Formal Charge

Start the process by drawing possible Lewis Structures.

1. Choose the central atom. Usually the least electronegative.
2. Count total valence electrons for the molecule.
3. Start by placing one pair of electrons for each bond.
4. Satisfy the octet rule. This may require making double or triple bonds (and removing lone pairs)
5. If you can draw multiple structures, check the formal charge. See below.

Formal Charge

- Formal charge is used to decide if a Lewis Structure is plausible.

$$\text{formal charge} = \left(\begin{array}{c}\text{number of}\\ \text{valence electrons}\end{array}\right) - \left[\left(\begin{array}{c}\text{number of}\\ \text{nonbonding electrons}\end{array}\right) + \frac{1}{2}\left(\begin{array}{c}\text{number of}\\ \text{bonding electrons}\end{array}\right)\right]$$

Formal Charge

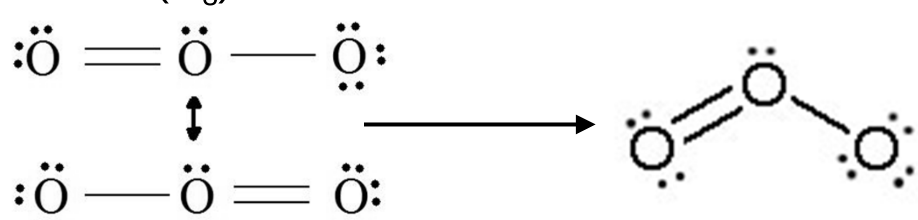
Rules for formal charges:

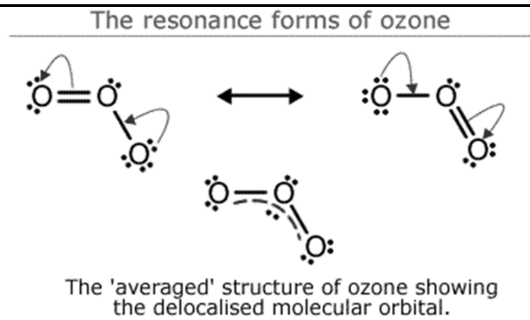
1. Formal charges in must add up to the charge of the molecule or ion.
2. We generally choose the Lewis structure in which the atoms bear formal charges closest to zero
3. We generally choose the Lewis structure in which any negative charges are on the more electronegative atoms.

Note: formal charges do not represent actual charge. It is merely a tool that helps us determine plausible Lewis structures.

Resonance

Ozone: (O_3)

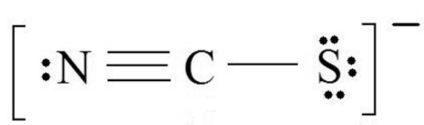




•If we were to freeze an individual molecule at a moment in time, we would not see one oxygen-oxygen single bond and one oxygen-oxygen double bond.
•Instead the two electrons which are needed to make a single bond into a double bond are shared equally between both oxygen pairs! This means both oxygen-oxygen bonds are equivalent. They are shorter and stronger than an oxygen-oxygen single bond, but longer and weaker than an oxygen-oxygen double bond.

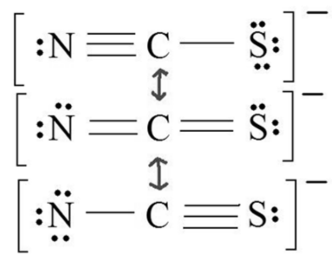
Resonance Continued

- Consider CNS^{-1}
- **1. Find the Lewis Structure of the molecule. (Remember the Lewis Structure rules.)**

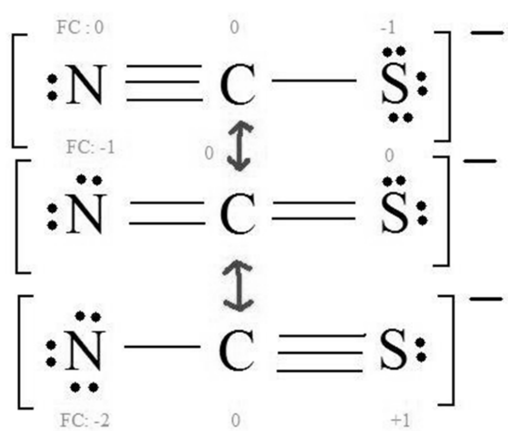


Resonance Cont.

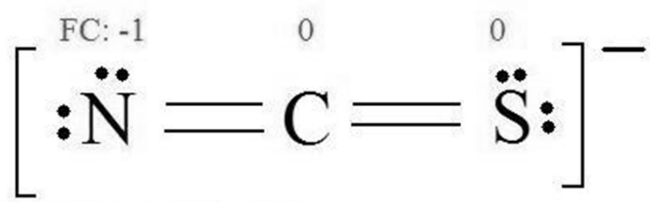
2. Resonance: All elements want an octet, and we can do that in multiple ways by moving the terminal atom's electrons around (bonds too).



- Assign formal charges



- Find the most ideal resonance structure.
  - It is the one with the least formal charges that adds up to zero or to the molecule's overall charge.)
  - The most electronegative atom should have a negative charge and least electronegative should have positive charge



Electronegatvity values:
N: 3.0 (-1) C: 2.5 S: 2.5

Is the "correct" Lewis structure out of all the other resonances because of the electronegativity values.

