Online Activity 3

Molecular Models

Introduction

The physical and chemical behavior of molecules and molecular compounds are determined by the intermolecular attractive forces that molecules can use to interact with other nearby molecules. The types of intermolecular attractive forces that are available to a molecule depend on the polarity of the molecule, which is determined by both the types of bonds present in the molecule and its overall shape, or geometry. Because geometry affects the overall polarity of a molecule, molecular geometry can provide important information about the physical and chemical behavior of both the individual molecule and the overall molecular compound. The geometry of a molecule is determined by the number of valence electrons present in the atoms that make up the molecule. **Valence electrons** are the electrons found in the outer shell of an atom; they are the only electrons that are involved in chemical reactions and that will form chemical bonds. A chemical bond is simply a force of attraction that holds the atoms together in a molecule. If you know the number of valence electrons in the atoms present in a molecule, you can determine how many and what type of bonds that molecule can have, its geometry, its polarity, and even whether it will be reactive or relatively non-reactive. Bonds will form to give an atom the most stable arrangement of valence electrons, which makes bond formation quite predictable. According to the **Octet Rule**, the most stable arrangement for most elements is 8 valence electrons around an atom. The Octet Rule provides a convenient basis for determining the geometries of most molecules. In this lab, you will study several different theories and methods of representing the geometry of molecules.

Lewis Structures

Lewis structures are pictures that show the covalent bonds in molecules. They are drawn using specific rules so that the atoms within the molecule are drawn with the correct connectivity and bond order. Lewis structures are useful for determining the structure of molecules and their polarity. The example below will take you through the rules for drawing a Lewis structure for the nitrate ion, NO_3^-.

Rules for Writing Lewis Structures

1. Count the number of valence electrons from all the atoms in the molecule. The number of valence electrons on an atom is equal to the group number of the atom, which is based on the column that the element is in on the Periodic Table.

3O: group 6	6 electron per O = 3x6 = 18 electrons
1N: group 5	5 electrons per N= 1x5 = 5 electrons

   Total valence electrons in the molecule: 18 + 5 = 23 valence electrons

2. If the molecule is an anion (negative ion), add the number of electrons that corresponds to its charge. If it is a cation (positive ion), subtract the electrons instead.

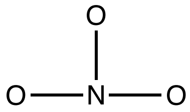
   Total valence electrons in the molecule: 23 + 1 = 24 valence electrons in anion

3. Select the least electronegative atom as your central atom. Hydrogen is the most notable exception. Since hydrogen atoms can only bond to one other atom (they only have one electron to share), they will always be located on the outside of the molecule. Outside atoms are referred to as **terminal** atoms. Arrange the terminal atoms around the central atom by keeping the atoms as far apart as possible.

O
O N O

There are a few exceptions that may arise when designating the location of the atoms. First, if you only have 2 atoms, your model will already be linear, so just draw 1 bond between the two atoms (note that depending on the total number of valance electrons, the bond might be a double or triple bond rather than a single bond). The second condition arises if you suspect you have 2 central atoms, as in the case of N_2H_4. In cases with more than one possible central atom, designate one of them the central atom and then do the Lewis structure based on that atom. You will then need to determine two separate geometries, one for each central atom.

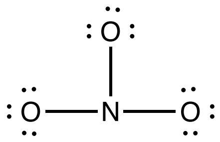
4. Use a dash (-) to designate a pair of electrons between each pair of bonded atoms. These electrons are called bonding pairs. There are 2 electrons in each bond.



5. Subtract the number of electrons used in bonding from the total number you need to place in the molecule.

24 valence electrons – 6 bonding electrons (3 bonds) = 18 electrons left

6. Place the remaining electrons in pairs around the terminal (outside) atoms until each atom contains an octet, (8 electrons), or in hydrogen, a duet (2 electrons). Do not split up the pairs.

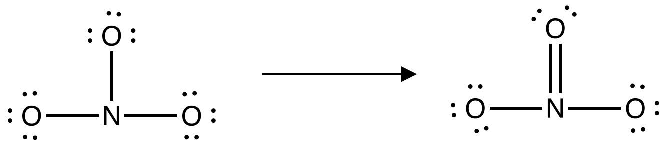


3 oxygen atoms X 6 electrons each = 18 electrons used around terminal atoms

7. If there are any electrons left over, place them around the central atom. All non-bonding electron pairs in the molecule are called **lone pairs**. Lone pairs have a high amount of negative charge and often provide a starting point for chemical reactions.

