UNIT-1

ATOMIC AND MOLECULAR STRUCTURE.

- **Lecture 1** : Molecular orbital theory : Introduction and postulates.
- **Lecture 2** : Application of molecular orbital theory to homonuclear diatomic molecules.
- **Lecture 3** : Application of molecular orbital theory to heteronuclear diatomic molecules.
- **Lecture 4**: Band theory of solids and its application to solids (Metals).
- **Lecture 5**: liquid crystals: classification, properties and applications.
- **Lecture 6**: crystal defects, Point defects in solids.
- **Lecture 7**: Structure, properties and applications of graphite and fullerene.
- **Lecture 8**: concepts, properties and applications of Nanoscience and nanomaterials.

Lecture-1

Molecular Orbital Theory: Introduction & Postulates

FUNDAMENTALS

- The Molecular Orbital Theory is one of the latest theory which explains the mixing of orbitas when forming a molecules and also describe the structure and properties of different molecules.

It overcomes all the drawbacks of Valence Bond theory. Valence-bond theory failed to explain the magnetic behaviour and stability of the molecule which was later explained by Molecular Orbital theory.

According to Molecular Orbital theory - Atomic orbitals with same energy ऊर्जा and symmetry समरूपता combine to form molecular orbitals in which ~~the~~ identity पहचान of both the atomic orbitals is lost खोना.

Two types of molecular orbitals are formed -

1) Bonding Molecular Orbital
2) Antibonding Molecular Orbital

→ The filling of molecular orbitals in a molecule take place in accordance with Aufbau Principle, Pauli's **exclusion Principle** and Hunds Rule.

→ Stability and Strength of a chemical bond is expressed in terms of bond order.

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Ques Discuss the postulates of Molecular Orbital Theory

OR

Outline the salient features of MOT on the basis of LCAO principle. (2016-17, 2018-19).

Ans Salient features of Postulates of MOT :

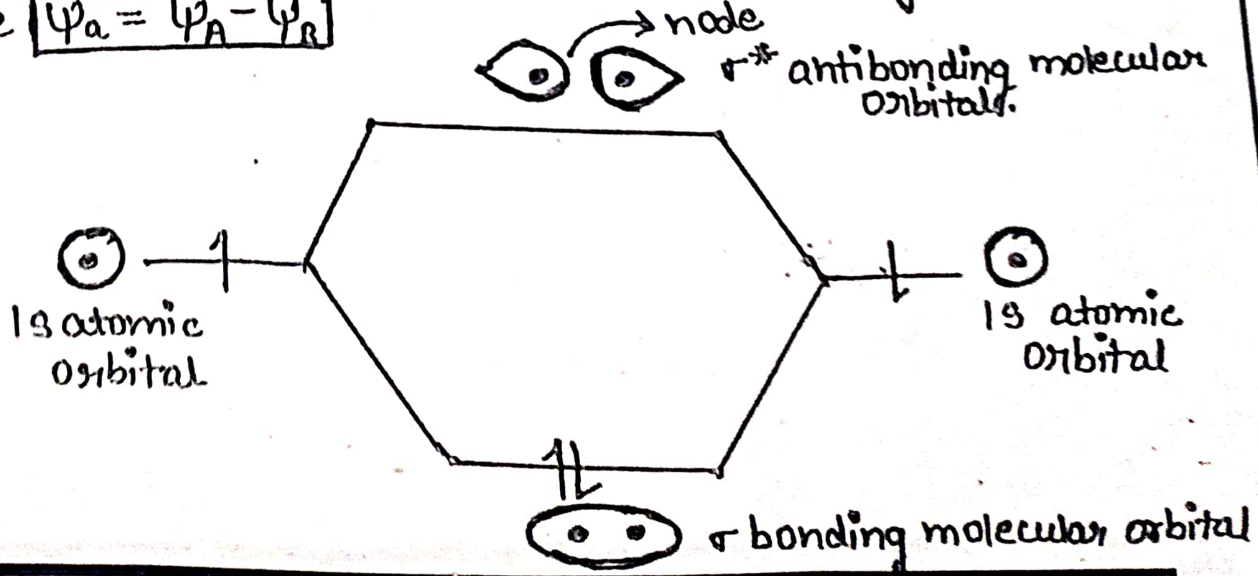
1. Atomic orbitals with same energy and symmetry (समरूप) combine to form molecular orbitals by LINEAR COMBINATION OF ATOMIC ORBITALS (LCAO)

If ψ_A and ψ_B are wave functions of atoms A & B then according to LCAO = $\psi_{MO} = \psi_A \pm \psi_B$

2. Two types of molecular orbitals are formed : bonding and antibonding molecular orbitals.

Molecular orbitals formed by additive overlap of two atomic wave functions is known as Bonding molecular orbitals. i.e $\boxed{\psi_b = \psi_A + \psi_B}$

Molecular orbitals formed by subtractive overlap of two atomic ~~wave~~ functions is called antibonding molecular orbital i.e $\boxed{\psi_a = \psi_A - \psi_B}$



3. The no. of molecular orbitals formed is always equal to the number of atomic orbitals taking part in bond formation.
4. Energy level of bonding molecular orbital is less than that of individual व्यक्तिगत atomic orbitals. So, e^- present in bonding molecular orbital **stabilizes** स्थिर the molecule.

   Energy level of antibonding molecular orbital is **more than** that of individual atomic orbitals. So, e^- present in antibonding Molecular orbital **destabilizes** अस्थिर the molecule.
5. Molecular orbitals that do not participate in bonding are called non bonding molecular orbital & their energy is equal to that of individual atomic orbitals.
6. Molecular orbitals are **polycentric.**
7. The atomic orbitals involved in the formation of molecular orbital completely lose their identity after the formation of molecular orbitals.
8. Electrons filling in the molecular orbitals follow **Aufbau principle**, **Pauli's exclusion principle** & **Hunds rule of maximum multiplicity.**
9. The electrons are filled in the molecular orbitals according to the following **order**:

   From H_2 to N_2: $\sigma 1s, \sigma^* 1s, \sigma 2s, \sigma^* 2s, \pi 2p_x = \pi 2p_y, \sigma 2p_z, \pi^* 2p_x = \pi^* 2p_y, \sigma^* 2p_z$

   From O_2 to Ne_2: $\sigma 1s, \sigma^* 1s, \sigma 2s, \sigma^* 2s, \sigma 2p_z, \pi 2p_x = \pi 2p_y, \pi^* 2p_x = \pi^* 2p_y, \sigma^* 2p_z$
10. Molecules or ions with one or more unpaired e^- in molecular orbitals are **paramagnetic** while those with all paired electrons in molecular orbital are **diamagnetic.**
11. Stability स्थिरता and strength ताकत of a chemical bond is expressed in terms of **bond order.**

12. Bond order - Bond order is equal to one half of the difference between the number of electrons in bonding MO & the no. of electrons in antibonding MO.

$$\boxed{BO = \frac{1}{2}(N_b - N_a)}$$

N_a = e(s) in ABMO
N_b = e(s) in BMO

$$\boxed{B.O \propto \frac{1}{\text{bond length}} \propto \underset{\text{स्थिरता}}{\text{Stability}} \propto \text{Bond Dissociation Energy.}}$$

Significance of bond order:

- Zero B.O molecule is unstable does not exist.
- Negative B.O is not possible.
- Positive value of BO molecule exists & is stable.
- B.O of +1, +2, +3 indicates the molecule has single, double or triple bond respectively.

Ques-1 Explain BMO and ABMO and differentiate between them. (2018-19).

Ans. BMO (bonding Molecular orbital) $\psi_b = \psi_A + \psi_B$

ABMO (antibonding Molecular orbital). $\psi_a = \psi_A - \psi_B$

BONDING MOLECULAR ORBITALS	ANTIBONDING MOLECULAR ORBITALS
1. They are formed by additive overlapping of atomic orbitals.	1. They are formed by subtractive overlapping of atomic orbitals.
2. $\psi_b = \psi_A + \psi_B$ (A and B are two atomic orbitals).	2. $\psi_a = \psi_A - \psi_B$ (A and B are two atomic orbitals.).
3. Electrons contribute (दान देना) to the formation of bond.	3. Electrons do not contribute to the formation of bond.
4. They have low energy and high stability.	4. They have high energy and low stability.
5. They are shown as σ, π etc.	5. They are shown as σ^*, π^* etc.
6. Maximum electrons are located in between the two nuclei.	6. Electrons are scattered.
7. Electron density (घनत्व) is higher.	7. Electron density is lower.

LECTURE-2

Molecular orbital diagram and its application to homo-nuclear diatomic molecule :

FUNDAMENTALS

- A homo nuclear diatomic molecule is on in which the molecule is formed from two atoms of the same element. eg- H_2, N_2, O_2 etc.
- Homo nuclear diatomic molecules formed from atoms having same electronegativity.
- Bonding and antibonding molecular orbitals are at equidistance from atomic orbitals.
- The electrons are filled in the molecular orbitals according to the following orders.

From H_2 to N_2 :

$\sigma 1s$, $\sigma^* 1s$, $\sigma 2s$, $\sigma^* 2s$, $\pi 2p_x = \pi 2p_y$, $\sigma 2p_z$, $\pi^*_{2p_x} = \pi^*_{2p_y}$, $\sigma^*_{2p_z}$

From O_2 to Ne_2

$\sigma 1s$, $\sigma^* 1s$, $\sigma 2s$, $\sigma^* 2s$, $\sigma 2p_z$, $\pi 2p_x = \pi 2p_y$, $\pi^*_{2p_x} = \pi^*_{2p_y}$, $\sigma^*_{2p_z}$

Ques-1 On the basis of MO theory explain why hydrogen forms diatomic molecule while helium remains monoatomic. (2014-15).

Ans Helium molecule (He_2) does not exist in nature

$H_2 \rightarrow \sigma 1s^2 \quad B.O = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(2-0) = 1$

$He_2 \rightarrow \sigma 1s^2 \, \sigma^* 1s^2 \quad BO = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(2-2) = 0$

As the bond order of He_2 is zero, the molecule (He_2) cannot be formed and it remains monoatomic.

Bond order of H_2 is 1, so it is a stable molecule.

Ques-2 Explain why bond energy of N_2 is greater than bond energy of O_2? (2015-16).

