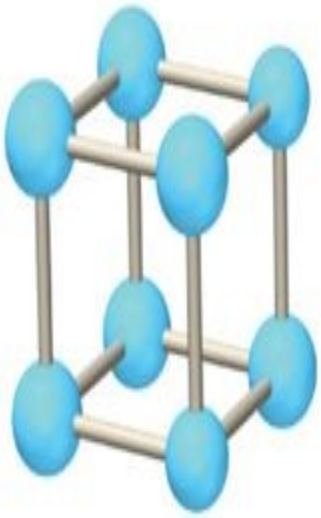
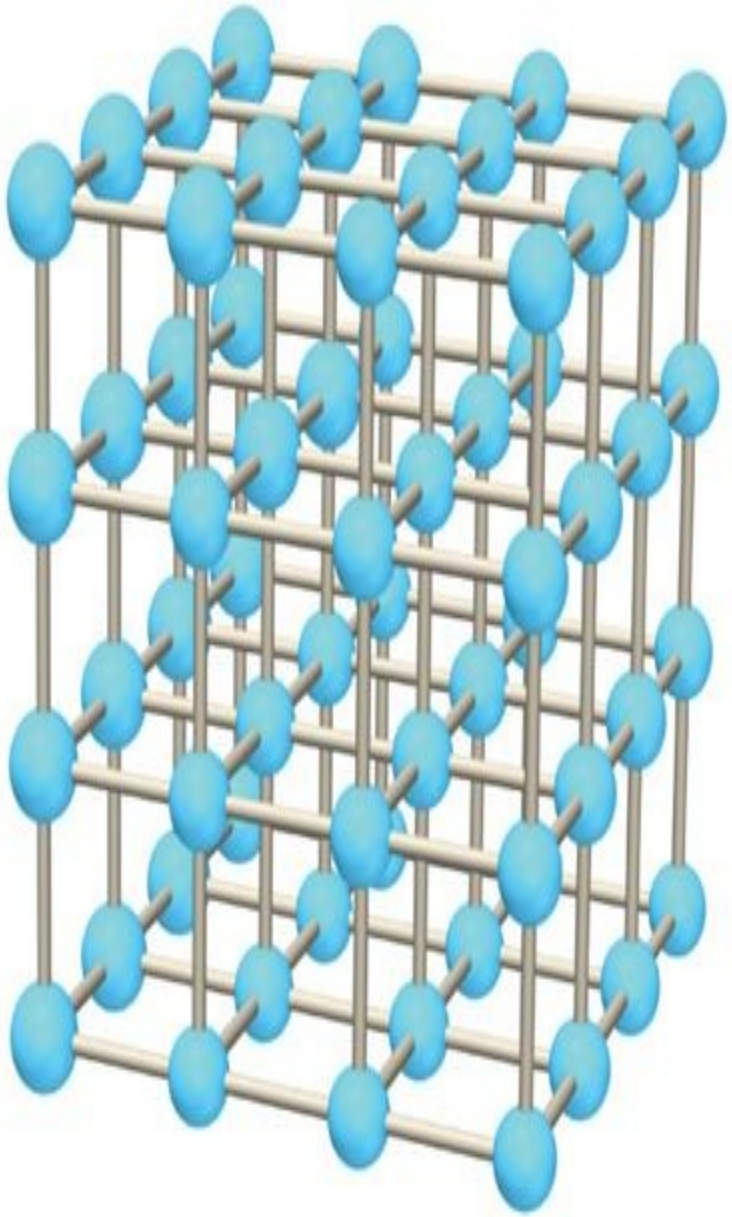
STRUCTURE OF MATTER

UNIT CELL, BRAVAIS LATTICE

- Primitive & Non-primitive Unit cells
- Different Lattice symbols
- Total no. of atoms in different unit cells
- Bravais lattice in three-dimensions



