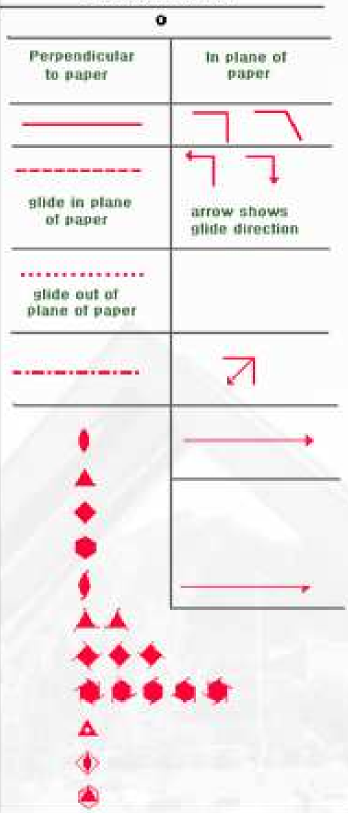
- Rotation by 60° around an axis → **symmetry operation**
- 6-fold rotation axis is a **symmetry element** which contains six rotational symmetry operations

- **Proper** symmetry elements
  - ✓Rotation axes, screw axes, translation vectors
- **Improper** symmetry elements
  - ✓Inverts an object in a way that may be imaged by comparing right & left hands
  - ✓Inverted object is called an **enantiomorph** of the direct object (right vs left hand)
  - ✓Center of inversion, roto-inversion axes, mirror plane, glide plane



Symmetry Element

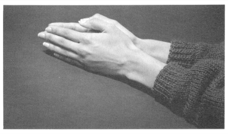
Type of symmetry element	Written symbol	Graphical symbol
Center of Symmetry	$\bar{1}$	o
		Perpendicular to paper / In plane of paper
Mirror plane	m	
Glide plane	a b c	glide in plane of paper; arrow shows glide direction; glide out of plane of paper
	n	
Rotation	2 3 4 6	
Screw Axis	2_1 3_1 3_2 4_1 4_2 4_3 6_1 6_2 6_3 6_4 6_5	
Inversion Axis	$\bar{3}$ $\bar{4}$ $\bar{6}$	

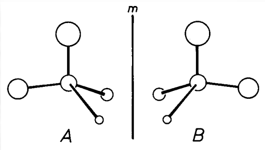


Ott Chap 15.2

Reflection

➢ reflection, a plane of symmetry or a mirror plane, m, | **(bold line)**, ⎾





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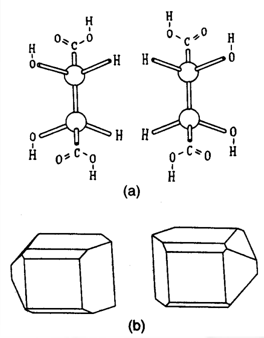
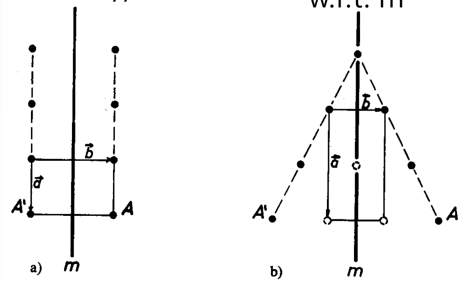


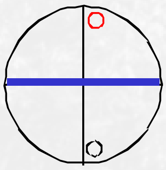
Lattice line // m

Lattice line tilted w.r.t. m

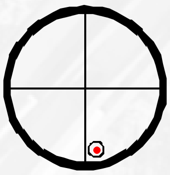


rectangular

centered rectangular



m_{yz} (m_x)



m_{xy} (m_z)

● down

○ up

Black & Red; enantiomorphs

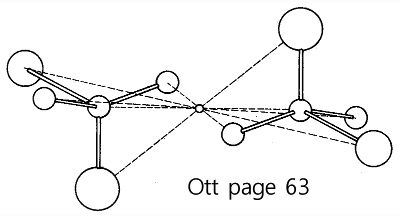
● down, left

○ up, right

Inversion

➢ inversion, center of symmetry or inversion center, $\bar{1}$ ○

Hammond page 82



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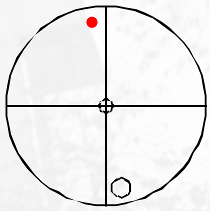

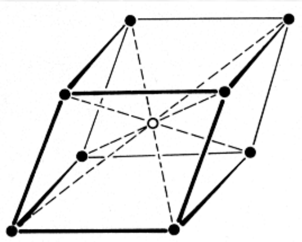

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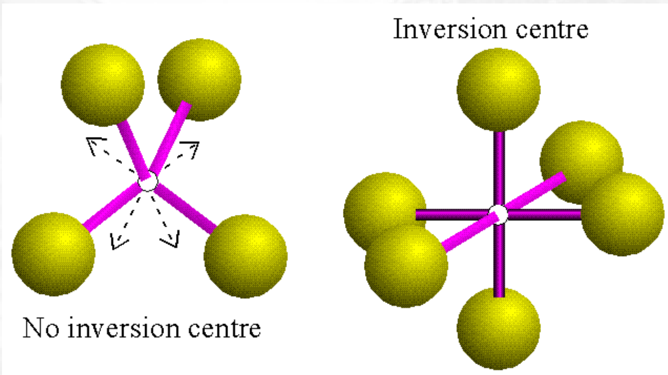


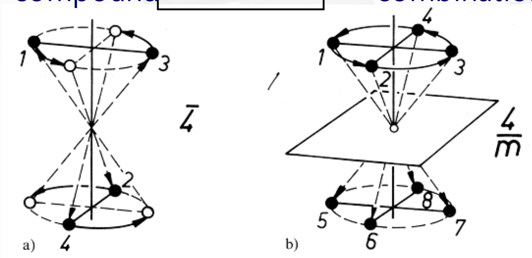
www.gh.wits.ac.za/craig/diagrams/

All lattices are centrosymmetric.

Compound Symmetry Operation

- compound symmetry operation
  - ✓ two symmetry operation in sequence as a single event
- combination of symmetry operations
  - ✓ 2 or more individual symmetry operations are combined, which are themselves symmetry operations.

compound **4 + 1bar** combination



4 & 1bar are not present

4 & m are present

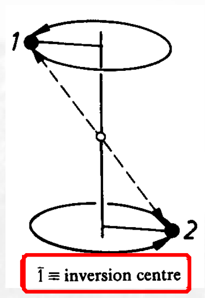
Table 5.1. Compound symmetry operations of simple operations. The corresponding symmetry elements are given in round brackets

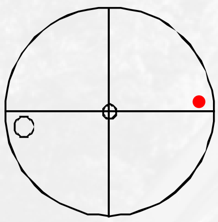
	Rotation	Reflection	Inversion	Translation
Rotation	×	Roto-reflection	Roto-inversion	Screw rotation
Reflection	(Roto-reflection axis)	×	2-fold rotation	Glide reflection
Inversion	(Roto-inversion axis)	(2-fold rotation axis)	×	Inversion
Translation	(Screw axis)	(Glide plane)	(Inversion centre)	×

Rotoinversion

- compound symmetry operation of rotation and inversion
- rotoinversion axis $\bar{n}$
- 1, 2, 3, 4, 6 → $\bar{\mathbf{1}}$ (=center of symmetry), $\bar{\mathbf{2}}$ (= mirror), $\bar{\mathbf{3}}$, $\bar{\mathbf{4}}$, $\bar{\mathbf{6}}$

