

Experiment 11 Molecular Modeling

version 5

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Now that we understand atomic structure, bonding, and a little about reactions, finally we come to molecular structure. Two models of aspirin are shown below: a perspective structural formula and a ball-and-stick representation (Figure 1). Models are useful for representing the three-dimensional shape and geometry of molecules, which will be important for predicting stability and reactivity in future chemistry endeavors.

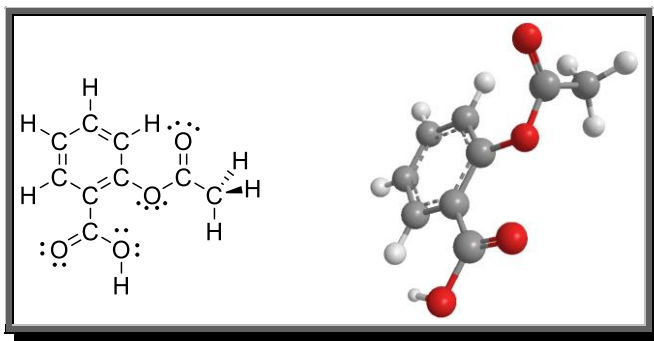


Figure 1. Molecular Model Representations of Aspirin, $C_9H_8O_4$. In the ball-and-stick model (on the right), grey indicates carbon, white indicates hydrogen, and red indicates oxygen.

Objectives

- Draw possible Lewis structures, calculate formal charges, and predict the most likely structure for a given molecular formula.
- Recognize and draw resonance structures.
- Apply the VSEPR model to predict molecular geometry.
- Relate molecular symmetry to its dipole moment and predict polarity of a molecule based on geometry and overall dipole moment.

Learning Outcomes

- Understand the nature and characteristics of a chemical bond.
- Understand the nature of molecular geometry as it relates to physical and chemical properties of molecules.

Definitions

- **Bond angle** – the angle formed by three atoms joined by bonds.
- **Electron group** – a negative region of space occupied by a group of electrons; the group can be a lone pair, single bond, double bond, or triple bond.
- **Electronegativity** – the ability of an atom to attract electrons in a bond.

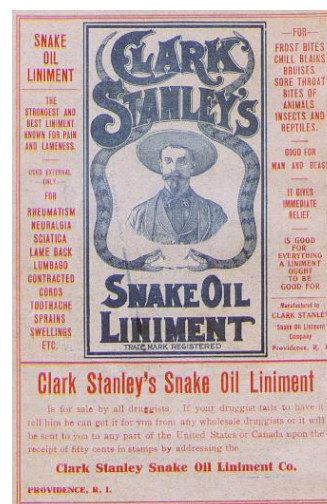
- **Electron-group geometry** – the arrangement of *electrons* around a central atom in a molecule or ion.
- **Formal charge** – the charge that an atom would have if all atoms in the molecule had the same electronegativity. While the formal charge is only a bookkeeping method for tracking valence electrons on an atom, it creates a representation of electron sharing in a molecule. The best Lewis structure will have small or zero formal charges.
- **Ionic bond** – an electrostatic attraction between ions of opposite charge. Often, ions are formed from transfer of electrons from metals to non-metals.
- **Lewis structures** – illustrate valence electrons surrounding an atom and how bonding occurs between atoms in a molecule.
- **Lone pairs (or nonbonding pairs)** – electrons around an atom that are not shared.
- **Molecular geometry** – the arrangement of *atoms* around a central atom in a molecule or ion.
- **Nonpolar bond** – a covalent bond between two atoms of similar electronegativity so that bonding electrons are shared relatively evenly.
- **Octet rule** – states that an atom will give up, accept, or share valence electrons to achieve a full valence shell.
- **Polar bond** – a covalent bond between two atoms with a large electronegativity difference so that electrons are held more tightly by one atom of the bond. This electronegativity difference creates a dipole, a partial negative charge area and a partial positive charge area on the molecule.
- **Resonance structures** – valid Lewis structures that differ in the placement of electrons for a molecule.
- **Valence electrons** – those in the outermost shell of an atom for main group elements, and those in the outermost shell plus the outermost *d* orbital electrons for transition metals.

