14 Bravais Lattices

Read

Ott Chapter 7, 8

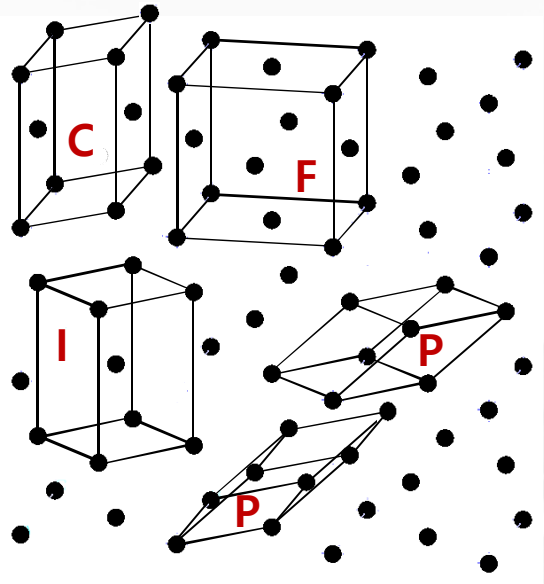
Krawitz Chapter 1.1 ~ 1.5

Hammond Chapter 2.1 ~ 2.4; 3.1 ~ 3.3; 5.1 ~ 5.6

Sherwood & Cooper Chapter 3.1~3.7

Brief but very good summary can be found here
https://unlcms.unl.edu/cas/physics/tsymbal/teaching/SSP-927/Section%2001_Crystal%20Structure.pdf

Lattice types - P, I, F, C, R



the number of lattice points in a unit cell (N)?

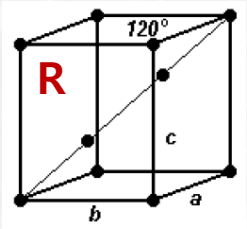
$$N = N_i + N_j/2 + N_c/8 + N_e/4$$

N_i = # of lattice points in cell interior (belong to 1 cell)

N_j = # of lattice points on cell faces (shared by 2 cells)

N_c = # of lattice points on cell corners (vertices) (shared by 8 cells)

N_e = # of lattice points on cell edges (shared by 4 cells)



- Primitive lattice; one lattice point per unit cell
- Non-primitive lattice; more than one lattice point per unit cell

Bravais lattices

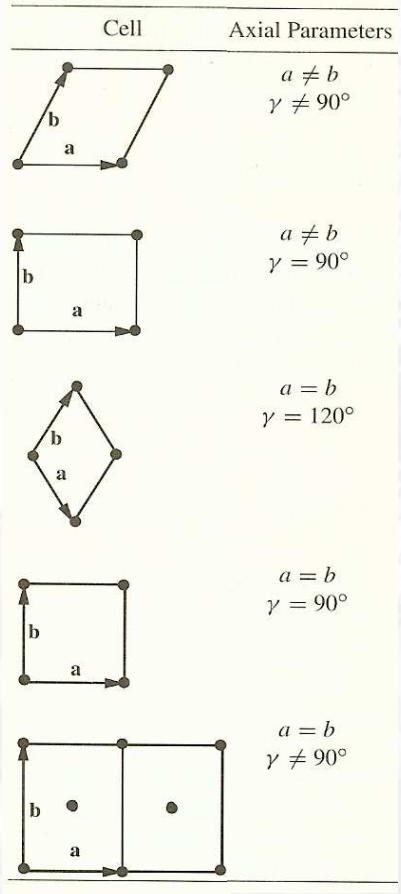
- In geometry and crystallography, a **Bravais lattice** is an infinite array of discrete points generated by a set of discrete translation operations described by: $\mathbf{R} = n_1\mathbf{a_1} + n_2\mathbf{a_2} + n_3\mathbf{a_3}$. This discrete set of vectors must be closed under vector addition and subtraction. For any choice of position vector **R**, the lattice looks exactly the same. (n_i ; any integer. $\mathbf{a_i}$; primitive vectors which lie in different directions and span the lattice.)

- A crystal is made up of a periodic arrangement of one or more atoms (*basis, motif*) repeated at each lattice point. Consequently, the crystal looks the same when viewed from any of the lattice points.

- Two Bravais lattices are often considered equivalent if they have isomorphic symmetry groups. In this sense, there are only 14 possible Bravais lattices in 3-dimensional space.

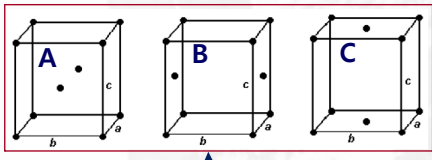
2D Bravais lattice (Plane lattice)

- In two dimensions, there are five Bravais lattices.



3D Bravais lattices

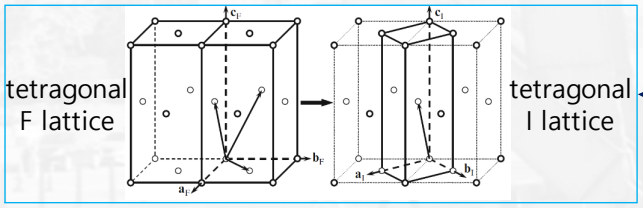
- The 14 Bravais lattices in 3 dimensions are obtained by coupling one of the 7 lattice systems (or axial systems) with one of lattice centerings. Each Bravais lattice refers to a distinct lattice type.



- 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



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

7 Crystal systems

- Combination of symmetry elements & their orientations w.r.t. one another defines the crystallographic axes → 7 crystal systems
- 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 element or specific combination of them** present in the point group symmetry
- 7 X 5 types of lattices → 14 different types of unit cells are required to describe all lattices (14 Bravais lattice)

7 Crystal systems, 6 Crystal family

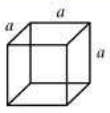
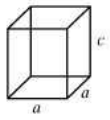
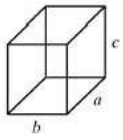
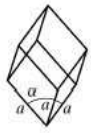
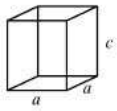
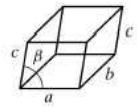
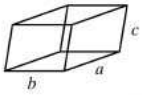
Table 2.6 Seven crystal systems and the corresponding characteristic symmetry elements.

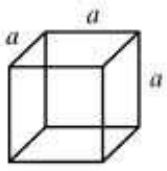
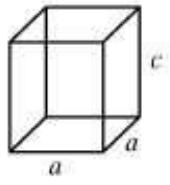
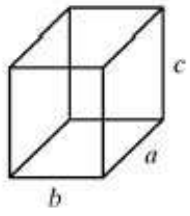
Crystal system	Characteristic symmetry element or combination of symmetry elements
Triclinic	No axes other than onefold rotation or onefold inversion
Monoclinic	Unique twofold axis and/or single mirror plane
Orthorhombic	Three mutually perpendicular twofold axes, either rotation or inversion
Trigonal	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

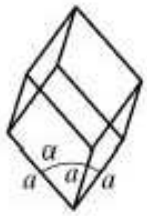
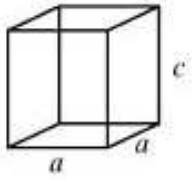
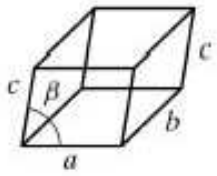
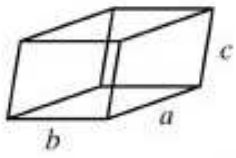
→ six crystal family

7 Crystal systems

System	Axial lengths and angles[a]	Unit cell geometry
Cubic	$a = b = c, \alpha = \beta = \gamma = 90°$	
Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90°$	
Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90°$	
Rhombohedral	$a = b = c, \alpha = \beta = \gamma \neq 90°$	
Hexagonal	$a = b \neq c, \alpha = \beta = 90°, \gamma = 120°$	
Monoclinic	$a \neq b \neq c, \alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90°$	

System	Axial lengths and angles[a]	Unit cell geometry
Cubic	$a = b = c, \alpha = \beta = \gamma = 90°$	
Tetragonal	$a = b \neq c, \alpha = \beta = \gamma = 90°$	
Orthorhombic	$a \neq b \neq c, \alpha = \beta = \gamma = 90°$	

[a]The lattice parameters a, b, and c are unit-cell edge lengths. The lattice parameters α, β, and γ are angles between adjacent unit-cell axes, where α is the angle viewed along the a axis (i.e., the angle between the b and c axes). The inequality sign ($\neq$) means that equality is not required. Accidental equality occasionally occurs in some structures.

Rhombohedral	$a = b = c, \alpha = \beta = \gamma \neq 90°$	
Hexagonal	$a = b \neq c, \alpha = \beta = 90°, \gamma = 120°$	
Monoclinic	$a \neq b \neq c, \alpha = \gamma = 90° \neq \beta$	
Triclinic	$a \neq b \neq c, \alpha \neq \beta \neq \gamma \neq 90°$	

Selection of a unit cell

- Trigonal & hexagonal can be described in the same type of the lattice → **six crystal family**
- Different types of crystal systems (lattices) can be identified by the presence of specific symmetry elements and their relative orientation

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	$m\bar{3}m$	$a = b = c; \alpha = \beta = \gamma = 90°$

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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

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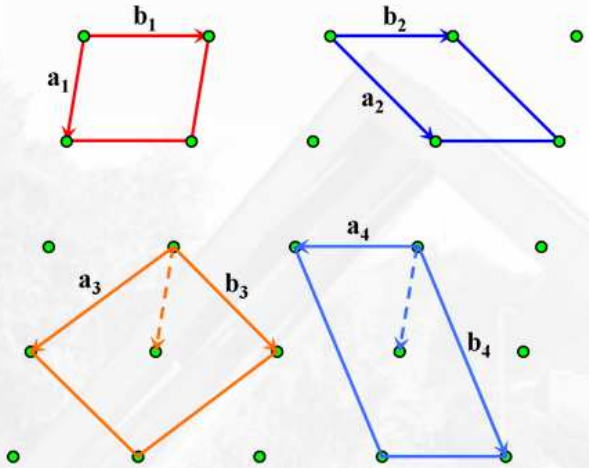
All lattices are centrosymmteric

Selection of a unit cell-1

- Rule #1 --- symmetry of the unit cell should be identical to the symmetry of the lattice, except for translation
- Choice of unit cell is arbitrary
  - ✓ It is not always possible to select a primitive cell



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Selection of a unit cell-2

Table 2.11 Rules for selecting the unit cell in different crystal systems.

