Formal Charge and Resonance

NAME:

Formal charge is an accounting procedure. It allows chemists to determine the location of charge in a molecule as well as compare how good a Lewis structure might be. The formula for calculating formal charge is shown below:

Formal Charge = # valence e^- - (# non-bonding e^- + ½ # bonding e^-)

Note: the formal charges must add up to the net charge of the molecule;

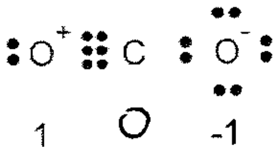
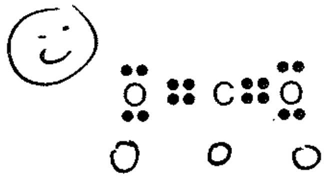
Generally, the Lewis structure with the smallest formal charges on individual atoms will be the "best" one.

EXAMPLES

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

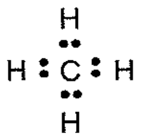
C: 4 - 4

O: 6 - (4 + 2)
= 0

Structure A	Structure B
 1 0 -1	 0 0 0

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.

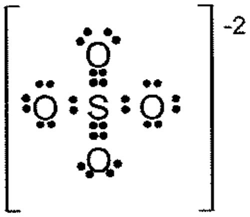
Calculate the formal charges on all of the atoms in the following molecules:



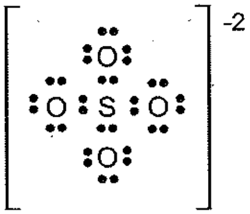
Carbon; FC = 4 – (0 + ½*8) = 0 each H; FC = 1 – (0 + ½ * 2) = 0

The molecule is neutral and has no formal charges

Choose the best structure based on formal charges



A



B

Structure A	
1-Sulfur	FC = 6 – (0 + ½*12) = 0
2-Oxygen (double bond)	FC = 6 – (4 + ½*4) = 0
2-Oxygen (single bond)	FC = 6 – (6 + ½*2) = -1

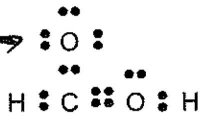
Net FC = -2

Structure B	
1-Sulfur	FC = 6 – (0 + ½*8) = +2
4-Oxygen	FC = 6 – (6 + ½*2) = -1

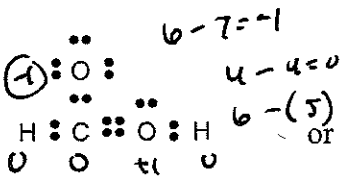
Net FC = -2

PROBLEMS

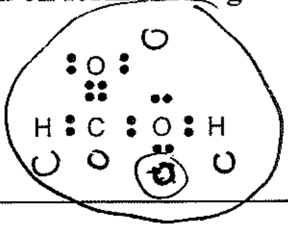
1)Assign formal charges to each atom in the following structures. Show your work.

			
C = 4-(2+3) = -1	C = 4-(2+5) = -1	H = 1-1 = 0	C = 4-(4) = 0
O = 6-(2+3) +1	H = 1-(1) = 0	C = 4-4 = 0	O_d = 6-(6+1) = -1
		N = 5-(2+3) = 0	O_s = 6-(2+3) = +1
			H = 1-1 = 0

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

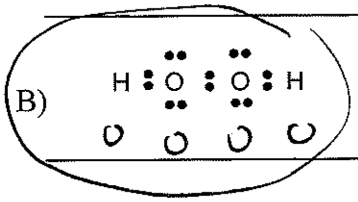
A) 

or



6-(4+2) = 0

O = 6-(4+2) = +0

B) 

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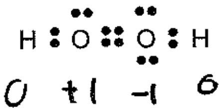
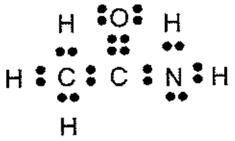


C) 

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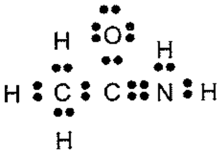
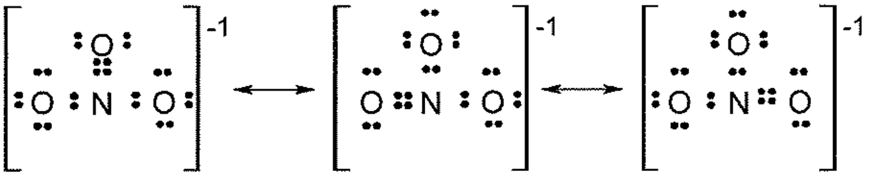


