

## SOLUTION MANUAL FOR HW # 9

### 11.5

A.  $1s^2 \ ^1S \rightarrow 1s2p \ ^1P \rightarrow \Delta l = +1 \ \& \ \Delta s = 0$  : Allowed

B.  $1s2p \ ^1P \rightarrow 1s3s \ ^1S \rightarrow \Delta l = -1 \ \& \ \Delta s = 0$  : Allowed

C.  $1s2s \ ^3S \rightarrow 1s2p \ ^3P \rightarrow \Delta l = +1 \ \& \ \Delta s = 0$  : Allowed

D.  $1s2p \ ^3P \rightarrow 1s3d \ ^3D \rightarrow \Delta l = +1 \ \& \ \Delta s = 0$  : Allowed

One peak is observed in each case.

### 11.13

Because of spin-orbit interaction the principal spectrum line of K is doublet.

### 13.5

$CF^+(14e^-)$  :  $\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \sigma_{2p}^2 \pi_{2p}^4$

$NO(15e^-)$  :  $\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \sigma_{2p}^2 \pi_{2p}^4 \pi_{2p}^{*1}$

$CF(16e^-)$  :  $\sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \sigma_{2p}^2 \pi_{2p}^4 \pi_{2p}^{*2}$

$CF^+$  : Bond Order:  $6/2 = 3$  &  $NO$  : Bond Order:  $(6-1)/2 = 2.5$  &  $CF$  : Bond Order :  $(6-2)/2 = 2 \rightarrow$  bond Dissociation Energy trend:  $CF^+ > NO > CF$

### 13.11

A)  $Li_2$  :  $1\sigma_g^2 1\sigma_u^{*2} 2\sigma_g^2$  &  $Li_2^+$  :  $1\sigma_g^2 1\sigma_u^{*2} 2\sigma_g^1$

$Li_2$  :  $B.O. = (4-2)/2 = 1$  &  $Li_2^+$  :  $B.O. = (3-2)/2 = 0.5 \Rightarrow \nu(Li_2) > \nu(Li_2^+)$

B)  $C_2$  :  $1\sigma_g^2 1\sigma_u^{*2} 2\sigma_g^2 2\sigma_u^{*2} 1\pi_u^4$  &  $C_2^+$  :  $1\sigma_g^2 1\sigma_u^{*2} 2\sigma_g^2 2\sigma_u^{*2} 1\pi_u^3$

$C_2$  :  $B.O. = (8-4)/2 = 2$  &  $C_2^+$  :  $B.O. = (7-4)/2 = 1.5 \Rightarrow \nu(C_2) > \nu(C_2^+)$

