

(10) Today

Sections 2.1 - 2.4
Polar Covalent Bonds, Formal Charges,
Resonance/Electron Delocalization

Bring Modeling Kits

Next Class (11)

Sections 2.1 - 2.4
Polar Covalent Bonds, Formal Charges,
Resonance/Electron Delocalization

Bring Modeling Kits

(12) Second Class from Today

Sections 2.7 – 2.11
Acids and Bases

Third Class from Today (13)

Sections 2.7 – 2.11
Acids and Bases

Section 2-12
Non-Covalent Interactions Between
Molecules

Polar Covalent Bonds and Electronegativity

Section 2.1

Electronegativity is a measure of an atom's ability to attract e^- 's that are part of a bond

"As a rough guide, bonds between atoms whose electronegativities differ by less than 0.5 are nonpolar covalent, bonds between atoms whose electronegativities differ by 0.5 to 2 are polar covalent, and bonds between atoms whose electronegativities differ by more than 2 are largely ionic."¹

$$|C_{\text{eneg}} - O_{\text{eneg}}| = 1.0 \text{ polar bond}$$

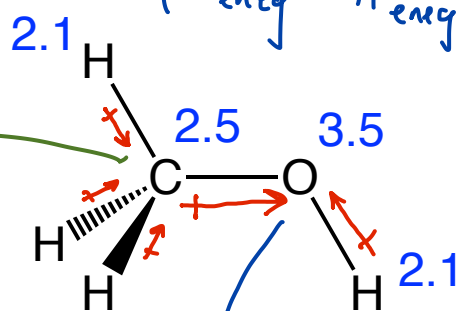
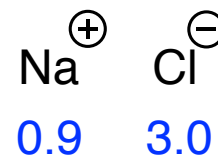
$$|O_{\text{eneg}} - H_{\text{eneg}}| = 1.4 \text{ polar bond}$$

$$|C_{\text{eneg}} - H_{\text{eneg}}| = 0.4$$

considered non polar

(in reality it is ever so slightly polar)

eneg dif > 2 ionic



- 2 σ bonds + 2 pair lp e^- 's
- tetrahedral geometry
- sp^3

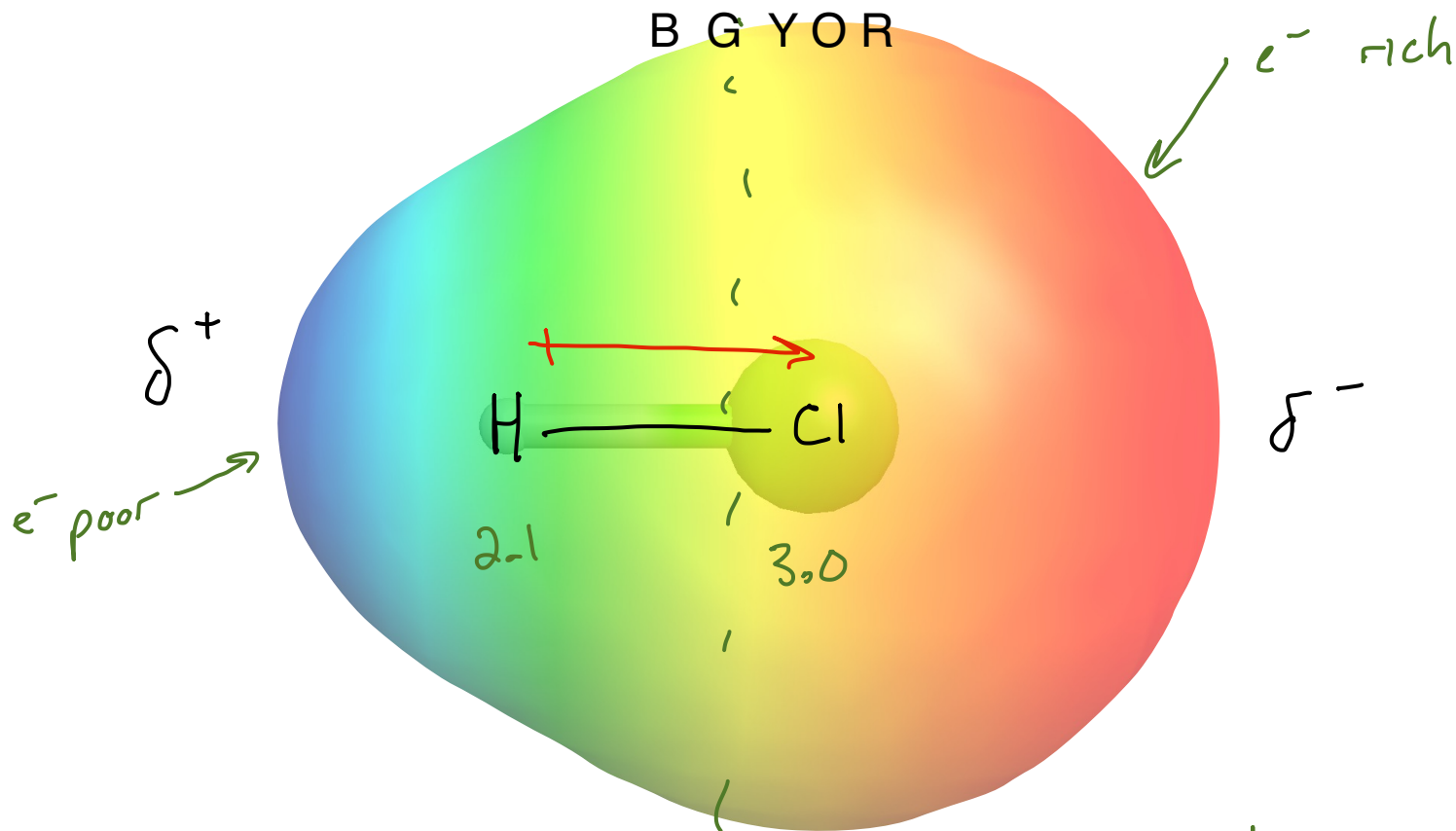
- 4 σ bonds around C
- tetrahedral
- sp^3 hybridized