$\bar{1}$

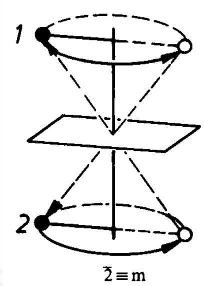


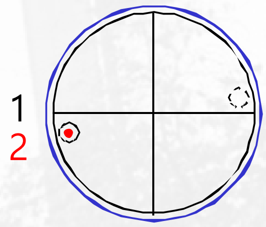


● down, left

○ up, right

$\bar{2}(\equiv m)$

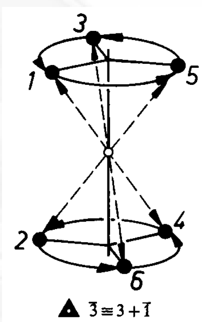


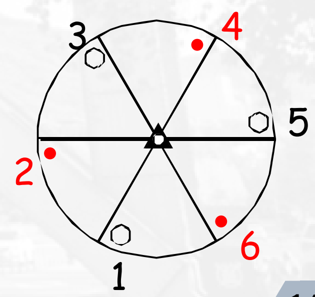


m_{xy} (m_z)

$\bar{3} \equiv 3 + \bar{1}$ ▲

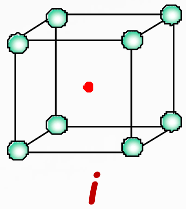
Rare case of "compound symmetry operation = combination of symmetry operation"

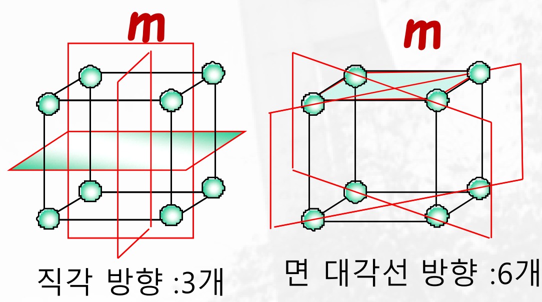


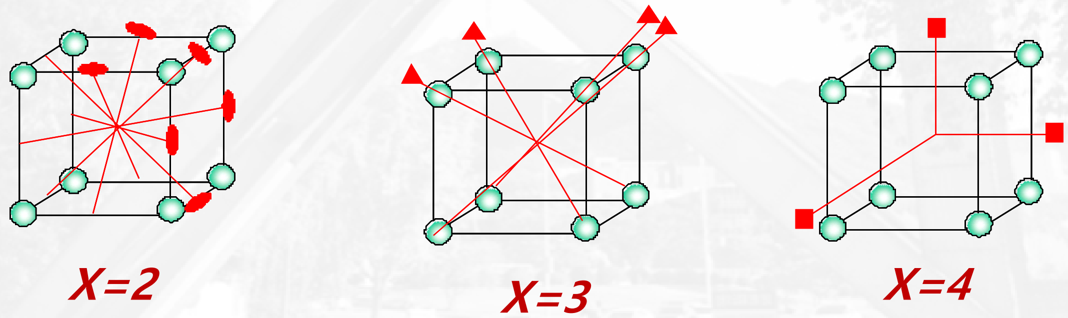


Symmetry elements of a Cube (정육면체)

- center of symmetry
- nine mirror planes
- six diad axis
- four triad axis
- three tetrad axis

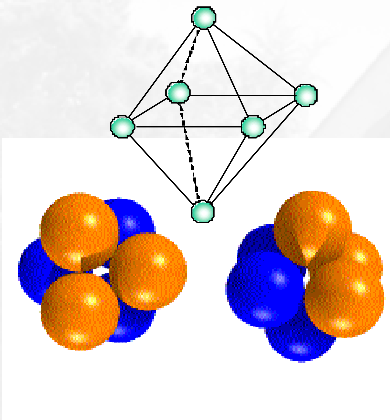


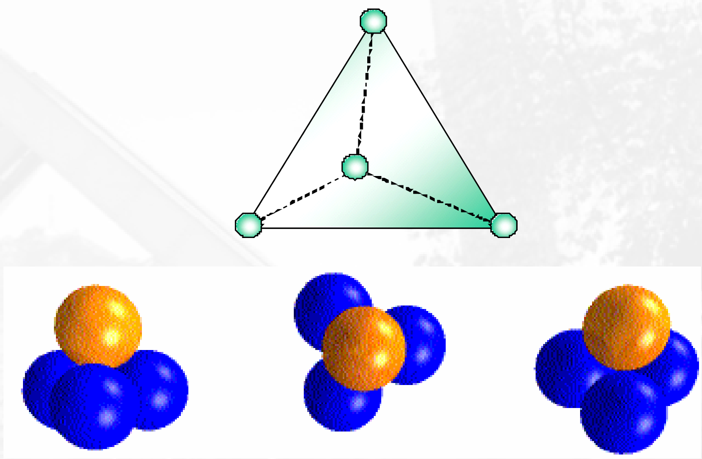




Symmetry elements of a Tetrahedron & Octahedron

- Symmetry elements of a octahedron ≡ those of a cube
- Symmetry elements of a tetahedron
  - ✓ six mirror planes
  - ✓ three $\bar{4}$ (inverse tetrad axis)
  - ✓ Four 3-fold rotation axis





Point group

- Complete set of symmetry elements → symmetry group
- Limited # of symmetry elements (ten) & all valid combination among them → 32 crystallographic symmetry groups → 32 point groups
- Limited # of symmetry elements (ten) + the way in which they interact with each other → limited # of completed sets of symmetry elements (32 symmetry groups = 32 point groups)

- Point group - a group of point symmetry operations whose operation leaves at least one point unmoved (lattice translation is not considered in point group.)
- Point group ← symmetry elements in these groups have at least one common point and, as a result, they leave at least one point of an object unmoved.

When a symmetry operation has a locus (that is a point, a line, or a plane) that is left unchanged by the operation, this locus is referred to as the **symmetry element.**

32 Point Groups

- The point groups are made up from point symmetry operation and combinations of them (translation is excluded).
- X : x-fold rotation axis
- m : mirror plane
- $\bar{1}$: inversion centre
- $\bar{X}$: rotoinversion axis
- X2 : X-fold rotation axis + 2-fold rotation axis (X⊥2)
- Xm(m) : X + m (X // m)
- $\bar{X}$2(2) : $\bar{X}$ + 2-fold axis (Xbar⊥2)
- $\bar{X}$m : $\bar{X}$ + m (X // m)
- X/mm : X + m1 + m2 (X ⊥ m1, X // m2)

32 point groups

Table 8.2. The 32 point groups

Crystal system	Point groups		
Triclinic	$\bar{1}$	1	2
Monoclinic	2/m	m, 2	3
Orthorhombic	2/m 2/m 2/m (mmm)	mm2, 222	3
Tetragonal	4/m 2/m 2/m (4/mmm)	$\bar{4}$2m, 4mm, 422 4/m, $\bar{4}$, 4	7
Trigonal	$\bar{3}$ 2/m ($\bar{3}$m)	3m, 32, $\bar{3}$, 3	5
Hexagonal	6/m 2/m 2/m (6/mmm)	$\bar{6}$m2, 6mm, 622 6/m, $\bar{6}$, 6	7
Cubic	4/m $\bar{3}$ 2/m (m$\bar{3}$m)	$\bar{4}$3m, 432, 2/m$\bar{3}$, 23 (m$\bar{3}$)	5

full symbols
(short symbols)

