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

Or

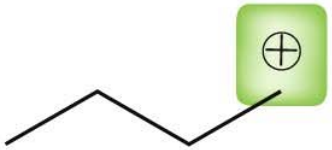
Functional Groups and Resonance

Formal Charges

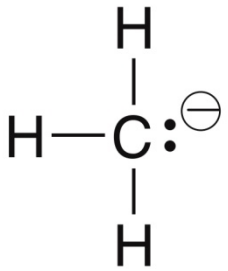
- Most carbon atoms will have FOUR covalent bonds and no lone pairs to avoid carrying a formal charge.

No hydrogen atoms on this C^+

One hydrogen atom on this C^+



Two hydrogen atoms on this C^+

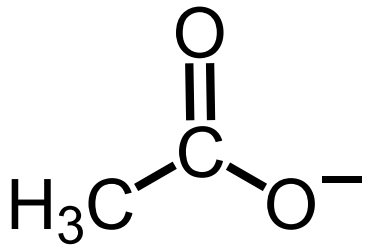


Lone Pair Electrons

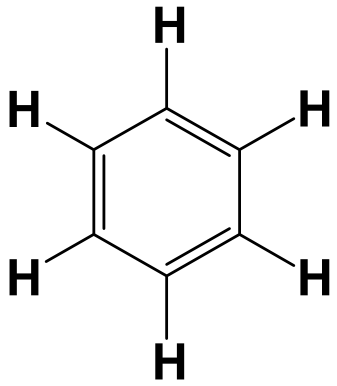
- How many lone pairs are on the oxygen atom below?

