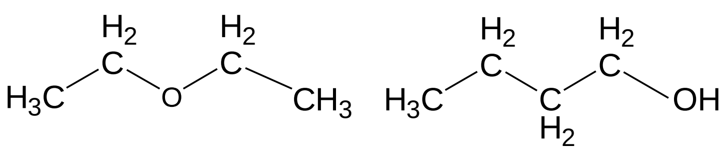
Experiment 2A: Molecular Models

The shape of simple molecules and ions

Background

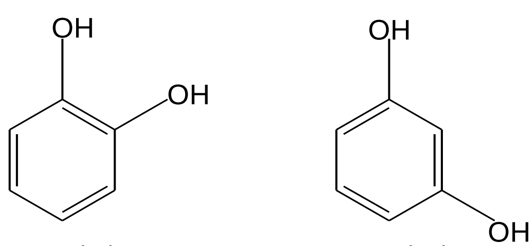
Part A. The shape of simple molecules and ions

The shape of a molecule is very important when investigating its properties and reactivity. This is true for both large molecules and small molecules. For example, compare diethyl ether (a compound that was used as an anesthetic) to *n*-butanol, which has the same chemical formula but with one of its oxygen atoms in a different position. The latter has no anesthetic properties.



diethyl ether n-butanol

Consider the following compounds, catechol and resorcinol. The first one is found in the skin irritants of poison ivy, whereas the second is used as an antiseptic and disinfectant. The only thing that is different between them is the position of an OH group.



catechol resorcinol

You can see why chemists are extremely interested in predicting the shape of the molecules they are working on.

We will use Lewis structures and the Valence-Shell Electron-Pair Repulsion (VSEPR) theory to predict the shape of small molecules and polyatomic ions. We will use the molecular kits to build 3-D models of these compounds.

Modeling Procedure

You will use a model set that consists of balls representing the nucleus and the core electrons of an atom and sticks representing the bonds between the atoms. In order to build the model of a molecule or an ion it is convenient to proceed in a systematic way.

The modeling procedure:
1. Calculate the number of valence electrons (ve) of the molecule (remember to add or subtract electrons if the molecule is an anion or a cation).
2. Draw the corresponding Lewis structure.
3. Use your knowledge of the VSEPR theory to determine the electron geometry and the molecular geometry of the molecule (ion).
4. **Build a model of the molecule (ion)** using the balls that correspond to the different atoms. In cases involving double bonds don't forget to use the longer, flexible sticks in your model.
5. Determine whether the molecule (ion) is polar or nonpolar and indicate the approximate location of the dipole moment on the 3D sketch of the molecule (ion) in the last column of the table.
6. Predict whether the structure has resonance forms.

What follows is a very brief reminder of how to draw Lewis structures and how to determine VSEPR geometries and resonance structures.

Lewis Structures

To draw the Lewis structure:
1. Determine how atoms are connected. Identify the central atom(s) and terminal atoms. H and F are always terminal atoms and form only one bond.
2. Draw a skeletal structure by joining atoms with single bonds.
3. Distribute the remaining electrons in pairs by completing the octets around the terminal atoms and then assigning the remaining electrons (if any) to the central atoms.
4. If there are too few electrons convert lone pairs from terminal atoms to form multiple bonds with central atoms.
5. There are some exceptions: 3^{rd} period or heavier elements may have 10 or 12 electrons around them (expanded valence shells). Atoms such as Be, B and Al may have 6 electrons around them. In species with an odd number of electrons the least electronegative atom carries the odd electron.

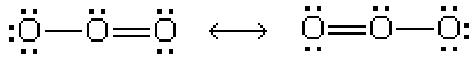
VSEPR Geometry

To determine the VSEPR geometry of a molecule (ion):
The central idea behind this method is that electron pairs in the valence shell try to get as far away from all other electron pairs in the valence shell (including non-bonding pairs)

1. Determine which element is the central atom.
2. Determine how many surrounding substituents that central atom has. **By substituents we mean not only atoms but also non-bonding pairs of electrons.**
3. Depending on the number of substituents (2, 3, 4, 5, or 6) we will have different 3D geometries so that the substituents are all as far apart as possible.

To draw resonance structures:

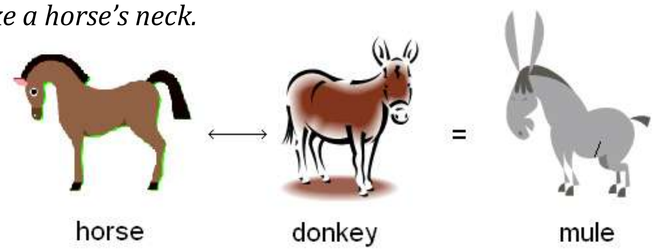
Resonance structures for a given molecule (ion) involve only changes in the electrons' positions (the nuclei stay fixed). Each of the resonance structures is considered to contribute to the "real structure" that can't be "drawn". The actual structure is called a resonance-hybrid and we represent it as follows, with a double-headed arrow between the two possible structures:



Resonance Structures

Most importantly, don't think that at a particular instant there is a single bond between the first two oxygens (and a double bond between the last two) and that in the next instant that bond becomes a double bond, with continual "flipping" back and forth. Both bonds in O_3 are identical, and the bonds are neither single nor double bonds. Each bond has properties intermediate between a single and double bond.

