Symmetry

CHAN PARK

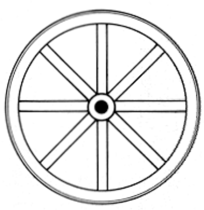
for animated images of point groups,

http://neon.mems.cmu.edu/degraef/pg/pg.html#AGM

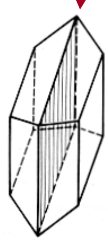
Symmetry

- 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

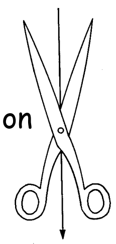


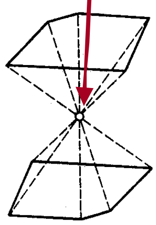
rotation



reflection

rotation





inversion

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Symmetry operation

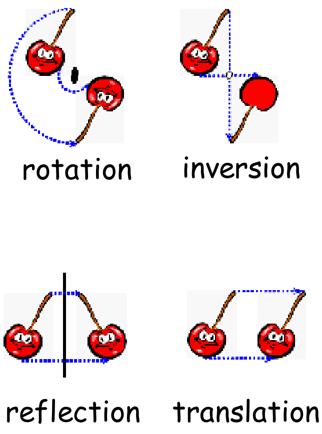
(1) Rotation; **1 2 3 4 6** (2) Reflection; **m** (= $\bar{2}$)

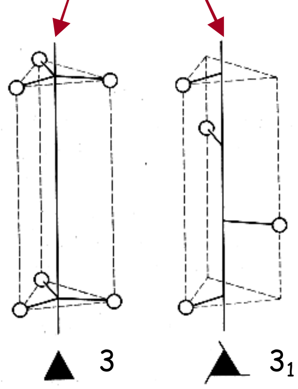
(3) Inversion (center of symmetry) (= $\bar{1}$)

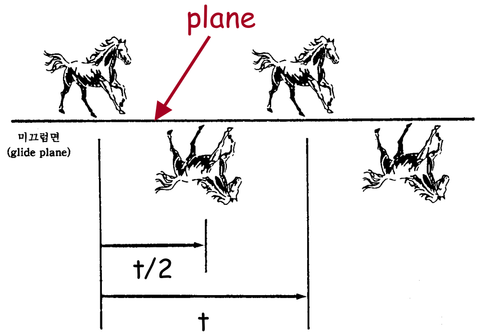
(4) Rotation-inversion; $\bar{1}$ (=center of symmetry), $\bar{2}$ (= mirror), $\bar{3}$, $\bar{4}$, $\bar{6}$

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

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







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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>

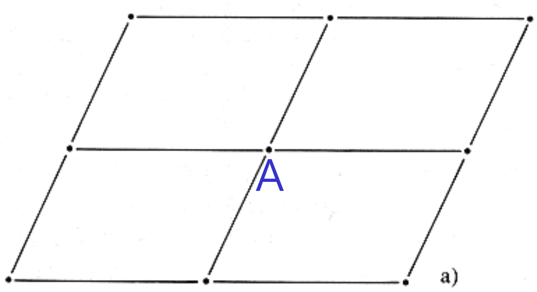
Fd3m
Face centered lattice
d ⊥ to a axis
3 fold axis along the <111>
m ⊥ to c axis

Rotation Axis

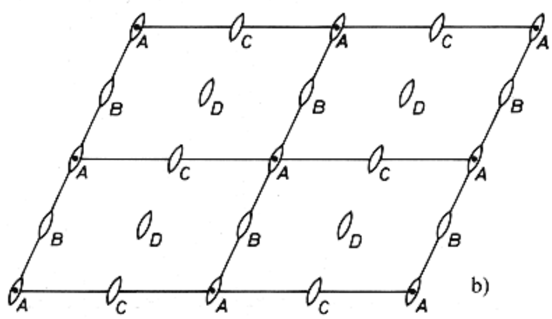
- general plane lattice
- 180° rotation about the central lattice point A → coincidence

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

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



a)



b)

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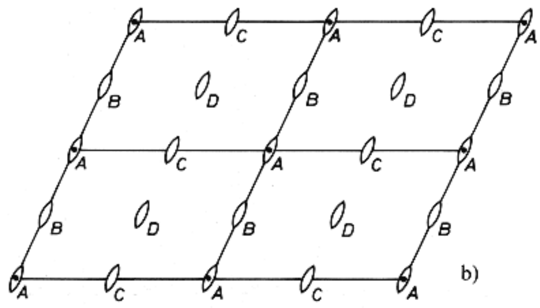
- Two objects are EQUIVALENT
  - ✓ When they can be brought into coincidence by application of a symmetry operation
- Two objects are IDENTICAL
  - ✓ When no symmetry operation except lattice translation is involved
  - ✓ equivalent by translation

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



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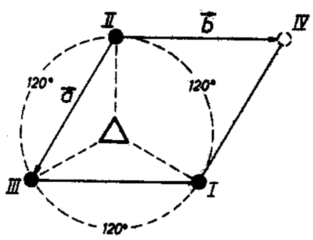
Rotation Axis

- 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 two other points lying in a plane $\perp$ to it
  - ✓ 3 non-colinear points define a plane → must be a lattice plane (translational periodicity)

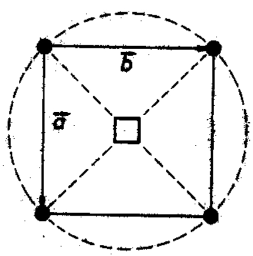
3-fold axis ▲

ϕ = 120°, n = 3



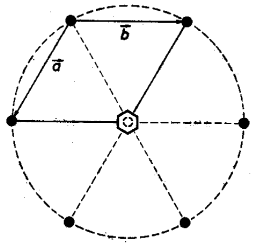
4-fold axis ■

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.

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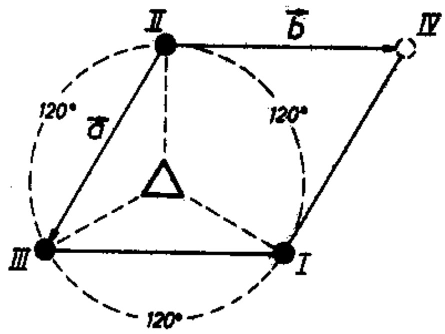
To be a lattice plane

- The points generated by rotation axis must fulfil the conditions for being a lattice plane --- parallel lattice lines should have the same translation period

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

→ 3 fold axes are compatible with space lattice



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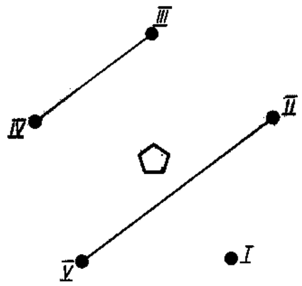
5-fold Rotation Axis



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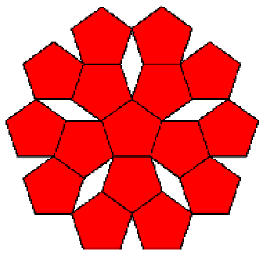

ϕ= 72°, n=5

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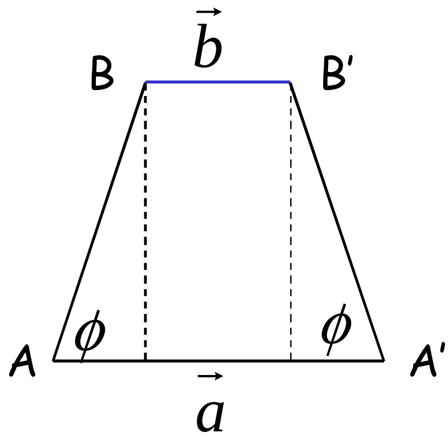
- II-V and III-IV parallel but not equal or integral ratio → no 5-fold axes in space lattice
- This structure does not have translational symmetry in 3-dimensions → do not have finite unit cell → called quasicrystal
  - ✓ Quasi – because there is no translational symmetry
  - ✓ Crystal – because they 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



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

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

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

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

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

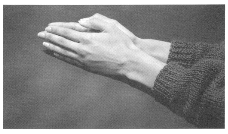
symmetry operation vs symmetry element, proper vs improper

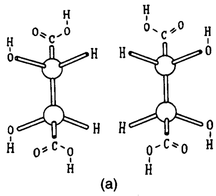
- Rotation by 60° around an axis → <u>symmetry operation</u>
- 6-fold rotation axis is a <u>symmetry element</u> which contains six rotational <u>symmetry operations</u>

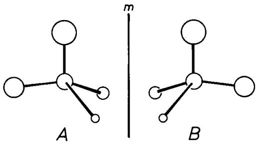
- <u>Proper</u> symmetry elements
  - ✓Rotation axes, screw axes, translation vectors
- <u>Improper</u> symmetry elements
  - ✓Inverts an object in a way that may be imaged by comparing <u>right & left hands</u>
  - ✓Inverted object is called an **<u>enantiomorph</u>** of the direct object (right vs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