18 electrons left from step 5 – 18 electrons used around terminal atoms = 0 leftover

8. Count the number of electrons around the central atom. If you do not have enough lone pair electrons to create an octet around the central atom, use some of the lone pairs that you placed on outside atoms to create a double or triple bond with the central atom. The type of bond used will depend on the number of electrons needed by the central atom. Two double bonds to the central atom is also possible for some molecules. Each bond counts as 2 electrons for **BOTH** atoms.



On N: 3 bonding pairs of electrons + 0 lone pairs = 6 electrons
The N needs 2 more electrons from an oxygen atom to form a double bond. It doesn't matter which oxygen you use. This is just one example that can be drawn.

9. Count all the electrons in the molecule to make sure you have accounted for all of the valence electrons. Count all the electrons around each atom to make sure each as an octet (H: duet). Occasionally the central atom will have more than 8 electrons. This is called an "expanded" octet, but is not seen in the majority of molecules. There are also a limited number of cases where the central atom (B or Be) will have less than 8 valence electrons.

24 valence electrons at start = 4 bonds + 8 lone pairs = 24 electrons
N: 4 bonds+ 0 lone pairs = octet
N–O: 1 bond + 3 lone pairs = octet
N=O: 2 bonds + 2 lone pairs = octet

Note: You could have placed a double bond on any one of the 3 oxygen atoms around the nitrogen atom. Because you could create 3 different structures, the actual molecule would be based on each of the 3 N–O bonds being identical with a bond strength of about 1 and 1/3 bonds. Because all of the bonds are identical, the molecule will be symmetrical and thus nonpolar. (See molecular polarity at the end of the introduction.)

VSEPR Model of Molecular Geometry

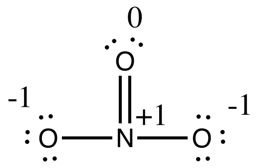
The **Valence-Shell Electron-Pair Repulsion (VSEPR)** model is a method of describing the geometry around a central atom in a molecule. VSEPR is based on the idea that pairs of valence electrons in bonded atoms repel one another and will attempt to get as far apart as possible. Thus, if placed at the maximum distance from each other around the nucleus, the atoms and lone pairs will conform to a particular molecular structure. Lone pairs of electrons will affect the shape of the molecule, and are included in the "**electron pair geometry**", but they are not included in the "**molecular geometry**", which only describes the locations of the bonded atoms with respect to each other. Like the method for drawing Lewis structures, VSEPR uses a series of rules that ultimately lead you to a specific geometry, which directly corresponds to a molecular shape.

Identifying VSEPR Geometries

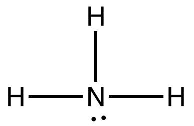
1. Draw out the Lewis Structure of the molecule, including all lone pairs.
2. Use the Lewis structure to count the number of lone pairs and the number of terminal atoms bonded to the central atom. The total number of regions of electron density (lone pairs + atoms) will tell you the electron pair geometry.
3. Once you have the electron pair geometry, identifying how many of the regions of electron density are lone pairs vs. bonded atoms will tell you the molecular geometry. If all of the regions of electron density are from atoms (i.e. no lone pairs on the central atom), then the molecular geometry and the electron pair geometry are the same.

Example1: Nitrate ion, NO_3^- Lewis Structure:

There are three regions of electron density around the nitrogen atom, corresponding to the three oxygen atoms. Three total regions of electron density = an electron pair geometry of trigonal planar. Since all of the regions of electron density are atoms (no lone pairs on the central atom), the molecular geometry is also trigonal planar.

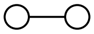
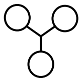
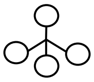


Example 2: Ammonia, NH_3 Lewis Structure

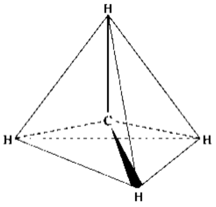


There are four regions of electron density around the nitrogen atom, corresponding to the three hydrogen atoms and the one lone pair. Four total regions of electron density = an electron pair geometry of tetrahedral. Since one of the regions of electron density is a lone pair, the molecular geometry is trigonal pyramidal (see charts p147 & 148).