sp^3 on C overlaps with sp^3 on O...
2 e^- 's shared to form bond

¹ Organic Chemistry, 10th ed., McMurray, OpenStax (2023) <https://openstax.org/details/books/organic-chemistry>

"The dipole moment, μ [...], is defined as the magnitude of the charge Q at either end of the [...] dipole times the distance r between the charges [...]."²

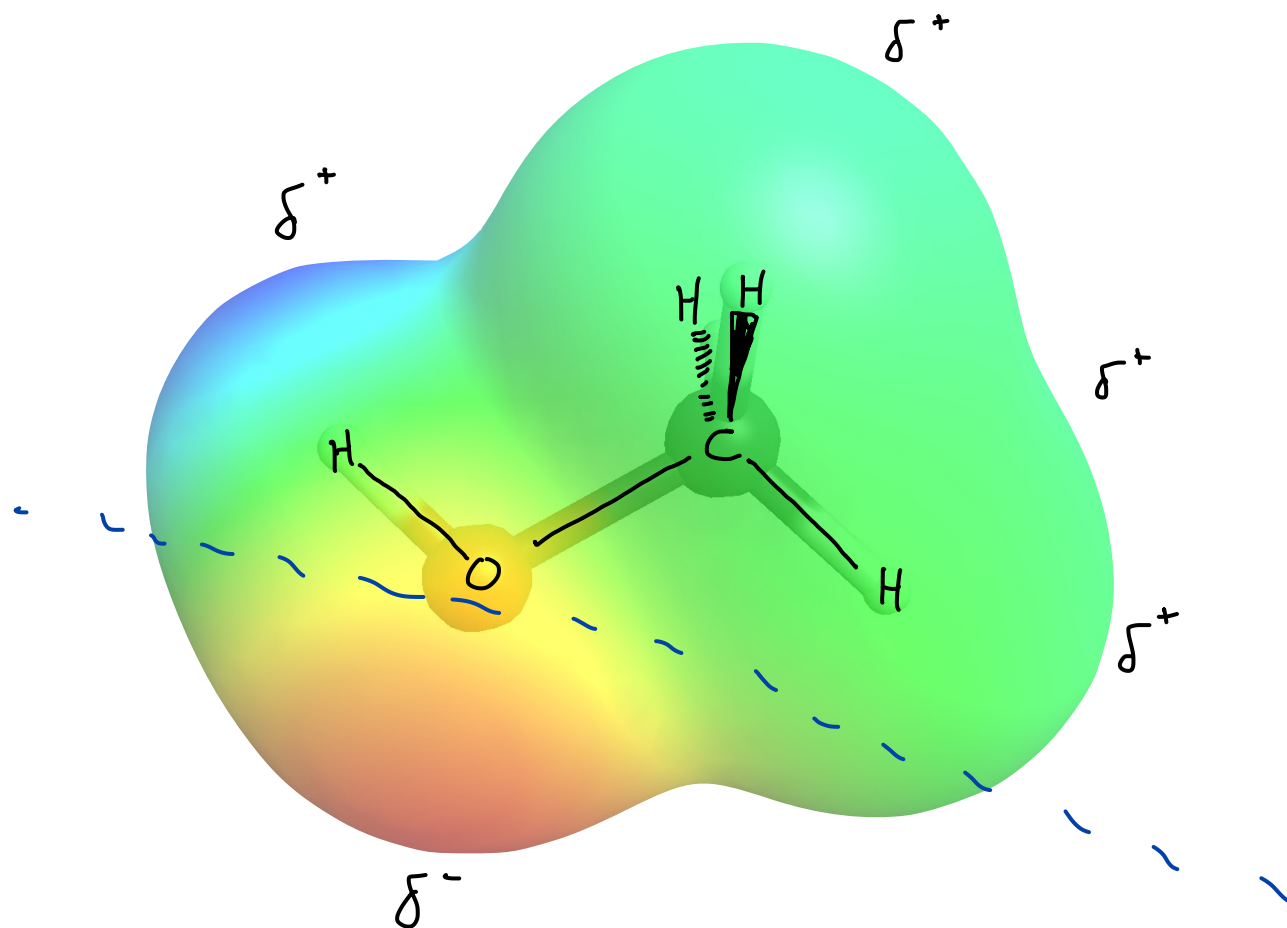