A good analogy for resonance: How do we describe a mule, the cross between a female horse and a male donkey? Do we say that the mule is 50% of the time a donkey and 50% of the time a horse? NOO! We can describe the mule with some of the characteristics of each parent. The mule has a thick short head and long ears like a donkey but its neck is shaped like a horse's neck.



To choose among the different resonance structures we can calculate the formal charge (FC) on the different atoms as follows:

Formal Charges

FC = (# of ve in an atom) – (# of lone pair e^-) – (½ # of bonding e^-)

Note: The formal charge is the charge a bonded atom would have if its bonding electrons were shared equally. It is a computed value and completely ignores the effect of electronegativity.

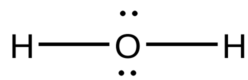
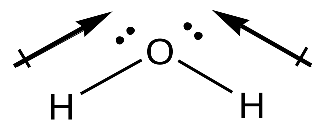
A simple mnemonic rule to remember how to calculate formal charge is the following one:

FC = # of ve in an atom – # of sticks – # of stones

The most important resonance structures have complete octets and low or no formal charges. When charges are unavoidable, then the more important resonance structures have like charges separated, unlike charges close and negative charges on the more electronegative atoms (positive charges on more electropositive atoms)

Experimental Procedure

For polar bonds, draw in the dipoles. See the example below.

	Lewis structure	3D structure (based on model)
Example: **Species = H_2O** valence electrons = 8 electron geometry = tetrahedral molecular geometry = bent polar bonds? O—H polar/nonpolar species? polar	**Example:** 	**Example:** 
Species = HF valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		
Species = N_2 valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		
Species = H_3O^+ valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		
Species = NH_3 valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		

	Lewis structure	3D structure (based on model)
Species = P_4 **(Hint: Every P is bonded to three others)** # of valence electrons = electron geometry of each P= molecular geometry of each P= polar bonds? polar/nonpolar species?		
Species = CH_3OH # of valence electrons = On your Lewis structure, note the electron and molecular geometry at each central atom. polar bonds? polar/nonpolar species?		
Species = H_2O_2 # of valence electrons = On your Lewis structure, note the electron and molecular geometry at each central atom. polar bonds? polar/nonpolar species?		
Species = NCl_3 # of valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		

	Lewis structure	3D structure (based on model)
Species = PCl_5 # of valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		
Species = BCl_3 # of valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		
Species = SF_4 # of valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		

	Lewis structure	3D structure (based on model)
Species = ICl_5 # of valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		
Species = SF_6 # of valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		
Species = ClF_3 # of valence electrons = electron geometry = molecular geometry = polar bonds? polar/nonpolar species?		

Species= SO_2 # of valence electrons= electron geometry= molecular geometry= polar bonds? polar/nonpolar species?	**Best** Lewis structure (Don't forget to assign formal charges!)
Other resonance structures (Don't forget to assign formal charges!)	
Species= CO_2 # of valence electrons= electron geometry= molecular geometry= polar bonds? polar/nonpolar species?	**Best** Lewis structure (Don't forget to assign formal charges!)
Other resonance structures (Don't forget to assign formal charges!)	
Species= $(S\underline{C}N)^{-1}$ **(carbon is central atom)** # of valence electrons= electron geometry= molecular geometry= polar bonds? polar/nonpolar species?	**Best** Lewis structure (Don't forget to assign formal charges!)
Other resonance structures (Don't forget to assign formal charges!)	

Species= SO_4^{2-} # of valence electrons= electron geometry= molecular geometry= polar bonds? polar/nonpolar species?	Lewis structure (Don't forget to assign formal charges!)
Other resonance structures (Don't forget to assign formal charges!)	
Species = $(NO_3)^-$ # of valence electrons= electron geometry= molecular geometry= polar bonds? polar/nonpolar species?	Lewis structure (Don't forget to assign formal charges!)
Other resonance structures (Don't forget to assign formal charges!)	
Species= $H\underline{N}O_3$ **(Hint: More than one central atom!)** # of valence electrons= On your Lewis structure, note the electron and molecular geometry at each central atom. polar bonds = polar/nonpolar species?	Lewis structure (Don't forget to assign formal charges!)
Other resonance structures (Don't forget to assign formal charges!)	

Pre-lab Assignment—To be completed BEFORE lab!

1. Using your text or the internet: Who was the scientist that came up with the octet rule?

2. State the *octet rule* in your own words.

3. How do you restate that rule for the element He?

4. What are two exceptions to the octet rule?

5. Which pair of compounds below represents a pair of resonance structures? ___________

Explain your choice: ____

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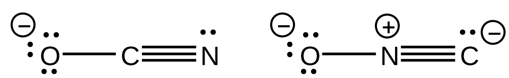
PAIR A



PAIR B

6. For the pair that you chose above, circle the best resonance structure. **Explain** your choice:

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7. Draw two resonance structures for each of the following polyatomic ions: CO_3^{2-}, SO_3^{2-}, CH_3COO^{-1}.

8. Calculate and display the formal charge for all atoms in every structure drawn above.

Verify how adding up the atomic formal charges within the ion results in its overall net charge.