CHE 1000: INTRODUCTORY CHEMISTRY
2019/2020

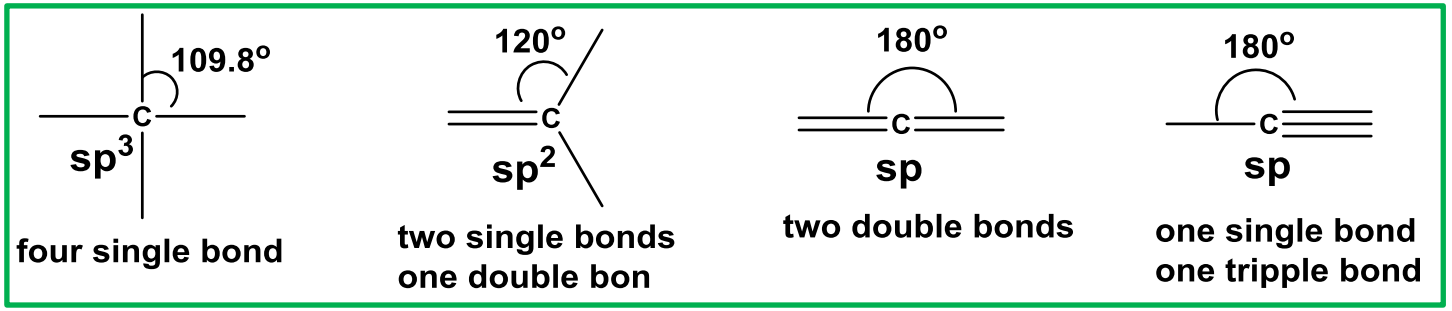
REPRESENTATION OF ORGANIC MOLECULES: 2

❑ Formal charge

Different ways by which Second Period Elements in Group C, N and O can attain the octet configuration and how the formal charge can be generated by inspection method

1. Carbon atom:

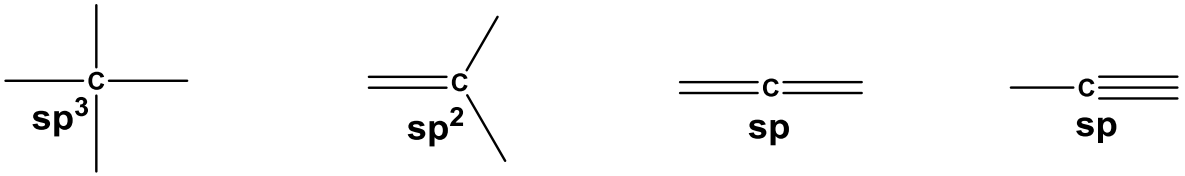
(a) Ways carbon atom can attain the octet



(b) Ways the formal charge can be generated

(i) If carbon is connected to three bonds and has no lone pair of electrons then formal charge is +1

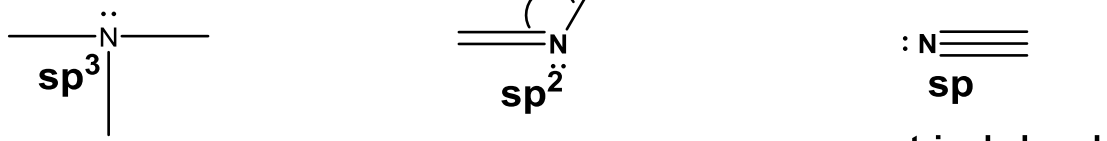
(ii) If carbon is normally connected to four bonds, then the formal charge is 0



(iii) If carbon is connected to three bonds and has a lone pair of electrons then formal charge is -1

2. Nitrogen atom:

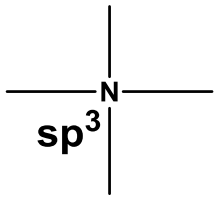
(a) Ways the nitrogen atom can attain the octet

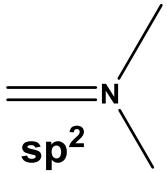


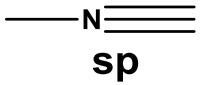
one tripple bond

(b) Ways the formal charge can be generated

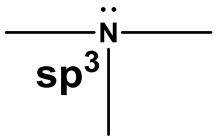
(i) If nitrogenatom is connected to four bonds the formal charge is +1