Total 32

Ott Chap 9

Symmetry directions

Xtal systems	Symmetry directions			
Triclinic	a	b	c	a1 ≠ a2 ≠ a3, α ≠ β ≠ γ ≠ 90º
Monoclinic	a	b	c	a1 ≠ a2 ≠ a3, α = γ = 90º ≠ β
Orthorhombic	a	b	c	a1 ≠ a2 ≠ a3, α = β = γ = 90º
Tetragonal	c	<a>	<110>	a1 = a2 ≠ a3, α = β = γ = 90º
Trigonal	c	<a>	-	a1 = a2 = a3, α = β = γ < 120º ≠ 90º
Hexagonal	c	<a>	<210>	a1 = a2 ≠ a3, α = β = 90º , γ = 120º
Cubic	<a>	<111>	<110>	a1 = a2 = a3, α = β = γ = 90º

7 crystal systems

- Combination of symmetry elements & their orientations w.r.t. one another defines the crystallographic axes.
- Axes can be chosen arbitrarily, but are usually chosen w.r.t. specific symmetry elements present in a group.
  - ✓ // rotation axes or ⊥ m
- All possible 3-D crystallographic point groups can be divided into a total of 7 crystal systems based on the presence of a specific symmetry elements or specific combination of them present in the point group symmetry.
- (7 crystal systems) X 5 (types of lattices) → 14 different types of unit cells are required to describe all lattices (14 Bravais lattices).

7 Crystal systems, 6 Crystal family

Table 2.6 Seven crystal systems and the corresponding characteristic symmetry elements.

Crystal system	Characteristic symmetry element or combination of symmetry elements
Triclinic	No axes other than onefold rotation or onefold inversion
Monoclinic	Unique twofold axis and/or single mirror plane
Orthorhombic	Three mutually perpendicular twofold axes, either rotation or inversion
Trigonal	Unique threefold axis, either rotation or inversion
Tetragonal	Unique fourfold axis, either rotation or inversion
Hexagonal	Unique sixfold axis, either rotation or inversion
Cubic	Four threefold axes, either rotation or inversion, along four body diagonals of a cube

Trigonal & hexagonal can be described in the same type of the lattice

→ six crystal family

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Characteristic symmetry elements of the 7 crystal systems

Table 8.9. Characteristic symmetry elements of the seven crystal systems

Crystal system	Point groups[a]	Characteristic symmetry elements
Cubic	$4/m\,\underline{\bar{3}}\,2/m$ $\bar{4}\underline{3}m$, $4\underline{3}2$, $2/m\underline{\bar{3}}$, $2\underline{3}$	4 ▲
Hexagonal	$\underline{6}/m\,2/m\,2/m$ $\underline{\bar{6}}m2$, $\underline{6}mm$, $\underline{6}22$, $\underline{6}/m$, $\underline{\bar{6}}$, $\underline{6}$	⬢ or (hexagon with triangle)
Tetragonal	$\underline{4}/m\,2/m\,2/m$ $\underline{\bar{4}}2m$, $\underline{4}mm$, $\underline{4}22$, $\underline{4}/m$, $\underline{\bar{4}}$, $\underline{4}$	1 ■ or 1 ◪ (3 ■ or 3 ◪ ⇒ cubic)
Trigonal	$\underline{\bar{3}}\,2/m$ $\underline{3}m$, $\underline{3}2$, $\underline{\bar{3}}$, $\underline{3}$	1 ▲ (remember that m normal to 3 gives $\bar{6}$ → hexagonal)
Orthorhombic	$\underline{2/m\,2/m\,2/m}$ $\underline{mm2}$, $\underline{222}$	2 and/or m in three orthogonal directions
Monoclinic	$\underline{2/m}$ $\underline{m}$, $\underline{2}$	2 and/or m in one direction
Triclinic	$\underline{\bar{1}}$ $\underline{1}$	$\bar{1}$ or 1 only

[a] Characteric symmetry elements are underlined.

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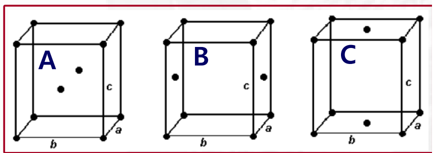
3D Bravais lattices

- The 14 Bravais lattices in 3 dimensions are obtained by coupling one of the 7 lattice systems (or axial systems) with one of lattice centerings. Each Bravais lattice refers to a distinct lattice type.

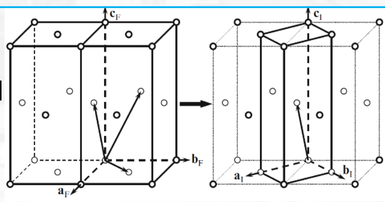


- The lattice centerings are
  - ✓ Body (I): one additional lattice point at center of the cell.
  - ✓ Face (F): additional lattice points at centers of all the faces of the cell.
  - ✓ Base (A, B or C): additional lattice points at centers of each pair of cell faces.

- Not all the combinations of crystal systems and lattice centerings are needed to describe the possible lattices.
- There are in total 7 × 5 (P, I, F, C, R) = 35 possible combinations, but many of these are in fact equivalent to each other.
  - ✓ For example, the tetragonal F lattice can be described by a tetragonal I lattice by different choice of crystal axes.

→ This reduces the number of combinations to 14. → 14 Bravais lattices

tetragonal F lattice

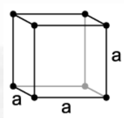
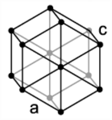
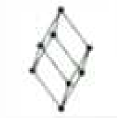
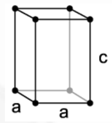
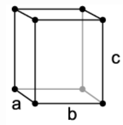
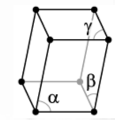
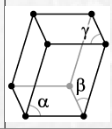
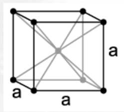
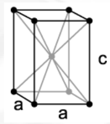
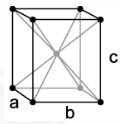
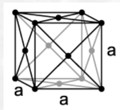
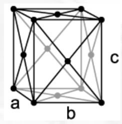
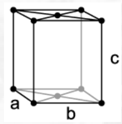
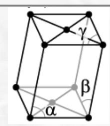


tetragonal I lattice

14 Bravais lattice

- 7 crystal systems (6 crystal families) X 5 types of lattices

→ only 14 different types of unit cells are required to describe all lattices using conventional crystallographic symmetry → 14 Bravais lattice

	cubic	hexagonal	rhombohedral (trigonal)	tetragonal	orthorhombic	monoclinic	triclinic
P							
I							
F				I			
C				P			

Pecharsky 2nd ed. 2.11 See Ott Chap 7

Space group

- Unit cell translations
- Centering operations (Lattices) (*A, B, C, I, F, R*)
- Glide planes (reflection + translation) (*a, b, c, n, d*)
- Screw axes (rotation + translation) (2_1, 3_1, 3_2)

- If translation operations are included with rotation and inversion → We have 230 three-dim. space groups
- Space group - symmetry of crystal lattices and crystal structures
- Bravais lattice + point group → 230 space groups
  + screw axis
  + glide plane
- Hermann-Mauguin symbols (4 positions)
  - ✓First position is Lattice type (P, A, B, C, I, F or R)
  - ✓Second, third and fourth positions as with point groups

$Cmm2$ (35) $P\frac{4}{m}\bar{3}\frac{2}{m}$ (225) $F\bar{4}3m$ (No.216)