Techniques

- Computer software modeling
- Ball-and-stick modeling

Introduction

John Ellis Water Machines (<http://johnellis.com/>) makes many promises to improve your health: using their water filtration system will ‘increase the bond angle in water from 104° to 114°, which will increase blood flow, grow back hair on bald heads, and prevent Ebola’.¹ Much like Clark Stanley’s Snake Oil Liniment, when claims sound too good to be true, they probably are! There are many websites, social media connections, and even brick-and-mortar stores that will take your money in exchange for unproven claims to improve health. Snake oil peddlers have been around for centuries; how can you protect yourself and your money from them? Being well-educated is one way. General chemistry can teach us about bond angles and why they occur. By the end of this lab, you should be able to predict the real bond angle of water.



Advertisement for Snake Oil Liniment
Circa 1905. By Clark Stanley
[Public domain], via
Wikimedia Commons.

Molecules are held together by covalent bonds created by sharing electrons between two atoms. First, we start building molecules by identifying the electrons. Only electrons in valence orbitals can be shared to form bonds. We can determine valence electrons from the periodic table. Main group elements have valence electrons in the outermost shell while transition metals include the outermost shell electrons plus the outermost *d* electrons. Recall that elements in a group will have the same number of valence electrons, leading to similar chemical properties (Figure 2).

Electron Configuration Table


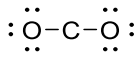
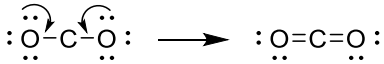
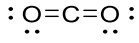
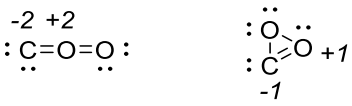
Period	Group	Electron Configuration Table																		
		1																	18	
		H																	He	
		1s																	1s	
		2	1	2											13	14	15	16	17	18
		Li	Be											B	C	N	O	F	Ne	
		2s	2s											← 2p →						
3	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
Na	Mg	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
3s	3s	← 3d →										← 3p →								
4	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr			
4s	4s	← 3d →										← 4p →								
5	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
Rb	Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe			
5s	5s	← 4d →										← 5p →								
6	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
Cs	Ba	La	Hf	Ta	W	Re	Os	Ir	Pt	Au	Hg	Tl	Pb	Bi	Po	At	Rn			
6s	6s	← 5d →										← 6p →								
7	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18		
Fr	Ra	Ac	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Cn	Uut	Fll	Uup	Lv	Uus	Uuo			
7s	7s	← 6d →																		
		* Ce 1 Pr 2 Nd 3 Pm 4 Sm 5 Eu 6 Gd 7 Tb 8 Dy 9 Ho 10 Er 11 Tm 12 Yb 13 Lu 14																		
		← 4f →																		
		** Th 1 Pa 2 U 3 Np 4 Pu 5 Am 6 Cm 7 Bk 8 Cf 9 Es 10 Fm 11 Md 12 No 13 Lr 14																		
		← 5f →																		

Name →	H	1	← Electrons
	1s		← Subshell

Figure 2. Periodic Table with Valence Electrons Indicated.² Image used under a [Creative Commons Attribution License \(by 4.0\)](#) from OpenStax, Chemistry.

Next, remember the driving force for sharing is achieving a full valence shell for atoms. For main group elements, the full shell contains eight electrons. In Lewis Theory, the octet rule states that an atom will give up, accept, or share electrons to have the filled outer shell. Note hydrogen and helium have a full shell with two electrons since they have a 1s orbital only. To show how the octet rule predicts molecules, Lewis structures illustrate all valence electrons surrounding an atom and how bonding occurs between atoms. Bonds are shown with a line that represents two electrons. Following are a set of steps that will help to get started drawing Lewis structures.

Example: Draw the Lewis structure for carbon dioxide.

