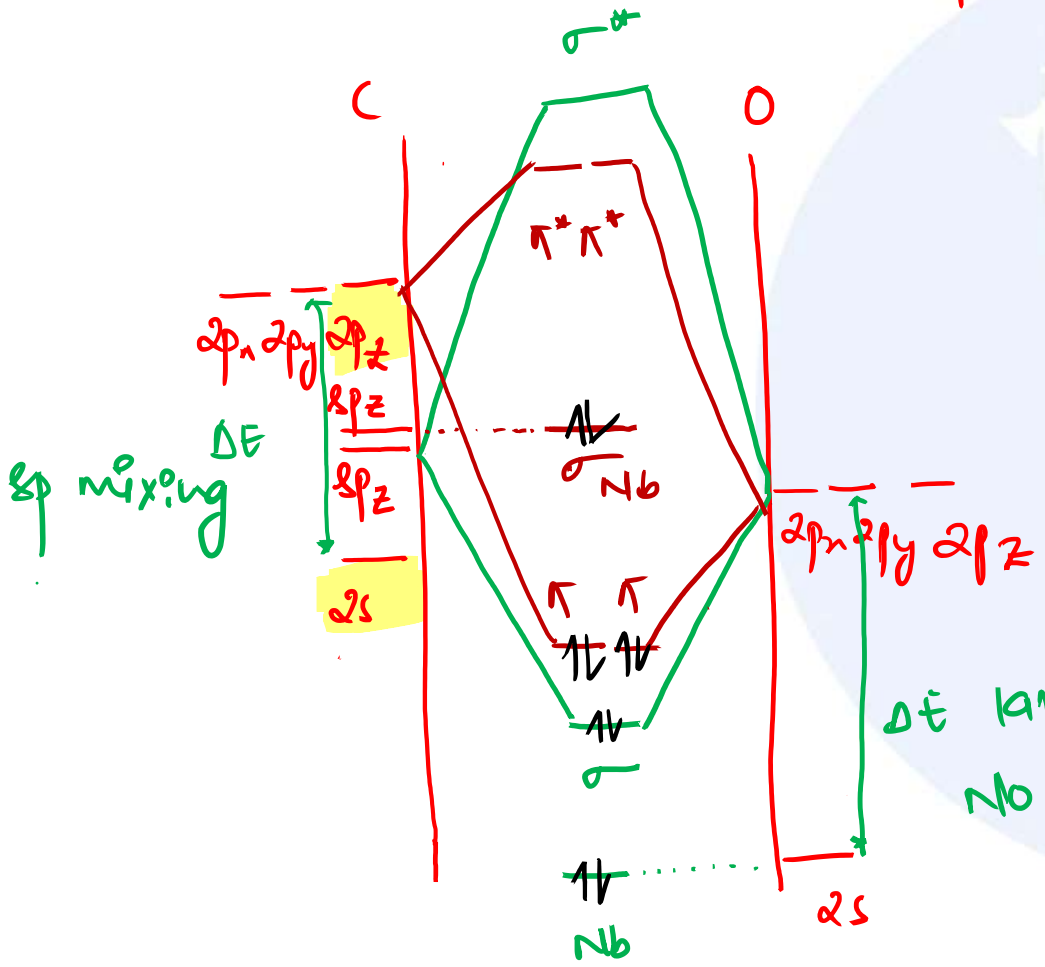
EN: C < O

CO: C : $2s^2 2p^2$

O : $2s^2 2p^4$



Mixing Condn. ① Symm. same

② Energy same

① Bond Order = $\frac{N_{BMO} - N_{ABMO}}{2}$

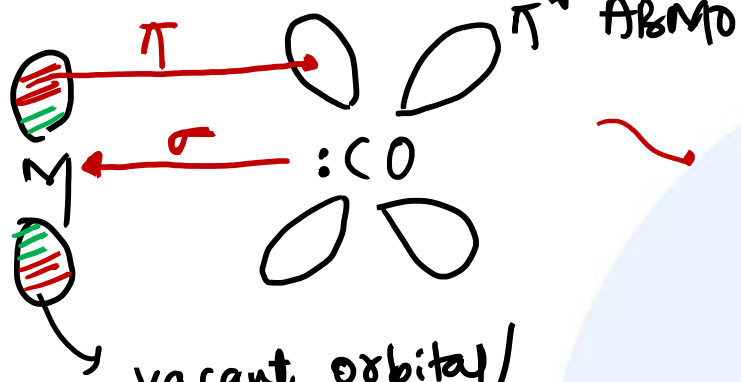
$= \frac{6-0}{2} = 3$

② HOMO : σ_{sp} (NBMO) (Small ABMO character)