Crystal family	Standard unit cell choice	Alternative unit cell choice
Triclinic	Angles between crystallographic axes should be as close to 90° as possible but greater than or equal to 90°	Angle(s) less than or equal to 90° are allowed
Monoclinic	*Y*-axis is chosen parallel to the unique twofold rotation axis (or perpendicular to the mirror plane) and angle β should be greater than but as close to 90° as possible	Same as the standard choice, but *Z*-axis in place of *Y*, and angle γ in place of β are allowed
Orthorhombic	Crystallographic axes are chosen parallel to the three mutually perpendicular twofold rotation axes (or perpendicular to mirror planes)	None
Tetragonal	*Z*-axis is always parallel to the unique fourfold rotation (inversion) axis. *X*- and *Y*-axes form a 90° angle with the *Z*-axis and with each other	None
Hexagonal and trigonal	*Z*-axis is always parallel to three- or sixfold rotation (inversion) axis. *X*- and *Y*-axes form a 90° angle with the *Z*-axis and a 120° angle with each other	In a trigonal symmetry,[a] threefold axis is chosen along the body diagonal of the primitive unit cell, then $a = b = c$ and $\alpha = \beta = \gamma \neq 90°$
Cubic	Crystallographic axes are always parallel to the three mutually perpendicular two- or fourfold rotation axes, while the four threefold rotation (inversion) axes are parallel to three body diagonals of a cube	None

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Selection of a unit cell-3

- Rule #3 --- minimum volume (or min # of lattice points inside the unit cell)

- Rule # 1, 2, 3, → 5 types of lattices (P, I, F, C, R)

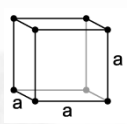
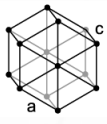
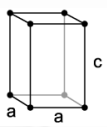
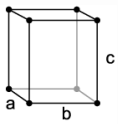
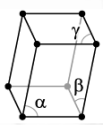
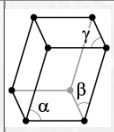
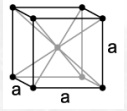
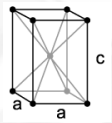
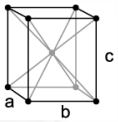
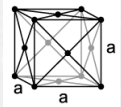
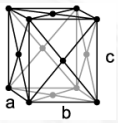
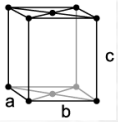
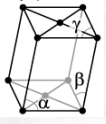
Table 2.12 Possible lattice centering.

Centering of the lattice	Lattice points per unit cell	International symbol	Lattice translation(s) due to centering
Primitive	1	P	None
Base-centered	2	A	$\frac{1}{2}(\mathbf{b}+\mathbf{c})$
Base-centered	2	B	$\frac{1}{2}(\mathbf{a}+\mathbf{c})$
Base-centered	2	C	$\frac{1}{2}(\mathbf{a}+\mathbf{b})$
Body-centered	2	I	$\frac{1}{2}(\mathbf{a}+\mathbf{b}+\mathbf{c})$
Face-centered	4	F	$\frac{1}{2}(\mathbf{b}+\mathbf{c}); \frac{1}{2}(\mathbf{a}+\mathbf{c}); \frac{1}{2}(\mathbf{a}+\mathbf{b})$
Rhombohedral	3	R	$\frac{1}{3}\mathbf{a}+\frac{2}{3}\mathbf{b}+\frac{2}{3}\mathbf{c}; \frac{2}{3}\mathbf{a}+\frac{1}{3}\mathbf{b}+\frac{1}{3}\mathbf{c}$

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			

➢ Why tetragonal F lattice is not one of 14?

✓ Because that lattice can be reduced to a lattice with different centering and/or a smaller unit cell (rule #3)

✓ Or Because they do not satisfy rule # 1 or #2

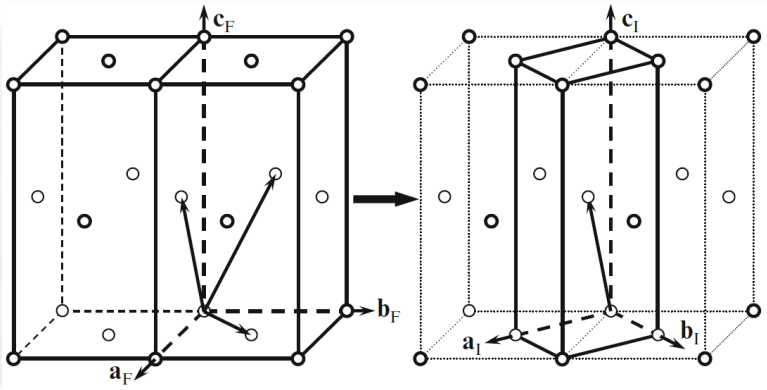


Fig. 2.21 The reduction of the tetragonal face-centered lattice (*left*) to the tetragonal body-centered lattice with half the volume of the unit cell (*right*). Small circles indicate lattice points.

See Hammond 3.2

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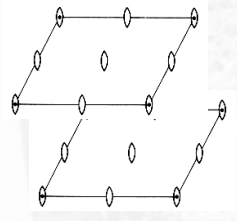
➢ general space lattice

✓ no symmetry elements except inversion center

All lattices are centrosymmteric



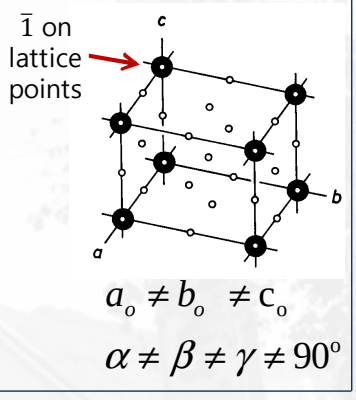
➢ special space lattice

✓ rotation axis and mirror plane

✓ restriction on the cell parameters

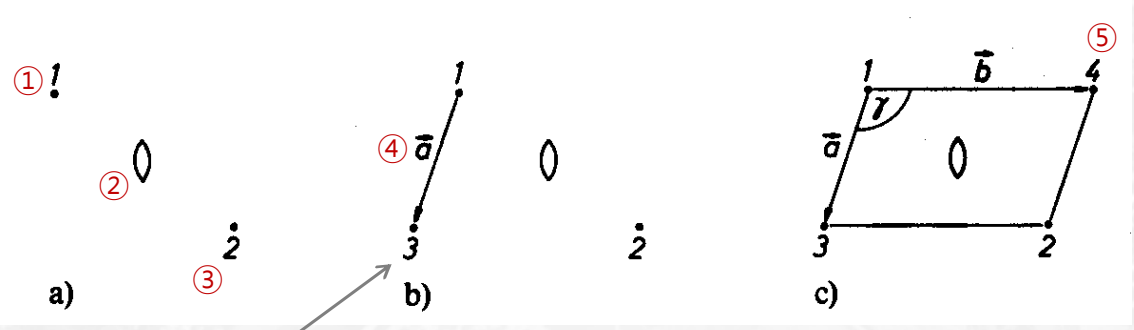
- ex) 4_z-fold rotation axis → a=b, γ=90°

✓ simplifications in the crystal morphology and in the physical properties



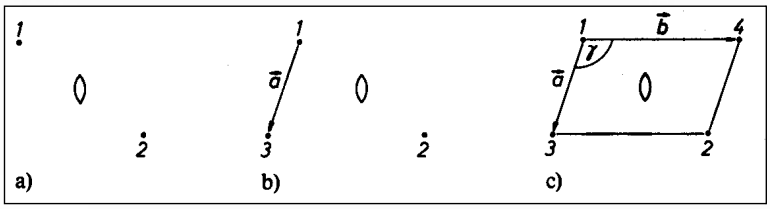
➢ plane lattices → space lattices

- general (oblique) lattice
  - ✓ 2 fold axis: 1 → 2
  - ✓ lattice translation $\vec{a}$: 1 → 3
  - ✓ 2 fold axis: 3 → 4
  - → oblique parallelogram, $a_0 \neq b_0$, $\gamma \neq 60^o, 90^o, 120^o$



Position of point 3 is general

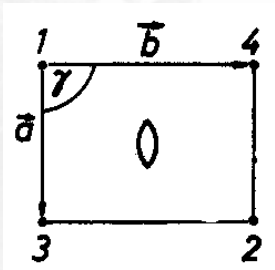
≠; need not be equivalent
=; are required to be equivalent by symmetry



Position of point 3 is general

$a_0 \neq b_0$, $\gamma \neq 60^o, 90^o, 120^o$

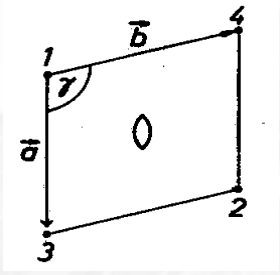
Position of point 3 is special



right triangle

$a_0 \neq b_0$
$\gamma = 90^o$

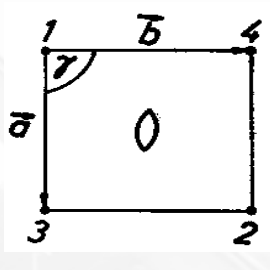
S1



Isosceles triangle

$a_0 = b_0$,
$\gamma \neq 60^o, 90^o, 120^o$

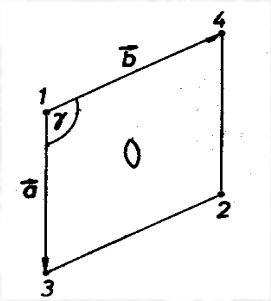
S2



Isosceles right triangle

$a_0 = b_0$
$\gamma = 90^o$

S3

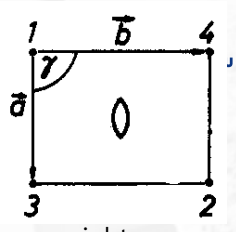


equilateral triangle

$a_0 = b_0$
$\gamma = 120^o$

S4

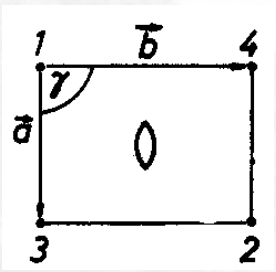
5 plane lattices > special plane lattice – 1 (S1)

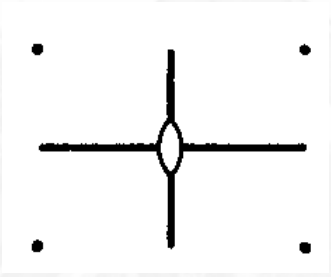


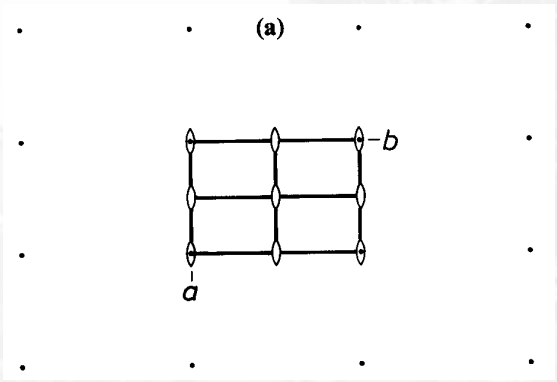
right triangle

$a_0 \neq b_0$
$\gamma = 90^o$

- special lattice ; $a_0 \neq b_0$, $\gamma = 90^o$
  - ✓ rectangular unit mesh
  - ✓ two perpendicular mirror planes // 2 fold axes

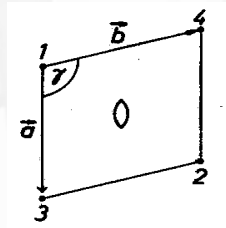






Position of point 3 is special (right angle 132)

5 plane lattices > special plane lattice - 2 (S2)



