ATOMS, MOLECULES & RESEARCH

COORDINATION CHEMISTRY -SPRING- WEEK 3

From the given HW sheet

① For all these complexes, the bonding MO's will be filled. Therefore the focus here will be on the HOMO & LUMO (t_{2g} & e_g) molecular orbitals.

$[Cr(CN)_6]^{4-}$ Cr is in the +2 oxidation state Cr^{2+}

CN^- is a strong field ligand. ∴ Δ_o is large. Low spin complex

$Cr = 4s^1\ 3d^5 = d^6$ case

$Cr^{2+} = d^4$ case

e_g — — $0.6\Delta_o$

Δ_o

t_{2g} ↿⇂ 1 1 $-0.4\Delta_o$

# of unpaired $\bar{e}$ = 2

$LFSE = -4(0.4\Delta_o) = -1.6\Delta_o$

$[Fe(H_2O)_6]^{3+}$ Fe^{3+} Δ_o is small, since H_2O is a weak field ligand. ∴ High-spin complex.

e_g 1 1

Δ_o

t_{2g} 1 1 1

$Fe\ \ 4s^2\ 3d^6 \Rightarrow d^8$ case

$Fe^{3+} \Rightarrow d^5$ case

$LFSE = 3(-0.4\Delta_o) + 2(0.6\Delta_o) = 0$

# of unpaired $\bar{e}$ = 5

$[Co(NO_2)_6]^{4-}$ Hogh spin complex since NO_2 is a weak field ligand.

e_g 1 1

t_{2g} ↿⇂ ↿⇂ 1

$Co = 4s^2\ 3d^7 = d^9$ case

$Co^{2+} = d^7$ case

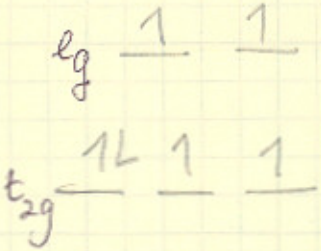
$LFSE = (-0.4\Delta_o)5 + 2(0.6\Delta_o) = -0.8\Delta_o$

# of unpaired $\bar{e}$ = 3

$[Co(NH_3)_6]^{3+}$ high spin complex since NH_3 is a weak field ligand. Co is in +3 oxidation state

$Co = 3d^7 4s^2 = d^9$ case

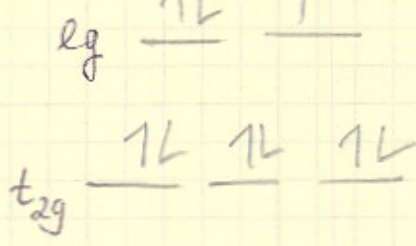
$Co^{3+} = d^6$ case



$LFSE = 4(0.4\Delta_o) + 2(0.6\Delta_o) = -0.4\Delta_o$

# of unpaired $\bar{e} = 4$

$[Cu(H_2O)_6]^{2+}$ high spin complex since H_2O is a neutral ligand. Cu is in the +2 oxidation state



$Cu = 4s^1 3d^{10} = d^{11}$ case

$Cu^{2+} = d^9$ case

$LFSE = 6(-0.4\Delta_o) + 3(0.6\Delta_o)$

$= -0.6\Delta_o$

# of unpaired $\bar{e} = 1$

(2)

element	Neutral atom	+1 ion	+2 ion	+3 ion
K	[Ar] $4s^1$	[Ar]	[Ne] $3s^2 3p^5$	[Ne] $3s^2 3p^4$
Ca	[Ar] $4s^2$	[Ar] $4s^1$	[Ar]	[Ne] $3s^2 3p^5$
Sc	[Ar] $4s^2 3d^1$	[Ar] $4s^1 3d^1$	[Ar] $3d^1$	[Ar]
Ti	[Ar] $4s^2 3d^2$	[Ar] $4s^1 3d^2$	[Ar] $3d^2$	[Ar] $3d^1$
V	[Ar] $4s^2 3d^3$	[Ar] $4s^1 3d^3$	[Ar] $3d^3$	[Ar] $3d^2$
Cr	[Ar] $4s^1 3d^5$	[Ar] $3d^5$	[Ar] $3d^4$	[Ar] $3d^3$
Mn	[Ar] $4s^2 3d^5$	[Ar] $4s^1 3d^5$	[Ar] $3d^5$	[Ar] $3d^4$
Fe	[Ar] $4s^2 3d^6$	[Ar] $4s^1 3d^6$	[Ar] $3d^6$	[Ar] $3d^5$
Co	[Ar] $4s^2 3d^7$	[Ar] $4s^1 3d^7$	[Ar] $3d^7$	[Ar] $3d^6$
Ni	[Ar] $4s^2 3d^8$	[Ar] $4s^1 3d^8$	[Ar] $3d^8$	[Ar] $3d^7$
Cu	[Ar] $4s^1 3d^{10}$	[Ar] $3d^{10}$	[Ar] $3d^9$	[Ar] $3d^8$
Zn	[Ar] $4s^2 3d^{10}$	[Ar] $4s^1 3d^{10}$	[Ar] $3d^{10}$	[Ar] $3d^9$
Ga	[Ar] $4s^2 3d^{10} 4p^1$	[Ar] $4s^2 3d^{10}$	[Ar] $4s^1 3d^{10}$	[Ar] $3d^{10}$
Se	[Ar] $4s^2 3d^{10} 4p^4$	[Ar] $4s^2 3d^{10} 4p^3$	[Ar] $4s^2 3d^{10} 4p^2$	[Ar] $4s^2 3d^{10} 4p^1$