B.Sc V Sem

Inorganic Chemistry (1) ①

* BIOINORGANIC CHEMISTRY *

* Introduction :-

- It describes mutual relationship between inorganic chemistry & bio chemistry
- Imp in function of inorganic substances in living systems & use of inorganics in medicinal therapy & diagnosis.
- Bioinorganic chemistry deals with study of structure, function, mechanism, dynamics of biologically relevant metal complexes & metal-containing proteins.
- Deals with understanding of function of biological relevant metal site its functions.
- Studies formation & development of organic 'life molecules'.
- Bioinorganic Chemistry is the field that examines the role of metals in biology.
- Biological processes like respiration depend upon molecules that fall within realm of inorganic chemistry.
- Is the field that examines role of metals in biology.

* Essential & Trace Elements In Biological Process :

Essential elements for life are :-

- Bulk elements → C, H, N, O
- Macronutrients → Na, K, Mg, Ca, S, P, Cl, Fe.
- Micronutrients (Trace elements) → Mn, Co, Ni, Cu, Zn, V, Cr, Mo, Se, F, I, Al, Pb, Sn, Si.
- Non essential → Al, Sr, Ba, Sn etc.
- Toxic → Cd, Pb, Hg etc. (disturb functioning of biological system)

Human body is made up of
H - 62.8%, C - 9.4%,
O - 25.4%, N - 1.4%.

* Significance of Biologically Important Elements :-

1. **Na^+ and K^+ :**
   - Contains free intra & extracellular cations.
   - Helps in regulation of osmotic pressure, membrane potentials, enzyme activity & signaling.

2. **Mg^{2+} :**
   - Chlorophyll
   - anaerobic energy metabolism (ATP)

3. **Ca^{2+} :**
   - Signalling, muscle contraction, enzyme regulation,
   - Main inorganic part of endoskeletons

(bones, teeth, enamel - hydroxyapatite.
- Exoskeletons - of muscles, shells, corals, sea urchins etc. - aragonite or calcite.

4. Mo, V, W, Mn, Fe, Ni, Cu:
These are active centres in electron-transport enzymes, oxygenases, dismutases.

5. Fe and Cu:
Transport of oxygen.

6. Fe (III): Iron storage proteins.

7. Fe (II) & Fe(III) in magnetite (Fe_3O_4):
- orientation of magnetobacteria, pigeons, bees in earth's magnetic field.

8. Co: Synthases & isomerases
(Cobalamines, eg: vitamin-B_{12})
Methylation of inorganics.

9. Zn^{2+}: - In active centre of hydrolases, carboanhydrase, alcohol dehydrogenase, synthase, genetic transcription, stabilisation of ter & quat. structures of proteins, repair enzymes

10. Si(IV): - Involved in built-up of bones, silica-gel support in monocotyledonous plants (grass) & shells of diatoms.
- energy metabolism (ATP), activation of organic substrate, phospholipids in cell

all membranes, phosphate esters (DNA, RNA).

11. Se (II): Selenocysteine is a special enzyme. (Selenium) (eg: glutathione peroxidase).

12. F⁻: Fluorapatite in dental enamel.

13. Cl⁻: Along with hydrogencarbonate it is most imp reaction

14. I⁻: Constituent of thyroid hormones (thyroxine)

* Medical Relevant Elements :-

1. Li⁺: Treatment of bipolar disorder (maniac depression) & hyperaction (mood swings)
2. Gd³⁺: Contrast agent in magnetic resonance tomography of soft tissues. (gadolinium)
3. $BaSO_4$: agent for x-ray tomography. Sun protection.
4. ^{99m}Tc: (metastable γ-emitter), Radio diagnostics - bone cancer, infarct risk.
5. Pt (II): Chemotherapy of cancer (ovaries, testis) — eg: cisplatin etc.
6. Au (I): Therapy of rheumatics - arthritis. (swelling of hands & feet)
7. Sb (III): Treatment of inflammatory skin pimples - acne. (antimony)
8. Bi (III): Treatment of gastritis.
9. Transition metal ions are complexed to ligands.

& this applies to metal (VI) ions in active centers of enzymes, peptides & proteins.

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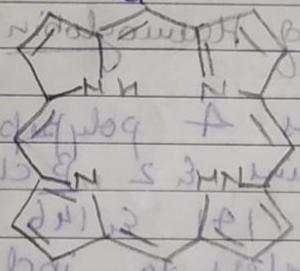
* Metalloporphyrins :-

It is a compound (heme) consisting of a porphyrin combined with a metal (Fe, Cu, Ag, Zn, Mg).

