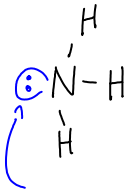
Notes 03/07

Friday, March 07, 2008
10:04 AM

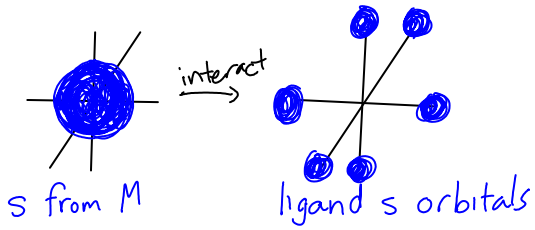
MO Orbitals

$[M(NH_3)_6]Cl_2$

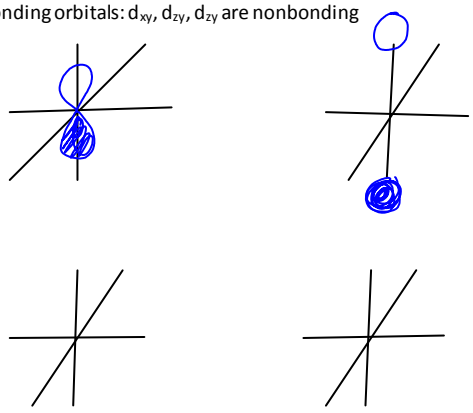


Homo - highest occupied molecular orbital. This is only point of interest in our MO

$6NH_3$



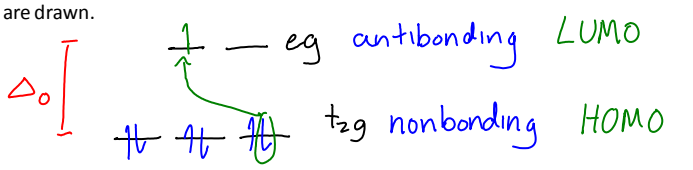
Nonbonding orbitals: d_{xy}, d_{zy}, d_{zy} are nonbonding



$[Co^{III}(NH_3)_6]Cl_3$

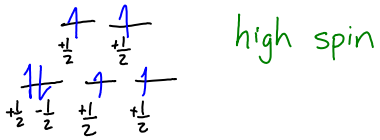
$Co^0 = 9e^-$ contributes $12e^-$

In octahedral MO orbital, all bonding orbitals are filled (assuming $12e^-$) so for simplicity, jus the eg and t2g are drawn.



Δ_o can change based on ligands

Small Δ_o



large Δ_o — — low spin

↿⇂ ↿⇂ ↿⇂

— — eg (antibonding)

— — — t_{2g} (nonbonding)

If have a strong bond between ML, bonding orbitals shift down and antibonding shifts up. 2tg is not affected, but eg goes up higher in energy.

SO:

- **strong field ligands gap is larger**
- **Weak field ligands gap is smaller**

Thus:

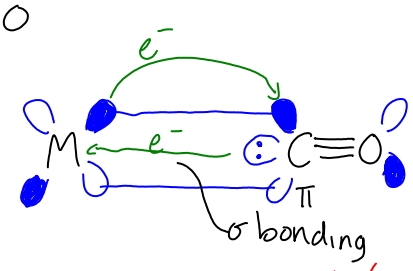
- **Strong field tends to be low spin**
- **Weak field tends to be high spin**

Which ligands are strong or weak field?

Halogens are clearly weak field
Contains water are in middle
CO, Cn etc are strong field
Increasing oxidation state or down the group increases strong field
See VOH for list of ligands.

Why is CO strong field?

M C O



Synergistic bonding or back bonding

CO is π-acid (accepting e^-)

Due to back bonding, the M-C is stronger but C-O is weaker

Tegragonal distortion. (characteristic of d^9 complex).

This type of distortion is Jahn-Teller distortion

D^8 is square planar

What is geometry of $Pd^{2+}NH_3$?

$[Pd(NH_2)_4]Cl_2$

d^8 – square planar

d^8 – square planar