What Is Resonance?

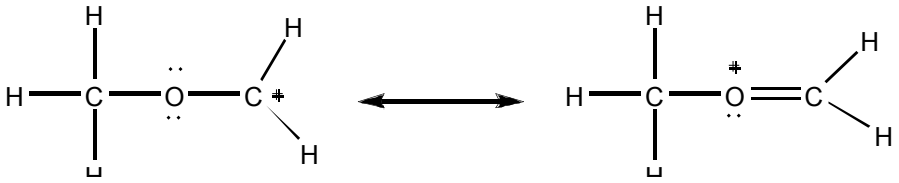
Introduction:

There are many occasions in which two or more valid Lewis structures are used to illustrate a compound's structure. Even though these Lewis structures differ in the placement of their electrons, they all represent the same compound. It is important to understand that none of these Lewis structures has a real physical existence, and the best representative of reality is the weighted average of these Lewis structures.

Key Terms and Concepts:

- **Resonance Contributor:** Each Lewis structure that represents a compound's real structure to a degree. Since these structures do not have a real physical existence it is wrong to assume that they are in equilibrium with each other.

Example 1: These are two valid Lewis structures for $CH_3OCH_2^+$

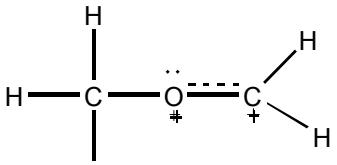


Contributor 1 **Contributor 2**

*The above structures are not in equilibrium with each other; therefore, the resonance sign ⟷ is used to illustrate their relationship with each other.

- **Resonance Hybrid:** The weighted average (blend) of resonance contributors which best represents the reality. Demonstrating the molecule the way it is observed in lab.

Example 2: This is the best representation of structure for $CH_3OCH_2^+$.

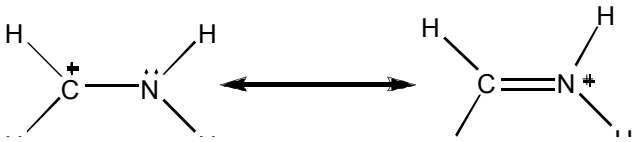


* The partial Pi bond that appears between the carbon atom and the oxygen atom is responsible for the energy barrier to rotation.
* The carbon atom and the oxygen atom are both partially positive due to the fact that each had a positive charge in different resonance contributors.
* If an atom has a positive charge in one and a negative charge in another resonance, no partial charges will be assigned to the atoms while drawing the resonance hybrid.

- **Delocalized Electrons:** These are electrons that are not limited to one atom or one covalent bond and are free to delocalize over several atoms. Electron

delocalization over larger volume gives longer wavelengths and lower energy to the electrons and stabilizes the molecule.

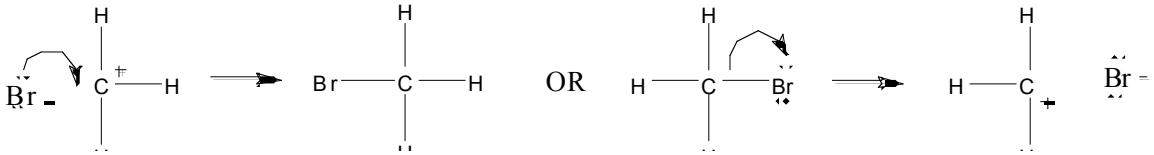
Example 3: The positive charge is delocalized due to the spread of electrons.



* In the above resonance forms the positive charge is delocalized (spread out) over the carbon atom and the nitrogen atom

- **Curved Arrow:** Arrows that are used to demonstrate the movement of electrons from a region of high electron density to a region of low electron density. If an arrow starts from a bond that bond is broken, and if it points to a space between two atoms a bond is formed.

Example 4: The curved arrows breaking and building bonds.[1]



* It is always helpful to draw the arrows while drawing the resonance contributors.

Major and Minor Resonance Contributors:

It is important to understand that resonance contributors do not contribute to the resonance hybrid equally. The more stable contributors which are represented in the resonance hybrid stronger are called Major Contributors. The less stable contributors which do not play a significant role in the structure of the Resonance hybrid are called the Minor Contributors. To determine whether a resonance is a major or minor contributor we get help from the "Resonance Contributor Preference Rule."[2]

Resonance Contributor Preference Rule:

These rules allow us to estimate the stability of the resonance contributors. Contributors that violate the majority of these rules are less stable and will not appear in the resonance hybrid as strongly as the contributors that violate only a few of these rules.

1. Contributors that have atoms with full octets are more stable than the ones with open octets.

   * The above rule has priority over the rest of the rules.

   * A contributor that violates two of these rules is still more stable than the ones that violate the first rule.

2. Contributors with the maximum number of covalent bonds are more stable.

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[1] . p.13, Steven Hardinger, PhD. *The Think Book.*

[2] P.17, Steven Hardinger, PhD. *The Think Book.*

* When counting the number of covalent bonds do not forget to count each Pi bond as two sigma bonds.

3. Contributors with the least number of Formal Charges are more stable.

* For calculating the Formal Charge of each atom one has to subtract the number of nonbonding electrons and _ of shared electrons from the atom's group number.

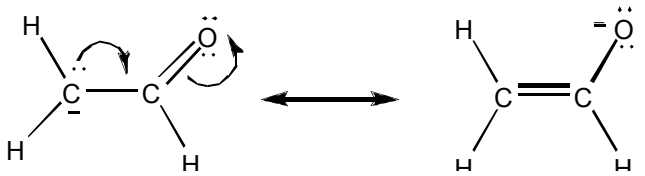
4. Contributors that have negative formal charges on the more electronegative atoms and positive charges on the least electronegative atoms are more stable.

* This is only if formal charges on the resonance contributors cannot be avoided.

5. Contributors that have bonds between atoms in the same row (especially C, N, O, and F) of the periodic table tend to be more stable.

* The violation of this rule is usually more important than the electronegativity consideration.

Example 5: Specify the major and minor contributors and explain why? [3]



Minor Contributor **Major Contributor**

* Both structures have full octets on all their atoms. The number of covalent bonds is 6 in both structures. However, since Oxygen is a more electronegative than Carbon, the structure with the negative charge on oxygen is more stable.

[3] . P.16, L.G.Wade, *Organic Chemistry*