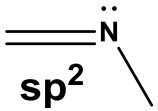


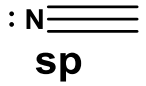




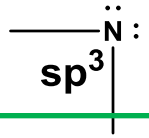
(ii) If nitrogen atom is connected to three bonds the formal charge is 0

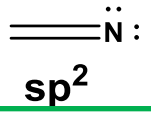






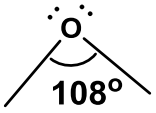
(iii) If nitrogen atom is connected to two bonds and has two pairs of electons the formal charge is -1



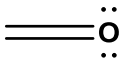


3. Oxygen atom:

(a) Ways the oxygen atom can attain the octet



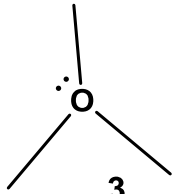
two single bond



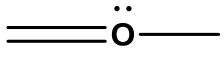
one doublebond

(b) Ways the formal charge can be generated

(i) If oxgen atom is connected to three bonds and a lone pair of electrons the formal charge is +1

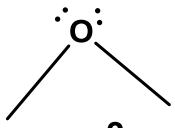


sp^3

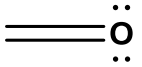


sp^2

(ii) If oxgyen atom is connected to two bonds and two pairs of electronsthe formal charge is 0

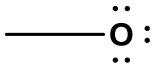


sp^3



sp^2

(iii) If nitrogen is connected to one bond and three pairs of electrons the formal charge is -1

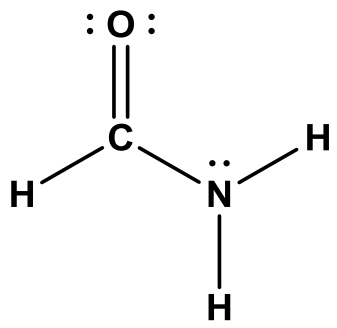


sp^2 or sp^3

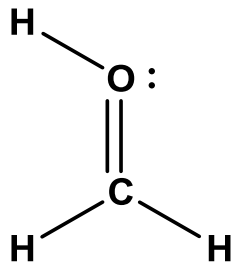
Take home problems:

1. Determine the formal charge of C, N and O atoms in the following molecules using the **inspection method?**

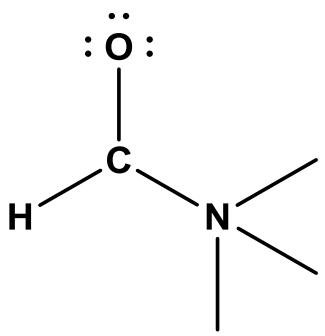
a



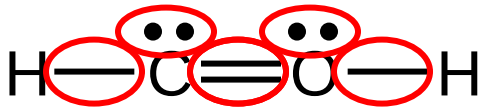
b



c



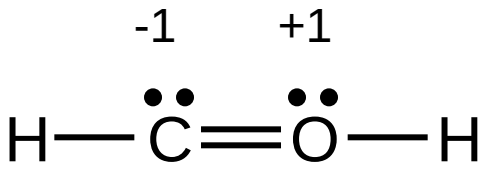
❖ **Alternatively formal charges can be calculated using the following formula;**



formal charge on an atom in a Lewis structure = total number of valence electrons in the free atom - total number of nonbonding electrons - $\frac{1}{2}$ (total number of bonding electrons)

