Resonance

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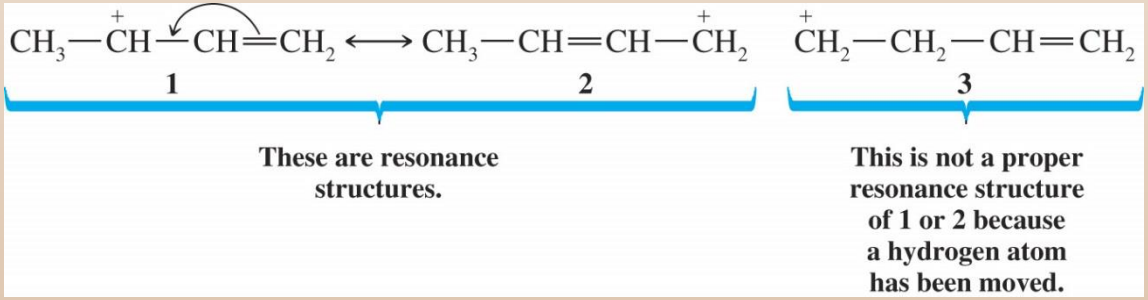
Resonance

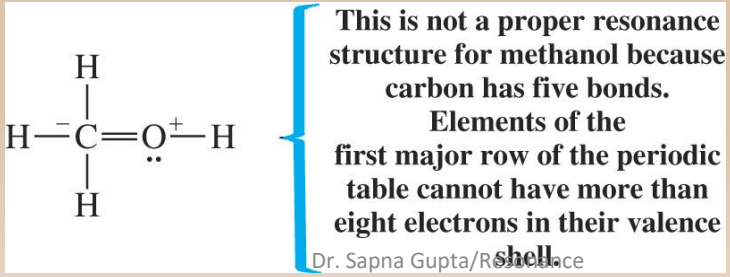
- Many molecules have more than one structure that represents the molecule.
- These structures are only on paper, i.e. they cannot be isolated. (If they can be isolated then the molecules are in equilibrium – resonance structures cannot be isolated)
- All structures that can be written out for one compound are called "contributing structures". One of them may contribute less or more to the overall stability of the molecule depending on its structure.
- The final molecule is considered to be a "hybrid" of all the structures.
- The more contributing structures there are, the more stable the molecule is.
- Resonance structures are shown by using curved arrows, which shows movement of electrons.

Rules for Writing Resonance Structures

- Individual resonance structures exist only on paper
  - The real molecule is a hybrid (average) of all contributing forms
  - Resonance forms are indicated by the use of double-headed arrows
- Only electrons are allowed to move between resonance structures
  - The position of nuclei must remain the same
  - Only electrons in multiple bonds and nonbonding electrons can be moved
- Example: 3 is not a resonance form because an atom has moved

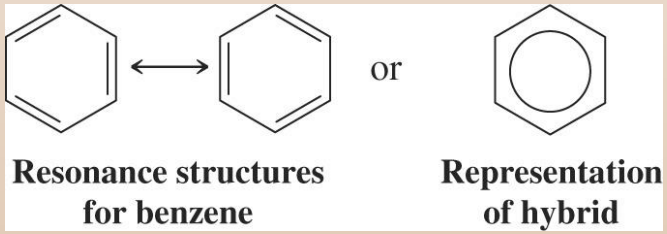


- All structures must be proper Lewis structures



Rules for Writing Resonance Structures..

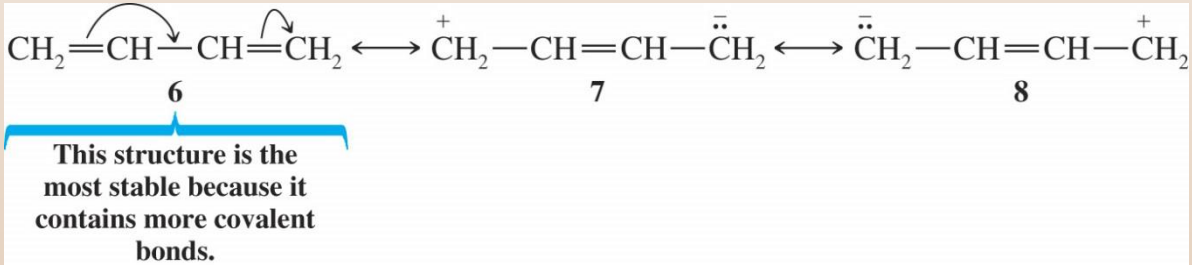
- The energy of the actual molecule is lower than the energy of any single contributing form
- Equivalent resonance forms make equal contributions to the structure of the real molecule
  - Structures with equivalent resonance forms tend to be greatly stabilized
  - Example: The two resonance forms of benzene contribute equally and greatly stabilize it