International Tables for Crystallography, Volume A: Space-group symmetry

Crystal symmetry, 14 Bravais lattice

Crystal System	Bravais Lattices	Symmetry	Symmetry	Axis System
Cubic	P, I, F	m3m	m**3**m	a=b=c, α=β=γ=90
Tetragonal	P, I	4/mmm	**4**/mmm	a=b≠c, α=β=γ=90
Orthorhombic	P, C, I, F	mmm	**mmm**	a≠b≠c, α=β=γ=90
Hexagonal	P	6/mmm	**6**/mmm	a=b≠c, α=β=90, γ=120
Rhombohedral	R	3m	**3**m	a=b=c, α=β=γ≠90
Monoclinic	P, C	2/m	**2**/m	a≠b≠c, α=γ=90, β≠90
Triclinic	P	1	1	a≠b≠c, α≠β≠γ≠90

Quartz
Crystal System: trigonal
Bravais Lattice: primitive
Space Group: $P3_221$
Lattice Parameters: 4.9134 x 4.9134 x 5.4052 A
Atom Positions:

	x	y	z
Si	0.47 0	0	0.667
O	0.414	0.268	0.786

$P3_221$
$P\ 3_2\ 2\ 1$

6/mmm
6/m m m

Symmetry directions, Space group

Xtal systems	**Symmetry directions**		
Triclinic			
Monoclinic	b		
Orthorhombic	a	b	c
Tetragonal	c	<a>	<110>
Trigonal	c	<a>	
Hexagonal	c	<a>	<210>
Cubic	<a>	<111>	<110>

Fmmm
Face centered lattice
m ⊥ to a axis
m ⊥ to b axis
m ⊥ to c axis

$P3_221$
Primitive lattice
3_2 along the c axis
2 fold rot axis along the a axis
1 fold rot axis along the <210>

Fd3m
Face centered lattice
d ⊥ to a axis
3 fold axis along the <111>
m ⊥ to <110>

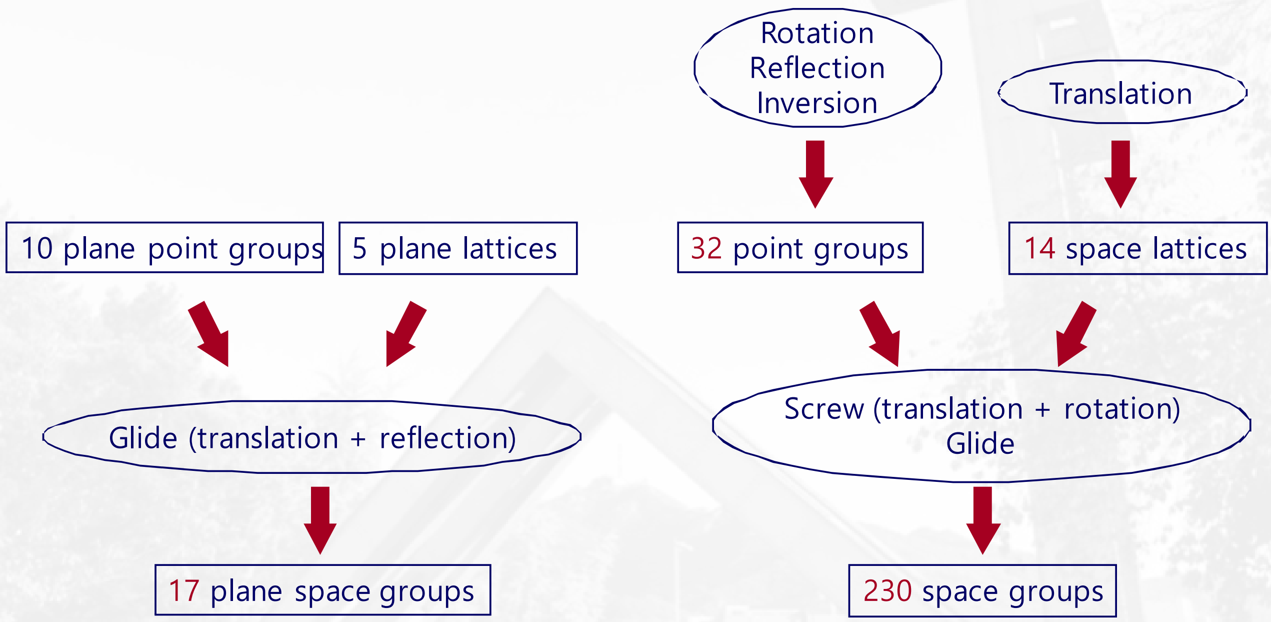
14 Bravais lattice > space group symbols

	P	C	I	F
Triclinic	$P\bar{1}$			
Monoclinic	$P2/m$	$C2/m$		
Orthorhombic	$P2/m2/m2/m$	$C2/m2/m2/m$	$I2/m2/m2/m$	$F2/m2/m2/m$
Tetragonal	$P4/m2/m2/m$		$I4/m2/m2/m$	
Trigonal	$P6/m2/m2/m$	$R\bar{3}2/m$		
Hexagonal				
Cubic	$P4/m\bar{3}2/m$		$I4/m\bar{3}2/m$	$F4/m\bar{3}2/m$

- The 14 Bravais lattice represent the 14 and only way in which it is possible to fill space by a 3-D periodic array of points.
- All crystals are built up on one of 14 Bravais lattices.
- Any crystal structure has only one Bravais lattice.
- **Number of lattice is fixed at 14.**
- **Infinite number of arranging atoms in a cell ← basis**

Ott Chap 7

plane groups vs. space groups



Krawitz page 25, page 28

International Tables for Crystallography

Short Hermann-Mauguin symbol | Schoenflies symbol | Point group | Crystal system symbol

Space group number

Full Hermann-Mauguin symbol

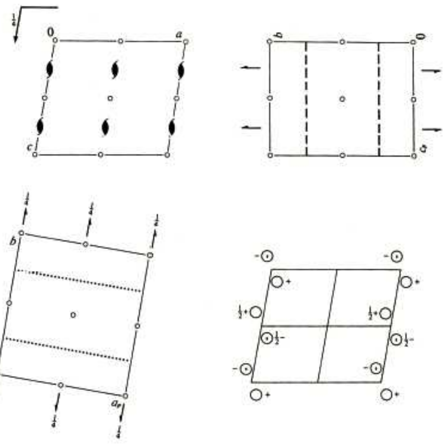
$P2_1/c$ C_{2h}^5 $2/m$ Monoclinic

No. 14 $P1\,2_1/c\,1$ Patterson symmetry $P1\,2/m\,1$

Patterson symmetry

UNIQUE AXIS b, CELL CHOICE 1

Projection of symmetry elements



Projection of a general position

Choice of origin
Asymmetric unit
Symmetry operations

Origin at $\bar{1}$

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

Symmetry operations

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

International Tables for Crystallography

General & special positions

CONTINUED   No. 14 $P2_1/c$

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	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$	$h0l$: $l=2n$ $0k0$: $k=2n$ $00l$: $l=2n$
							Special: as above, plus
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$			hkl : $k+l=2n$
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$			hkl : $k+l=2n$
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$			hkl : $k+l=2n$

General position

Special position

Symmetry of special projections

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

Along [100] $p2gg$ $\mathbf{a}'=\mathbf{b}$ $\mathbf{b}'=\mathbf{c}_p$ Origin at $x,0,0$

Along [010] $p2$ $\mathbf{a}'=\frac{1}{2}\mathbf{c}$ $\mathbf{b}'=\mathbf{a}$ Origin at $0,y,0$

Maximal non-isomorphic subgroups

I   [2] $P1c1$ (Pc, 7)   1; 4
[2] $P12_11$ ($P2_1$, 4)   1; 2
[2] $P\bar{1}$ (2)   1; 3