③ LUMO : π^* (ABMO) (C-character)

④ $CO^{\oplus}$ (B.O = 3.5) > CO (B.O = 3)

Synergetic Effect:

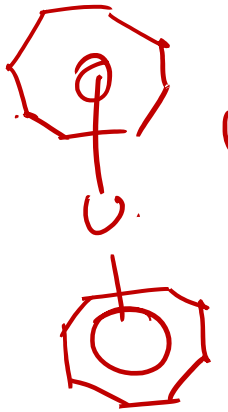


σ bond is stabilised by Back donation from metal to C≡O (π*) ABMO.

OMC

① Metal & Organic compounds / ligands are interacting.

② Apart from T.M, p-block, s block, f block can also form OMC.

Ex: $Cr(CO)_6$, $Mn(CO)_5Cl$, $Ni(CO)_4$, $B(Ph)_3$,  Uranocene.

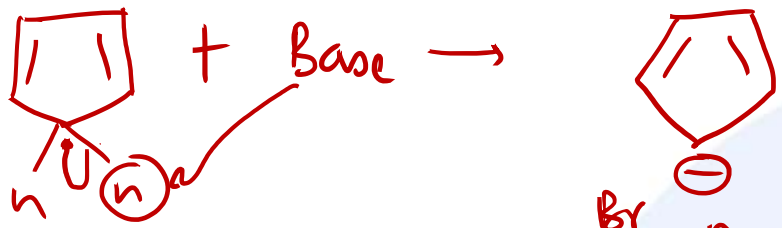
③ Generally OMC have lower O.S state.

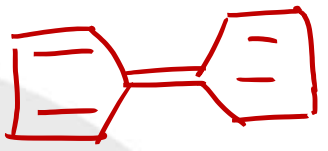
④ Wilkinson Catalyst : $[RhCl(PPh_3)_3]$

Ye bhi OMC hai, Jab ye T.S banata hai.

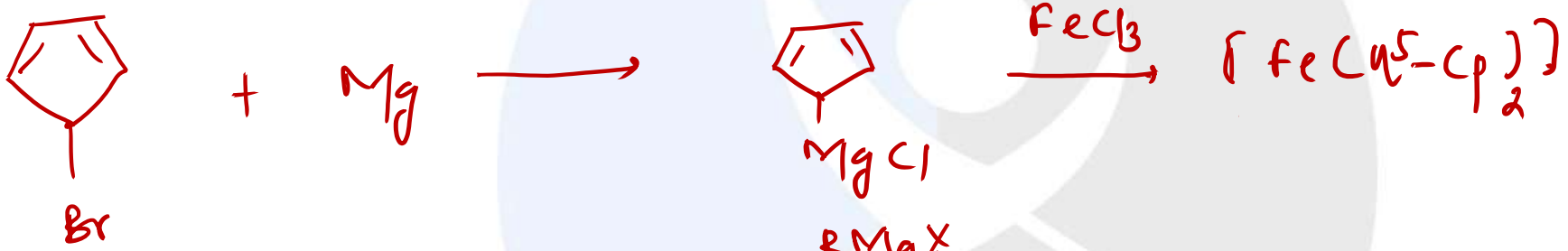
Tab ye organic ligand k sath coordinate karta hai.

(5)





fulvalene



ferrocene

Supprisingly stable ← OMC

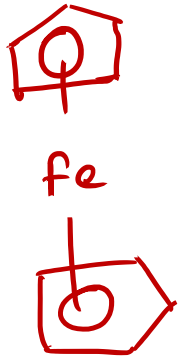
Orange.

Ferrocene

Staggered Rings (D_{5d})
(Solid)

Eclipsed Rings (Gaseous)
(D_{5h})

Skew (D_5) (H.T)



★ Generally OMC are stable in 18 $e^{\ominus}$ complexes

Why?