Isosceles triangle

$a_0 = b_0$,
$\gamma \neq 60^o, 90^o, 120^o$

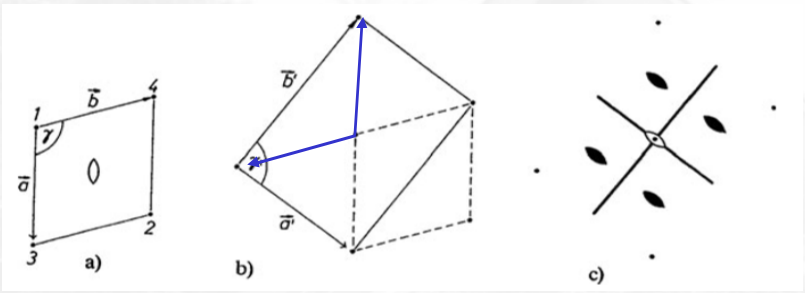
Position of point 3 is special (13 = 32)

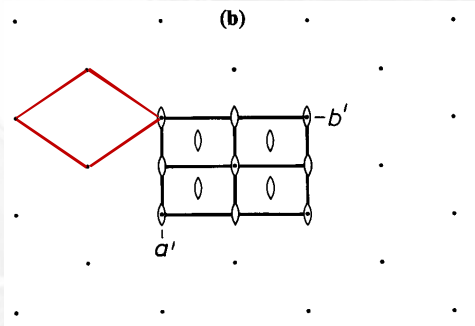
$a_0 = b_0$, $\gamma \neq 60^o, 90^o, 120^o$

extension of the edges 1-3 & 1-4

→ alternative unit mesh, $a'_0 \neq b'_0$, $\gamma' = 90^o$

→ centered rectangular ; 2-fold axes, mirror plane





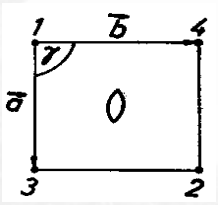
5 plane lattices > special plane lattice – 3 (S3), 4 (S4)

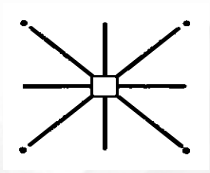
Position of point 3 is special (1, 2, & 3 make an isosceles right triangle)

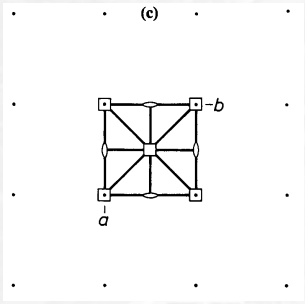
$\overline{13} = \overline{23}$

$a_0 = b_0$, $\gamma = 90^o$ square mesh

4-fold axes, 4 mirror planes





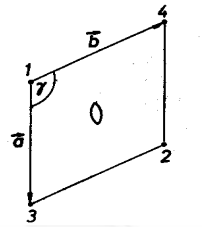


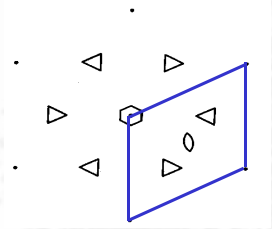
Position of point 3 is special (1, 2, & 3 make an equilateral triangle)

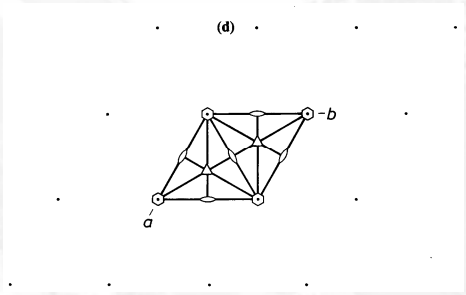
$\overline{13} = \overline{23}$

$a_0 = b_0$, $\gamma = 120^o$ hexagonal mesh

2, 6, 3-fold axes, mirror planes







5 plane lattices

		Shape of unit mesh	Lattice parameters	Characteristic symmetry elements
General plane lattices		Parallelogram	$a_0 \neq b_0$ $\gamma \neq 90°$	2
Special plane lattice	a	Rectangle (primitive)	$a_0 \neq b_0$ $\gamma = 90°$	m
	b	Rectangle (centred)	$a_0 \neq b_0$ $\gamma = 90°$	m
	c	Square	$a_0 = b_0$ $\gamma = 90°$	4
	d	120° Rhombus	$a_0 = b_0$ $\gamma = 120°$	6 (3)

Any two-dimensionally periodic array can be assigned to one of the 5 lattice types

See Hammond 2.4

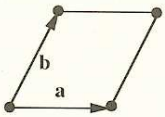
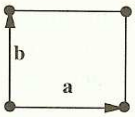
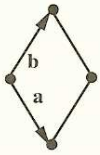
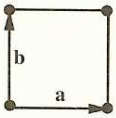
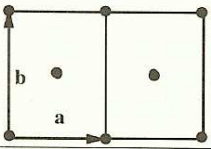
5 plane lattices

Five 2-D lattice types

Ten 2-D point groups
Ten plane point groups

See Hammond 2.3

Table 1.3. Plane Lattice Types, Axial Parameters and Associated Two-Dimensional Point Groups

Cell	Name	Axial Parameters	Point groups
	Oblique	$a \neq b$ $\gamma \neq 90°$	1, 2
	Rectangular	$a \neq b$ $\gamma = 90°$	m, $2mm$
	Hexagonal	$a = b$ $\gamma = 120°$	3, $3m$ 6, $6mm$
	Square	$a = b$ $\gamma = 90°$	4, $4mm$
	Centered Rectangular	$a = b$ $\gamma \neq 90°$	m, $2mm$

- Stack plane lattices → space lattice

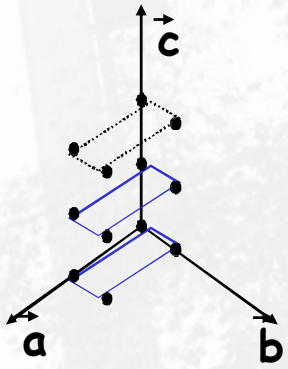
Primitive space lattice (P-lattice)

- 5 space lattices with primitive unit cells from the 5 plane lattices

  → primitive space lattices

  - Congruent lattice planes are stacked above one another

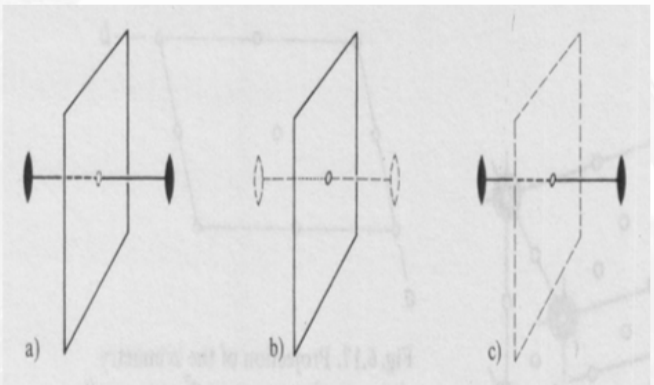
Shape of unit mesh in stacked layers	Interplanar spacing	Lattice
Parallelogram[a] ($a_0 \neq c_0$)	b_0	Monoclinic P
Rectangle ($a_0 \neq b_0$)	c_0	Orthorhombic P
Square ($a_0 = b_0$)	$c_0 \neq (a_0 = b_0)$	Tetragonal P
Square ($a_0 = b_0$)	$c_0 = (a_0 = b_0)$	Cubic P
120°-Rhombus ($a_0 = b_0$)	c_0	Hexagonal P

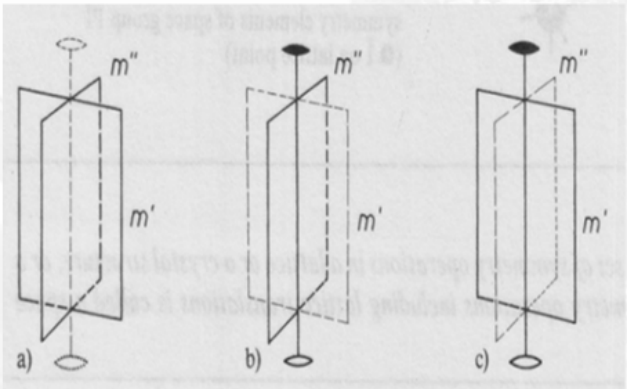


[a] Note that for historical reasons, the description $a_0 \neq b_0$, $\gamma \neq 90°$ has been changed in this case to $a_0 \neq c_0$, $\beta \neq 90°$. (See slide # 14; standard unit cell choice of monoclinic)

Symmetry of P-lattices

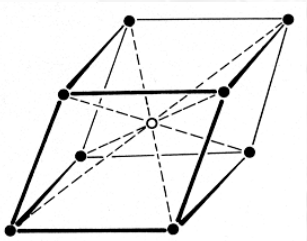
- The presence of any two of the following symmetry elements implies the presence of the third
- Rule 1 : A rotation axis of even order (X_e = 2, 4, 6), a mirror plane normal to X_e, and an inversion center at the point of intersection of X_e and m
- Rule 2 : Two mutually perpendicular mirror planes and a 2-fold axis along their line of intersection





$2 \perp m \rightarrow \bar{1}$ $\quad \bar{1}$ on $m \rightarrow 2$ $\quad \bar{1}$ on $2 \rightarrow m$ $\quad m' \perp m'' \rightarrow 2$ $\quad 2$ on $m' \rightarrow m''$ ($\perp m'$) $\quad 2$ on $m'' \rightarrow m'$ ($\perp m''$)

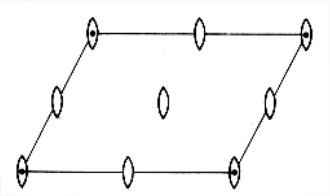
- Every lattice has inversion centers on the lattice point and midway between any two of them



All lattices are centrosymmteric

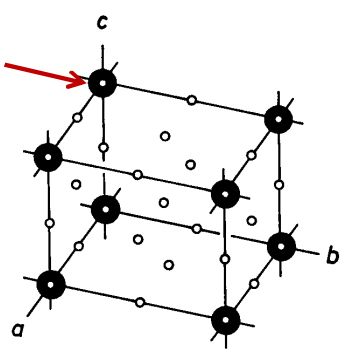
- Space group
  - ✓ the complete set of symmetry operations in a lattice or a crystal structure
  - ✓ a group of symmetry operations including lattice translations
  - ✓ 230 space groups

Space lattice > Triclinic P-lattice (general lattice)

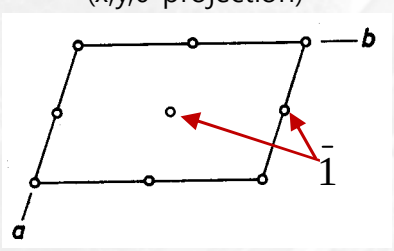


- When stacked directly above one another → monoclinic P lattice
- When lattice points of stacked plane do not coincide → lose 2-fold axis → triclinic P lattice → The only point symmetry elements are inversion centres

