

Assignment - 01

Section A

① Write down any five postulates of molecular orbital Theory.

- Ans ① When atomic orbitals overlap molecular orbitals are formed.
② the rule of overlapping is linear combination of Atomic orbitals (CAO)
③ the atomic orbitals loses their identity after overlapping.
④ the no. of molecular orbital formed is equal to total no. of atomic orbital overlapping.
⑤ Due to overlapping the system become polycentric.

② Why Li_2 exists but He_2 does not?

Ans The electronic configuration of $\text{Li}_2 = \sigma 1s^2 \sigma^* 2s^2$

\therefore the Bond order of $\text{Li}_2 = \frac{1}{2} (N_b - N_a)$

$$BO \Rightarrow \frac{1}{2} (4-2) = \frac{2}{2}$$

$$BO = 1$$

So, Li_2 exist with a single bond.

The electronic configuration of $\text{He}_2 = \sigma 1s^2 \sigma^* 1s^2$

\therefore the Bond order of $\text{He}_2 = \frac{1}{2} (2-2)$

$$BO = 0$$

So, no net bonding

$\rightarrow \text{He}_2$ does not exist

③ Why are liquid crystals anisotropic?

Ans Liquid crystals are anisotropic because their elongated molecules align in specific direction (director) instead of being randomly arranged. This partial orientational order causes properties like refractive index and electrical conductivity to vary with direction.

④ Classify nanomaterials based on their dimension. Give examples for each.

Ans Classifications of Nanomaterials :-

(i) Zero-Dimensional (0D) :- All three dimensions (length, width & height) are in the nanoscale.

Ex :- Fullerenes (C_60), Metal nanoparticles (gold, silver).

(ii) One-Dimensional (1D) :- Two dimensions are in the nanoscale, while the third dimension (length) is larger.

Ex :- Carbon nanotubes, Nanowires (ZnO , silicon nanowires)

(iii) Two-Dimensional (2D) :- Only one dimension (thickness) is in the nanoscale, while the other two dimensions are much larger.

Ex :- Graphene, MoS_2 nanosheets, metal/oxide thin films

(iv) Three-Dimensional (3D) :- Materials with nanostructures in all three dimensions, but the overall size is bulk-like.

Eg:- Nanocomposites, Dendrimers.

Q) Why are green solvents preferred over traditional solvents?

A) Green solvents are preferred because they are environment friendly, non-toxic, and biodegradable, which reduces pollution and health hazards. They also help in safer chemical processes, lower energy consumption, and minimize harmful waste compared to traditional organic solvents.

Section-B

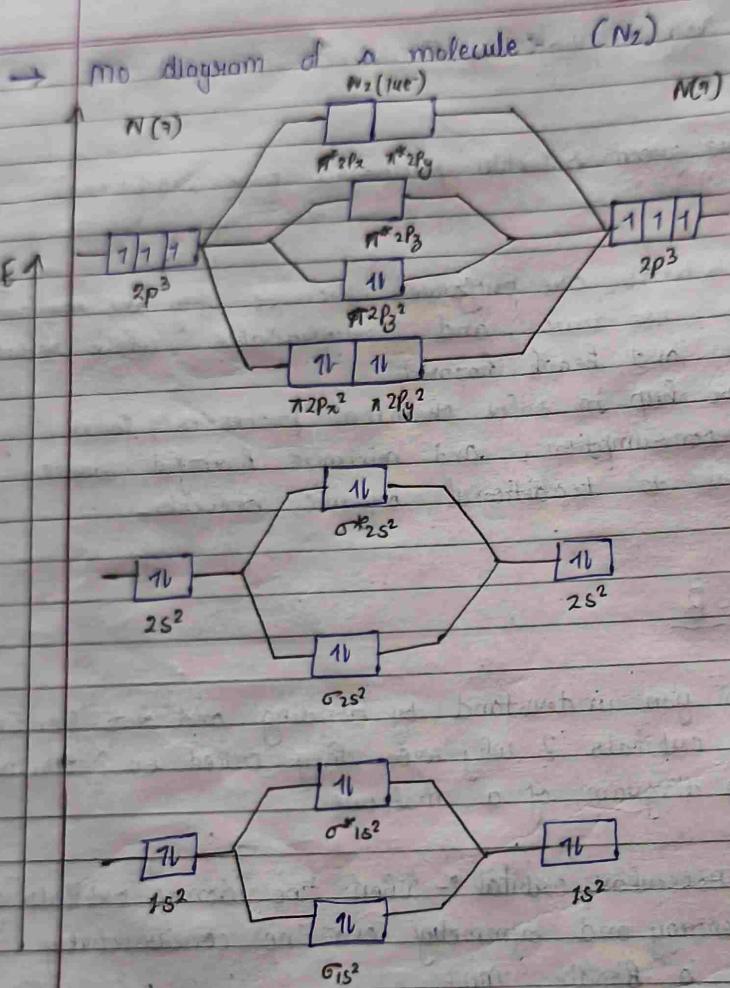
Q) What do you understand by Bonding and Anti-bonding molecular orbitals? Why are they called so? Illustrate with MO diagram of a molecule.

