What’s in Chapter 9:

Shapes of molecules affect:
- reactivity
- physical properties

Shapes of molecules explained by:
- VSEPR
- Valence bond theory

Why molecules form:
- Molecular orbital theory

Can atomic orbitals explain these shapes or angles?

VSEPR: sections 9.1-9.2
- bonding and non-bonding e\(^{-}\) (e\(^{-}\) domains) take up space around atom
- Lowest PE state has e\(^{-}\) domains far apart
- non-bonding pairs of e\(^{-}\) affect molecular geometry

You are responsible for shapes and bond angles of:
1. Linear/bent
2. Trigonal
3. Tetrahedral
4. Trigonal bipyramidal
5. Octahedral
Valence Bond Theory:

- Mixture of Lewis dots and orbitals
- Bonds form via overlap of half-full orbitals
- PE is lowered when e\(^{-}\) are shared between 2 orbitals
- In VBT, s, p and d orbitals allowed to mix
- Does it work for BeH\(_2\)?

Atomic orbitals can’t explain the geometry of real molecules
Use electron configuration of central atom to determine hybridization

Molecules are not stationary, bonds are always moving

For H\(_2\): Will this model work for HCl?

Table 9.2

<table>
<thead>
<tr>
<th>Number of Electron Domains</th>
<th>Electron-Donating Groups</th>
<th>Bonding Domains</th>
<th>Nonbonding Domains</th>
<th>Molecular Geometry</th>
</tr>
</thead>
<tbody>
<tr>
<td>4</td>
<td>4</td>
<td>0</td>
<td></td>
<td>Tetrahedral</td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td></td>
<td></td>
<td>Trigonal pyramidal</td>
</tr>
</tbody>
</table>

Figure 9.15

Figure 9.14

http://teaching.shu.ac.uk/hwb/chemistry/tutorials/molspec/irspec1.htm
Summary of VBT:

To determine the hybrid orbital scheme:

1. Draw Lewis structure
2. One hybrid orbital for every e⁻ domain
   one per single bond or e⁻ pair
3. Use 1 atomic orbital for each hybrid orbital
Multiple Bonds

- Sigma (σ)-Bonds: $e^-$ density between nuclei.
  - single bonds
- π-Bonds: $e^-$ density above and below σ-bonds (from regular atomic p orbitals)
  - double bond = $1\, \sigma + 1\, \pi$
  - triple bond = $1\, \sigma + 2\, \pi$

Draw Lewis structure for acetylene, C$_2$H$_2$

- Geometry?
- Bond angles?
- Hybridization?

C$_2$H$_2$

Two lobes of one π bond

One π bond
Bonding in Benzene

- For benzene, C₆H₆, what is geometry and hybridization?
- 6 C-C σ bonds, 3 pi bonds
- each C atom:
  - sp²
- How many atomic p orbitals are left?

Molecular Orbital Theory (MOT)

- MO Theory compliments Lewis structures, VSEPR theory and hybridization.
- Basics:
  - e⁻ are in atomic orbitals in atoms,
  - e⁻ are in molecular orbitals in molecules
- two MO’s form when two AO’s overlap
Molecular Orbitals

- For every 2 AO’s, 2 MO’s form
  - 1 higher in E
  - 1 lower in E

- all e− from both atoms go into the MO’s
- Bonding e− are in MO’s lower in E than AO’s
- **Antibonding** e− are in MO’s higher in E than AO’s

MO’s for H₂ and He

- σ bonding
- σ* antibonding

Bond Order

- Bond order = ½ * (bonding e− − antibonding e−)

- Bond order of 1 = single bond, 2 = double bond, etc.

- Fractional bond orders are possible.
- Bond order >0 means stable molecule
- Higher bond order means stronger (shorter) bond

H₂ has a single bond, stable molecule, according to MO theory

H₂ has a single bond, stable molecule, according to MO theory

He₂ has no bond, not a stable molecule, according to MO theory

Draw e− for Li₂

What is bond order of Li₂?

Is Li₂ stable?

What is bond order of Li₂?

Is Li₂ stable?
How many MO's for 2nd row non-metals?

- 2p
- 2s

Boron - nitrogen
Oxygen-Neon

Magnetic behavior

- magnetic behavior:
  - paramagnetism (unpaired e\(^{-}\) in molecule): strong attraction between magnetic field and molecule;
  - diamagnetism (no unpaired e\(^{-}\) in molecule): weak repulsion between magnetic field and molecule.
- Can predict with MO theory, not VBT
VSEPR problems
State the geometry, angles and hybridization for each:

If the bonds were polar, are the molecules polar?

1. The bond length in C₂ is measured by neutron diffraction to be 131 pm (100 pm = 1Å). Using your information about carbon-carbon bonds from the computer modeling lab, does the C₂ bond resemble a C−C, a C=C, or a C≡C?

2. Predict the bond order of C₂ via MO theory.

3. Calcium and carbon form an ionic compound, CaC₂. Draw the lewis structure of the C₂ anion. What is the MO orbital configuration and the bond order of this anion? Do VBT and MO theory agree?

4. The ionization energy of O₂ is lower than the IE of atomic O. Explain this in terms of the where the electrons are in atomic and MO’s of O₂.

5. Do you expect the IE of N₂ to be higher or lower than that of atomic N?
Cascade:
1. Light $E (h\nu)$ is absorbed, cis $\rightarrow$ trans
2. Protein 1 changes shape (metarhodopsin II)
3. Protein 2 activates enzyme 1 (transducin)
4. Enzyme 1 activates enzyme 2 (phosphodiesterase).
5. Enzyme 2 catalyzes the hydrolysis of cyclic GMP:

$$\text{Guanine} + H_2O \rightarrow \text{Guanine}$$

6. cGMP keeps Na$^+$ channels open
7. Closed Na$^+$ channels lead to build up of charge
8. Nerve signal is generated
Cis and Trans fats

cis-Oleic acid

trans-Oleic acid

Nutrition Facts

Serving Size: 1 cup (229 g)
Servings Per Container: 2

Amount Per Serving
Calories 200
Calories from Fat 110

% Daily Value
Total Fat 12g 18%
Saturated Fat 3g 15%
Trans Fat 1.5g

Acid group

Trans fatty acid
cis fatty acid