Lecture 1
Crystal Structure

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Chapter 4
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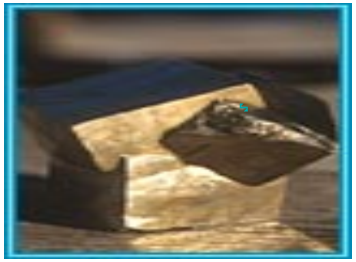
ELEMENTARY CRYSTALLOGRAPHY

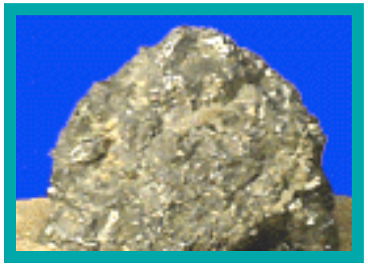
SOLID MATERIALS

CRYSTALLINE



LONG RANGE ORDER

AMORPHOUS (NON-CRYSTALLINE)



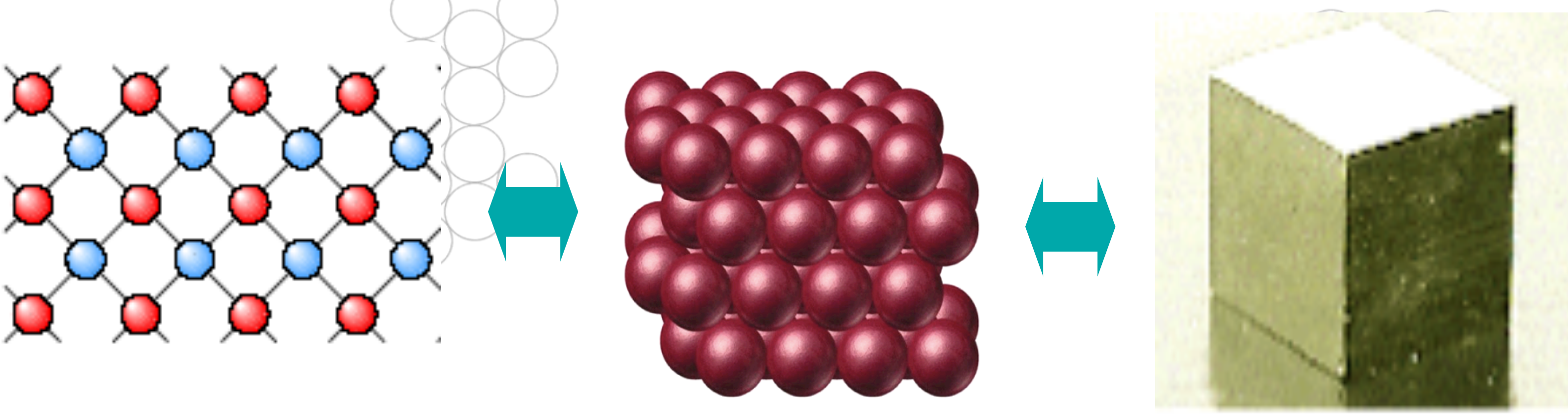
SHORT RANGE ORDER

Glass, plastic, and gel

- *Distinguished by size of ordered region.*
- *Structure of materials decides mechanical, thermal , electrical and magnetic properties.*
- ***Crystal is a solid composed of atoms or other microscopic particles arranged in an orderly repetitive array***