A) → Bonding Molecular orbital :- When two atomic orbitals of similar energy and symmetry combine constructively, they form a bonding MO.

Anti-bonding MO :- When the same atomic orbitals combine destructively, they form an anti-bonding MO.

→ They are called BMO & ABO because :-

Bonding MOs stabilize the molecule (favourable bonding). Anti-bonding MOs destabilize it (oppose bonding).



AO of N -atom MO of N_2 molecule AO of N -atom

→ orbital

- ② With the help of MOT, explain why bond order of N_2^+ is less than N_2 but bond order of O_2^+ is more than O_2 .

Ans For N_2 ($Z=7$)

Total $e^- = 14$

MO configuration of $N_2 = \sigma_{1s}^2 \sigma^*_{1s}^2 \sigma_{2s}^2 \sigma^*_{2s}^2 \pi(2p_x)^2 = \pi(2p_y)^2 \sigma(2p_z)^2$

$$BO = \frac{1}{2} [16 - 4] = \frac{6}{2} = 3$$

For N_2^+

Total $e^- = 13$

MO configuration of $N_2^+ = \sigma_{1s}^2 \sigma^*_{1s}^2 \sigma_{2s}^2 \sigma^*_{2s}^2 \pi(2p_x)^2 = \pi(2p_y)^2 \sigma(2p_z)$

$$BO = \frac{1}{2} [9 - 4] = \frac{5}{2} = 2.5$$

The bond of N_2^+ is less than N_2 bcoz 1 e^- is removed from the highest energy orbital $\sigma(2p_z)$, a bonding MO.

for O_2

Total $e^- = 16$

MO configuration of $O_2 = \sigma_{1s}^2 \sigma^*_{1s}^2 \sigma_{2s}^2 \sigma^*_{2s}^2 \sigma(2p_x)^2 \sigma(2p_y)^2 = \pi(2p_z)^2$
 $\pi^*(2p_x) = \pi^*(2p_y) \sigma^* 2p_z$