Resonance

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

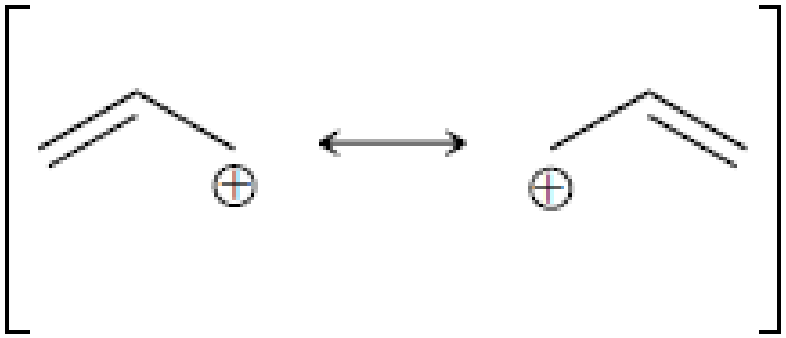


Kekulé Formulation of Benzene

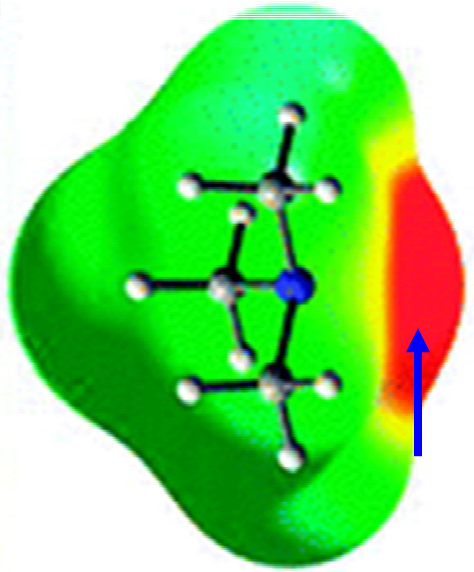


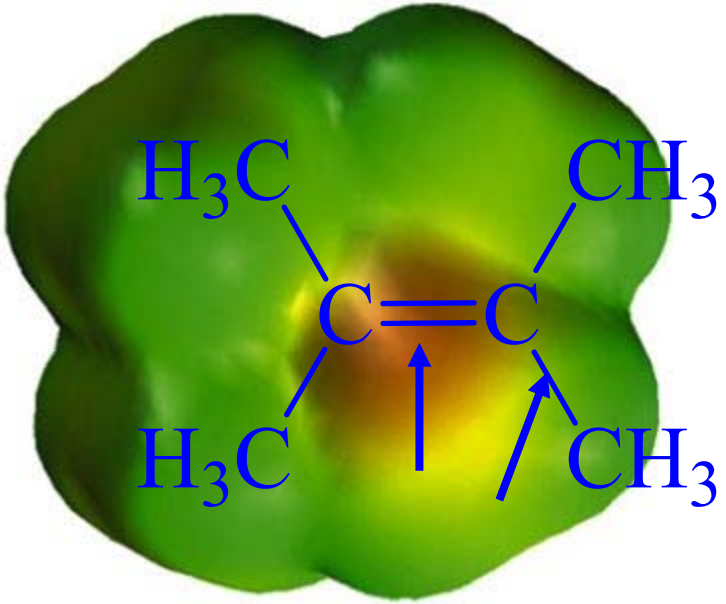
Resonance

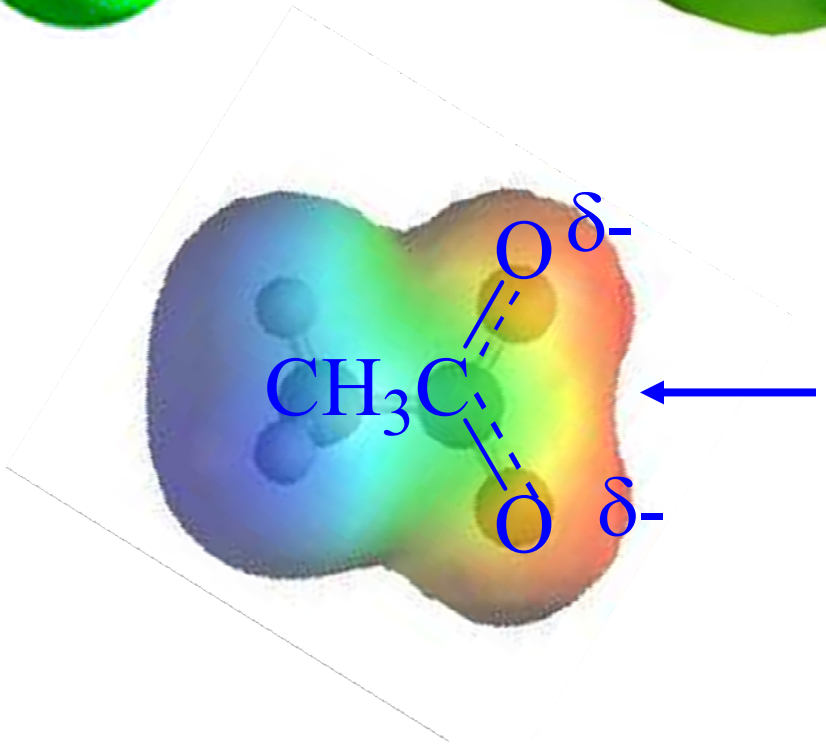
- How do we represent the complete picture of the allyl carbocation provided by valence orbital and MO theories using a bond-line structure?



Localized Versus Delocalized Electrons

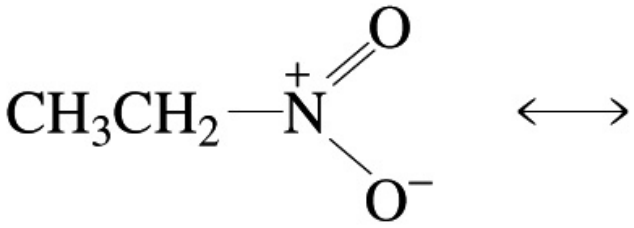




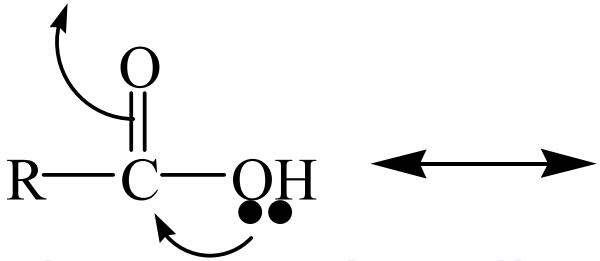


Electrons can be moved in one of the following ways:

