TYPES OF UNIT CELL IN CRYSTAL SYSTEMS

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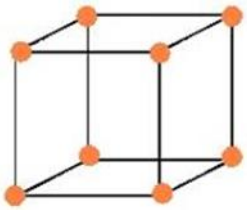
There are basically two types of unit cells constituting different crystal systems. These are:

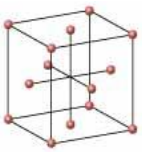
Primitive unit cells: The unit cells which have point (or particles) only at the corners. These are also called simple unit cells.



Primitive Unit Cell

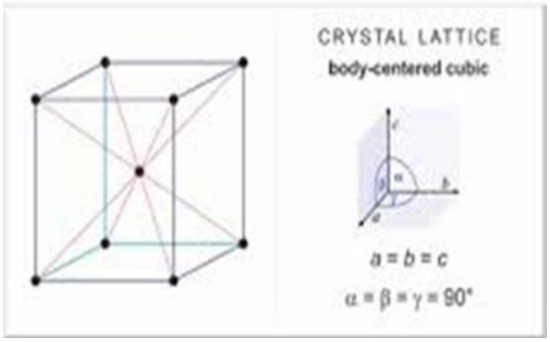
Primitive cubic

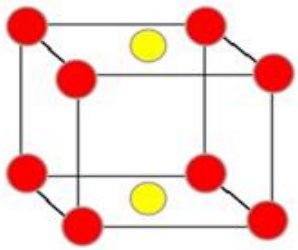
Body-centered cubic



Face-centered cubic

Centered unit cells: These are unit cells which have points (or particles) at the corner as well as at some other positions. The centered unit cells are of three types:
(a) Face Centered unit cells in which the points are present at all corners as well as at the centre of each face.
(b) Body Centered unit cells in which the points are present at all corners as well as body centre of the unit cell.

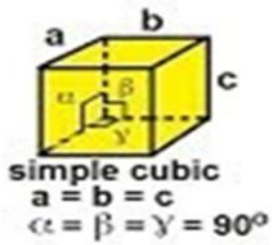




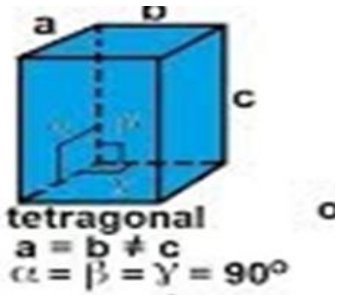
(c) End Centered unit cell in which the points are present at all corners and at the centre of two opposite faces

Seven Crystal Systems: When a unit cell in a crystal lattice has lattice points only at its corners, it is called a simple or primitive unit cell. In all, there are seven types of simple or primitive unit cells among crystals. These unit cells are characterized by the **length a, b and c and the angles α, β and ϒ**. These are called seven crystal systems or crystal habits. All crystals can be placed in one of these seven crystal systems. These are:

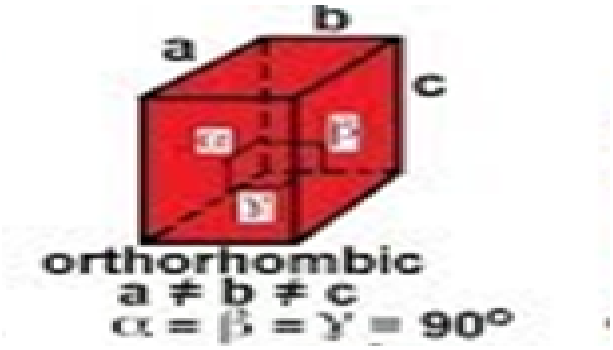
Cubic: all the three axes are of equal length and are at right angles to each other (a= b=c, all angles = 90º). E.g. NaCl, KCl, Zinc blende, Cu, Ag