Note: Double or triple bonds do not matter in counting bonded atoms. All covalent bonds count once, regardless of bond type. Also, electrons are counted IN PAIRS, not singly when determining the regions of electron density. You also do not count any electron pairs on terminal atoms, only those that are directly on the central atom.

Electron pairs	Electron Geometry	Molecular Shape	Bond Angles
2	Linear		180°
3	Trigonal Planar		120°
4	Tetrahedron		109.5°

Bond Angles



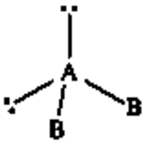
VSEPR notation: AX_4

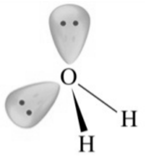
The approximate bond angles in a structure can be determined directly from the molecular geometry. If you assume that all of the attachments to the central nucleus are spaced a maximum distance apart in three-dimensional space, then the bond angles can be determined based on relative locations of the atoms and lone pairs present in the structure. For example: CH_4 has 4 atoms spread out in three-dimensional space. The maximum distance for these atoms to be apart will be 109.5°. Since lone pairs have greater repulsion than bonding electrons, the bond angles may be slightly different in molecules that have lone pairs around the central atom.

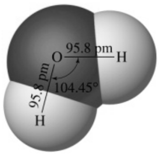
Molecular Geometry vs. Electron Pair Geometry

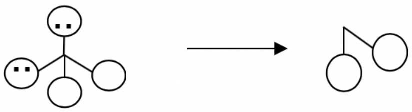
If there are no lone pairs associated with the central atom, then the molecular geometry will be identical to the electron pair geometry. However, many molecules do have one or more lone pairs of electrons located on the central atom that will also need space, because the repulsion between electrons is still present. While the effect of the lone pair(s) is felt by the central atom, since the electrons cannot be seen, the shape of the molecule will be different from that determined from the electron pair geometry.

For example, the water molecule, H_2O, has a tetrahedral electron pair geometry. However, since only atoms are visible in a molecule, the molecular geometry just consists of the portion of the molecule that is visible. Thus, instead of a tetrahedron, the H_2O molecule is considered to have a bent structure. One way to determine the molecular geometry in a molecule is to draw the Lewis structure in pencil and then erase any electron pairs on the central atom. The remaining figure would represent the shape of the molecule. You can also draw the Lewis Structure, count the number of lone pairs and atoms bonded to the central atom, and then use a table similar to the one on page 148 to determine the molecular geometry based on the total number of regions of electron density around the central atom and how many of those regions are atoms vs. lone pairs.









See Table 1 for some molecular geometries that can be formed for molecules with lone pairs on the central atom.

Table 1: Summary of VSEPR data for molecules with lone pairs on the central atom.

Regions of electron density (lone pairs + atoms)	Bonding pairs (atoms)	Lone Pairs	Electron Pair Geometry	Molecular Geometry	Example
3	2	1	Trigonal Planar	Bent	SO_2
4	3	1	Tetrahedral	Trigonal Pyramidal	NH_3
4	2	2	Tetrahedral	Bent	H_2O

Hybridization

The VSEPR theory tells us that electron pairs, regardless of where the electrons originally came from, repel each other. All electrons are treated equally and no distinction is made as to their original atomic source. A second theory, the **Molecular Orbital (MO) theory** addresses the differences between s and p electrons when forming a bond and better predicts the bond energy that will be associated with a particular bond. MO theory states that a bond will form if the valence electrons in both atoms combine in such a way that the electrons in the bond are lower in energy, and thus more stable than valence electrons in the original atoms. The molecular orbital associated with the bond must have 1 electron from the central atom and the second electron from the terminal atom to make a bond. So, for example, when looking at the hydrogen molecule, the 1s electrons from each hydrogen atom form a stable bond by filling the molecular orbital with 2 electrons rather than having 2 half-filled atomic orbitals.

