Example: Polar Bonds in Hydrides

Identify which you would expect to be the most polar:

- [ ] H – C
- [x] H – F Maximizes charge & minimizes bond length
- [ ] H – Cl
- [ ] H – S

Example: The I F Bond

Answer the following questions given the ~~following~~ the bonding energy (kJ/mol) data:

I-I: 150
F-F: 160
C-C: 350
H-H: 435

(a): Calculate the energy of the I-F Bond in kJ/mol.

$$E_{IF} = \sqrt{E_{II} E_{FF}} + 96.2(2.66 - 3.98)^2$$

$$= \sqrt{150 \cdot 160} + 167.619$$

$$= 322.538 \text{ kJ/mol}$$

(b): Calculate the ionic character:

$$\% \text{ ionic char.} = \left(1 - \exp\left(-\frac{1}{4}(\chi_F - \chi_I)^2\right)\right) \cdot 100\%$$

$$= \left(1 - \exp\left(\frac{-1}{4}(1.742)\right)\right) \cdot 100\%$$

$$= 35.3\%$$

Example: Oxygen and the superoxide ion

Use molecular orbital theory to predict whether the bond order in the superoxide ion, O_2^-, should be higher or lower than the bond order of O_2.

Recall Bond order $= \frac{1}{2}$(bonding e^- − non bonding e^-)

Note that Bond order decreases as more non-bonding e^- are present; O_2 has the same bonding e^- as O_2^-, but one less non-bonding. Thus, lower.

Example: Ozone depletion

CFCs are organic compounds that have been implicated in ozone depletion. When the CFC known as Freon 12 (CCl_2F_2) is exposed to UV radiation (wavelength in the range of 10 - 400 nm, a bit shorter than visible light), a chlorine atom breaks off from the rest of the molecule. Prove that this is possible by calculating the maximum ~~wave length~~ wavelength (in meters) capable of breaking the Cl-C bond.

Bond energies

C-C : ~~242~~ 347

Cl-Cl: 242 kJ/mol

(a): Calculate:

$$E_{C-Cl} \cong -\sqrt{E_{CC} E_{ClCl}} + 96.2 (X_C - X_{Cl})^2$$

$$= -\sqrt{242 \cdot 347} + 96.2 (2.55 - 3.16)^2$$

$$\frac{1000\,J}{kJ} \cdot \frac{kJ}{mol} = 325.579\ kJ/mol$$

$$\frac{5.406 \cdot 10^{-19}\,J}{bond} = 325\,579\ J/mol \cdot \frac{\frac{1}{avo}}{\frac{1}{avo}}$$

$$5.406 \cdot 10^{-19}\,J = h\,\nu$$

$$\nu = 8.159 \cdot 10^{14}\ Hz$$

$$\Rightarrow$$

$3.67 \cdot 10^{-7}\,m = \lambda = 367.448$, thus UV light breaks this bond

Example: Cyanide Anion

Select each compound below that is isoelectronic with CN^- ($2s^2 2p^{\cancel{3}2} + 2s^2 2p^3 + e^- \Rightarrow$ or Val $e^- = 10$)

X	O_2^{2-}	Val e^- = ~~12~~ no	10 yes
	NO^+	" = 12	no
X	HF	" = 10	yes
	ClO^-	" =	no
	NO	" = 11	no
X	CO	" =	10 yes