Ans. $\boxed{\text{Bond Energy} = \text{Bond Order.}}$

$BO \text{ of } N_2 = \frac{1}{2}(N_b - N_a)$ [illegible] $\frac{1}{2} \times 6 = 3$

$BO \text{ of } O_2 = \frac{1}{2}(N_b - N_a)$ [illegible] $\frac{1}{2} \times 4 = 2$

Since, bond order of N_2 is greater than that of O_2, hence its bond energy is greater than that of O_2.

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Ques. 3 Calculate the bond order of N_2^- and O_2^+. (2015-16).

Ans. B.O of N_2^-

Electronic configuration - $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2, \pi^* 2p_x^1 = \pi^* 2p_y^0$

$BO = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-5) = \frac{1}{2} \times 5 = 2.5$

BO of O_2^+

Electronic configuration - $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^0$

$BO = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-5) = \frac{1}{2} \times 5 = 2.5$

Ques-4 Calculate the bond order of N_2. (2016-17).

Ans N_2 (14 electrons).

Electronic configuration = $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2$

$B.O$ of $N_2 = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-4) = \underline{3}$

Ques-5 Calculate the bond order of N_2^+. (2017-18).

Ans N_2^+ (13 electrons)

Electronic configuration = $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^1$

BO of $N_2^+ = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(9-4) = \frac{1}{2} \times 5 = \underline{2.5}$

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Ques-6 Arrange the following in the increasing order of their bond energy O_2, O_2^{2+}, O_2^{2-}. (2017-18)

Ans. $B.O$ of $O_2 = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-6) = \frac{1}{2} \times 4 = 2$

$B.O$ of $O_2^{2+} = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-4) = \frac{1}{2} \times 6 = 3$

$B.O$ of $O_2^{2-} = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(8-6) = \frac{1}{2} \times 2 = 1$

Since $B.O \propto$ Bond energy. So, the order will be $\boxed{O_2^{2+} > O_2 > O_2^{2-}}$

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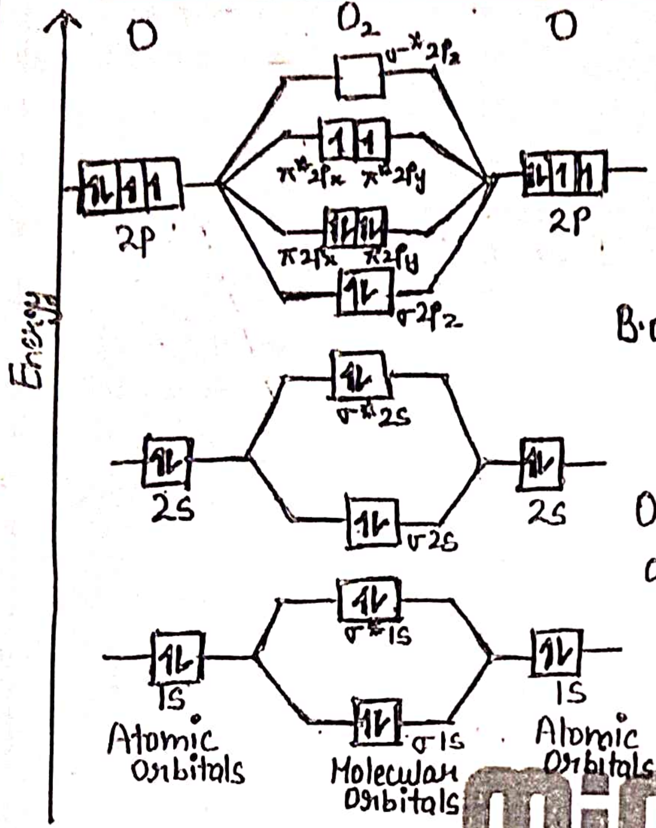
Ques-7 Draw the molecular orbital diagrams of N_2 and O_2. Calculate their bond orders and write its magnetic behaviour. (2016-17, 2017-18).

Ans. Molecular Orbital Diagram of O_2

Electronic configuration of O_2 ($16e^-$)

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1$

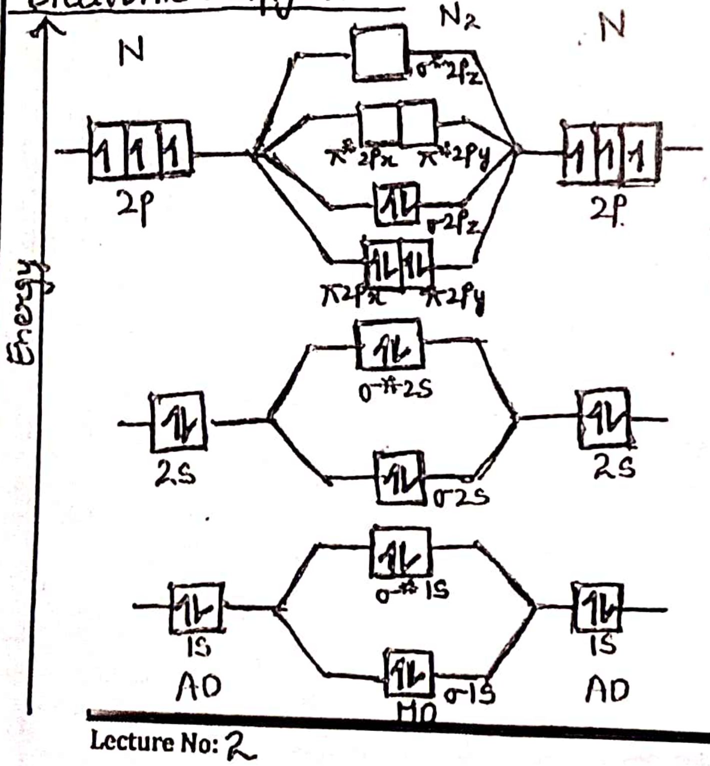


$$\text{B.O of } O_2 = \frac{1}{2}(N_b - N_a)$$
$$= \frac{1}{2}(10-6)$$
$$= 2$$

Oxygen is <u>Paramagnetic</u> in nature as there are two unpaired electrons in π^*2p_x and π^*2p_y

Molecular Orbital Diagram of N_2

Electronic configuration → $\sigma1s^2, \sigma^*1s^2, \sigma2s^2, \sigma^*2s^2, \pi2p_x^2 = \pi2p_y^2, \sigma2p_z^2$



$$\text{B.O of } N_2 = \frac{1}{2}(N_b - N_a)$$
$$= \frac{1}{2}(10-4)$$
$$= 3$$

Nitrogen is <u>diamagnetic</u> as all the electrons in its molecular orbital diagram are paired.

Ques-8 Explain why O_2 is paramagnetic in nature. (2017-18) (2018-19)

Ans. Molecular orbital electronic configuration of O_2 ($16e^-$)

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1$

There are two unpaired electrons in $\pi^* 2p_x$ & $\pi^* 2p_y$ orbitals. So, O_2 is paramagnetic.

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Ques-9 Arrange the following molecules/ions in order of their increasing bond length N_2, N_2^- and N_2^{2-}. (2018-19) (2019-20).

Ans. : B.O of $N_2 = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-4) = 3$

B.O of $N_2^- = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-5) = 2.5$

B.O of $N_2^{2-} = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-6) = 2$

$\boxed{\text{Bond order} \propto \frac{1}{\text{Bond length}}}$

So, the order will be $N_2 < N_2^- < N_2^{2-}$

Ques-10 Why O_2 is Paramagnetic and N_2 is diamagnetic? (2020-21)

Ans N_2 (14 electrons)

Electronic Configuration - $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2$

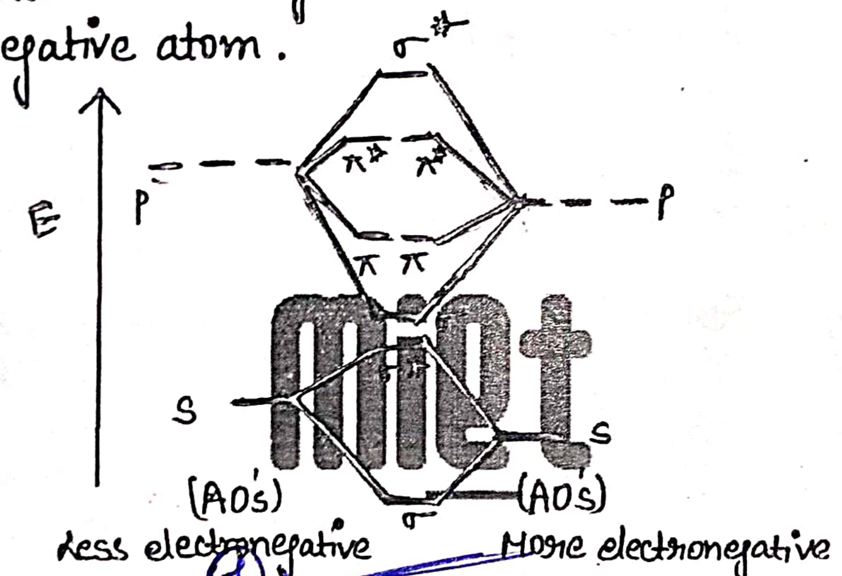
Nitrogen is diamagnetic as all the electrons in its molecular orbital diagram are paired.

Oxygen is paramagnetic in nature as there are two unpaired electrons in $\pi^* 2p_x$ and $\pi^* 2p_y$ orbitals. (Refer to L-2, Page-7 Qu-7)

LECTURE-3 FUNDAMENTALS

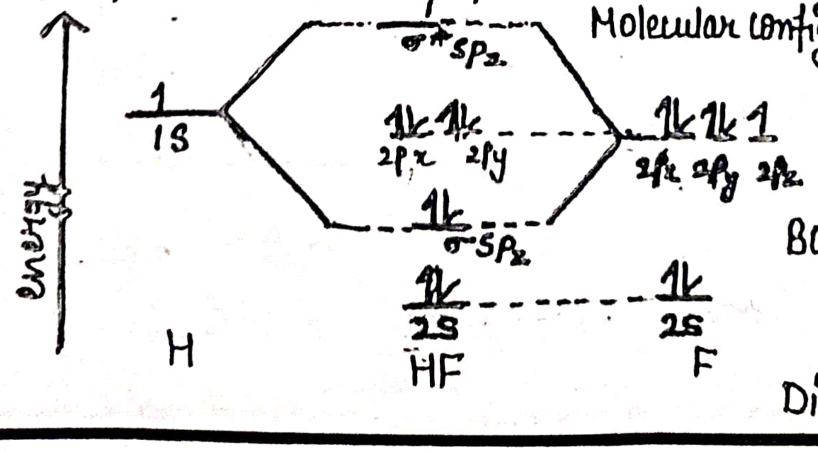
Molecular orbital theory and its application to hetronuclear diatomic molecule.

