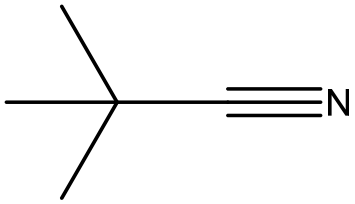
Chapter 2:
Molecular Representations
Chapter 2 (2.7-2.12)

Or

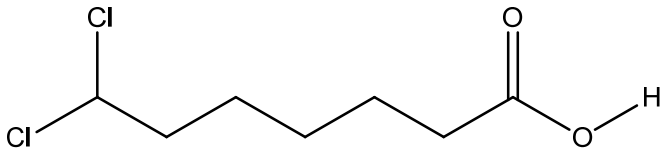
Functional Groups and Resonance

Additional Practice Problems

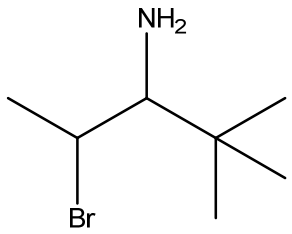
- Draw the bond-line structures from the following formulas:
- $C(CH_3)_3CN$



- $Cl_2CH(CH2)_5CO_2H$



- $CH_3CHBrCH(NH_2)C(CH_3)_3$

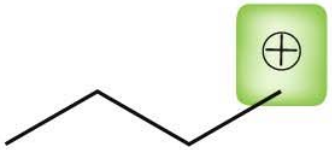


Formal Charges

- Most carbon atoms will have FOUR covalent bonds and no lone pairs to avoid carrying a formal charge.
  - Sometimes carbon will have a +1 charge. In such cases, the carbon will only have THREE bonds.

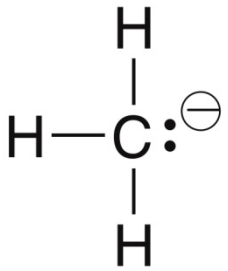
No hydrogen atoms on this C^+

One hydrogen atom on this C^+



Two hydrogen atoms on this C^+

  - Sometimes carbon will have a -1 charge.



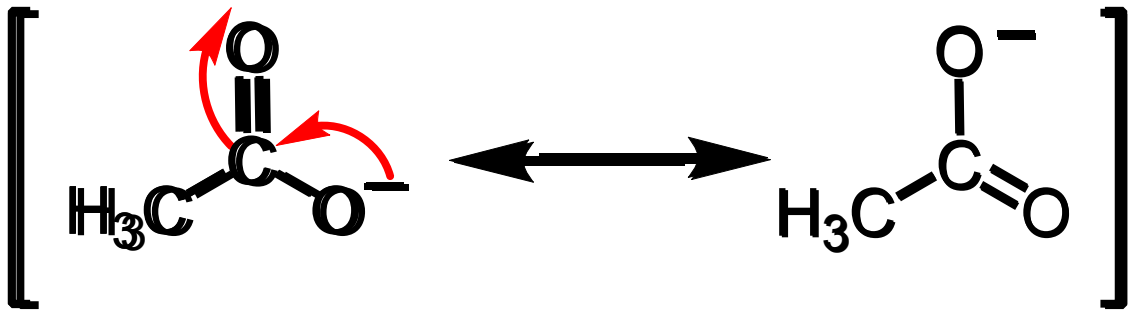
Lone Pair Electrons

- How many lone pairs are on the oxygen atom below?

- Oxygen SHOULD have 6 valence electrons assigned to it because it is in Group VIA on the periodic table.
- It is carrying a -1 charge, so it must ACTUALLY have one additional electron (6 + 1 = 7) assigned.
- HOW many lone pairs should it have?