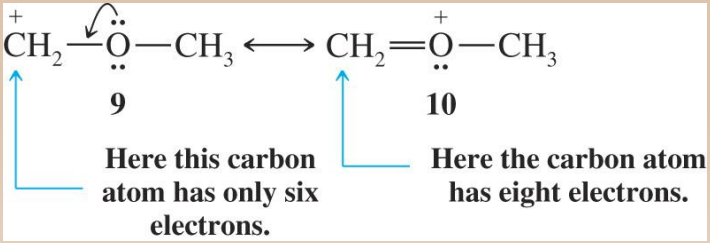
- Unequal resonance structures contribute based on their relative stabilities
  - More stable resonance forms contribute more to the structure of the real molecule

Rules for Resonance Structures

- A resonance form with more covalent bonds is more important than one with less
  - Example: 6 is more stable and more important because it has more total covalent bonds

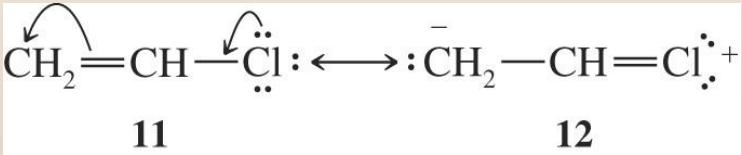


- Resonance forms in which all atoms have a complete valence shell of electrons are more important
  - Example: 10 is more important because all atoms (except hydrogen) have complete octets



Rules for Resonance Structures....

- Resonance forms with separation of charge are less important
- Separation of charge cost energy and results in a less stable resonance contributor
  - Example: 12 is less important because it has charge separation



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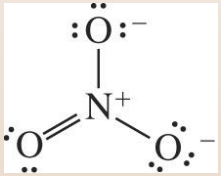
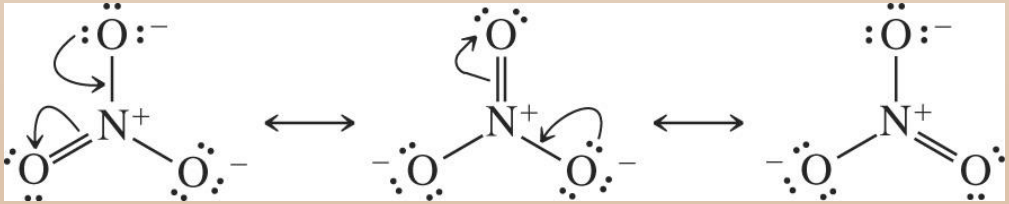
- Forms with negative charge on highly electronegative atoms are more important
- Those with positive charge on less electronegative atoms are also more important

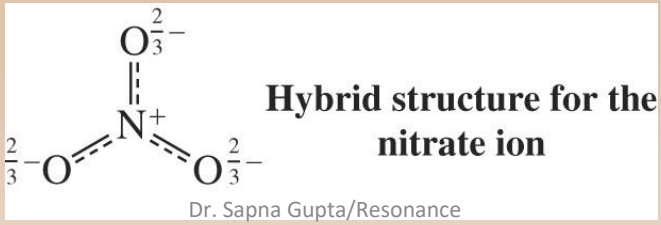
Examples – 1: Nitrate Ion

- The nitrate ion is known to have all three nitrogen-oxygen bond lengths the same and the negative charge spread over all three atoms equally



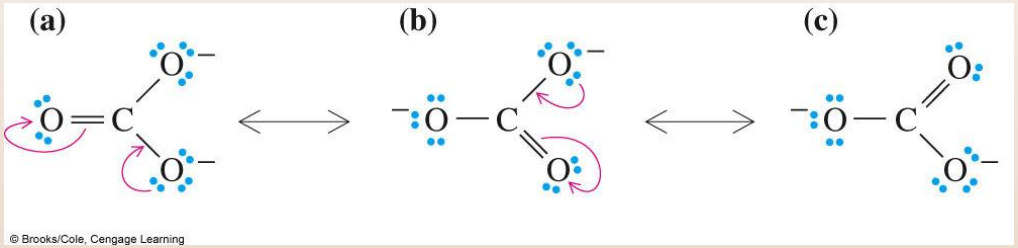
- Resonance theory can be used to produce three equivalent resonance forms
  - Curved arrows show the movement of electrons between forms
  - When these forms are hybridized (averaged) the true structure of the nitrate ion is obtained



