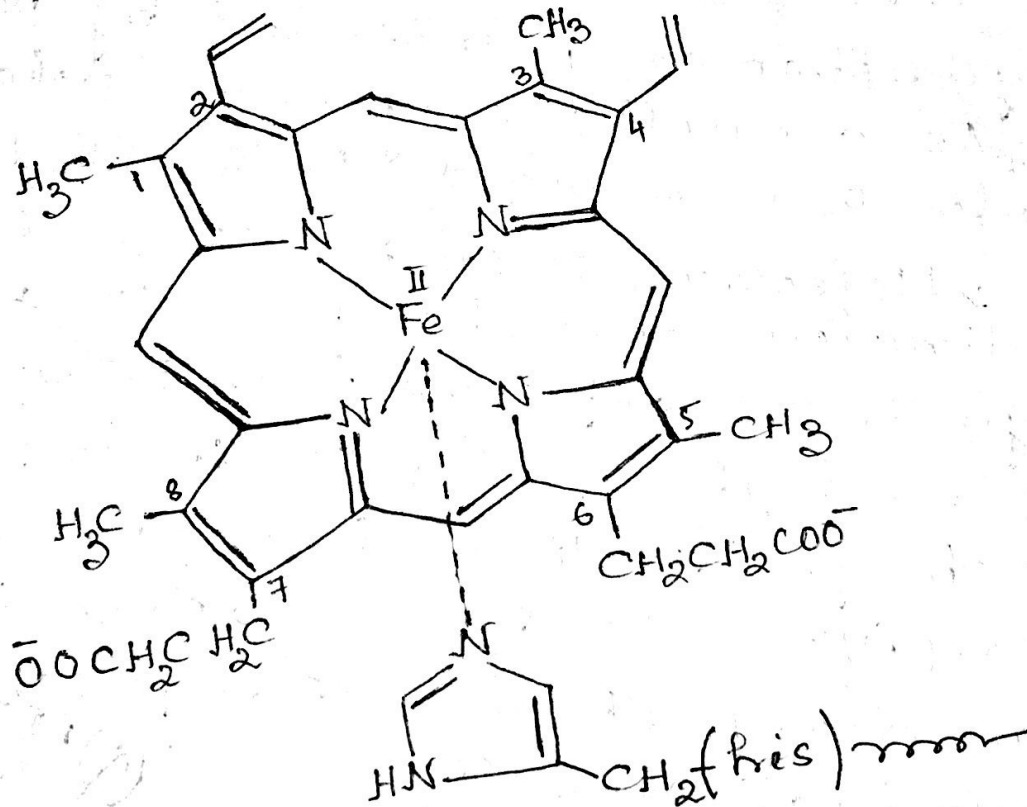


2. Depict the structure of heme group in Hb and Mb. Explain clearly what is meant by co-operative interaction as prevails in Hb. Explain the change in Fe(II) coordination sphere during oxygenation of Hb and Mb.



Active site structure of heme group in Hb and Mb.

Oxygen binds to the Fe(II) heme at vacant 6th position and the resulting octahedral field is sufficiently strong to transform high spin Fe(II) to low spin Fe(II) . Hence a conformational change throughout the peptide occurs which causes to rupture some one of the $-\text{COO}^{\ominus} \cdots \text{NH}_3^{\oplus}$ salt-bridge interaction. The constrained Hb tetramers then relax exposing the 6th positions of the remaining heme groups to oxygenation. This phenomenon is known as "cooperative interaction".

The active sites of both Hb and Mb contain the heme group in which Fe(II) is equatorially coordinated by the four porphyrin nitrogen atoms of porphyrin ring. The 5th position is coordinated by the imidazole nitrogen atom of a histidine of the protein chain i.e. globin. The 6th position is vacant but hydrophobically shielded by protein chain. As a result, only non-polar neutral molecules O_2 can bind to the 6th position.

Moreover, Fe(II) in Hb and Mb is 5-coordinated and hence Fe(II) is present in high spin configuration. $\text{Fe(II)}-\text{N}$ bond lengths in high spin $\text{Fe(II)}-\text{N}$ compounds is much greater than the mean radius of the porphyrin cavity. Pentacoordinated Fe(II) in deoxy-Hb and deoxy-Mb has sq. pyramidal geometry and Fe is situated about 0.8 \AA out of the porphyrin plane being shifted towards the apically coordinated histidine. Oxygen binds to the Fe(II) heme at the vacant 6th position and the resulting octahedral field is sufficiently strong to transform high

Spin Fe(II) to low spin Fe(II) . As a result of the Fe(II) radius is contracted by about 0.17 \AA and Fe(II) in the active site of oxy-Hb and oxy-Mb moves towards the porphyrin plane and ultimately sits in the porphyrin cavity. This movement of Fe(II) causes the coordinated histidine to move towards the porphyrin ring plane. This brings about a conformational change throughout the peptide chain amounting to rupture of some or all the $\text{CO} \cdots \text{NH}_2$ salt bridge interactions. The constrained Hb tetramer then relaxes by exposing the 6th positions of the remaining heme groups to oxygenation. This phenomenon is known as cooperative interaction. Oxygenation of Hb is autocatalytic due to this cooperative interaction. But such effects are absent in Mb due to its monomeric nature.