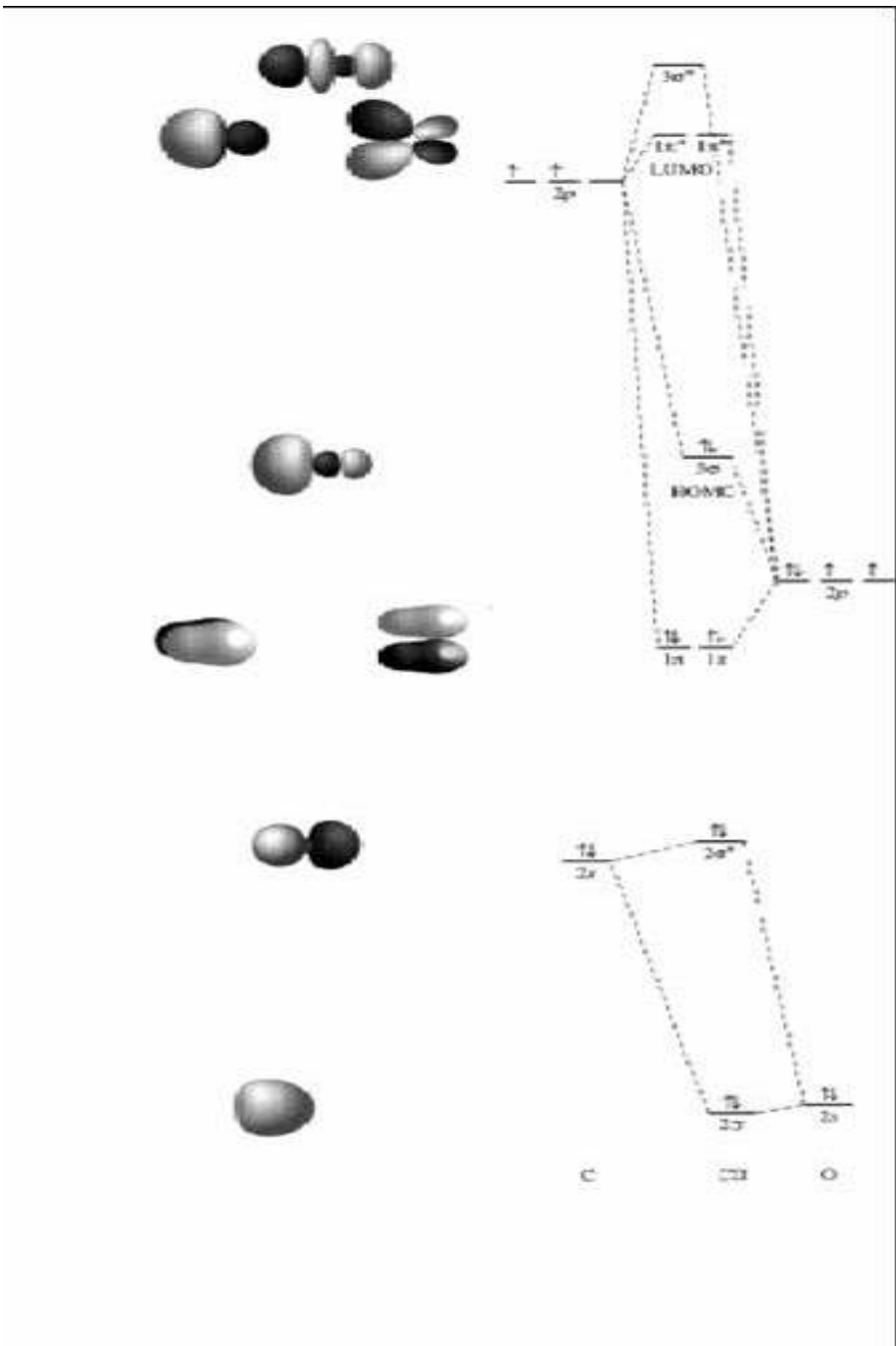
C)  $O_2$  :  $1\sigma_s^2 1\sigma_s^{*2} 2\sigma_s^2 2\sigma_s^{*2} 2\sigma_p^2 1\pi_u^4 1\pi_u^{*2}$  &  $O_2^+$  :  $1\sigma_s^2 1\sigma_s^{*2} 2\sigma_s^2 2\sigma_s^{*2} 2\sigma_p^2 1\pi_u^4 1\pi_u^{*1}$

$O_2$  :  $B.O. = (10-6)/2 = 2$  &  $O_2^+$  :  $B.O. = (10-5)/2 = 2.5 \Rightarrow \nu(O_2^+) > \nu(O_2)$

D)  $F_2$  :  $1\sigma_s^2 1\sigma_s^{*2} 2\sigma_s^2 2\sigma_s^{*2} 2\sigma_p^2 1\pi_u^4 1\pi_u^{*4}$  &  $F_2^-$  :  $1\sigma_s^2 1\sigma_s^{*2} 2\sigma_s^2 2\sigma_s^{*2} 2\sigma_p^2 1\pi_u^4 1\pi_u^{*4} 2\sigma_p^{*1}$

$O_2$  :  $B.O. = (10-8)/2 = 1$  &  $O_2^-$  :  $B.O. = (10-9)/2 = 0.5 \Rightarrow \nu(F_2) > \nu(F_2^-)$

### 13.13



AO Energy= Ionization Level (0)-AO Ionization Energy

→ O2s = -32.3 eV & O2p = -15.8 eV

→ C2s = -19.4 eV & C2p = -10.9 eV