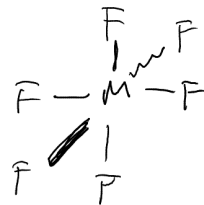
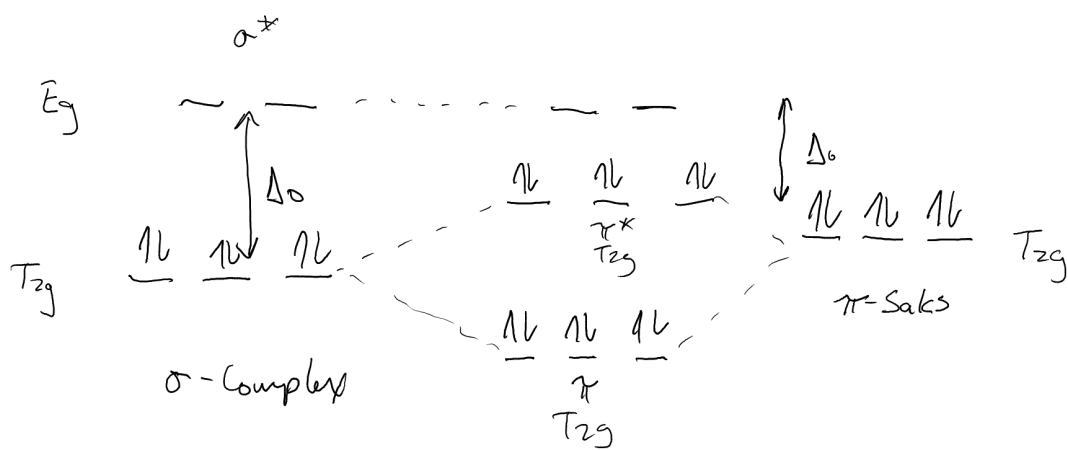
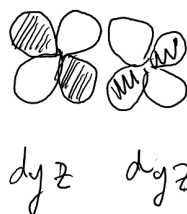
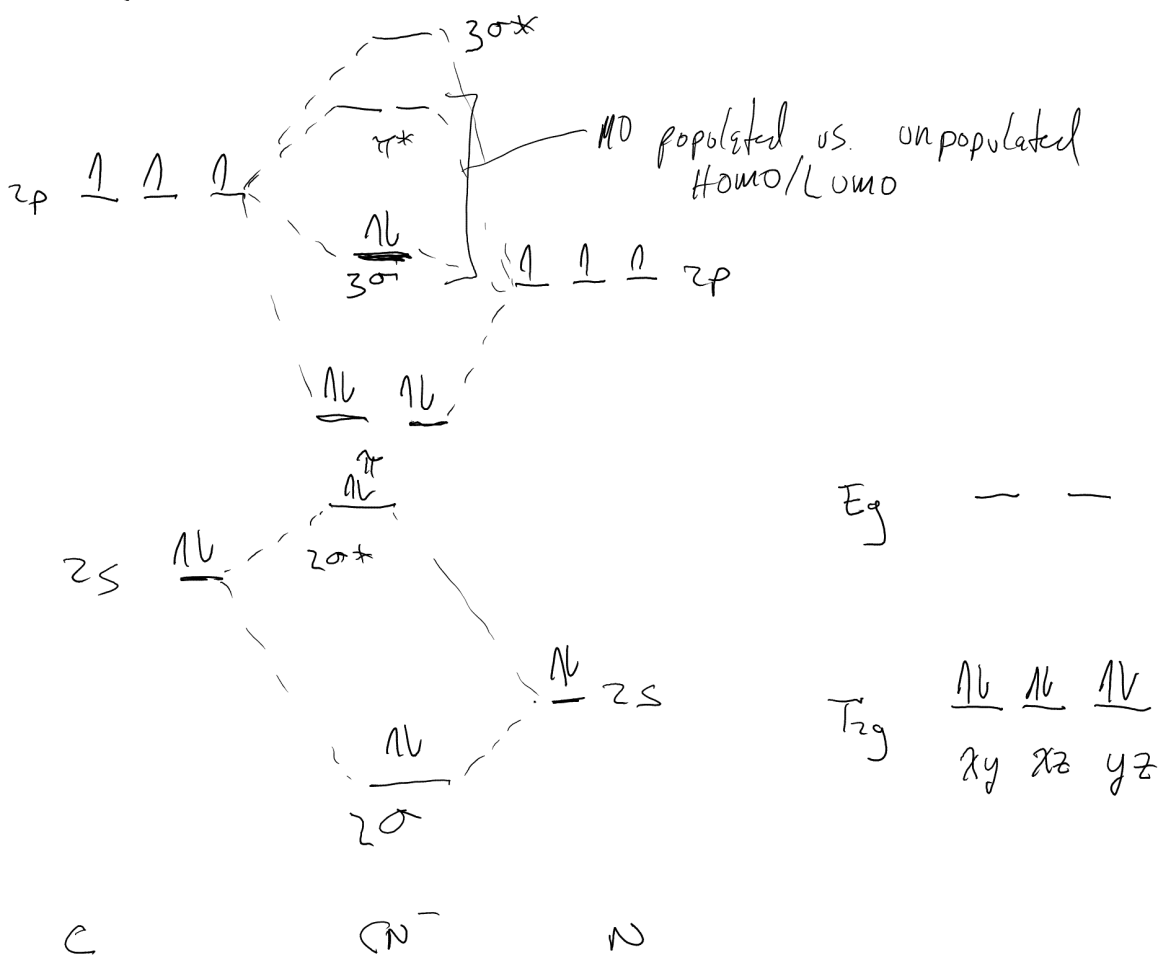