$\bar{1}$ on lattice points



(x,y,0 projection)



point group: $\bar{1}$

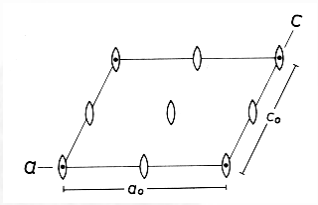
space group: $P\bar{1}$

$a_o \neq b_o \neq c_o$

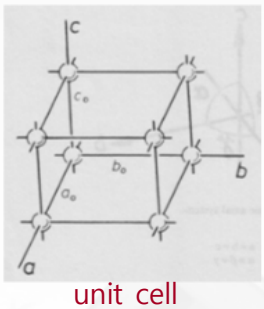
$\alpha \neq \beta \neq \gamma \neq 90^o$

Space lattice > Monoclinic P-lattice

- set of 2-fold axes // b
- mirror planes normal to b at x,0,z and x,½,z
- inversion center

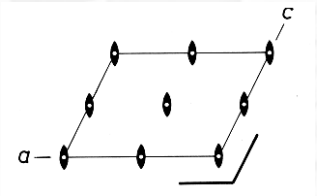


unit mesh



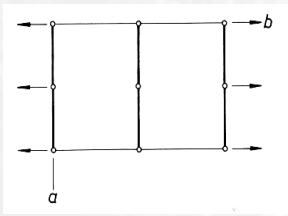
unit cell

stack with inter-planar spacing b_0



(x,0,z projection)

_/ indicates a mirror plane // to the plane of the page at heights of 0 and ½



(x,y,0 projection)

The b-axis (// to 2 and ⊥ to m) is called symmetry direction ("2nd setting")

1st setting; c // 2, c ⊥ m

$a_o \neq b_o \neq c_o$

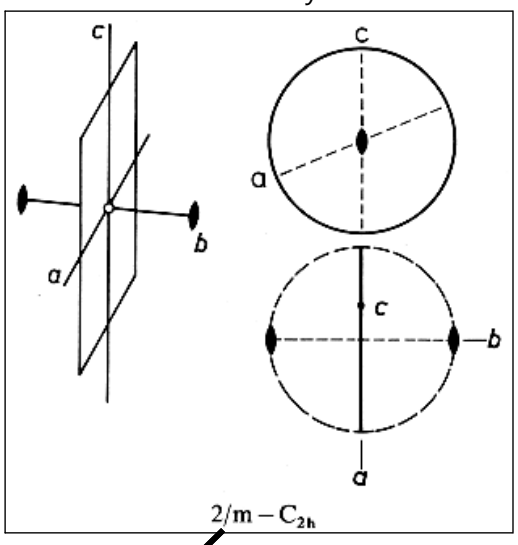
$\alpha = \gamma = 90^o,\ \beta > 90^o$

point group: $\frac{2}{m}$

space group: $P\frac{2}{m}$

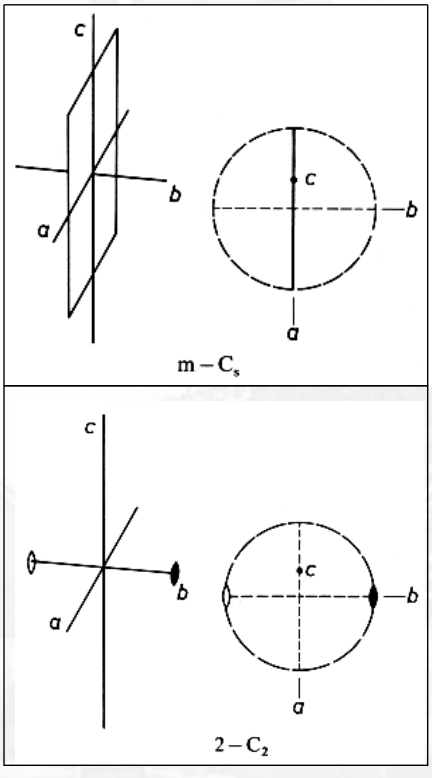
Space lattice > Monoclinic P-lattice

Highest symmetry point group in monoclinic system



along b direction
along symmetry direction

lower symmetry

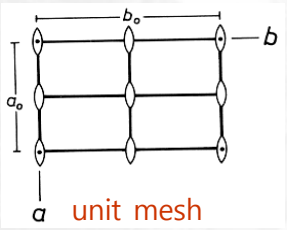


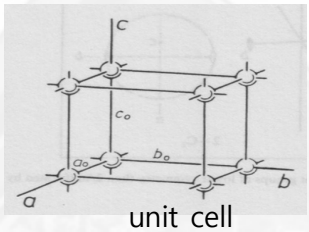
monoclinic point groups of lower symmetry

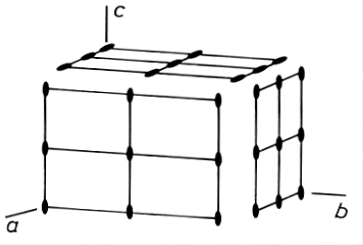
Space lattice > Orthorhombic P-lattice

- rectangular plane lattice
- set of 2-fold axes // c
- symmetry of stacked plane + (mirror planes ⊥ c at x,y,0 and x,y,½) + (inversion centres)
- rule I* ($\bar{1}$ on m → 2⊥m) or rule II* (m⊥m → 2) generates

  2-fold axes at x,0,0; x,0,½; x,½,0; x,½,½; 0,y,0; 0,y,½; ½,y,0; ½,y,½



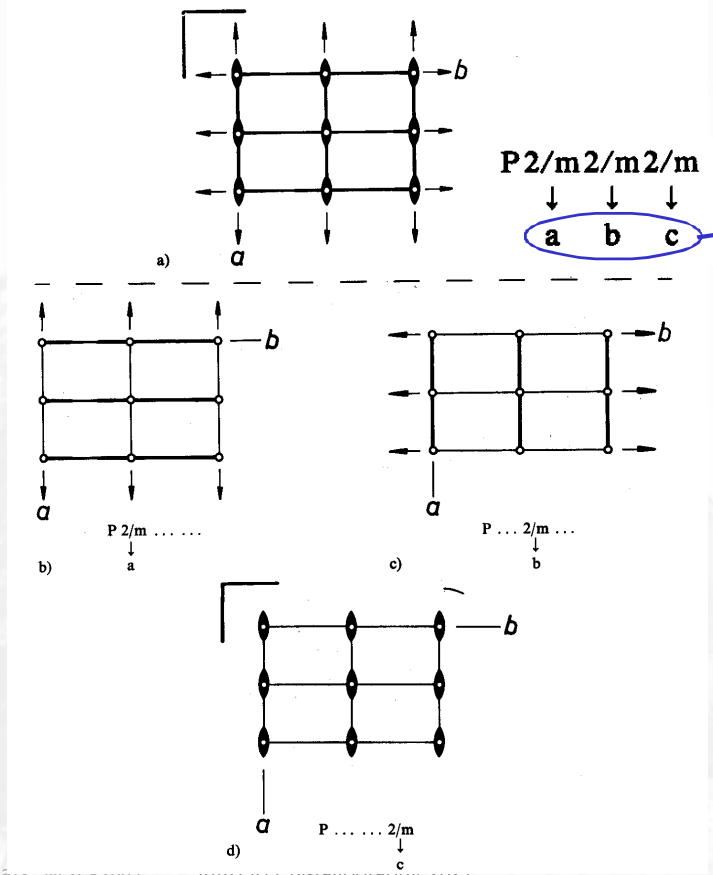




stack with inter-planar spacing c_0

* rule I or rule II ; see slide # 28

Space lattice > Orthorhombic P-lattice



P2/m2/m2/m
↓ ↓ ↓
a b c

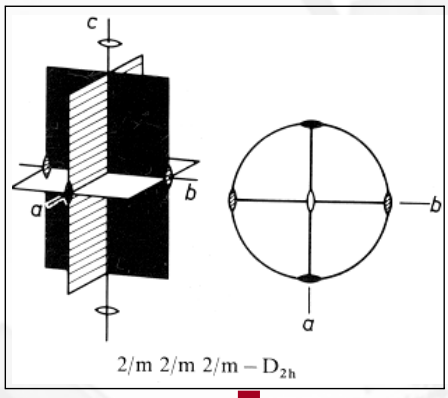
symmetry directions of orthorhombic

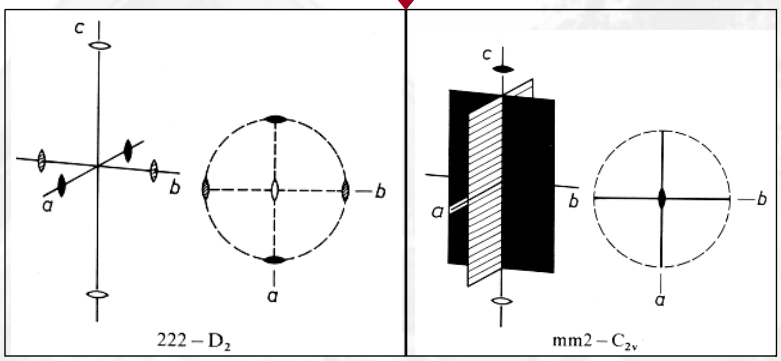
$a_o \neq b_o \neq c_o$

$\alpha = \beta = \gamma = 90^o$

point group: $\frac{2}{m}\frac{2}{m}\frac{2}{m}$

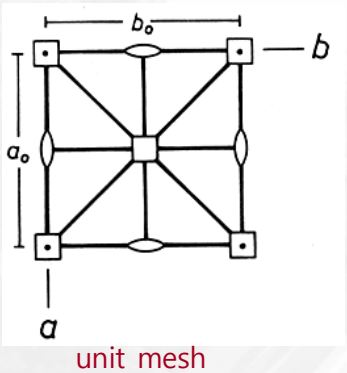
space group: $P\frac{2}{m}\frac{2}{m}\frac{2}{m}$



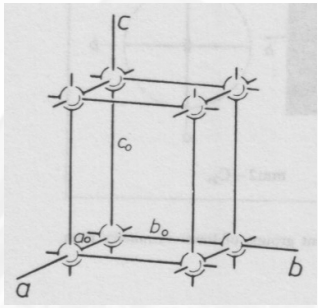


orthorhombic point groups of lower symmetry

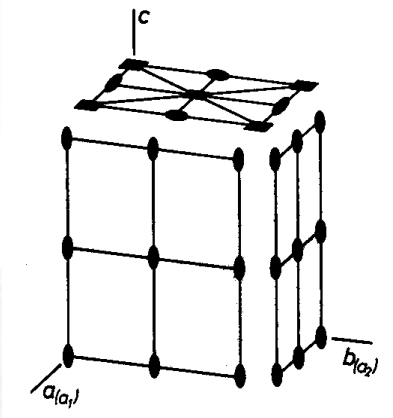
- symmetry of stacked plane + (mirror planes ⊥ c at x,y,0 and x,y,½) + (inversion centres)
- rule I* ($\bar{1}$ on m → 2⊥m) or rule II* (m⊥m → 2) generates several 2-fold axes