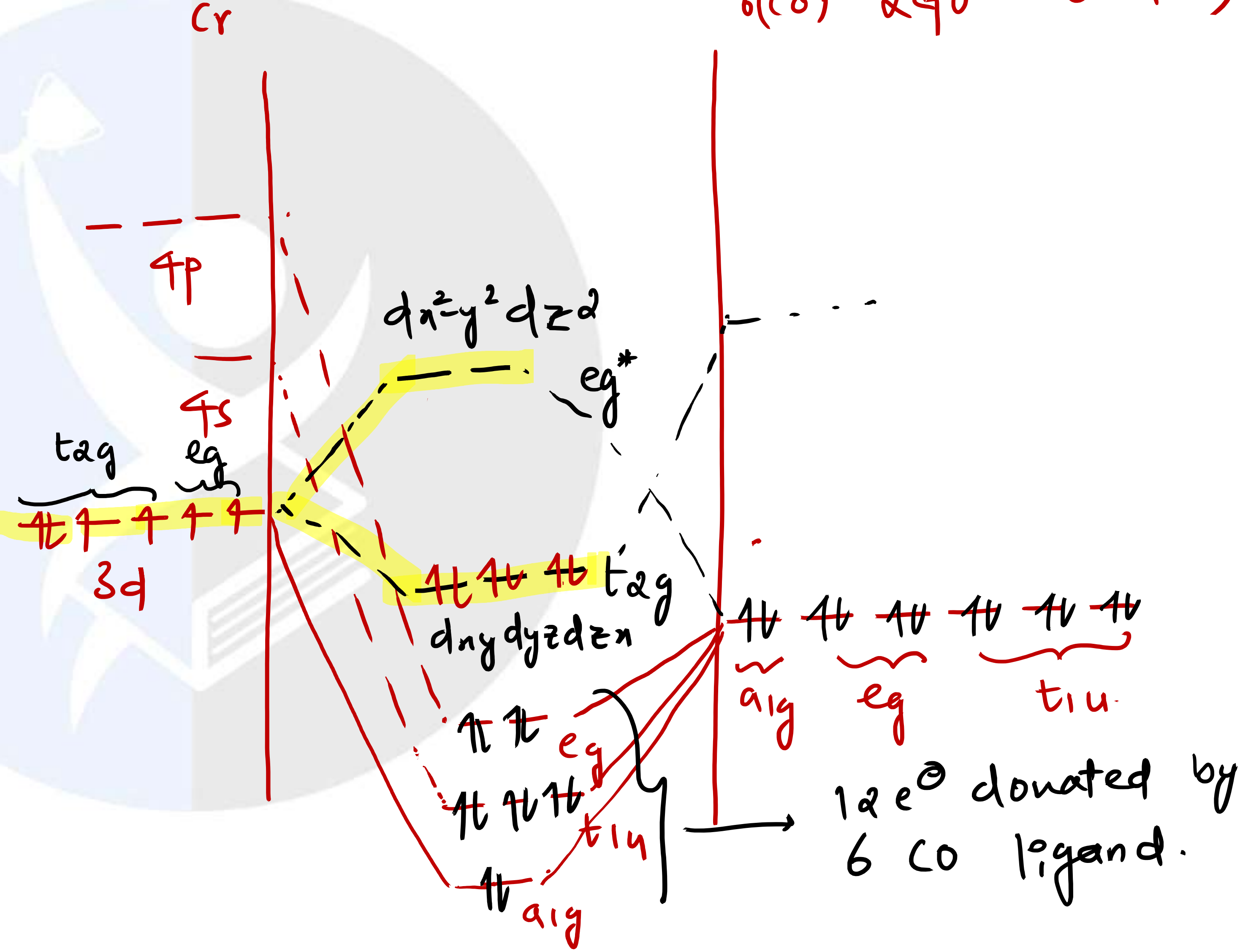
Ex: O_h complex ; $Cr(CO)_6$

Types of Interactn :

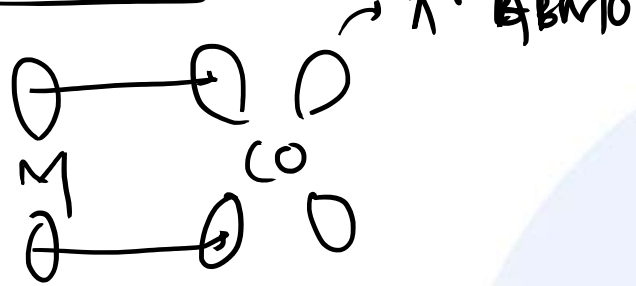
① σ Interactn

$M \xleftarrow{\sigma} :CO$

This interactn ↑es energy of eg orbitals making it ABMO



② π interaction :



π interaction decreases energy of tag set of orbitals of metal making the BMO.

