# Molecular Bonding

**Unit 10B:** Advanced Lewis Dot Structures and Resonance

### Knowledge/Understanding:

* Predicting bonding

### Write and discuss resonance forms where appropriate

### Determine formal charges for atoms within molecules and ions

### Use formal charges to predict the relative stabilities for several resonance forms

### Skills:

* Draw proper Lewis Dot structures

### Notes:

### Resonance

Try drawing out the Lewis Dot structure of a carbonate group; CO32-

How did you determine which oxygen should have the double bond? Which should have formal charges?

In reality, it makes no difference which of the 3 oxygen you gave the double bond to, or which 2 oxygen received the -1 charge, as each of the bonds experiences resonance. For such molecules, the various resonance forms are typically written as connected by double-headed arrows to show their relationship.

Ex: CO32-

Some molecules can be represented by more than one Lewis dot structure. Two (or more) different Lewis dot structures for a given species are called resonance structures or resonance forms. It is important to understand that these resonance forms do not exist, even briefly, but are simply the best approximations to the actual molecular structure that can be made within the constraints of the Lewis theory.

Resonance forms are useful, however, because the structure of a molecule described by resonance is intermediate between the structures of its resonance forms.

Ex: CO32-

Note that resonance can be predicted with electron pushing, where a pair of unbound e- are used to create a new bond, forcing e- in an adjacent bond to become unbound.

Ozone, a high energy allotrope of oxygen with the formula O3, provides a good example of resonance. In order to provide each of the three oxygen atoms in ozone with an octet of electrons (as required by the Lewis theory), two of the oxygen atoms must be connected by a single bond and the other by a double bond. There are, however, two different ways this can be done, depending on where the double bond is placed.

Experiments indicate that the two bonds in the O3 molecule do not have different properties, as they would if the single and double bonds were fixed in position. Rather, the two bonds are equivalent with properties intermediate between those of a single and a double bond.

Double bond shared over 2 bonds (O3)

Carbon dioxide, CO2, is another molecule for which a number of resonance forms can be written. First, there is the most familiar form of CO2 in which the two oxygen atoms are bonded to the carbon by two double bonds. In addition, two other resonance forms can be written, each containing a single and a triple bond.

**Formal Charge**

Formal charge represents the difference between the number of valence electrons an atom possesses in its free state (before bonding) and the number assigned to it in a given Lewis structure (after bonding).

The number of valence electrons assigned to an atom in the bonded state can be found by counting all of the electrons belonging exclusively to that atom (i.e., nonbonding electrons) and one-half of the electrons in the bonds to it. The formal charge is obtained by subtracting the number obtained in this way from the number in the free atom. This is summarized in the following equation:

Formal charge = Number of original valence – Number of final valence

= Number of original valence – (nonbonding + ½ bonding e-)

The formal charge concept is a very useful one because:

1. It provides a means for 2nd period elements to obey the octet rule

Ex: NO3-

1. It may be helpful in determining the best, or most stable, of several resonance structures. The best structure is the one which:
   1. Has the lowest number of assigned formal charges
   2. Has negative/positive charges placed on the proper elements based upon their relative electronegativity values

The cyanate ion, NCO-, with two reasonable resonance forms (labeled a = cyanate and and b = isocyanate) provides a useful example.



The formal charge for each of the atoms in structure (a) would be:

N = 5 e- - [2 nonbond e- + ½ (6 bond e-)] = N = 5 - 5 = -0

C = 4 e- - [ ½ (8 bond e-)] = C = 4 - 4 = 0

O = 6 e- - [6 nonbond e- + ½ (2 bond e-)] = O = 6 -7 = -1

Similarly, the formal charge for each of the atoms in structure (b) would be:

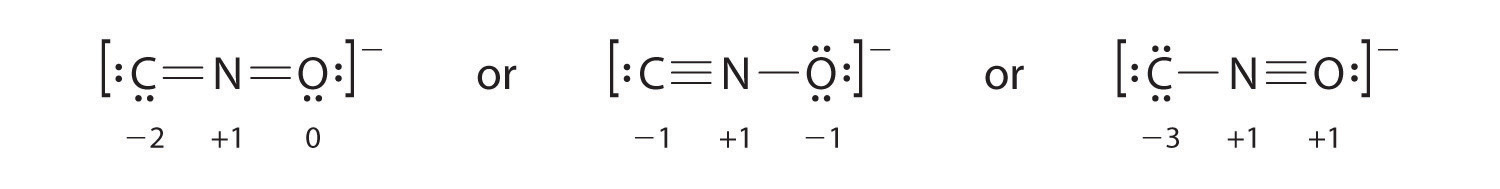
N = 5 e- - [4 nonbond e- + ½ (4 bond e-)] = N = 5 - 6 = -1

C = 4 e- - [ ½ (8 bond e-)] = C = 4 - 4 = 0

O = 6 e- - [4 nonbond e- + ½ (4 bond e-)] = O = 6 - 6 = 0

Which would be more stable (preferred)?

Why?

Now examine the fulminate ion: 

The fulminate ion has a similar molecular formula to the cyanate ion even though its structural formula is different. When it is analyzed in terms of formal charge, a determination as to why it is unstable can be made.

Which of the above is the preferred (stable) structure?

Again, in evaluating the stabilities of resonance forms, the following rules apply:

1. minimize nonzero formal charges
2. avoid nonzero formal charges on adjacent atoms
3. place negative formal charges on atoms with greater electronegativity and positive formal charges on atoms with lower electronegativity.

Determine the formal charges on the atoms in the hypothetical species with the atomic arrangement CON- and use these to explain why this ion is unknown.