- Diatomic molecules with two different atoms e.g NO, CO, HF etc.
- Have difference in electronegativity. विद्युत ऋणात्मकता
- The diagram is distorted (विकृत) because more electronegative atom lies near the bonding molecular orbital.
- Bonding molecular orbital lies close to more electronegative atom and antibonding molecular orbital lies close to less electronegative atom.



① **Molecular orbital diagram of HF:** $(10e^-)$ 1s and 2s electrons as well as 4 electrons of p orbital of flourine do not participate in the formation of molecular orbital of HF and exist as lone pair. 1s of hydrogen pairs up with 2p unpaired electron of flourine to form σsp molecular orbital.

Molecular configuration $= \sigma sp_z^2$



$$BO = \frac{1}{2}(N_b - N_a)$$
$$= \frac{1}{2}(2-0)$$
$$= 1$$

Diamagnetic

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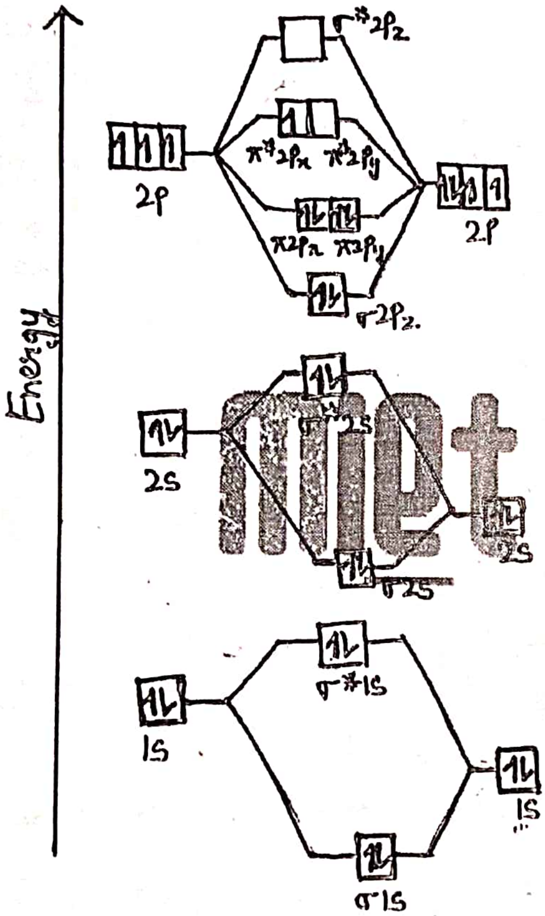
Ques-1 With the help of molecular orbital diagram explain the formation of NO and CO. Also calculate their bond order and predict their magnetic behaviour? (2015-16, 2018-19, 2019-20).

Ans Molecular orbital diagram of NO

$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^0$

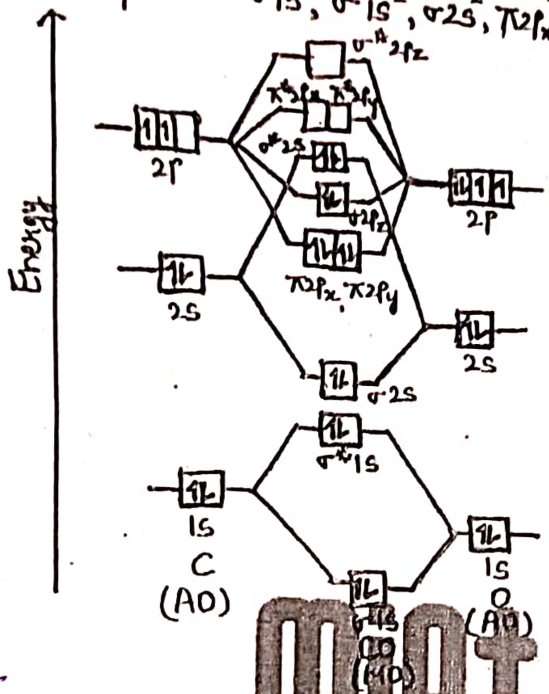


$$\text{BO of NO} = \frac{1}{2}(N_b - N_a)$$
$$= \frac{1}{2}(10-5)$$
$$= 2.5$$

NO is paramagnetic in behaviour as it contains an unpaired electron in $\pi^* 2p_x$ orbital.

Molecular orbital diagram of CO:

MO configuration of CO is- $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \pi 2p_x^2 = \pi 2p_y^2, \sigma 2p_z^2, \sigma^* 2s^2, \pi^* 2p_x^0 = \pi^* 2p_y^0$



B.O of CO $= \frac{1}{2}(N_b - N_a)$
$= \frac{1}{2}(10-4)$
$= 3$

CO is diamagnetic in behaviour as all electrons are paired in it.

v.imp ②

Ques-2 Calculate bond order, magnetic behaviour & order of stability of NO, NO^- and NO^+. (2020-21).

Ans $\boxed{NO}$ → Molecular orbital configuration of NO is -
$\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^0$
$B.O = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-5) = 2.5$

The molecule of NO is paramagnetic as it contains one unpaired electron.

$\boxed{NO^-}$ → $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^1 = \pi^* 2p_y^1$
$B.O = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-6) = 2$

NO^- is paramagnetic since there are two unpaired electrons in it.

$\boxed{NO^+}$ → $\sigma 1s^2, \sigma^* 1s^2, \sigma 2s^2, \sigma^* 2s^2, \sigma 2p_z^2, \pi 2p_x^2 = \pi 2p_y^2, \pi^* 2p_x^0 = \pi^* 2p_y^0$
$B.O = \frac{1}{2}(N_b - N_a) = \frac{1}{2}(10-4) = 3$, NO^+ is diamagnetic.

$\boxed{\text{Bond order} \propto \text{Stability}}$ Order of stability = $NO^- < NO < NO^+$

LECTURE-4 BAND THEORY OF SOLIDS AND APPLICATIONS

X. FUNDAMENTALS

Metallic Bond - "The force of attraction that holds the metal Kernels and the free electrons within its sphere of influence is known as metallic bond.

the atomic orbitals of the metals having the same energy combine to form molecular orbitals which are close in energy to each other to form a Baud.

In case of solids there are three bands -

→ Valence Band
→ Conduction Band
→ Forbidden Gap

Band theory differentiates solids into conductors, semiconductors and insulators. This classification depends upon the width of energy gap or band gap or forbidden gap.

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Ques-1 Explain Molecular Orbital theory in case of metals.

OR

Explain band theory in solids and on its basis differentiate between conductors, semiconductors and insulators. (2017-18, 2020-21)

Ans <u>Explanation of Metallic bond on the basis of MOT or band theory of solids.</u>

* According to this theory electron in the metal cover the whole crystal lattice.

* Metallic bond is formed by the delocalization of all the orbitals containing free electrons.

* According to M.O.T when two atomic orbitals combine two molecular orbitals are formed i.e bonding and anti-bonding.

* When three atomic orbitals combine, three MO's are formed i.e bonding, nonbonding & anti-bonding.

* Similarly when 'n' atomic orbitals combine 'n' molecular orbitals are formed. (In case of metals 'n' is of the order of 10^{23}.)

So, 10^{23} molecular orbitals are formed and these are so closely spaced that they form a continuous energy band. That is why the theory is known as band theory.

for eg - Bonding in Sodium Metal

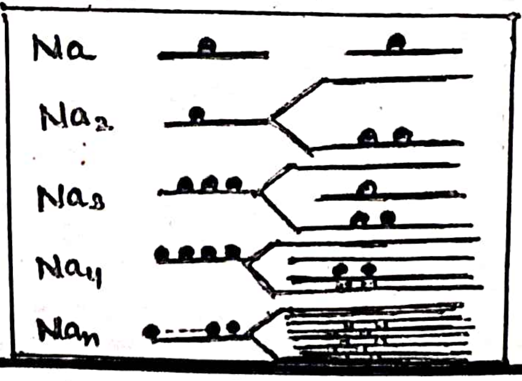
$Na = 1s^2, 2s^2, 2p^6, 3s^1$

$Na_2 = Na + Na$

$Na_3 = Na + Na + Na$

$Na_4 = Na + Na + Na + Na$

$Na_n = Na + Na + Na + \text{------} Na_n$



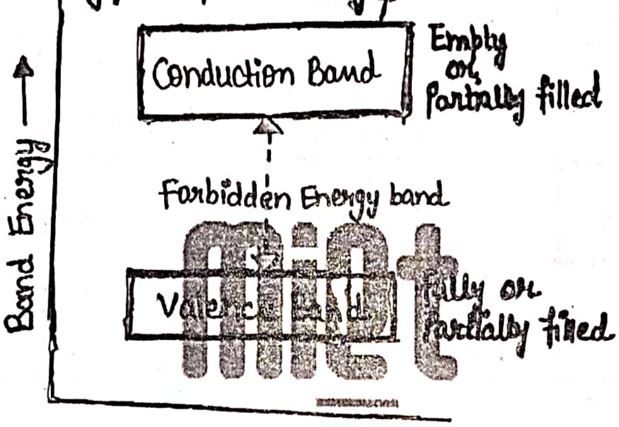
Application of band theory in solids: Formation of conductors, semi-conductors and insulators on the basis of band theory -

With the help of band theory we can classify solids into conductors, semi-conductors and insulators. In case of solids there are three bands-

* The outermost completely filled or partially filled (eg Lithium) energy band is known as Valence band.

* The band above the Valence band that is empty at 0K is known as **Conduction band**.