Color coded, based on the colors of the rainbow, red negative to blue positive



polar molecules have opposite charges on opposite sides

² Ibid.

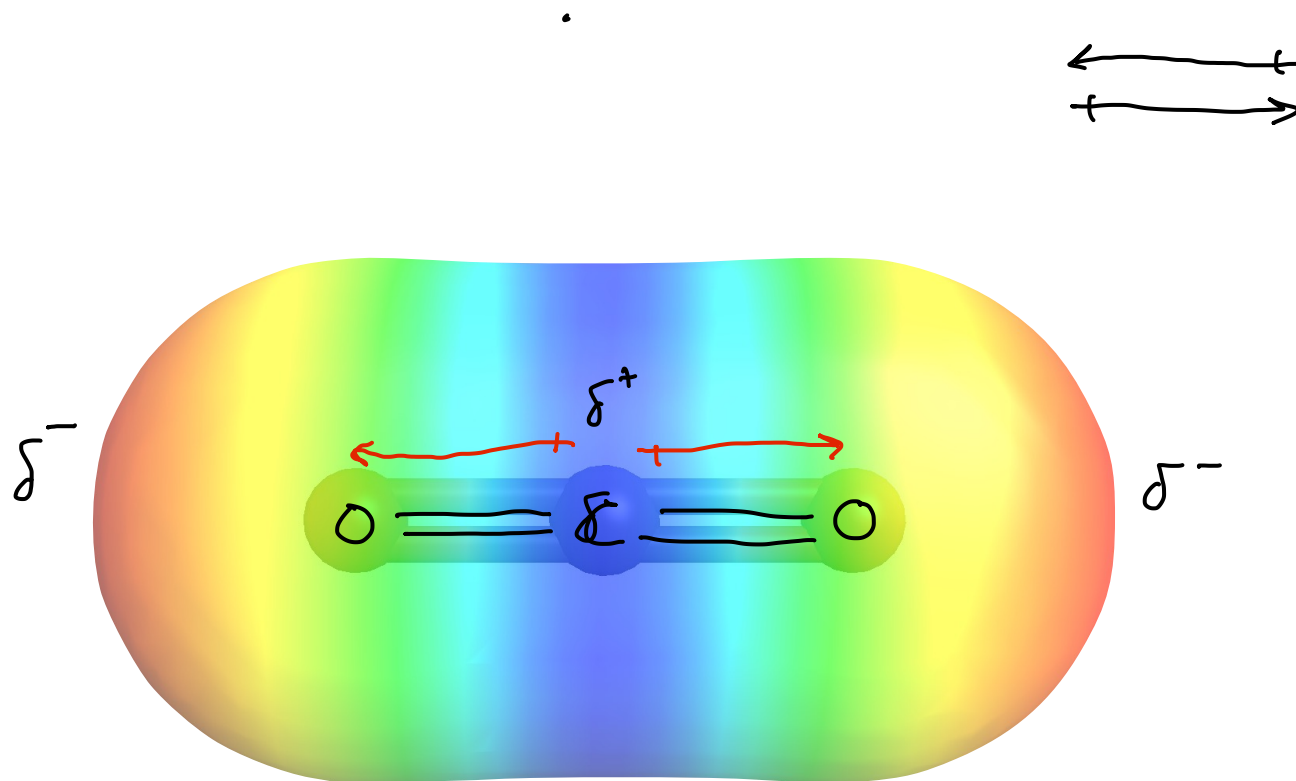
"The dipole moment, μ [...], is defined as the magnitude of the charge Q at either end of the [...] dipole times the distance r between the charges [...]." ³