∴ we call CO ligand as σ donor & π acceptor.

Q. But do all OMC follow 18 e⊖ rule ?

→ NO, only complexes having strong π acceptor obey 18 e⊖ rule.

→ If complexes have weak σ donor (weak field ligands) / moderate σ donor only. They do not follow 18 e⊖ rule.

Ex: $[Zn(en)_3]^{2+}$

$[Zn(en)_3]^{2+}$

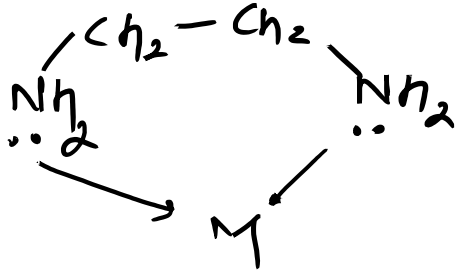
$Zn^{+2} \rightarrow 10\ e^{\ominus}$

$3en \rightarrow 12\ e^{\ominus}$

$22\ e^{\ominus}$

en → 4 $e^{\ominus}$ donor

Moderate σ donor



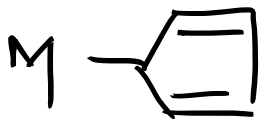
Although $[Zn(en)_3]^{2+}$ has 22 TVE but it is stable

→ Square planar Complexes follow 16 $e^{\ominus}$ rule generally.

→ 18 $e^{\ominus}$ rule is very important, through this we can find no. of M–M bond in metal clusters, no. of bridging ligands. etc.

Electron Count & Hapticity :-

Hapticity : No of atom of ligand attached to metal.

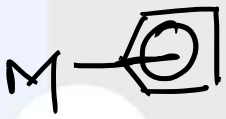


η^1

1 $e^\ominus$ donor

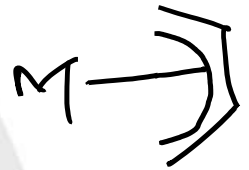
η^3

3 $e^\ominus$ donor



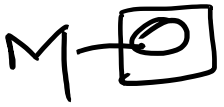
η^5

5 $e^\ominus$ donor



η^4

4 $e^\ominus$ donor

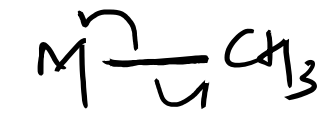


η^4

Electron Count :- 2 Methods

4

Neutral Method

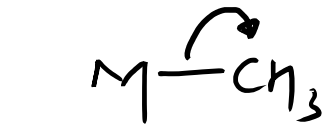
Ex: 

$M^{\cdot}$ $\quad$ $\cdot CH_3$

1 $e^{\ominus}$ donor

→ Here Ligands are considered in neutral form.

Donor Pair method

Ex: 

$M^{\oplus}$ $\quad$ $CH_3^{\ominus}$

2 $e^{\ominus}$ donor / 1 $e^{\ominus}$ pair

→ Here Ligands are expected to donate pair of electron.

① TiF_6^{2-} TVE : 4+6+2 = 12 $e^{\ominus}$

Stable ✓ as F is weak field ligand. M — F: ↳ 1 $e^{\ominus}$ donor

★ Application of 18 $e^{\ominus}$:-

→① Metal- Metal Bonds :-

ML_6 → 18 $e^{\ominus}$

M_2 → TVE : 36

M-M M_2 → TVE = 34

M=M M_2 → TVE = 32

M≡M M_3 → TVE = 30

M-M bond = 0

M-M bond = 1

M-M bond = 2

M-M bond = 3

M_3 → TVE = 54 M-M = 0

M_3 → TVE = 52 M-M = 1

M_3 → TVE = 50 M-M = 2

M_3 → TVE = 48 M-M = 3.