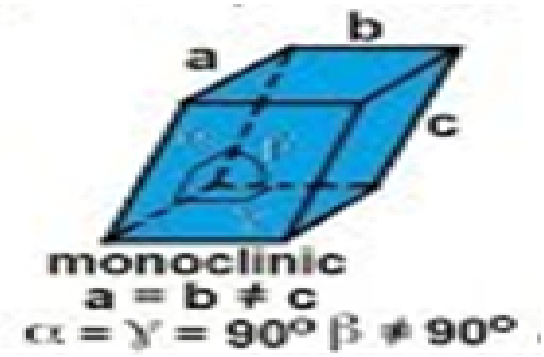
Tetragonal: The three axes are at right angle to each other but only the two axes are equal (a=b≠ c, all angles= 90º). E.g. white tin, SnO_4, TiO_2, $CaSO_4$



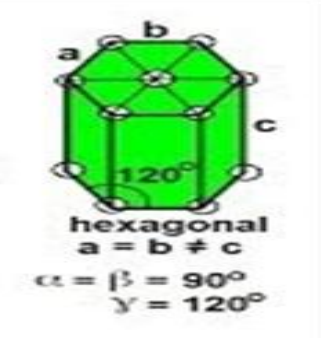
Orthorhombic: It has three unequal axes which are at right angles to each other (a≠ b≠ c, all angles = 90º).
E.g., rhombic sulphur, $BaSO_4$, KNO_3, $PbCO_3$



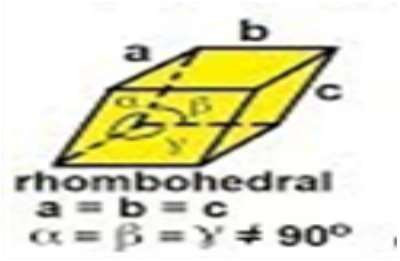
Monoclinic: The three axes are of unequal length and two angles are of 90º (a≠ b≠ c, two angles = 90º and one ≠ 90º)e.g. monoclinic sulphur, $PbCrO_4$, Na_2SO_4



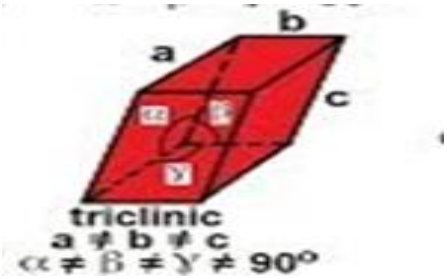
Hexagonal: It has two edges of equal length (a=b) and two angles of 90º and one angles of 120º (a = b ≠c, two angles of 90º and one angle of 120º).e.g. graphite, ZnO, CdS



Rhombohedral: The three axes are of equal length which are inclined at the same angle but the angle is not equal to 90º (a= b= c, all three angles equal but not equal to 90º). E.g. $CaCO_3$, quartz, and cinnabar (HgS) Sb.