$$BO = \frac{1}{2} (16 - 6) = \frac{10}{2} = 5$$

for O_2^+

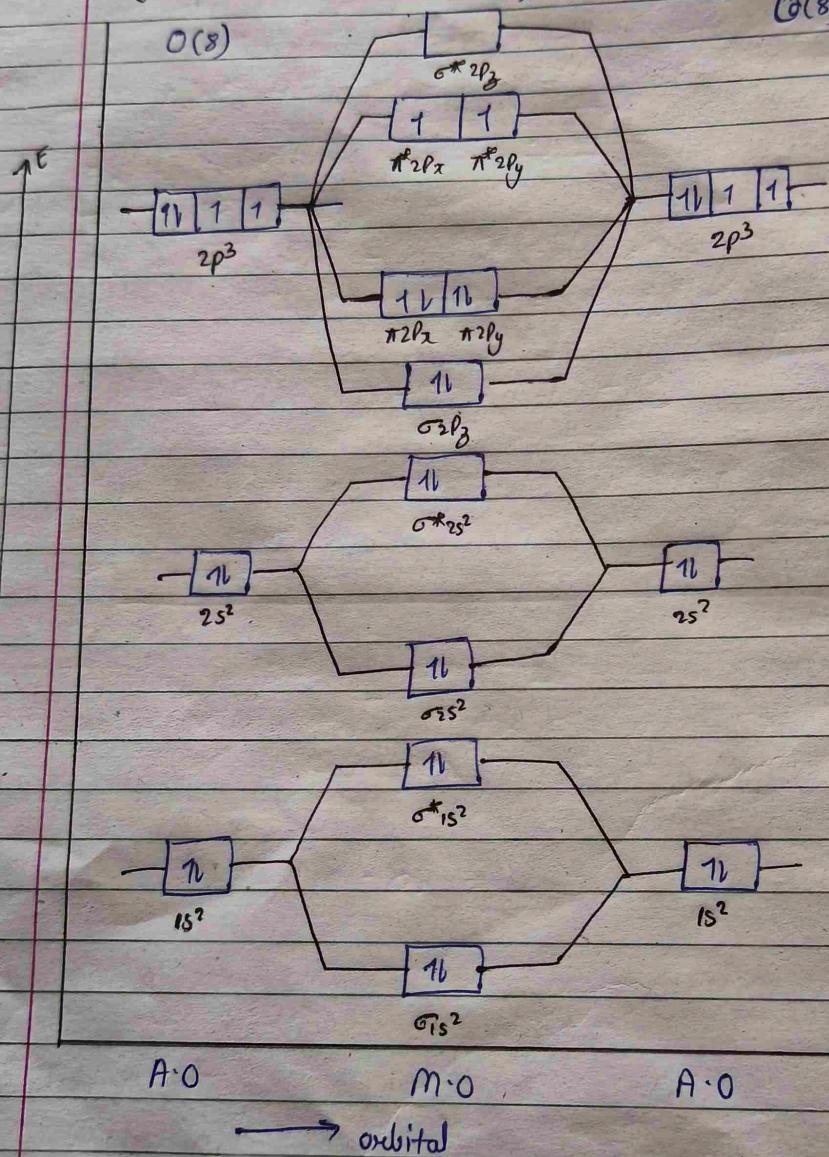
Total $e^- = 15$

MO configuration of $O_2^+ = \sigma_{1s}^2 \sigma^*_{1s}^2 \sigma_{2s}^2 \sigma^*_{2s}^2 \sigma(2p_x)^2 \pi(2p_y)^2 = \pi(2p_z)^2$
 $\pi^*(2p_x) = \pi^*(2p_y) \sigma^* 2p_z$

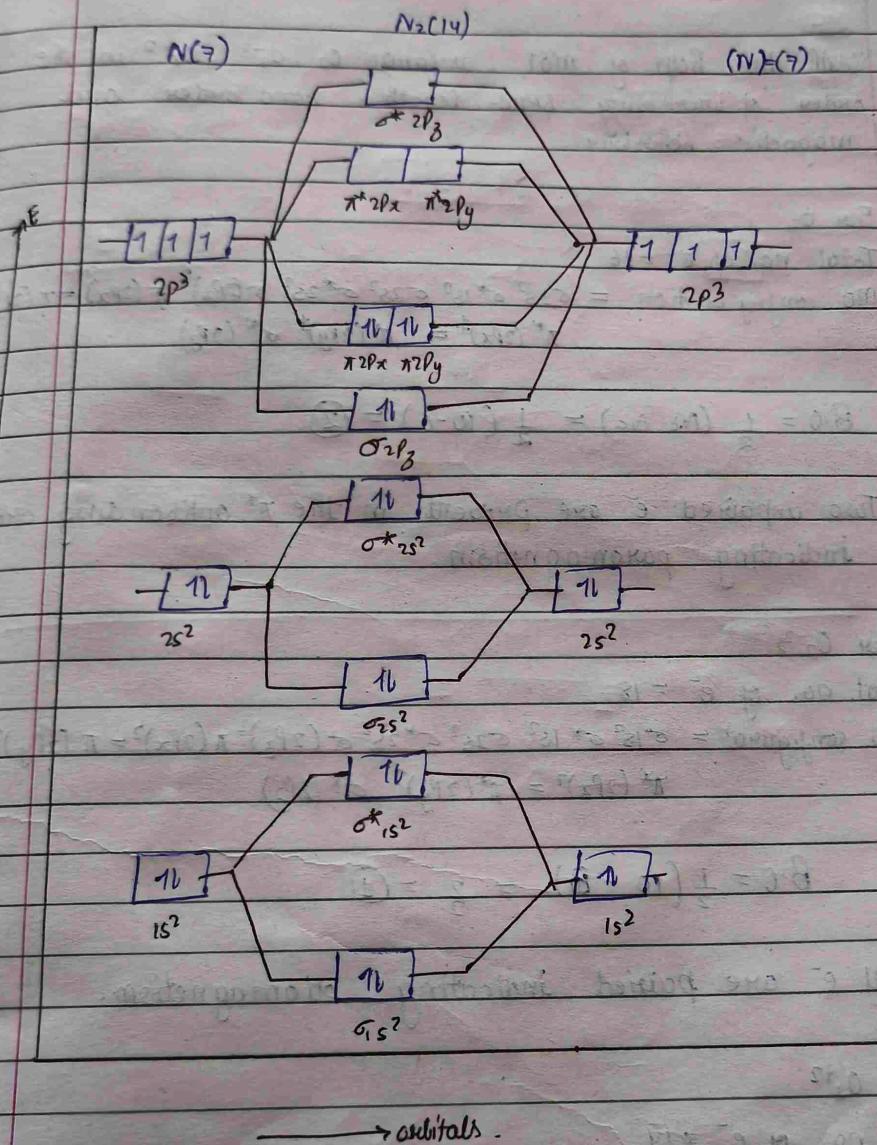
$$BO = \frac{1}{2} (16 - 5) = \frac{11}{2} = 5.5$$

The bond order of O_2^+ is more than O_2 bcoz 1 e^- is removed from the highest energy orbital $\pi^*(2p_z/2p_y)$, an antibonding MO.

