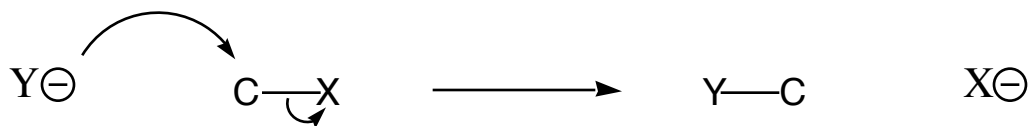


Representing Organic Compounds and Chemical Reactions

Organic chemists have developed an arrow pushing formulation to depict organic compounds and organic chemical reactions

It is important to become proficient with this arrow pushing in order to depict where the electrons are located and how they are moving



direction of arrows and placement of arrows (relative to atoms) are critical to correctly depict what is occurring in the reaction

Resonance Structures

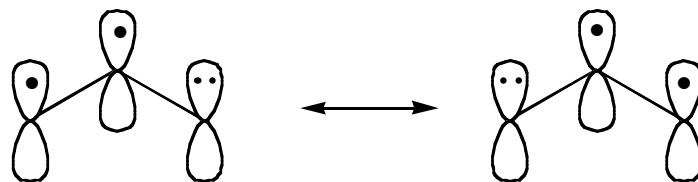
Resonance structures are valuable for organic chemists to understand where the electron density is located

none of the resonance structures alone is an accurate depiction of the compound, but instead the compound's properties are due to a "hybrid" of all possible resonance structures

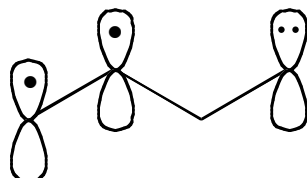
rules for resonance structures:

- 1) all resonance structures must be valid Lewis structures
- 2) only electrons move
- 3) must maintain same number of paired electrons in each resonance structure

In resonance structures, electrons move across conjugated p orbitals

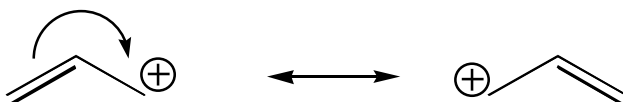


cannot move across saturated atoms



Only Push Electrons

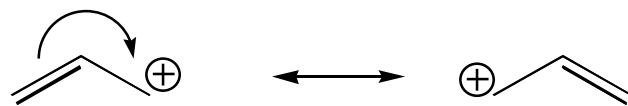
Since only electrons move, the bonds and bond angles do not change



the electrons moved, not the positive charge

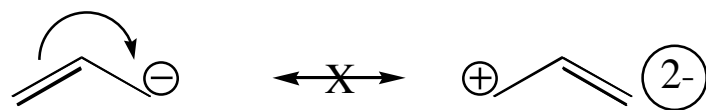
therefore the arrow represents the two electrons which were forming a π bond between the two carbons on the left, moved to now form a π bond between the two carbons on the right

Move Electrons Toward Positive Charge



as seen, electrons move toward positive (or partial positive) charge

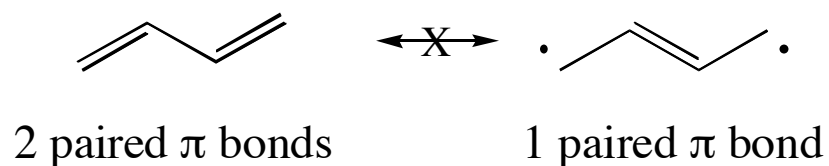
do not move electrons toward a negative charge



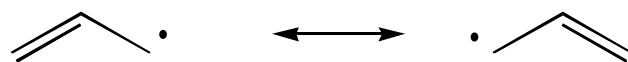
violates octet rule!!!

Must Have Same Number of Paired Electrons

Cannot break up paired electrons to create resonance structure



does not mean you cannot have resonance structures with a radical present



have one paired π bond in each structure,
these are correct resonance structures

Radicals: One-Headed Arrows

When only one electron is moving a one-headed arrow is used



one-headed arrow, one electron is moving



two-headed arrow, two electrons are moving

observed this previously in halogenation reactions

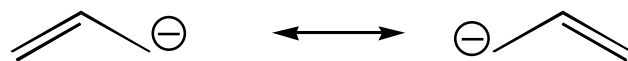


Overall Charge Must be the Same

-the formal charge for each structure must be the same

-if the charge did change, then that means the number of electrons has changed

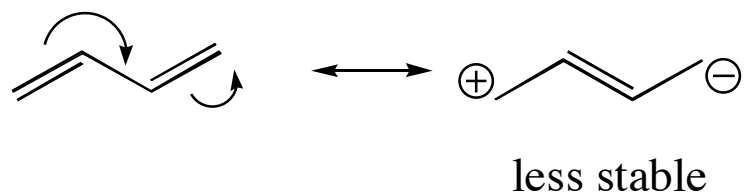
-don't lose or gain electrons, only move electrons within the structure