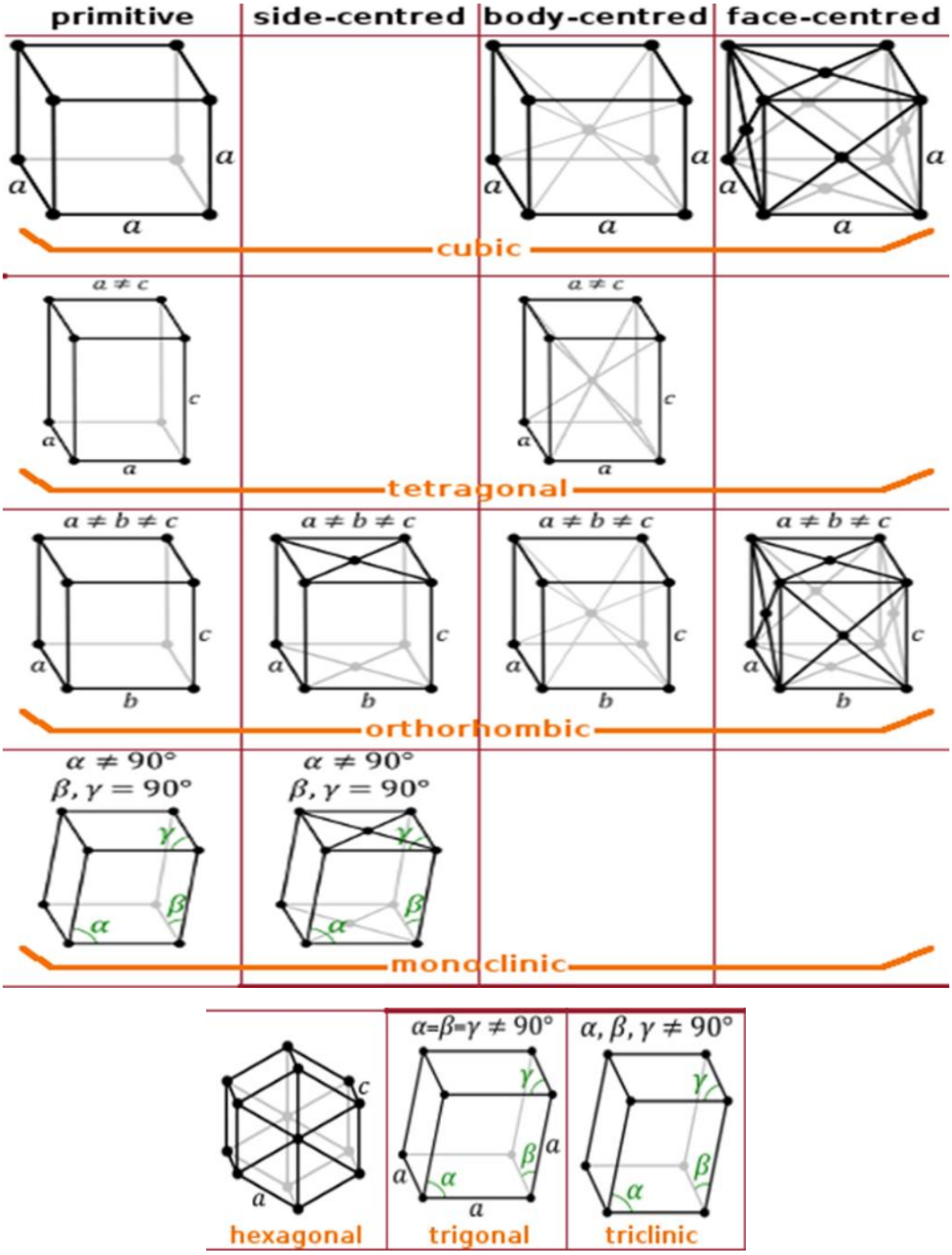


Triclinic: The three axes are of unequal length, and all angles are different but none is perpendicular to any of the others(a≠ b≠ c, all angles different and none equal to 90º) $CuSO_4.5H_2O$, $K_2Cr_2O_7$, H_3BO_3

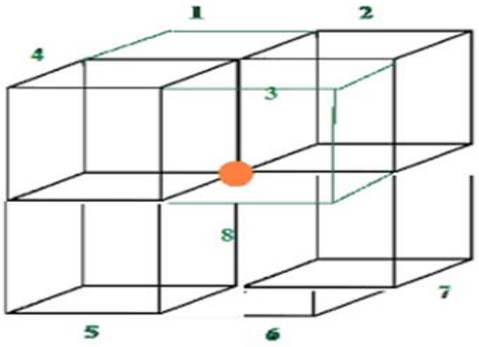


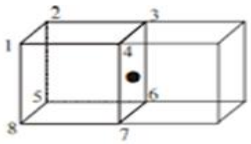
A French mathematician, Bravais, showed that there are only 14 possible three-dimensional lattices. These are called Bravais lattices. Cubic is most symmetrical while triclinic is most unsymmetrical system