Q(3) Why O_2 is paramagnetic while N_2 is diamagnetic.



$\therefore O_2$ is paramagnetic due to unpaired e^- in last orbital.

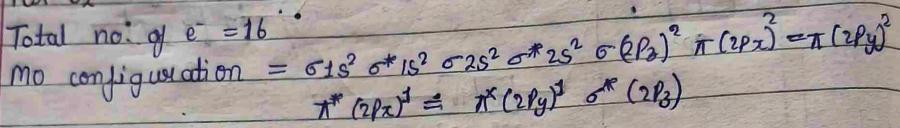


$\therefore N_2$ is diamagnetic due to paired e⁻ in last orbital.

- (4) With the help of MOT, arrange O_2 , O_2^{-2} , O_2^{+2} in the order of increasing bond length, bond order and magnetic behaviour.

For O_2

$$\text{Total no. of } e^- = 16$$

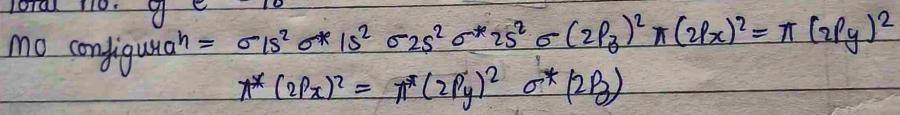


$$B.O = \frac{1}{2} (N_b - N_a) = \frac{1}{2} (10 - 6) = 2$$

Two unpaired e^- are present in the π^* antibonding orbital, indicating paramagnetism.

For O_2^{-2}

$$\text{Total no. of } e^- = 18$$

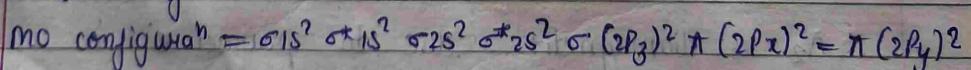


$$B.O = \frac{1}{2} (10 - 10) = \frac{0}{2} = 0$$

All e^- are paired, indicating diamagnetism.

For O_2^{+2}

$$\text{Total no. of } e^- = 14$$



$$B.O = \frac{1}{2} (10 - 4) = \frac{6}{2} = 3$$

All e^- are paired, indicating diamagnetism.

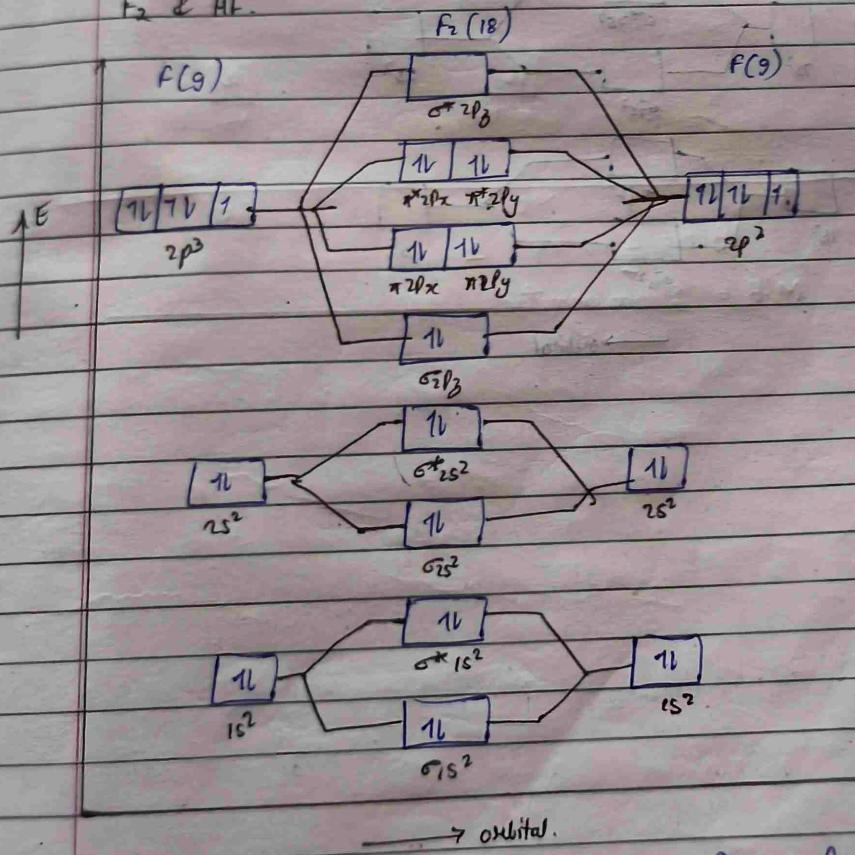
Bond order :- $O_2^{+2} > O_2 > O_2^{-2}$

