(2) Discuss the magnetic property and spin states of metal ion in deoxygenated and oxygenated species of Hb.

It has long been known that $Mb(O_2)$ and $Hb(O_2)_4$ complexes are diamagnetic. But Hb and Mb are paramagnetic consisting of HS Fe(II) with $t_{2g}^4 e_g^2$ configuration.

Fe(II) state → $t_{2g}^4 e_g^2$ (High spin)

↑↑ ↑↓ ↑ ↑

Paramagnetic ⇐ 4 unpaired $e^\ominus$

Fe(II) is bonded to 4 'N' atoms from pyroll ring in a porphyrin system, fifth Co-ordination site through a N atom of hystidine residue of globin part and sixth position by a H_2O molecule.

Hb and Mb are paramagnetic for 4 unpaired $e^\ominus$.

When Co-ordination takes place with dioxygen (O_2) then resulting oxy-species viz, $Mb(O_2)$ and $Hb(O_2)_4$ become diamagnetic.

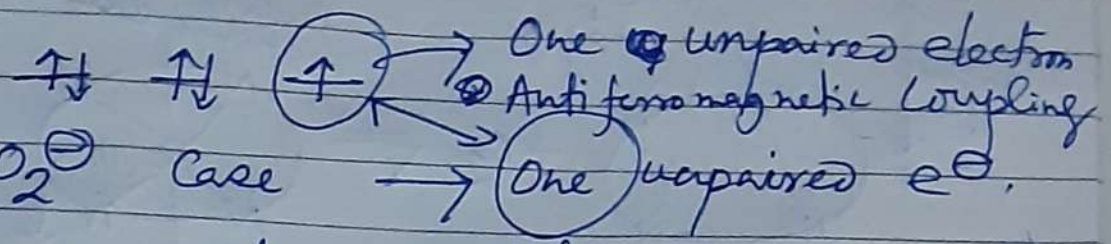
Two explanations can be made here.

I) Singlet oxygen molecule coordinate with LS Fe(II)

II) Low spin (LS) Fe(III) – $O_2^\ominus$ (Super Oxide)

I) Fe(II) LS → paired t_{2g} → t_{2g}^6 → } diamagnetic
Singlet Oxygen → paired

II) Fe(III) LS state



$O_2^{\ominus}$ Case →

There occurs a strong antiferromagnetic Coupling between unpaired spin state of Fe(III) LS and $O_2^{\ominus}$.

This antiferromagnetic Coupling mechanism is well supported by the fact that $[Cr(TPP)(Py)(O_2)]$

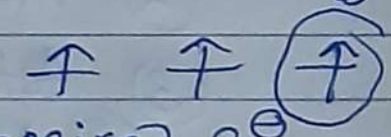
Where, TPP → Tetraphenyl phenyl porphyrin

The magnetic moment of $[Cr(TPP)(Py)(O_2)]$ is 2.7 BM which indicates 2 unpaired electrons in the system.