Resonance

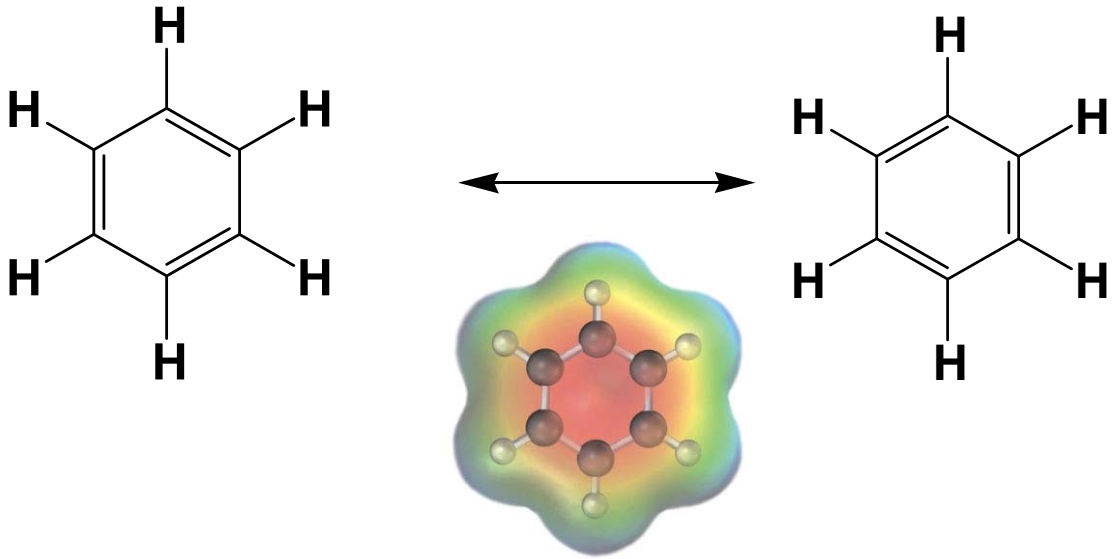
Some compounds are not sufficiently described by a single Lewis structure. Consider acetate anion. $[CH_3COO]^-$



- These different structures are called RESONANCE structures.
- The real structure is a combination of the resonance forms, and is called a RESONANCE HYBRID.

Kekulé Formulation of Benzene

- Kekulé proposed a cyclic structure for C_6H_6 with alternating single and double bonds.

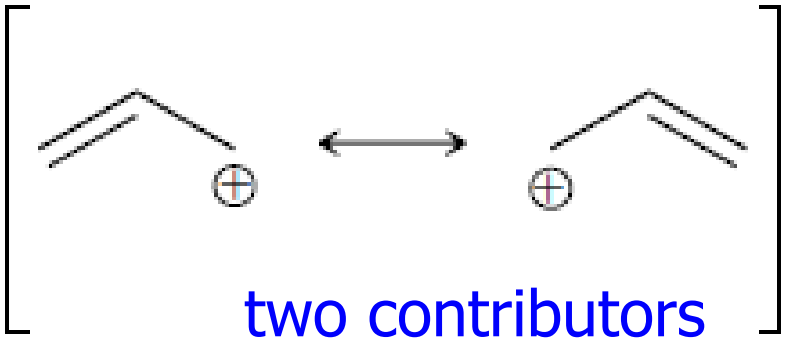


- Later, Kekulé revised his proposal by suggesting a rapid equilibrium between two equivalent structures.

- Electrons are not in alternating single and double bonds, but are delocalized over all six ring carbons.

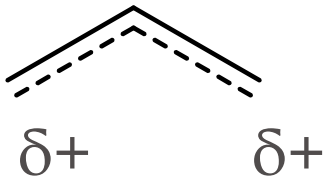
Resonance

- How do we represent the complete picture of the allyl carbocation provided by valence orbital and MO theories using a bond-line structure?
  - The pi electrons can move freely to both sides of the molecule, so we can use two resonance contributors to represent the structure.



two contributors

vs.



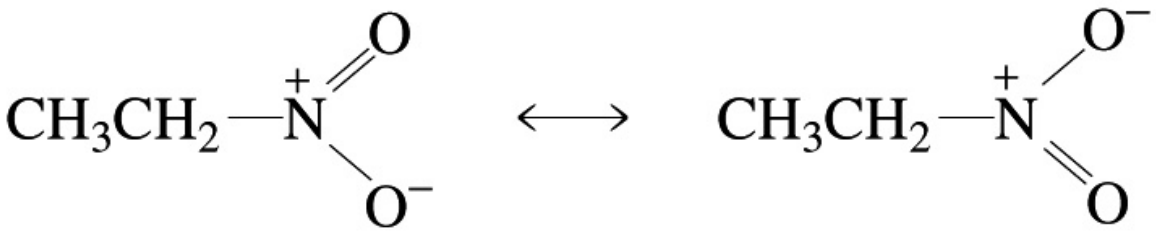
resonance hybrid

Delocalization of charge:

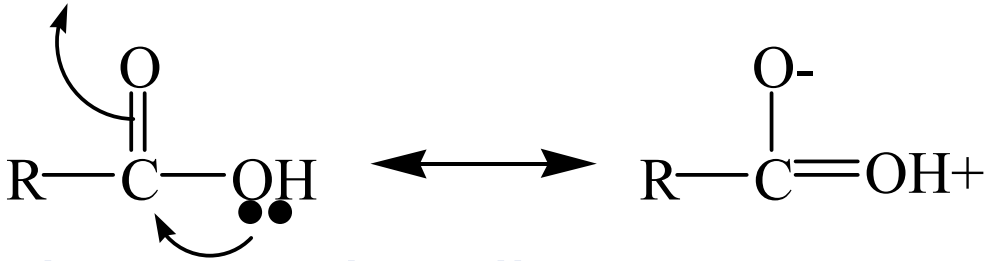
The charge is spread out over more than one atom. The resulting partial charges are more stable than a full +1 charge.

