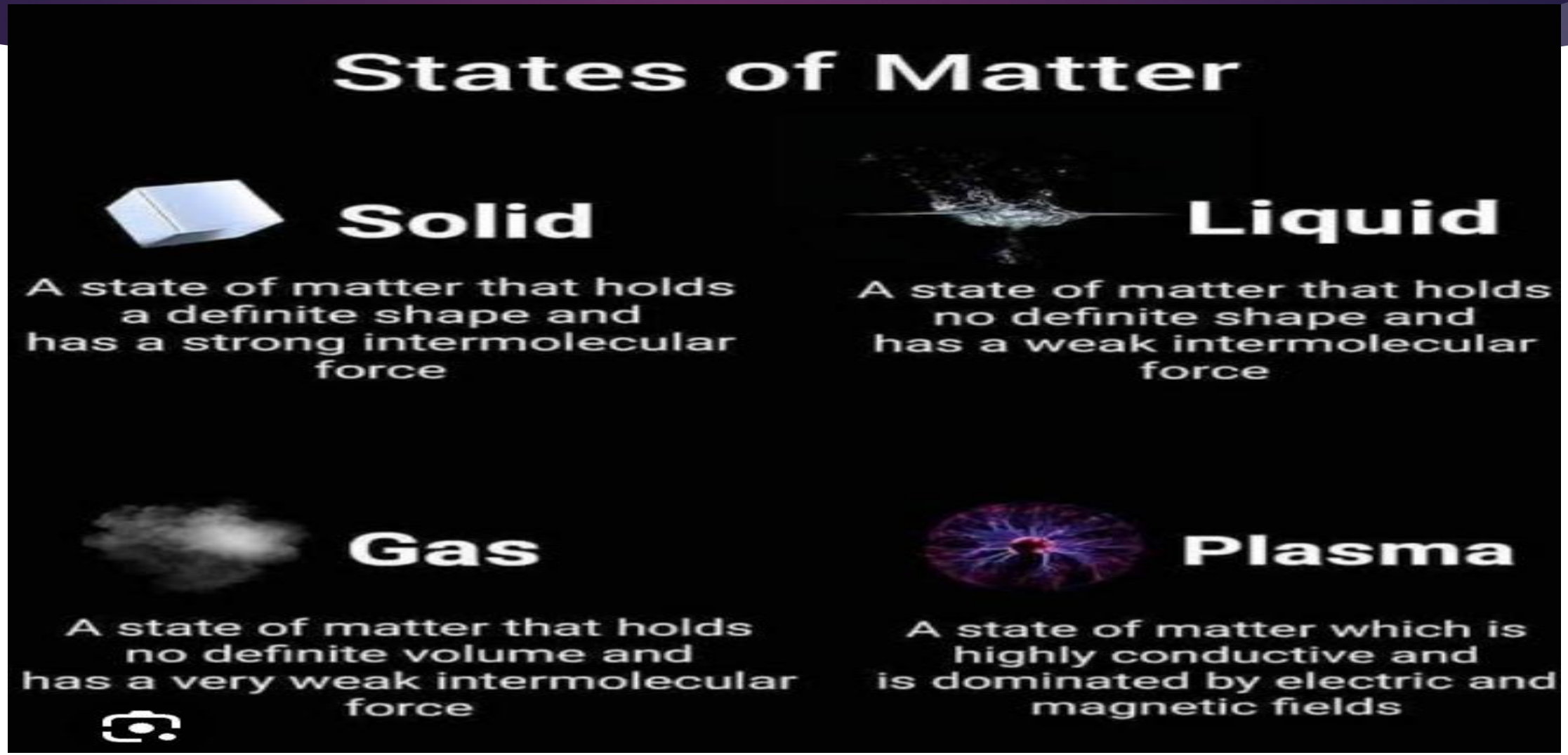
# Crystal Structure

# INTRODUCTION



## Crystalline Solids

- Crystalline Solids have a highly ordered and repeating three-dimensional atomic structure.