methanol is polar
the dipoles add up to place δ^+
on one side and δ^- on the other

³ Ibid.

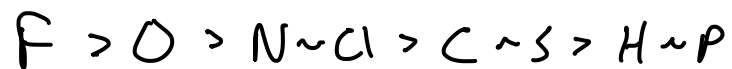
"The dipole moment, μ [...], is defined as the magnitude of the charge Q at either end of the [...] dipole times the distance r between the charges [...]." ⁴



not polar because the dipoles cancel each other out

⁴ Ibid.

Polar Molecules



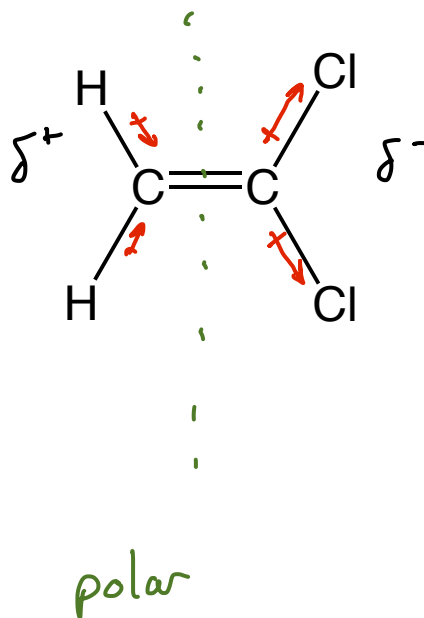
Section 2.2

Draw Lewis Structure

Draw VSEPR Structure

Draw Dipole arrows on polar bonds

If (+) and (-) are on opposite sides (front and back, left and right, top and bottom, upper left and lower right) then the molecule is polar otherwise it isn't.