Reflection

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







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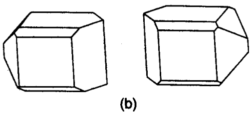
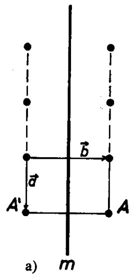
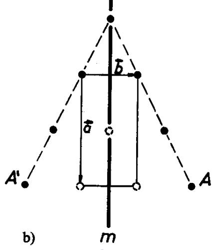


Lattice line // m

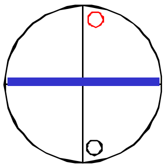


rectangular

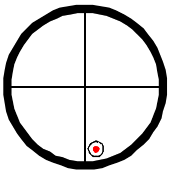
Lattice line tilted w.r.t. m



centered rectangular



m_{yz} (m_x)



m_{xy} (m_z)

■ down

○ up

Black & Red; enantiomorphs

■ down, left

○ up, right

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Inversion

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

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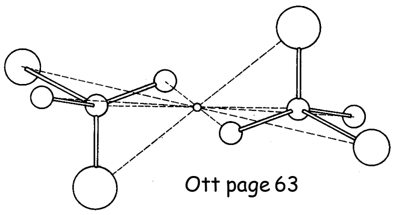

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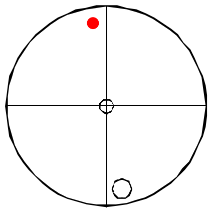

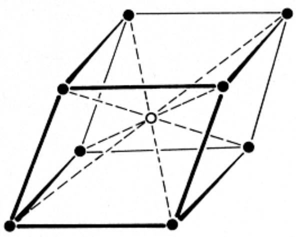

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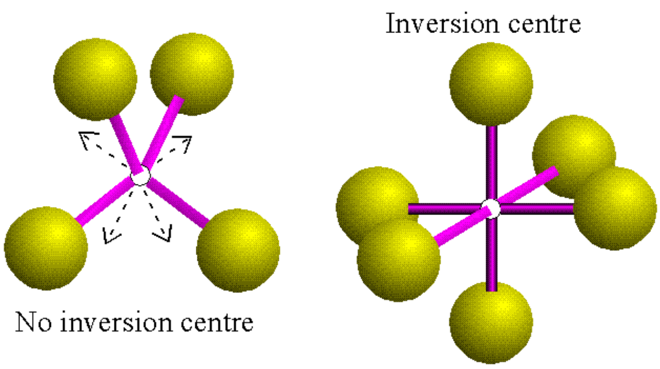
All lattices are centrosymmetric.



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

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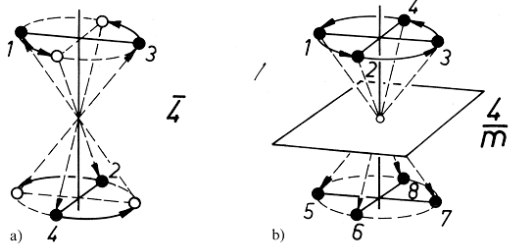
Hammond Chap 4

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 $\boxed{4 + 1bar}$ 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)	×

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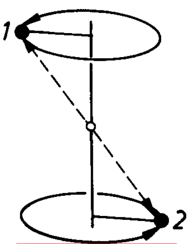
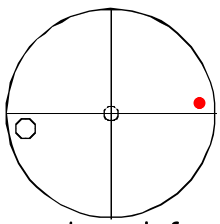
Rotoinversion

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

$\boxed{\bar{1}}$



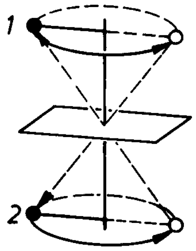
$\bar{1} \equiv$ inversion centre



● down, left

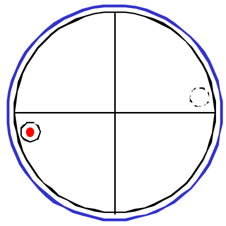
○ up, right

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



$\bar{2} \equiv m$

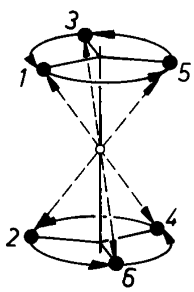
1
2



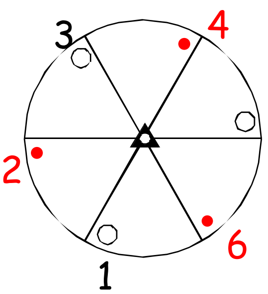
m_{xy} (m_z)

$\boxed{\bar{3} \equiv 3 + \bar{1}}$ ▲

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



▲ $\bar{3} \equiv 3 + \bar{1}$



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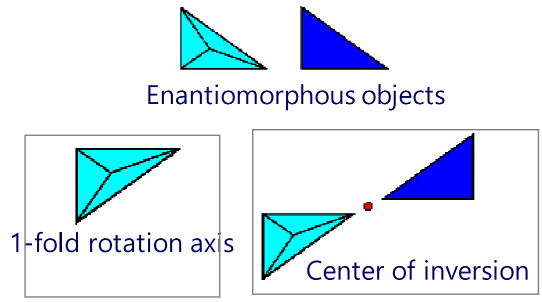
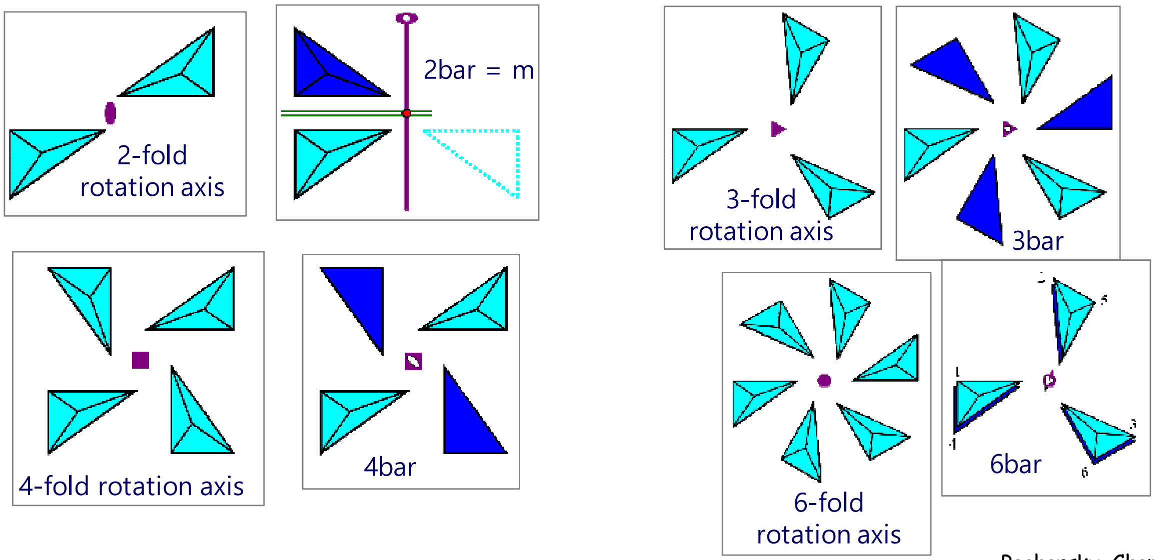
Symmetry elements

- 1, 2, 3, 4, 6 (proper rotation axes)
- $\bar{1}$ = inversion center, $\bar{2}$ = m, $\bar{3}$, $\bar{4}$, $\bar{6}$ (improper axes; right & left hands → enantiomorph)
- Screw axes (rotation + translation)
- Glide planes (reflection + translation)





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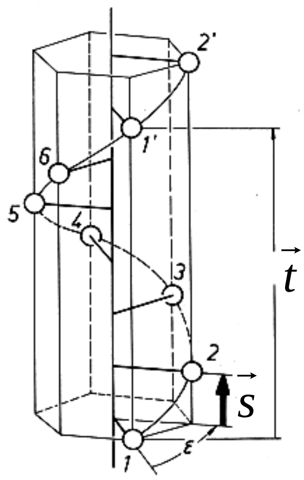
Screw axes
(rotation + translation)



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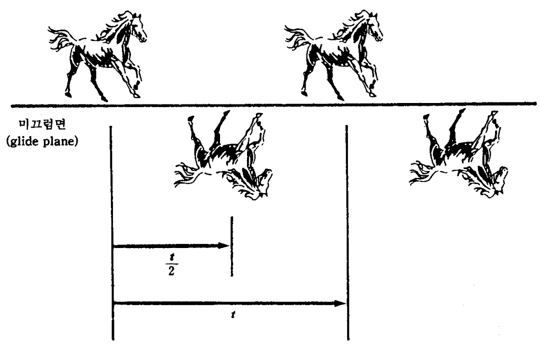
Glide planes
(reflection + translation)