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

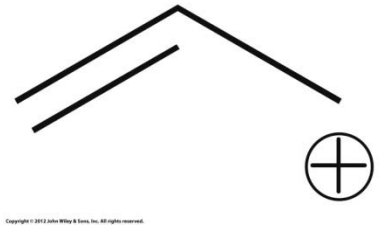
Resonance Structure Rules:

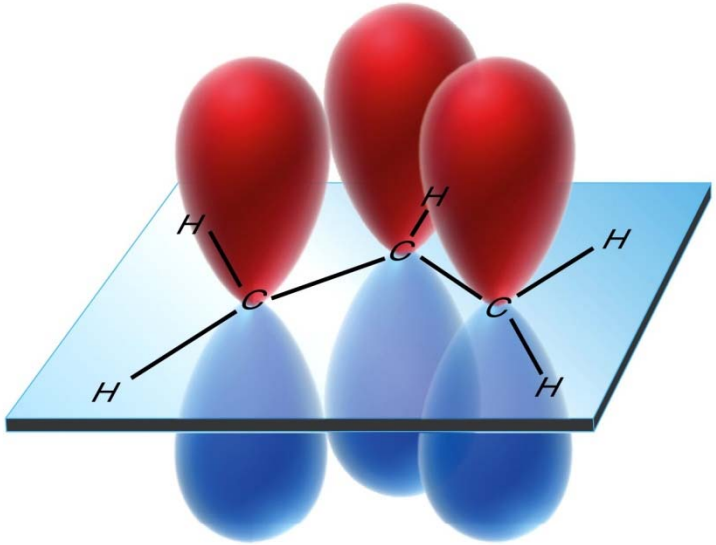
1. All resonance structures must be valid Lewis structures.

Resonance

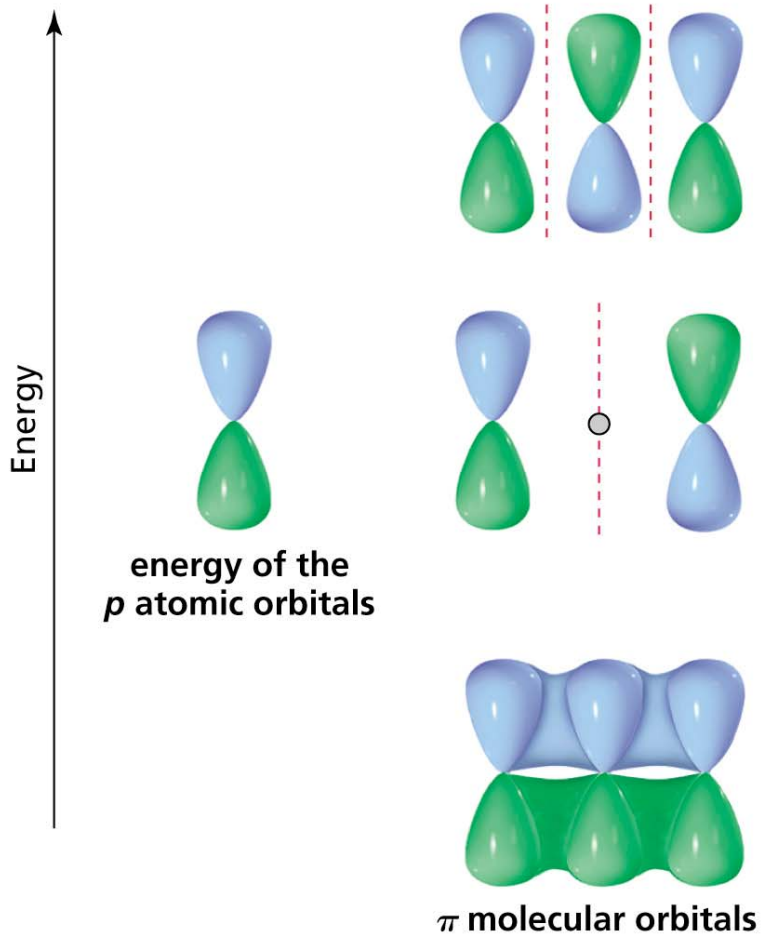
Let's look at the hybridization in the allyl carbocation:

- 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.