Vs

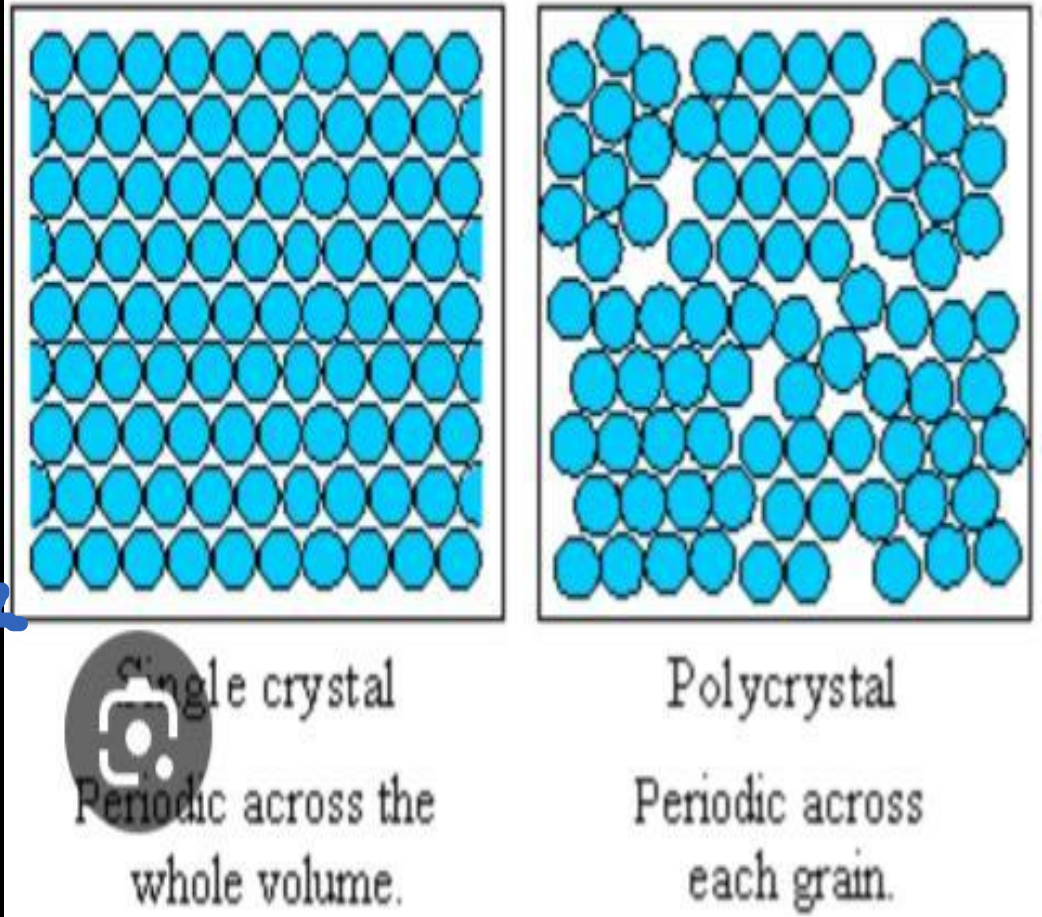
## Amorphous Solids

- Amorphous Solids lack a long-range order in their atomic structure and have a disordered arrangement of atoms.