Separate atoms H: ↑ ↑:H Molecular Hydrogen H_2: ↑↓

The filled molecular orbital will be more stable than 2 half-full atomic orbitals

While this works well for hydrogen, other atoms such as carbon are more complex. A carbon atom has 4 valence electrons and forms 4 identical bonds with 4 different hydrogen atoms to form the methane molecule, CH_4. However, the energies associated with the 4 valence electrons in carbon are not equal. Carbon has the electronic configuration of $1s^2 2s^2 2p^2$ with the 2s valence electrons already paired and not available for bonding, leaving only the 2p electrons with openings in their shells to form bonds. However, we know that methane has 4 identical C-H bonds, so there must be 4 open spaces available in the carbon atom to allow for bonding. If we add energy to the carbon atom to bounce one of the 2s electrons into the empty $2p_z$ orbital we now have 4 openings ready to accept an electron from each of the 4 hydrogen atoms.

C: ↑↓ ↑↓ ↑ ↑ ___
1s 2s $2p_x$ $2p_y$ $2p_z$

C: ↑↓ ↑ ↑ ↑ ↑
1s 2s $2p_x$ $2p_y$ $2p_z$

This does give us the space to put in the 4 electrons from the hydrogen atoms to make 4 molecular orbitals, but the s and p orbitals are significantly different in energy, which would not result in 4 **identical** bonds. We need a way to make 4 **identical** molecular orbitals. The presence of 4 identical orbitals is explained by creating hybrid orbitals that are a mixture of the atomic orbitals on the central atom. This process is called hybridization and can be thought of as averaging the energies of the 4 atomic orbitals together, so that instead of 1 low energy molecular orbital and 3 higher energy molecular orbitals, we now have something in the middle. The name associated with the new "hybridized" orbitals comes directly from the type of atomic orbitals used to form the bonds. For the carbon atom which used one s and three p atomic orbitals to bond, we call the 4 new hybridized orbitals sp^3 orbitals. All molecular structures which require 4 regions of electron density (bonds or lone pairs) around the central atom will have sp^3 hybridized orbitals. If you need only 3 spaces around the central atom, you only need 3 atomic orbitals, one s and two p orbitals (sp^2), and finally if you only need 2 regions of electron density, your molecule will be considered to be sp hybridized. Extra electrons found in the p shells stay there and may be involved with double or triple bonding of the atoms, but will not be considered to be part of the hybridization. For example, in acetylene, H–C≡C–H, the extra 2 central bonds are formed using the $2p_y$ and $2p_z$ electrons, but those electrons are not be in hybridized orbitals.

C: ↑↓ ↑ ↑ ↑ ↑ (used in second and third bond in H–C≡C–H)
1s 2s $2p_x$ $2p_y$ $2p_z$

Only the bonds associated with the shape of the molecule as obtained from the VSEPR are considered hybridized, so both carbon atoms in acetylene would have a linear structure (2 bonded atoms, no lone pairs) and thus would be sp hybridized. One way to determine the hybridization is to draw out the Lewis Structure. The number of regions of electron density around the central atom will be the same as the number of atomic orbitals needed in the hybridization.

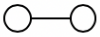
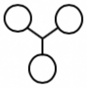
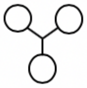
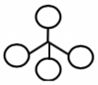
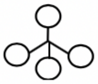
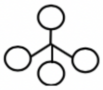
2 regions of electron density = sp
3 regions of electron density = sp^2
4 regions of electron density = sp^3, etc.

Note that hybridized orbitals can be occupied by lone pairs of electrons, not just bonding electrons. For elements in the first row of the periodic table, there are only three hybridization options, which are shown in Table 2.

