HETERONUCLEAR DIATOMICS:
HF
H(ls) F [He] 2s^2 2p^5

MO: LINEAR COMBO OF
ls(H) \( \frac{\text{H}}{+} \) \( \infty \) \( \frac{\text{F}}{-(2p_z(F))} \)

However, there will not be equal contributions
1e
\( \Phi = (a^2 + b^2)^{-1/2} (a \text{ls}(H) - b 2p_z(F)) \)

What does HF look like? \( H^+ F^-; H^- F^+; H: F ? \)

Nature of bond is determined by \( b/a \)

Ionic vs. Covalent? Dipole moment \( \mu \)

\( \mu = \sum_{i} q_i \epsilon_i \) \( \sum_{j} Z_j \epsilon_j \)

Electrons Nuclei

Example NaCl Ionic \( \text{Na}^+ \text{Cl}^- \)

Can approximate \( \mu \) from 2 point charges
\[ 2 \xrightarrow{\text{Na}^+} \text{Cl}^- \]  
\[ r_e = 2.304 \text{ Å} \]

\[ 1 \mu = 1.2 \times 10^{-10} \text{ cm} \]  
\[ 1 \text{ D} = 10^{-18} \text{ esu cm} \]

**Units of \( \mu \) are Debye (D)**

**Electronic charge =** \[ 4.8 \times 10^{-10} \text{ esu (CGS units)} \]

**Pt. Charge Approx. To NaCl:**  
\[ \mu = (4.8)(2.301) = 11.34 \text{ D} \]

**Expt. \( \mu = 9.0 \text{ D} \Rightarrow \text{Close to Pt. Charge Treatment} \)**

**Approx. an Ionic Bond**

**HF: \( \mu = 1.82 \text{ D} \); For \( H^+ F^- \Rightarrow \mu_{\text{ionic}} = 4.4 \text{ D} \) (\( r_e = 0.928 \))**

**HF has Partial Ionic/Covalent Bonding**

**Why \( H^+ F^- \) instead of \( H^- F^+ \)?**

**Electronegativity**

\[ x = \frac{1}{2} (IP + EA) \]

**IP:**  
\[ A \rightarrow A^+ + e^- \]

**EA:**  
\[ A + e^- \rightarrow A^- \text{ (Exothermic)} \]

**H:**  
\[ IP = 13.595 \text{ eV} \]

\[ EA = 0.764 \text{ eV} \]

\[ X_H = 7.17 \text{ eV} \]

**F:**  
\[ 1s^2 2p^5 \]

\[ IP = 20.96 \text{ eV} \]

\[ EA = 3.47 \text{ eV} \]

\[ X_F = 12.22 \text{ eV} > X_H \]

**Because**  
\[ X_H < H \Rightarrow H-F \]

**Because**  
\[ X_F > H \Rightarrow H-F \]
MO's in Heteronuclear Diatomics:

Flower: More Electronegative

HF

$1A^*$

$1S_H$

$2P_F^R, 2P_F$

$1A$

$1A$ has more F character,
$1A^*$ has more H character,

$1A$

$H_F, 1A$

$H_F^*$

2nd Row Species

$A_B, X_A > X_B$

$2P_A, 2p^X$

$2P_B, 2p^B$

$2S_A, 2S_B$

$1S_A, 1S_B$

Ordering is always true for 2nd row species:

No $g/u$ Symmetry

$BIC$ is a part of inversion

Term Symbols: Same as before: No $g/u$ Symmetry

$Co: (2s^2)(2s^*^2)(2p^6)(2p^4)^2(2p^6)^2: \frac{1}{2}^+$

$No: (2s^2)(8s^*^2)(2p^6)(2p^4)^2(2p^6)^2(2p^6)^2: 2^+$
**Electronic Excitation:**

Occupied MO $\rightarrow$ Unoccupied MO (Electronic Spectroscopy)

$H_2$: Ground State $(15\sigma_g)^2 (15\sigma_u)^0$

Lowest excited state: $(15\sigma_g)(15\sigma_u)$

$\Rightarrow$ 2 excited states

$15\sigma_g - t$

$3\tilde{\sigma}^+ \quad 1\tilde{\pi}^+$

$E(R)$ for $1\tilde{\sigma}^+, 3\tilde{\sigma}^+, 1\tilde{\pi}^+$

Diagram:
- $H(15) + H(2\tilde{\sigma})$
- Repulsive
- $H(15) + H(1\tilde{\sigma})$

Labeling:
- $X$ is ground state
- $A$ is 1$^{st}$ excited state with same spin multiplicity
- $a$ is 1$^{st}$ excited state with different spin multiplicity
$O_2$: Ground State MO Config.

$\pi^* - 2\pi^* + 2\pi^+ + \pi$

Lowest Excited MO Config.

$\pi^* \rightarrow \pi^+_g$

$\pi^* + 3\Delta_u + \Sigma_u^+$

Can have $S=0$ or $S=1$

All term symbols will be $\Omega (3 \text{ \text{ } u \text{ \text{ } electrons})$

$3\Delta_u, \Sigma_u, \Sigma_u^+, \Sigma_u^-$

Have to distinguish between states of different spin multiplicity.