IIa none

IIb none

Maximal isomorphic subgroups of lowest index

IIc [2] $P12_1/c1$ ($\mathbf{a}'=2\mathbf{a}$ or $\mathbf{a}'=2\mathbf{a}, \mathbf{c}'=2\mathbf{a}+\mathbf{c}$) ($P2_1/c$, 14); [3] $P12_1/c1$ ($\mathbf{b}'=3\mathbf{b}$) ($P2_1/c$, 14)

Minimal non-isomorphic supergroups

I [2] $Pnna$ (52); [2] $Pmna$ (53); [2] $Pcca$ (54); [2] $Pbam$ (55); [2] $Pccn$ (56); [2] $Pbcm$ (57); [2] $Pnnm$ (58); [2] $Pbcn$ (60); [2] $Pbca$ (61); [2] $Pnma$ (62); [2] $Cmce$ (64)

II [2] $A12/m1$ ($C2/m$, 12); [2] $C12/c1$ ($C2/c$, 15); [2] $I12/c1$ ($C2/c$, 15); [2] $P12_1/m1$ ($\mathbf{c}'=\frac{1}{2}\mathbf{c}$) ($P2_1/m$, 11); [2] $P12/c1$ ($\mathbf{b}'=\frac{1}{2}\mathbf{b}$) ($P2/c$, 13)

International Tables for Crystallography

- Positions
  - ✓ Multiplicity (rank); # equivalent points in the unit cell
  - ✓ Wyckoff letter
  - ✓ Site symmetry (point symmetry of the position)
  - ✓ Coordinates of the equivalent positions

a set of equivalent points with point symmetry (site symmetry) 1

General position

Special position

a set of equivalent points with point symmetry higher than 1

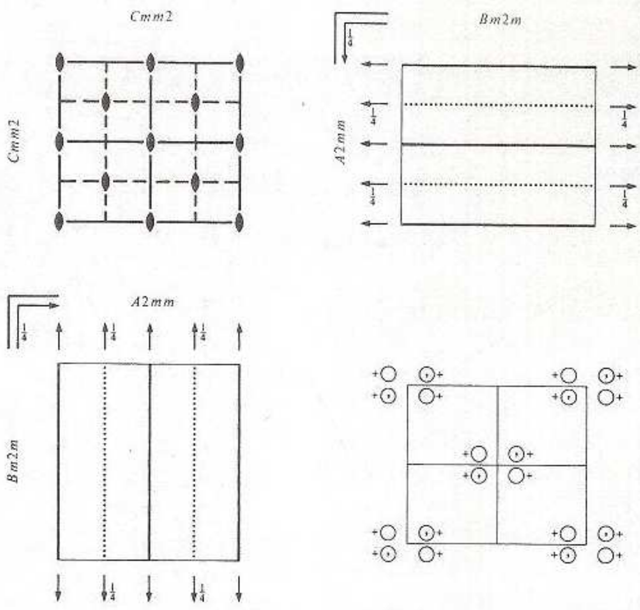
Positions

Multiplicity	Wyckoff letter	Site symmetry	Coordinates			
4	e	1	(1) x,y,z	(2) $\bar{x},y+\frac{1}{2},\bar{z}+\frac{1}{2}$	(3) $\bar{x},\bar{y},\bar{z}$	(4) $x,\bar{y}+\frac{1}{2},z+\frac{1}{2}$
2	d	$\bar{1}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$		
2	c	$\bar{1}$	$0,0,\frac{1}{2}$	$0,\frac{1}{2},0$		
2	b	$\bar{1}$	$\frac{1}{2},0,0$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
2	a	$\bar{1}$	$0,0,0$	$0,\frac{1}{2},\frac{1}{2}$		

① *Cmm2* C_{2v}^{11} *mm2* Orthorhombic

② No. 35 *Cmm2* Patterson symmetry *Cmmm*

③



④ **Origin** on *mm2*

⑤ **Asymmetric unit** $0\le x\le\frac{1}{4};\quad 0\le y\le\frac{1}{2};\quad 0\le z\le 1$

⑥ **Symmetry operations**

For (0,0,0)+ set

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

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

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

① *Headline*: Section 2.2.3.

Short Hermann–Mauguin symbol (Section 2.2.4 and Chapter 12.2)	Schoenflies symbol (Chapters 12.1 and 12.2)	Crystal class (Point group) (Section 10.1.1 and Chapter 12.1)	Crystal system (Section 2.1.2)

② Number of space group [Same as in *IT* (1952)] — Full Hermann–Mauguin symbol (Section 2.2.4 and Chapter 12.3) — Patterson symmetry (Section 2.2.5)

③ *Space-group diagrams*, consisting of one or several projections of the symmetry elements and one illustration of a set of equivalent points in general position. The numbers and types of the diagrams depend on the crystal system. The diagrams and their axes are described in Section 2.2.6; the graphical symbols of symmetry elements are listed in Chapter 1.4.

For monoclinic space groups see Section 2.2.16; for orthorhombic settings see Section 2.2.6.4.

④ *Origin* of the unit cell: Section 2.2.7. The site symmetry of the origin and its location with respect to the symmetry elements are given.

⑤ *Asymmetric unit*: Section 2.2.8. One choice of asymmetric unit is given.

⑥ *Symmetry operations*: Section 2.2.9 and Part 11. For each point $\bar{x}, \bar{y}, \bar{z}$ of the general position that symmetry operation is listed which transforms the initial point x, y, z into the point under consideration. The symbol describes the nature of the operation, its glide or screw component (given between parentheses), if present, and the location of the corresponding symmetry element.

The symmetry operations are numbered in the same way as the corresponding coordinate triplets of the general position. For centred space groups the same numbering is applied in each block, *e.g.* under 'For $(\frac{1}{2}, \frac{1}{2}, 0)+$ set'.

[*Continued on inside back cover*]

① CONTINUED No. 35 *Cmm*2

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

③ **Positions**

Multiplicity, Wyckoff letter, Site symmetry			Coordinates $(0,0,0)+$ $(\frac{1}{2},\frac{1}{2},0)+$				Reflection conditions
							General:
8	*f*	1	(1) x,y,z	(2) $\bar{x},\bar{y},z$	(3) $x,\bar{y},z$	(4) $\bar{x},y,z$	hkl : $h+k=2n$ $0kl$: $k=2n$ $h0l$: $h=2n$ $hk0$: $h+k=2n$ $h00$: $h=2n$ $0k0$: $k=2n$
							Special: as above, plus
4	*e*	*m* . .	$0,y,z$	$0,\bar{y},z$			no extra conditions
4	*d*	. *m* .	$x,0,z$	$\bar{x},0,z$			no extra conditions
4	*c*	. . 2	$\frac{1}{4},\frac{1}{4},z$	$\frac{1}{4},\frac{3}{4},z$			hkl : $h=2n$
2	*b*	*m m* 2	$0,\frac{1}{2},z$				no extra conditions
2	*a*	*m m* 2	$0,0,z$				no extra conditions

④ **Symmetry of special projections**

Along [001] *c*2*mm*
a′ = **a** **b**′ = **b**
Origin at $0,0,z$

Along [100] *p*1*m*1
a′ = $\frac{1}{2}$**b** **b**′ = **c**
Origin at $x,0,0$

Along [010] *p*11*m*
a′ = **c** **b**′ = $\frac{1}{2}$**a**
Origin at $0,y,0$

⑤ **Maximal non-isomorphic subgroups**

I [2] *C*1*m*1 (*Cm*, 8) (1; 3)+
[2] *Cm*11 (*Cm*, 8) (1; 4)+
[2] *C*112 (*P*2, 3) (1; 2)+