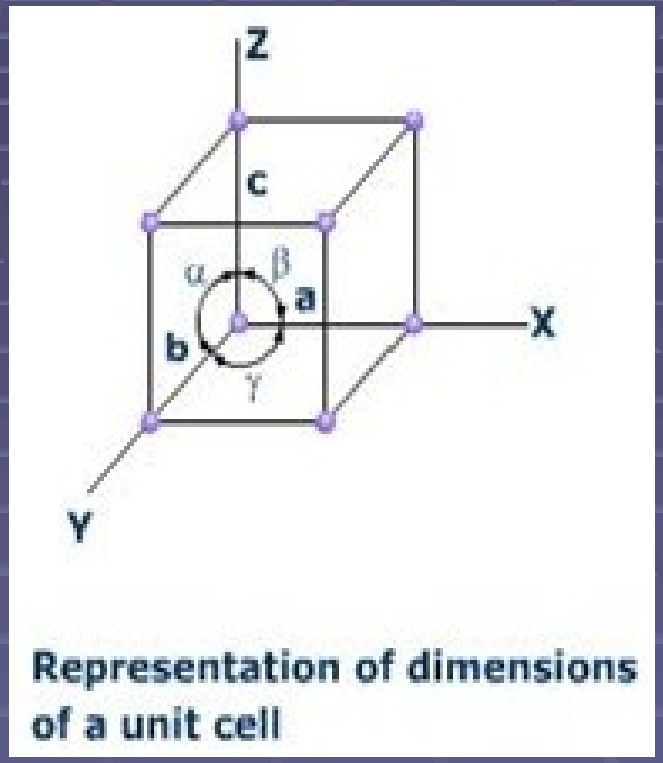
(a) Unit cell



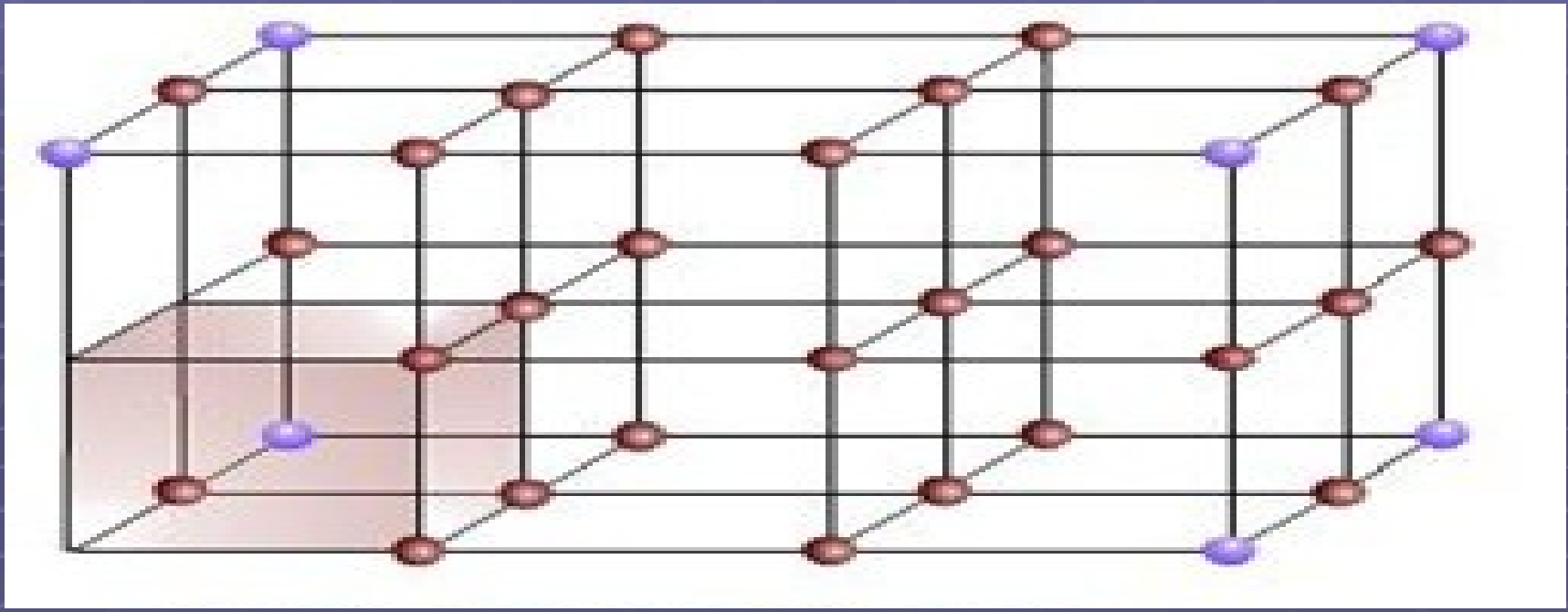
(b) Crystal Structure

Lattice Parameters

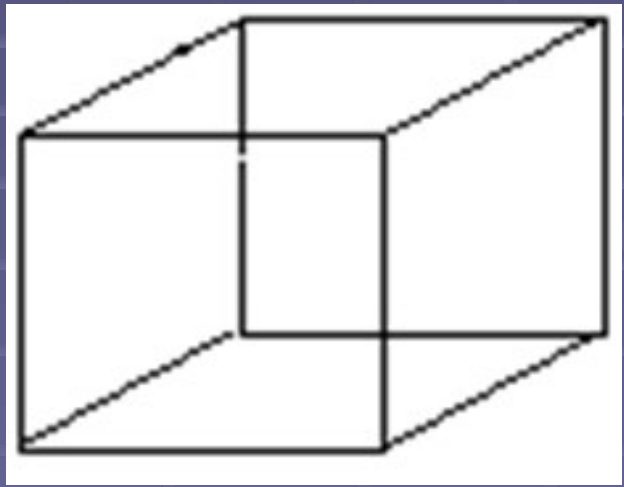
- **The three sides of a unit cell are called the *crystallographic axes.* The angles between the three axes α, β and γ are called the axial angles.**
- **The intercepts *a, b, c* define the dimensions of a unit cell and are known as *lattice parameters of the unit cell*.**



Representation of dimensions of a unit cell

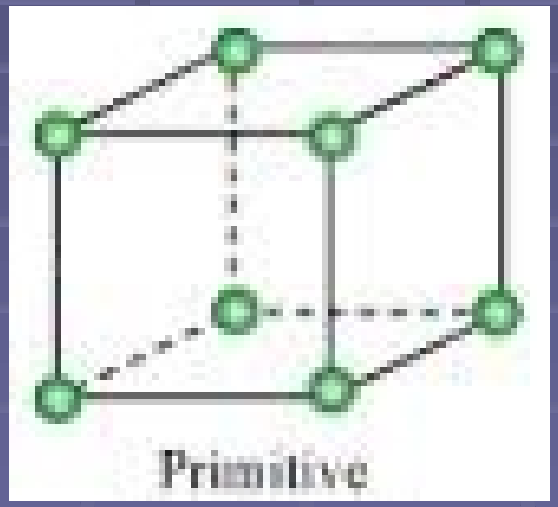


A parallelepiped shaped volume which reproduced by close packing in three dimension gives the whole crystal, is called the unit cell.



Primitive Unit cell

- **The unit cell occupying the smallest volume in a given lattice is called the primitive unit cell.**
- **It contains only one lattice point.**



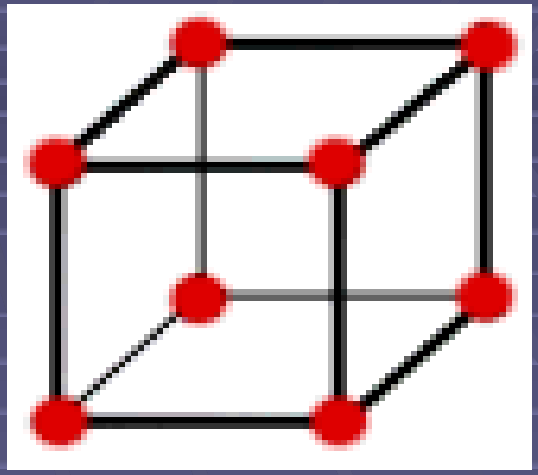
Non-Primitive unit cell: **The unit cell which is larger than the minimum volume unit cell is defined as a non-primitive unit cell. A non-primitive unit cell contains more than one lattice point. The volume of a non-primitive unit cell is an integral multiple of a primitive cell.**

Distinguish between primitive unit cell & unit cell:

Primitive Cell	*Unit Cell*
1. The unit cell occupying the smallest volume in a given lattice is called the primitive unit cell.	1. A parallelepiped shaped volume, which reproduced by close packing in three dimensions gives the whole crystal is called the unit cell.
2. It always contains only one lattice point.	2. It may contain more than one lattice point.
3. A primitive cell is the smallest cell in crystal. A cell smaller than it is never possible.	3. A unit cell may be smallest or not.
4. It is always a unit cell.	4. But a unit cell is not always a primitive cell.