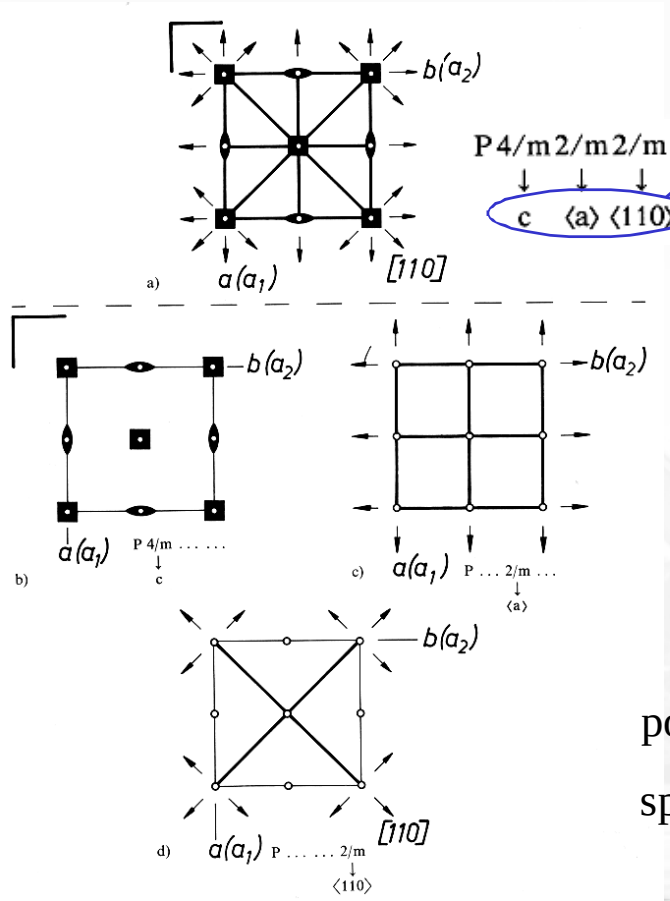
unit mesh



unit cell



* rule I or rule II ; see slide # 28



point group: $\frac{4}{m}\frac{2}{m}\frac{2}{m}$

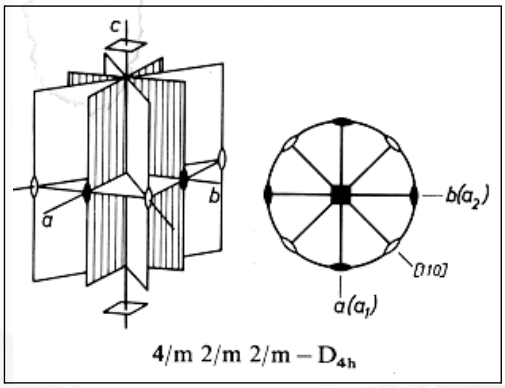
space group: $\mathrm{P}\frac{4}{\mathrm{m}}\frac{2}{m}\frac{2}{m}$

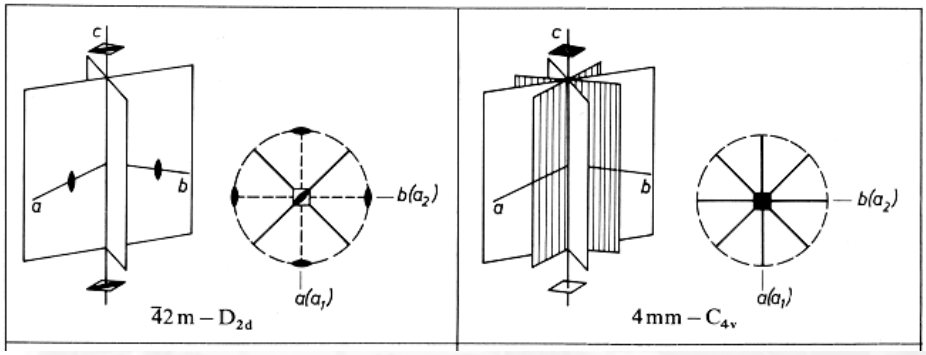
$a_o = b_o \neq \mathrm{c_o}$

$\alpha = \beta = \gamma = 90^{\mathrm{o}}$

point group: $\frac{4}{m}\frac{2}{m}\frac{2}{m}$

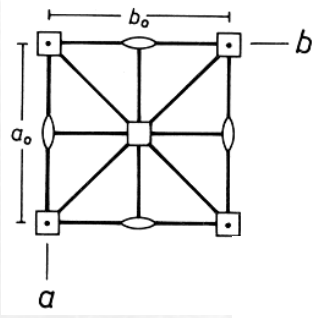
space group: $\mathrm{P}\frac{4}{\mathrm{m}}\frac{2}{m}\frac{2}{m}$

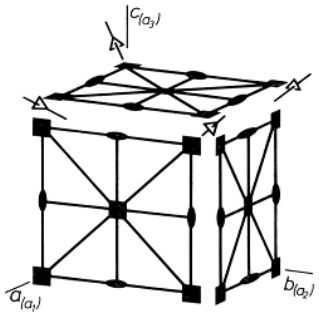




tetragonal point groups of lower symmetry

- $a_0=b_0=c_0$ → four 3-fold axes along the body diagonals of unit cell as well as inversion center → $\bar{3}$
- Rule I* or II* generates 2-fold axes // [110] and equivalent directions





symmetry directions of cubic

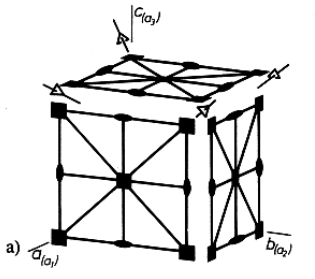
d Space group

P 4/m $\bar{3}$ 2/m (Pm$\bar{3}$m)

⟨a⟩ ⟨111⟩ ⟨110⟩

Symmetry elements (incomplete) of the cubic P-lattice. This is one of the space groups of highest symmetry in the cubic system

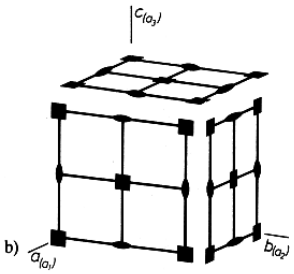
* rule I or rule II ; see slide # 28



symmetry directions of cubic

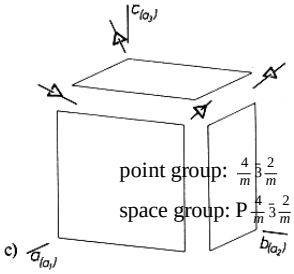
P 4/m $\bar{3}$ 2/m

⟨a⟩ ⟨111⟩ ⟨110⟩



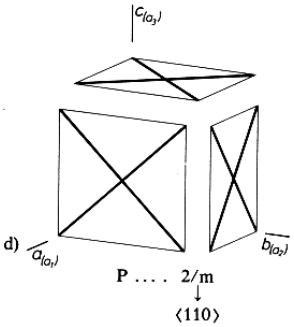
P 4/m . . . .

⟨a⟩



P . . . $\bar{3}$ . . .