Electrons can be moved in one of the following ways:

1. Moving a nonbonding pair of electrons toward a π bond



2. Move lone-pair electrons toward a π bond



3. Move a single nonbonding electron toward a π bond

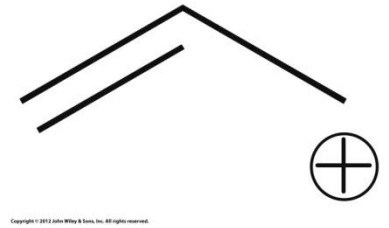
Resonance Structure Rules:

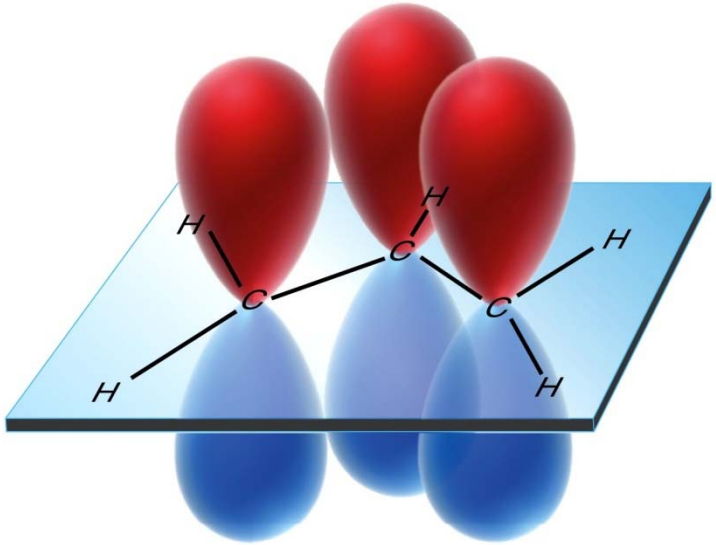
1. All resonance structures must be valid Lewis structures.
2. Only the placement of electrons can be changed (atoms cannot be moved).
3. The number of unpaired (not lone pairs) electrons must stay the same.
4. The major resonance contributor is the one of lowest energy.
5. Resonance stabilization is best when delocalizing a charge over 2 or more atoms.

Resonance

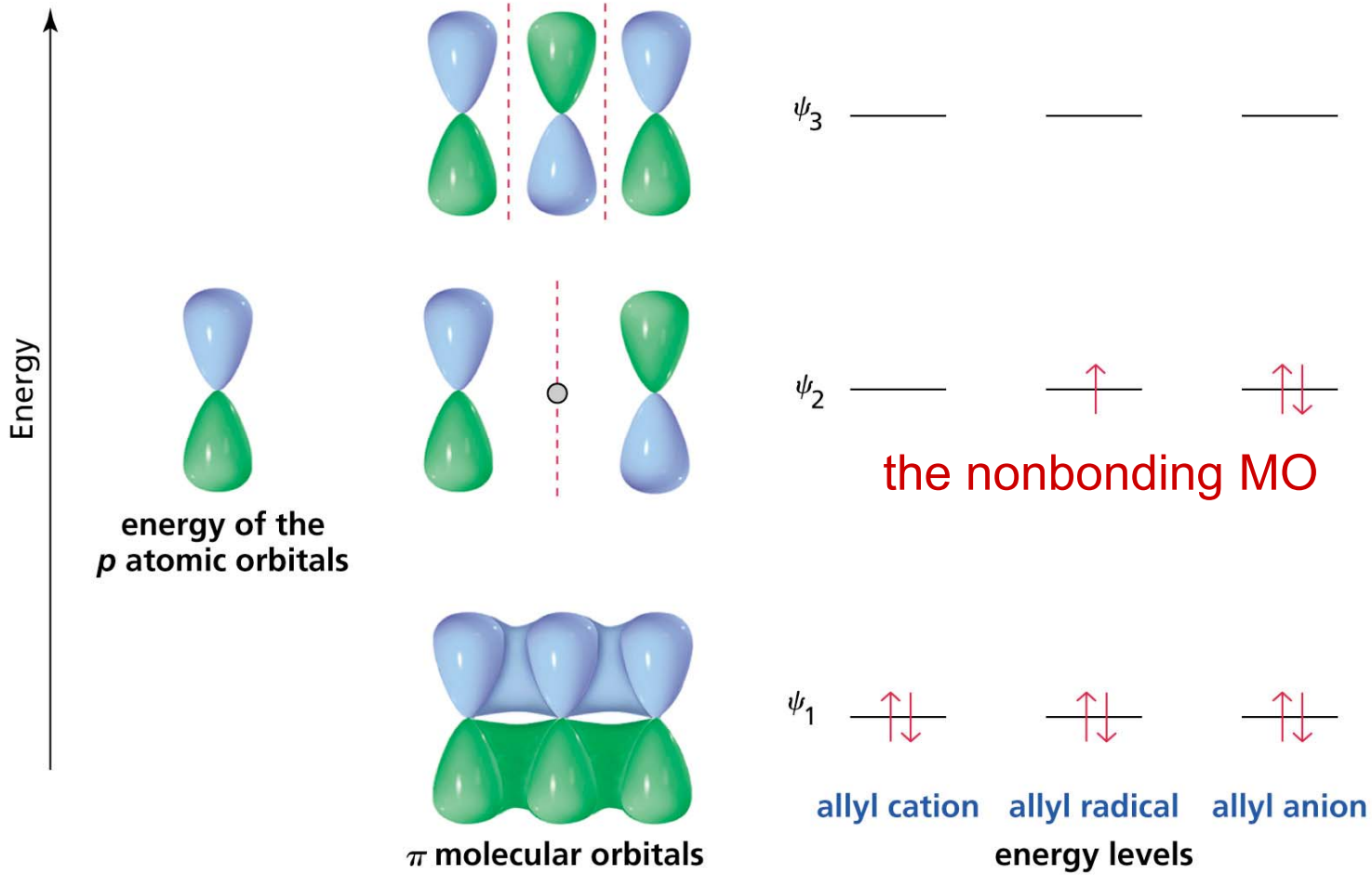
Let's look at the hybridization in the allyl carbocation:

