Resonance, Resonance, Resonance
Everything you need to know about Resonance

Topics Covered:
- Vocabulary
- Resonance
- Resonance contributors
  - Drawing resonance contributors
  - Four common electron shift patterns
  - Resonance contributor preference rules
    - Major or minor resonance contributor?
- Resonance hybrid
- Drawing resonance hybrid
- Importance of resonance
- Consequences

What is **Resonance**?
- A molecule representation that cannot be portrayed by just one Lewis structure
- Need two or more Lewis structures

![Lewis structures]

**Resonance contributors**
- Lewis structures that are only different in how electrons are delocalized.
- The number of electrons are the same. Only the formal charges, number of lone pairs, and number and covalent bonds can be different.
- Use these arrows to show the relationship between resonance contributors.

![Arrows]

- HELPFUL: Use curved arrows to show electron delocalization to help draw resonance contributors.

![Curved arrow]

- Each resonance contributor is NOT the “real” representation of the molecular structure.
The best (most accurate) representation is the “weighted average” of these resonance contributors—**resonance hybrid**.

**Resonance Contributors**

**Drawing Resonance Contributors**

- **Four Common Electron Pair Shift Patterns**
  1. **Switch the lone pair with the pi bond.**

```
\[ \text{H}_3\text{C} - \text{C} - \text{CH}_2 \quad \text{H}_3\text{C} - \text{C} = \text{CH}_2 \]
```

  2. **If there is an open valence shell, interchange it with the pi bond.**

```
\[ \text{H}_2\text{C} = \text{C} - \text{BH}_2 \quad \text{H}_2\text{C} - \text{C} = \text{BH}_2 \]
```

  - **Open valence shell**

  3. **Change the bond with the lone pair and open valence shell.**

```
\[ (\text{CH}_3)_2\text{N} - \text{C}(\text{CH}_3)_2 \quad (\text{CH}_3)_2\text{N} - \text{C}(\text{CH}_3)_2 \quad \text{Pi bond formed} \]
```

```
\[ (\text{CH}_3)_2\text{C} = \text{O} \quad (\text{CH}_3)_2\text{C} - \text{O} : \quad \text{Pi bond broken} \]
```

  4. **Switch the pi bonds.**

```
```

```
Resonance Contributor Preference Rules

**Rule 1:** Atoms prefer to have full valence shells (octets or expanded octets depending on the atom)—more stable

- Avoid open valence shells
  - Open valence shells—less stable

\[
\begin{align*}
H_2C\equiv\mathrm{OH} & \quad \text{All valence shells filled} \\
\text{More important contributor} & \\
& \\
H_2C\equiv\mathrm{OH}^+ & \quad \text{Open valence shell on carbon} \\
\text{Less important contributor} & \\
\end{align*}
\]

★ This rule outweighs all other rules!
(Remember: as Professor Hardinger says, Rule 1 is the “Ring of Power”)

**Rule 2:** The more covalent bonds, the more significant the contributor.

\[
\begin{align*}
H & \quad \text{Four covalent bonds} \\
\text{More important contributor} & \\
& \\
H & \quad \text{Three covalent bonds} \\
\text{Less important contributor} & \\
\text{(violates two rules)} & \\
\end{align*}
\]

**Rule 3:** Avoid formal charges. The less, the better!

\[
\begin{align*}
H & \quad \text{No formal charges} \\
\text{More important contributor} & \\
& \\
H & \quad \text{Two formal charges} \\
\text{Less important contributor} & \\
\text{(violates Rule 1, Rule 2, Rule 3 (twice))} & \\
\end{align*}
\]

**Rule 4:** If a contributor cannot avoid formal charges, then make sure negative formal charges are on the most electronegative atoms and positive formal charges are on the least electronegative atoms.
Electronegativity trend: EN↓ with ↑distance from fluorine

Rule 5: Atoms in the same row of the periodic table have stronger pi bonds.
- Since carbon, nitrogen, oxygen, fluorine are in the same row, their interactions will be stronger → more important contributor
- This rule overpowers electronegativity (Rule 4)!

Rule 6: Resonance contributors that are aromatic (closed loop of p orbitals with 4n+2 pi electrons, where n is an integer) are more significant than ones that are not aromatic.
Resonance hybrid

1. Draw all resonance contributors.

2. Draw a core structure that includes the same characteristics from each resonance contributor.
   - Include sigma and pi bonds, lone pairs, and formal charges

3. Add whatever is left from each contributor to the core structure shown in the representation above by using:
   - ----- to represent partial pi bonds
   - δ⁺ or δ⁻ to represent partial charges

Importance of Resonance

Consequences
- Electron delocalization increases stability.
- Resonance affects the molecular structure→planarity.
- Resonance can influence:
  - Planarity
  - Electron delocalization
  - Increase in stability
  - Increase or decrease in barrier to rotation
  - p orbital overlap
Works Cited:
• Professor Hardinger’s Chemistry 14C Lecture Supplement (p.17-27)
• Previous Midterm 1 Exams
• All images (found in Lecture Supplement or Illustrated glossary)
• http://www.chem.ucla.edu/harding/index.html
  • Illustrated glossary