The unpaired electrons in Cr(III) is

$Cr \rightarrow 4s^2 3d^5$

$Cr(III) \rightarrow 3d^3$

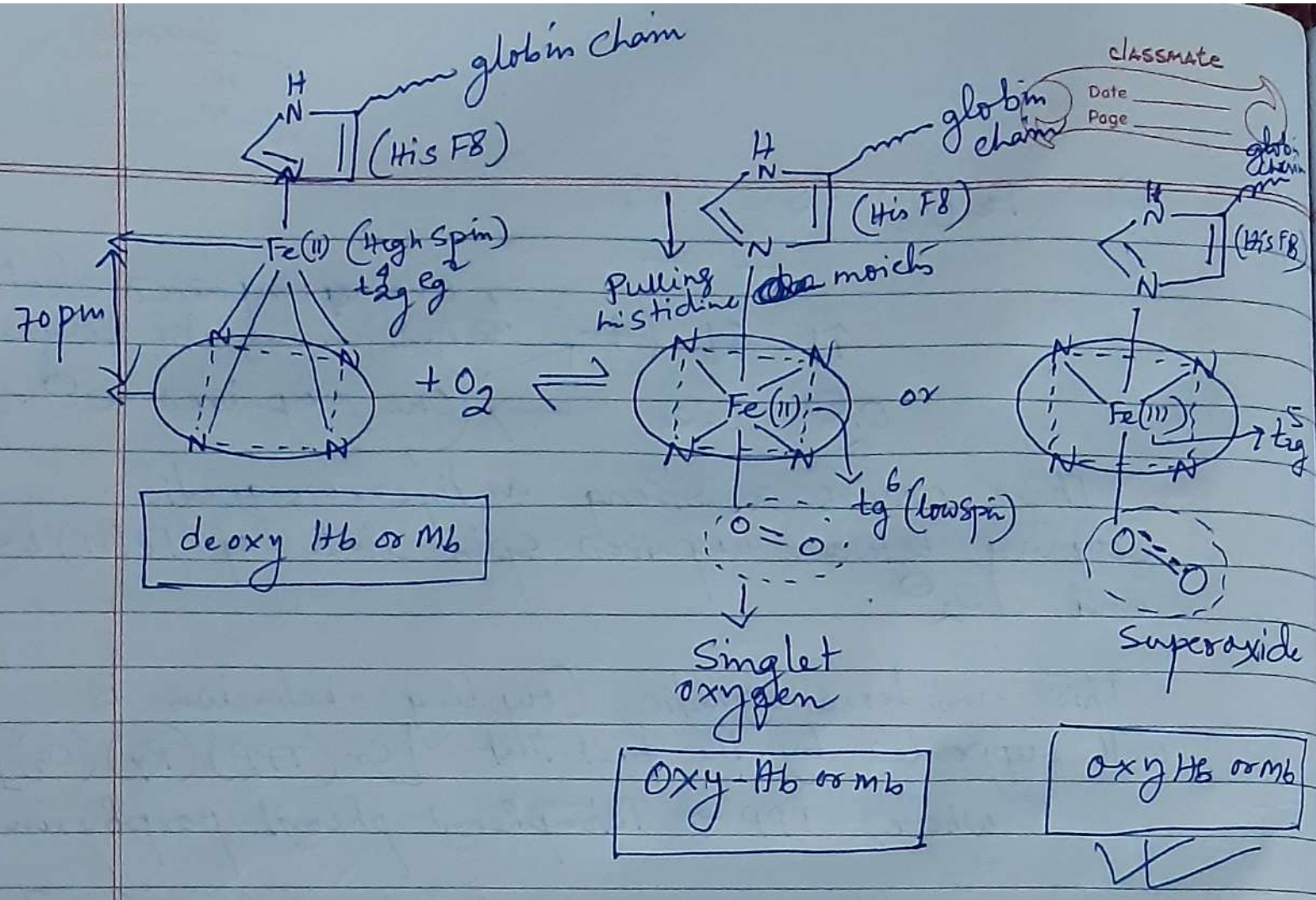


3 unpaired $e^{\ominus}$

$O_2^{\ominus}$ has (1) unpaired electron.

Experimetally it has been obsored that two unpaired electrons in the system. That means from that observation it Can be Conclude that there exist a strong antiferro-magnetic Coupling between one unpaired $e^{\ominus}$ of Cr(III) and the unpaired $e^{\ominus}$ of $O_2^{\ominus}$. The net magnetic moment coming from 2 unpaired electrons.

Another evidance is that O-O bond stretching frequency is 1106 cm^{-1} which holds good for superoxide mechanism.



Related lecture topics :-

1. Bohr effect (pH dependance) CO_2 Liberation in tissue
2. Thermodynamic & Kinetic inertness
3. Activation of Dioxygen Through Complexes
4. Naming of F8 - ? How ?

* Note :- (Video lecture will be provided when all the home tasks and other related topics are finished. End of the this Week.)