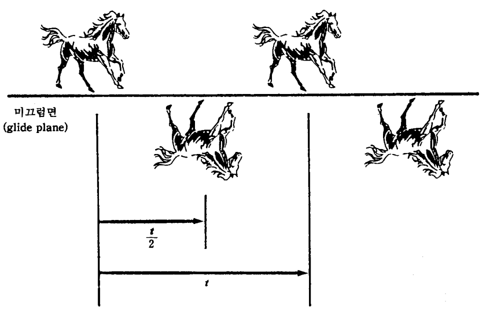
Glide Plane

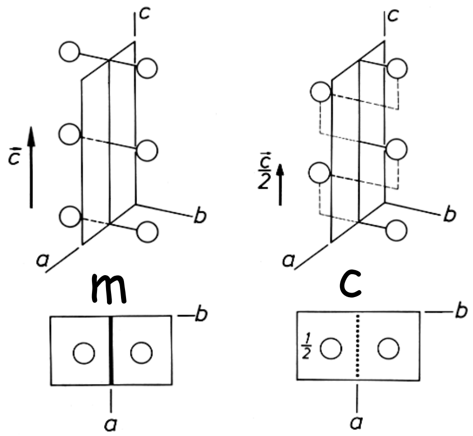
i) reflection

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 only occur in an orientation that is possible for a mirror plane

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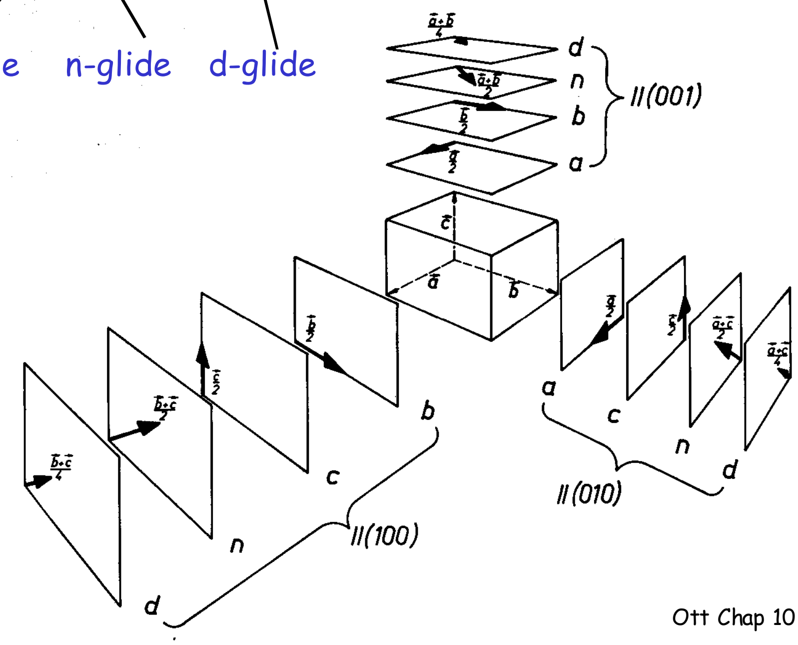
Glide Plane

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



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Glide Plane

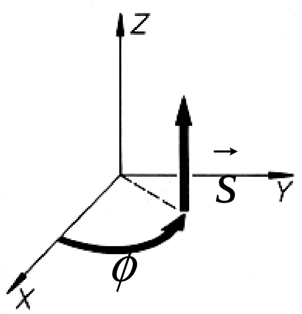
Reflection plus ½ cell translation

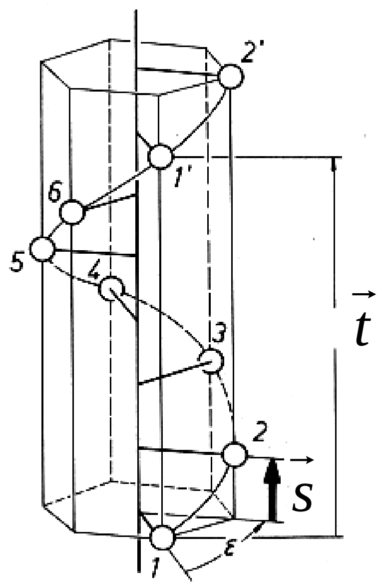
- *a* - glide: *a*/2 translation
- *b* - glide: *b*/2 translation
- *c* - glide: *c*/2 translation
- *n* – glide (normal to *a*): *b*/2+*c*/2 translation
- *n* – glide (normal to *b*): *a*/2+*c*/2 translation
- *n* – glide (normal to *c*): *a*/2+*b*/2 translation
- *d* - glide : (*a* + *b*)/4, (*b* +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

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





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

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

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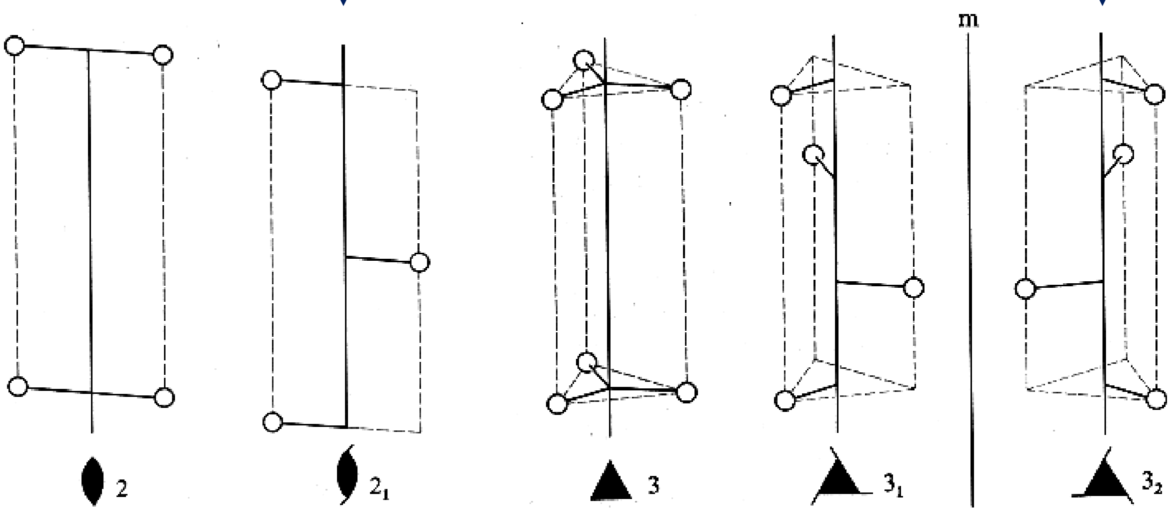
Screw Axis

2_1 is a 180° rotation plus $\frac{1}{2}$ cell translation

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



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

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Screw tetrads

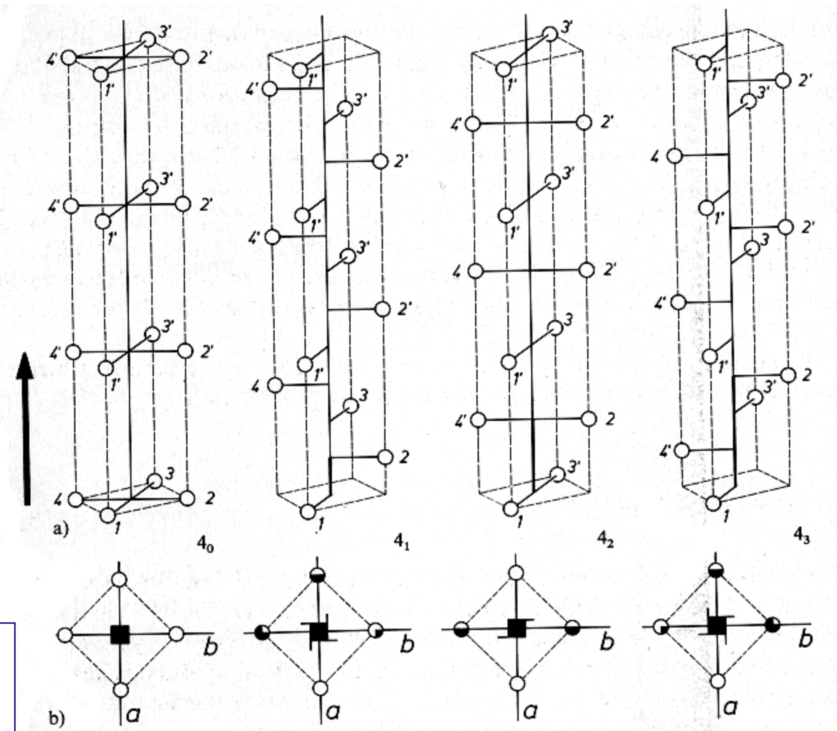
4_0 is 4-fold rotation axis

4_1 is a 90° rotation plus $\frac{1}{4}$ cell translation (right-handed)