* The energy gap between Valence & Conduction band is known as **Energy gap or band gap or forbidden gap.**

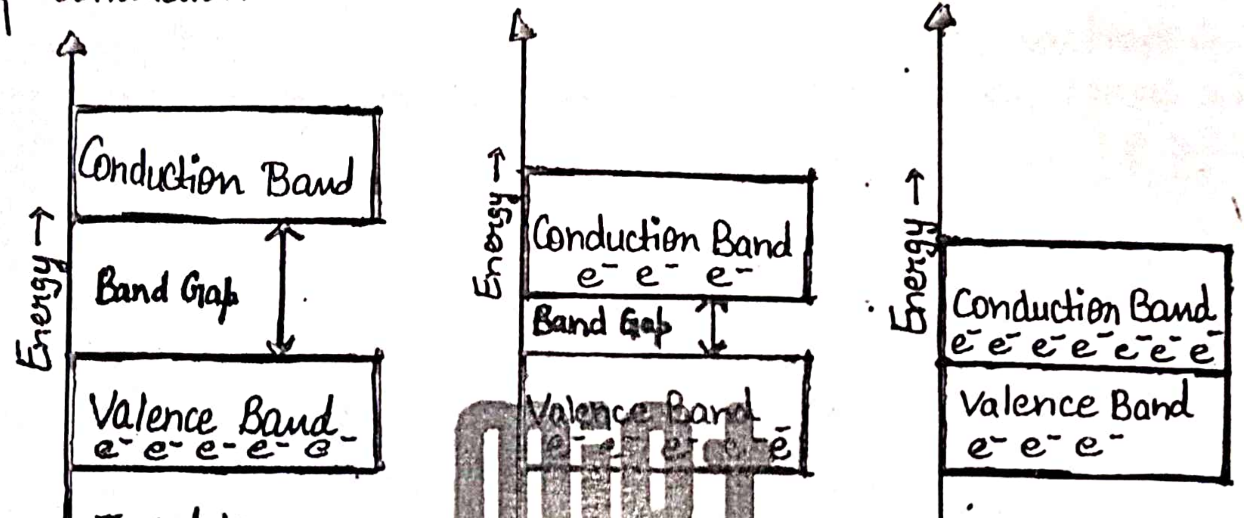


Conductors: No forbidden gap between Valence band and conduction band. The two bands overlap. Hence even at room temperature, a large number of electrons are available for conduction.
eg. Iron.

Insulators: Large forbidden gap in between the conduction band and the valence band (about 7eV)
Electrons can not jump from the valence band to the conduction band. Hence, such materials cannot conduct electricity.
Example: diamond, glass, wood, mica, paper etc.

Semiconductors: The forbidden gap is in between conductors and insulators (1 eV). Doping or the energy provide by the heat at room temperature can move the electrons from the Valence band to conduction band.

Therefore at room temperature, Semiconductors are capable of conduction.



Property	Insulators	Semiconductors	Conductors.
Electrical conductivity	Negligible 10^{-13} mho/m	B/w those of conductors & Insulators i.e- 10^{-7} mho/m to 10^{-13} mho/m	very high 10^{-7} mho/m
Resistivity	Very High more than 10^{5} Ω-m	b/w those of conductors & Insulators i.e- 10^{-5} to 10^{5} mho/m	Negligible less than 10^{-5} Ω-m
Energy-gap	Very large e.g. in diamond ΔE_g = 7e.v.	More that in conductors but less than that in Insulators eg in Ge, ΔE_g = 0.72 eV, in Si, ΔE_g = 1.1 eV in Ga. As ΔE_g = 1.3eV	Zero or very small.

LECTURE-5 Liquid Crystals : Classification, properties & application

V. Imp

FUNDAMENTALS

Discovery of Liquid Crystal :

- began in 1888 when an Austrian botanist named Friedrich Reinitzer observed that the material known as cholesteryl benzoate had two distinct (अलग) melting point.

$$\underset{\text{(Solid)}}{\text{P-chloesteryl benzoate}} \xrightleftharpoons[\text{Transition Temp}]{145^\circ c} \underset{\text{(Liquid Crystal)}}{\text{P-chloesteryl benzoate}} \xrightleftharpoons[\text{Melting Temp}]{178^\circ c} \underset{\text{(Liquid)}}{\text{P-chloesteryl benzoate}}$$

Liquid Crystals are state of matter which has properties between those of conventional liquids and those of solid crystals. The liquid-crystalline state is often called mesomorphic state (meso meaning "intermediate"), and the liquid crystals are called mesophase.

Liquid crystals are a fourth state of matter : LC flows like a liquid and has long-range order like solids.

Classification of liquid crystals ~~:~~ LC's are classified into

1. Thermotropic Liquid crystals
2. Lyotropic Liquid crystals.

1.) Thermotropic liquid crystals - They are formed by change in temperature. These liquid crystals are further classified into

a) Nematic Liquid Crystals
b) Smectic Liquid Crystals
c) Cholesteric Liquid Crystals
d) Discotic Liquid Crystals

2.) Lyotropic Liquid Crystals - These are made on change in the concentration of mesogen and/or change in temperature.

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~~Ques~~ What is liquid crystalline state? Describe the various types of liquid crystals. Give the application of liquid crystals.

OR.

What do you mean by mesomorphic state? Discuss its classification. Give their important applications. Differentiate between nematic and smectic liquid crystals.

(2014-15, 2016-17, 2017-18, 2019-20, 2020-21)

Ans. Liquid crystals are state of matter that has properties between those of conventional liquids and solid crystals. The liquid crystalline state is often called Mesomorphic State (mezos means intermediate), and the substance itself is called Mesophase.

Properties of liquid crystals.

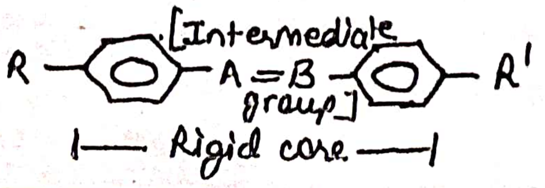
- The molecules are rod shaped or disc shaped.
- All liquid crystals are mesogens but all mesogens are not liquid crystals.
- Molecules are anisotropic in nature.
- Molecules possess very strong dipole moment.

The molecules prefer to align parallel to each other due to strong intermolecular attraction (π-π interaction).

Assuming the direction of preferred orientation in a liquid crystal to be ↑, (the direction is represented by an arrow, called the director of the L.C) each molecule is oriented at some angle to the director.

A typical L.C. molecule is represented by a central rigid part, known as mesogen (generally aromatic) and the flexible ends (generally aliphatic groups).

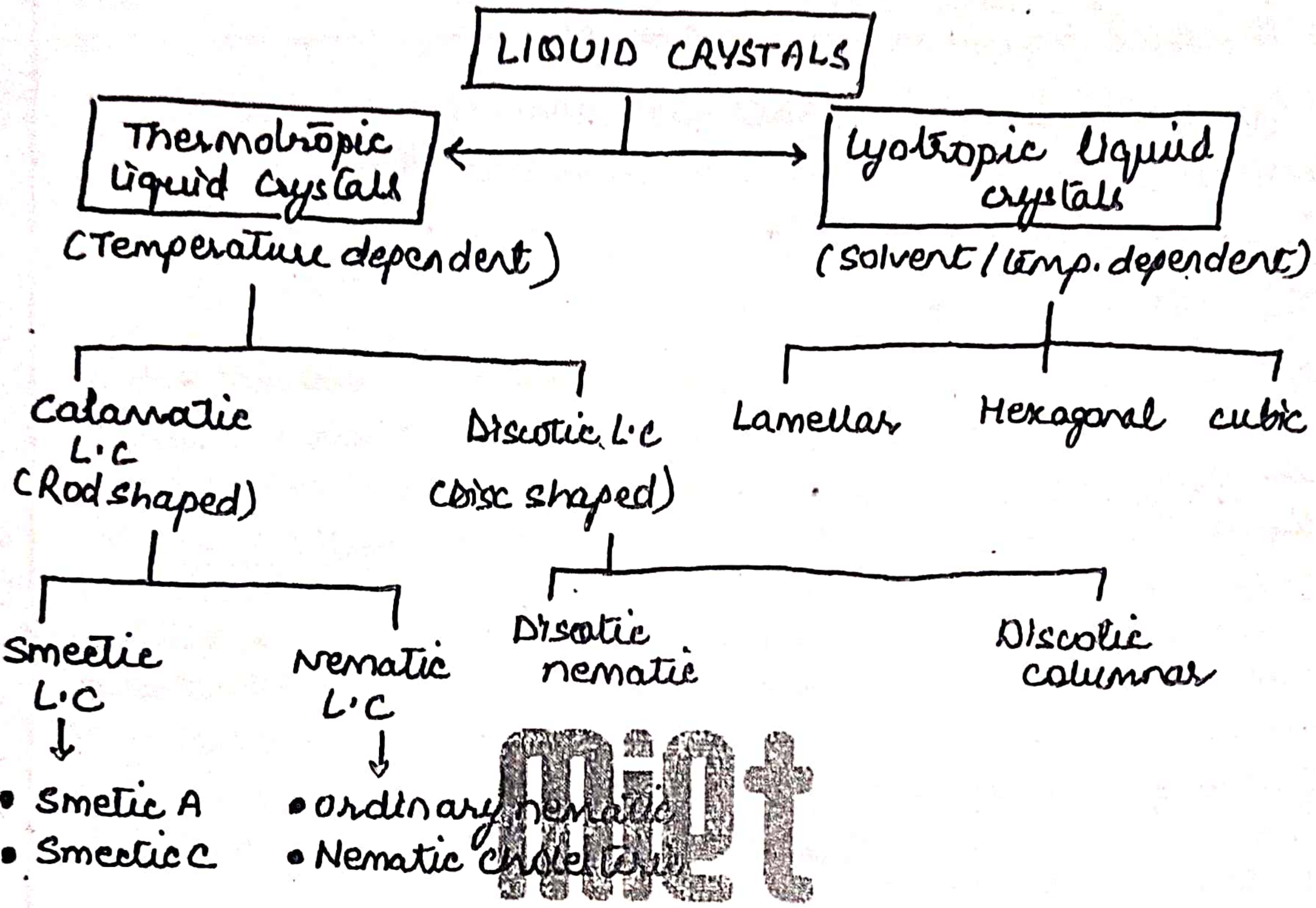
It consists of 2 or more ring systems connected by a central linkage group.



(R, R' - semiflexible end chains)

(A=B → Intermediate group).