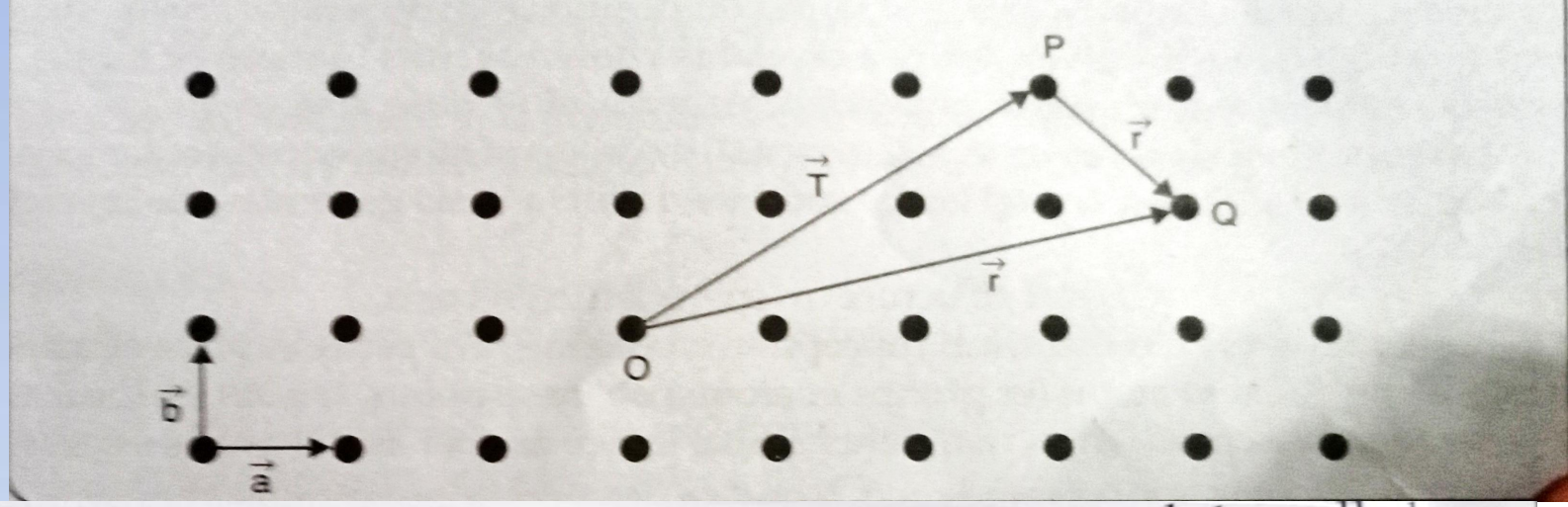
# Crystalline solids dividend into two types:- SINGLE CRYSTAL AND POLYCRYSTALLINE SOLIDS

A single crystal refers to a solid state in which molecules (atoms or ions) contained in the sample are regularly and periodically arranged in a three-dimensional space.

Polycrystals are composed of many small grains that have the same arrangement but are inconsistent in



- **Lattice:** defined as a regular periodic array of point in space. Each point in a lattice has identical surrounding everywhere. Lattice is basically imaginary points on space with a periodic manner.




To define space lattice, let us consider point O as origin and two vectors $a$ and $b$, called fundamental translational vectors in two dimensions. To obtain any point P, we draw a vector T from O to P. Then

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b},$$

where $n_1$ and $n_2$ are integers.

Similarly, in three dimensional lattice

$$\vec{T} = n_1 \vec{a} + n_2 \vec{b} + n_3 \vec{c} \qquad \text{.....(1.1)}$$

The application of this operation (1.1) to any point Q results in the point □

$$\vec{r}' = \vec{r} + \vec{T}$$

or

$$\vec{r}' = \vec{r} + n_1 \vec{} + n_2 \vec{} + n_3 \vec{} \qquad \text{.....(1.2)}$$

Such translational vectors which produce a translation operation containing integral coefficients are called *primitive translational vectors*.

If point Q is obtained by using equation

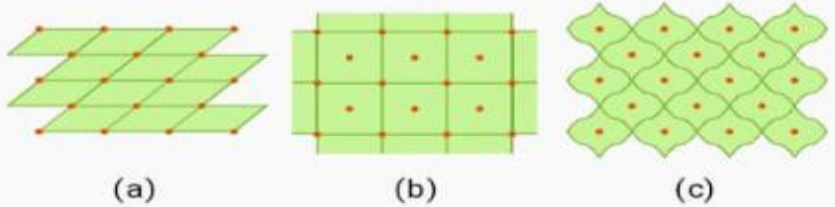
## 1. Unit Cell

These elements are called **unit cells** and fulfil the following requirements:[1][2]

- A repetitive arrangement (pure translation) of them can build up the whole crystal without overlaps/gaps.
- There is no further partition of the unit cell that could itself be used as a unit cell.

One finds varying definitions of this term in the literature.[3][4] On this website the definition above will be used consistently.