IIa [2] *Pba*2 (32) 1; 2; (3; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] *Pbm*2 (*Pma*2, 28) 1; 3; (2; 4) + $(\frac{1}{2},\frac{1}{2},0)$
[2] *Pma*2 (28) 1; 4; (2; 3) + $(\frac{1}{2},\frac{1}{2},0)$
[2] *Pmm*2 (25) 1; 2; 3; 4

IIb [2] *Ima*2 (**c**′ = 2**c**) (46); [2] *Ibm*2 (**c**′ = 2**c**) (*Ima*2, 46); [2] *Iba*2 (**c**′ = 2**c**) (45); [2] *Imm*2 (**c**′ = 2**c**) (44); [2] *Ccc*2 (**c**′ = 2**c**) (37); [2] $Cmc2_1$ (**c**′ = 2**c**) (36); [2] $Ccm2_1$ (**c**′ = 2**c**) ($Cmc2_1$, 36)

⑥ **Maximal isomorphic subgroups of lowest index**

IIc [2] *Cmm*2 (**c**′ = 2**c**) (35); [3] *Cmm*2 (**a**′ = 3**a** or **b**′ = 3**b**) (35)

⑦ **Minimal non-isomorphic supergroups**

I [2] *Cmmm* (65); [2] *Cmme* (67); [2] *P*4*mm* (99); [2] *P*4*bm* (100); [2] $P4_2cm$ (101); [2] $P4_2nm$ (102); [2] $P\bar{4}2m$ (111); [2] $P\bar{4}2_1m$ (113); [3] *P*6*mm* (183)

II [2] *Fmm*2 (42); [2] *Pmm*2 (**a**′ = $\frac{1}{2}$**a**, **b**′ = $\frac{1}{2}$**b**) (25)

① *Headline* in abbreviated form.

② *Generators selected*: Sections 2.2.10 and 8.3.5. A set of generators, as selected for these *Tables*, is listed in the form of translations and numbers of general-position coordinates. The generators determine the sequence of the coordinate triplets in the general position and of the corresponding symmetry operations.

③ *Positions*: Sections 2.2.11 and 8.3.2. The general Wyckoff position is given at the top, followed downwards by the various special Wyckoff positions with decreasing multiplicity and increasing site symmetry. For each general and special position its multiplicity, Wyckoff letter, oriented site-symmetry symbol, as well as the appropriate coordinate triplets and the reflection conditions, are listed. The coordinate triplets of the general position are numbered sequentially; *cf. Symmetry operations*.

Oriented site-symmetry symbol (third column): Section 2.2.12. The site symmetry at the points of a special position is given in oriented form.

Reflection conditions (right-most column): Section 2.2.13.

[*Lattice complexes* are described in Part 14; Tables 14.2.3.1 and 14.2.3.2 show the assignment of Wyckoff positions to Wyckoff sets and to lattice complexes.]

④ *Symmetry of special projections*: Section 2.2.14. For each space group, orthographic projections along three (symmetry) directions are listed. Given are the projection direction, the plane group of the projection, as well as the axes and the origin of the projected cell.

⑤ *Maximal non-isomorphic subgroups*: Sections 2.2.15 and 8.3.3.

Type **I**: *translationengleiche* or *t* subgroups;
Type **IIa**: *klassengleiche* or *k* subgroups, obtained by 'decentring' the conventional cell; applies only to space groups with centred cells;
Type **IIb**: *klassengleiche* or *k* subgroups, obtained by enlarging the conventional cell.

Given are:
For types **I** and **IIa**: Index [between brackets]; 'unconventional' Hermann–Mauguin symbol of the subgroup; 'conventional' Hermann–Mauguin symbol of the subgroup, if different (between parentheses); coordinate triplets retained in subgroup.
For type **IIb**: Index [between brackets]; 'unconventional' Hermann–Mauguin symbol of the subgroup; basis-vector relations between group and subgroup (between parentheses); 'conventional' Hermann–Mauguin symbol of the subgroup, if different (between parentheses).

⑥ *Maximal isomorphic subgroups of lowest index*: Sections 2.2.15, 8.3.3 and 13.1.2.

Type **IIc**: *klassengleiche* or *k* subgroups of lowest index which are of the same type as the group, *i.e.* have the same standard Hermann–Mauguin symbol. Data as for subgroups of type **IIb**.

⑦ *Minimal non-isomorphic supergroups*: Sections 2.2.15 and 8.3.3.
The list contains the reverse relations of the subgroup tables; only types **I** (*t* supergroups) and **II** (*k* supergroups) are distinguished. Data as for subgroups of type **IIb**.

Symmetry operations, Point groups, Space groups

- Symmetry operations – Translation, Rotation, Reflection, Inversion
- Shape of the unit cell, symmetry within the unit cell, translation of the unit cell → define a repeating pattern.
- Point groups (32) – set of symmetry operations about a point in space (except for translation)
- Space groups (230) ← (32 point groups + 7 crystal systems)
- Space (plane) lattice; 3 (2)-dimensional arrays of points in space that have a basic repeating pattern, a unit cell, that can be translated to fill all space

- 3-D, 14 possible lattices, 7 different axis systems
- The application and permutation of all symmetry elements to patterns in space give rise to **230 space groups** (instead of 17 plane groups) distributed among **14 space lattices** (instead of 5 plane lattices) and **32 point group symmetries** (instead of 10 plane point group symmetries).
- Point group symmetry & space group symmetry has to be distinguished.
- Space group symmetry – the way things are packed together and fill space
- Space group – translational component = point group

Point group vs. Space group

Point groups: A group of point symmetry operations, whose operation leaves at least one point unaltered. Any operation involving lattice translations is thus excluded	Space groups: A group of symmetry operations which include lattice translations
1 $\bar{1}$ 2 m 3 $\bar{3}$ 4 $\bar{4}$ 6 $\bar{6}$	1 $\bar{1}$ 2 m 2_1; a, b, c, n, e, d 3 $\bar{3}$ $3_1, 3_2$ 4 $\bar{4}$ $4_1, 4_2, 4_3$ 6 $\bar{6}$ $6_1, 6_2, 6_3, 6_4, 6_5$ lattice translations
a, b, c α, β, γ	a_0, b_0, c_0 α, β, γ
Order of the symmetry operations e.g. 4/m 2/m 2/m c < a > < 110 >	Order of the symmetry operations e.g. $P4_2/m$ 2/m 2/m c < a > < 110 >
General form: Set of equivalent faces each with face symmetry 1	General position: Set of equivalent points each with site symmetry 1
$f_{\text{asymmetric face unit}} = \dfrac{f_{\text{sphere}}}{\text{multiplicity of general form}}$	$V_{\text{asymmetric unit}} = \dfrac{V_{\text{unit cell}}}{\text{multiplicity of general point}}$
Multiplicity of general form of the point group	Multiplicity of the general position in all space groups with a P-lattice that are isomorphous with that point group
Special form: Set of equivalent faces each with face symmetry >1	Special position: Set of equivalent points each with site symmetry >1

Ott Chap 10

Laue class, Laue group; 11 point groups with center of symmetry

Table 2.9 The 11 Laue classes and six "powder" Laue classes.