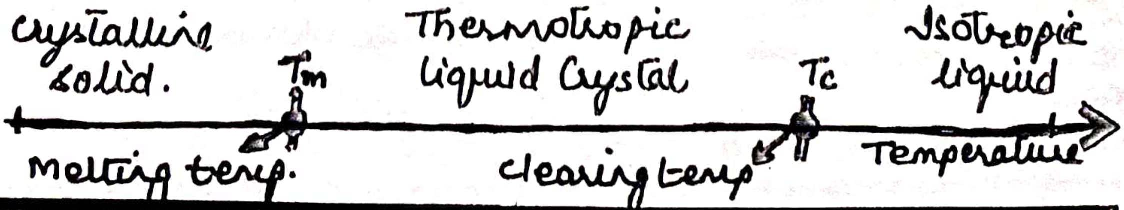
Classification of liquid crystals



1. Thermotropic liquid Crystals :

Thermotropic L.C are formed by change of temperature. They occur घटित as liquid crystals over a certain temperature range between solid and liquid phase. Example - LCD TV's, alarm clocks

$$\text{Solid crystal} \underset{\text{cool}}{\overset{\text{Heat}}{\rightleftharpoons}} \text{Thermotropic Liquid crystals} \underset{\text{cool}}{\overset{\text{Heat}}{\rightleftharpoons}} \text{liquid}$$



Thermotropic L.C. are further classified into:
a) calamatic liquid crystals (Rod shaped elongated molecules)
b) Discotic liquid crystals (Disc shaped molecules)

a) Calamatic liquid crystals are elongated rod shaped molecules which are further classified into:
i) Nematic liquid crystals
ii) Smectic liquid crystals

i) Nematic liquid crystals: Word 'nematic' is derived from the Greek word 'Nema' which means thread. These molecules are essentially (आवश्यक रूप से) rod like i.e elongated in shape. Nematic liquid crystals are divided into ordinary nematic L.C and cholesteric Nematic crystals depending on their structure. Ordinary nematic L.C have no ordered structure of molecule whereas cholesteric L.C have the molecules in a twisted and chiral arrangement.

(I) Ordinary Nematic liquid crystals:
- The molecules does not have any positional order but has orientational order.
- It is the simplest form of liquid crystals and the molecules are free to move any where
- They flow like normal liquids and have low viscosity.
- Do not have layered structure.
- Molecules can be aligned by the application of electric or magnetic field.
- only liquid crystals which do not have any translational order.
- Eg- P-azoxy anisole (first synthetic liquid crystal to be produced.

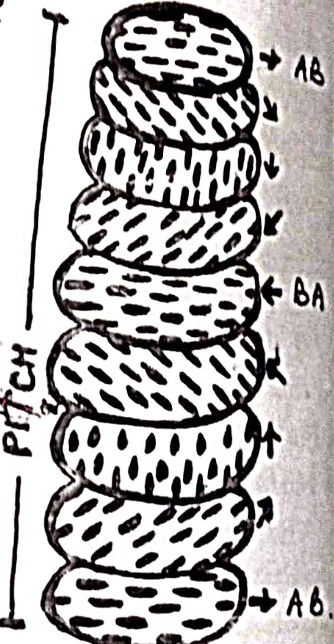
Nematic Liquid crystals.

II Cholesteric Nematic liquid crystals:
The cholesteric phase is also known as chiral nematic phase.
These are formed by adding chiral twisting agents to

nematic liquid crystals.

- This phase is typically composed of nematic mesogenic Molecu containing a chiral centre.
- The molecules are organized in layers with positional orde within layers but a director axis which varies with layers.
- Each layer in cholesteric liquid crystal is tilted with respect to the other one, and in this way molecules take a complete turn of 360° to make a helix.
- The distance covered by the director to make a one complete turn of 360° by the molecules is known as pitch.
- Pitch is inversely proportional to the temperature

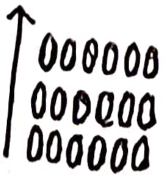
  Pitch is affected by the change of temperature, pressure, electric and magnetic field
- This phase is usually observed in cholesterol derivatives so is the name cholesteric L·C
- Example : Cholesteroyl benzoate (It was the first liquid crystal to be identified)



cholesteric L·C

ii Smectic liquid Crystals

- They are soap like (smectic means cleaning or having soap like properties) and are clayey or greasy.
- Molecular are rod shaped, elongated and cigar like.
- found at lower temperature than nematic L·C
- They are arranged in layers
- Do not flow like normal liquids and have high viscosity.
- Not affected by external electric or magnetic field.



Smectic A

smectic C

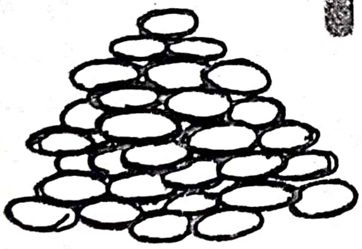
- Molecules are free to move within the layers, but not from one layer to another.
- Different layers can slide over one another
- Have short range orientational as well as positional order.
- Are of two types Smectic A & Smectic C.
- Smectic A molecules are aligned parellel to the director while that of smectic C are slightly tilted at some angle to the director.
- Eg - Ethyl-p-azoxy phenetole.

b) Discotic liquid crystals

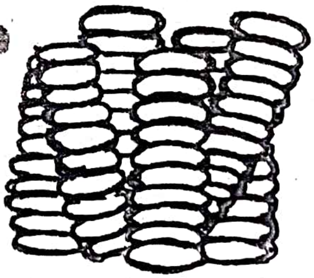
Molecules are essentially disc shaped. They are classified into:

i) **Discotic nematic**: The molecules are disc shaped. They have orientational order but no positional order.

ii) **Discotic columnar**: The [illegible] are packed in stacks the phase is called discotic columnar.



Discotic nematic



Discotic columnar

2 Lyotropic Liquid Crystals

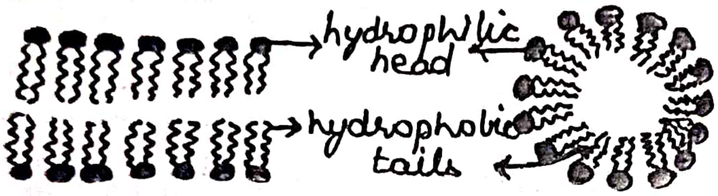
These are made by change in the concentration of solvent and/or change in temperature.

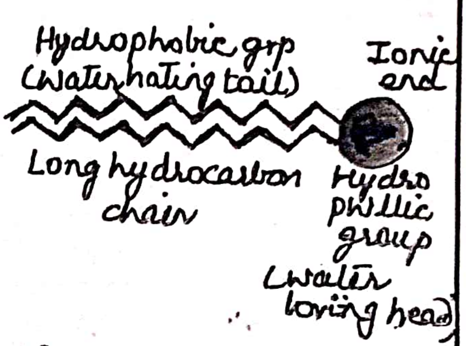
The mesogen is added to the solvent until critical मिसेल micelle concentration (CMC) is reached. On further addition of solvent LLC changes to liquid phase.

$$\text{Solid crystals} \xrightarrow{\text{solvent}} \text{Lyotropic liquid crystals (Critical Micelle conc.)} \xrightarrow{\text{solvent}} \text{Liquid.}$$

- Many amphiphilic molecules show lyotropic liquid crystal phase.
- These amphiphiles are made up of two immiscible hydrophilic and hydrophobic parts.

The hydrophilic part is polar part (head) and the hydrophobic part is called tail.





Lyotropic liquid crystals

Lyotropic liquid crystals are classified into lamellar, hexagonal and cubic liquid structures depending on their structure. If LLC have hexagonal structure, then they are called hexagonal if they have lamellar structure, then called lamellar and if cubical structure then known as cubic LLC. Eg. detergent, soap, phospho lipids

Uses
Applications of liquid crystals

- Used in cosmetics
- Due to their colour effect, cholesteric L.C are used in nail paints, eye shadows etc.
- Used for displays in LCD's, calculators, wrist watches etc
- Used in coloured thermometers.
- Used in research work.
- Used in electronic industries.
- Used for localized drug delivery.

Difference between Nematic and Smectic liquid crystals.

Nematic Liquid Crystal	Smectic Liquid Crystal.
1. They are thread like.	1. They are soap like and are clayey or greasy.
2. Molecules have elongated rod like shape.	2. Molecules are cigar shaped.
3. Do not have layered structure.	3. They have layered structure.
4. Flow like normal liquids.	4. They do not flow like normal liquids and has limited mobility.
5. They have low viscosity.	5. They have high viscosity.
6. Formed at relatively higher temperature.	6. Formed at comparatively lower temperature.
7. Flow in all directions & not in layers.	7. Flow in layers and different layers can slide over one another.
8. Can be aligned by the application of electric or magnetic field.	8. Not affected by external electric or magnetic field.
9. E.g P-azoxy anisol	9. E.g - Ethyl-p-azoxyphenetole.

M. Imp

Ques-2 Define the term Pitch. What is it significance? (2016-17)

Ans Pitch is defined as distance travelled by the director when it gets turned by 360°. It is affected by temperature, pressure and electric or magnetic field. It is inversely proportional to the temperature. This property of cholesteric liquid crystals finds the application in coloured thermometers, in nail paints, eye shadows etc.

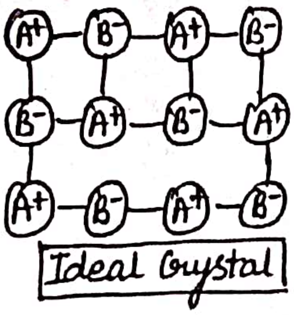
X LECTURE-6

Point defects in solids : Zero Dimensional Defects - FUNDAMENTAL

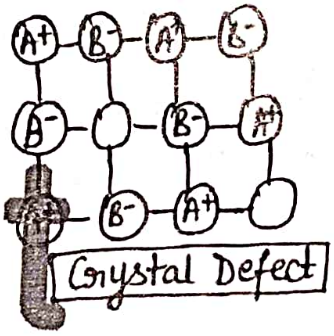
Ideal Crystal - An ionic crystal which has the same unit cell containing the same lattice points throughout the whole crystal.

Ideal Crystal exists only at absolute zero (0K) temperature.

Crystal Defect - Any deviation from a perfectly ordered arrangement of constituents (ions or atoms) in a crystal is known as crystal imperfection or defect.