Table 2: Relationship between electron pairs and hybridization

Electron pairs	**Electron Geometry**	**Hybridization**	**Example**
2	Linear	sp	C_2H_2
3	Trigonal planar	sp^2	SO_2
4	Tetrahedral	sp^3	H_2O, CH_4, NH_3

Table 3: Molecular Geometry Summary

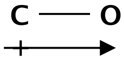
Electron Pairs	Bonding Pairs	Lone Pairs	Molecular Shape	Bond Angles	Electron Geometry	Molecular Geometry	Hybridization	Example
2	2	0		180°	Linear	Linear	sp	CO_2
3	3	0		120°	Trigonal Planar	Trigonal Planar	sp^2	CH_2O
3	2	1		120°	Trigonal Planar	Bent	sp^2	NOCl
4	4	0		109.5°	Tetrahedral	Tetrahedral	sp^3	CH_4
4	3	1		109.5°	Tetrahedral	Trigonal Pyramidal	sp^3	NH_3
4	2	2		109.5°	Tetrahedral	Bent	sp^3	H_2O

Polarity

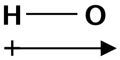
Bond polarity arises when atoms with differing electronegativity values bond. **Molecular polarity** occurs when **bond dipoles** do not cancel out in the molecule. The measurement of the degree of bond polarity is called the dipole moment and it is a function of the magnitude of the charge difference and the distance between the positive and negative "poles" of the molecule. Lone-pair electrons contribute to dipole moments by increasing the negative charge in an area and causing bending of a molecule, thus, polarity must be determined from both bond polarity & molecular shape. Use the following method to determine if a molecule is polar or nonpolar.

1. Use electronegativity values to predict bond dipoles. Use an arrow with a + on one end to designate the direction of higher electronegativity. The arrow should point towards the more electronegative atom. (That's why the +sign is on the other end!)

CO_2

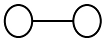


H_2O

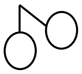


2. Determine the molecular geometry.

CO_2
Linear

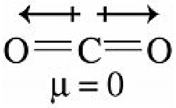


H_2O
Bent

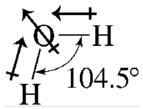


3. Determine if bond dipoles cancel (equal & opposite) or combine

Cancel:
Nonpolar



Combine:
Polar

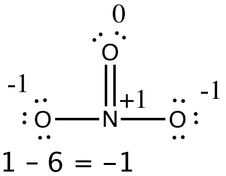


Formal Charge

Formal charge is a means of determining the relative stability of each atom in a molecule. It is a comparison of the number of valence electrons (group number) in each atom to the number of bonds and lone pair electrons present on each atom in the molecule. If the number of valence electrons equals the number of bonds and lone pair electrons (counted as individuals, not as a pair), the formal charge is zero for that atom and the atom is in a stable state. If some formal charge is present, the most negative charge should be on the most electronegative atoms. If it is not, then there is probably an error in the Lewis structure. Traditionally the formal charge is written near the upper corner of each atom in the Lewis structure.

The formal charge is easily calculated using the following equation.
FC= (# valence electrons – # bonds – # lone electrons)

Example 3: Formal charges on each atom in one resonance structure of the nitrate ion, NO_3^-



Nitrogen (N) is in column 15 (5A) and has 5 valence electrons. In nitrate:
Nitrogen has 4 bonds and no lone pairs. Formal charge = 5 – 4 – 0 = +1

Oxygen (O) is in column 16 (6A) and has 6 valence electrons. In nitrate:
2 oxygens have 1 bond and 6 lone pair electrons. Formal charge on each = 6 – 1 – 6 = –1
1 oxygen has 2 bonds and 4 lone pair electrons. Formal charge = 6 – 2 – 4 = 0.

Overall formal charge for the molecule = +1 –1 –1 = –1

For a polyatomic ion, the overall formal charge on the molecule must equal the charge on the ion. For neutral molecules, the overall formal charge on the molecule must equal 0.

In this simulation

During this activity, you will use another one of the phet simulations, called "molecule shapes" (https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html) to build each of the 10 structures given. Some of the molecules may be pre-built under the real molecules section of the simulation, but others you will need to build yourself under the model section. Once you have built the model of a molecule, you will draw the Lewis structure with all the bonds and electrons present and then determine the electron pair and molecular geometries for the compound. Once you have determined the geometries, you will then sketch both the molecular geometry, which will be exactly like the model, and also the electron geometry, which will be similar, but will also show where lone pairs are located on the central atom. Include the name of the geometry below your sketch. Draw arrows along the bonds in your sketch in the molecular geometry box to demonstrate the polarity of each bond Finally, if the molecule is polar, draw an arrow to the right of the molecule showing the direction of the overall polarity. If it is nonpolar, just make the notation, NP. There is a polarity simulation that may help you with the polarity portion of this activity if you would like to use it.