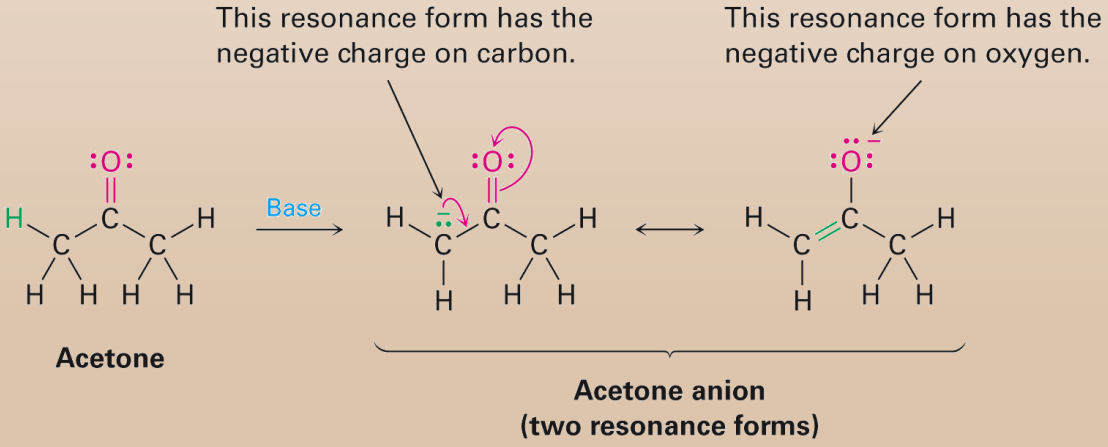


More Examples

- Carbonate Ion

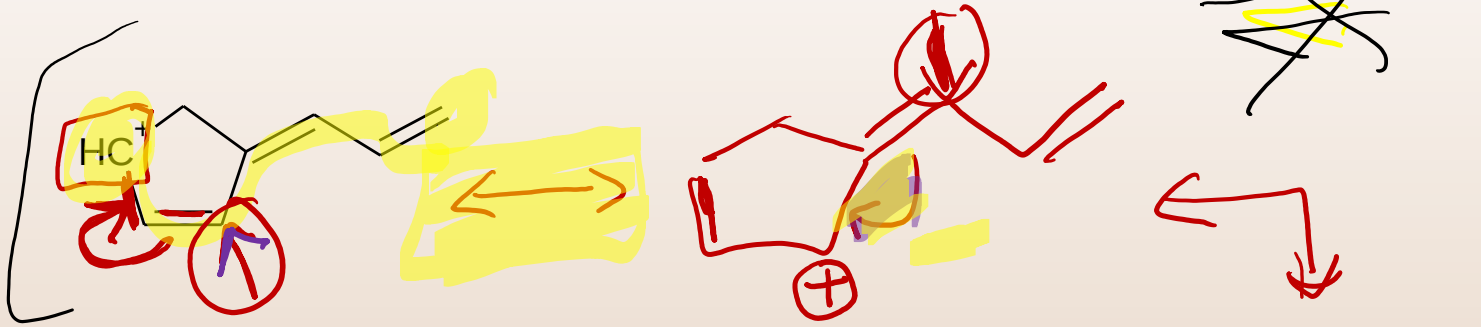


- Acetone

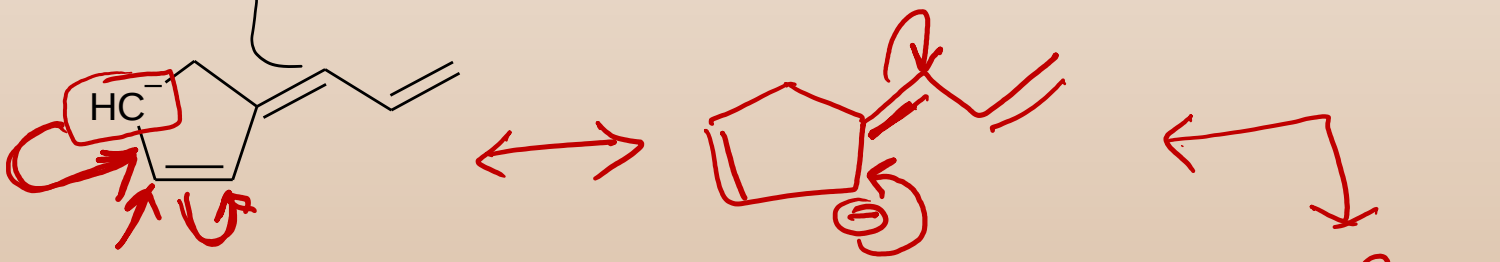


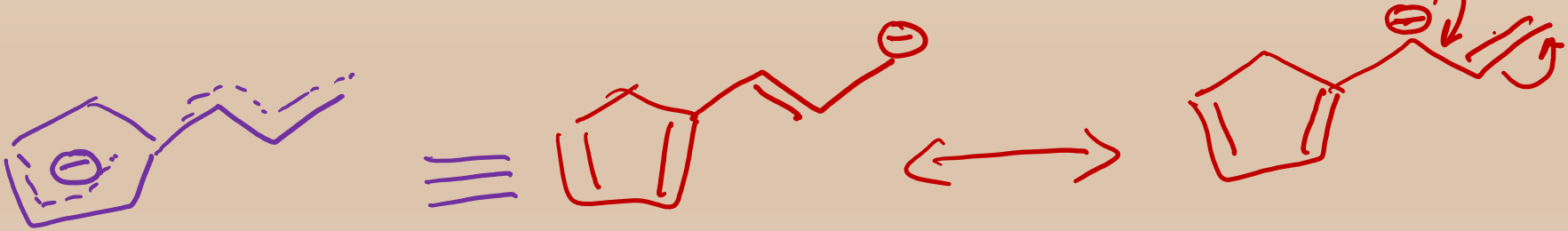
Organic Molecules and Resonance

- Cation