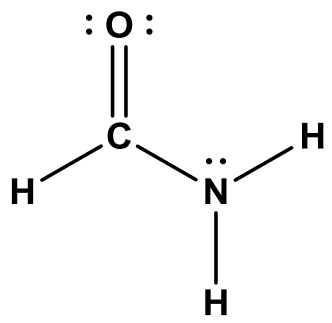
formal charge on C = 4 - 2 - ½ x 6 = -1

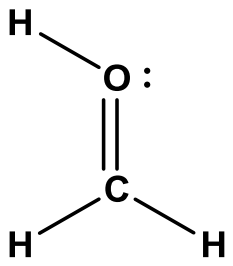
formal charge on O = 6 - 2 - ½ x 6 = +1

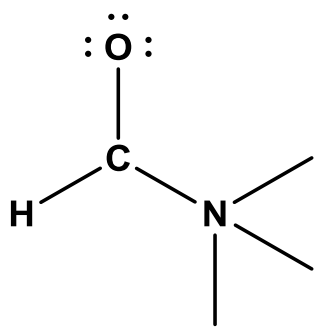


Take home problems:

1. Determine the formal charge of C, N and O atoms in the following molecules using the formula;

a 

b 

c 

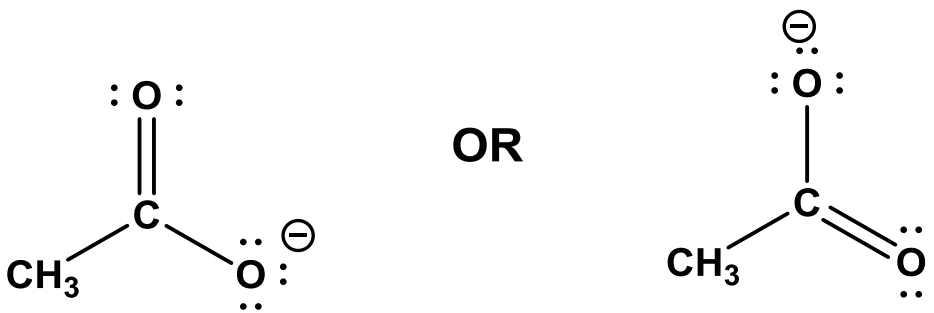
❑ Resonance Theory

Its a theory which states that a molecule or ion can be represented by two or more Lewis structures that differ only in the positions of the electrons

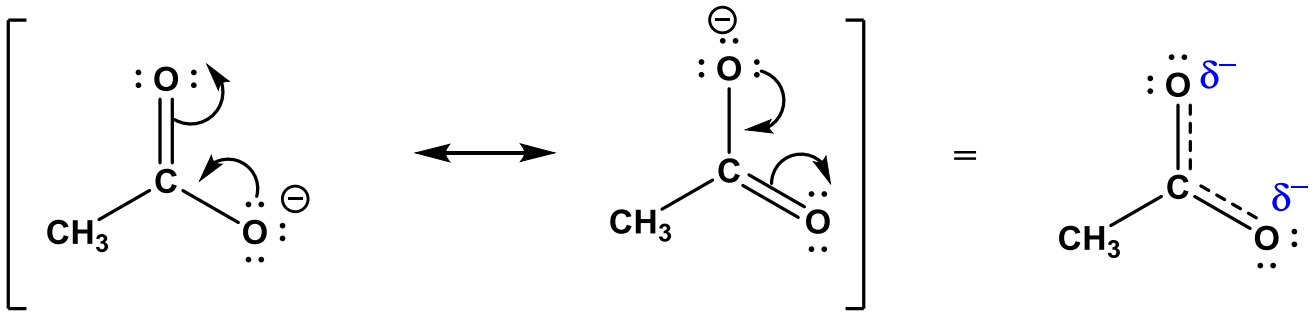
Note;

- **None of these structures, which we call resonance structures or resonance contributors, will be a realistic representation for the molecule or ion**
- **Resonance structures are not real structures for the actual molecule or ion; they exist only on paper**
- **When resonance structures are drawn, they are connected by double-headed arrows (↔)**

Consider the two Lewis structures for acetate , CH_3COO^-. Which structure is correct?