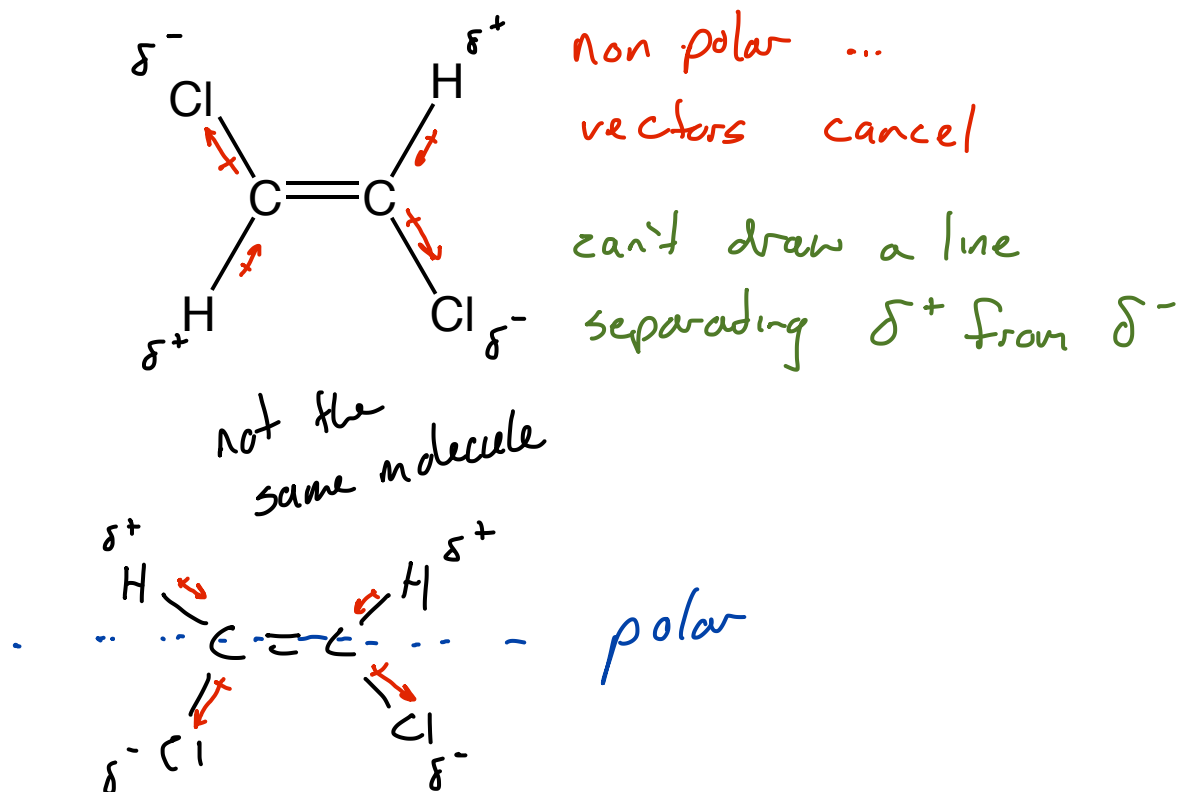


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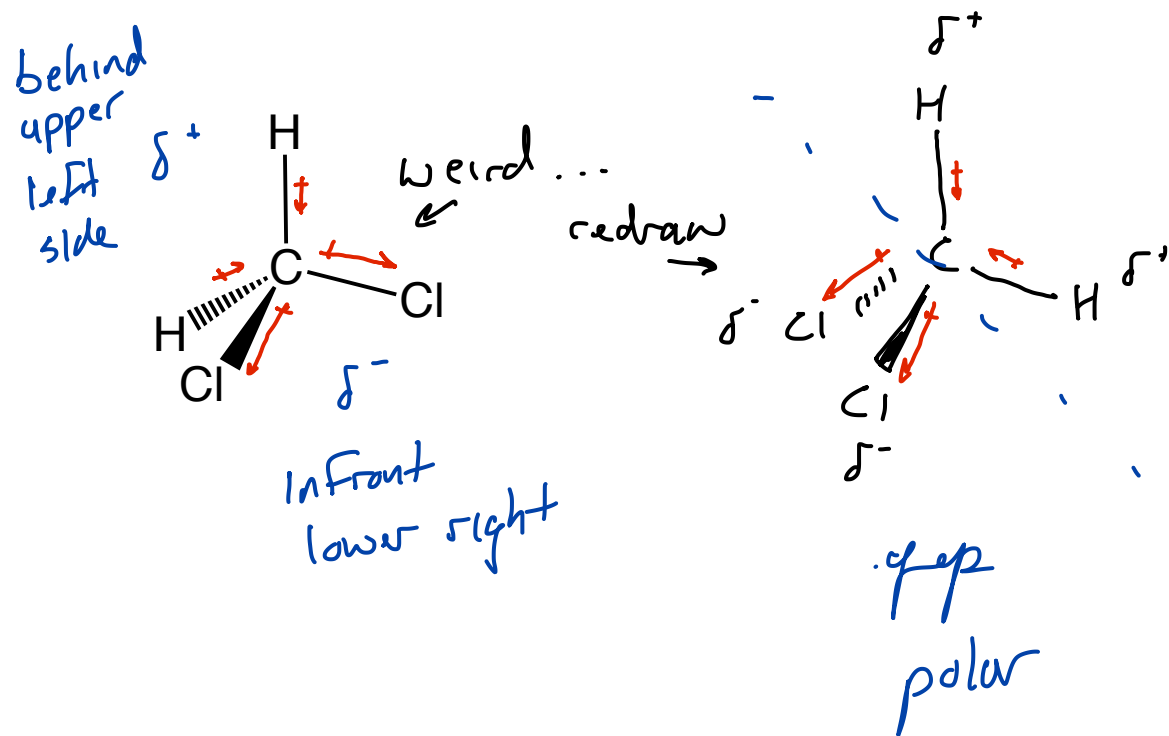