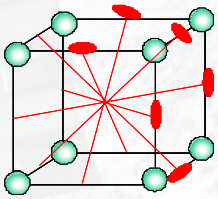
⟨111⟩



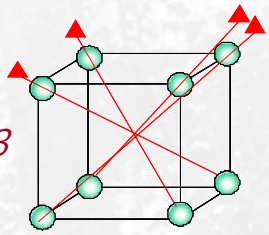
P 2/m

⟨110⟩

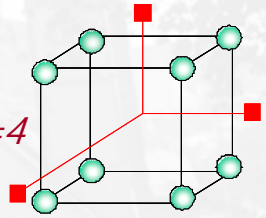
X=2



X=3



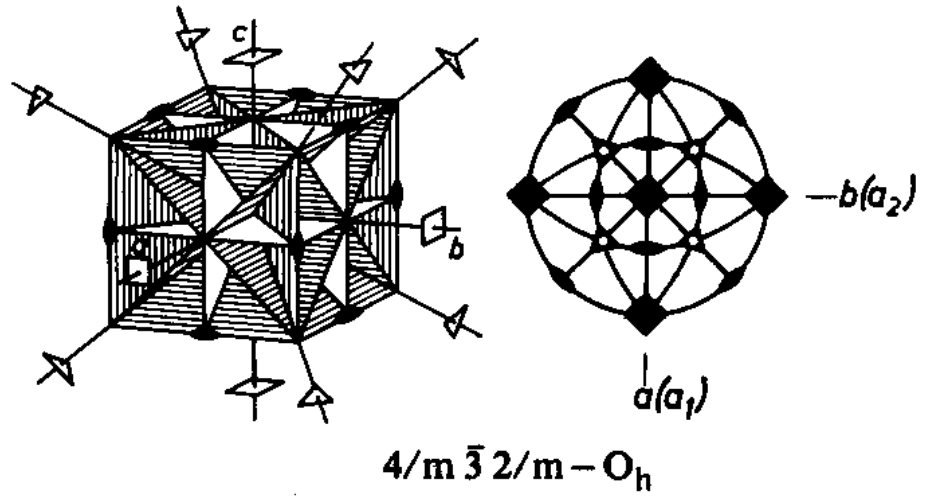
X=4



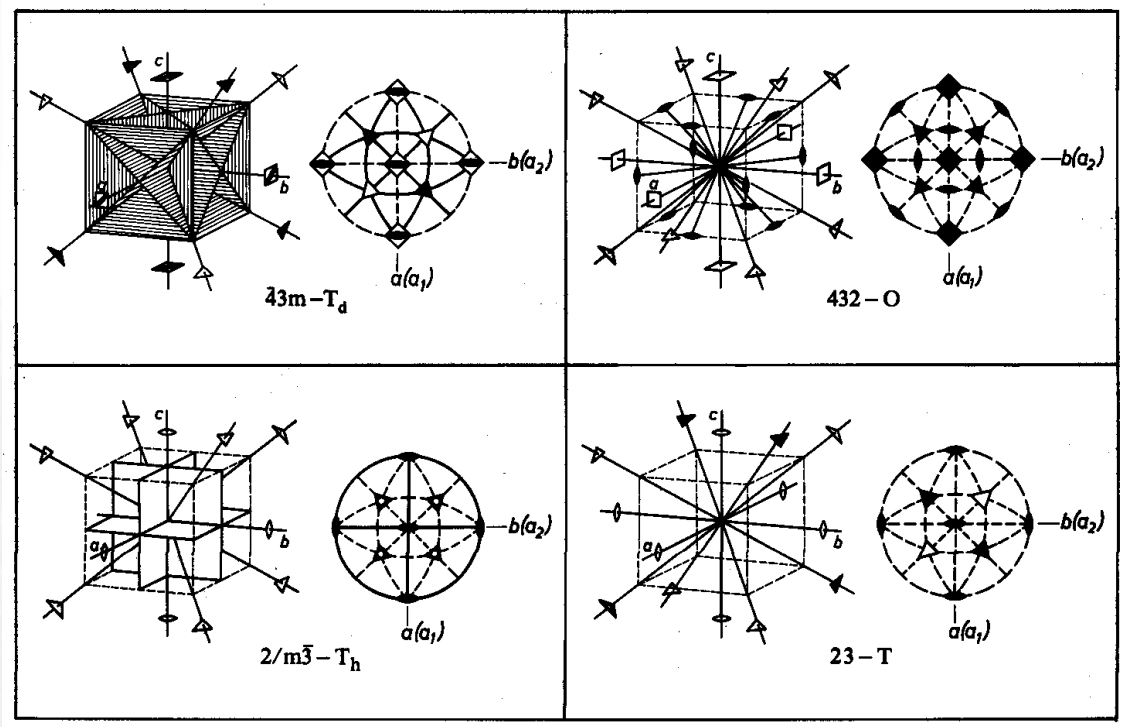
$a_o = b_o = c_o$
$a = b = g = 90^o$

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

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

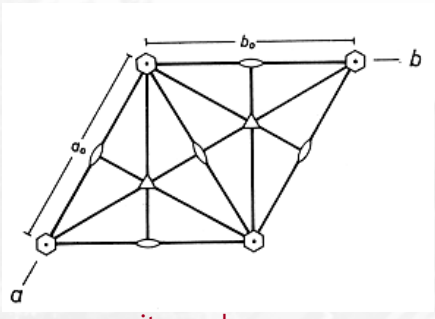


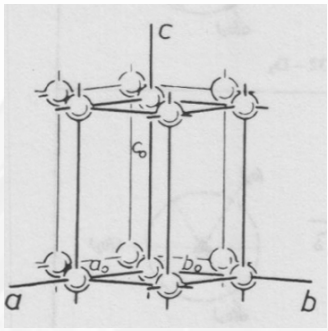
Highest symmetry point group in cubic system

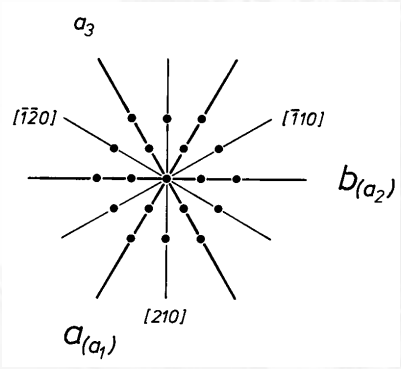


cubic point groups of lower symmetry

- symmetry of stacked plane + (mirror planes ⊥ c at x,y,0 and x,y,½) + (inversion centres)
- rule I* ($\bar{1}$ on m → 2⊥m) or rule II* (m⊥m → 2) generates several 2-fold axes



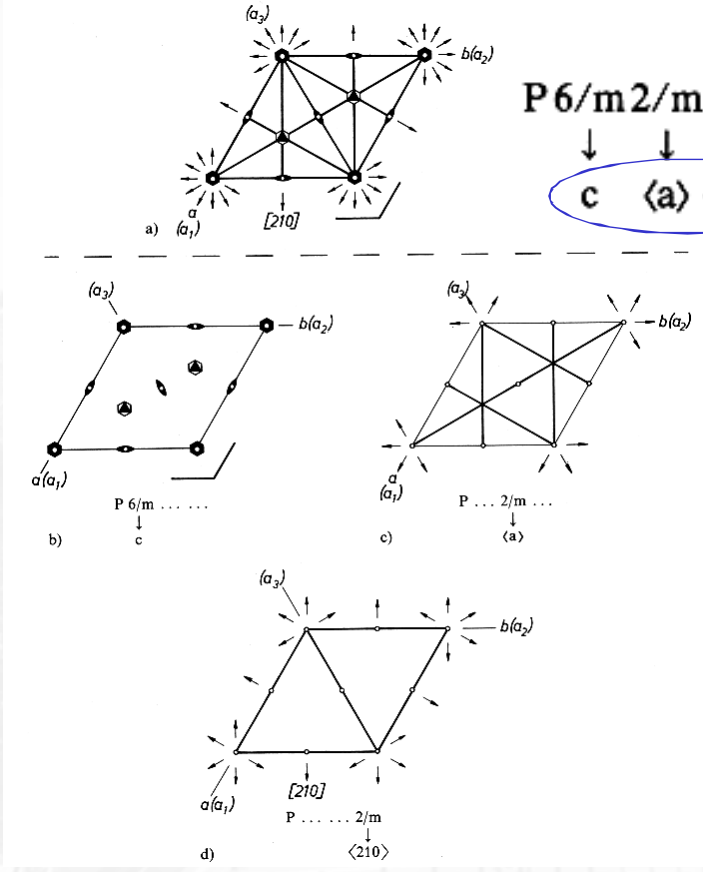




unit mesh → unit cell

stack with inter-planar spacing c_0

* rule I or rule II ; see slide # 28



P 6/m 2/m 2/m

c ⟨a⟩ ⟨210⟩

symmetry directions of hexagonal

point group: $\frac{6}{m}\frac{2}{m}\frac{2}{m}$

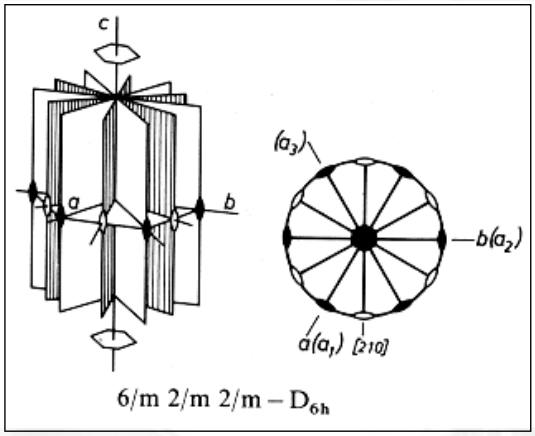
space group: P $\frac{6}{m}\frac{2}{m}\frac{2}{m}$

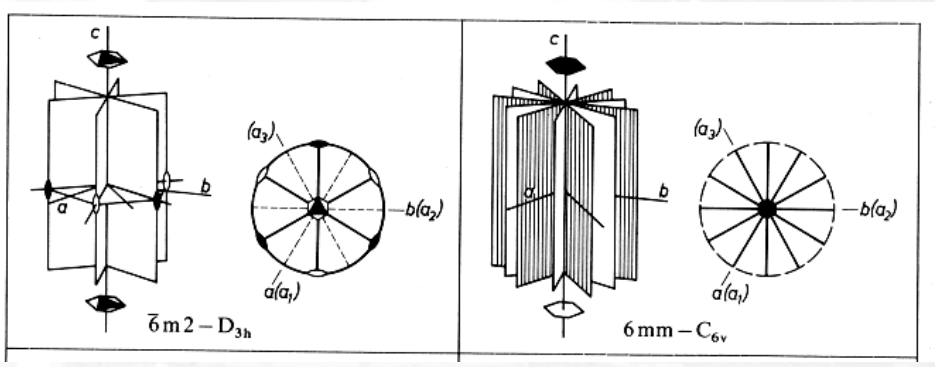
$a_o = b_o \neq c_o$

$\alpha = \beta = 90^o, \gamma = 120^o$

point group: $\frac{6}{m}\frac{2}{m}\frac{2}{m}$

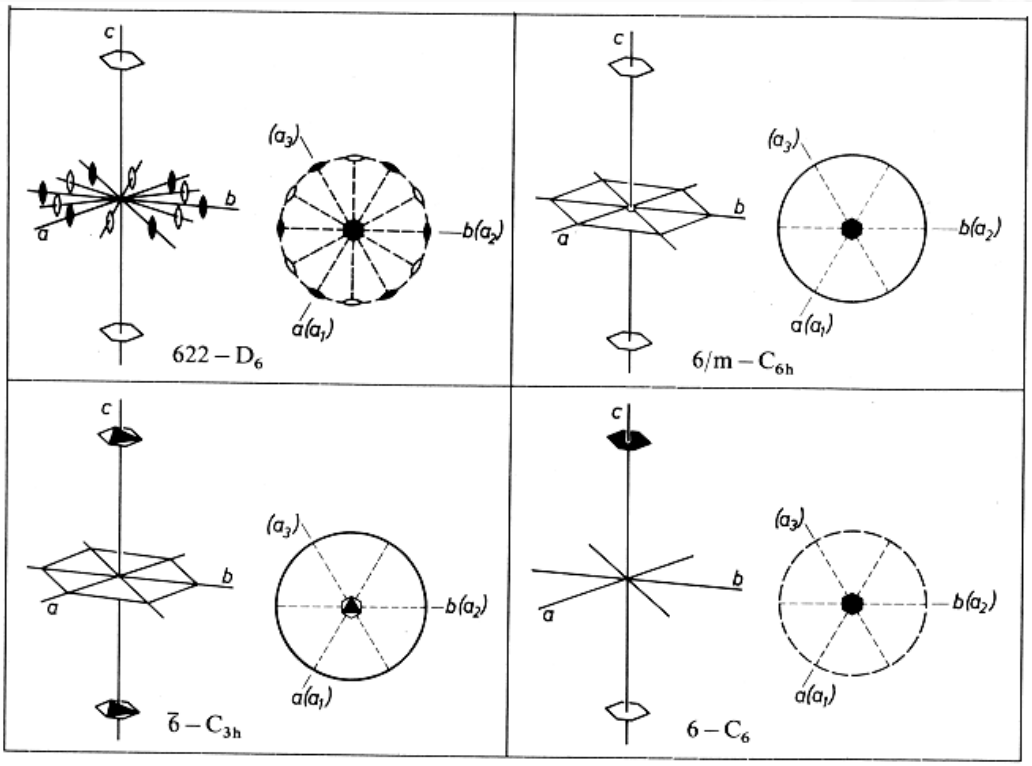
space group: $P\frac{6}{m}\frac{2}{m}\frac{2}{m}$



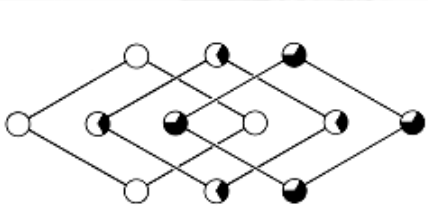


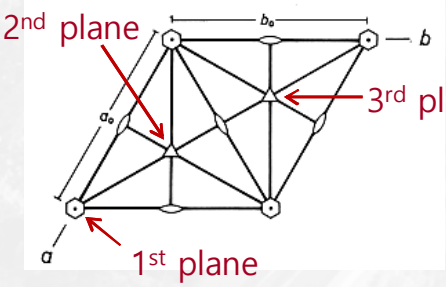
hexagonal point groups of lower symmetry

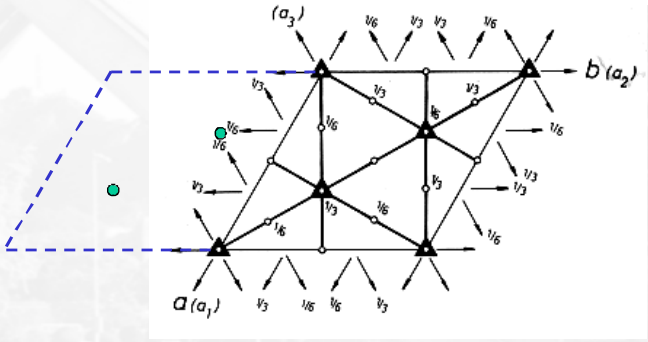
hexagonal point groups of lower symmetry