π -Donor Ligands

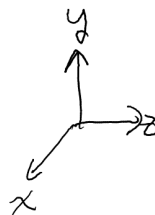


π -Acceptors

Cyanide CN^- $:\overset{\ominus}{C}\equiv N:$

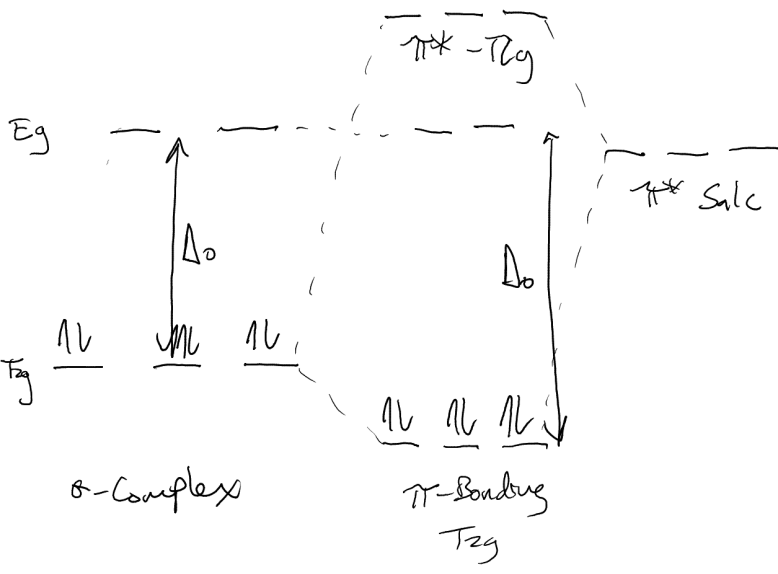


= $m-m$ π -bond

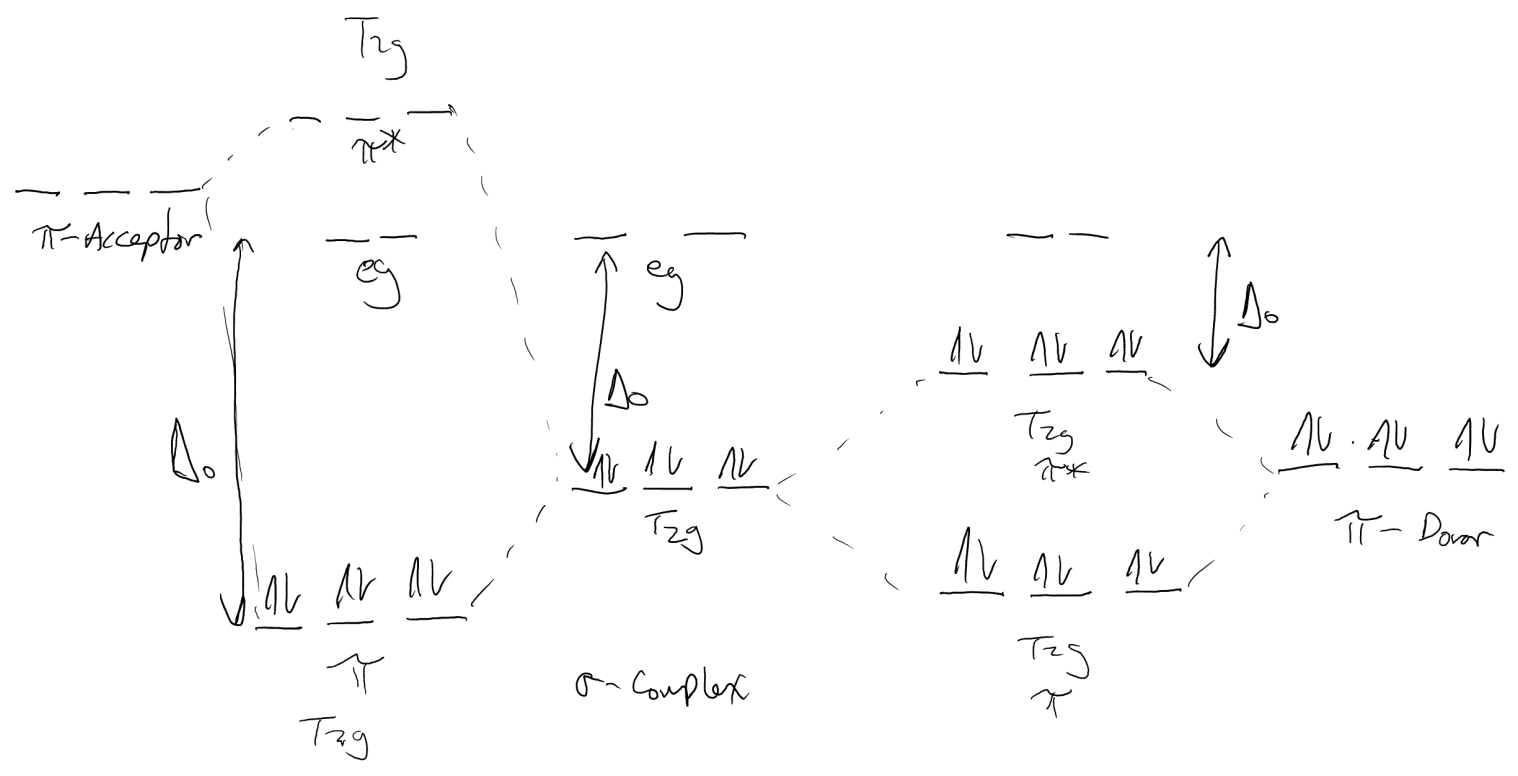




HOMO $\rightarrow$ LUMO



Strongest Field Ligands
 CN^- , CO , NO^+
 Ligands that are π -acceptors

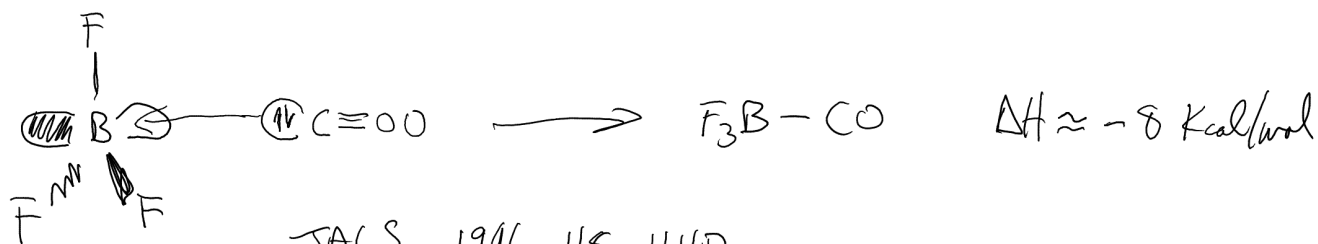


π -Acceptor Ligands
 Strong Field

π Donor Ligands
 Weak Field

- ① Predicting Rxn Mechanisms
- ② Understanding Stability of DMs

③ CO is such an excellent ligand



JACS 1996, 118, 440

Lewis
Acid



Lewis Base ΔH (Kcal/mol)

NEt_3	-135
Py	-128
MeCN	-60
Et_2O	-79
THF	-96
Acetone	-76
EtOAc	-75
DMSO	-105
PMe_3	-97
CO	-8

CO is typically a very poor Lewis base w/ organics...