Crystalline Solid

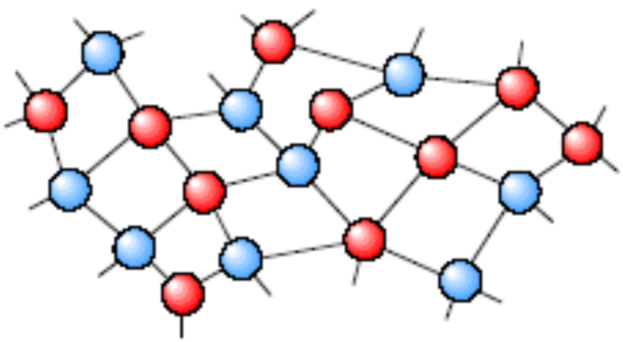
- <u>Crystalline Solid</u> is the solid form of a substance in which the *atoms or molecules* **are arranged in a definite, repeating pattern in three dimension.**
- **Single crystals, ideally have a high degree of order, or regular geometric periodicity, throughout the** ***entire volume of the material*****.**

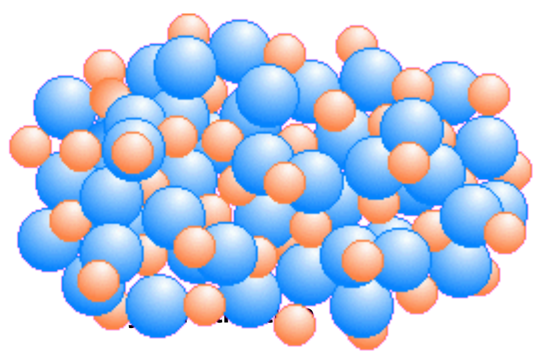


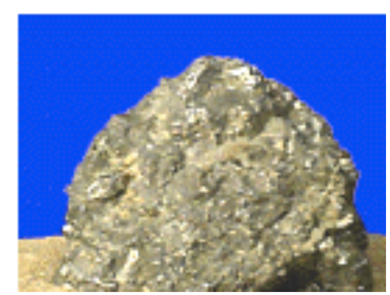
(a) Crystalline solid

Amorphous Solid

- **Amorphous (Non-crystalline) Solid** is composed of randomly orientated atoms , ions, or molecules that do not form defined patterns or lattice structures.
- **Amorphous materials have order only within a few atomic or molecular dimensions.**
- **Amorphous materials do not have any long-range order, but they have varying degrees of short-range order.**
- **Examples to amorphous materials include amorphous silicon, plastics, and glasses.**
- **Amorphous silicon can be used in solar cells and thin film transistors.**

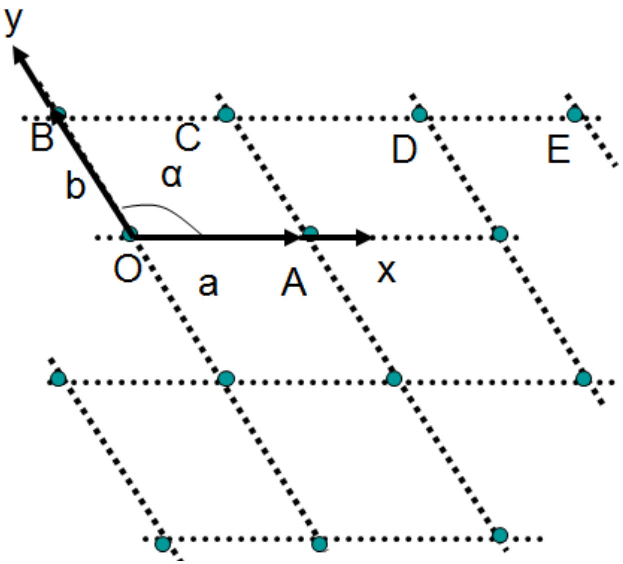






Crystal Lattice

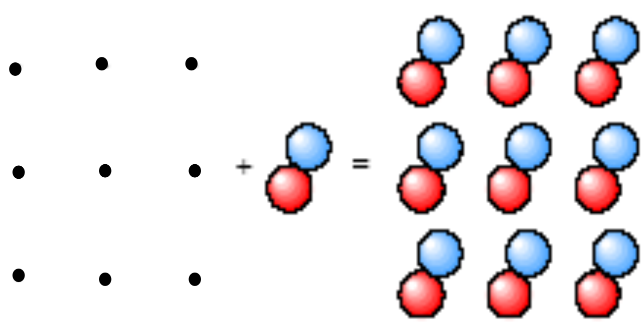
- An infinite periodic array of imaginary points in space with identical surroundings →Lattice points