$$BO \propto \frac{1}{BL}$$

Bond length :- $O_2^{-2} > O_2 > O_2^{+2}$

Magnetic behaviour :- $O_2^{+2} = O_2^{-2} < O_2$ (diamagnetic < paramagnetic)

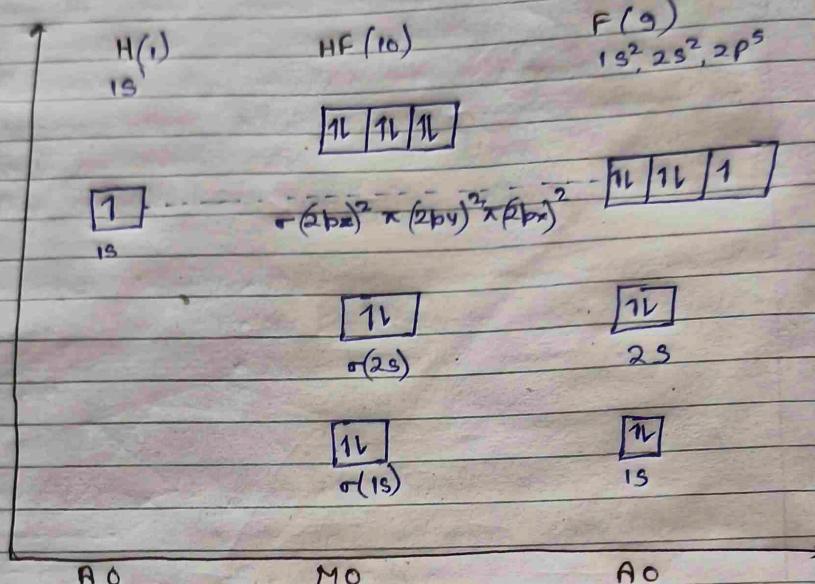
(5) Find out the bond order and magnetic behaviour of F_2 & HF .



$\therefore F_2$ is diamagnetic due to paired e⁻ in last orbital.

$$BO = \frac{1}{2} [10 - 8] = \frac{2}{2} = 1$$

HF



$$B.O = \frac{1}{2} (2 - 0) = 1$$

M.B = Diamagnetic

- ⑥ Arrange the bond length of the NO, NO^+ and NO^- in decreasing order.

MO configuration of NO (16) :- $\sigma_1s^2 \sigma^*1s^2 \sigma_2s^2 \sigma^*2s^2 \sigma(2p_3)^2 \pi(2p_x)^2 = \pi(2p_y)^2$
 $\pi^*(2p_x)^2 = \pi^*(2p_y) \sigma^*2p_2$

$$B.O = \frac{1}{2} [10 - 5] = \frac{5}{2} = (2.5)$$

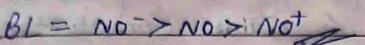
MO configuration of NO^+ (14) :- $\sigma_1s^2 \sigma^*1s^2 \sigma_2s^2 \sigma^*2s^2 \sigma(2p_3)^2 \pi(2p_x)^2 = \pi(2p_y)^2$

$$B.O = \frac{1}{2} [10 - 4] = \frac{6}{2} = (3)$$

MO configuration of NO^- (16) :- $\sigma_1s^2 \sigma^*1s^2 \sigma_2s^2 \sigma^*2s^2 \sigma(2p_3)^2 \pi(2p_x)^2 = \pi(2p_y)^2$
 $\pi^*(2p_x)^2 = \pi^*(2p_y)^2$

$$BO = \frac{1}{2} [10 - 6] = 4 = ②$$

$$BL \propto \frac{1}{BO}$$



① Classify liquid crystals based on their behaviour under temperature and concentration: Give their applications.

Liquid crystals are classified mainly into two types depending on temperature and concentration.

① Thermotropic liquid crystals (Temperature-dependent)

These lig. crystals show mesophase behaviour (intermediate b/w solid crystal and liq) only within a certain temp range.

