Chemistry 2141 Homework #2 (74 pts) Due Feb 3. Friday 5:00 PM

Use a pencil (not pen). Use your own paper; ***explicitly show all work****, and sign your name!.*

{Note: K = Kilo = 10^3, d = deci = 10^{-1}, m = milli = 10^{-3}, ? = micro = 10^{-6})

Length units: 1 $\mathring{A}$ = 10^{-8} cm, 1 in = 2.54 cm, 1 mi. = 1.609 km

Energy units: 1 Joule (J) = 1 Kg m^2 s^{-2}, 1 Lit atm = 101.325 J, 1 erg = 1 g cm^2 s^{-2}, 1 cal = 4.184 J, 1 wavenumber (cm^{-1}) = 1.987×10^{-23}J, 1 eV = 8065.5 cm^{-1}

Force (F = ma) units: 1 Newton (N) = 1 Kg m s^{-2}, 1 dyne = 1 g cm s^{-2}

1 mole (mol) = 6.02×10^{23} {particles, bodies, molecules, etc. actually dimensionless}

1. (15 pts) For the molecules below state the electron-domain geometry, hybridization, and molecular geometry?

Molecule	electron-domain geometry	Hybridization (i.e. sp, sp^2, …)	Molecular Shape
CF_2			
CS_2			
XeF_4			
SF_4			
SF_6			

2. (5 pts) Please explain why the overall process of bonding via hybrid orbitals results in a net energy release (more stable), although electron promotion requires an input of energy.

3. (4 pts) Please draw the other two resonance structures with "+" and "– " charges that are resonant with the neutral resonant structure 2,4-hexadiene:

H_3C-CH=CH-CH=CH-CH_3

4. (10 pts) An anion of "**–1**" charge of a homonuclear diatomic has the following electron configuration

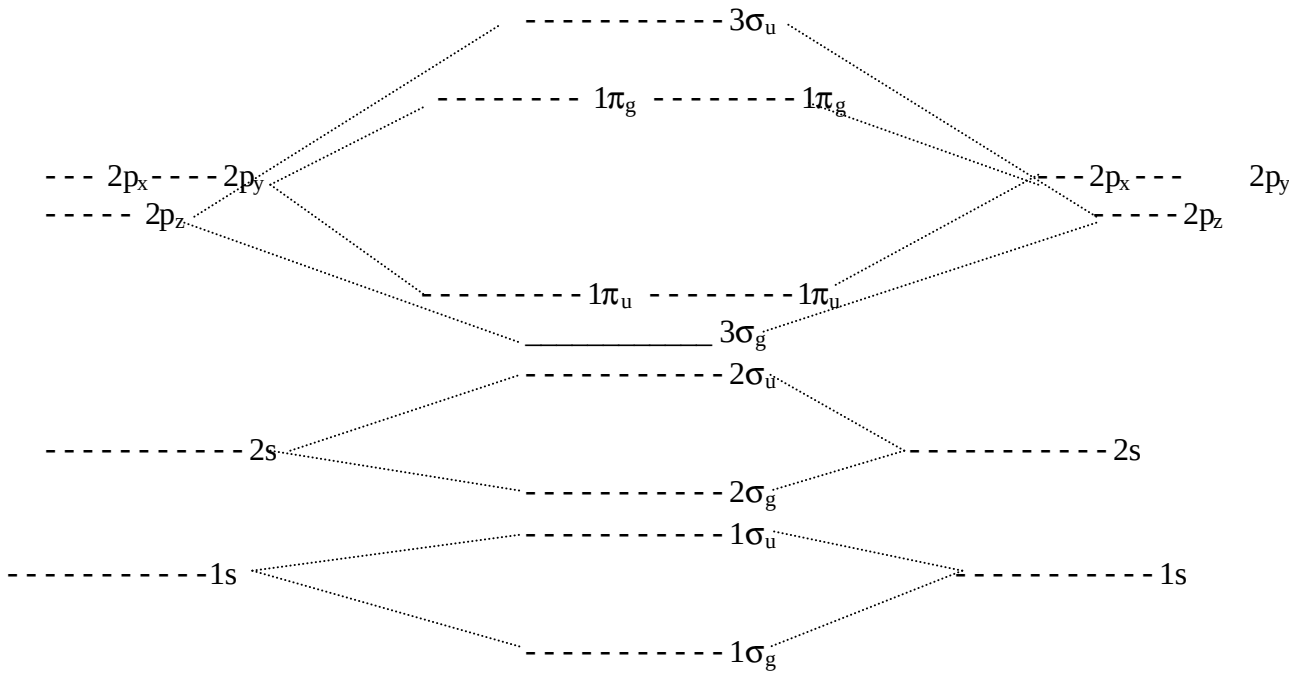
$$(s_g1s)^2(s_u1s)^2(s_g2s)^2(s_u2s)^2(s_g2p_z)^2(p_u2p_x)^2(p_u2p_y)^2(p_g2p_x)^2(p_g2p_y)^2(s_u2p_z)^1$$

a. (8 pts) State (i) the bond order (ii) the parity (iii) whether it is paramagnetic or diamagnetic and (iv) write the chemical formula for this homonuclear diatomic anion (make sure we can identify the element!).

b. (2 pts) Would you expect the anion to be energetically more stable or less stable than the corresponding neutral diatomic. (*Justify your answer!*)

5. (14 pts) Using the figure below answer the following questions.

For the oxygen anion $O_2^{?}$ (a) place electrons as ↑ or ↓ into the M.O. levels shown. (b) write the electronic configuration utilizing the M.O. designations shown below, i.e. $(1\sigma_g)^2(1\sigma_u)^1$, (c) state the bond order, (d) state the parity, (e) state the HOMO (f) state the LUMO and (g) state whether this species should be paramagnetic or diamagnetic.



6. (8 pts) Using Fig. 14.25 as a guide sketch a π-bonding and π-antibonding molecular orbital composed of two "d" atomic orbitals.

7. (10 pts) For ethene ($H_2C=CH_2$): (a) what is the predicted H-C-H bond angle if hybridiztion had not occurred. (b) If hybridization does occur for each CH_2 fragment describe the molecular orbitals that account for the bonding between the two carbon atoms and specify the type of "hybrid orbitals".

8. (8 pts) Tetraene $CH_2=CHCH=CHCH=CHCH=CH_2$ can be treated as box of length 8R where R = 140 pm. Utilizing the free-electron molecular orbital (FEMO) theory calculate the maximum wavelength for the HOMO-LUMO transition in nm units.