Molecular Orbitals of the Allyl System



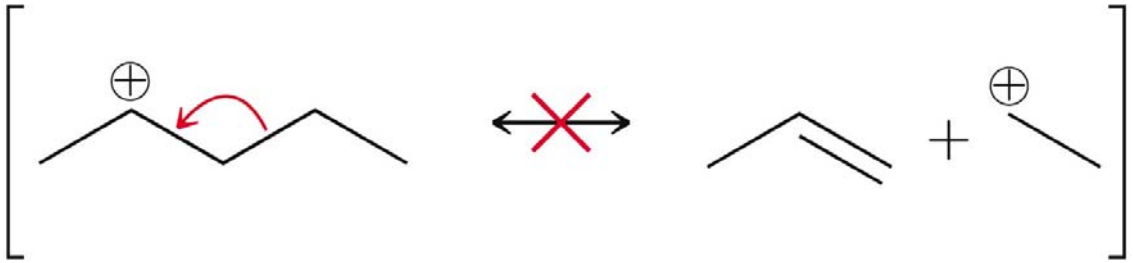
Curved Arrows in Resonance

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

- Curved arrows generally show electron movement for PAIRS of electrons:

Curved Arrows in Resonance

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

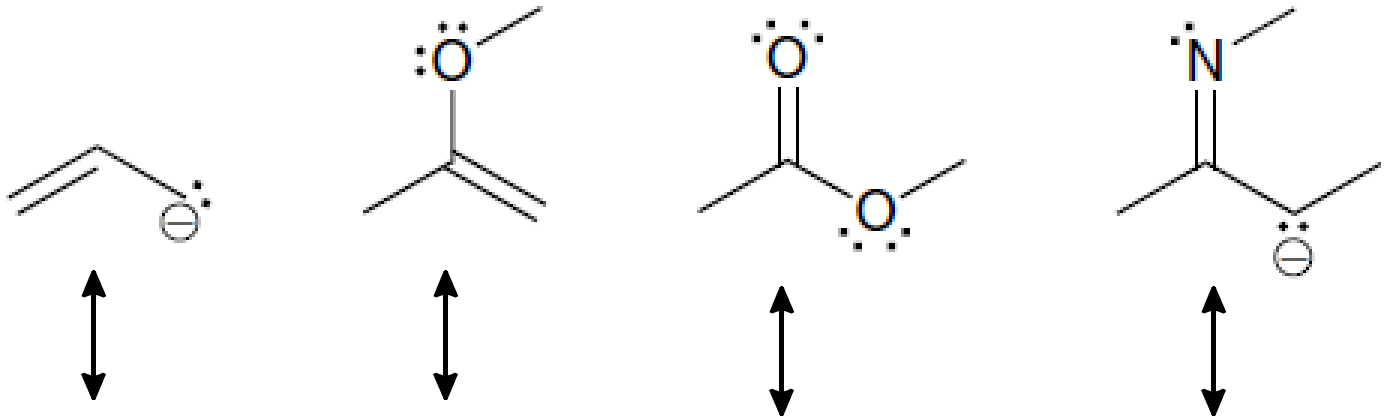


Patterns in Resonance

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

Patterns in Resonance

1. Identifying allylic lone pairs:
   - For each of the following, show the resulting resonance contributor and all formal charges.



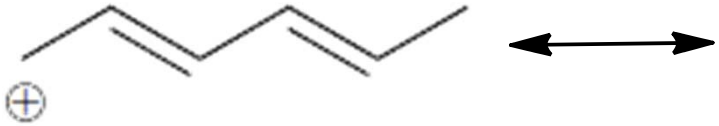
Patterns in Resonance

2. Dealing with allylic positive charge

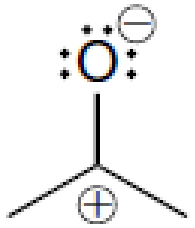
Allylic positive charge

- Only one curved arrow is needed.