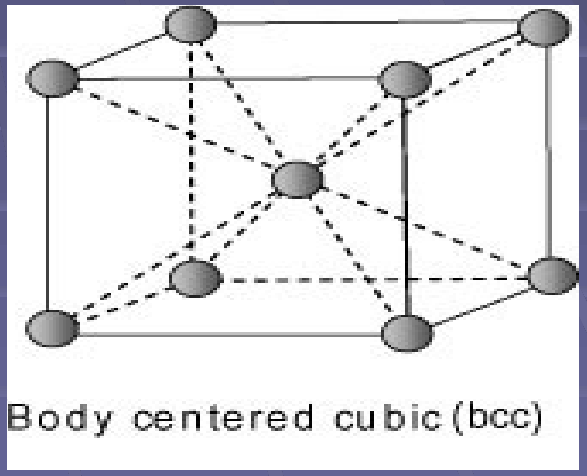
Lattice Symbols

'P': ***It*** **means the primitive cell where lattice points are at the corners of the cell. A primitive cell is always a unit cell.**



Simple cubic (sc)

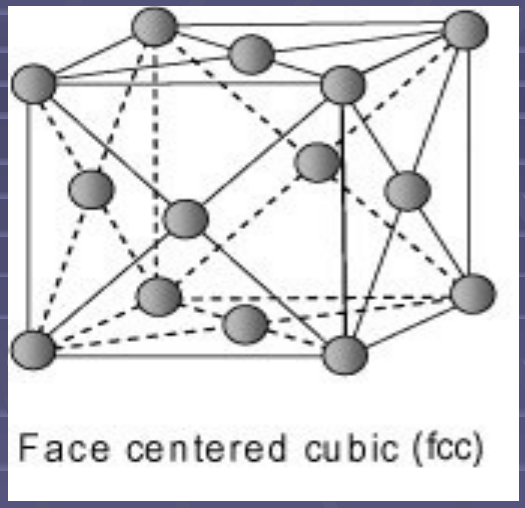
'I': **It means the body centered lattice. In the body centered lattice, the lattice points are at the corners and inside the cell.**



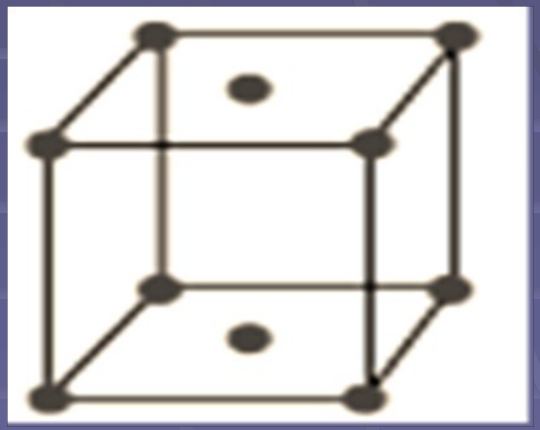
Body centered cubic (bcc)

Lattice Symbols

'F': ***It*** **means the face-centered lattice. In the face centered lattice, the lattice points are at the corners and all the faces centered.**



'C': **It means the lattice is base centered or C-face centered. In the base centered lattice, the lattice points are at the corners and at the face centered of opposite sides.**



(bcc)

Total Number of atoms in different unit cells

The formula for the total number of atoms in a unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where, N_i = Points inside the cell

N_f = Points on the faces

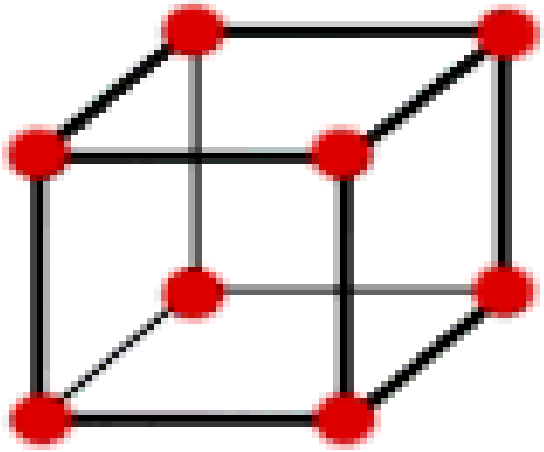
N_c = Points at the corners

Primitive cell: For a primitive cell, the lattice points are at the eight corners of the cell. So for primitive cell $N_i = 0$, $N_f = 0$ *and* $N_c = 8$.