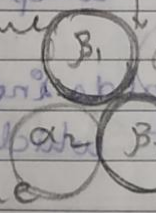
Exs: Haemoglobin, Chlorophyll etc.

⇒ Porphyrins:
- Naturally occuring group of organic compounds. Greek word for purple.

eg: Heme →
- pigment in RBC
- It is a cofactor of protein hemoglobin.
- have very intense absorption bands in Visible region
- Deep coloured.



* Function & Structure of Haemoglobin:



- Haemoglobin is a protein in RBC.
- Transports Oxygen from lungs to tissues.
- Responsible for red colour of RBC.
- Haemoglobin tightly binds oxygen from

lungs, carries from lungs to tissues, after unloading oxygen at tissues it binds CO_2 & returns it to lungs to be exhaled.

- Haemoglobin is composed of two proteins subunits i.e α & β.
- Abnormalities in subunits causes disorder.
- Abnormal Hb structure / function results in disorders like sickel cell & thalassemia
- O_2 does not oxidize Hb. Reversible binding of O_2 in Hb is due to porphyrin ring system & hydrophobic blocking of globin (protein) A porphyrin ring system with coordinated iron (heme group).

Structure of Haemoglobin:-

- Hb contains 4 polypeptide subunits: 2 α chains & 2 β chains. each with 141 & 146 amino acids.
- globin refers to individual protein subunits.
- Each subunit is comprised of α-helias & not β.
- Each subunit folds into 8 α helical segments for pocket which holds heme.
- Heme molecule is cyclic molecule which consists of C, H, N with Fe^{2+} ion located at center.
- 4 N-atoms holds iron in center.
- Fe ion bonds with histidine side chain from one subunit to form pocket.

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- Fe ion bonds to histidine 87 in α-chain & histidine 92 part of F helix in each subunit.
- Molar mass of Hb is 64,500

* CHLOROPHYLL :

- Is a molecule which absorbs sunlight & uses its energy to synthesize carbohydrates from CO_2 & H_2O. This process is called photosynthesis.
- Reaction :

$$6CO_2 + 6H_2O + \text{light energy} \longrightarrow C_6H_{12}O_6 + 6O_2$$

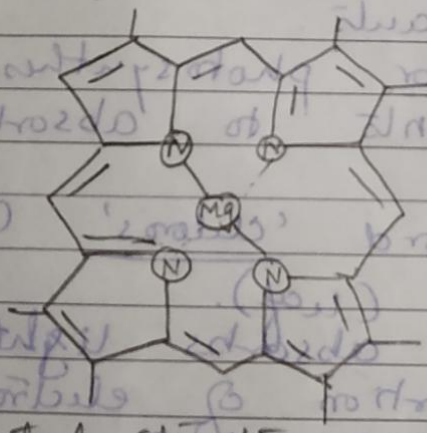
- Chlorophyll is green pigment found in cyanobacteria & chloroplasts of algae & plants.
- Is imp for photosynthesis which allows plants to absorb energy from light.
- Greek word 'chloros' (green) & phyllon (leaf).
- Chlorophyll absorbs light strongly in blue portion of electromagnetic spectrum followed by red portion.

Chlorophyll as a Photoreceptor →

- Chlorophyll traps most elusive of all powers so called as photoreceptor.
- Is cause for green colour in plants.
- It's structure is a porphyrin ring co-ordinated to central atom.
- Similar to structure of Hb., except

central atom is Magnesium.

- Two types of chlorophyll's
  a & b
  differ in side chain
  a is $-CH_3$ b is CHO.
- Both are very effective photo receptors as they contain network of alternate single & double bonds
- orbitals can delocalise stabilising structure.
- These delocalised polyenes have strong absorptions bands in visible regions & hence allows plants to absorb energy from sunlight.



Central structure of Chlorophyll

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* Metal Ions in Biological Systems

⇒ Biological role of Na:

- Adult human has 105g Na, 24% located in bone & 65% in extracellular waste.
- 9s maintained by kidney.
- Na, K, Cl occur in fluids & soft tissues of body.
- Na controlling osmotic pressures & acid-base equilibrium.
- Na- imp role in water metabolism.
- 93% of ions of Na found in blood stream.
- absorption of carbohydrate.
- NaCl salt is a dietary source - excessive Na intake results in hypertension (B.P.), increased K intake Reduce high B.P.
- - Extracellular fluid
- Osmotic balance 'sodium pump'
- Acid-base balance
- Conformation of proteins & nucleic acids.
- Electrical impulse of nerve system.