Crystal Structure

- *Crystal structure can be obtained by attaching atoms, groups of atoms or molecules which are called basis to the lattice sides of the lattice point.*

Crystal Structure = Crystal Lattice • + Basis 

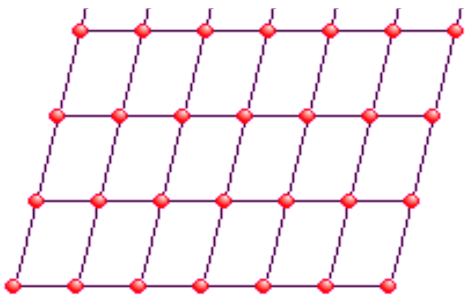


Ex : 1. Cu and Na *(basis is a single atom)*
2. NaCl, CsCl *(basis is diatomic)*
3. CaF_2 *(basis is triatomic)*

Crystal Lattice

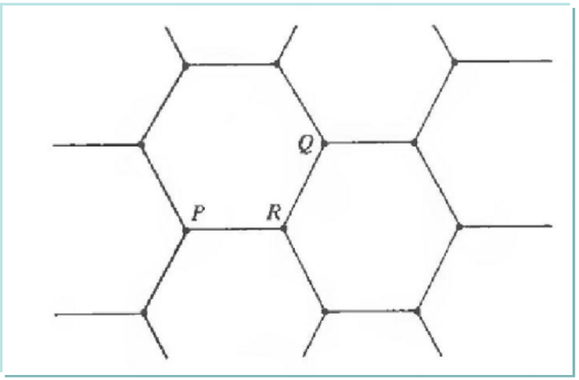
Bravais Lattice (BL)

- *All atoms are of the same kind*
- *All lattice points are equivalent*



Non-Bravais Lattice (non-BL)

- *Atoms can be of different kind*
- *Some lattice points are not equivalent*
- *A combination of two or more BL*



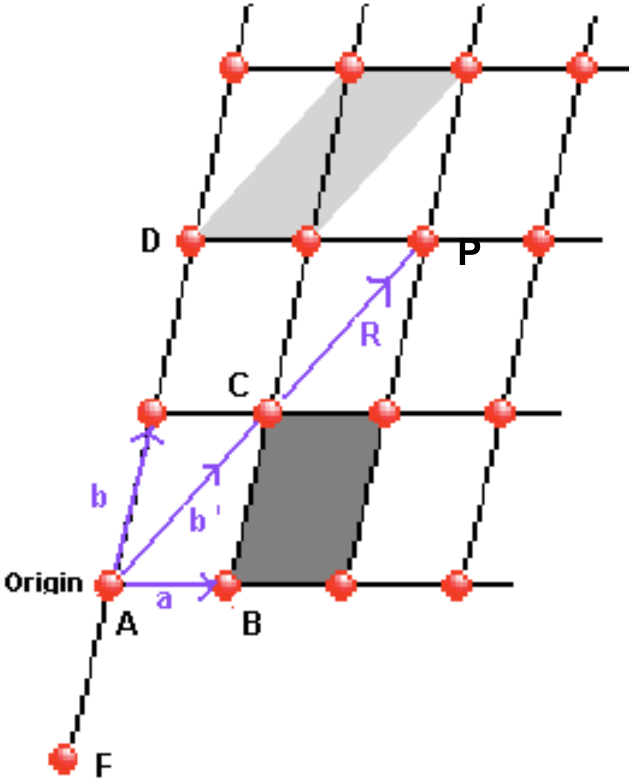
Bravais lattice:

Translational & orientational (rotational) symmetry

Non-Bravais (Space) Lattice:

Only translational symmetry.