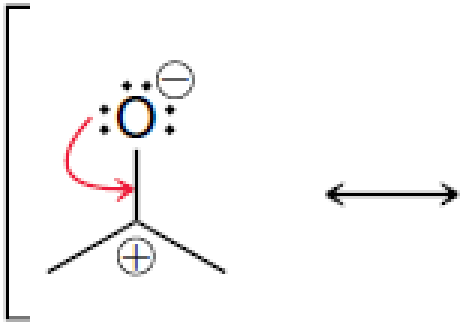
- If there are multiple conjugated double bonds, then multiple contributors are possible. Show the resonance contributors and curved arrows below.

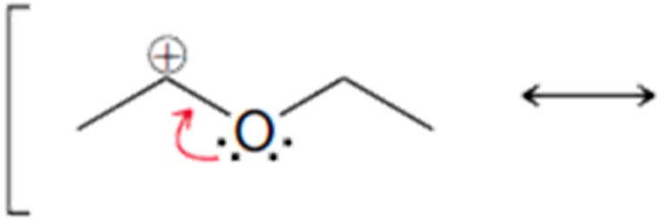


Patterns in Resonance



3. A lone pair adjacent to a positive charg
   - Only one arrow is needed.
   - Show the resonance contributors and curved arrows below. Draw a resonance hybrid.



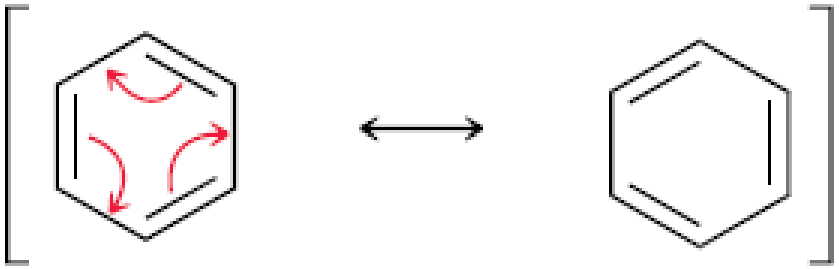


Patterns in Resonance

4. A pi bond between atoms of different electronegativity:
   - The pi electrons will be more attracted to the more electronegative atom.

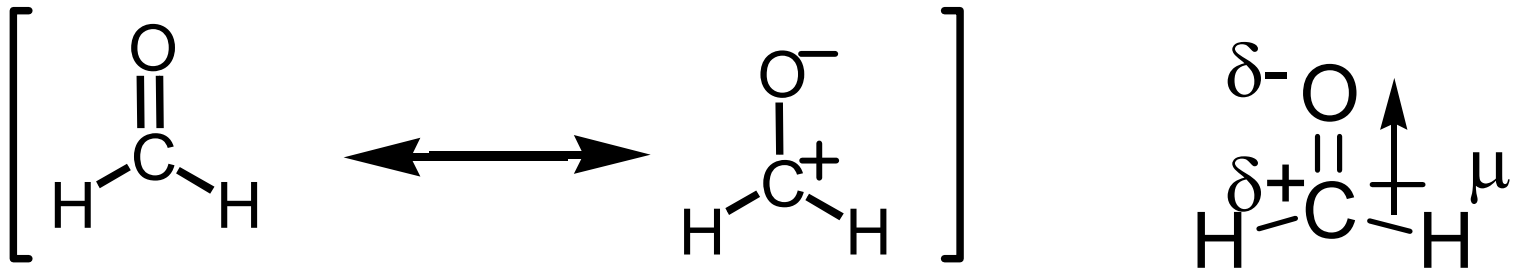
Patterns in Resonance

5. Conjugated pi bonds in a ring:
   - Each atom in the ring MUST have an unhybridized p orbital that can overlap with its neighbors.



Major and Minor Contributors

- Certain resonance structures are more stable than others (i.e. of lower energy).



Consider formaldehyde, even though the minor contributor is of higher energy than its double bonded counterpart, its contribution helps explain the polarization of the double bond.