$$\text{M-M bond} = \frac{18n - TVE}{2}$$

① n = no. of metal

② $(n \leq 4)$

Ex ① $[(\eta^5-C_5H_5)_2 Fe_2(CO)_4]$

TVE = $5\times2 + 8\times2 + 8 = 34$

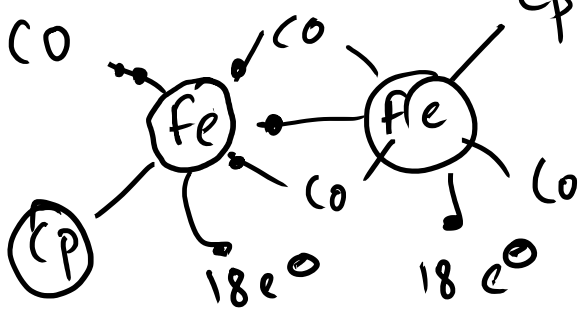
M–M bond = $\frac{18n - TVE}{2}$

= $\frac{18\times2 - TVE}{2}$

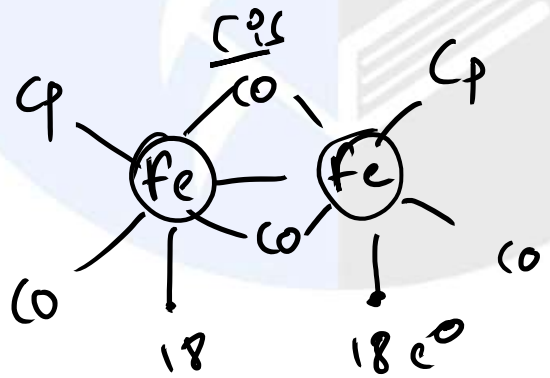
= $\frac{36 - 34}{2}$ = 1 M–M bond.

(MPS)
Most probable structure

trans



cis



② $[(\eta^5-Cp)Mo(CO)_2]_2^{-2}$

10 + 12 + 8 + 2 = 32

M–M bond = $\frac{18n - TVE}{2}$

= $\frac{36 - 32}{2}$ = 2 M–M bond

M.P.S

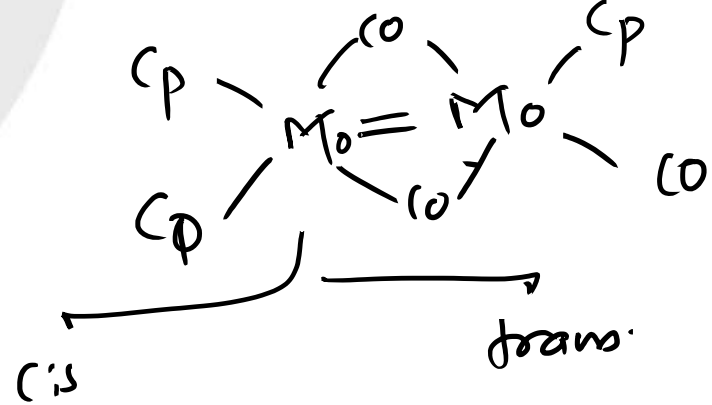


TABLE 13.1 Electron Counting Schemes for Common Ligands

Ligand	Method A	Method B
H	2 (H^-)	1
Cl, Br, I	2 (X^-)	1
OH, OR	2 (OH^-, OR^-)	1
CN	2 (CN^-)	1
CH_3, CR_3	2 (CH_3^-, CR_3^-)	1
NO (bent M—N—O)	2 (NO^-)	1
NO (linear M—N—O)	2 (NO^+)	3
CO, PR_3	2	2
NH_3, H_2O	2	2
=CRR′ (Carbene)	2	2
$H_2C{=}CH_2$ (Ethylene)	2	2
CNR	2	2
=O, =S	4 (O^{2-}, S^{2-})	2
η^3-C_3H_5 (π-allyl)	4 ($C_3H_5^-$)	3
≡CR (Carbyne)	3	3

$\equiv N$	6 (N^{3-})	3
Ethylenediamine (en)	4 (2 per nitrogen)	4
Bipyridine (bipy)	4 (2 per nitrogen)	4
Butadiene	4	4
η^5-C_5H_5 (Cyclopentadienyl)	6 ($C_5H_5^-$)	5
η^6-C_6H_6 (Benzene)	6	6
η^7-C_7H_7 (Cycloheptatrienyl)	6 ($C_7H_7^+$)	7


Thank you