Resonance Structures

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^{-1}

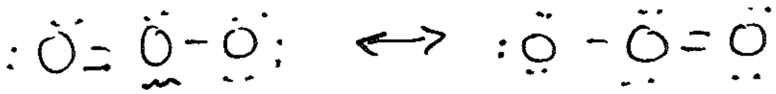


Note that because all three oxygen atoms are really equivalent, the double bond could be written between the nitrogen atom and any of the three oxygen atoms. The actual molecule is a hybrid of all three structures, meaning that all three bonds are equivalent with each N-O bond being about 1 and 1/3 (rather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

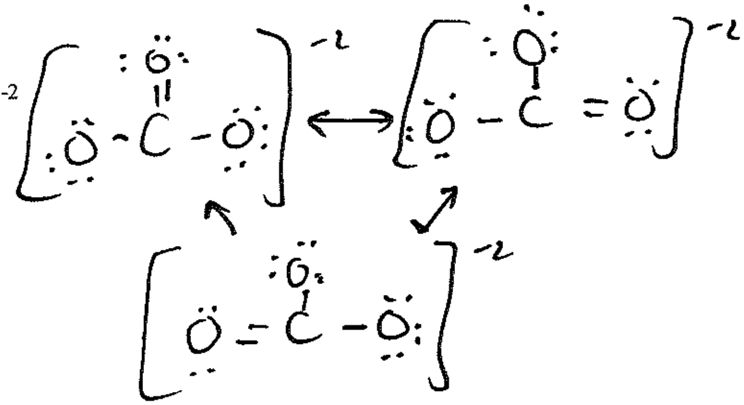
PROBLEMS

1)Write the required equivalent resonance structures for the following molecules and ions:

O_3 18

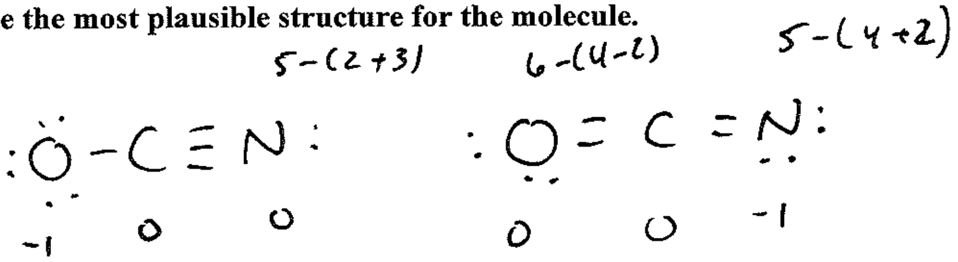


CO_3^{-2}



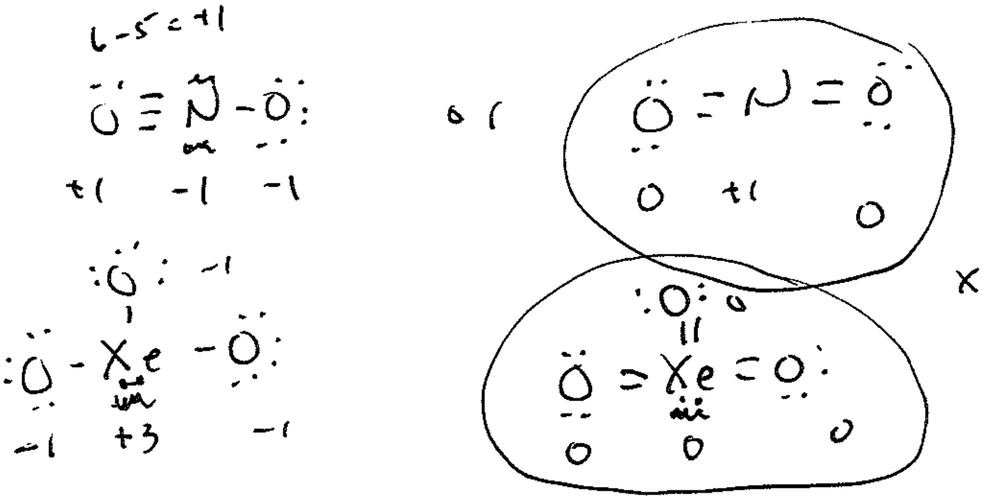
2) For each, draw the possible resonance structures that the molecule can have. Assign formal charges in each and circle the most plausible structure for the molecule.

OCN^-



N_2O
16

XeO_3



6-(4+2)=0

Xe: can violate octet rule