Translational Lattice Vectors – 2D



Point D(n1, n2) = (0,2)

Point F (n1, n2) = (0,-1)

*What is **T** for point **P** in terms of **a,b** and **b'**?*

A space lattice is a set of points such that a translation from any point in the lattice by a vector;

$$\vec{T} = n_1\vec{a} + n_2\vec{b} \qquad \text{In 2-D}$$

$$\vec{T} = n_1\vec{a} + n_2\vec{b} + n_3\vec{c} \qquad \text{In 3-D}$$

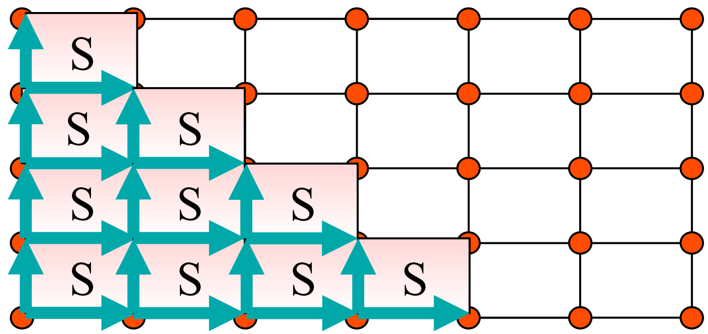
locates an exactly equivalent point, i.e. a point with the same environment as P . This is translational symmetry. The vectors a, b are known as lattice vectors and (n_1, n_2, n_3) is a pair of integers whose values depend on the lattice point.

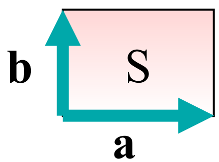
- *The two vectors a and b form a set of lattice vectors for the lattice.*
- ***The choice of lattice vectors is not unique**. Thus one could equally well take the vectors a and b' as a lattice vectors.*

Unit Cell in 2D (Building block)

- *The smallest component of the crystal (group of atoms, ions or molecules), which when stacked together with pure translational repetition reproduces the whole crystal.*

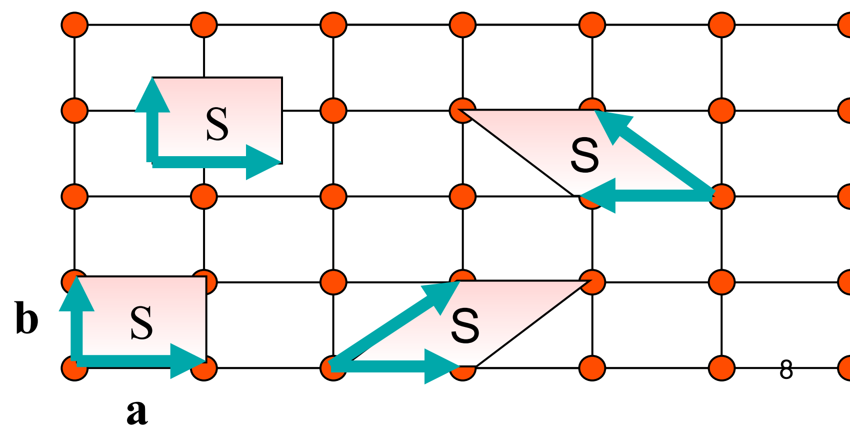
2D-Crystal



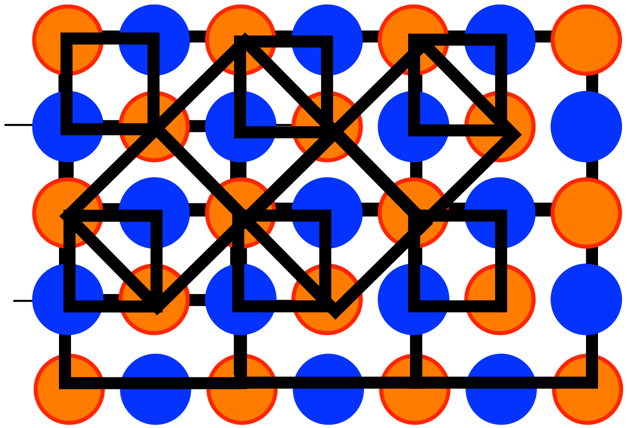


Unit Cell

The choice of unit cell is not unique.