For a given crystal there are always quite a few possible unit cells:




## 2. Primitive Cell

A **primitive cell** is a unit cell that contains exactly one lattice point. It is the smallest possible cell.[5] If there is a lattice point at the edge of a cell and thus shared with another cell, it is only counted half. Accordingly, a point located on the corner of a cube is shared by 8 cubes and would count with $\frac{1}{8}$.

There is a special type of primitive-cells known as Wigner-Seitz cell. The **Wigner-Seitz cell** of a lattice point is defined as the volume that encloses all points in space which are closer to this particular lattice point than to any other. It can be constructed as depicted below.[6][7]

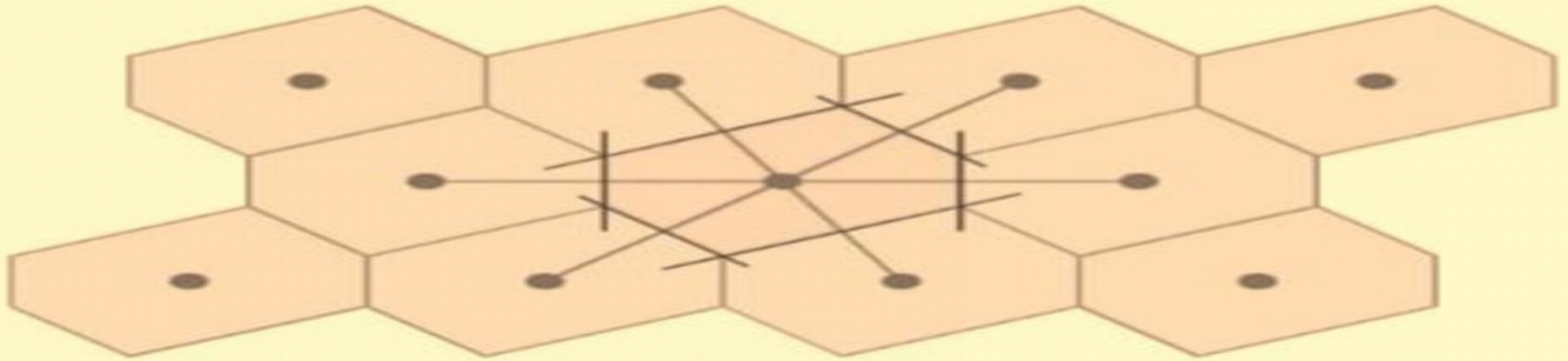


**Fig. 2** - 2D-construction of a Wigner-Seitz cell: One chooses any lattice point and draws connecting lines to its closest neighbours. In a second step one constructs the perpendicular bisectors of the connecting lines. The enclosed area is the

**CRYSTAL SYMMETRY:-** A symmetry operation is one which carries the crystal Structure into itself i.e. leaves the crystal and its environment invariant.

**(*i*) Rotation axes of symmetry.** If a body remains invariant after a rotation through an angle $\phi$ (known as throw of an axis), the body is said to possess rotational symmetry. If a crystal retains its identity after a rotation of $360/n$ about an axis, the crystal is said to possess $n$-fold rotational symmetry.