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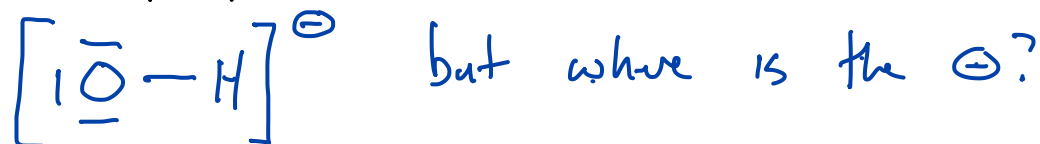
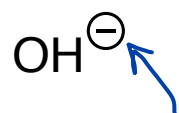
Formal Charges

1. can help us understand where molecules are δ^- rich

Formal Charge of an atom	=	# valence e ⁻ 's in the neutral atom	-	(# of lone pair electrons	+	1/2 of the e ⁻ 's in the bonds)
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- 2. communicating structures
- 3. whether molecules might be more reactive

Lewis structure



$$\begin{array}{r} 1e^- \\ 6e^- \\ 1e^- \\ \hline 8e^- \\ \hline 2 \end{array} = 4 \text{ pairs}$$

Kekule structure



$FC_H = 1 - (0 + 1) = 0$

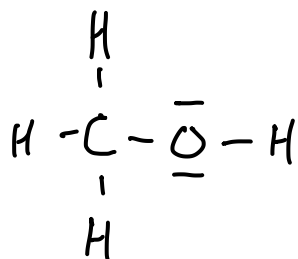
$FC_O = 6 - (6 + 1) = -1$

by indicating that the O is negative you know that the O must have 6 lp e⁻'s



↖ what's up with this O? without a charge we assume neutral, but then this wouldn't be OH⁻

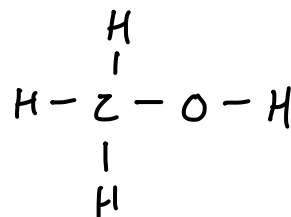
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-----------------------------	---	--	---	---	-----------------------------	---	--	---

CH₃OH

Lewis

$$\begin{aligned}
 & \left(\right. \\
 & \text{FC}_O = 6 - (4 + 2) \\
 & \quad = 0
 \end{aligned}$$

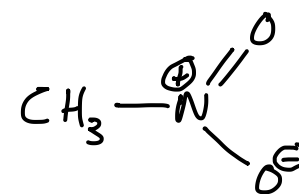
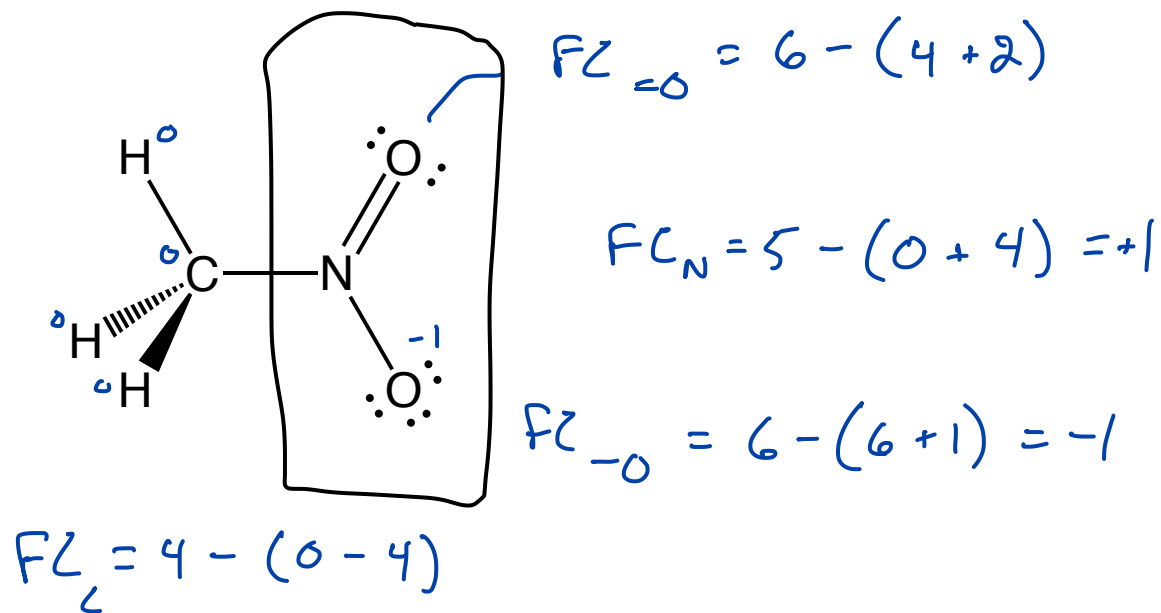
$$\begin{aligned}
 \text{FC}_C &= 4 - (0 + 4) \\
 &= 0
 \end{aligned}$$