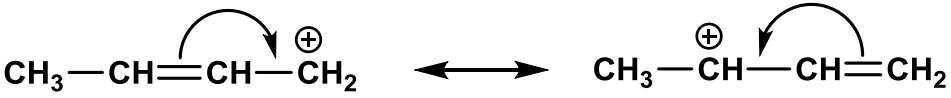
The two Lewis structures for acetate , CH_3COO^- are both correct.



resonance contributors hybrid

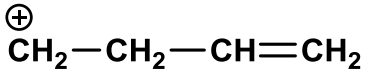
➢ Rules for writing resonance structures

1. Only lone pairs or π- electrons are moved not breaking of σ-bonds between atoms



1 2

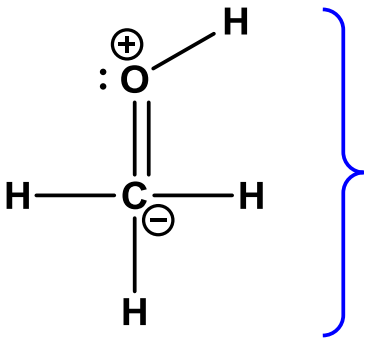
1 & 2 are resonance structures



3

3 is not a proper resonace structure of 1or 2 because a hydrogen atom has been moved

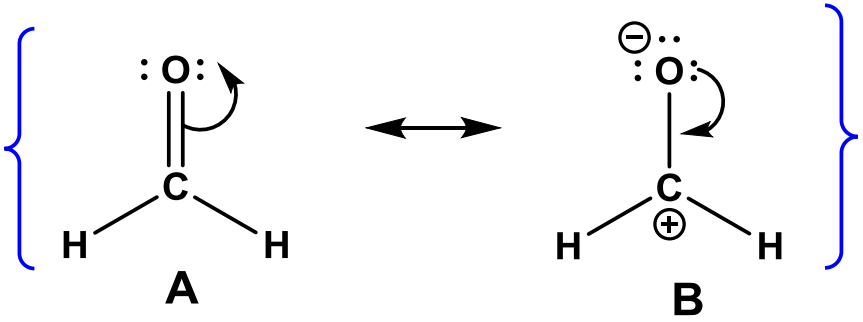
2. All of the structures must be proper Lewis structures



This is not a proper resonance structure of methanol because carbon has five bonds. Elements of the second row cannnot have more than eight electrons in their valence shell

3. The more covalent bonds (noble gas configuration) a structure has, the more stable it is, and the more it contributes to the resonance hybrid, contrary charge separation decreases stability and the less it contributes to the hybrid

Four covalent bonds and neutral



three covalent bonds and charge separated

A

more stable

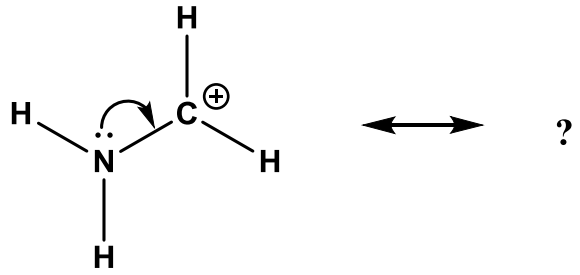
B

less stable

Take home problems:

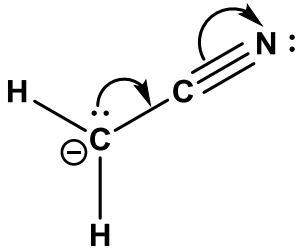
1. **Write the resonance structure that would result from moving the electrons as the curved arrows indicate. Be sure to include formal charges if needed.**

(a)



?

(b)



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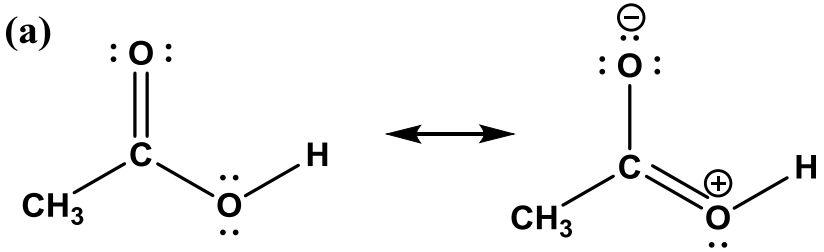
2. **From each set of resonance structures that follow, designate the one that would contribute most to the hybrid and explain your choice:**

(a)



(b)