Answers HW #8. Chem 1410

9-12. Why is $De(N_2) > De(N_2^+)$, but $De(O_2^+) > De(O_2)$?

N_2: ... $\underbrace{2\sigma_g^2 2\sigma_u^2}_{2s}\ \underbrace{3\sigma_g^2 1\pi_u^4}_{2p}$

N_2^+: one of the electrons is removed from the $3\sigma_g$ or $1\pi_u$ orbitals which are bonding.

$BO(N_2) = 3$, $BO(N_2^+) = 2.5$

$\Rightarrow De(N_2) > De(N_2^+)$

O_2: ... $2\sigma_g^2 2\sigma_u^2 3\sigma_g^2 1\pi_u^4 1\pi_g^2$

O_2^+: An electron is removed from the $1\pi_g$ orbital which is antibonding.

$BO(O_2) = 2$, $BO(O_2^+) = 2.5$

$\Rightarrow De(O_2) < De(O_2^+)$

9-17 Compare NO and NO^+

NO^+: $\underbrace{1\sigma^2 2\sigma^2}_{1s}\ \underbrace{3\sigma^2 4\sigma^2}_{2s}\ \underbrace{5\sigma^2 1\pi^4}_{2p}$ B.O. = 3

isoelectronic with N_2.

NO: $1\sigma^2 2\sigma^2 3\sigma^2 4\sigma^2 5\sigma^2 1\pi^4 2\pi$ B.O. = 2.5

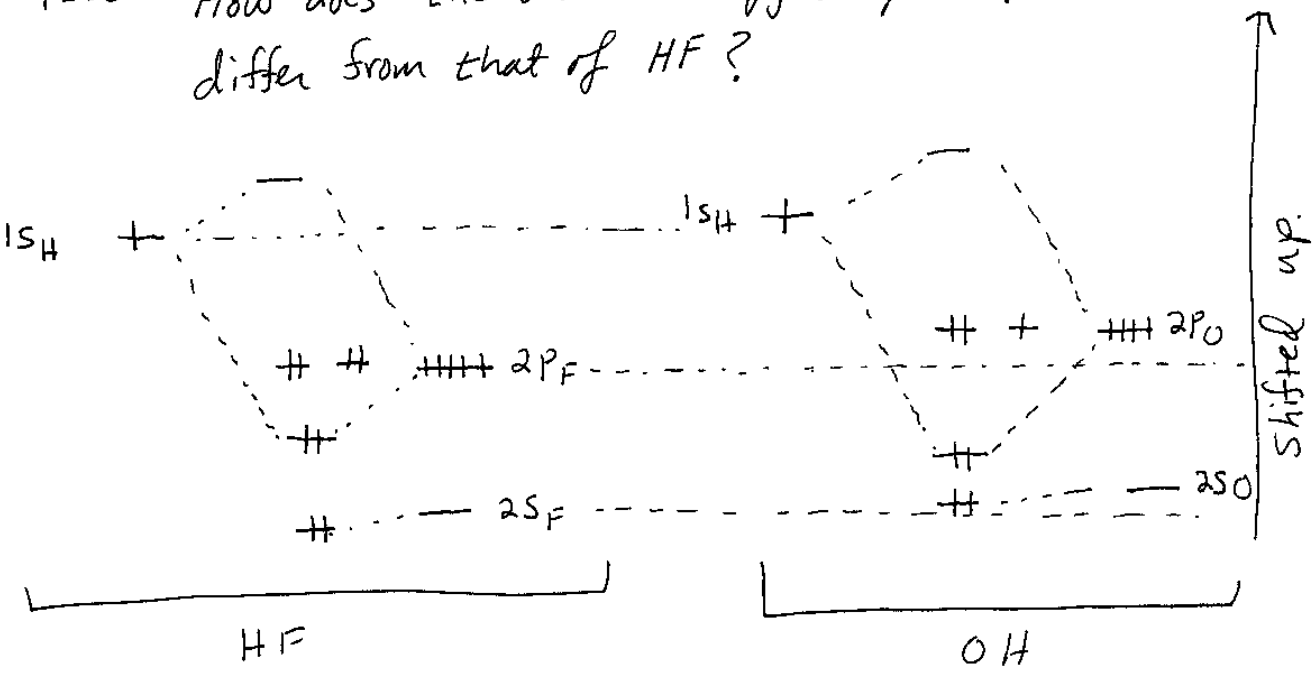
(1π: bonding; 2π: antibonding)

9-19.

Molecule	k (N/m)	BO
B_2	350	1
C_2	930	2
N_2	2260	3
O_2	1140	2
F_2	450	1

The force constants correlate with the bond orders as expected.

9-22 How does the orbital energy diagram of OH differ from that of HF?



BO = 1

BO = 1

OH also has a bond order = 1, since the electron that is "missing" (relative to HF) has been emoved from a non-bonding orbital.

9-31 What are the term symbols of O_2, N_2, O_2^+, N_2^+?

O_2 $\underbrace{1\sigma_g^2 1\sigma_u^2}_{1s}\ \underbrace{2\sigma_g^2 2\sigma_u^2}_{2s}\ \underbrace{3\sigma_g^2 1\pi_u^4 1\pi_g^2}_{2p} \rightarrow {}^3\Sigma_g^-$

O_2^+ $\underbrace{1\sigma_g^2 1\sigma_u^2}_{1s}\ \underbrace{2\sigma_g^2 2\sigma_u^2}_{2s}\ \underbrace{3\sigma_g^2 1\pi_u^4 1\pi_g}_{2p} \rightarrow {}^2\Pi_g$

N_2 $\underbrace{1\sigma_g^2 1\sigma_u^2}_{1s}\ \underbrace{2\sigma_g^2 2\sigma_u^2}_{2s}\ \underbrace{3\sigma_g^2 1\pi_u^4}_{2p} \rightarrow {}^1\Sigma_g^+$

N_2^+ $\underbrace{1\sigma_g^2 1\sigma_u^2}_{1s}\ \underbrace{2\sigma_g^2 2\sigma_u^2}_{2s}$ $\begin{cases} 3\sigma_g^2 1\pi_u^3 \rightarrow {}^2\Pi_u \\ 3\sigma_g 1\pi_u^4 \rightarrow {}^2\Sigma_g^+ \end{cases}$ } give credit for either since these state are close in energy.

9-36 dipole moment of LiH if 100% ionic?

$$\mu = qR = (1.602 \times 10^{-19}\ C)(1.59 \times 10^{-10}\ m)$$
$$= 25.5 \times 10^{-30}\ C \cdot m$$

What is the percentage of ionic character?

$$\frac{\text{Expt. dipole}}{\text{ideal dipole}} = \frac{q_1 R}{q_2 R} = \frac{q_1}{q_2} = \frac{19.62}{25.5}$$

$q_1 = 0.77\ |e|$ 77% ionic character.