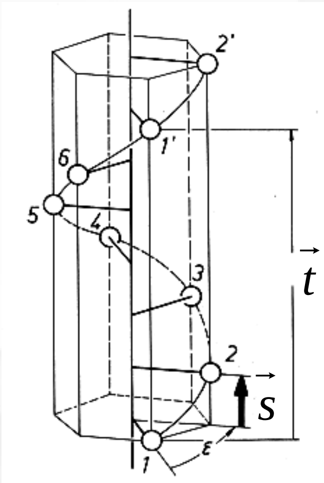
Crystal system	Laue class	"Powder" Laue class	Point groups
Triclinic	$\bar{1}$	$\bar{1}$	1, $\bar{1}$
Monoclinic	2/m	2/m	2, m, 2/m
Orthorhombic	mmm	mmm	222, mm2, mmm
Tetragonal	4/m	4/mmm	4, $\bar{4}$, 4/m
	4/mmm	4/mmm	422, 4mm, $\bar{4}$m2, 4/mmm
Trigonal	$\bar{3}$	6/mmm	3, $\bar{3}$
	$\bar{3}$m	6/mmm	32, 3m, $\bar{3}$m
Hexagonal	6/m	6/mmm	6, $\bar{6}$, 6/m
	6/mmm	6/mmm	622, 6mm, $\bar{6}$m2, 6/mmm
Cubic	m$\bar{3}$	m$\bar{3}$m	23, m$\bar{3}$
	m$\bar{3}$m	m$\bar{3}$m	432, $\bar{4}$3m, m$\bar{3}$m

- Laue class → Pecharsky page 40
- Laue index → Hammond page 138

Pecharsky Chap 2

Glide planes & Screw Axis

Screw axes
(rotation + translation)



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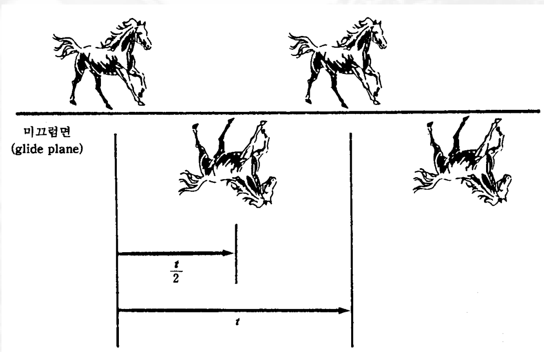
Glide planes
(reflection + translation)



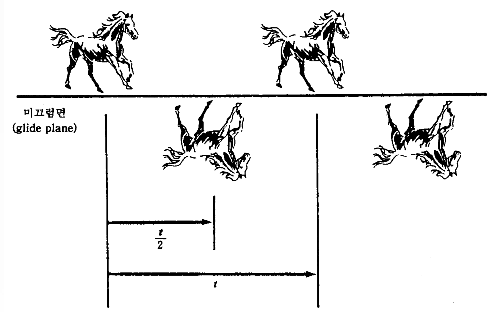
i) reflection

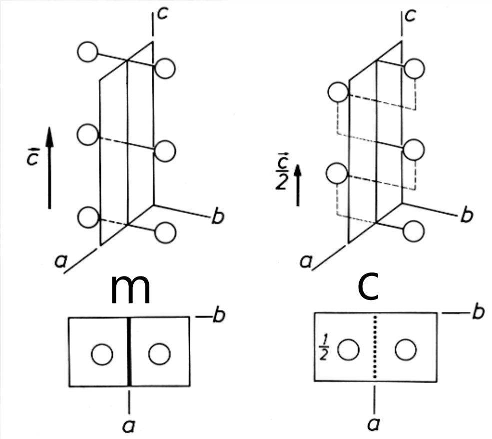
ii) translation by the vector $\vec{g}$ parallel to the plane of reflection

where $|\vec{g}|$ is called glide component

$\vec{g}$ Is one half of a lattice translation parallel to the glide plane.

$$|\vec{g}| = \frac{1}{2}|\vec{t}|$$





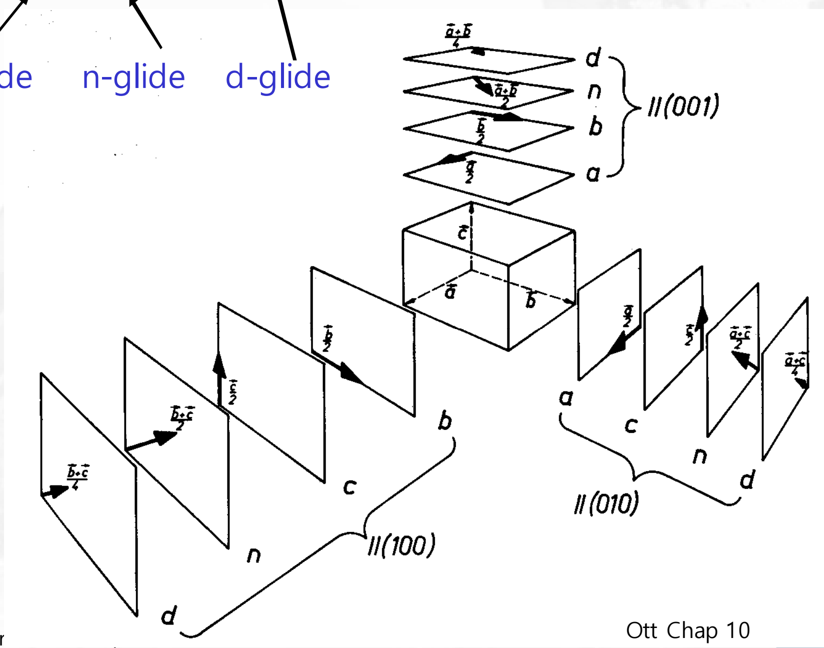
- Glide plane can <u>only</u> occur in an orientation that is possible for a mirror plane.

Orthorhombic **P2/m2/m2/m**

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

Glide plane // (100) → $\frac{1}{2}|\vec{b}|$, $\frac{1}{2}|\vec{c}|$, $\frac{1}{2}|\vec{b}+\vec{c}|$, $\frac{1}{4}|\vec{b}\pm\vec{c}|$

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



Glide Plane

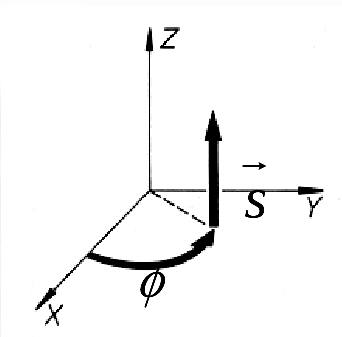
Reflection plus ½ cell translation

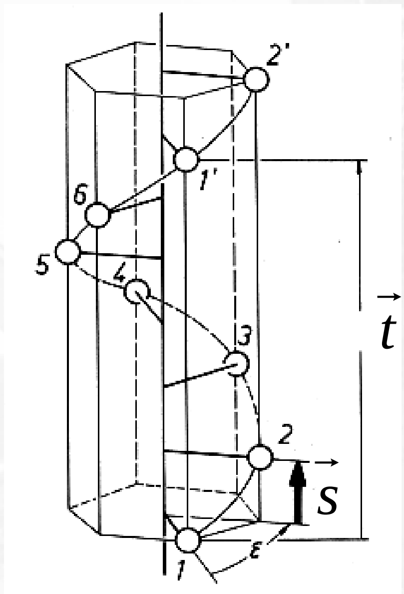
- *a* - glide: *a*/2 translation
- *b* - glide: *b*/2 translation
- *c* - glide: *c*/2 translation
- *n* – glide (normal to *a*): *b*/2+*c*/2 translation
- *n* – glide (normal to *b*): *a*/2+*c*/2 translation
- *n* – glide (normal to *c*): *a*/2+*b*/2 translation
- *d* - glide : (*a* + *b*)/4, (*b* + *c*)/4, (*c* + *a*)/4
- *g* - glide line (two dimensions)

