

CHEMISTRY STUDY MATERIALS FOR CLASS 12 (NCERT BASED NOTES OF CHAPTER- 01)

GANESH KUMAR

DATE:- 29/07/2020

The Solid State

Unit cell

A unit cell is the smallest repeating unit of a crystal lattice which, when repeated in three dimension we get a whole crystal. Or, it is the building block of a crystal. A unit cell is characterized by its edge lengths (a, b and c) and angle between the edges – α (between b and c), β (between a and c) and γ (between a and b). Thus a unit cell is characterized by 6 parameters – a, b, c, α , β and γ .

Unit cells can be broadly divided into two - primitive and centred unit cells.

1. Primitive Unit Cells:

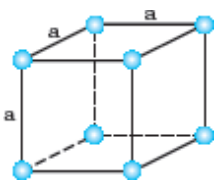

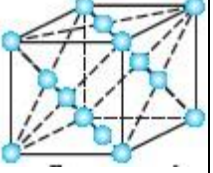
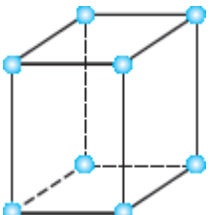
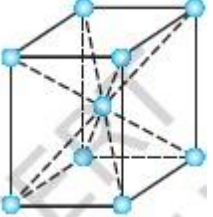
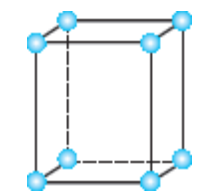
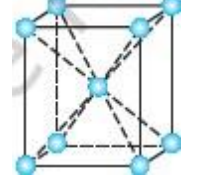
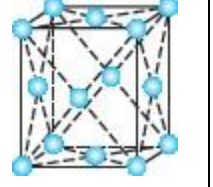
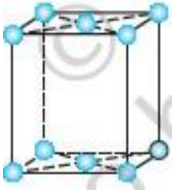
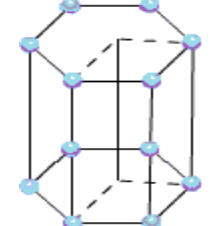
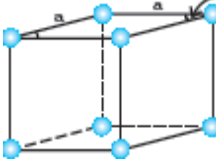
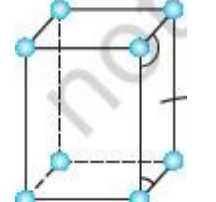
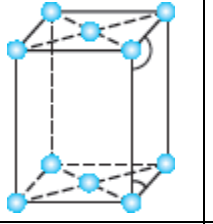
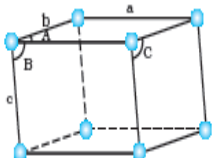
Here the constituent particles are present only at the corners of the unit cell.

2. Centred Unit Cells:

Here the constituent particles are present at the corners and other positions of the unit cell. These are of three types:

- i. *Body-centred unit cells*: Here the constituent particles are present at the body centre and at the corners of the unit cell.
- ii. *Face-centred unit cells*: Here the constituent particles are present at the centre of each faces and at the corners of the unit cell.
- iii. *End-centred unit cells*: Here the constituent particles are present at the centre of any two opposite faces and at the corners of the unit cell

Seven types of crystal systems and their possible variations

Crystal	Possible variations				Examples
1. Cubic $a = b = c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive 	Body-centered 	Face-centered 		NaCl, Zinc Blende, Cu
2. Tetragonal $a = b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive 	Body-centered 			White tin, SnO_2 , TiO_2 , CaSO_4
3. Orthorhombic (Rhombic) $a \neq b \neq c$ $\alpha = \beta = \gamma = 90^\circ$	Primitive 	Body-centered 	Face-centered 	End-centered 	Rhombic sulphur, KNO_3 , BaSO_4
4. Hexagonal $a = b \neq c$ $\alpha = \beta = 90^\circ$, $\gamma = 120^\circ$	Primitive 				Graphite, ZnO, CdS
5. Rhombohedral / Trigonal $a = b = c$ $\alpha = \beta = \gamma \neq 90^\circ$	Primitive 				Calcite (CaCO_3), HgS (Cinnabar)
6. Monoclinic $a \neq b \neq c$ $\alpha = \gamma = 90^\circ$, $\beta \neq 90^\circ$	Primitive 			End-centered 	Monoclinic sulphur, $\text{Na}_2\text{SO}_4 \cdot 10 \text{H}_2\text{O}$
7. Triclinic $a \neq b \neq c$ $\alpha \neq \beta \neq \gamma \neq 90^\circ$	Primitive 				$\text{K}_2\text{Cr}_2\text{O}_7$, $\text{CuSO}_4 \cdot 5\text{H}_2\text{O}$, H_3BO_3

Calculation of Number of atoms in a unit cell (z)

1. Primitive cubic (Simple Cubic) unit cell:

Here atoms are present only at the corners of the cube. Each corner atom is shared by 8 unit cells. Therefore, contribution to one unit cell = $1/8$

Since each unit cell has 8 atoms at the corners, the total number of atoms in one unit cell = $8 \times 1/8 = 1$ So for a primitive (simple cubic) unit cell, $z = 1$

2. Body-centred cubic (bcc) unit cell:

Here the particles are present at the corners of the cube and also one atom at the body centre. The number of atoms at the corner = $8 \times 1/8 = 1$

The atom present at the centre of the body is not shared by other atoms. So the number of atoms at the body-centre = 1

Therefore, total number of atoms in the unit cell = $1+1=2$, so for a bcc, $z = 2$

3. Face-centred cubic (fcc) unit cell:

Here the atoms are present at the corners and also at the centre of each faces. Each corner atom is shared by 8 unit cells and each face centre atom is shared by 2 unit cells.

Number of corner atoms = $8 \times 1/8 = 1$

Number of face-centre atoms = $6 \times 1/2 = 3$

Therefore, total number of atoms = $1+3=4$ so, for an fcc, $z = 4$