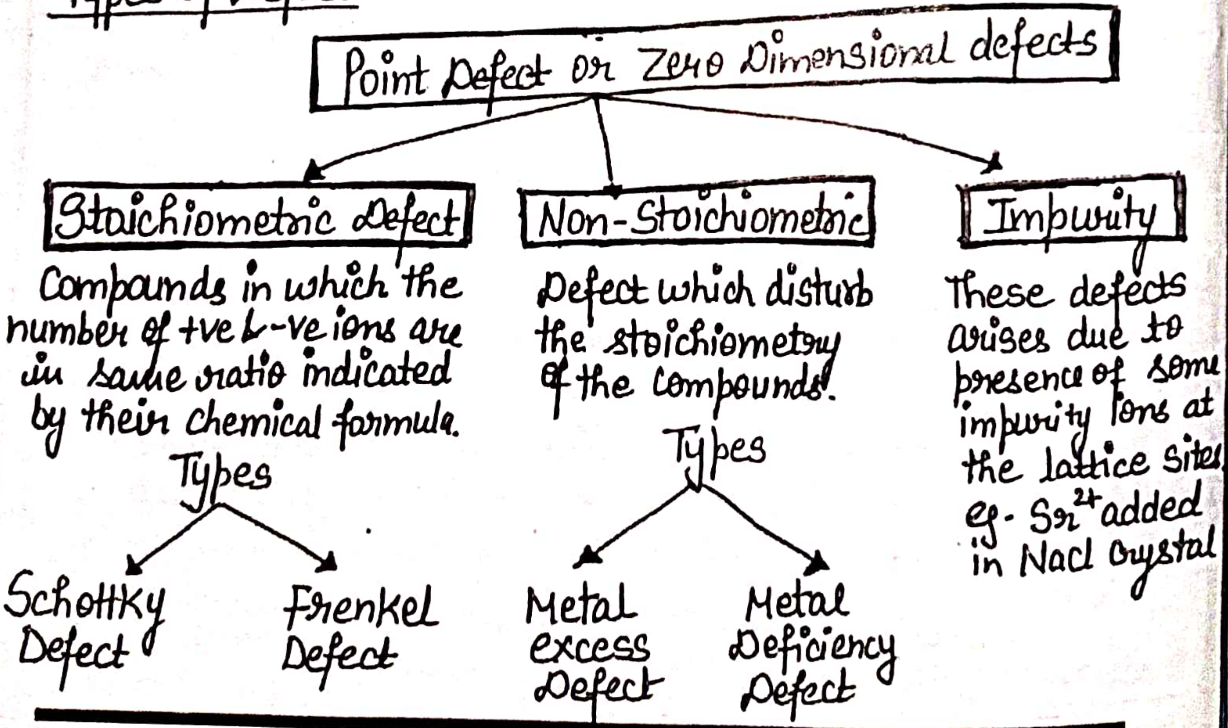


Ideal Crystal



Crystal Defect

Types of Defect -



Point Defect or Zero Dimensional defects

Stoichiometric Defect - Compounds in which the number of +ve & -ve ions are in same ratio indicated by their chemical formula.

Types

- Schottky Defect
- Frenkel Defect

Non-Stoichiometric - Defect which disturb the stoichiometry of the compounds.

Types

- Metal excess Defect
- Metal Deficiency Defect

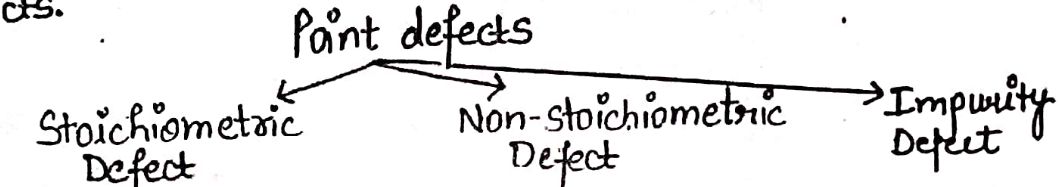
Impurity - These defects arises due to presence of some impurity ions at the lattice sites eg- Sr^{2+} added in NaCl crystal

M.Imp
ues-1 What is crystal imperfection ? Explain the one dimensional imperfection in solid. (2015-16)

ns Crystal defect or Crystal imperfection.-

Any deviation from a perfectly ordered arrangement of constituents (ions or atoms) in a crystal is known as crystal imperfection or defect.

Point defect or one dimensional defect - When the deviation exists from the regular or periodic arrangement around an atom or a group of atom in a crystalline substance, the defects are called point defects.



) Stoichiometric Defect - The compound in which the number of +ve & -ve ions are exactly in the ratios indicated by their chemical formulas are called stoichiometric defects.

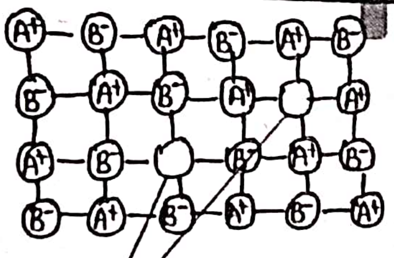
These defects do not disturb the stoichiometry (ratio of +ve & -ve ions) of solids.

Also known as thermodynamic defects as these occur due to increase in temperature.

These are of following types :

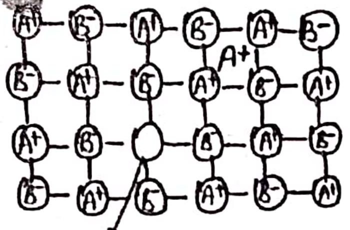
- Vacancy defects : Occurs when one or more atoms are completely missing from the lattice site creating a vacancy or hole. It decreases the density of the crystal E.g. Schottky defect.
- Interstitial defects : Occurs when an atom occupies a position other than its normal lattice position. The density of the crystal remains the same E.g. Frenkel defect.

Schottky defect	Frenkel Defect
1. Equal no. of cations and anions are missing from crystal lattice.	1. An ion is missing from the lattice site and occupies interstitial position.
2. It is a Vacancy defect.	2. It is a hybrid of Vacancy defect & interstitial defect.
3. Occurs in highly ionic compound, which have high coordination number.	3. Occurs in compounds with low coordination number.
4. Occurs in crystals having same size of anions & cations.	4. Occurs in crystal where cations & anions are of difference sizes (cations are smaller.
5. It decreases the density of crystal.	5. Density of the crystal remains the same as before.
6. Found in pure alkali metal halides.	6. Not found in pure alkali metal halides as in them cations are large in size
7. E.g - $NaCl$, $AgBr$	E ZnS, $AgCl$, AgI, $AgBr$.



Pair of ions missing from lattice

Schottky Defect



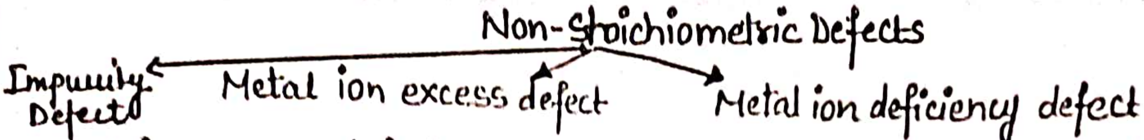
A cation missing from the lattice

Frenkel Defect

b) Non-stoichiometric Defect - The defect which disturb the stoichiometry of the compounds are called non-stoichiometric Defects.

These are either due to the presence of excess metal ions or deficiency of metal ions.

Electrical neutrality of ionic crystal is maintained due to the presence of either extra positive charge on one of the neighbouring cation or presence of extra free electron in crystal lattice.



Metal ion excess defect - May be due to anionic vacancy or due to extra interstitial cation.

Due to Anionic Vacancy	Due to extra Interstitial Cation
1. Arises when some of the negative ions (anions) are missing from the lattice site.	1. Arises when the voids or interstitial sites are occupied by additional metal ion.
2. Absence of anion from the crystal lattice leaves a hole which is occupied by an electron to maintain electrical neutrality.	2. Electrical neutrality is maintained by corresponding number of electrons present in same interstitial site.
3. Crystals which are likely to show Schottky defects show anionic vacancy defects.	3. Crystals which are likely to show Frenkel defects show such defects.
4. F centres or colour centres are created.	There are no F centres
5. Eg. Nacl	Eg Zno

Metal ion deficiency defect :

Due to cationic Vacancy	Due to extra interstital anion
1. Arises when a cation is missing from its lattice.	1. Arises due to presence of extra anion at the interstitial site.
2. Occurs in ionic solids where metal ion can exhibit variable Valency	2. Not practically possible (Anion being larger in size cannot fit in voids.
3. To maintain electrical neutrality one of the nearest metal ion acquires the positive charge.	3. The extra negative charge is balanced by one extra positive charge on adjacent metal ion.
4. Eg. Transition metal compounds like NiO, FeO, FeS etc.	4. No example known so far.

Ans:-6

$$GCV = \frac{(W+w)(t_2-t_1+C_c)-(C_A+C_F+C_{cr})}{x}$$

$$= \frac{(2200+550)(2.42)-(50+10)}{0.92}$$

$$= \frac{(2750)(2.42)-(60)}{0.92}$$

$$= \frac{6595}{0.92} = 7168.48$$

$$= \boxed{7168.48\ cal/gm}$$

Ans:-

$$NCV = HCV - 0.09 \times H\% \times 580\ cal/gm$$

$$= 7168.48 - 0.09 \times 6 \times 580$$

$$= 7168.48 - 313.2$$

$$= 6855.28\ cal/gm.$$

Imp

Ques 7 A sample of coal contains C = 93%, H = 6% + ash = 1%. The following data were obtained when the above coal was tested in Bomb's calorimeter:

(i) weight of coal burnt = 1.029 gm

(ii) weight of water taken = 2200 gm

(iii) water equivalent of calorimeter = 570 gm

(iv) Rise in temprature = 2.3°C

(v) Cooling correction = 0.047°C

(vi) Acid correction = 62.6 cal

(vii) Fuse wire correction = 3.8 cal

(viii) Cotton thread = 1.6 cal

Imp

Qu-1. The voltage of the cell $Pb/PbSO_4/Na_2SO_4/Hg$ is 0.9647V at 25°C. The temprature cofficient is 1.74×10^{-4} VK^{-1} calculate the value of $\Delta G, \Delta S, \Delta H$ (2018-19)

Ans- $\Delta S = nF\left(\frac{\partial E}{\partial T}\right)_P$

$n = 2$; $F = 96500 \, C/mol$ $\left[\frac{\partial E}{\partial T}\right]_P = 1.74 \times 10^{-4}$.