3 Exceptions to the Octet Rule

1. Molecules with an odd number of electrons (i.e. NO_2).

- If you have an odd number of electrons there is no way to satisfy the octet rule. Try it if you don't believe me.

3 Exceptions to the Octet Rule

2. Molecules where an atom has less than an octet (i.e. BF_3, BeH_2, $AlCl_3$). BORON is most common exception for less than octet.

- This only happens to atoms near the boundary between metals and non-metals, such as Be, B, Al and Ga. The electronegativity of these atoms is not high enough to force more electronegative non-metals into forming double and triple bonds. When working with such atoms never draw multiple bonds and you will be able to get the correct Lewis dot structures.

3 Exceptions to the Octet Rule

3. Molecules where an atom has more than an octet of electrons (i.e. ClF_3, PCl_5, XeF_2).
 SULFUR is most common exception for more than an octet.
   - This is fairly common for elements in the 3rd period (row) and below. However, elements in the first two periods, H – Ne, cannot violate the octet rule in this way.

Determining Molecular Shape

Examples:

1. **H_2O**
2. Oxygen will be central. Assign it a number of 6
3. |charge x quantity| of hydrogens = 2
4. Not an ion so don't need to add or subtract anything
5. Total = 8
6. divide by 2 = 4 (so for water there are 2 bonds and 2 lone pairs)

Determining Molecular Shape

Examples:

NO_3^{-1}

1. Nitrogen will be central. Assign it a number of 5
2. Ignore other atoms because they are oxygen
3. A -1 ion (add 1 electron)
4. Total = 6
5. Divide 6 by 2 = 3 (so 3 bonds and no lone pairs – note that one of the bonds is a double bond)

Determining Molecular Shape

A trick to determine the number of bonds + lone pairs in a molecule (from Sherry Berman Robinson)

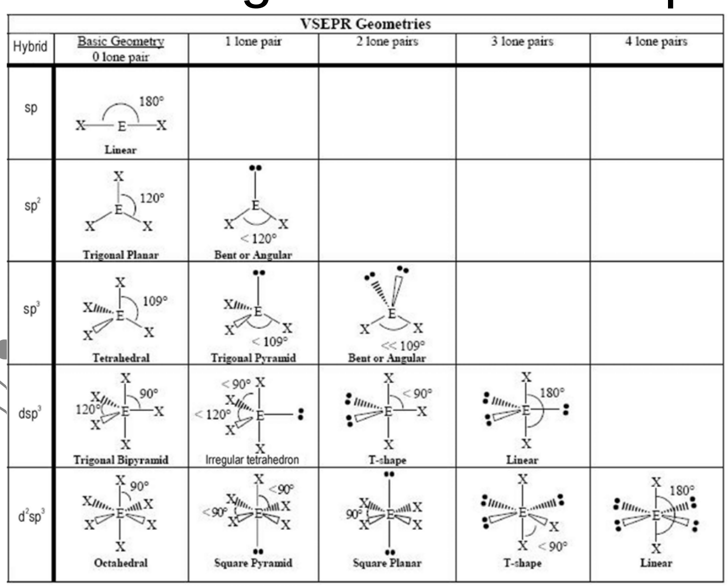
1. Determine the central atom. Assign it a number the same as its Group number (number of valence electrons). (ex. Oxygen would be 6, phosphorus would be 5, etc.)
2. If the other atoms are Sulfur or Oxygen, ignore them. If not, then assign them a number equal to the absolute value of |charge x quantity|
3. If a negative ion, add number of electrons equal to charge
4. If a positive ion, subtract number of electrons equal to charge
5. Add up numbers from steps 1-3. This is equal to the total number of electrons available for bonding
6. Divide the total by 2. This is your number of bonds + lone pairs.

Determining Molecular Shape

Hybrid	sp	sp^2		sp^3			dsp^3				d^2sp^3		
# bonds	2	3		4			5				6		
Bonded pairs	2	3	2	4	3	2	5	4	3	2	6	5	4
Lone pairs	0	0	1	0	1	2	0	1	2	3	0	1	2
Shape	linear	Trigonal	Bent	Tetrahedral	Pyramidal	Bent	Trigonal bipyramidal	Irregular tetrahedron	T-Shaped	Linear	Octahedron	Square pyramid	Square planar
Mnemonics	Love Live	To To	Be Be	The The	Play Perfect	Boy Brother	Toy That	In Ignores	Toy The	Land Life	On Of	Square Strange	Ships Siblings
Bond Angle	180	120	105	109.5	107	105	90 & 120	90 & 120	90 & 120	90 & 120	90	90	90
Example Molecule	$HgCl_2$	$AlCl_3$	$SnCl_2$	CH_4	NCl_3	SCl_2	PCl_5	$TeCl_4$	ClF_3	XeF_2	SF_6	BrF_5	XeF_4

See handout!

Determining Molecular Shape



Modified from diagram found at: Http://en.wikipedia.org/wiki/AXE_method

Formal Charge References

- Examples: see the following websites:
- http://en.wikipedia.org/wiki/Formal_charge#Formal_Charge
- http://wine1.sb.fsu.edu/chm1045/notes/Bonding/Drawing/Bond06.htm
- http://www.chem.ucalgary.ca/courses/351/Carey5th/Ch01/ch1-3depth.html
- http://www.science.uwaterloo.ca/~cchieh/cact/c120/dotstruc.html
- References: Chemistry 7th ed., Chang; http://en.wikipedia.org/wiki/Formal_charge#Formal_Charge