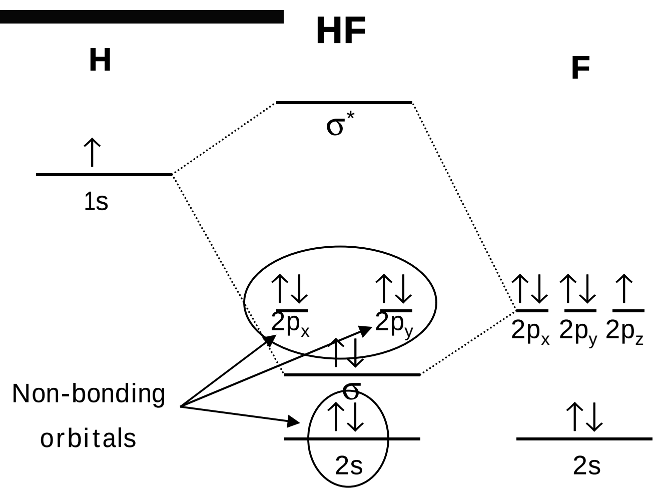
Announcements – 11/13/00

- **Exam #3** - Wed., 11/15/00, 7pm
  -see me ASAP about alternate times!

- ***Quiz post mortem***

Example: HF



Orbital Mixing

- Mixing of orbitals depends on *symmetry* and on *energy* matches
- The extent to which an atomic orbital contributes to the molecular orbital wavefunction is represented in the mixing equation:

$$\psi_{mol} = \sigma = C_H \psi_{1s}(H) + C_F\, \psi_{2p}(F)$$

- The magnitudes of C_H and C_F will reflect the degree to which these *atomic orbitals* contribute to the resulting *molecular orbital* wavefunction

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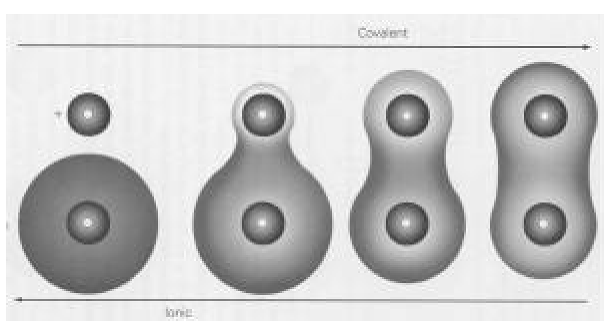
Polar Covalent Continuum

- Replacing **H** with ***Na*** pushes its *s-orbital* to higher energy, decreasing the mixing with the p_z-orbital on F
- $C_{Na} < C_H$ so resulting MO will have more electron density on **F** (more polar)



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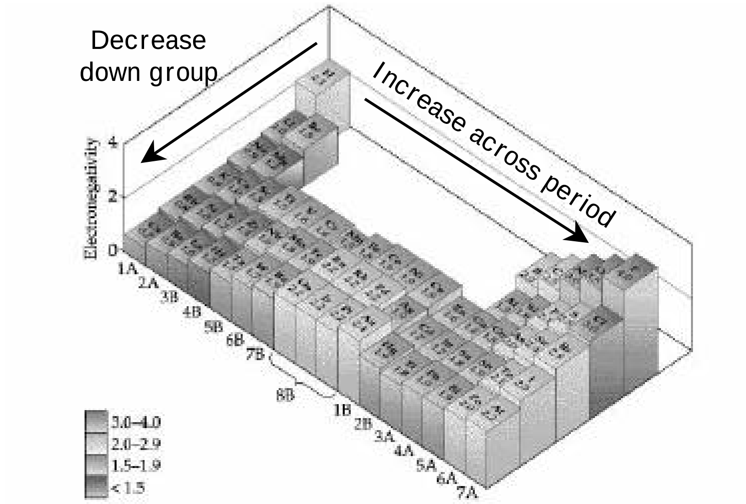
Electronegativity: Periodic Trends



Determining %-Ionic Character

- If we know a molecule's *dipole moment* and **bond length**, then we can assess the degree of charge separation (ionic character) across the bond:

% - Ionic character = δ x 100, where:

$$\delta = \mu/(e \times d)$$

μ - dipole moment
e - charge on an electron
d - bond length

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%-Ionic Character Examples

- So, for **HCl:** μ **=** 1.08 D d = 1.27 Å

$$\delta = \frac{1.08\ \text{D}}{(1.602 \times 10^{-19}\ \text{C})(1.27 \times 10^{-10}\ \text{m})} \times \frac{3.336 \times 10^{-30}\ \text{C-m}}{}$$

δ = **0.177086** $\Rightarrow$ *17.7 % ionic character*

- For **NaCl**: μ **=** 9.001 D d = 2.36 Å

δ = **0.794223** $\Rightarrow$ *79.4 % ionic character*

Dipole Moments and Bond Properties

- Trends in the *Hydrogen Halides:*

Compound	**d (Å)**	**μ (D)**	**%-δ**	**ΔEN**
HF	0.92	1.82	41.2	1.9
HCl	1.27	1.08	17.7	0.9
HBr	1.41	0.82	12.1	0.7
HI	1.61	0.44	5.7	0.4