4_2 is a 90° rotation plus $\frac{1}{2}$ cell translation (no handedness)

4_3 is a 90° rotation plus $\frac{3}{4}$ cell translation (right-handed) = a 90° rotation plus $\frac{1}{4}$ cell translation (left-handed)

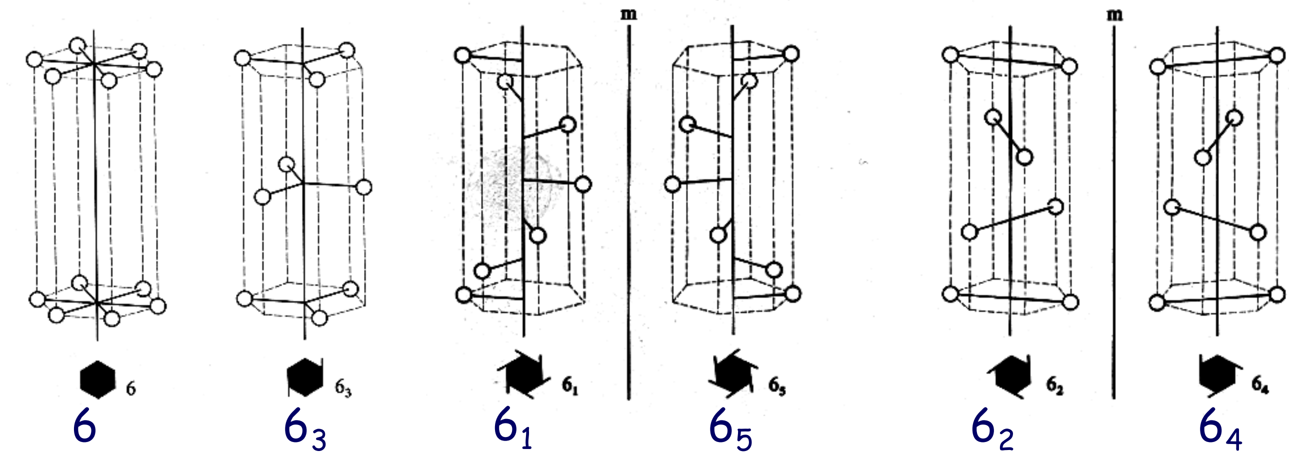
Sets of points generated by 4_1 and 4_3 are a pair of enantiomorphs (mirror images of one another)



4_0 4_1 4_2 4_3

Ott Chap 10

Screw hexads



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

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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	slide in plane of paper	arrow shows glide direction
		slide 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	$\bar{3}$		
	$\bar{4}$		
	$\bar{6}$		

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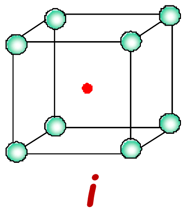
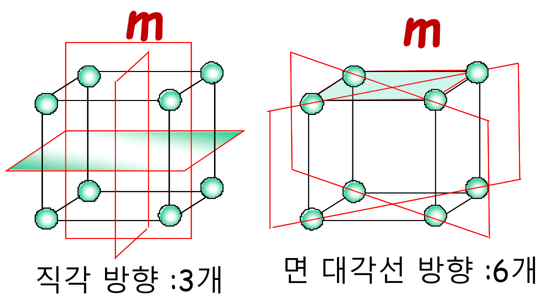
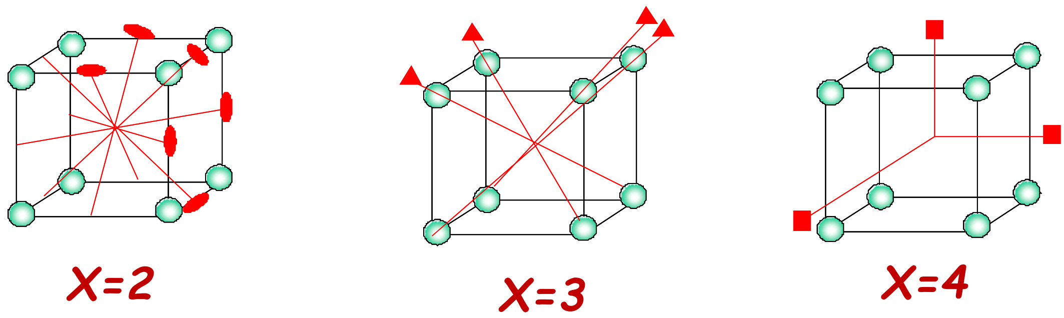
Cube(정육면체)의 대칭요소

- ➢ 대칭심(center of symmetry)
- ➢ 9개의 거울면(mirror plane)
- ➢ 6개의 2회전축(diad axis)
- ➢ 4개의 3회전축(triad axis)
- ➢ 3개의 4회전축 (tetrad axis)

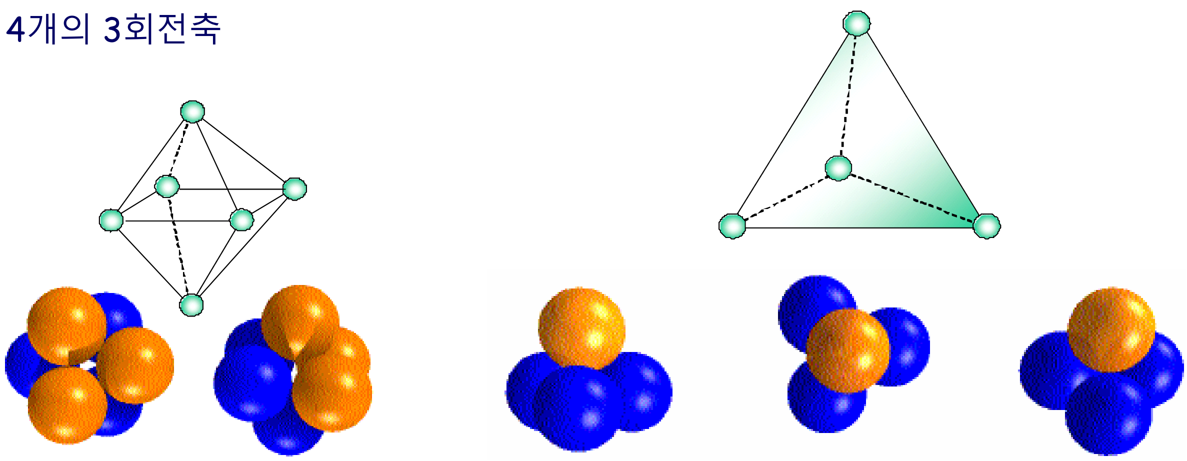






Tetrahedron과 Octahedron의 대칭

- ➢ 정8면체(octahedron)의 대칭요소 ≡ 정6면체의 대칭요소
- ➢ 정4면체(tetahedron)의 대칭요소
  - ✓ 6개의 거울면
  - ✓ 3개의 4회반축(inverse tetrad axis)
  - ✓ 4개의 3회전축



Point groups

- Lattice – an array of points in space in which the environment of each point is identical
- Basis (motif) – repeating unit of pattern
- Lattice + basis → crystal structure

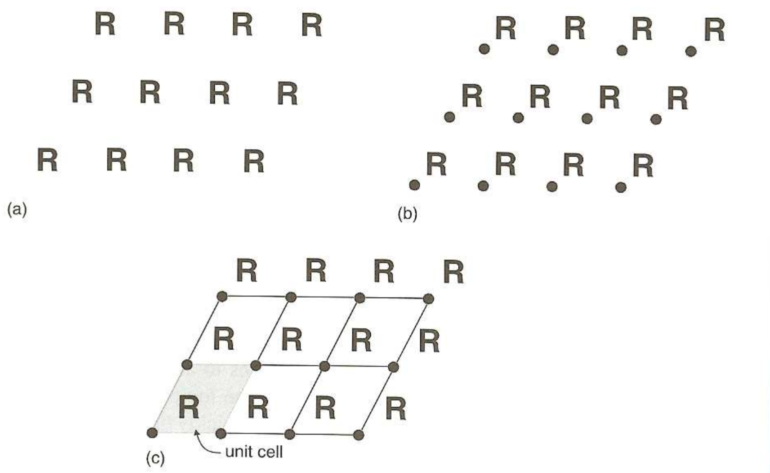


Fig. 2.1. (a) A pattern with the motif **R**, (b) with the lattice points indicated and (c) the lattice and a unit cell outlined (Drawn by K. M. Crennell).