S.No.	Name of crystal system	Bravais Space lattices	Edge Lengths	Axial Angles
1.	Cubic	Primitive, Cubic Body Centered, Cubic face Centered	a =b =c	α = β = γ = 90°
2.	Tetragonal	Tetragonal Primitive, Tetragonal Body Centered	a=b≠c	α = β = γ = 90°
3.	Hexagonal		a=b≠c	α = β = 90°, γ = 120°
4.	Rhombohedral			α = β = γ ≠ 90°
5.	Orthorhombic	Orthorhombic Primitive, Orthorhombic body centered, Orthorhombic face centered, Orthorhombic End Centered	a≠b≠c	α = β = γ ≠ 90°
6.	Monoclinic	Monoclinic Primitive, Monoclinic End Centered	a≠b≠c	α = β = 90°, γ ≠ 90°
7.	Triclinic		a≠b≠c	α ≠ β ≠ γ ≠ 90°

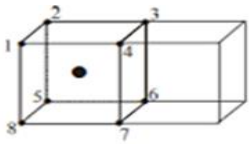


Types of cubic crystals and number of atoms per unit cell: We know that a crystal lattice is made up of a very large number of unit cells and every lattice point is occupied by one constituent particles (atom, molecules or ion). In different types of unit cells, the particles may be at the corner, at the body Centre, or at the centre of faces. Since every unit cell in a crystalline solid is adjacent to other unit cells, most of the atom (or constituent particles) are shared by neighboring unit cells. As a result, only some portion of each atom belongs to a particular unit cell. For example, in all types of cubic cells, each corner atom belongs to eight adjacent unit cells as shown in figure, four units in the lower layer and four unit cells of the upper layer. Therefore, only 1/8th of an atom (or molecule or ion) actually belongs to a particular unit cell.





Point at Face Centre



Point at body Centre

Type of Lattice Point	Contribution per unit cell
Corner	1 / 8
Edge	1 / 4
Face Centre	1 / 2
Body Centre	1

Similarly, each face centered atom is shared by two-unit cells and only ½ of an atom belongs to a particular unit cell. An atom at the body centre of a unit cell is not shared by other units and it completely belongs to the unit cell. For simplicity assume that the constituent particles are atoms. The unit cell may be represented in three different ways.

(a) each small sphere in figure represents only the centre of the particle occupying that position and not its actual size. Such type of structures are called open structures. It is easier to follow the arrangement of particles in open structures.
(b) space filling representation of the unit cell with actual particle size. This gives a more realistic picture showing how particles actually back within the solid.
(c) actual portion of different atoms present in unit cell.

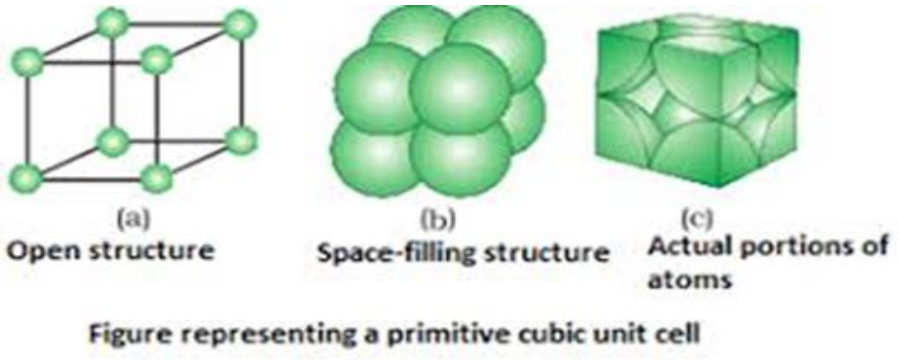
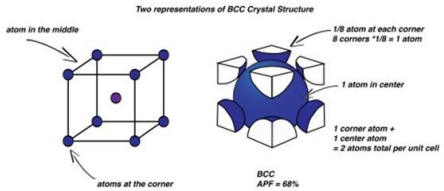