Kekulé

Sum of formal charges
must equal the
charge of the molecule

Formal Charge of an atom	=	# valence e ⁻ 's in the neutral atom	-	(# of lone pair electrons	+	1/2 of the e ⁻ 's in the bonds)
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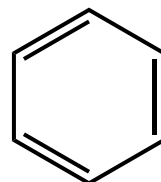
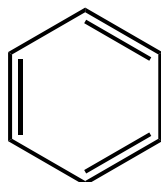


$$0 + 0 + 0 + 0 + 0$$

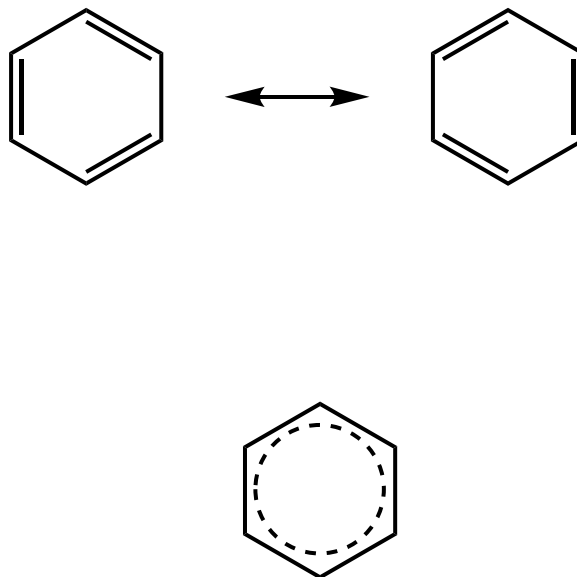
$$+1 \quad -1$$

Also a way to move charge around a molecule...

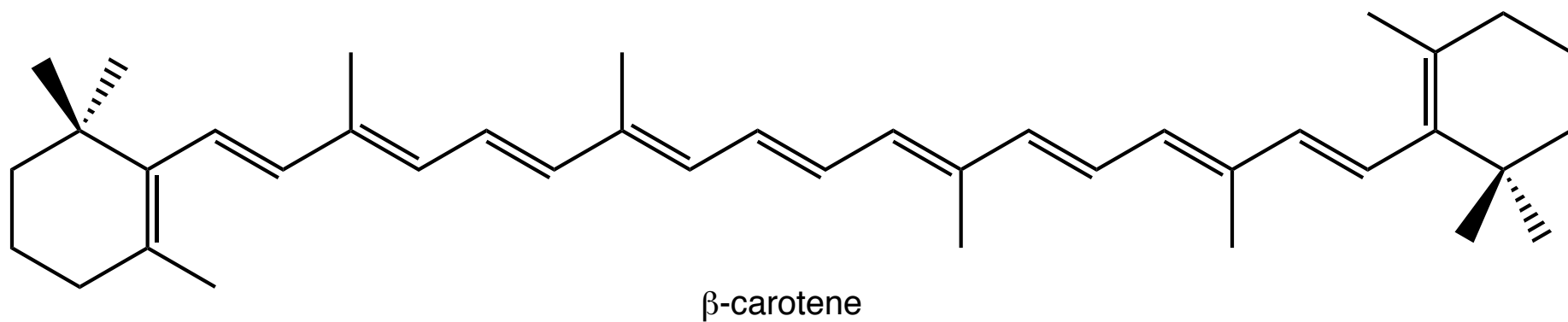
Which one is correct?