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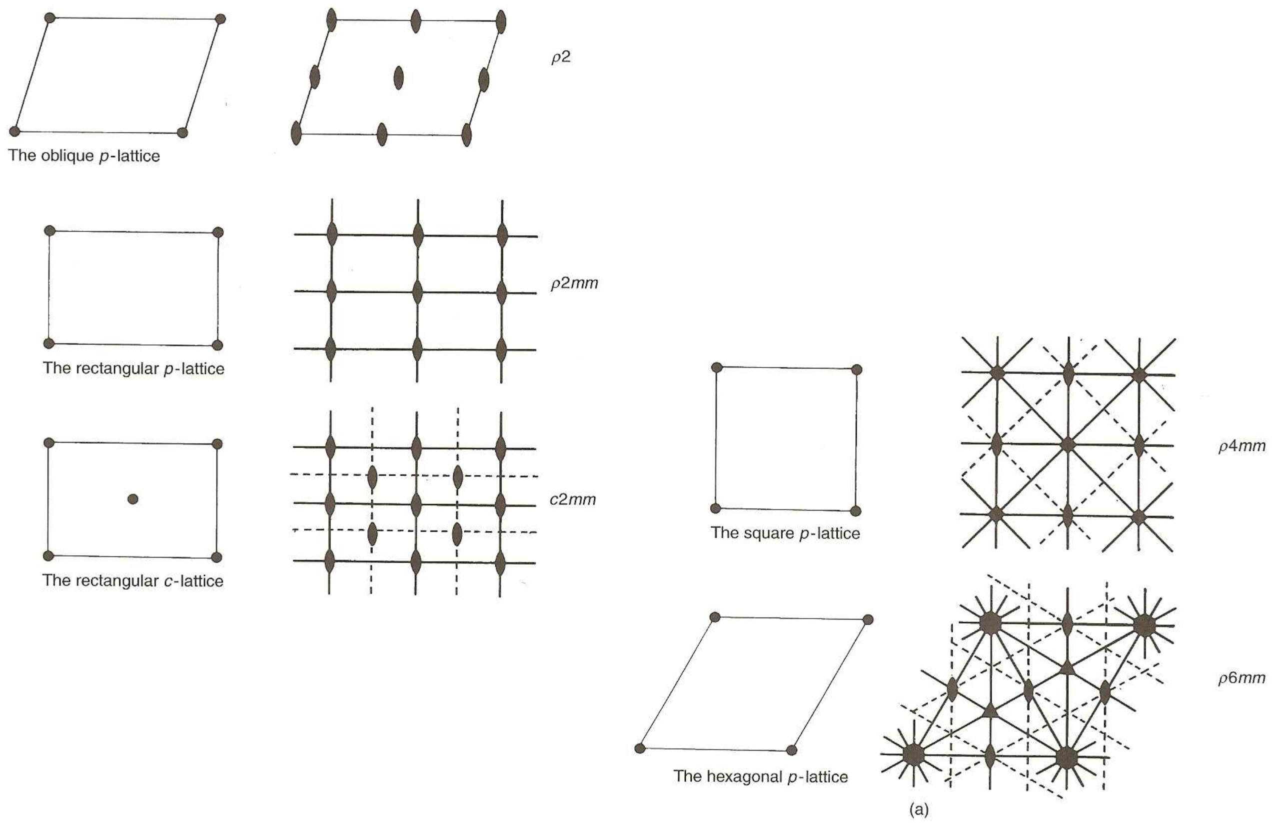
- Ten 2-D point groups (plane point groups)
  - 1, 2, 3, 4, 6, m, 2mm, 3m, 4mm, 6mm
  - Only these combinations of axes & mirror lines can occur in regular repeating patterns in two dimensions
- 5 lattices in 2-D (5 plane lattices)
- A basis can possess one of ten point group symmetries in two dimension
- There are only ten different types of two-dimensional patterns, distributed among the five plane lattices (10 plane point groups)
- 17 plane groups
  - p1, p2, p3, p4, p6, pm, pg, cm, p2mm, p2mg, c2mm, p2gg, p4mm, p4gm, p31m, p3m1, p6mm

- 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)

- Space group symmetry – the way things are packed together and fill space
- Space group – translational component = point group

5 plane lattices



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17 plane groups

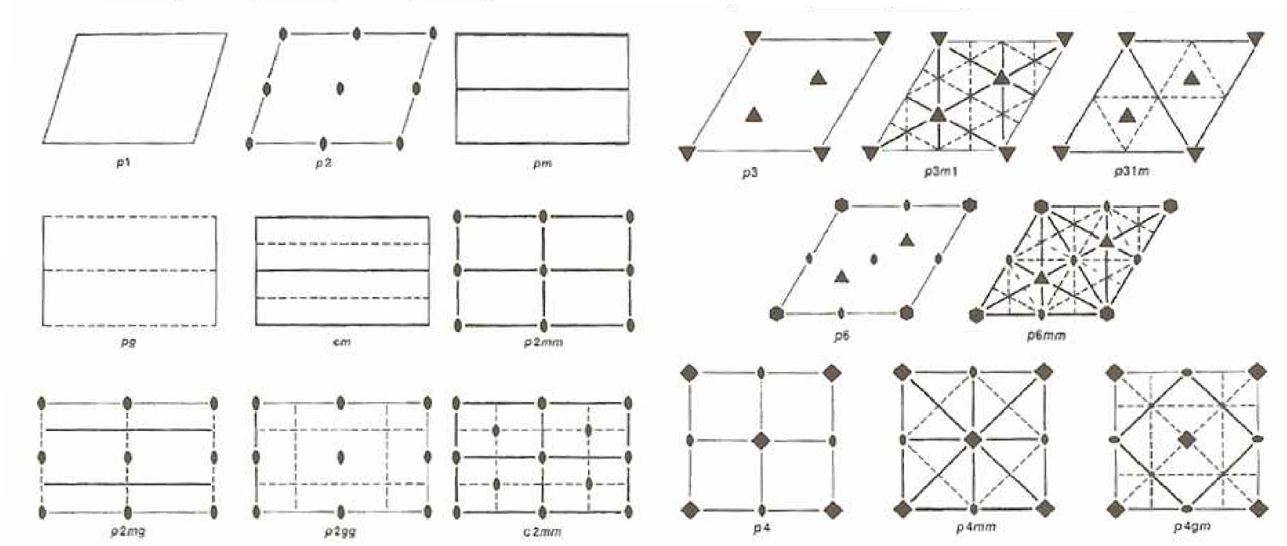

Fig. 2.6. (a) The seventeen plane groups (from *Point and Plane Groups* by K. M. Crennell). The numbering 1–17 is that which is arbitrarily assigned in the International Tables. Note that the 'shorthand' symbols do not necessarily indicate all the symmetry elements which are present in the patterns. (b) The symmetry elements outlined within (conventional) unit cells of the seventeen plane groups, heavy solid lines and dashed lines represent mirror and glide lines respectively (from *Manual of Mineralogy* 21st edn, by C. Klein and C. S. Hurlbut, Jr., John Wiley, 1999).

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plane groups vs. space groups

Rotation
Reflection
Inversion

Translation

10 plane point groups | 5 plane lattices

32 point groups | 14 space lattices

Glide (translation + reflection)

Screw (translation + rotation)
Glide

17 plane space groups

230 space 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)

- 32 unique combination of symmetry operations about a point in space → **32 point groups** (32 three-dimensional point groups; ten two-dimensional point groups)

