

**HW#4 CHEM 281 Your Name:** \_\_\_\_\_

**Valence Shell Electron Pair Repulsion Theory**

1. Determine the electron pair arrangement and the molecular shape (geometry and angles) according to VSEPR theory.
- a)  $\text{CCl}_4$
  - b)  $\text{BH}_3$
  - c)  $\text{PCl}_3$
  - d)  $\text{PF}_5$
  - e)  $\text{XeO}_3$

**Polarity of molecules**

2. Predict the polarity of following molecules:

- a.  $\text{CCl}_4$
- b.  $\text{BH}_3$
- c.  $\text{PCl}_3$
- d.  $\text{PF}_5$
- e.  $\text{XeO}_3$

**Hybridization**

3. Predict the hybridization in the central atom:

- a.  $\text{CCl}_4$
- b.  $\text{BH}_3$
- c.  $\text{PCl}_3$
- d.  $\text{PF}_5$
- e.  $\text{XeO}_3$
- f.  $[\text{Fe}(\text{CN})_6]^{-3}$

**Valence-Bond Theory**

4. What is valence bond(VB) theory and use following as examples

- a.  $\text{PF}_5$
- b.  $\text{XeO}_3$
- c.  $[\text{Fe}(\text{CN})_6]^{-3}$

5. Define the following terms:
  - a) Hybridization (LCAO)
  - b) Molecular orbitals (LCAO)
  - c) What are the main features of the molecular orbital theory?
  
6. Outline the main differences between VB theory and MO theory
  
7. Define the following terms:
  - a.  $\sigma$  molecular orbital:
  
  - b.  $\pi$  molecular orbital:
  
8.  $\delta$  molecular orbital and quadruple bonding:
  
9. Use a molecular orbital diagram to determine the bond order of the  $H_2$
  
10. Would you expect  $Be_2$  to exist? Use a molecular orbital energy diagram to explain your reasoning.

### **Molecular Orbitals for Period 2 Homonuclear Diatomic Molecules**

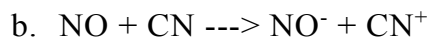
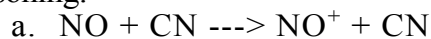
11. Are there any differences in molecular orbital diagrams of  $B_2$ ,  $C_2$ ,  $N_2$ ,  $O_2$  and  $F_2$ ?
  
12. Draw a molecular orbital diagram for  $O_2$  determine the bond order and magnetic properties.

13. Use a molecular orbital diagram to determine the bond order in the  $O_2^+$  ion. Write an electron configuration  $[KK(\sigma_{2s})^2, \dots]$  for this ion. Draw a molecular orbital diagram for CO and determine the bond order and magnetic properties.

14. Assuming that it has similar molecular orbital energies to those of carbon monoxide, deduce the bond order of the  $NO^+$  ion.

15. Assuming that it has similar molecular orbital energies to those of carbon monoxide, deduce the bond order of the  $NO^-$  ion.

16. Predict which of the following gas-phase reactions are the more favored and give your reasoning.



### Intermolecular Forces

17. What are the main differences in following intermolecular forces?

a. Hydrogen bonding

b. Dipole-Dipole forces

c. Dispersion (London) Forces

18. Predict the intermolecular forces in following

a)  $N_2$

b)  $CO_2$

c)  $CCl_4$

d)  $H_2O$

e)  $HCl$