- Calculate the steric number (# of σ bonds + lone pairs).
- When the steric number is 3, it is sp^2 hybridized.
- If all of the carbons have unhybridized p orbitals, they can overlap.
- All three overlapping p orbitals allow the electrons to move throughout the overlapping area simultaneously.
- THAT'S RESONANCE.





Molecular Orbitals of the Allyl System



From a molecular orbital point of view, when the THREE unhybridized p orbitals overlap, THREE new MOs are formed.

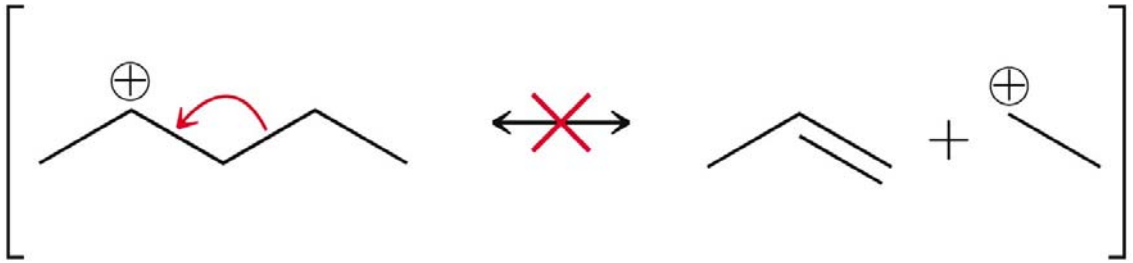
Curved Arrows in Resonance

- Throughout organic chemistry, we will be using curved arrows to show electron movement.

- Curved arrows generally show electron movement for PAIRS of electrons:
  - The arrow starts where the electrons are currently located.
  - The arrow ends where the electrons will end up after the electron movement.
  - A double-headed arrow shows the movement of one pair of electrons

Curved Arrows in Resonance

- Rules for using curved arrows to show RESONANCE:
  1. Avoid breaking a single bond.



  - Single bonds can break, but NOT in RESONANCE.
  - Resonance occurs for electrons existing in overlapping p orbitals, while electrons in single bonds are overlapping sp, sp^2, or sp^3 (sigma) orbitals.

Patterns in Resonance

There are 5 main bonding patterns in which resonance occurs. Recognize these patterns to predict when resonance will occur:

1. Allylic lone pairs
2. Allylic positive charge
3. Lone pair of electrons adjacent to a positive charge
4. A pi bond between two atoms with different electronegativities
5. Conjugated pi bonds in a ring

For Next Time….

- Friday Chapter 3.1-3.4

- Homework Practice Problems Chapter 2

  #1,5,12,16,25,34,40,47,48,54,55,64, 66

  *know the functional groups in table 2.1