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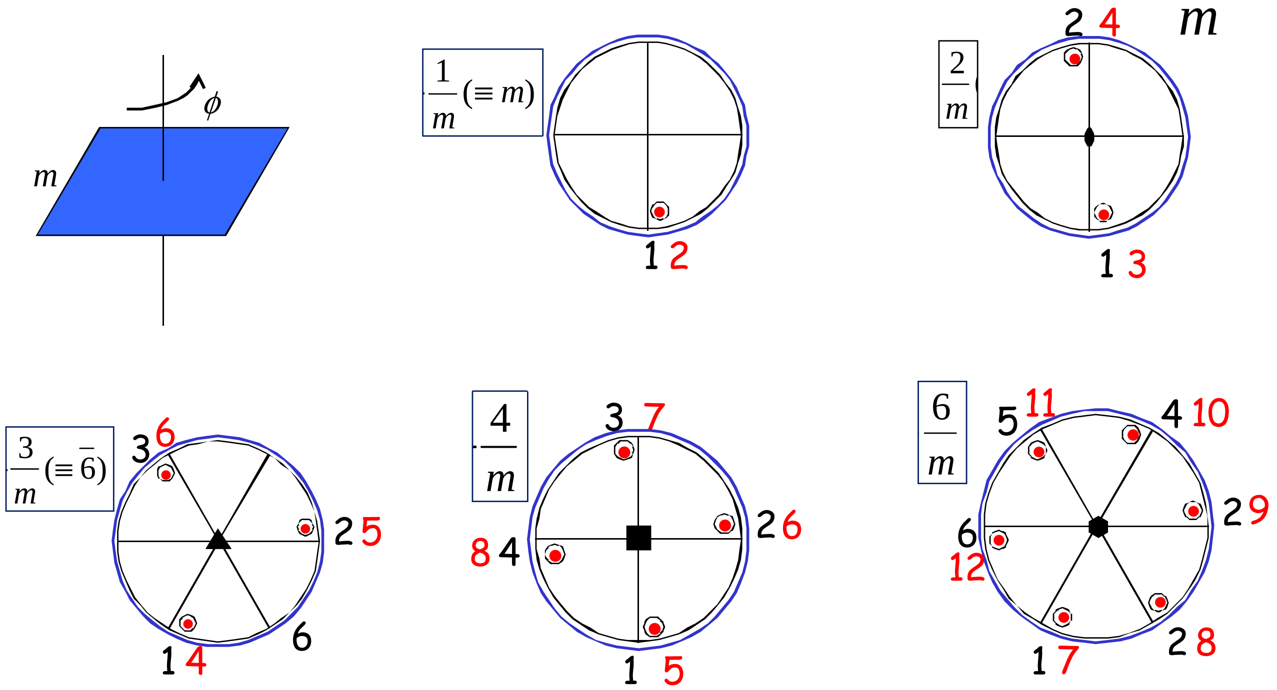
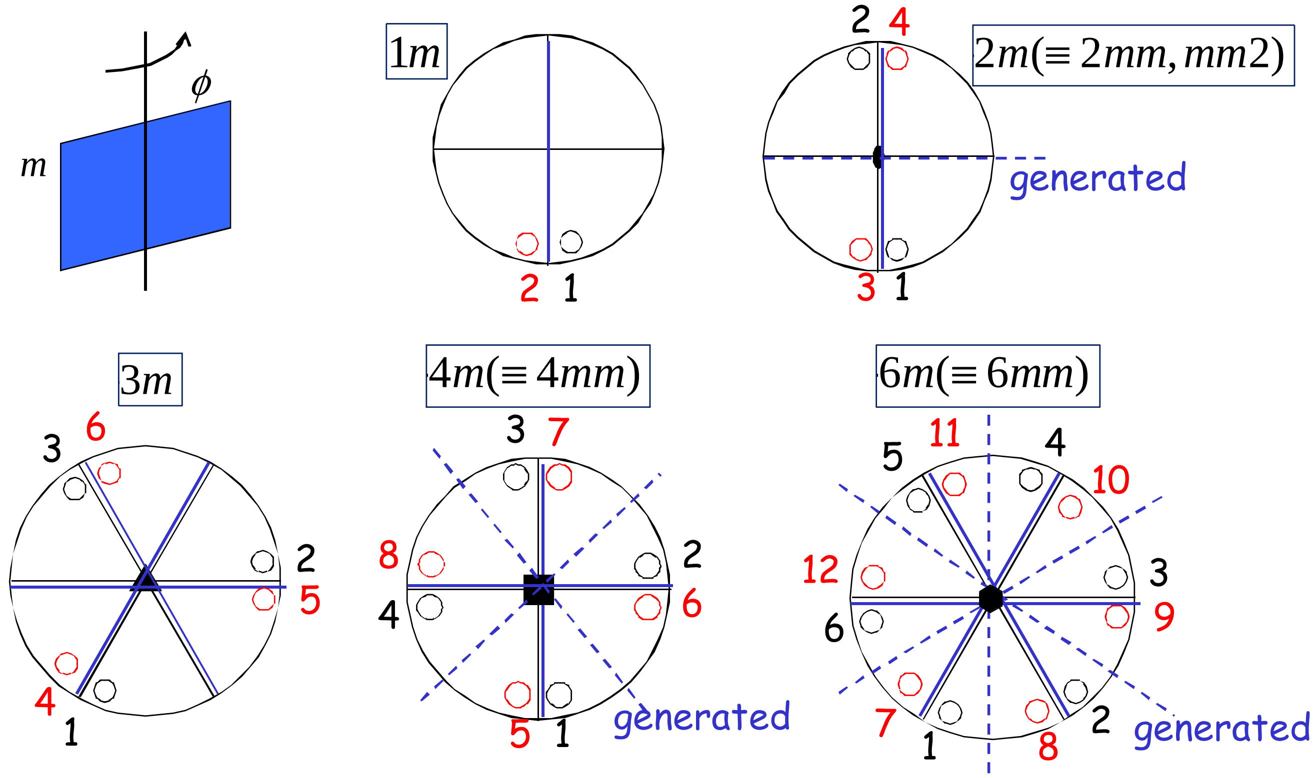
Combination > X/m

- a mirror plane is added normal to the rotation axis, $\frac{X}{m}$



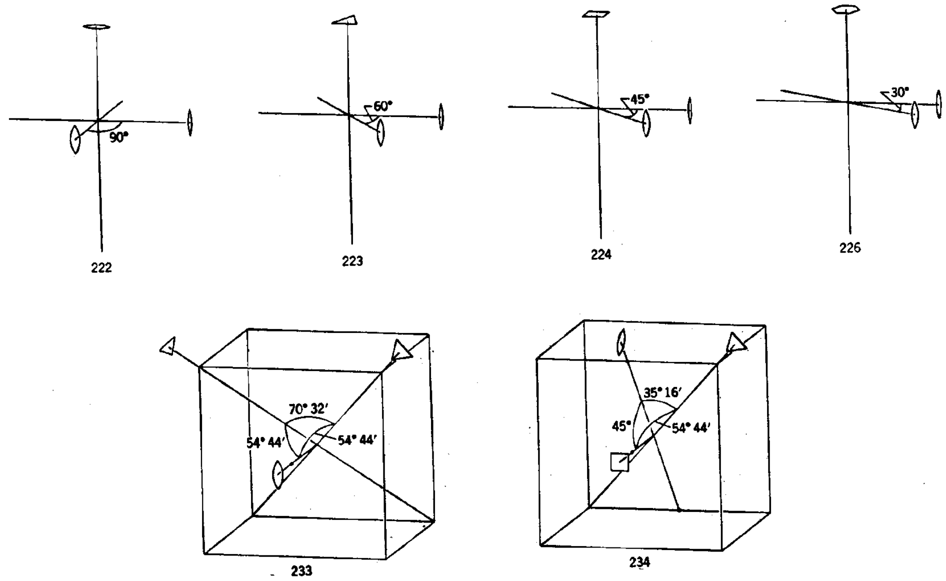
Combination > Xm

- a mirror plane is added parallel to the rotation axis, Xm



Combination of rotation axes – should be mutually consistent

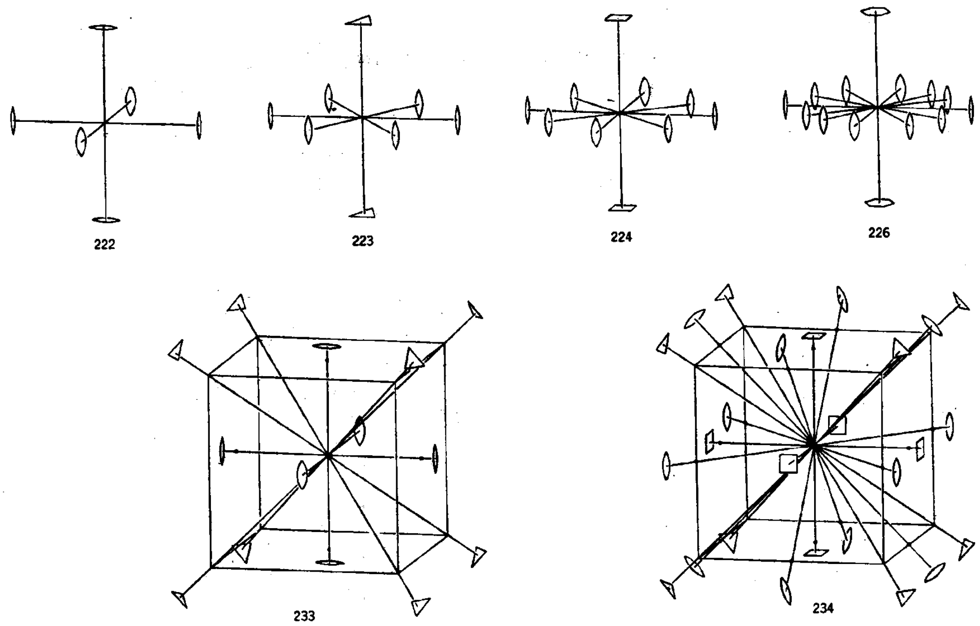
Allowed sets of simultaneous rotational symmetries passing thru a point



Spatial arrangements for the six permissible combinations of 3 rotational symmetry axes passing through a point in crystals

Page 149, Allen & Thomas, The Structure of Materials (MIT Series in Materials Science and Engineering) (1999)
Page 43, Buerger, Elementary Crystallography: An introduction to the fundamental geometric features of crystals (1978)