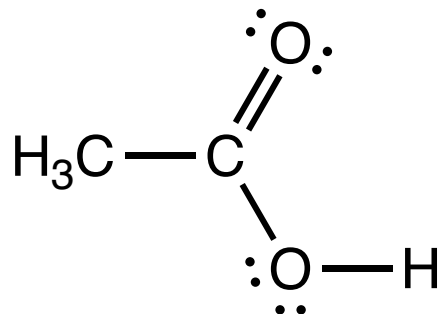
Whenever 3 or more p orbitals are in a row experiments and MO theory say that the electrons are delocalized over all of the p orbitals.



Resonance: Where else do we see extended π systems/electron delocalization

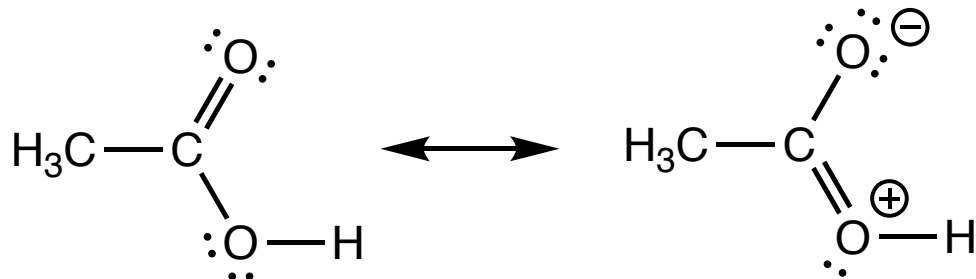


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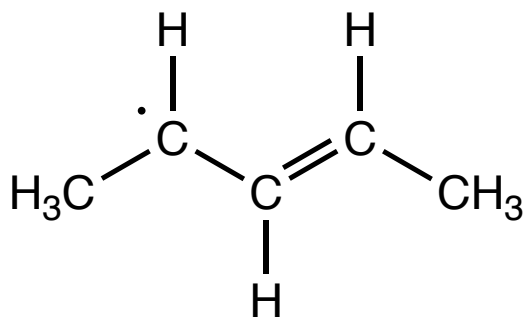


The more stable the resonance contributor is, the more it contributes to the resonance hybrid

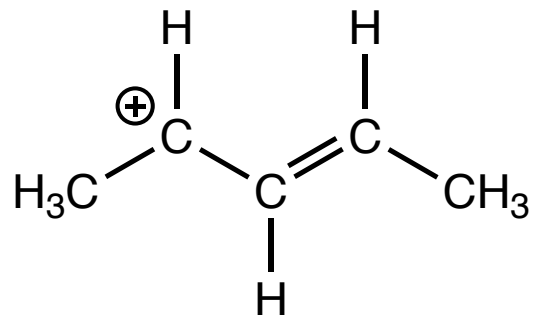
1. Incomplete octets
2. "Wrong" charges
 - negative charge is not on the most electronegative element
 - a positive charge on an electronegative element
3. charge separation



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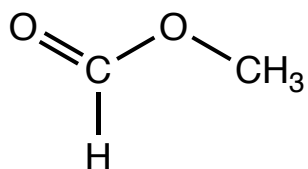


Drawing Resonance Contributors

Section 2.4

Rules for drawing Resonance Contributors

1. **atoms don't move**, only electrons
2. **don't move σ bonds**, only π bonds, lone pair e⁻'s, or unpaired e⁻'s (radicals)
3. the total number of electrons must stay the same, **don't change the net charge**
4. p orbitals must be able to line up parallel to each other

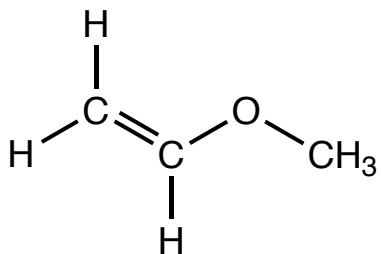


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