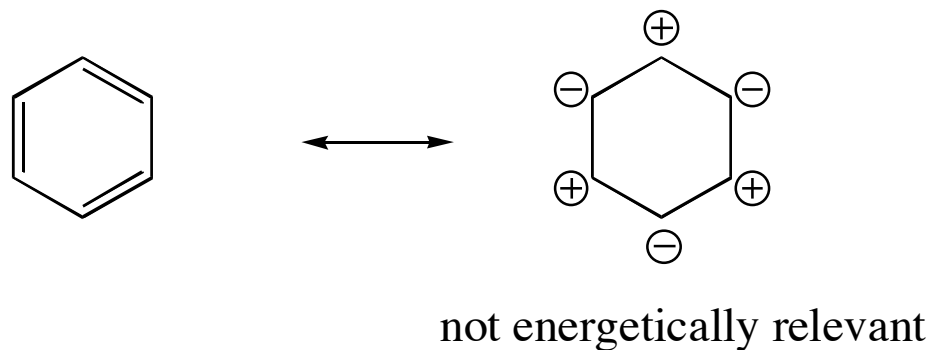
formal negative charge in each structure

Relative Energy

As number of formal charge sites increase in a structure, the energy of resonance structure generally decreases



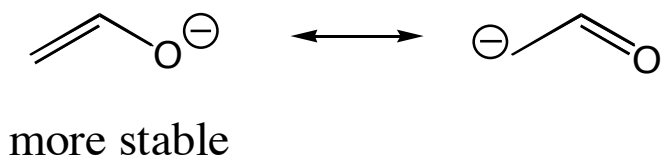
at some point, the structures become energetically irrelevant



Stability Dictated by Where Charge is Located

In unsymmetrical resonance structures, each structure will have a different energy (the relative energy determines the percentage of the hybrid the resonance contributes to the "actual" structure)

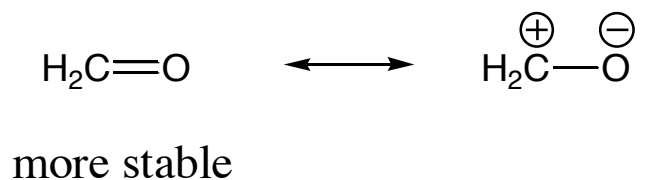
most stable resonance structure is one with charge that is most stabilized



placing negative charge on more electronegative oxygen is more stable

Octet Rule

When resonance structures differ in number of electrons in outer shell of each atom,
structure that satisfies octet rule is favored

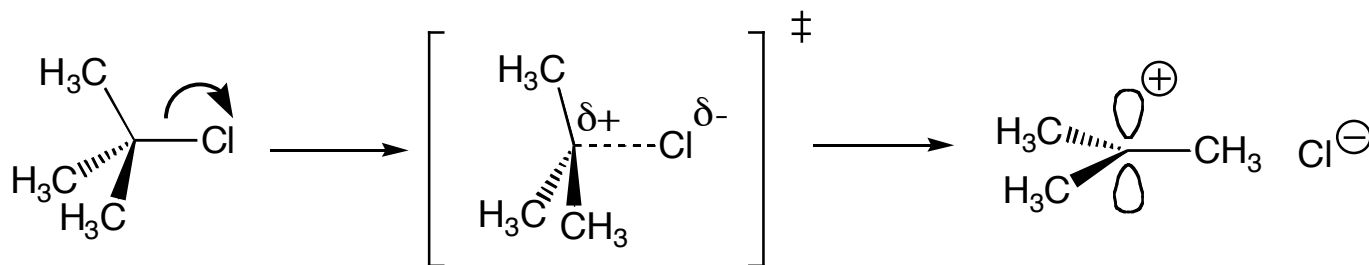


-applies even if negative charge can be placed
on more electronegative atom in other structures

Reaction Mechanisms

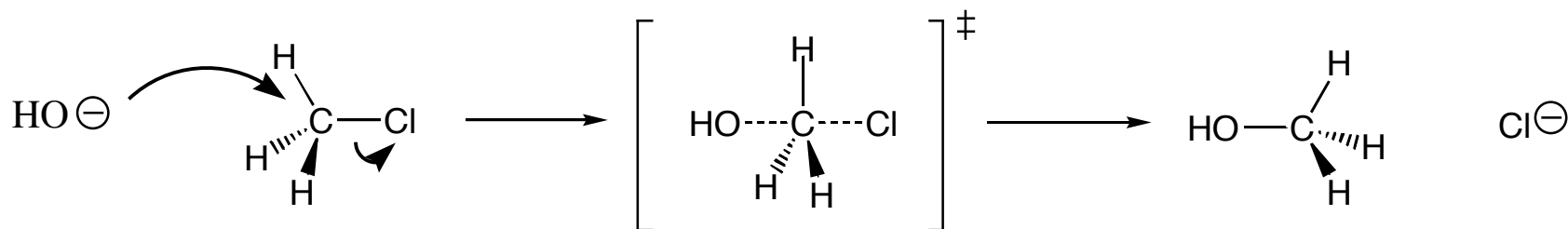
Understanding movement of electrons aids in predicting organic reactions

S_N1 :



electrons move to chlorine leaving group in rate determining step

Differs from S_N2



same considerations for arrow pushing:

- 1) arrows represent movement of electrons
- 2) electrons move toward positive (or partially positive) charged sites
- 3) cannot write invalid Lewis structures for any structure or intermediate
- 4) rate of reaction is dependent on relative stability of starting material(s) and intermediate(s) for rate determining step (hence activation energy)