Bonding Hybrid Orbitals

Orbital Shapes

- s orbitals and p orbitals have different shapes.
- An s is sphere, p is pear shaped.
- 2 of the valence electrons in C are found in s orbitals, and the other 2 are found in p orbitals
- For carbon to from 4 bonds we assume there is one electron in each of the 4 orbitals.
- Therefore, one electron must move out of the s orbital an into a p orbital to make room for all bonding electrons.

- Of course, given the different shapes of the orbitals it makes sense that one bond (the s) would be different from the other 3 (the p's)

That does NOT happen!!

- Experiments show that methane (CH_4) has **4 identical C-H bonds.**
- VSEPR theory predicts the tetrahedral shape with a 109.5° bond angle.
- **No consideration** is given to the different types of orbitals.
- To account for this chemists describe what is called a *hybrid* orbital
- A hybrid is mixing dissimilar things, like a gas and electric car or a lion and tiger to make a liger.

Hybrid orbital

- The hybrid orbital in methane is called an sp^3 hybrid orbital
- There is a blend of s and p orbitals for each bonding electron.
- Each orbital is experimentally shown to have a large lobe and a smaller lobe

Orbitals shape

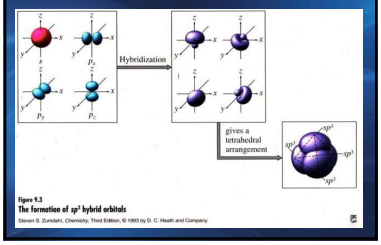
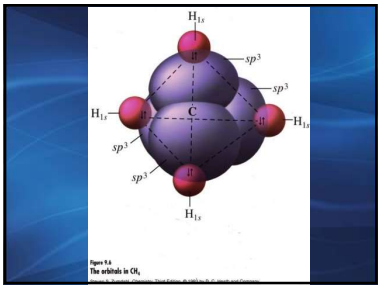


Figure 9.3
The formation of sp^3 hybrid orbitals



There are other hybrid orbitals

- sp hybridization- two groups around an atom (linear).
- sp^2 hybridization- three groups around an atom (trigonal planar).

sp hybrid

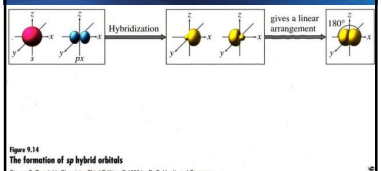
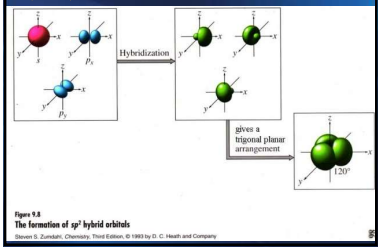


Figure 9.14
The formation of *sp* hybrid orbitals

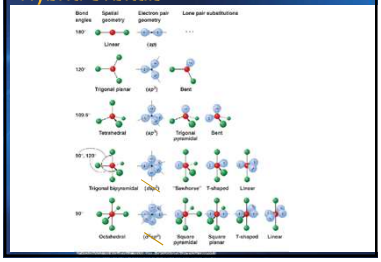
sp^2 hybrid



d hybrid orbitals

- The book makes several mention of d hybrid orbitals
- Like sp^3d hybrid orbital necessary for a trigonal bipyramidal shape
- There is new research disputing the existence of d hybrid orbitals
- d hybrid orbitals have been removed from the AP curriculum.
- You still have to know the VSEPR shapes, but they won't ask about the hybrid orbital

Hybrid Orbitals



Problems

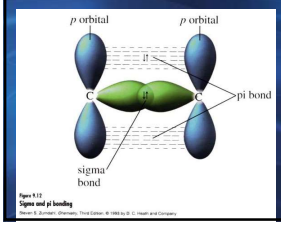
- For each of the following molecules or ions, predict the hybridization of each atom, and describe the molecular shape.
- NH_3
- CO_2
- BF_4^-
- XeF_2 (ignore hybridization)

Locations of electrons in a bond

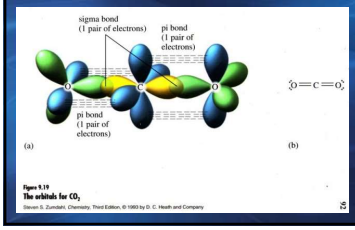
- A single pair of electrons shared between atoms is found centered in a line between the two nuclei.
- This type of bond is called a sigma bond (σ bond)
- For a double bond the other pair of electrons is found in the space above and below the sigma bond.
- This bond is called a pi bond (π bond)

Sigma and pi bonding

- C_2H_4

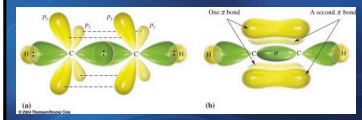


Sigma and pi bonding



Triple bonds

- Triple bonds have 1 sigma and 2 pi bonds
- C_2H_2

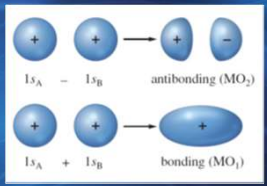


Molecular orbital model

- **Assumes molecules have orbitals**. Not atoms with intertwined orbitals but molecules as a collection of nuclei and orbitals that extend over the entire molecule.
- The electrons are assumed to be **delocalized** rather than always located between a given pair of atoms.
- Delocalized means the electrons belong to the molecule not individual atoms. They can flip from one orbital to another within that molecule.

- The electron probability of orbitals is centered along the line passing through the two nuclei for sigma (σ) molecular orbitals (MOs)
- In a molecule, only the molecular orbitals are available for occupation by electrons.

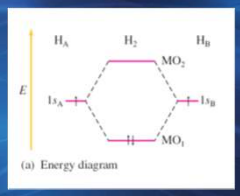
Combination of Hydrogen 1*s* Atomic Orbitals to form MOs



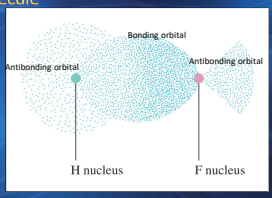
MO Model

- The molecular orbital model produces electron distributions and energies that agree with our basic ideas of bonding.
- The labels on molecular orbitals indicate their symmetry (shape), the parent atomic orbitals, and whether they are bonding or antibonding.
- Antibonding means not bonding. There is a node between the two nuclei.

MO Energy-Level Diagram for the H_2 Molecule



The Electron Probability Distribution in the Bonding Molecular Orbital of the HF Molecule



Sigma Bonding and Antibonding Orbitals

AP Test

- There is a lot more information on Moleculear Orbitals in the book, and possibly needed to go further on in chemistry.
- However, most of it is not on the the AP test so I don't want to cover it extensively given the exceptionally large amount of material we do need to cover in a short amount of time.