Screw Axis

i) rotation $\phi = \frac{2\pi}{X}$ $(X = 1,2,3,4,6)$

ii) translation by a vector $\vec{s}$ parallel to the axis where $|\vec{s}|$ is called the screw component





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

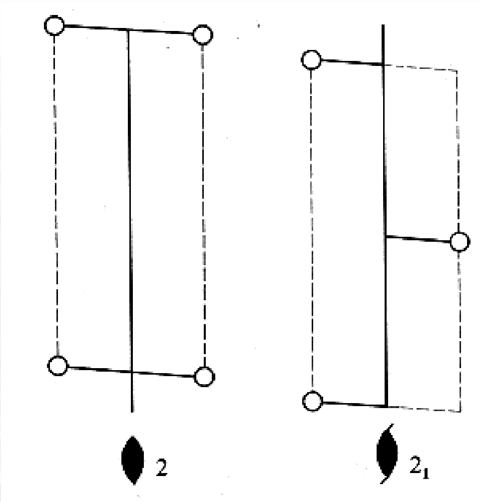
$$X_p = X_0, X_1, \ldots X_{X-1}$$

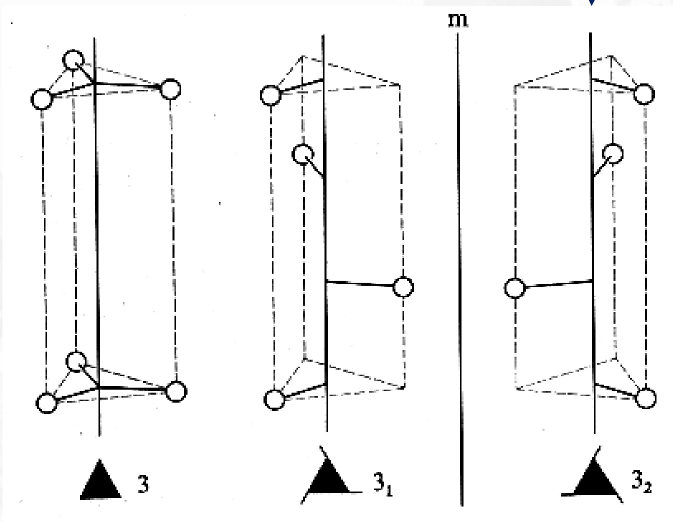
Ott Chap 10

Screw Axis

2_1 is a 180° rotation plus ½ cell translation

3_2 is a 120° rotation plus (2/3) cell translation





3_1 is a 120° rotation plus (1/3) cell translation

Ott Chap 10

Screw tetrads

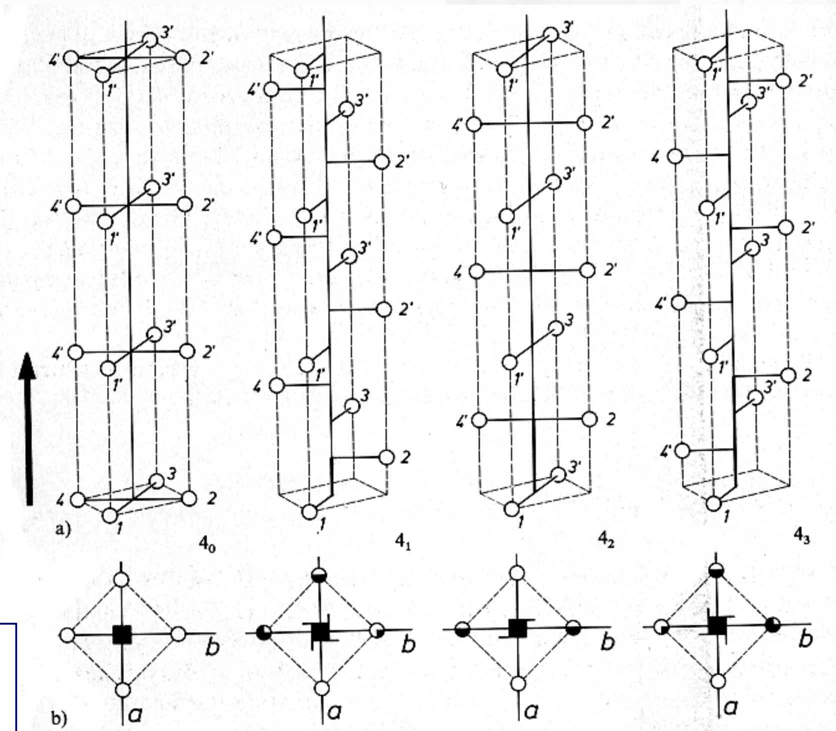
4_0 is 4-fold rotation axis.

4_1 is a 90° rotation plus ¼ cell translation (right-handed).

4_2 is a 90° rotation plus ½ cell translation (no handedness).

4_3 is a 90° rotation plus ¾ cell translation (right-handed) = a 90° rotation plus ¼ cell translation (left-handed).

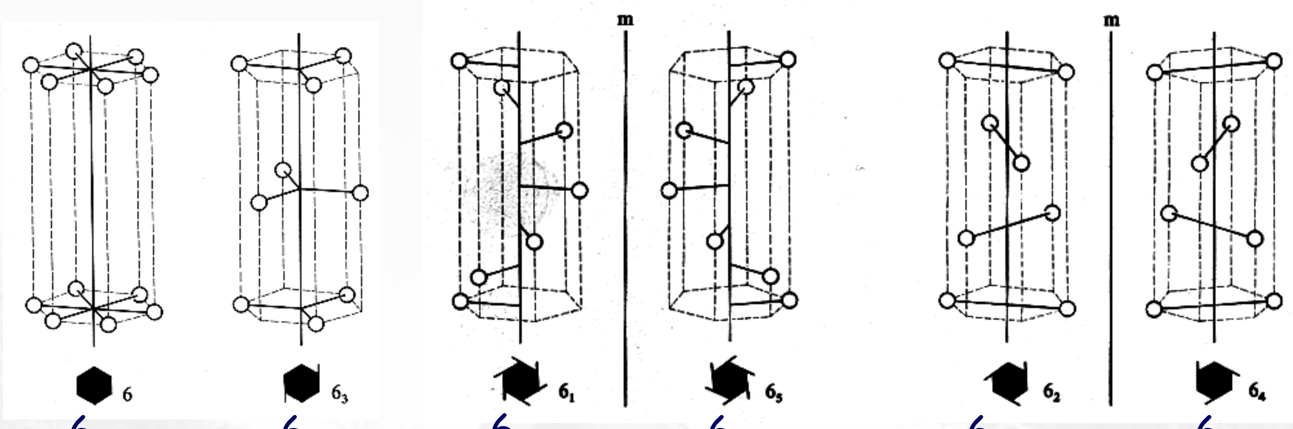
Sets of points generated by 4_1 and 4_3 are a pair of enantiomorphs (mirror images of one another).



4_0 4_1 4_2 4_3

Ott Chap 10

Screw hexads



- **6_1** 60º rotation + 1/6 cell translation (right-handed)
- **6_2** 60º rotation + 1/3 cell translation (right-handed)
- **6_3** 60º rotation + ½ cell translation (no handedness)
- **6_4** 60º rotation + 2/3 cell translation (right-handed) = (1/3 left-handed)
- **6_5** 60º rotation + 5/6 cell translation (right-handed) = (1/6 left-handed)

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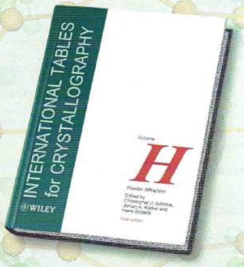

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