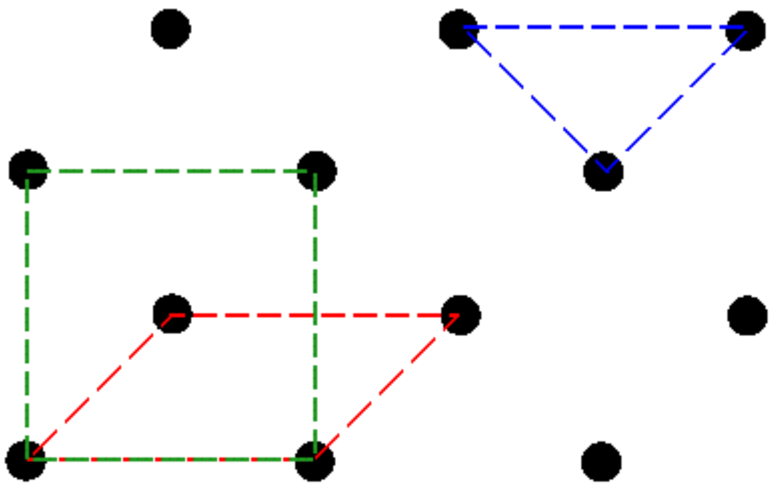
2D Unit Cell example -(NaCl)



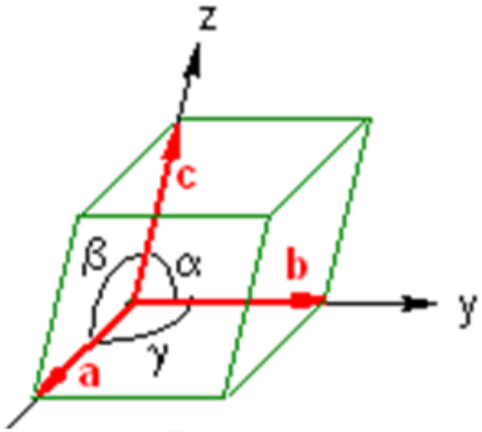
We define **lattice points** ; these are points with *identical environments*

In 2D, this IS a unit cell
In 3D, it is NOT

Which one is not a unit cell.
Why can't the blue triangle be a unit cell?



Unit Cell



- The unit cell and, consequently, the entire lattice, is *uniquely* determined by the six lattice constants: a, b, c are lattice parameters in x, y, and z directions **respectively**. α, β and γ are angle between bc, ca and ab.
- Only 1/8 of each lattice point in a unit cell can actually be assigned to that cell.
- Each unit cell in the figure can be associated with 8 x 1/8 = 1 lattice point.

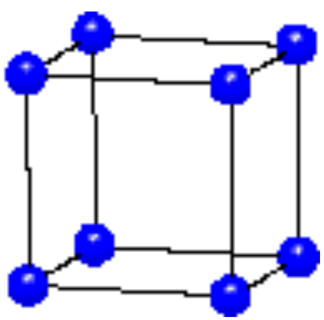
UNIT CELL

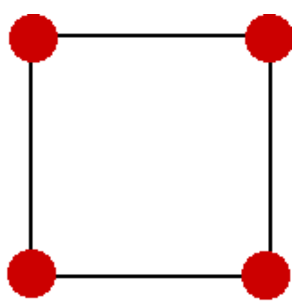
Primitive

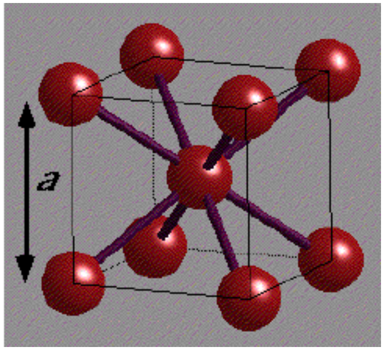
- Single lattice point per cell
- Smallest area in 2D, or
- Smallest volume in 3D