$\Delta S = 96500 \times 2 \times 1.74 \times 10^{-4} = 33.58 \, JK^{-1}$

$\Delta H = nF\left[T\left(\frac{\partial E}{\partial T}\right)_P - E\right] = 96500 \times 2 [298 \times 1.74 \times 10^{-4} - 0.9647]$

$= -1.76 KJ$

$\Delta G = \Delta H - T\Delta S = -176 - 298 \times 33.58 = -176 - 10$

$= -186 \, KJ \, mol^{-1}$

M. Imp

Qu-2 The emf of a cell measured by means of hydrogen electrodes against a saturated colonal electrodes at 298 K is 0.4100V. If the presence of H_2 was maintained at 1 atm, calculate the pH of the unknown solution. Give potential of reference electrodes is 0.2415V (2019-20)

$E_{cell} = 0.4100V$

Cell. $Pt / H_2(g) / H^+ \| KCl(salt), HgCl_2(s) / Hg(l) \; Pt$; Given
(anode) (cathode)

$E^\circ_{Hg^{+2}/Hg} = 0.2415V$

$E^\circ_{H^+/H_2} = 0V$

Cell Reaction:-

at anode:- $HgCl_2 + 2e^- \longrightarrow Hg(l) + 2Cl^-$

at cathode- $\left[\frac{1}{2}H_2 + Cl^- \longrightarrow HCl + e^-\right] \times 2$

Netcell Reaction:

$HgCl_2(s) + H_2(g) \longrightarrow 2HCl(aq) + Hg(l)$

or

$Hg^{+2}(s) + H_2(g) \longrightarrow 2HCl(aq) + Hg(l)$

Then $Q = \dfrac{[H^+]^2 [Hg(l)]}{[Hg^{+2}_{(s)}] [H_2(g)]}$

Since

$[Hg(l) = [Hg^{+2}_{(s)}] = 1$ and $H_2(g) = 1$ atm

Thus $Q = \dfrac{[H^+]^2}{[Hg(g)]} = [H^+]^2$

Now

$E^\circ_{cell} = E_{cathode} - E_{anode} = 0.2415V - 0.0V$
$= 0.2415V$

Now Nernst Equation,

$E_{cell} = E^\circ_{cell} - \dfrac{0.0592}{n} \log Q$

$E_{cell} = E^\circ_{cell} - \dfrac{0.0592}{n} \log [H^+]^2$

$0.4188 = 0.2415 - \dfrac{0.0592}{2} \log [H^+]^2$

$0.4188 - 0.2415 = -\dfrac{0.0592}{2} \times 2 \log H^+$

$0.1773 = 0.0591\ pH$

Note $\boxed{pH = -\log[H^+]}$

Thus

$pH = \dfrac{0.1773}{0.0591}$

$\boxed{pH \simeq 3}$ Ans

Imp
Ques-2 Explain Impurity defects (2020-2021)

Ans. Impurity defects arises when foreign atoms i.e atoms different from host atoms, are present in the crystal lattice. Germanium is common impurity in silicon. There are two types of impurity defects:

Substitutional defects: when the host atom is substituted by some other atom.

Interstitial defects: when the atoms different from host atoms are present in the interstitial spaces.

⁂

Imp
F-centers:- The e^- occupying holes, created by missing of anions from the lattice sites are called F-centers. There F-centers are responsible for colour of compound. eg:- When crystals of NaCl are heated in an atmosphere of sodium vapour, the sodium atoms are deposited on the surface. The Cl ions diffuse from the crystal to the surface & combine with Na atoms forming NaCl. During this process, the Na atoms on the surface of the crystal lose electrons & these diffuse electrons occupy the vacant anionic sites.

LECTURE - 7

Structure and Applications of Graphite & fullerene

FUNDAMENTAL

Allotrope : Allotropy or allotropism is the property of some chemical elements to exist in two or more different forms, known as allotropes of these elements.

Allotropes of Carbon :

1. **Diamond** - It is the hardest known natural mineral and finds applications in cutting, drilling & jewellery.
2. **Graphite** - Graphite is a 2D covalent solid and has planar structure.

→ It is the most stable form of the carbon.

→ Thermodynamically more stable than diamond.

→ Unlike diamond, graphite is an electrical conductor.

→ Graphene is a single layer of carbon atoms arranged in one plane; layers of graphene make up graphite and its possible applications in electronics.

3. **Fullerene** (Discovered by Kroto & Smalley)

→ It is an allotrope of carbon, also called buckminster fullerene or Bucky Ball.

→ Fullerenes are a class of carbon allotropes in which carbon takes the form of a hollow sphere.

→ C_{60} is the most stable member of fullerene family.

→ It is an allotrope of carbon with truncated icosahederon geometry. It is highly symmetrical & is said as zero dimensional.

Structure - There are 12 pentagons & 20 hexagons of C atoms.

Preparation of Fullerene : Fullerene are prepared by Arc Discharge Method.

⑦

I.M.P

Ques What are lubricants? Give the structure, properties and uses of graphite. Explain its lubricating properties.

OR

With the help of neat diagram describe the structure of graphite. Also give atleast five applications of graphite.
(2014-15, 2016-18, 2017-18).

Ans A lubricant is a substance that helps to reduce friction between surface in mutual contact, which ultimately reduces the heat generated when the surfaces move.

GRAPHITE : AN ALLOTROPE OF CARBON

Structure of graphite -

Graphite is an allotrope of carbon. (it is made up बना of only pure carbon atoms).

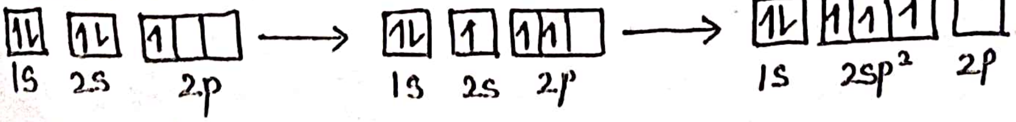
Each carbon atom in graphite is sp^2 hybridised. संकरण

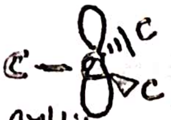
6 such carbon atoms join with the covalent सहसंयोजक bonds to form hexagons षट्भुज. थर्मोडायनामिक

In hexagons each carbon atom forms three covalent bond (C-C distance is 1.42 A°) with the other carbon atoms.

- Fourth electron of each carbon ~~atom~~ is free to move within the layer.
- Various hexagons षट्भुज join together to form a plane or sheet called नाम graphene.
- Various sheets (graphenie) are arranged one above the other.
- Different layers of graphite are attached to each other with weak Vander Waals forces.
- Distance between two successive लगातार आते sheets is 3.41 A°.
- Graphite has planar, two dimensional आकार structure.

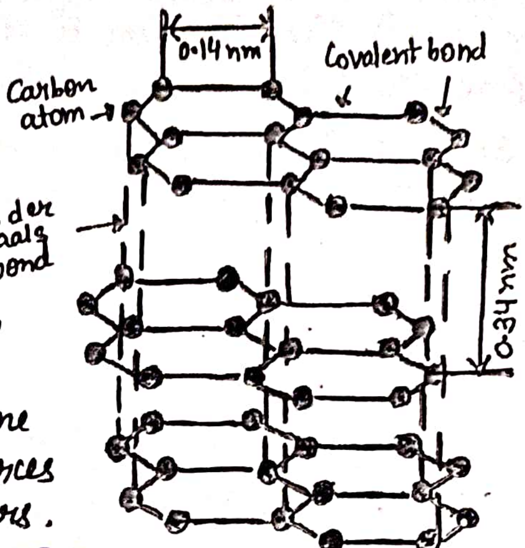
Hybridisation संकरण of C in graphite:





Trigonal Planar Carbon in graphite

Properties of Graphite :



1. It is greyish black and greasy substance. धूसर पदार्थ चिकना
2. Has metallic lustre and its opaque to light. धात्विक चमक अपारदर्शी
3. High melting point because the strong covalent bonds take long time to break. उच्च गलनांक
4. Slippery nature / layers can slide one another due to weak Vander Waal forces of attraction between the two layers.
5. Low coefficient of friction. – घर्षण गुणांक
6. Ineffective in vaccum conditions. अप्रभावी निर्वात
7. Thermodynamically more stable than diomond. ऊष्मागतिक स्थिर
8. Graphite exists in two forms: α-graphite and β-graphite.
9. Graphite is a conductor due to the presence of free electron in P_z orbital of each carbon
10. Density $1.25 g/cm^3$

Applications of Graphite :

- Used as lubricants as layers can slide over one another due to weak Vander waal forces. स्नेहक परत ऊपर खिसके
- Used in pencil leads due to soft, slippery nature and it leaves a black mark on paper when rubbed against it.
- It is used in preparation of electrods as it conduct electricity. तैयारी
- Due to high melting point it is used to prepare crucible. घरिया
- It is used as moderator in nuclear reactors as it absorbs fast moving neutrons. मंदक परमाणु रिएक्टर
- Used as a conduction of electricity.

Imp

Ques-2 Explain the structure of graphite. (2014-15, 2016-17).

Ans.
- Graphite is an allotrope of carbon. Each carbon atom in graphite is sp^2 hybridised and is bonded to three other carbon atoms covalently to form hexagons.
- The hexagons join together to form layer. Several layers are arranged one above the other in a series.
- Strong covalent bonding between carbon atoms within the layer and C-C distance is 1.42A°.
- Different layers held together by weak vander waal forces and the distance between two successive sheet is 3.41 A°.

Ques-3 Graphite is good conductor of electricity. Why? (2017-18)

Ans Graphite is good conductor of electricity because in graphite all the carbon atoms are sp^2 hybridised and each carbon has one free electron to conduct the electricity.

Imp

Ques-4 Why graphite is used as lubricant? (2018-19)

Ans. Graphite is used as lubricant because it is soft and slippery. Its layers can slide over one another due to presence of weak Vanderwaals forces between them.

M.M.Imp (S)

~~Ques~~-5 Discuss the preparation, properties and application of an allotrope of carbon having truncated icosahedrons geometry. (2014-15, 2015-16, 2016-17, 2019-20, 2020-21).

Ans FULLERENE (Discovered by Kroto & Smalley)

अपररूप

- It is an allotrope of carbon, also called buckminster fullerene or Bucky Ball.
- C_{60} is the most Stable & widely use member of fullerene family.