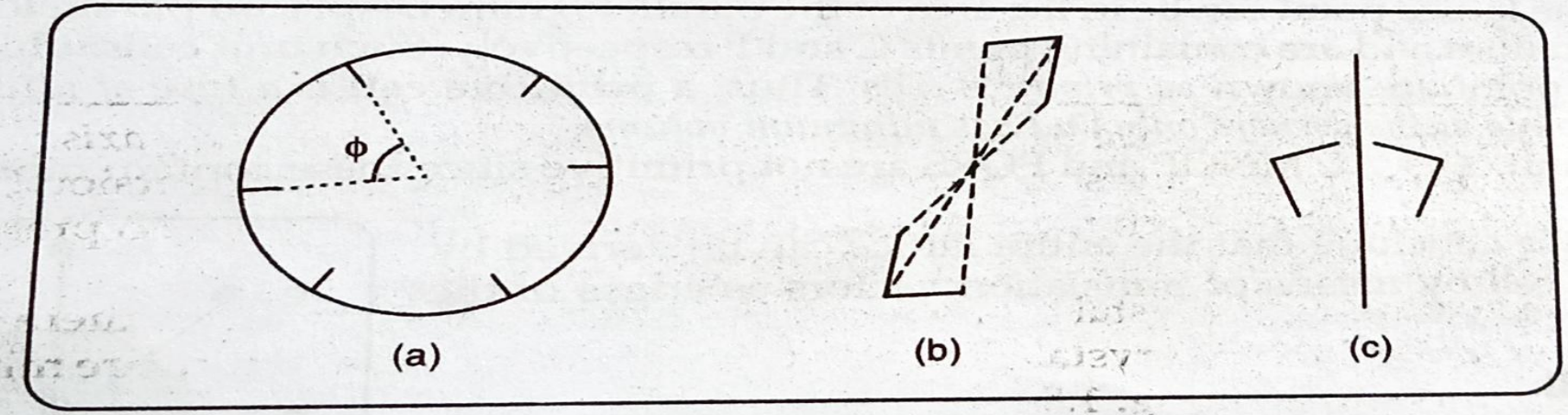



**Fig. 1.5:** (a) Rotational (b) Inversion symmetries, (c) Reflection

Let us now discover which are permissible throws that rotation axes can have. Consider a row of lattice points A, B, C, D as shown in fig. 1.6. Let the system possess $n$-fold rotation symmetry, then rotation by an angle $\phi$ either clockwise or anti-clockwise leads us to same new lattice points P and Q. Let $t$ be the translation vector. The distance BP and CQ will also

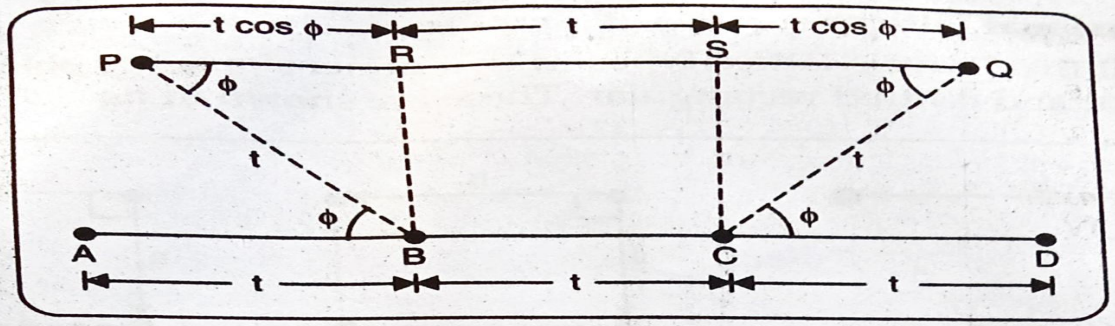



**Fig. 1.6:** To show 5- fold symmetry is incompatible

be $t$ by construction. Also P and Q must be joined by the same translation or some integral multiple of $t$ say $mt$. Where $m$ is an integer.
Therefore, from the geometry of fig. 1.6, we find that

$$PQ = PR + RS + SQ$$
$$mt = t\cos\phi + t + t\cos\phi$$
$$(m-1)\ t = 2t\cos\phi$$
$$\frac{m-1}{2} = \cos\phi$$

Since $m$ is an integer, so $(m-1)$ will also be an integer say N. Hence

$$\cos\phi = N/2 \qquad \text{.....(1.3)}$$

$\cos\phi$ has values lying between + 1 and – 1 and hence $-2 \le N \le 2$ *i.e.*, N has values – 2, – 1, 0, 1 and 2, only five values. For other values of N eq. (1.3) does not hold good. Following table gives the values of $\phi$ corresponding to these values of N :

| N | $\cos\phi$ | $\phi$ | $n = 360°/\phi$ |
|---|---|---|---|
| – 2 | – 1 | 180° | 2 |
| – 1 | $-\frac{1}{2}$ | 120° | 3 |
| 0 | 0 | 90° | 4 |
| 1 | $\frac{1}{2}$ | 60° | 6 |
| 2 | 1 | 360° or 0° | 1 |