- start with hexagonal plane lattice
  - ✓ second plane $\frac{1}{3}c_o$ with a lattice point on 3-fold at $\frac{2}{3}, \frac{1}{3}, c_o$
  - ✓ third plane $\frac{2}{3}c_o$ with a lattice point on 3-fold at $\frac{1}{3}, \frac{2}{3}, z$
  - ✓ → reduce 6-fold to 3-fold axis,
    - remove mirrors $x, 0, z;\ 0, y, z;\ x, x, z$
    - remove 2-fold axis // c

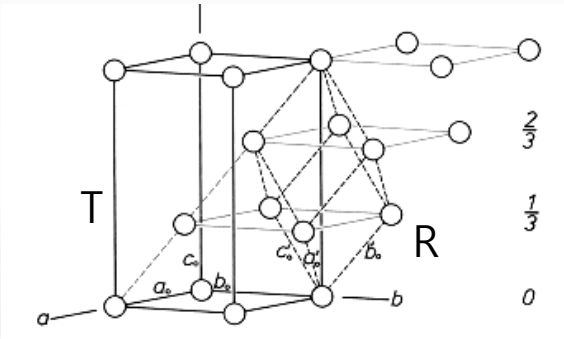


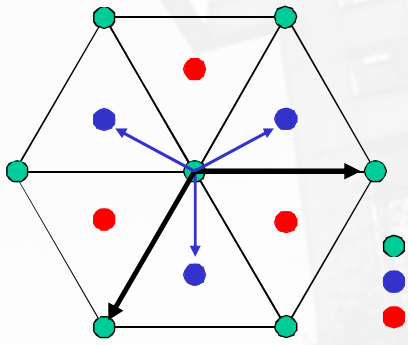




What is the difference between hexagonal and trigonal (rhombohedaral) lattice? Starting 2D mesh is same, but difference in stacking.

- Two unit cells





Trigonal R-lattice

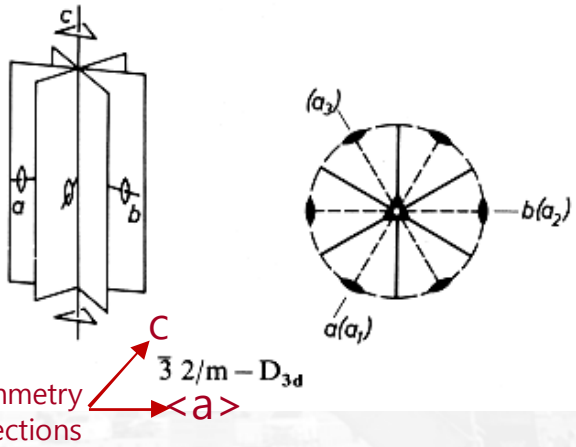
$a_o = b_o \neq c_o$

$\alpha = \beta = 90^o \quad \gamma = 120^o$

Rhombohedral P-lattice

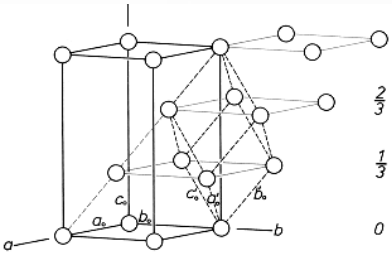
$a_o' = b_o' = c_o'$

$\alpha = \beta = \gamma$



See Hammond page 68 ~74

- Primitive cells of cubic I and cubic F are rhombohedral (Fig 3.2 of Hammond)
- α = 90° → cubic P lattice
- α = 60° → cubic F lattice
- α = 109.47° → cubic I lattice



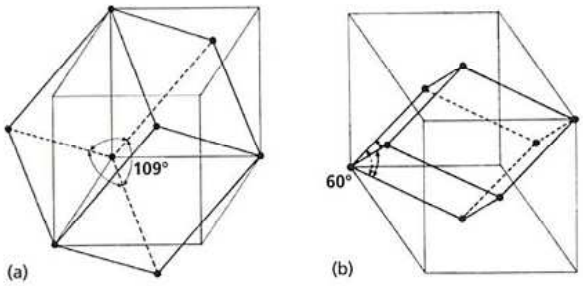
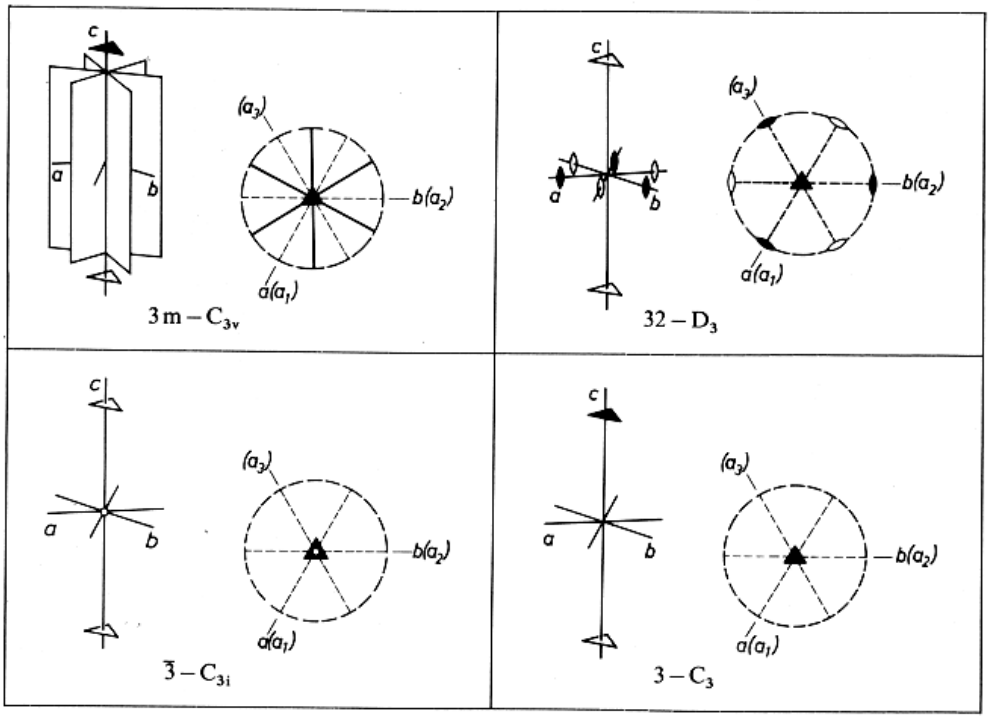


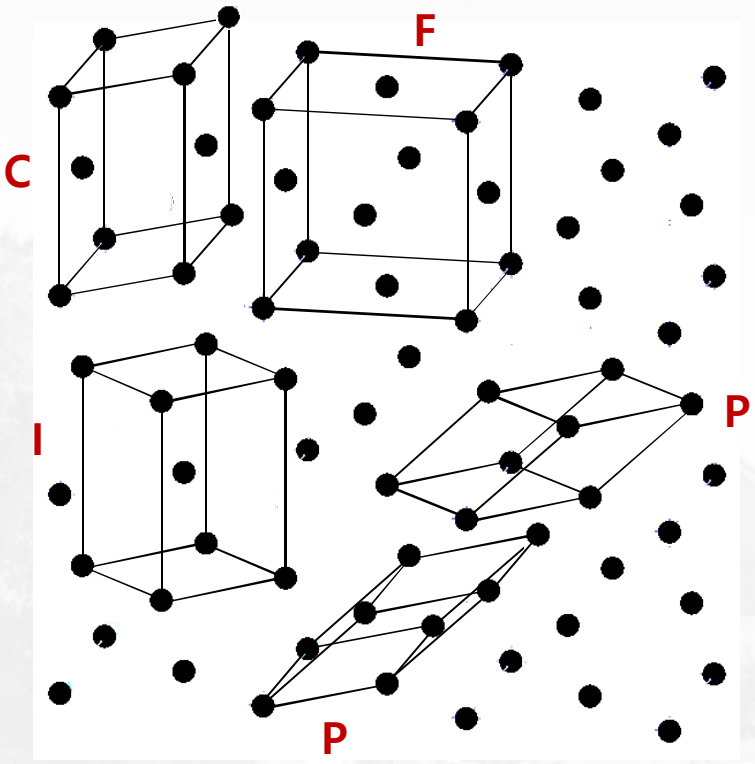
Fig. 3.2. (a) The cubic *I* and (b) the cubic *F* lattices with the primitive rhombohedral cells and inter-axial angles indicated.

- When hexagonal layers of lattice points in the rhombohedral lattice are spaced apart in such a way that α = 90°, 60°, or 109.47°, then cubic symmetry results.
- What is the difference between hexagonal and trigonal (rhombohedaral) lattice?
  - ✓ Hexagonal --- AAAAAA
  - ✓ Rhombohedral --- ABCABC

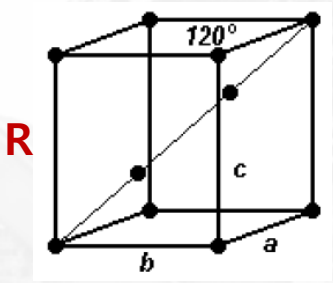


trigonal point groups of lower symmetry

Lattice types - P, I, F, C, R



the number of lattice points in a unit cell?

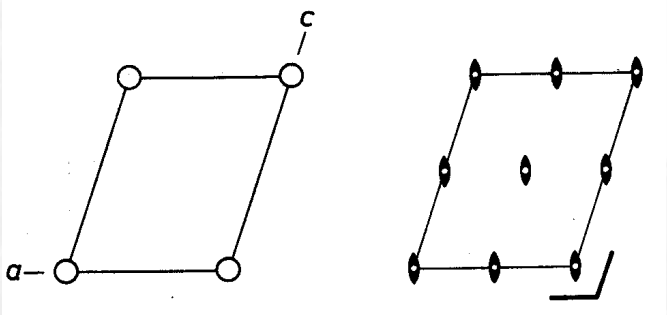


14 Bravais lattice > Non-primitive lattice

➢What happens when we add extra lattice planes into monoclinic P-lattice?

