Exercise 08.5b
Formal Charges

Name: _____

Date: _____ Per: _____

A **formal charge** is an accounting procedure that allows chemists to evaluate the locations of electrons/atoms in a Lewis structure. Formal charge is calculated for each atom in a Lewis structure by comparing the number of valence electrons an atom normally has to the number it would have in a bonded structure by assuming bonded electrons are equally shared. The formula is:

$$\text{Formal Charge} = \#e^-_{\text{valence}} - \#e^-_{\text{unshared}} - \tfrac{1}{2}\,\#e^-_{\text{shared}})$$

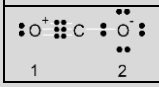
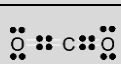
The sum of the formal charges in the structure must be equal to the charge of the structure.
Adjacent atoms in the structure should NOT have like signs (pos – pos or neg – neg).

Ranking the importance of resonance structures:

- Those with at least an octet, barring exceptions, and no charge separation are favored over
  - Those that exhibit a charge separation, which are favored over
    - Those that exhibit a charge separation *against* that predicted by electronegativity.
- **Summary: Most # of bonds for least formal charges are most important**

Generally, the Lewis structure with the smallest formal charges on individual atoms will be the "best" one.

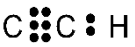
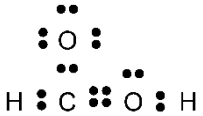
Example: **Which of the following is a better Lewis dot structure for carbon dioxide (CO_2)?**

Structure A	Structure B
	

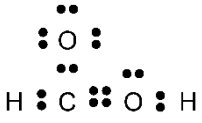
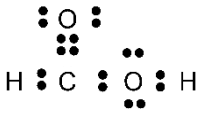
The answer is Structure B because it has the least formal charges even though both structures satisfy all octets and have the correct number of valence electrons.

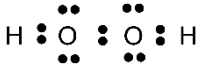
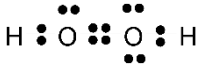
DIRECTIONS: Answer the following in the space provided:

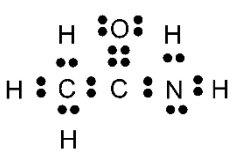
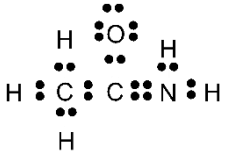
1. Assign formal charges to each atom in the following structures. Show your work.

			
C =	C =	H =	C =
O =	H =	C =	O_d =
		N =	O_s=
			H =

2. Choose the best structure based on formal charges. Show your work and explain.

a)  or 

b)  or 

c)  or 

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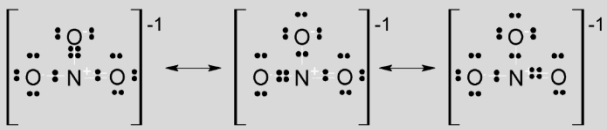
Resonance Structures

When more than one **valid** Lewis structure can be written for a molecule, the true structure is generally a mixture or hybrid of all of the possibilities. This most commonly occurs when a double bond could be written between a central atom and two or more identical attached atoms. Under these circumstances, all of the possible structures are shown with a double arrow between each as shown in the examples below. These are called resonance structures. This is not to imply that the molecule flips around between the possibilities, but instead that the real molecule is an average of them.

Example: Write resonance structures for the following: NO_3^-



Because all three oxygen atoms are really equivalent, the double bond could be written between the N atom and any of the three O atoms. The actual molecule is a hybrid of all three structures, meaning all three bonds are equivalent with each N-O bond being about 1 and 1/3 (rather than two single bonds and 1 double bond.)

DIRECTIONS: For each, draw the possible resonance structures that the molecule can have. Assign formal charges in each and circle the most plausible structure for the molecule.

1. OCN^-

2. BrF_3

3. SO_4^{2-}

4. O_3

5. POF_3