स्थिर व्यापक रूप

Structure : There are 12 Pentagons (पन्चकोण) & 20 hexagons (षट्कोण) of C atoms.

- No two Pentagons touch each other.
- Diameter of C_{60} 7A°; geometry - geodesic dome.
- There are 30 CC=C) double bonds in C_{60}.
- There are 60 vertices, 32 faces. भागने
- C-C Single bond length - 1.43 A°, C=C double bond length = 1.38A°
- It is highly symmetrical (सममित) molecular & is said as zero dimensi (आकार)
- Fullerene crystal structure is FCC.
- Its density is 1.65 gm/cc.

Preparation of Fullerene : Fullerenes are Prepared as Arc Dischar

Method :

Graphite rods kept in an inert (निष्क्रिय) atmosphere (He gas) (0.05 to 1 atm Pressure)

↓ Electric current

Rods evaporate to give fullerene soot containing 5 to 15% fulleren

↓ Sublimation

Fullerene mixture

↓ chromatography using alumina hexane

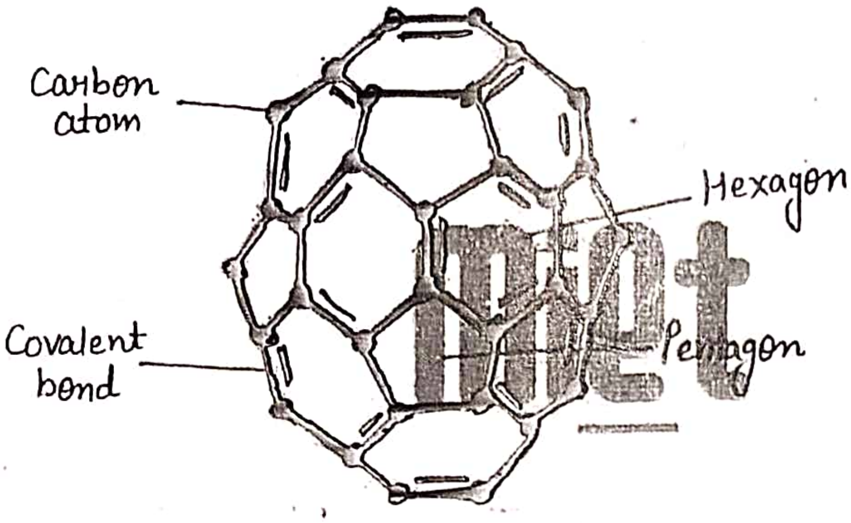
C_{60}

Properties :

- Mustard colored solid and looks brown and black as its thickness increases.
- Basically semiconductors but on doping with alkani metals can be Converted into Conductor or super conductor.
- Shows poor aromatic nature.
- Strongest known material to man.
- Exists as discrete molecule unlike graphite or diamond.
- Pentagon of a fullerene are more strained than the hexagon.
- It is possible to trap some ions inside fullerene cage.
- Can be compressed to lose 30% of its original volume, without destroying the Carbon edge structure.

Uses:/ APPLICATION.

- Have powerful antioxidant properties, so used in health & personal care areas.
- C_{60} shows Catalytic process.
- Act as drug delivery agent.
- C_{60} derivatives act as potential inhibitors to HIV.
- Used in preparation of Superconductors
- In optical devices.
- Used in batteries as charge carriers.



Fullerene Structure

LECTURE-8

Concepts, Properties & applications of Nono-Science & Nano-material.

(10) FUNDAMENTAL फन्डा-मेन्टल

Nanomaterials: Materials having at-least one of its dimensions in the nanometre scale ($1 nm = 10^{-9} m$).

Nanotechnology: is the technology of manipulating a material and its properties at the nanoscale (atomic or molecular scale) for target-specific applications.

Nanostructured materials: Nano materials can be zero, one, two or three dimensional.

- Nanoparticles
- Nanowires
- Nanotubes
- Nanorods
- Nanopourous materials

Nanomaterial synthesis Approach -

1. **Top down approach** (ऊपर): Breaking of bulk material.
2. **Bottom up approach** (नीचे): Building up of material: Atom → molecule → cluster

In major view nanomaterials has found their applications in many major areas like Electronics, Medicine, Engineering and technology, industries etc.

Method For the Preparation of Nanomaterials by Top down approach:-
Grinding, Milling, Laser ablation, Thermal decomposition.

Method For the preparation of Nanomaterials by bottom-up approach:
chemical Reduction, Precipitation, Collaidal dispersion.

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Ques-1 Give five applications of nanomaterials.

OR

Give applications of nanomaterials in electronic and medicines. (2017-18, 2018-19).

Ans In major view nanomaterials has found their applications in many major areas :

- Electronics : Used to prepare nano chips.
- Medicine : Used for centralized drug delivery.
- Engineering and technology
- Industries
- Environment
- Sensors
- Catalysis

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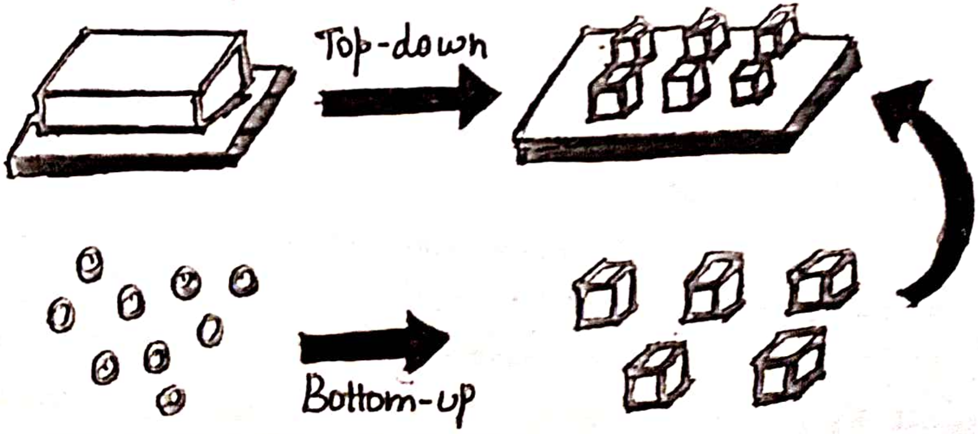
Ques-2 Give the approaches used for the preparation of nanomaterials. (2018-19)

Ans Approach for synthesis of nanomaterial can be either of the two -

Top down Approach - It involves the production of very small structures from larger piece of material.

Bottom Up Approach - It involves atom by atom or molecule by molecule production of nanomaterials.

Buildup of material : Atom → molecule → cluster.



5 Year's

University Previous Questions

(Questions Bank)

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5 Years AKTU University Examination Questions		Unit-1	
S. No	**Questions**	**Session**	**Lecture No**
1	Discuss the postulates of Molecular Orbital Theory OR Outline the salient features of MOT on the basis of LCAO principle.	(2016-2017) (2018-2019)	L 1
2	Explain BMO and ABMO and differentiate between them.	(2018-2019)	L 1
3	On the basis of MO theory explain why hydrogen forms diatomic molecule while helium remains monoatomic	(2014-2015)	L 2
4	Explain why bond energy of N_2 is greater than bond energy of O_2?	(2015-2016)	L 2
5	Calculate the bond order of N_2^- and O_2^+	(2015-2016)	L 2
6	Calculate the bond order of N_2	(2016-2017)	L 2
7	Calculate the bond order of $N2^+$.	(2017-2018)	L 2
8	Arrange the following in the increasing order of their bond energy O_2, O_2^{2+}, O_2^{2-}.	(2017-2018)	L 2
9	Draw the molecular orbital diagrams of N_2 and O_2 Calculate their bond orders and write its magnetic behavior	(2016-2017) (2017-2018)	L 2
10	Explain why O_2 is paramagnetic in nature	(2017-2018) (2018-2019)	L 2
11	Arrange the following molecules/ions in order of their increasing bond length: N_2, N_2^- and N_2^{2-}	(2018-2019) (2019-2020)	L 2
12	Why O_2 is paramagnetic and N_2 is diamagnetic?	(2020-2021)	L 2
13	With the help of molecular orbital diagram explain the formation of NO and CO. Also calculate their bond order and predict their magnetic behavior?	(2015-2016) (2018-2019) (2019-2020)	L 3
14	Calculate bond order, magnetic behavior and order of stability of NO, NO^-, NO^+	(2020-2021)	L 3
⑮	Explain Molecular Orbital theory in case of metals or Explain band theory in solids and on its basis differentiates between conductors, semiconductors and insulators.	(2017-2018) (2020-2021)	L 4
16	What is Liquid crystalline state? Describe the various types of liquid crystals. Give the applications of liquid crystals OR What do you mean by mesomorphic state? Discuss its classification on basis of temperature and give their important applications Differentiate between nematic and smectic liquid crystals.	(2014-2015) (2016-2017) (2017-2018) (2018-2019) (2019-2020) (2020-2021)	L 5
17	Define the term pitch. What is its significance?	(2016-2017)	L 5

18	What is Crystal imperfection? Explain the one dimensional imperfection in solid.	(2015-2016)	L 6
19	What are stoichiometric and non-stoichiometric defects? Explain Frenkel and Schottky defects found in solids.	(2014-2015) (2016-2017) (2017-2018) (2019-2020) (2020-2021)	L 6
20	Define schottky defect? Give example	(2019-2020)	L 6
21	Explain impurity defects.	(2020-2021)	L 6
22	What are lubricants? Give the structure, properties and uses of graphite. Explain its lubricating properties OR With the help of neat diagram describe the structure of graphite. Also give at-least five applications of graphite.	(2014-2015) (2016-2018) (2017-2018)	L 7
23	Explain the structure of graphite.	(2014-2015) (2016-2017)	L 7
24	Graphite is a good conductor of electricity. Why?	(2017-2018)	L 7
25	Why Graphite is used as lubricant?	(2018-2019)	L 7
26	Discuss the preparation properties and application of an allotrope of carbon having truncated icosahedrons geometry.	(2014-2015) (2015-2016) (2016-2017) (2019-2020) (2020-2021)	L 7
27	Give five applications of nanomaterials. OR Give applications of nanomaterials in electronics and medicines	(2017-2018) (2018-2019)	L 8
28	Give the approaches used for the preparation of nanomaterials.	(2018-2019)	L 8