⇒ Biological Role of K:

- K is found in most animal & vegetable foods.
- Humas has appr. 140g of K.
- K is major cation of intracellular fluid & regulate intracellular osmotic pressure & acid-base balance.
- K has stimulating effect on muscle irritability.
- K necessary for synthesis of glycogen &

& protein & breakdown of glucose.
- K is enzyme activator.
- Conformation of proteins & RNA replication
- Secretion of gastric acid
- Transmembrane potentials.

⇒ Biological Role of Fe:
- Human has 4-5g Fe. of this 60-70% is present in Hb in RBC, 3-5% is in muscle myoglobin, 15% - bound to Fe storage cellular protein ferritin, 0.2-1% - occurs in critical respiratory enzymes, 0.004% - bound to serum transport protein - transferin.
- Fe deficiency causes anemia,
- Acute Fe poisoning leads to vomiting, shock, circulatory collapse & coma.
- Siderosis ⇒ Chronic conditions in which iron is deposited in tissues & organs of body.
- Fe is for respiratory pigments Hb & myoglobin.
- Fe is essential for O₂ & ē transport within body.

⇒ Role of Fe, Cu, Mo:
- Electron-transfer
- Redox proteins & enzymes
- O₂ carrying proteins
- Nitrogen fixation.

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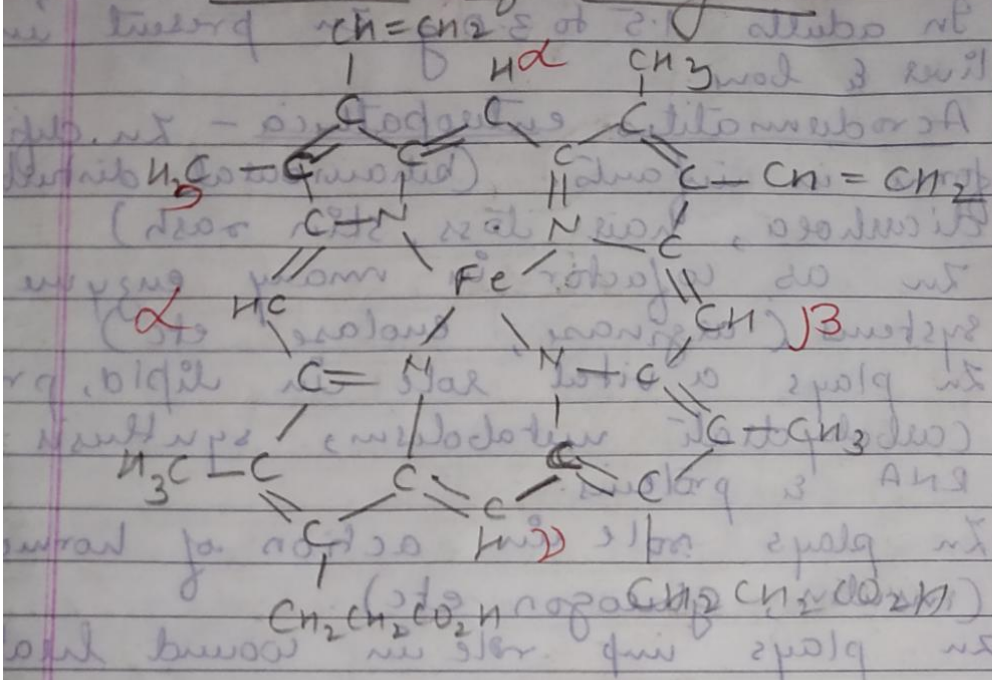
⇒ Biological Role of Zn :-

- In adults 1.5 to 3.0 g Zn present in liver & bone.
- Acrodermatitis enteropathica - Zn deficiency form in infants. (behavioural disturbances, diarrhoea, hair loss, skin rash)
- Zn as cofactor in many enzyme systems (arginase, enolase etc)
- Zn plays a vital role in lipid, protein carbohydrate metabolism, synthesis of RNA & proteins.
- Zn plays role in action of hormones (insulin, glucogon etc).
- Zn plays imp role in wound healing

Role of Zn →

- Metalloenzymes
- Structure promoters
- Lewis acid
- Not a redox catalyst.

Structure of Hemoglobin