➢ monoclinic P-lattice

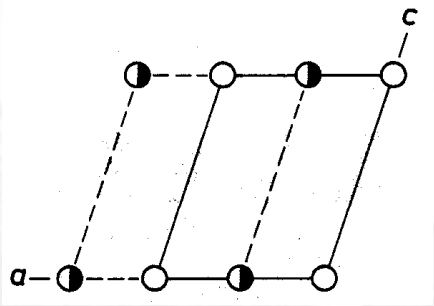
- ✓ lattice point: $\frac{2}{m}$
- ✓ new lattice points to be added also should have 2/m
  - ½,0,0 ; 0,½,0 ; 0,0,½ ; ½,½,0 ; ½,0,½ ; 0,½,½ ; ½,½,½



Consider all the possibilities for introducing extra lattice planes into the monoclinic P lattice (next 3 slides) → all these can be represented as P or C lattice

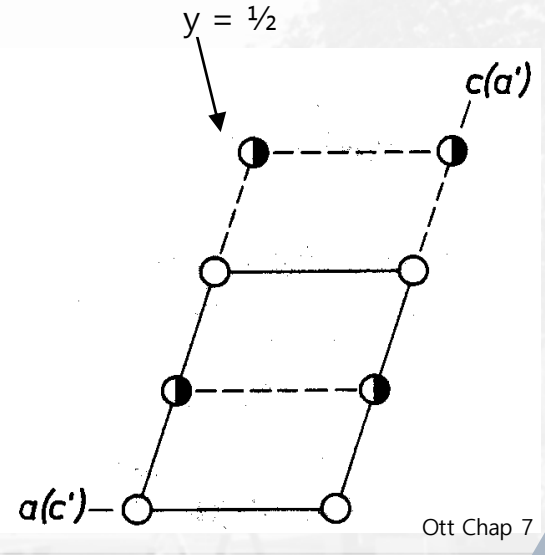
➢ Introduce extra lattice planes into monoclinic P-lattice

(a) new lattice point @ ½,½,0 → C-centered lattice or C-lattice

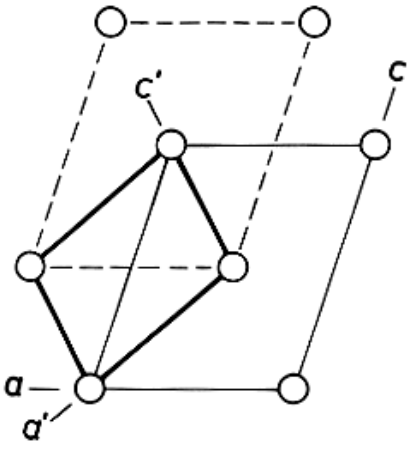


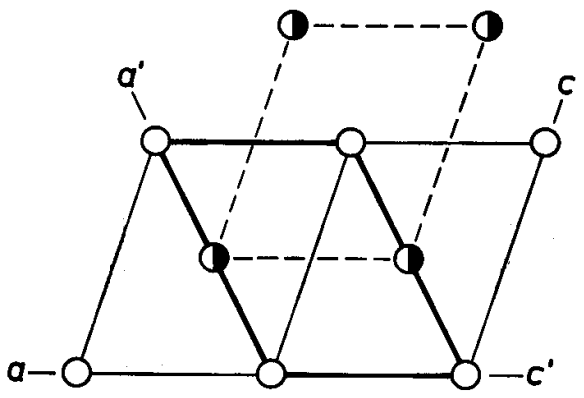
(b) @ 0,½,½ → A-lattice → C-lattice

(a & c can be swapped)



(c) at ½,0,½ → B-lattice → smaller primitive unit cell (P-lattice)



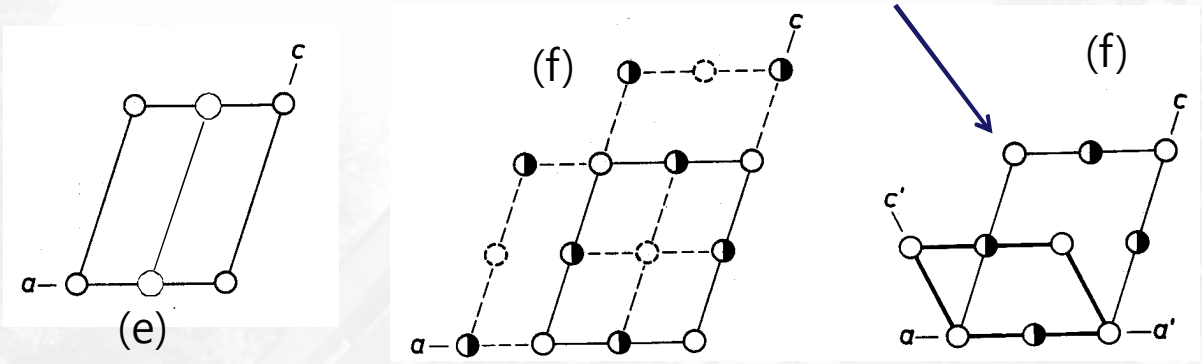


(d) at ½,½,½ → I-lattice → C-lattice

➢ monoclinic lattice

(e) at ½,0,0; 0,½,0 or 0,0,½ → half the cell → P-lattice

(f) at ½,½,0 & 0 ½,½ → further lattice point @ ½,0,½ (because all lattice points should have the same environment) → F-lattice → can be reduced to C-lattice of half the volume



➢In last 3 slides, considered all the possibilities for having non-primitive monoclinic lattice → P or C monoclinic lattice can exist

➢monoclinic lattice can only be either P or C

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

➢ The 14 Bravais lattice represent the 14 and only way in which it is possible to fill space by a 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.

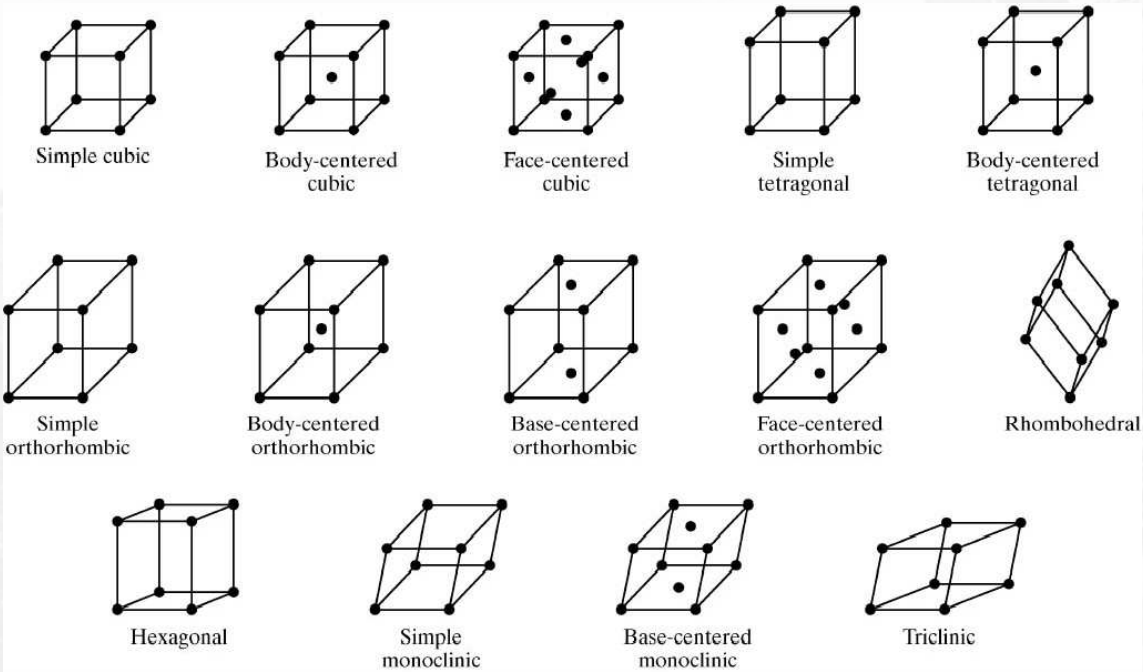
➢ **Number of lattice is fixed at 14.**

➢ **Infinite number of arranging atoms in a cell ← basis**

Symmetry directions

Xtal systems	Symmetry directions			Axial system
Triclinic				a1 ≠ a2 ≠ a3, α ≠ β ≠ γ ≠ 90°
Monoclionic	b			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°

14 Bravais lattice



Numbers & coordinates of the lattice points in the unit cells of the Bravais lattices

Lattice	No. of lattice points in unit cell	Coordinates of lattice points in unit cell
P	1	$0,0,0$
A	2	$0,0,0;\ 0,\frac{1}{2},\frac{1}{2}$
B	2	$0,0,0;\ \frac{1}{2},0,\frac{1}{2}$
C	2	$0,0,0;\ \frac{1}{2},\frac{1}{2},0$
I	2	$0,0,0;\ \frac{1}{2},\frac{1}{2},\frac{1}{2}$
R	3	$0,0,0;\ \frac{2}{3},\frac{1}{3},\frac{1}{3},\ \frac{1}{3},\frac{2}{3},\frac{2}{3}$
F	4	$0,0,0;\ \frac{1}{2},\frac{1}{2},0;\ \frac{1}{2},0,\frac{1}{2};\ 0,\frac{1}{2},\frac{1}{2}$

7 Xtal systems	a, b, c, α, β, γ	**14 Bravais lattice**	Lattice symbol
Cubic	a = b = c α = β = γ = 90°	Simple	P
		Body-centered	I
		Face-centered	F
Tetragonal	a = b ≠ c α = β = γ = 90°	Simple	P
		Body-centered	I
Orthorhombic	a ≠ b ≠ c α = β = γ = 90°	Simple	P
		Body-centered	I
		Base-centered	C
		Face-centered	F
Rhombohedral	a = b = c, α = β = γ < 120° , ≠ 90°	Simple	R
Hexagonal	a = b ≠ c, α = β = 90° , γ = 120°	Simple	P
Monoclinic	a ≠ b ≠ c, α = γ = 90° ≠ β	Simple	P
		Base-centered	C
triclinic	a ≠ b ≠ c, α ≠ β ≠ γ ≠ 90°	Simple	P

Table 8.9. Characteristic symmetry elements of the seven crystal systems

Crystal system	32 Point groups[a]	Characteristic symmetry elements
Cubic	$4/m\ \bar{3}\ 2/m$ $\bar{4}3m, 432, 2/m\bar{3}, 23$	4 ▲
Hexagonal	$6/m\ 2/m\ 2/m$ $\bar{6}m2, 6mm, 622,$ $6/m, \bar{6}, 6$	⬢ or ⬟
Tetragonal	$4/m\ 2/m\ 2/m$ $\bar{4}2m, 4mm, 422,$ $4/m, \bar{4}, 4$	1 ■ or 1 ◪ (3 ■ or 3 ◪ ⇒ cubic)
Trigonal	$\bar{3}\ 2/m$ $3m, 32, \bar{3}, 3$	1 ▲ (remember that m normal to 3 gives $\bar{6}$ → hexagonal
Orthorhombic	$2/m\ 2/m\ 2/m$ $mm2, 222$	2 and/or m in three orthogonal directions
Monoclinic	$2/m$ $m, 2$	2 and/or m in one direction
Triclinic	$\bar{1}$ 1	$\bar{1}$ or 1 only

[a] Characteric symmetry elements are underlined.

todos

- Read
  - ✓ Ott Chapter 7, 8
  - ✓ Krawitz Chapter 1.1 ~ 1.5
  - ✓ Hammond Chapter 2.1 ~ 2.4; 3.1 ~ 3.3; 5.1 ~ 5.6
  - ✓ Sherwood & Cooper Chapter 3.1~3.7

- Bravais HW (due in 1 week)
  - ✓ Hammond 1.9; 3.1, 3.2