Thus the total number of atoms in a primitive cell is

$$N = 0 + \frac{0}{2} + \frac{8}{8} = 1$$

So, the primitive cell has only one lattice point.



Total Number of atoms in different unit cells

The formula for the total number of atoms in a unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where, N_i = Points inside the cell

N_f = Points on the faces

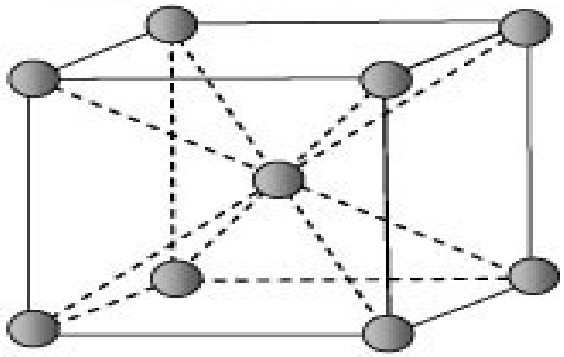
N_c = Points at the corners

Body centered cubic: For a body centered cubic lattice, the lattice points are at the eight corners and inside the cell. So, for body centered cubic lattice $N_i = 1$, $N_f = 0$ *and* $N_c = 8$.

Thus the total number of atoms in body centered cubic lattice is

$$N = 1 + \frac{0}{2} + \frac{8}{8} = 2$$

So, the body centered cubic lattice has only two lattice points.



Body centered cubic (bcc)

Total Number of atoms in different unit cells

The formula for the total number of atoms in a unit cell is

$$N = N_i + \frac{N_f}{2} + \frac{N_c}{8}$$

Where, N_i = Points inside the cell

N_f = Points on the faces

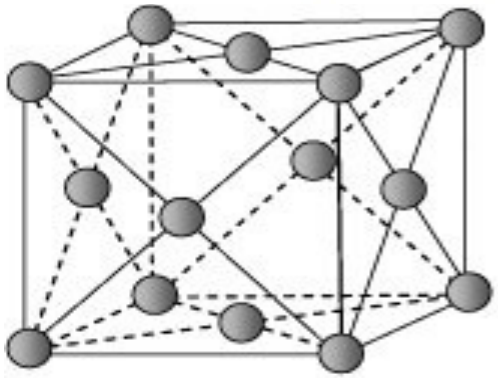
N_c = Points at the corners

Face-centered cubic: For a face centered cubic lattice, the lattice points are at the eight corners and all (six) the faces centered. So, for face centered cubic lattice $N_i = 0$, $N_f = 6$ *and* $N_c = 8$.

Thus the total number of atoms in a face centered cubic lattice is

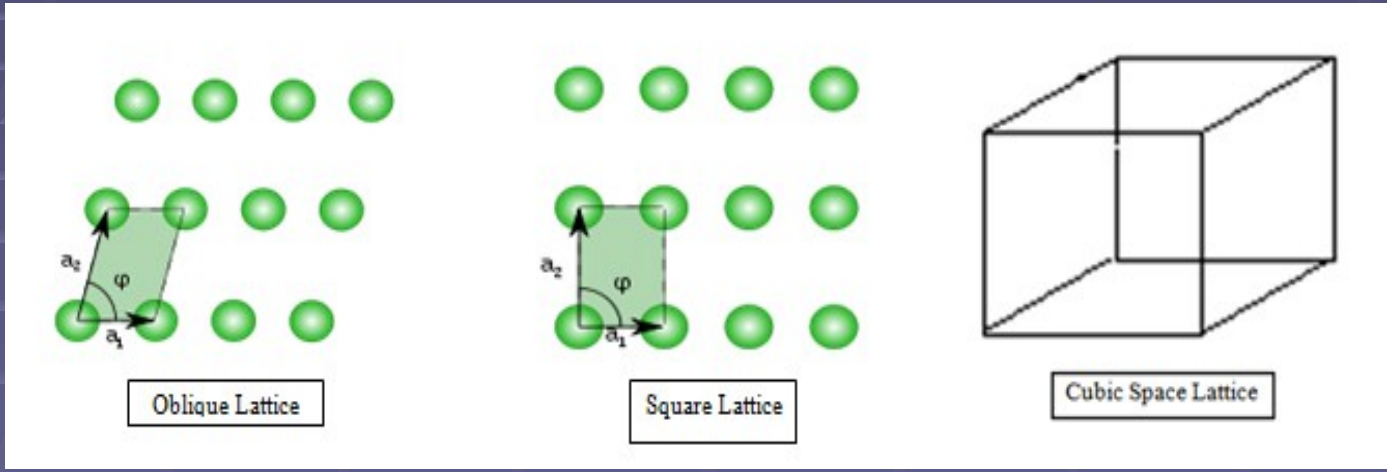
$$N = 0 + \frac{6}{2} + \frac{8}{8} = 4$$