Applications:-

- (i) Lig. crystal displays (LCDs) in calculators, TVs, watches etc.
- (ii) Temp. sensors & thermometers (color change with temp).
- (iii) Optical switches and tunable lasers.

② Lytotropic liquid crystals (Concentration-dependent).

These appear when amphiphilic molecules (like soaps, detergents, surfactants) are mixed with a solvent (usually water) at specific concentrations.

Applications:-

- (i) Nanotechnology (templating materials)
- (ii) Biological membranes (cell membranes are naturally lyotropic)
- (iii) Drug delivery systems (controlled release of medicines)
- (iv) Detergents, soaps and cosmetics

Q) Classify thermo tropic liquid crystal into Isotropic, Nematic, Smectic, and Chiral Nematic phase. Give diagrams.

Ans) Thermotropic lig. crystals are materials that exhibit a lig crystalline phase depending on temperature - they show properties b/w lig & solids (anisotropic behaviour). They are classified into the following main types:-

(i) Isotropic phase :-

- Molecules are randomly oriented
- No long-range order (completely lig-like)
- Occurs at high temp, above the lig-crystal phase.



(2) Nematic phase :-

- Molecules are oriented in the same direction along a preferred axis (director), but their posn are not ordered.
- Show fluidity like a lig. but directional order like a crystal.



(3) Smectic phase :-

- Molecules are layered in parallel planes
- Within a layer, they can move freely (like a lig) but the layers are stacked (positional order)
- More ordered than nematic



(4) Chiral Nematic (or Cholesteric) phase:-

- Similar to nematic but molecules are chiral (asymmetric)
- Molecules are oriented in layers, & the orientation twists gradually from layer to layer, forming a helical structure.
- Exhibits selective reflection of light (used in displays)

(g) Differentiate b/w graphite and fullerenes. Explain with the help of well-labeled structures.

Ans Difference b/w Graphite and Fullerenes:-

Graphite :-

- (i) Consists of layered sheets of carbon atoms arranged in a 2D hexagonal network. Layers are held by weak van der Waals forces.
- (ii) Each carbon is sp^2 hybridized and bonded to three other carbon atoms.
- (iii) 2-D allotrope of carbon (extended sheets).
- (iv) Good conductor of electricity due to delocalized electrons moving freely b/w layers.
- (v) Soft and slippery because layers can slide over each other (used as lubricant).
- (vi) Used in pencils, lubricants, electrodes, nuclear reactors.

Diagram:-

Show layered hexagonal sheets with arrows for weak forces b/w layers.



Graphite layers.

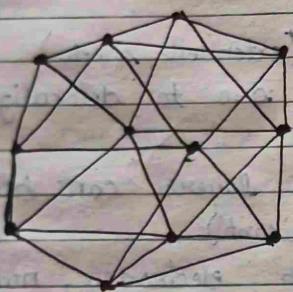
Fullerenes :-

- (i) Consists of carbon atoms arranged in closed cage-like structures made of hexagons and pentagons.
eg - C_{60} , buckyball.

- (ii) Carbon atoms are also sp^2 hybridized, but arranged in a curved spherical / cylindrical form.
- (iii) O-D allotrope of carbon (molecule-like, discrete).
- (iv) Poor conductor or behaves as a semiconductor.
- (v) Hard molecules, but not as soft / slippery as graphite.
- (vi) Used in drug delivery, superconductors, catalysts, nanotechnology.

Diagram :-

Show a spherical football-like structure made up of 12 pentagons and 20 hexagons.



Fullerene (C_{60} approx.)

- (10) Give reasons for the following properties of graphite :-
- (i) Lustrous (ii) Lubricating, (iii) Conducting and (iv) High strength.

(i) Lustrous

- Graphite has a layered structure with delocalized π -e⁻ above the carbon sheets.
- These free electrons reflect light, giving graphite a shiny or metallic lusture, especially on freshly cut surfaces.

(ii) Lubricating

- Graphite layers are held together by weak van der Waals forces.

- The layers can easily slide over one another.
- This slippery nature makes graphite an excellent solid lubricant.

(i) Conducting

- Each carbon atom in graphite is bonded to three others via sp^2 hybridization, leaving one e⁻ delocalized in the π -system.
- These delocalized electrons are free to move along the layers, allowing graphite to conduct electricity & heat.

(ii) High Strength

- Within each layer, carbon atoms are bonded by strong covalent bonds forming hexagonal networks.
- These C-C covalent bonds are very strong, giving each sheet high strength and stability.
- Although layers slide, the in-phase strength of graphite is very high.

(1) Explain why the following properties of nanomaterials are different than bulk material.

