CHEM 223 (2024) SI Session #1

Learning Objectives: By the end of this session, students should be able to:

- Describe the formal charges of atoms within organic compounds using the bonding patterns table and the formal charge equation
- Turn condensed structures into lewis structures and line-angle diagrams
- Describe the hybridization of the atoms within organic compounds
- Draw resonance structures with accurate arrow pushing

Section 1: Formal Charges & Bonding Patterns

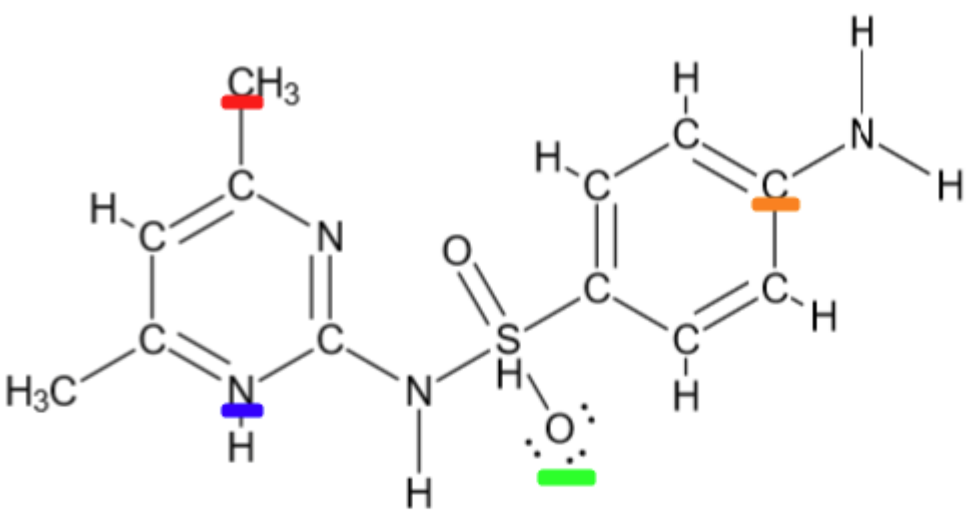
1. What is "formal charge"? Write the formula we use to calculate it.

   ↳ the "charge" attributed to an atom in an organic molecule.

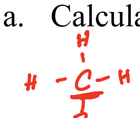
   $$FC = \underbrace{\text{group \#}}_{\text{\# of valence } e^{\ominus}} - \underbrace{\left(\text{\# of nonbonding } e^{\ominus} + \tfrac{1}{2}\cdot \text{\# of bonding } e^{\ominus}\right)}_{\text{\# of current valence } e^{\ominus}}$$

   note: I've just factored out a −1 from the equation

2. Use the structure to answer the following questions.

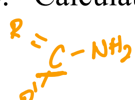


   a. Calculate the formal charge of the atom underlined in **red**

   $4 - (0 + \frac{1}{2}\cdot 8) = \emptyset$, neutral

   b. Calculate the formal charge of the atom underlined in **orange**

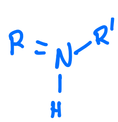
   $4 - (0 + \frac{1}{2}\cdot 8) = \emptyset$, neutral

   c. Calculate the formal charge of the atom underlined in **green**

   $6 - (6 + \frac{1}{2}\cdot 2) = -1$, −1

   d. Calculate the formal charge of the atom underlined in **blue**

   $5 - (0 + \frac{1}{2}8) = 1$, +1

3. In each of the blanks, draw the atom with the amount of bonds and/or lone pairs required to achieve the formal charge listed (Note: there are multiple valid ways to do this, but we will focus on the most "common" ones for now).

	Formal Charge		
Atom	**+1**	**0**	**-1**
Hydrogen	H^{+} no bonds no lone pairs	H–R 1 bond no lone pairs	$H:^{-}$ no bonds 1 lone pair
Carbon	3 bonds no lone pairs	4 bonds no lone pairs	3 bonds 1 lone pair
Oxygen	3 bonds 1 lone pair	2 bonds 2 lone pairs	1 bond 3 lone pairs
Nitrogen	4 bonds no lone pairs	3 bonds 1 lone pair	2 bonds 2 lone pairs
Halogens	2 bonds 2 lone pairs	1 bond 3 lone pairs	no bonds 4 lone pairs

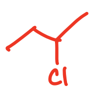
Section 2: Condensed Structures & Hybridization

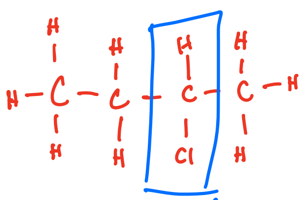
4. What is "hybridization"? How do we determine an atom's hybridization state?

