

HW 2
CHEM 362

Available: Jan. 25, 2008

Due: Feb. 1, 2008

1. Why are the sign and magnitude of overlap between orbitals on adjacent atoms good indications of whether atoms are bonded and how strongly they are bonded?
2. Take Atom A with one s orbital, three p orbitals and five d orbitals and show with drawings how each of these orbitals overlaps with:
 - a. an s orbital located on atom B (nine drawings)
 - b. the p_x orbital located on atom B (nine drawings)
 - c. the d_{xy} orbital located on atom B (nine drawings)
 - d. the d_{z^2} orbital located on atom B (nine drawings)Be certain to label your coordinate axes on Atoms A and B (which must be the same).
3. Draw an energy-level diagram for the interaction of two atoms that both have an s orbital. Show how the M.O.'s would be occupied if the two atoms in question were H atoms and if they were He atoms. What conclusions are to be drawn about the formation of bonds in the two cases?
4. When a bond is formed between two atoms, they are drawn together. What limits their internuclear distance so that they do not coalesce into one big atom?
5. What is meant by a node and a nodal plane? How do these terms relate to the characteristics of σ , π and δ bonding?
6. How is a bond order defined for a diatomic molecule in MO theory?
7. Are the $2s$ and $2p$ orbitals in a N atom *higher* or *lower* than those of O? Explain your answer?
8. State the geometric arrangement of bonds produced by each of the following sets of hybrid orbitals: dsp^2 , d^2sp^3 , dsp^3 . For each one, state explicitly which d and p orbitals are required for each geometric arrangement.
9. Explain by M.O. theory why the NO bonds in NO_3^- have a bond order of $1\frac{1}{3}$.
10. Why is the use of hybrid orbitals preferable to the use of single atomic orbitals in forming bonds? Illustrate.
11. Draw a qualitatively correct energy-level diagram for the CO_2 molecule. Show that it accounts correctly for the presence of double bonds.
12. Explain why there is $2s$ - $2p$ mixing in the M.O. energy-level diagram of Li_2 , but none for F_2 .
13. For the series of diatomics: O_2^+ , O_2 , O_2^- , O_2^{2-} , determine from an M.O. diagram how the bond lengths will vary and how many unpaired electrons each will have.
14. Draw Lewis Diagrams and predict the structures of $(\text{CH}_3)_2\text{S}$ (dimethyl sulfide) and $(\text{CH}_3)_2\text{SO}$ (dimethylsulfoxide). How will the C-S-C bond angles differ?

15. Draw Lewis Diagrams for each of the molecules or ions in the series: OCO, NNO, ONO⁻, NCO⁻, NNN⁻ and NCN²⁻. What is the same in all of these molecules?
16. Describe the geometry and hybridization in [PtCl₆]²⁻.
17. Use VSEPR to predict the shapes (bond angles) in the following:
- OF₂
 - BrF₅
 - OPCl₃
 - OIF₅
 - PCl₄⁺
 - OSF₄
 - B₂H₆
18. Identify the molecules in problem 17 that are:
- electronically saturated
 - electronically unsaturated
 - electron deficient
19. The structure of the pentafluorotellurate monoanion, [TeF₅]⁻, has been determined by X-ray techniques (see attached journal article: S. H. Mastin *et. al. Inorg. Chem.*, 1970, 9, 2100-2103.)
- What is the oxidation state of Te in this anion?
 - Draw the Lewis Diagram for this anion.
 - Determine the occupancy and formula AB_xE_y for Te in this anion and explain any deviations from ideal geometry using VSEPR theory.