(i) Surface area (ii) Optical (iii) Mechanical and (iv) Electrical

Ans (1) Surface area:-

- Nanomaterials have a very high surface area-to-volume ratio.
- More atoms are present on the surface \rightarrow higher reactivity than bulk materials.

(2) Optical properties:-

- Due to quantum confinement, band gap changes with size.
- Nanomaterials show different colors, fluorescence, and absorption compared to bulk.

- (3) Mechanical properties
- Nanomaterials are often stronger, harder, and more elastic.
 - This is because they are nearly defect-free and restrict dislocation motion.
- (4) Electrical properties
- Electron movement is confined at nanoscale.
 - They show effects like tunneling, quantized conductance, Coulomb blockade.
 - Hence, electrical conductivity is different from bulk material.

(12) Classify Carbon Nano Tubes. Why do they possess high tensile strength, electrical conductivity, and ductility?

Ans Classification of carbon Nanotubes (CNTs).

(1) Based on layers :-

- (a) Single-Walled Carbon Nanotubes (SWCNTs) :- Consist of a single graphene sheet rolled into a tube.
- (b) Multi-Walled Carbon Nanotubes (MWCNTs) :- Made of multiple concentric graphene cylinders nested inside each other.

(2) Based on Structure (chirality) :-

- Armchair ($n=m$) :- Highly conductive.
- Zigzag ($n, 0$) :- Can be metallic or semiconducting.
- Chiral (n, m where $n \neq m$) :- Usually semiconducting, with twisted structure.

Reason for their properties :-

(1) High tensile strength

- CNTs are made of sp^2 hybridized carbon bonds, the strongest type of covalent bond in nature.
- Their tubular, defect-free structure allows efficient load transfer and stress distribution.

(2) High Electrical conductivity

- In armchair and some zigzag CNTs, delocalized π -e⁻ move freely along the tube axis.
- This gives CNTs metallic or semi-metallic conductivity depending on chirality.

(3) High Ductility

- CNTs can undergo significant elastic deformation without breaking due to strong carbon-carbon bonding.
- Their cylindrical geometry allows them to bend & twist without fracture.

(13) What are the applications of Nanomaterials and Carbon Nanotubes?

Ans Applications of Nanomaterials :-

(1) Electronics - Used in high-speed transistors, memory devices, and miniaturized circuits.

(2) Medical field - Drug delivery, cancer therapy, imaging & biosensors.

(3) Energy - Solar cells, fuel cells, hydrogen storage & batteries.

(4) Catalysis - Nanoparticles act as excellent catalysts due to high surface area.

- (5) Textiles & Coatings - stain-resistant fabrics, UV protective coatings, and scratch-proof paints.
- (6) Environment - Water purifications, air filters, and pollutant removal.
- (7) Optics - Anti-reflective coatings, smart windows & optical sensors.

Applications of Carbon Nanotubes (CNTs)

- (1) Electronics - Used in nanoscale transistors, conductive films, and field-emission displays.
- (2) Energy storage - CNTs improve efficiency of batteries, supercapacitors, and fuel cells.
- (3) Medical - Targeted drug delivery, biosensors, tissue engineering scaffolds.
- (4) Mechanical reinforcement - Added to polymers, metals, and ceramics to enhance strength & toughness.
- (5) Aerospace & automotive - lightweight, high-strength composites for aircraft and vehicles.
- (6) Sensors - Gas sensors, chemical sensors, and pressure sensors due to high sensitivity.
- (7) Environment - CNT filters for water purification and pollutant removal.

- (14) Write down the 12 principles of green chemistry. What is atom economy? Write down the formula and explain with an example.

12 Principles of Green chemistry:

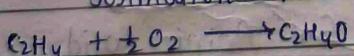
- (1) Prevention of wastes
- (2) Atom Economy
- (3) Avoiding the generation of hazardous chemical
- (4) The design of safe chemical
- (5) Design of safe solvent
- (6) Energy efficiency
- (7) Incorporation of renewable feedstocks
- (8) Reduction in the generation of derivatives
- (9) Incorporation of catalyst
- (10) Designing of chemicals for degradation
- (11) Incorporation real-time analysis
- (12) Safe chemical & prevention of accidents

Atom Economy :- The rxn or the synthesis is considered to be green if there is max incorporation of the starting material and reagents in the final product to minimise the waste.

% atom Economy :- $\frac{\text{Molecular mass of desired product}}{\text{Total molecular weight of all reactant}} \times 100$

Example:-

Formation of Ethylene oxide from Ethylene.



