Interaction Between Light & Matter

Problem Set #2 — Diatomics: Solutions

1. a. 4
   b. 3 (a triplet)
   c. (1) increase, (2) decrease
   d. 2 (a doublet)

2. a. $(1s\sigma_g)^2(1s\sigma_u*)^2(2s\sigma_g)^2(2s\sigma_u*)^2(2p\sigma_g)^2(2p\pi_u)^4(2p\pi_g*)^1$
   b. 5
   c. O_2^+ has a larger dissociation energy.
   d. All σ MOs.

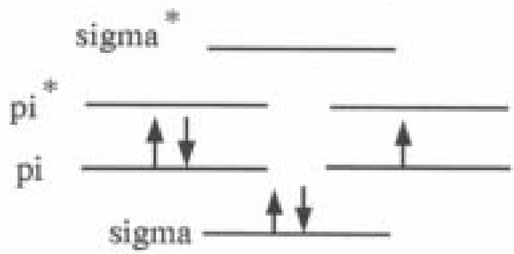
3. The ionization energy represents energy that must be expended to remove the electron from potassium and the electron affinity represents energy that is gained by adding an electron to iodine. The difference between these two energies, 1.28 eV, represents that which must be supplied by the Coulomb energy so as to conserve energy. The Coulomb energy is

$$E = \frac{e^2}{r}$$

where e is the charge on the electron and r is the distance between the potassium and iodide ions. Rearranging and substituting gives

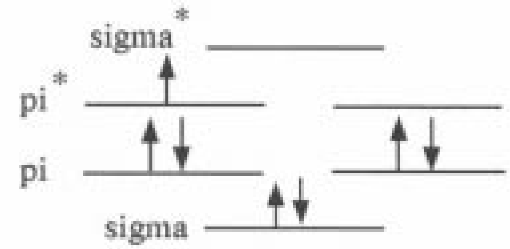
$$r = \frac{143.8 \times 10^{-9} eV \cdot cm}{1.28 eV} = 1.12 nm$$

4. N_2^+ would have the following MO energy level diagram



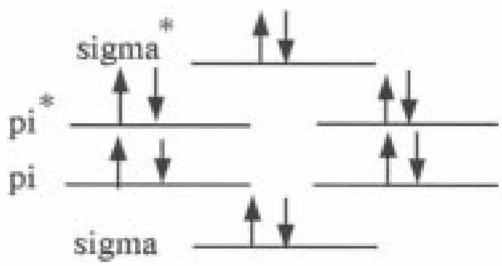
This molecule would have 2.5 bonds and would have a lower bond energy than the triply bonded N_2

O_2^+ would have the following MO energy level diagram



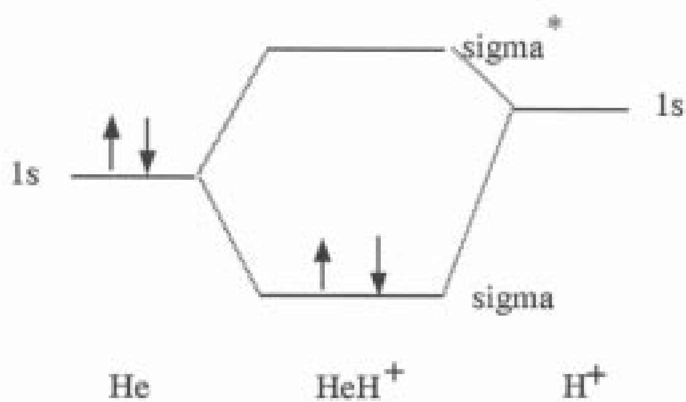
This molecule would have 2.5 bonds and would have a higher bond energy than the doubly bonded O_2.

5. Ne has the following atomic structure $1s^2 2s^2 2p^6$. Thus Ne_2 has 12 p electrons.



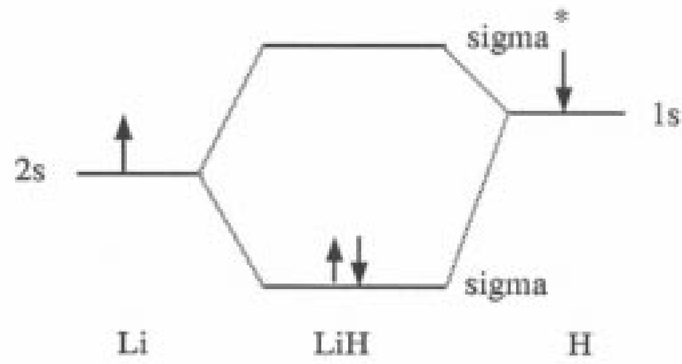
Therefore, Ne_2 is unstable, no net bonding.

6. a.



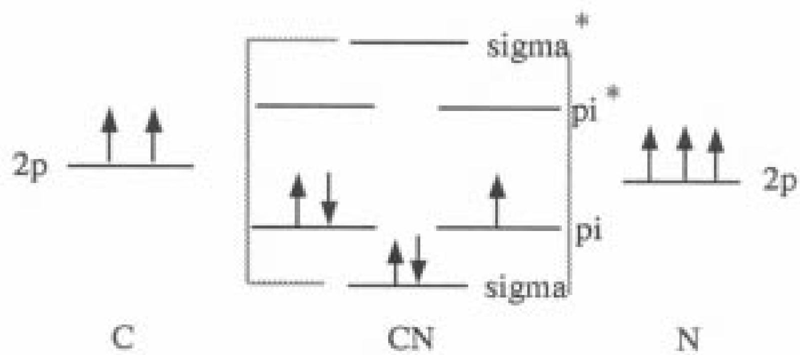
One σ bond

b.



One σ bond

c.



One σ bond, 1.5 π bonds