Figure representing a primitive cubic unit cell

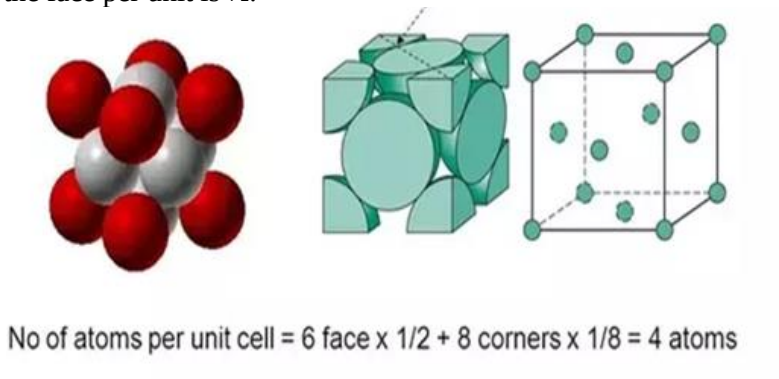
Let us now calculate number of atoms in different types of unit cells. We know that cubic system is the simplest system. There are three common types of cubic system:
(i) simple or primitive cubic unit cell
(ii) body centred cubic unit cell
(iii)face centred cubic or close packing unit cell.

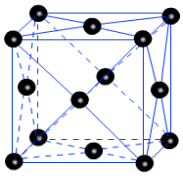
(i) Simple primitive cubic unit cell: In this unit cell, the points (atoms, ions or molecules) are present at all the corners of a cube. It is clear from the figure that atom present at each corner contributes 1/8 to each cube because it is shared by 8 cubes. Now, there are 8 atoms at the corners. Thus, the number of atoms present in each unit cell = 8 corner atoms X 1/8 atom per unit cell = 1 atom.
Thus, the simple or primitive cubic unit cell has only one atom per unit cell.

(ii) Body centred cubic unit cell: It has atoms at all the corners as well as at the body centre of the cube. It is clear from the figure that there are 8 atoms at the corners and each is shared by 8-unit cells so that the contribution of each atom at corner is 1/8. In addition, there is one atom in the body of the cube which is not shared by any other cube.
Thus, number of atoms present at the corners per unit cell= 8 corner atoms X 1/8 atom per unit = 1 .
The number of atoms present at the centre of the cube =1
Total number of atoms in bcc arrangement = 1 + 1=2



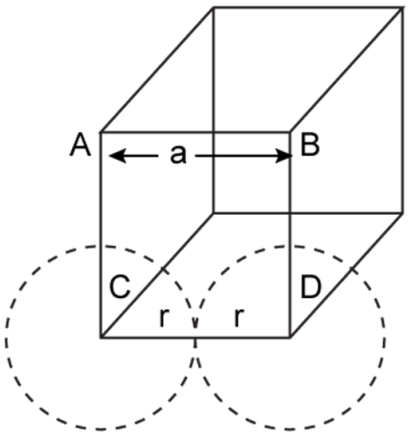
(iii) Face centered cubic unit cell**: T**his is also called cubic close packed unit cell. It has points at all the corners as well as at the centre of each of the six faces. In this arrangement, there is one atom at each of the eight corners. It is clear from the figure that atom present at each corner contributes 1/8 to each cube because it is shared by eight cubes. In addition, there are 6 atoms at the faces of the cube and each is shared by two-unit cells. Therefore, the contribution of each atom at the face per unit is ½.





Thus, the number of atoms present at the corners per unit cell = 8 corner atoms X 1/8 atom per unit cell = 1.
The number of atoms present at faces per unit cell = 6 atoms at the faces X ½ atom per unit cell =3.
Total number of atoms in ccp or fcc arrangement = 1 + 3= 4

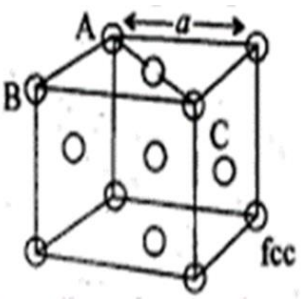
Relation between the nearest neighbor distance (d) and radius of atom (r):
1. **Simple cubic structure**: distance between the nearest neighbors, d= AB =a radius, r= a/2