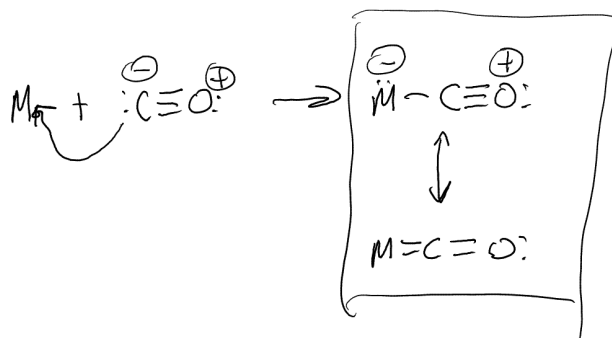


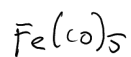
<u>M</u>	<u>BDE (ΔH)</u>
Fe	40 Kcal/mol
Ru	28 Kcal/mol
Os	30 Kcal/mol

Interaction dominated by π -back donation from d-orbital on metal to π^* on CO



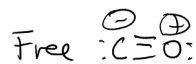
<u>M</u>	<u>BDE (ΔH)</u>
Cr	40 Kcal/mol
Mo	40 Kcal/mol
W	45 Kcal/mol





Fe-C distance = 1.81 Å

C-O distance = 1.15 Å

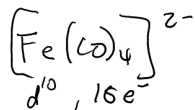
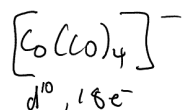
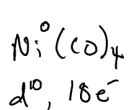


C-O distance = 1.13

CO is an excellent IR Probe



$\nu_{\text{CO}} \Rightarrow 2143 \text{ cm}^{-1}$



ν_{CO}

2060 cm^{-1}

1890 cm^{-1}

1790 cm^{-1}

← CO Bond Strength

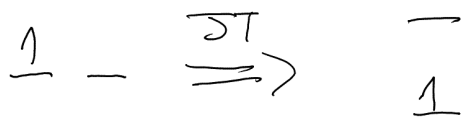
→ CO Bond Length

→ e^- rich metal center

Jahn Teller Effect

Jahn Teller Theorem states that there cannot be unequal occupation of degenerate orbitals

↳ To avoid this unequal occupation, molecules can deform.



First Order JT distortion - most pronounced for e or e_g

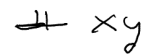
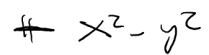
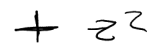
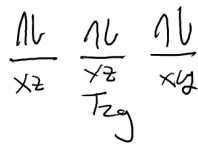
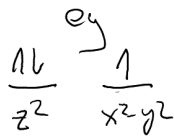
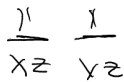
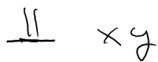
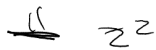
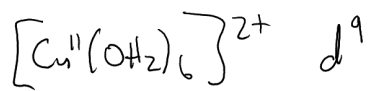


d-electrons
HS
LS

	1	2	3	4	5	6	7	8	9
HS	w	w	/	S	/	w	w	/	S
LS	w	w	/	w	w	/	S	/	S

E_g $\underline{1}$ $\underline{1}$

T_{2g} $\uparrow\downarrow$ $\underline{1\downarrow}$ $\underline{1\downarrow}$



Elongation
along
z-axis

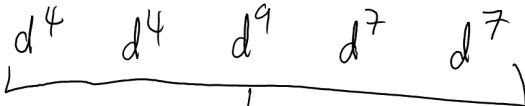
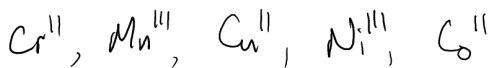
O_h

Compression
along
z-axis

D_{4h}

D_{4h}

Common ions to observe JT distortion



→ Unequal occupation of E_g