Some important structural features of Hb & Mb ⇒
(Only specific topic will be discussed here)

Important functions of Heme proteins are –
a) Transport & storage of dioxygen. (Hb & Mb)
b) Electron transport ($cyt\ b_5$)
c) Catalysis in redox reactions (Catalase, Cytochrom P-450, peroxidase etc.)

The most common hemoglobin in adults contains two α-units (141 aminoacid residues) and two β units (146 aminoacid residues):

Amino acid Sequence → protein chain → α, β, δ, γ

Common hemoglobin → $\alpha_2\beta_2$, $\alpha_2\delta_2$ (very less, only 2%.)

Fetal hemoglobin → $\alpha_2\gamma_2$

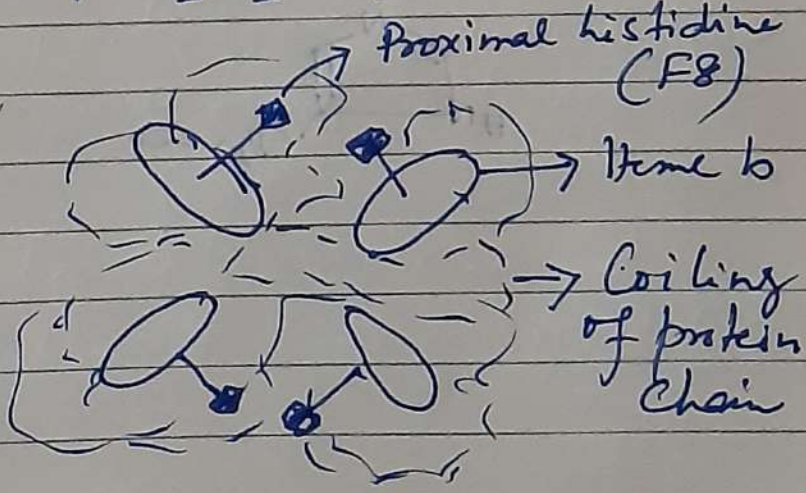
Salt bridge interaction

$-COO^{\ominus}\cdots\overset{\oplus}{H}N-$

In protein chain

↳ deoxy-Hb form

But oxy-Hb, these interaction destroyed.

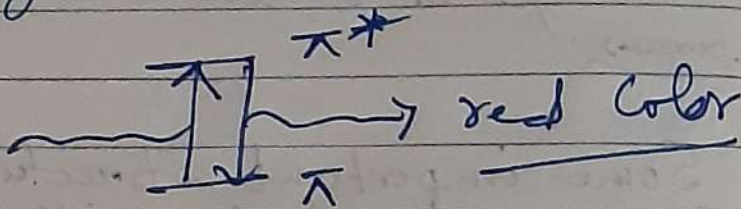


Porphyrin ring ⇒

Porphyrin ring is planar.
Extended double bond (Conjugated)

* $\pi - \pi^*$ (Charge transfer transition)
(origin of red color of blood)

extended Conjugation decrease the HOMO-LUMO gap and red color generates (visible range)



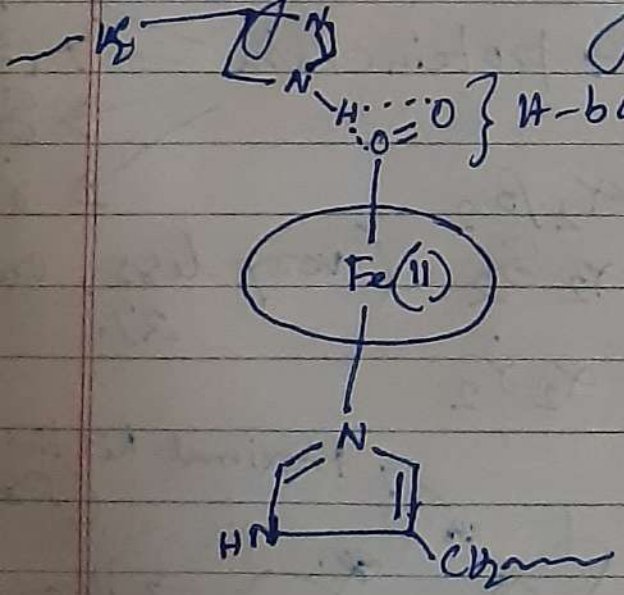
→ Blue region band
Soret → 400-500 nm
α, β bands → 500-600 nm

Deoxy form → Sixth Co-ordination site occupied by H_2O.

Oxy form → Sixth co-ordination site occupied by O_2.

Distal Histidine ⇒ (E7)

Distal histidine stabilises the oxy form through H-bonding.



* CO poisoning can be protect.

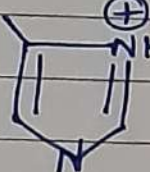
Salt bridge interactions :- (Details)

(β_2) $H_3N^{\oplus}$ — Asp-94 — His-146 ⟶ $COO^{\ominus}$

(α_1) $^{\ominus}OOC$ ← Arg-141 — Asp-126 — Lys-40 — $NH_3^{\oplus}$

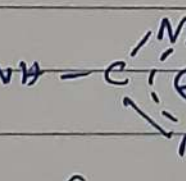
(α_2) $H_3N^{\oplus}$ — Lys-40 — Asp-126 — Arg-141 — $COO^{\ominus}$

(β_1) $^{\ominus}OOC$ — His 146 — Asp-94 — $NH_3^{\oplus}$

1, 8 ⇒  (Histidine) — (Aspartate)

2, 7 ⇒ $-NH_3^{\oplus}$ ..... $^{\ominus}OOC-$ (Lysine) — (Terminal)

3, 6 ⇒ $-NH_3^{\oplus}$ ..... $^{\ominus}OOC-$ (Terminal) — (Terminal)

4, 5 ⇒  (Arginine) — (Aspartate)

These interactions are favourable as per their pka values.

T-State in de-oxy Hb

But on oxygenation these interaction destroyed.

R-State

a) Interactions are $\beta_2-\beta_2$, $\alpha_1-\alpha_2$, $\beta_2-\alpha_1$, $\alpha_2-\beta_1$, $\beta_1-\beta_1$

b) Interaction between BPG and $NH_3^{\oplus}$ — site (β_1 & β_2 unit).

Next lecture topic (Final lecture topic on Hb & Mb)
Role of Distal (E7) and Proximal Histidine :-

Related topic ⇒

① Amino acid sequence (for advance study)
② Charge transfer transition ? Why it is intense ? Color in C-T ; How it differ from d-d transition ? Types of Basic charge transfer transition ? Any symmetry rule concept for charge transfer applied ?
Condition for charge transfer transition.
③ Porphirin ring aromatic or not ? (Home tasks)