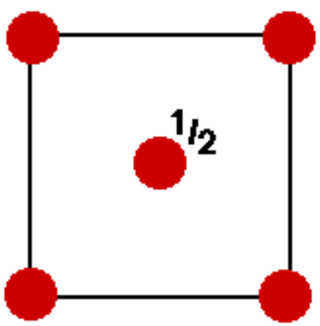
Conventional & Non-primitive

- More than one lattice point per cell
- Integral multibles of the area of primitive cell









Simple cubic(sc)

Conventional = Primitive cell

Body centered cubic(bcc)

Conventional ≠ Primitive cell

Primitive Unit Cell

- The primitive unit cell must have only one lattice point.
- There can be <u>different choices</u> for lattice vectors , <u>but the volumes of these primitive cells are all the same.</u>

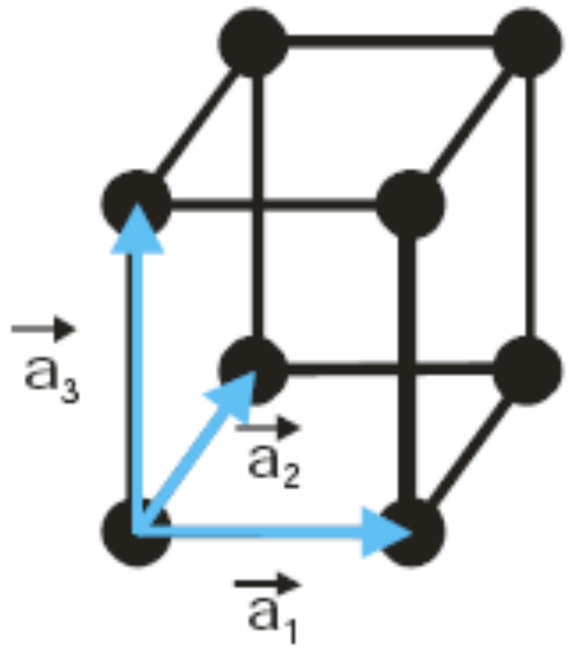
P = Primitive Unit Cell
NP = Non-Primitive Unit Cell

Primitive Unit Cell and vectors

- A primitive unit cell is made of primitive translation vectors a_1 ,a_2, and a_3 such that there is no cell of smaller volume that can be used as a building block for crystal structures.

- A primitive unit cell will fill space by repetition of suitable crystal translation vectors. This defined by the parallelepiped a_1, a_2 and a_3. The volume of a primitive unit cell can be found by

- $V = a_1.(a_2 \times a_3)$ (vector products)



Cubic cell volume = a^3

TYPICAL CRYSTAL STRUCTURES

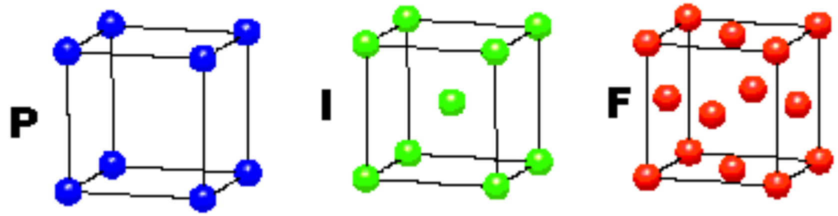
- There are only seven different shapes of unit cell which can be stacked together to completely fill all space (in 3 dimensions) without overlapping. This gives the *seven crystal systems*, in which all crystal structures can be classified.