So, the face centered cubic lattice has only four lattice points.



Face centered cubic (fcc)

Bravais lattice: **There are various ways of positioning points (lattice) in space such that all points have same identical surroundings, *i.e.* all points are of same kind and equivalent. These lattices are known as Bravais lattices. Bravais showed that, there exist no more than 14 space lattices in three dimensions. In order to specify the arrangements of points in a space lattice, he introduced 7-system of axes or crystal system.**



Non-Bravais lattice: **All points are not identical compared to each other known as non-Bravais lattices.**

Seven crystal system

The names of seven crystal system are: Triclinic, Monoclinic, Orthorhombic, Tetragonal, Cubic, Trigonal and Hexagonal.

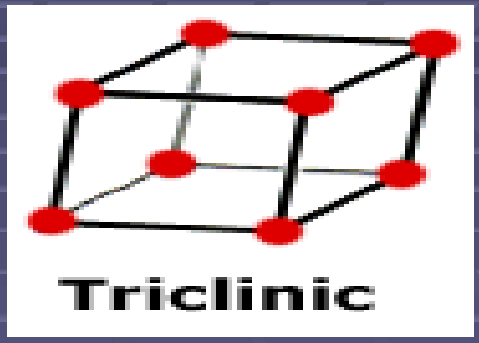
Restrictions on conventional cell axex and angles:

System	No. of lattice in the system	Lattice Symbol	Restrictions on	
			Conventional cell axes	Conventional axial angles
Triclinic	1	P	$a \neq b \neq c$	$\alpha \neq \beta \neq \gamma$
Monoclinic	2	P, C	$a \neq b \neq c$	$\alpha = \gamma = \frac{\pi}{2} \neq \beta$
Orthorhombic	4	P, C, I, F	$a \neq b \neq c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$
Tetragonal	2	P, I	$a = b \neq c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$
Cubic	3	P, I, F	$a = b = c$	$\alpha = \beta = \gamma = \frac{\pi}{2}$
Trigonal	1	R	$a = b = c$	$\alpha = \beta = \gamma < \frac{2\pi}{3} \neq \frac{\pi}{2}$
Hexagonal	1	P	$a = b \neq c$	$\alpha = \beta = \frac{\pi}{2}, \gamma < \frac{2\pi}{3}$

Triclinic: **In the triclinic system, the single lattice type has a primitive unit cell (P) with three crystallographic axes of unequal lengths and unequal angles between them. *i.e.***