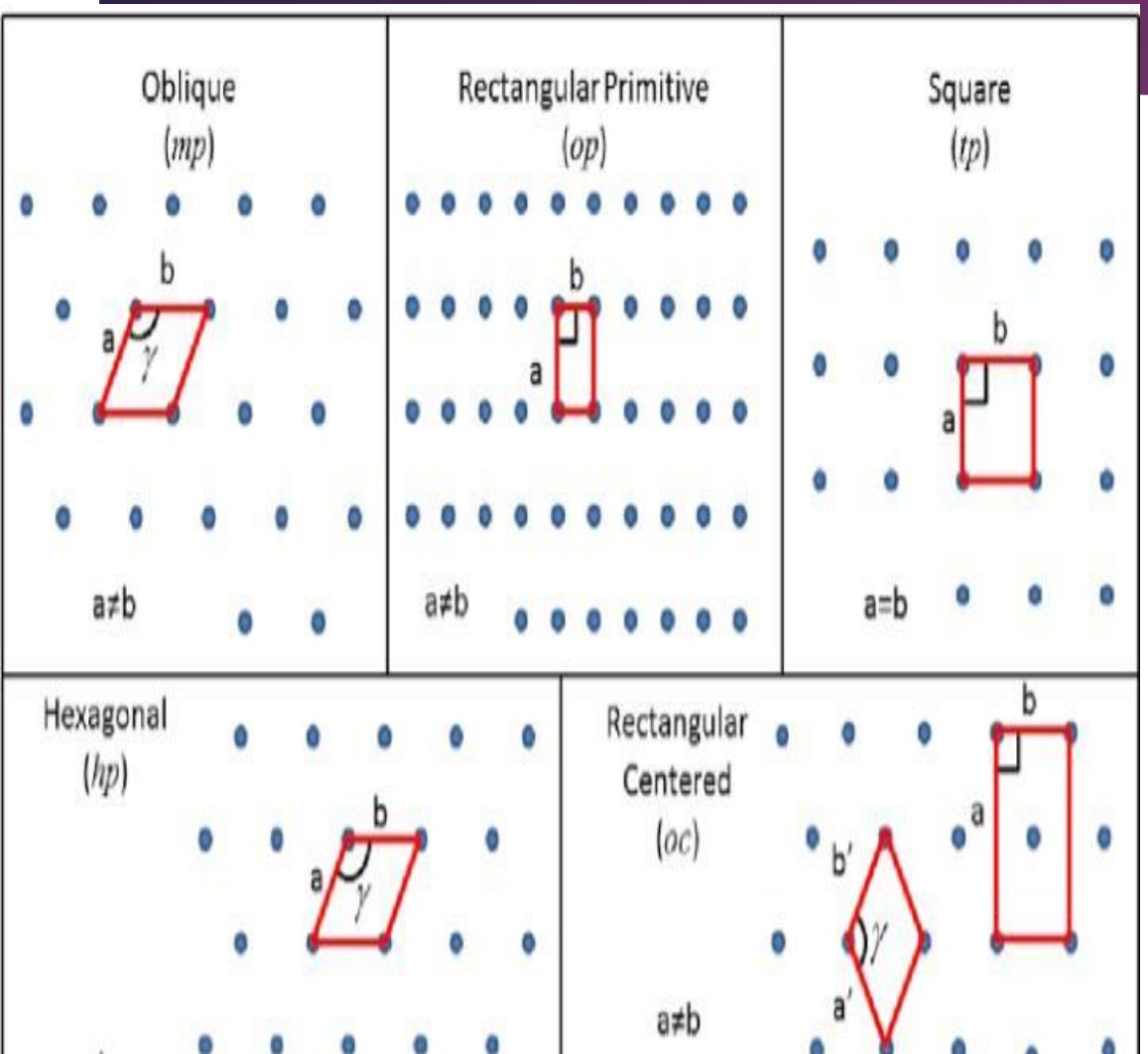
*It is also clear from this table that there does not exist 5-fold or 7-fold symmetry axis.*

(*ii*) **Inversion centre.** A crystal is said to possess centre of symmetry or inversion centre if for every lattice point at position $r$, another lattice point at position $-r$ is also present. This is shown in fig. 1.5. (b).