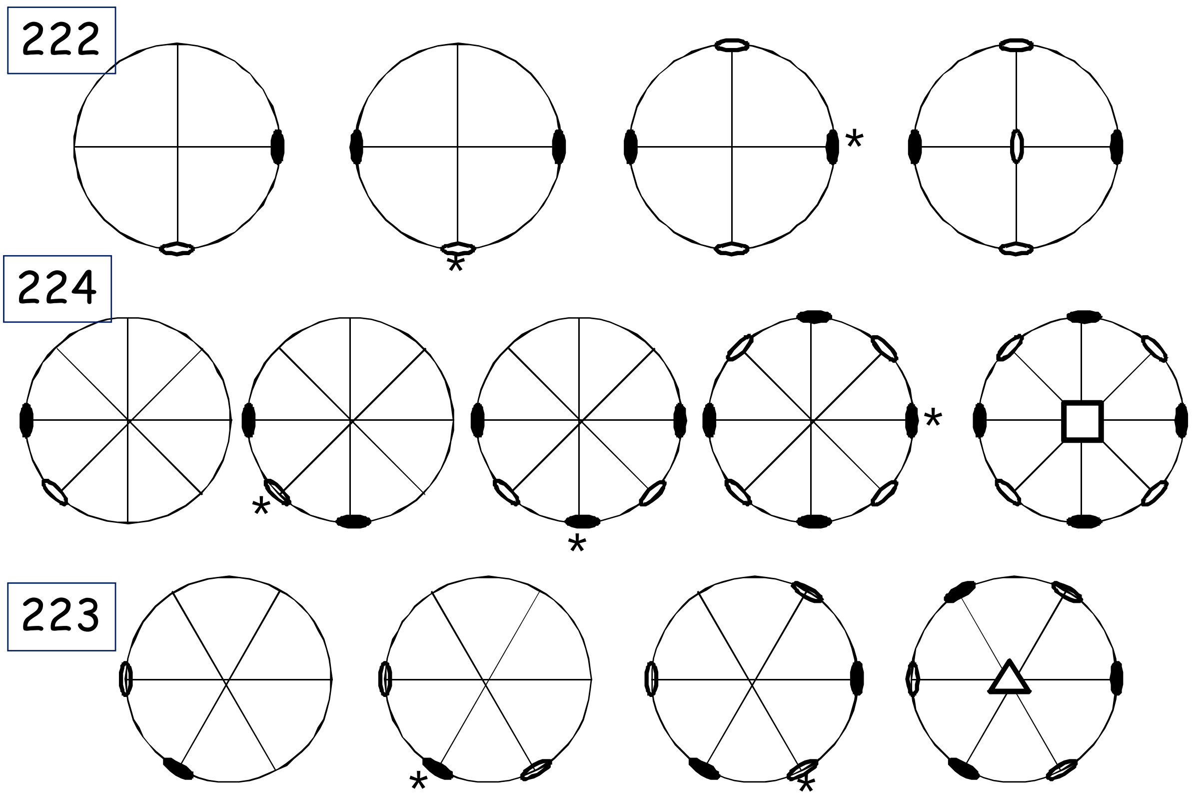
Combination of rotation axes



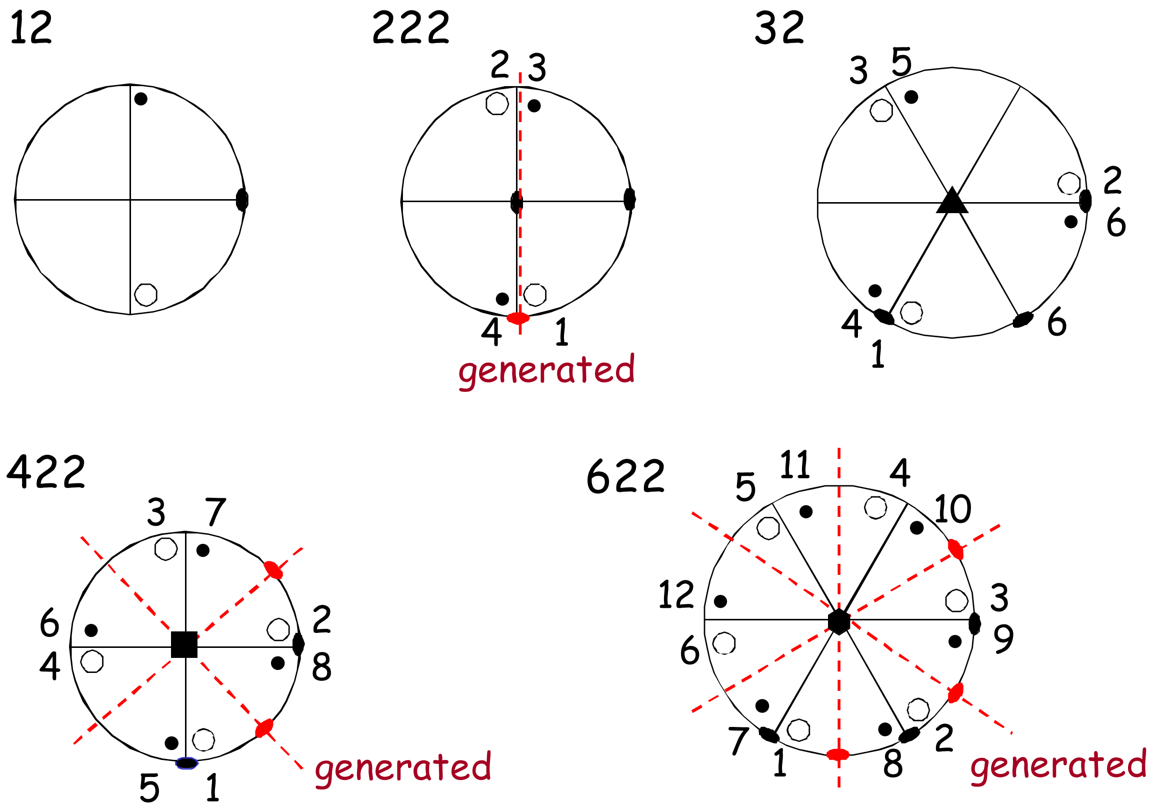
Spatial arrangements for the 6 permissible combinations of rotational symmetry axes passing through a point in crystals after allowing all rotational repetitions

Page 150, Allen & Thomas, The Structure of Materials (MIT Series in Materials Science and Engineering) (1999)
Page 44, Buerger, Elementary Crystallography: An introduction to the fundamental geometric features of crystals (1978)