$$a \neq b \neq c$$

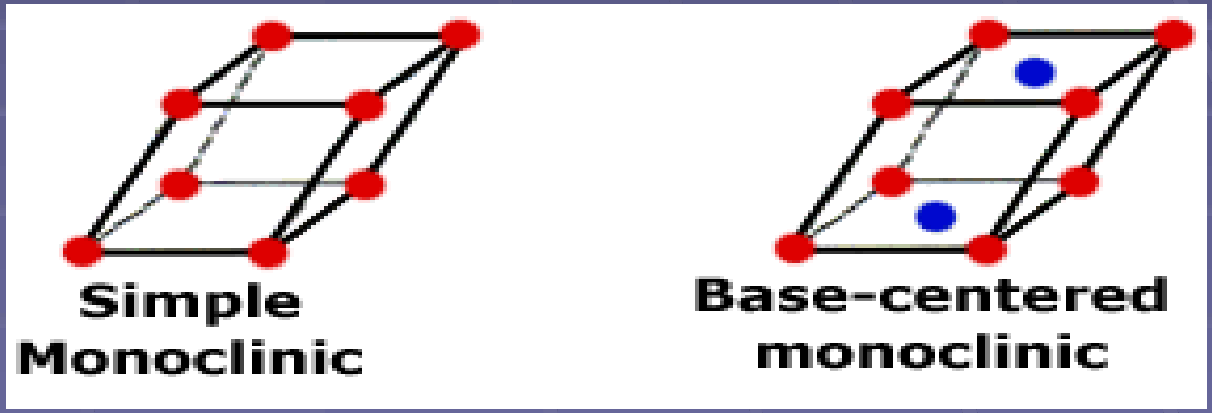
$$\alpha \neq \beta \neq \gamma$$



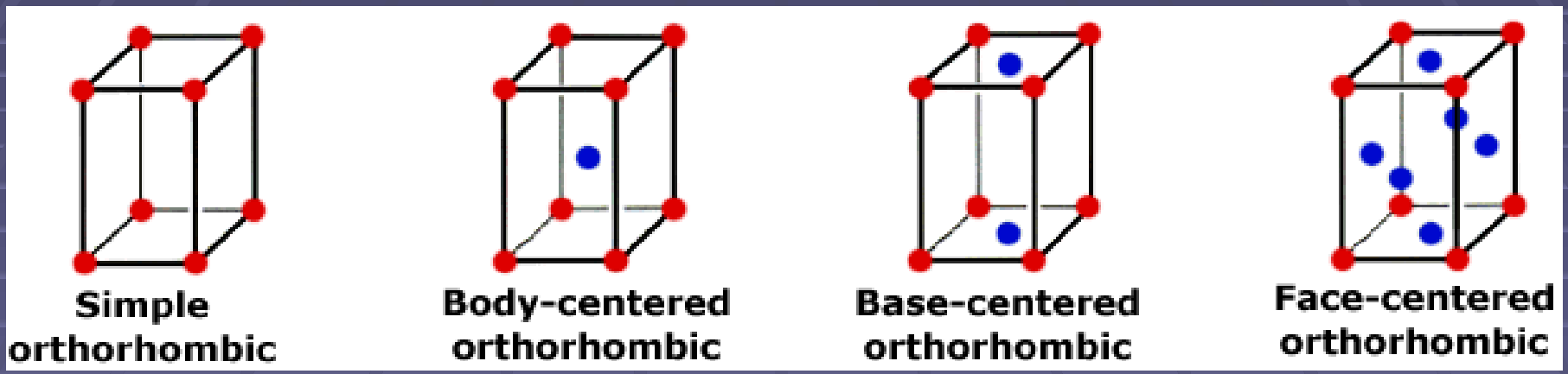
Monoclinic: **In the monoclinic system, there are two lattice types: one with a primitive unit cell (P) and other with a non-primitive conventional cell which may be base centred (C) with the lattice point at the centre of the rectangular cell faces. Where**

