

Chem 315, Fall 2000
Answers to Problem Set #3

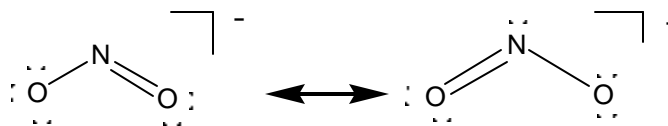
3.3. The (HeHe*) molecule has the following configuration: $\sigma_g^2 \sigma_u^1 \sigma_g^1$ (here σ_u is the antibonding orbital).

3.8. Band gap energy is 4eV, based on this Al_2O_3 is an insulator and would have higher density next to the band edges. Based on O having more electrons in p-orbs than Al, p-peak has more oxygen characteristics.

3.9. The first two values at $T = 273$ K and $T = 373$ K describe the electrical conductivity of solid bismuth. The third point, $T = 573$ K, is not relevant, since it's given for liquid bismuth. (Melting point of Bi is $271^\circ C = 544$ K). Both decrease in the electric conductivity upon heating and it's value, are quite typical for normal metals. Therefore, bismuth can be classified as a metallic conductor.

3.11 The ground state configuration for a neutral fragment NH_2 (bent) is $a_1^2 2a_1^2 1b_2^2 1b_1^1$. The configuration of the first excited state would be $a_1^2 2a_1^2 1b_2^1 1b_1^2$. In this case, there would be two electrons on the nonbonding orbital, which would not significantly decrease the stability of the fragment. Therefore, the lowest total energy would be obtained in the case of angular molecule.

Ex. 3.3



Formal Charges	-1						-1
Oxidation No.	-2	+3	-2				-2

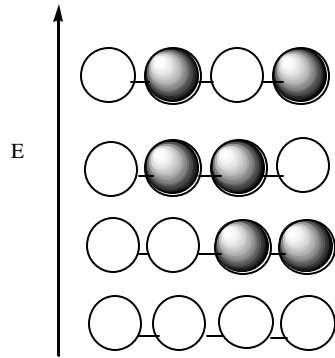
Ex. 3.14

a) s_2 , 12 valence electrons: $\sigma_g^2 \sigma_u^2 \sigma_g^2 \sigma_u^4 \sigma_g^2$. 8 electrons on the bonding orbitals, 4 - on the antibonding. Bond order (B.O.) = $\frac{1}{2}(8-4)=2$, as expected.

b) Cl_2 , 14 valence electrons: $\sigma_g^2 \sigma_u^2 \sigma_g^2 \sigma_u^4 \sigma_g^4$. 8 electrons on the bonding orbitals, 6 - on the antibonding. B.O. = $\frac{1}{2}(8-6)=1$, as expected.

c) NO^- , 12 valence electrons, similar to a): $\sigma_g^2 \sigma_u^2 \sigma_u^2 \sigma_g^2 \sigma_g^2$. 8 electrons on the bonding orbitals, 4 - on the antibonding. B.O. = $\frac{1}{2}(8-4)=2$, as expected.

Ex. 3.16



Ex. 3.23

- a) Ge adds an electron , so it is n-type
- b) Ge removes an electron, so it is p-type
- c) Ge doesn't add or remove so not doped