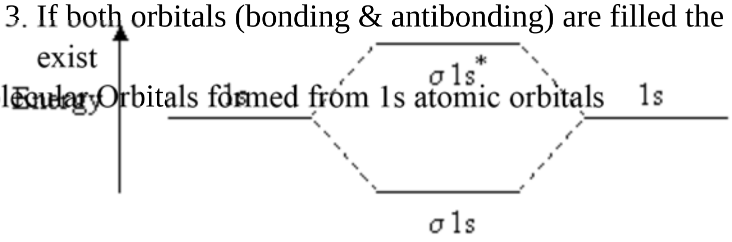
Covalent Bonding Orbitals

Chapter 9

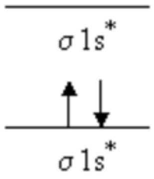
- I. Localized Electron Model (Hybridization) Explained in Chapter 8
  - A. Electrons are shared in orbitals that are specifically associated with one or the other of the bonded atoms
  - B. these are called atomic orbitals
  - C. the shape of the molecule is determined using VSEPR
  - D. Hybridization of Orbitals
    - 1. s,p, & d orbitals in an atom change to form a new type of orbital
    - 2. the new orbitals are all identical in shape
    - 3. the total number of hybrid orbitals formed is equal to the total number of atomic orbicats used
      - a. ex. C shows sp^3 hybridization
  - E. Double and Triple Bonds
    - 1. first bond forms from hybridized orbitals
    - 2. second and third bonds form from unhybridized p orbitals (not accounted for directly)
      - a. **Sigma Bonds –** any bond where the electron pair is shared on the line between the two bonded atoms from a hybridized orbital
      - b. **pi bond –** a bond where the electron pair is shared in the area above and below the line joining the atoms.
        - 1. always formed by unhybridized p orbitals
        - 2. ***a double bond is always a combination of a sigma bond and a pi bond.***
        - 3. ***a triple bond is always a combination of a sigma bond and 2 pi bonds***
- II. Molecular Orbital Model
  - A. When bonding, overlapping atomic orbitals change and become orbitals encompassing the entire molecule
  - B. the number of molecular orbitals formed is the same as the number of atomic orbitals used
  - C. each pair of atomic orbitals forms on bonding molecular orbital and one antibonding molecular orbital
    - 1. Bonding Molecular Orbital – greatest probability of finding the shared electrons is between the two nuclei + : +
      - a. Because both nuclei attract the electrons, filling a bonding orbital provides a force to hold the molecule together.
    - 2. Antibonding Orbital
      - a. Greatest probability of finding the shared electrons is outside of the space between the two nuclei × + + ×
        - 1. when electrons are in this type of orbital the nuclei repel each other
        - 2. this tends to break the molecule apart
        - 3. in each pair, the antibonding orbital is more effective than the bonding orbital
    - 3. If both orbitals (bonding & antibonding) are filled the molecule will break apart and not exist
  - D. Molecular Orbitals formed from 1s atomic orbitals



1. For a given formula
    a. Determine the total number of valence electrons in the molecule
    b. Fill molecular orbitals from lowest to highest energy level

Ex. H_2

Antibonding orbital is empty

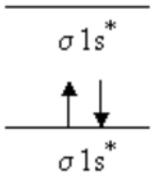


Bonding orbital is full
Therefore the atoms bond and the molecule exists

III. Bond Order
  A. An indicator of bond strength
    1. 1= single bond, 2 = double bond, 3 = triple bond
    2. Bond order = bonding e$^-$ - antibonding e$^-$ /2
      a. For H_2, Bond order (BO) = 2-0/2 = 1

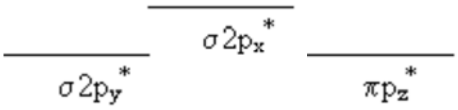
Ex. He_2

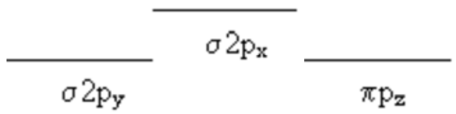
Antibonding orbital is full

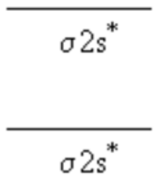


Bonding orbital is full
BO = 2-2/2=0
Therefore He_2 does not exist

  B. Bond Order for 2nd Principal Energy Level
    1. Diagram now uses s & p orbitals
    2. 8 molecular orbitals are formed from 8 atomic orbitals
    3. Antibonding orbitals are at higher energy levels than bonding orbitals
    4. sp_x has more energy than pp_{y} and pp_{z}







IV. Paramagnetism and Diamagnetism

- A. Paramagnetism is a slight attraction to magnets
  - 1. results from uncancelled magnetic fields of unpaired electrons
  - 2. any substance with unpaired electrons will be paramagnetic
    - a. odd atomic numbers, even atomic numbers with ½ filled orbitals
- B. Diamagnetism – a slight repulsion to magnets
- C. Occurs when all electrons are paired
  - 1. Practice with Li_2, Be_2, B_2, C_2, N_2, O_2, F_2, Ne_2
  - 2. Using Molecular orbital diagrams, determine the bond orders and magnetism in each of the following: O_2, O_2^+, O_2^-
  - 3. Determine the Bond Order & magnetism for: Ne_2, P_2
- C. Heteronuclear Diatomic Molecules
  - 1. Certain molecules cannot be addressed in the localized electron model because of the odd

number of valence electrons

a. Using molecular orbitals, predict the bond order and magnetism of: NO, NO^+, CN^-

V. Molecular Orbital Theory

- A. Strengths
  - 1. correctly predicts bond strengths and magnetism for diatomic molecules
  - 2. portrays electrons as being delocalized in polyatomic molecules
- B. Weakness
  - 1. very difficult to apply to polyatomic molecules