- *Cubic Crystal System (SC, BCC,FCC)*
- *Hexagonal Crystal System (S)*
- *Triclinic Crystal System (S)*
- *Monoclinic Crystal System (S, Base-C)*
- *Orthorhombic Crystal System (S, Base-C, BC, FC)*
- *Tetragonal Crystal System (S, BC)*
- *Trigonal (Rhombohedral) Crystal System (S)*

3D – 14 BRAVAIS LATTICES AND THE SEVEN CRYSTAL SYSTEM

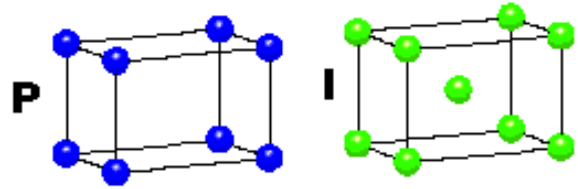
CUBIC

$a = b = c$
$\alpha = \beta = \gamma = 90°$



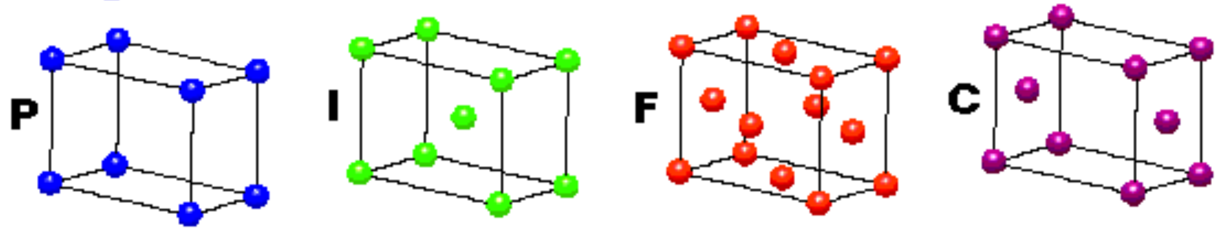
TETRAGONAL

$a = b \neq c$
$\alpha = \beta = \gamma = 90°$



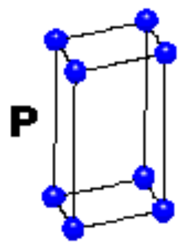
ORTHORHOMBIC

$a \neq b \neq c$
$\alpha = \beta = \gamma = 90°$



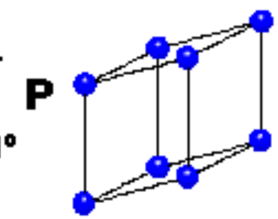
HEXAGONAL

$a = b \neq c$
$\alpha = \beta = 90°$
$\gamma = 120°$



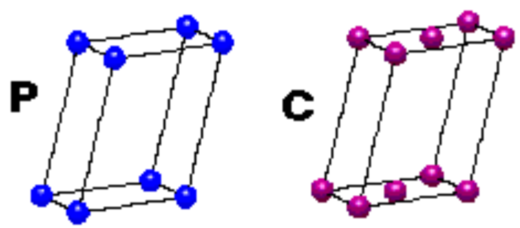
TRIGONAL

$a = b = c$
$\alpha = \beta = \gamma \neq 90°$



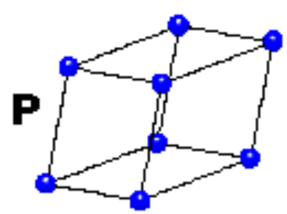
MONOCLINIC

$a \neq b \neq c$
$\alpha = \gamma = 90°$
$\beta \neq 120°$



TRICLINIC

$a \neq b \neq c$
$\alpha \neq \beta \neq \gamma \neq 90°$



4 Types of Unit Cell
P = Primitive
I = Body-Centred
F = Face-Centred
C = Side-Centred
+
7 Crystal Classes
→ 14 Bravais Lattices