2. **Face centred cubic**: distance between the nearest neighbors d= AC/2

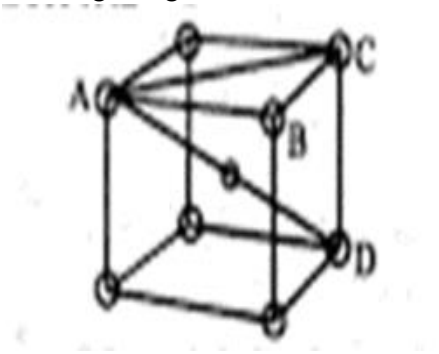
Now in right angled ΔABC : $AC^2 = AB^2 + BC^2$; $AC^2 = a^2 + a^2 = 2a^2$; AC = √2.a ;

Radius, r = d/2 = $\frac{a}{2\sqrt{2}}$



3. **Body centred cubic**: Distance between nearest neighbors
d = $\frac{AD}{2}$

In right angled ΔABC



$AC^2 = AB^2 + BC^2$

$AC^2 = a^2 + a^2 = 2a^2$ $AC = \sqrt{2}.a$

Now in right angled ΔADC,

$AD^2 = AC^2 + DC^2$

$AD^2 = (\sqrt{2}.a)^2 + a^2 = 3a^2$

$AD = \sqrt{3}.a$

d = √3.a/2 Radius, r = d/2 = √3.a/4

Multiple Choice Questions (MCQ)

1. The most unsymmetrical and symmetrical systems are respectively.
(A) tetragonal, cubic (B) triclinic, cubic (C) rhombohedral, hexagonal (D) orthorhombic, cubic

2. The unit cell with dimensions $\alpha = \beta = \Upsilon = 90^o$, $a = b \neq c$ is ----
(A) cubic (B)triclinic (C) hexagonal (D) tetragonal

3. The number of atoms in bcc arrangement is ------
(A) 1 (B) 2 (C) 4 (D) 6

4. A compound formed by elements A and B crystallizes in cubic structure where A atoms are at the corners of a cube and B atoms are at the face centres. The formula of the compound is -----
(A) AB_3 (B) A_2B (C) AB_2 (D) A_2B_3

5. In a face -centred cubic unit cells of close packed atoms, the radius of atom (r) is related to the edge length (a) of the unit cell by the expression------
(A) r= a/√2 (B) r= a/2 (C) r= a/2√2 (D) r= √3a/4

6. In a fcc arrangement of P and Q where P atoms are at the corners of the unit cell, Q atoms at the face centres and two atoms are missing from two corners in each unit cell, then the formula of the compound is -------
(A) P_2Q (B) PQ_4 (C) P_4Q_5 (D) PQ_4

7. Sodium atom specializes in body centred cubic with cell edge (a) = 4.29Å. The radius of sodium atom is -----
(A) 18.6Å (B) 1.86Å (C) 1.86pm (D) 1860 pm

8. How many kinds of space lattice are possible in a crystal?
(A) 23 (B) 7 (C) 230 (D) 14

9. The edge length of fcc unit cell is 508 pm. If the radius of cation is 110 pm, the radius of anion is ------
(A) 144 pm (B) 288 pm (C) 618 pm (D) 398 pm

10. The crystal system of a compound with unit cell dimensions, a= 0.387, b= 0.387 and c= 0.504 nm and α=β=90 and $\Upsilon=120^o$ is -----
(A) cubic (B) hexagonal (C) orthorhombic (D) rhombohedral

11. In a triclinic crystal:
(A) a=b=c, $\alpha=\beta=\Upsilon\neq 90^o$ (B) a≠ b=c, $\alpha=\beta=\Upsilon\neq 90^o$ (C) a≠ b≠ c, $\alpha\neq\beta\neq\Upsilon\neq 90^o$ (D) a≠ b≠ c, $\alpha=\Upsilon=90^o\neq\beta$

Answers

1. (B) 2. (D) 3. (B) 4. (A) 5. (C) 6. (D) 7. (B) 8. (D) 9. (A) 10. (B) 11. (C)

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