

ANSWERS TO MOLECULAR ORBITALS PROBLEM SET

1. (a) $N_2^+(13 e^-): \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^1$
 $N_2^{2+}(12 e^-): \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2$
 $N_2(14 e^-): \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2$
 $N_2^-(15 e^-): \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2 \pi_{2p}^{*1}$
 $N_2^{2-}(16 e^-): \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2 \pi_{2p}^{*1} \pi_{2p}^{*1}$
 - (b) Bond orders are: $N_2^+ = 2.5$; $N_2^{2+} = 2.0$; $N_2 = 3.0$; $N_2^- = 2.5$; $N_2^{2-} = 2.0$
 - (c) Longest bond (N_2^{2+} & N_2^{2-}) > (N_2^+ & N_2^-) > (N_2) Shortest bond
 - (d) Strongest bond (N_2) > (N_2^+ & N_2^-) > (N_2^{2+} & N_2^{2-}) Weakest bond
 - (e) Paramagnetic (N_2^+ , N_2^- , N_2^{2-})
Diamagnetic (N_2 and N_2^{2+})
2. (a) $O_2^+: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2 \pi_{2p}^{*1}$
(b) $NF: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2 \pi_{2p}^{*1} \pi_{2p}^{*1}$
(c) $CO: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2$
(d) $C_2: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2$
(e) $BN: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2$
(f) $Be_2: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2}$
(g) $H_2: \sigma_{1s}^2$
(h) $F_2^-: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2 \pi_{2p}^{*2} \pi_{2p}^{*2} \sigma_{2p}^{*1}$
(i) $OF^-: \sigma_{1s}^2 \sigma_{1s}^{*2} \sigma_{2s}^2 \sigma_{2s}^{*2} \pi_{2p}^2 \pi_{2p}^2 \sigma_{2p}^2 \pi_{2p}^{*2} \pi_{2p}^{*2}$
3. (a) 1 σ -bond and 2 π -bonds
(b) 5 σ -bonds and 1 π -bond
(c) sp^2
(d) 6 electrons in 3 π -bonds
4. (a) CCl_4 : London or Dispersion forces
(b) CH_2Cl_2 : Dipole-Dipole and London forces
(c) CH_3OH : H-bonding, Dipole-Dipole and London forces
(d) CO_2 : London forces
(e) SCl_4 : Dipole-Dipole and London forces
(f) SCl_6 : London forces