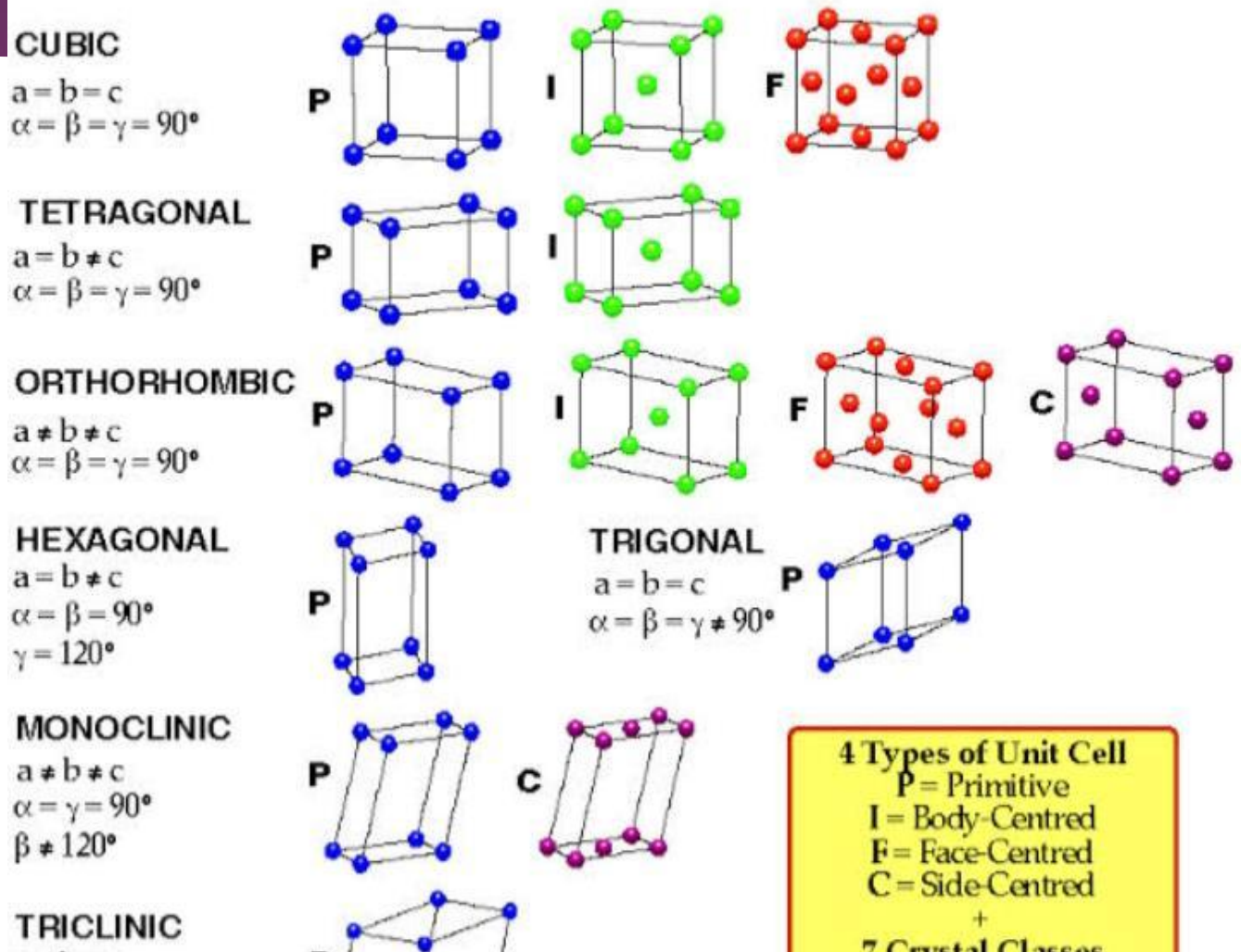
(*iii*) **Reflection symmetry.** A crystal is said to possess a reflection symmetry if there exists a line or plane which divides the crystal into two exactly identical halves which are mirror images of each other as shown in fig. 1.5 (c).

# TYPES OF LATTICES:-

## 2-D LATTICES 👇




## 3D LATTICES 👇



Thank
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