Molecular mass ($\text{C}_2\text{H}_4\text{O}$) = 44 g/mol
of desired product

Molecular mass of (C_2H_4) = 44 g/mol
Reactants

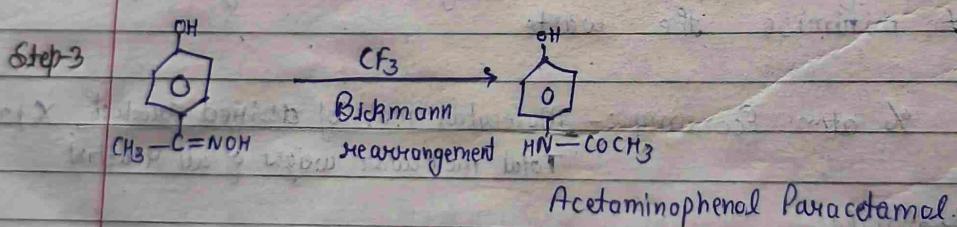
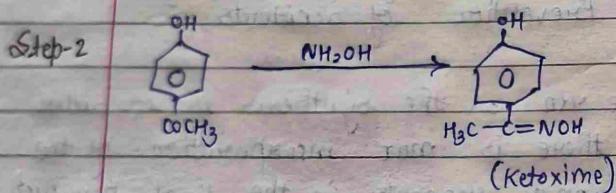
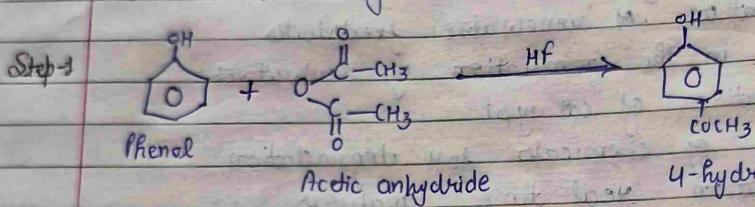
$$\text{Atom Economy} = \frac{44}{44} \times 100 = 100\%$$

This rxn has 100% atom economy

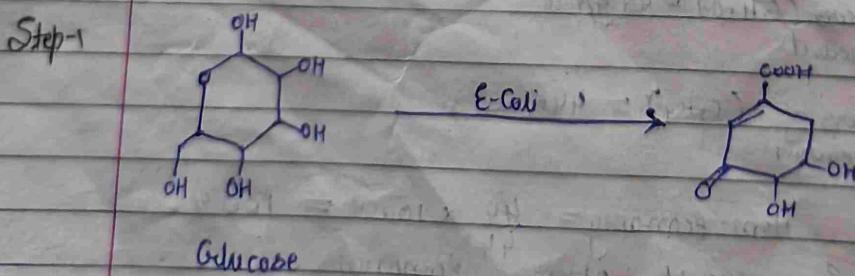
(B) Write down the green route for synthesis of Paracetamol and Adipic acid. What challenges exist in fully replacing conventional method with green method?

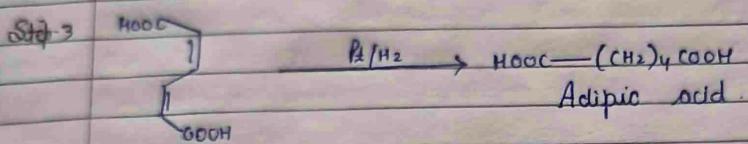
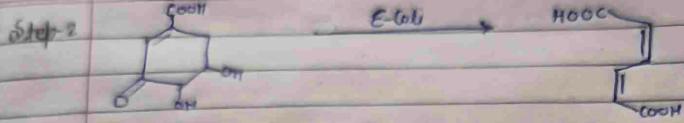
Ans \Rightarrow Green Route Synthesis for Paracetamol :-

In Green route Paracetamol is produced from phenol and acetic anhydride in presence of strong acid HF.



\Rightarrow Green Route Synthesis for Adipic acid :-





Challenges in fully replacing conventional with green method.

- (1) Cost-factor - Green catalysts / biocatalysts are expensive compared to conventional acids and nitration methods.
- (2) Scalability - Industrial-scale green processes are not yet as efficient or reliable as conventional ones.
- (3) Reaction rate - Green methods often have slower kinetics compared to harsh chemical processes.
- (4) Catalyst stability - Many eco-friendly catalysts / enzymes lose activity over time.
- (5) Feedstock supply - Renewable raw materials (like glucose or biomass) need sustainable and continuous supply.
- (6) Industrial infrastructure - Current plants are built for conventional methods; switching requires huge investment.
- (7) Market acceptance - Industries prefer proven, high-yield methods; risk in adopting newer routes.