You will also be required to draw resonance structures for one of the compounds.

Once you have created your drawings you will fill out the data sheets for the second portion of the lab, in which you will show the hybridization and formal charges on each compound. You must include a formal charge for each atom, even if the formal charge is zero.

When you open the simulation it will show a molecule with a central atom and two single bonds. Click on the bonds under "Bonding" to add additional bonds. Click on the red square with the x to remove types of bonds. Once you add a double or triple bond, you can remove the single bonds if needed. Click on the lone pair in the "Lone Pair" box to add lone pairs. If you have added a lone pair, it will give you the red square with the x to remove it if needed. Click in the box next to "Show Bond Angles" to have the program show you the bond angles. Remember that molecular geometries do not show lone pairs, electron pair geometries do show lone pairs.

Online Activity 3: Data Sheets for Lewis Structures and Geometries

Refer to the “In this simulation” section for instructions
Submit as part of your online activity report

Name: ____ Date: ________ Section: ________

Perform the following for all 10 structures.

Use the instructions in the introduction to fill in the information in the following table.

Include the following information on the Lewis structures when needed:

1. Show all double or triple bonds that may be present.
2. Show all lone pair electrons on all atoms.
3. Use arrows on the Lewis structure to demonstrate polarity.
4. Indicate bond angles on structures.

Formula	Lewis Structure	Electron Group Geometry	Molecular Geometry
CO_2		Sketch: Name:	Sketch:
CO_3^{2-}		Sketch: Name:	Sketch: Name:
H_2O		Sketch: Name:	Sketch: Name:
H_3O^+		Sketch: Name:	Sketch: Name:
HCN		Sketch: Name:	Sketch: Name:

Formula	Lewis Structure	Electron Group Geometry	Molecular Geometry
NH_3		Sketch: Name:	Sketch: Name:
NO_3^- 3 resonance structures		Sketch: Name:	Sketch: Name:
N_2H_4 (2 central atoms)		Sketch: Name:	Sketch: Name:
C_2H_4 (2 central atoms)		Sketch: Name:	Sketch: Name:
CH_3OH 2 central atoms		Sketch: Name:	Sketch: Name:

Online Activity 3: Data Sheets for Hybridization and Formal Charges

Refer to the "In this simulation" section for instructions

Submit as part of your online activity report

Use the instructions in the introduction to fill in the information in the following table.

Include the following information when needed:

1. If more than one central atom, show hybridization for all central atoms.
2. Include formal charges for each atom in structure.

Formula	Number of Regions of Electron Density	Hybridization	Formal Charges
CO_2			
CO_3^{2-}			
H_2O			
H_3O^+			
HCN			
NH_3			
NO_3^-			
N_2H_4			
C_2H_4			
CH_3OH			

Online Activity 3: Grading Rubric

Points

All molecular data are present and correct from Table 1	3pts each molecule
All molecular data are present and correct from Table 2	3pts each molecule

Molecule	Total Points
CO_2	
CO_3^{2-}	
H_2O	
H_3O^+	
HCN	
NH_3	
NO_3^-	
N_2H_4	
C_2H_4	
CH_3OH	

Grade for models ________pts

Online Activity 3 Questions

Submit as part of your online activity report (4 points each)

Name: ______________________________ Date: ________ Section: ________ Grade: ________

1. How many valence electrons are in an atom of phosphorus?

____

2. If an ion has a −2 charge, how many extra electrons do you add to the Lewis structure?

____

3. Identify the terminal atoms in a water molecule.

____

4. How do you designate a double bond in a Lewis structure?

____

5. How many regions of electron density (atoms and lone pairs) are connected to the central atom in a molecule that is sp^2 hybridized?

____

6. Draw an arrow to represent the direction of polarity in the hydroxide ion below.

$(O-----H)^-$

7. How many electrons do you want around each atom in a Lewis structure? Include all the electrons contained in both lone pairs and bonds.

____

8. What is the formal charge of the N atom in NH_3? Show your work

____

9. Give the hybridization of the central atom in CO_2.

____

10. Show both resonance structures for HCO_2^-. All atoms are on the central carbon.

________________ ________________