$$a \neq b \neq c$$

$$\alpha = \gamma = \frac{\pi}{2} \neq \beta$$

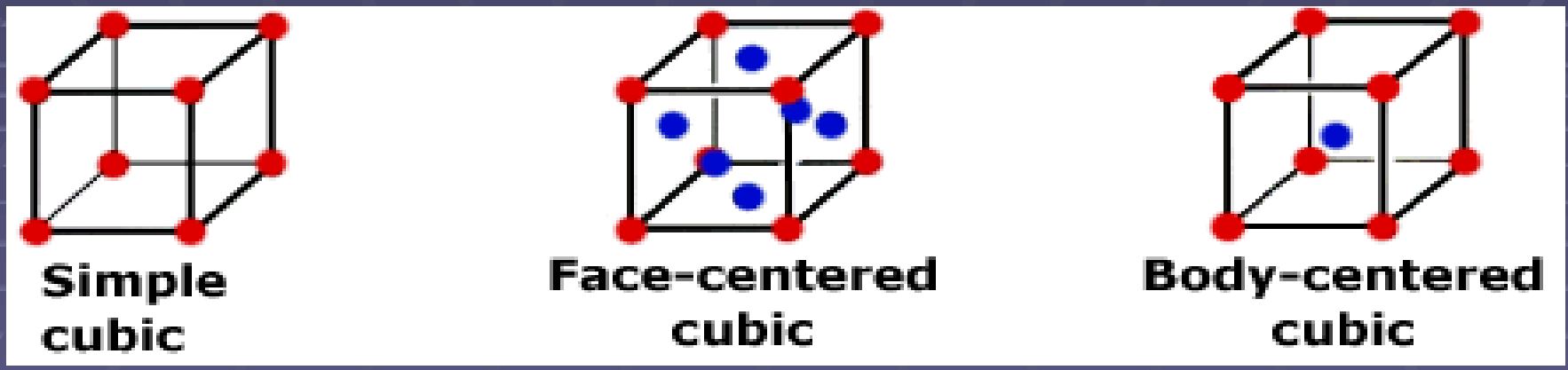


Orthorhombic: In the orthorhombic system, there are four lattice types: one lattice has a primitive unit cell (P), one lattice is base centered (C), one lattice is body centered (I), and one lattice is face centered (F). Here, $a \neq b \neq c$ $\alpha = \beta = \gamma = \frac{\pi}{2}$

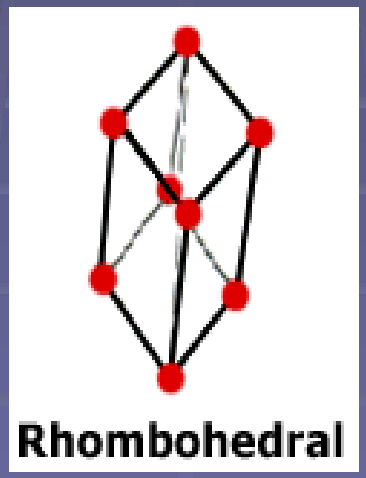


Tetragonal: In the tetragonal system, there are two lattice types: one is primitive unit cell (*P*) and another is body centered (*I*). In this case $a = b \neq c$ $\alpha = \beta = \gamma = \frac{\pi}{2}$

Cubic: **In the cubic system, there are three lattice types: the simple-cubic lattice (sc), the body centered cubic (bcc), and the face centered cubic (bcc).Here,** $a = b = c$ $\alpha = \beta = \gamma = \frac{\pi}{2}$



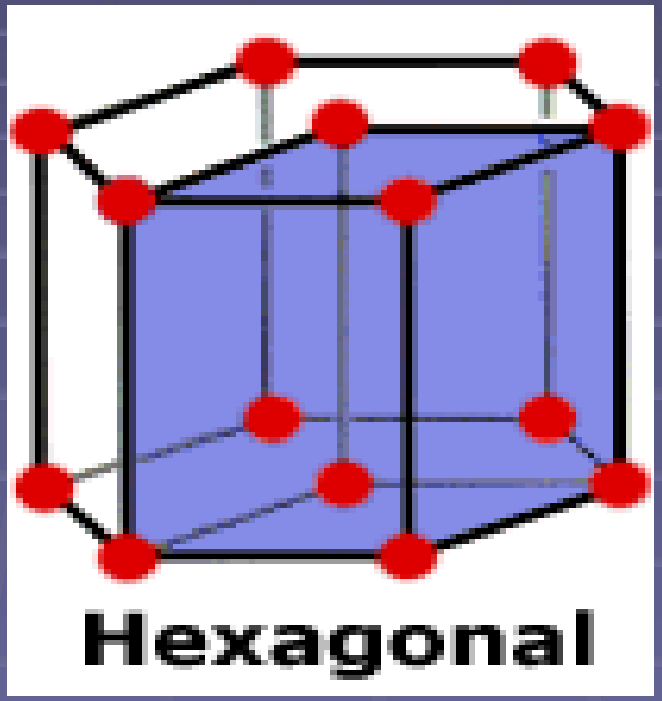
Trigonal: **In the Trigonal system, a rhombohedron is usually chosen as the primitive cell. In this case** $a = b = c$ $\alpha = \beta = \gamma < \frac{2\pi}{3} \neq \frac{\pi}{2}$



Hexagonal: In the Hexagonal system, the lattice is primitive and for this

$$a = b \neq c$$

$$\alpha = \beta = \frac{\pi}{2}, \gamma < \frac{2\pi}{3}$$




Physics is hopefully simple but Physicists are not