↳ combining orbitals on the <u>same atom</u>. Hybridization is determined by counting the # of areas of $e^{\ominus}$ density.
(sp mainly)

5. For each of the following condensed structures: (1) convert them into lewis structures, (2) convert them into line-angle diagrams, (3) write out the formal charge of any atom that has **non-zero formal charge**, and (4) write out the hybridization of all atoms.

 a. $CH_3CH_2CH(Cl)CH_3$

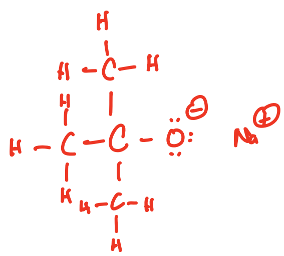




All Hydrogens: No hybridization (has no p orbitals)
All Carbons: sp^3
Chlorine: sp^3

<u>Follow-up Question (FQ)</u>: does the orientation of the Cl matter?
A: No! → sp^3 bonds have free rotation.

 b. $(CH_3)_3CONa$

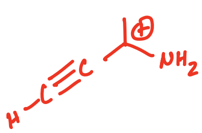


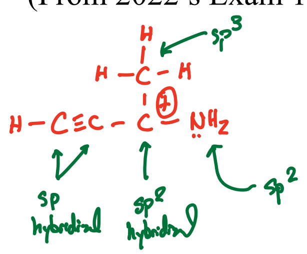
All carbons: sp^3
Oxygen: sp^3

<u>FQ</u>: type of bond between O and Na?
A: Ionic → nonzero formal charges. Do <u>not</u> draw a line between them!

 c. (From 2022's Exam 1) $HCCC(CH_3)_2NH_2$

C≡C





all carbocations are sp^2 hybridized.

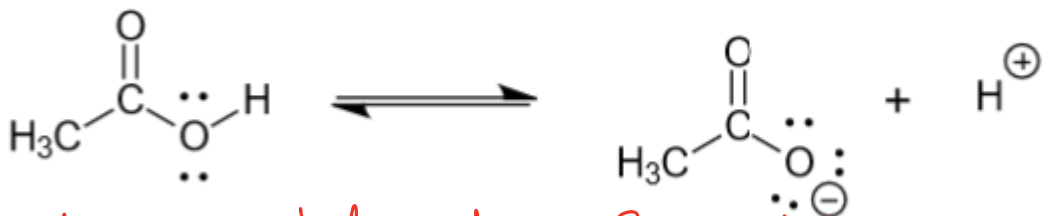
Section 3: Resonance & Arrow Pushing

6. What is "resonance?"

Lewis structures that can be interconverted by moving $e^{\ominus}$ only
↳ π and lone pairs $e^{\ominus}$

FQ: why is resonance important? → stability → $e^{\ominus}$ distribution

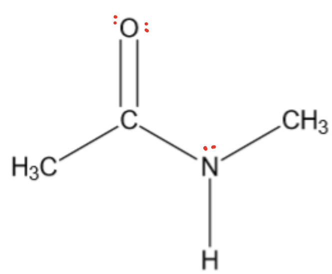
7. (From 2022's Exam 1) Are the following structures resonance structures? Explain



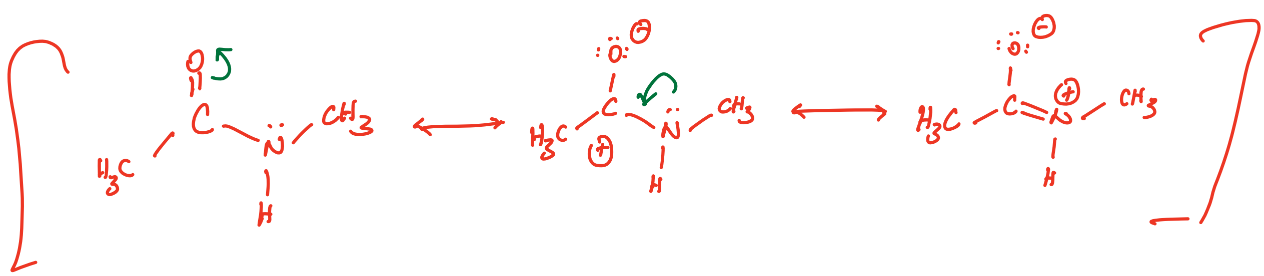
No, a σ bond is broken. Resonance structures only modify lone pairs and π bonds.