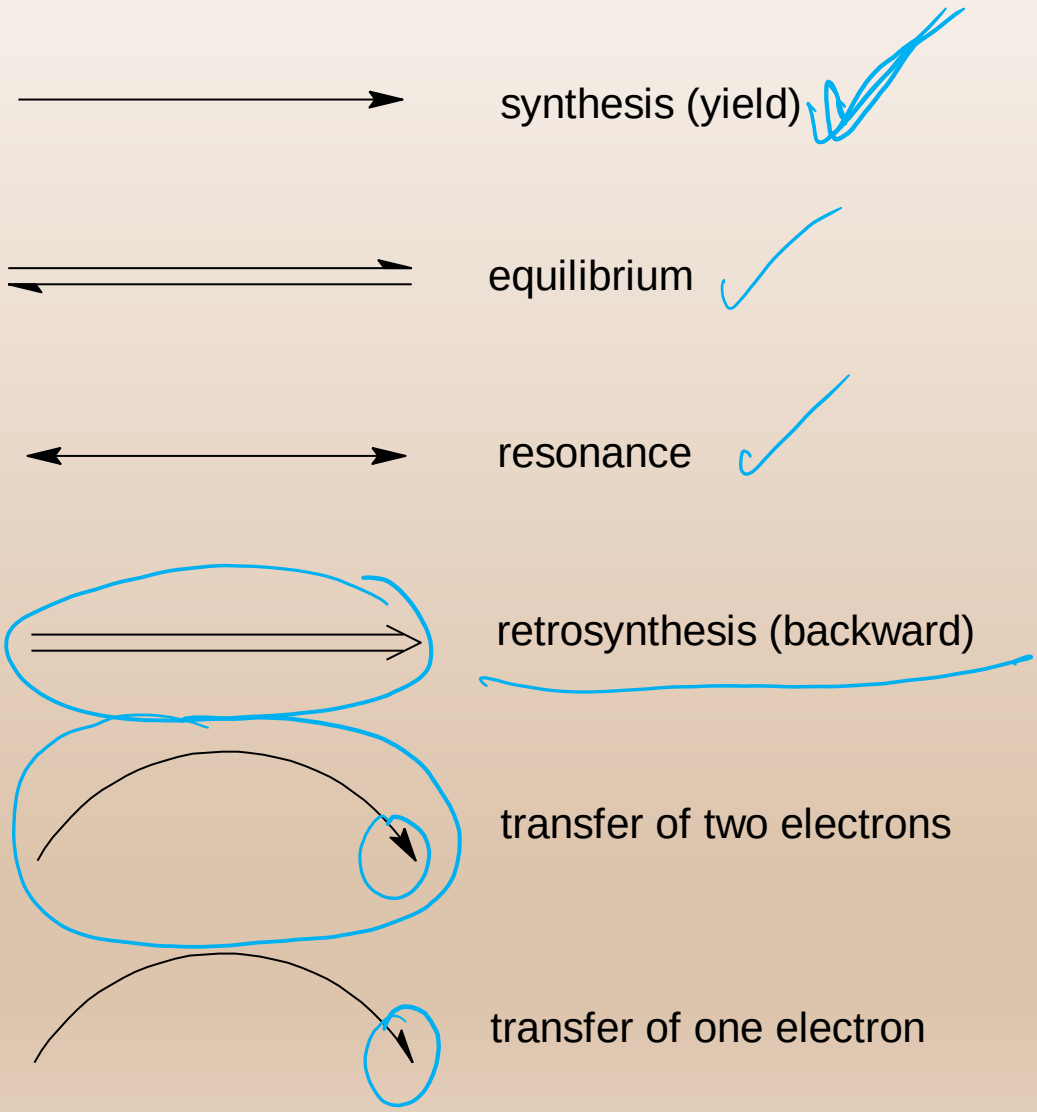


- Anion





Arrows in Organic Chemistry



Key Words/Concepts

- Writing resonance structures by moving electrons in the correct direction.
- Learning the rules of resonance.
- Learning different arrows.