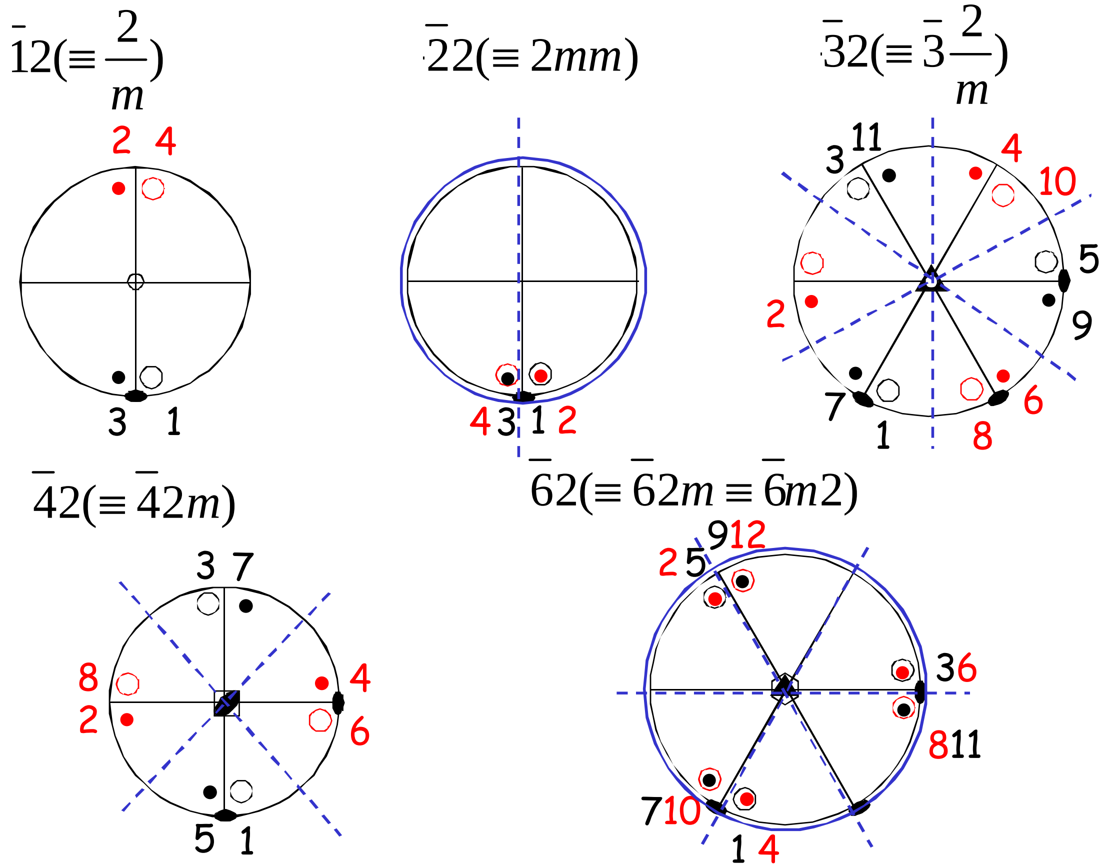
Combination of rotation axes



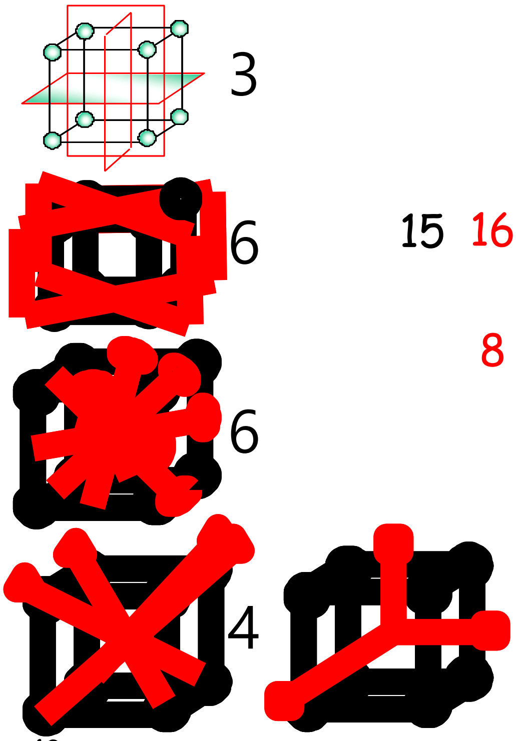
Combination of rotation axes, n2

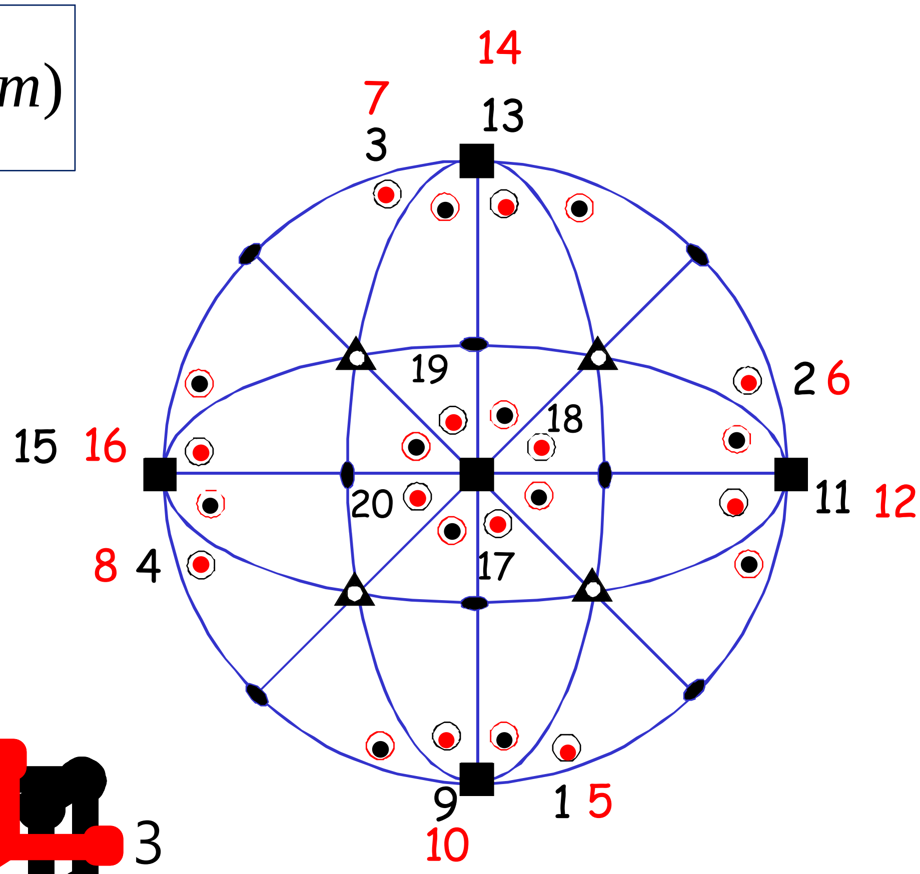


Combination of rotation axes, $\bar{n}2$



$$\frac{4}{m}\bar{3}\frac{2}{m}(\equiv m\bar{3}m)$$





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 Group

➢ Schönflies symbol vs. International (Hermann-Mauguin) symbol

C_n: n-fold rotation axis; identical with X

C_n	C_1	C_2	C_3	C_4	C_6
X	1	2	3	4	6

C_{ni}: odd-order rotation axis and inversion centre $i \equiv \bar{X}$ (odd)
C_s: (s for German Spiegelebene) = mirror plane;
S_n: n-fold rotoreflection axis (only S_4 and S_6 used)

	C_i	C_s	$C_{3i} \equiv S_6$	S_4	
$\bar{X}$	$\bar{1}$	$(\bar{2} \equiv)$ m	$\bar{3}$	$\bar{4}$	

C_{nh}: n-fold axis normal to mirror plane $\equiv$ X/m

C_{nh}		C_{2h}	C_{3h}	C_{4h}	C_{6h}
X/m		2/m	$(3/m \equiv) \bar{6}$	4/m	6/m

Symmetry directions

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

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

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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

Table 2.10 Lattice symmetry and unit cell shapes.

Crystal family	Unit cell symmetry	Unit cell shape/parameters
Triclinic	$\bar{1}$	$a \neq b \neq c;\ \alpha \neq \beta \neq \gamma \neq 90°$
Monoclinic	2/m	$a \neq b \neq c;\ \alpha = \gamma = 90°, \beta \neq 90°$
Orthorhombic	mmm	$a \neq b \neq c;\ \alpha = \beta = \gamma = 90°$
Tetragonal	4/mmm	$a = b \neq c;\ \alpha = \beta = \gamma = 90°$
Hexagonal and Trigonal	6/mmm	$a = b \neq c;\ \alpha = \beta = 90°, \gamma = 120°$
Cubic	m$\bar{3}$m	$a = b = c;\ \alpha = \beta = \gamma = 90°$

Pecharsky Chap 2

Notations in the "International Tables for Crystallography"

Table 1.1. Notation for Asymmetric Units Used to Represent Point Group Symmetry

Notation	Description
	Asymmetric unit in the plane of the page
	Asymmetric unit above (+) or below (−) the plane of the page
	Apostrophe indicating a left-handed asymmetric unit and clear circle indicating righthandedness.
	Two asymmetric units directly on top of one another, with the "+" meaning above the plane and the "−" meaning below the plane.
	Two asymmetric units directly on top of one another, one left-handed and the other right-handed

Note: The notation derives from the *International Tables for Crystallography*.

■ down
○ up

Black & Red; enantiomorphs
■ down, left
○ up, right

Krawitz page 10

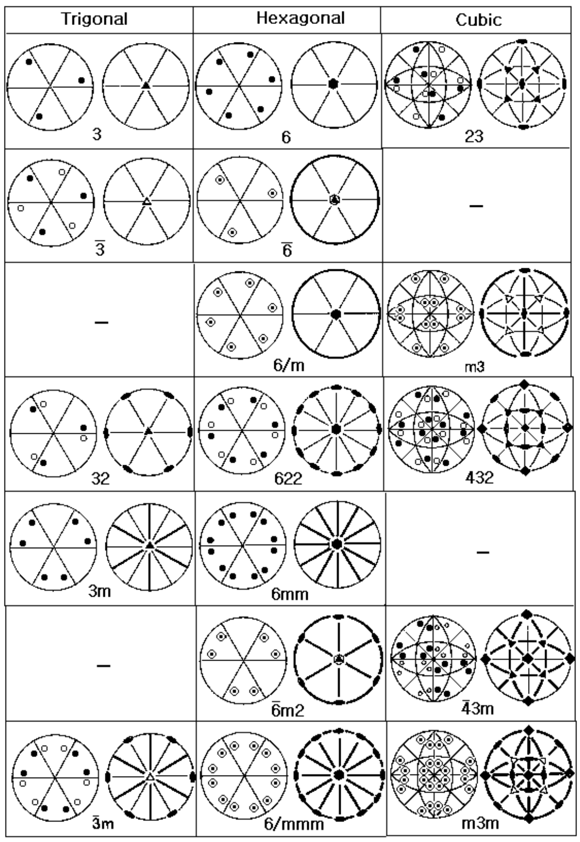

Fig. The 32 crystallographic point group. Each pari of stereograms shows (left) the poles of a general form , (righr) the symmetry elements of the point group