8. For each of the structures, draw the resonance structures **with arrow pushing**.

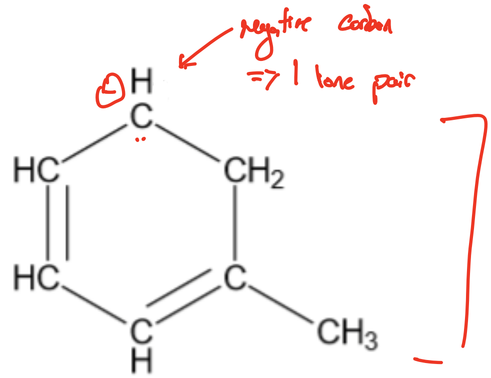
Tip: Draw lone pairs; they contribute to resonance

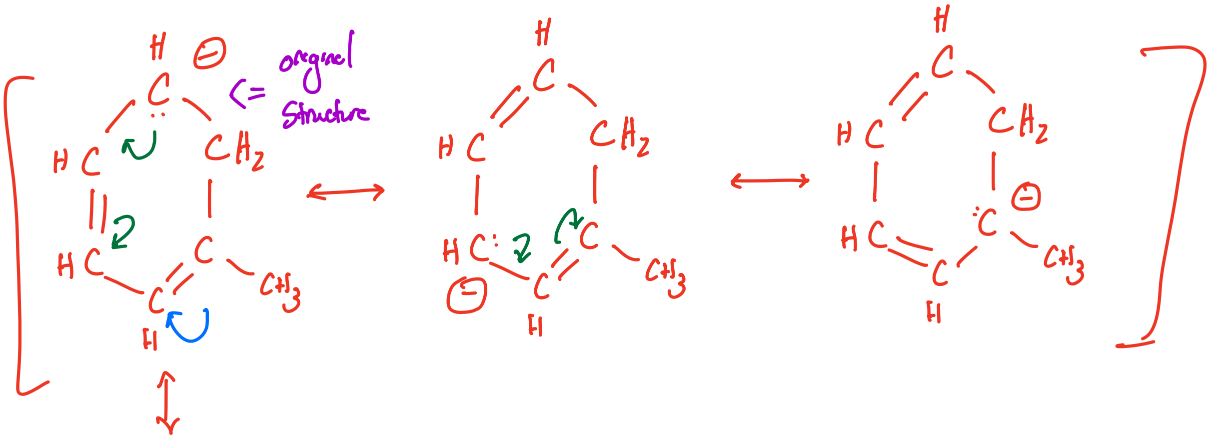


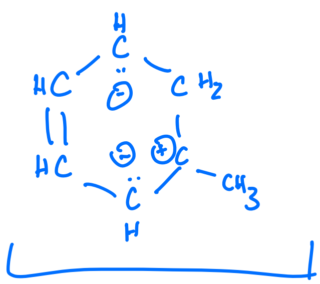
a. (From 2022s Exam 1)



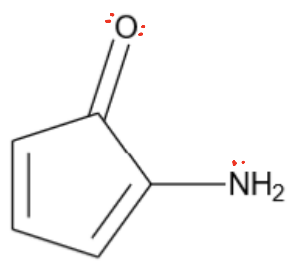
b. (From 2022's Exam 1)

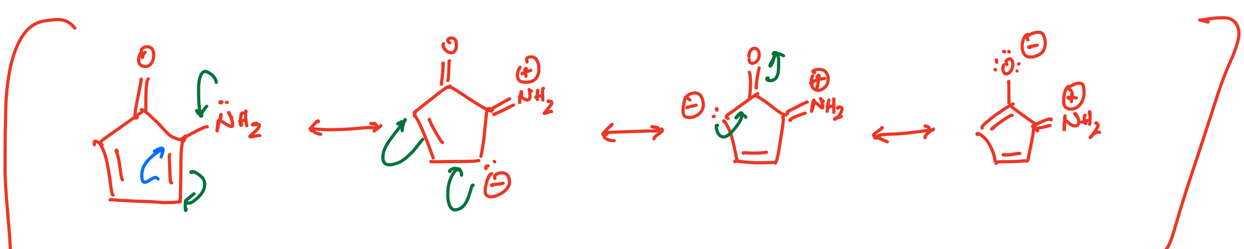






c.





Note: for this structure, there are more — these 4 are the "most important."

We will re-visit this structure later.

Next Session: 1/29, Sears 548. Electronic Structure, Hybridization & Molecular Orbitals will be covered.