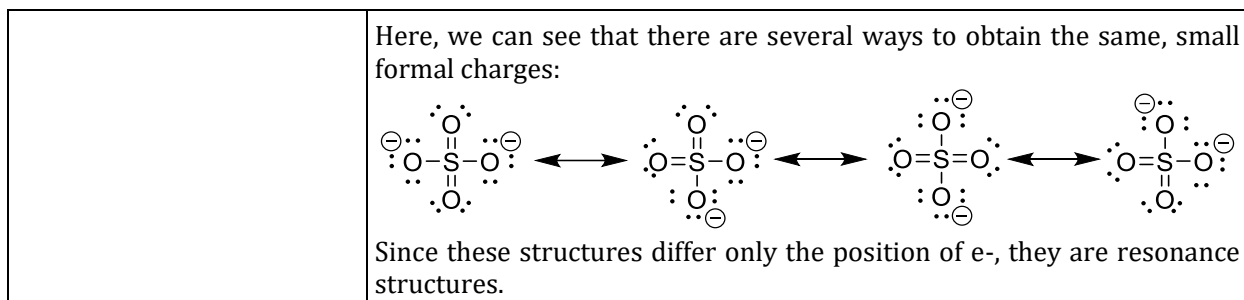
<p>1. Determine the total number of valence electrons in the whole molecule. For formulas with a negative charge, the charge should be added to the number of e- while for formulas with a positive charge, the charge should be subtracted from the number of e-.</p>	<p>Carbon dioxide has the formula CO₂. From the periodic table, C has 4 valence e-, O has 6 valence e-. Sum the e- to obtain the total in the molecule: $1 \times 4e^- + 2 \times 6e^- = 16e^-$</p>
<p>2. Write a plausible Lewis structure by drawing each atomic symbol, and connecting them with line bonds. Often molecules take a symmetrical shape with the less electronegative atom at the central position. Hydrogens will never be central since they only form one bond.</p>	<p>There are a few possible structures for CO₂: O-C-O C-O-O</p> <p style="text-align: center;">  </p> <p>Let's choose the first since it places the carbon (least electronegative atom) in the center.</p>
<p>3. Count the electrons in the line bonds and determine the remaining electrons to place in the structure.</p> <ol style="list-style-type: none"> Place pairs of electrons as lone pairs around the terminal atoms to give each terminal atom an octet (except hydrogen that only needs two since it has a complete octet with one bond). Assign any remaining electrons as lone pairs around the central atom. If necessary, move one or more lone pairs of electrons from a terminal atom to form a multiple bond to the central atom. <ul style="list-style-type: none"> One shared pair forms a single bond. Two shared pairs form a double bond. Three shared pairs form a triple bond. 	<p>Each line bond represents two shared e- for 4 e- placed in total: O-C-O</p> <p>Twelve e- remain. Begin to place them on the terminal atoms. Remember that e- are most stable paired:</p> <p style="text-align: center;">  </p> <p>All 16 e- are placed, so we do not add more. Checking for octet, the oxygens have 8 e- each, but the carbon only has four. Share terminal e- by forming two double bonds:</p> <p style="text-align: center;">  </p>
<p>4. Finally, to verify the correct Lewis structure, use a formal charge calculation on each atom. <i>Formal charge =</i> <i>(valence e-) - (lone pair e-) - 1/2(bonding e-)</i></p> <ol style="list-style-type: none"> Usually, the most plausible Lewis structure is one with no formal charges or very small formal charges. Negative formal charges are most stable on the most electronegative atom. Adjacent atoms should never carry formal charges with the same sign. Charges other than 0 should be indicated on the atom since they help to indicate the distribution of electrons on a molecule. The sum of formal charges should total the charge on a formula. 	<p>Now that all atoms have eight e-, double-check that this is the <i>best</i> Lewis structure by using formal charge: $O = (6 \text{ val } e^-) - (4 \text{ lp } e^-) - \frac{1}{2}(2 \text{ bonding } e^-) = 0$ $C = (4 \text{ val } e^-) - (0 \text{ lp } e^-) - \frac{1}{2}(4 \text{ bonding } e^-) = 0$</p> <p style="text-align: center;">  </p> <p>Both oxygens have 0 formal charge since they have the same bonding pattern. We can double-check the other possible skeletal structures too:</p> <p style="text-align: center;">  </p> <p>Since first Lewis structure has 0 formal charges, it is considered the most plausible structure over either of the others above.</p>

There are a few exceptions to the octet rule when drawing Lewis structures. A few atoms tend to have incomplete octets, namely boron, beryllium, and aluminum, since they have few valence electrons. Atoms below period 2 may have expanded octets with 10 or 12 electrons since they have *d* orbitals to use in bonding. In either of these exceptions, following the steps for drawing the Lewis structure and verifying it with formal charge calculations will lead to the most correct Lewis structure.

Occasionally, molecules have more than one reasonable Lewis structure. If these structures have the same connectivity of atoms, but differ in the placement of electrons, they are called resonance structures. The sulfate anion is a good example of both an expanded octet and resonance structures.

Example: Draw the Lewis structure for the sulfate ion.

<p>1. Determine the total number of valence electrons in the whole molecule.</p>	<p>Sulfate ion has the formula SO_4^{2-}. From the periodic table, S has 6 valence e-, O has 6 valence e-, add 2 e- for 2- charge. Sum the e- to obtain the total in the molecule: $1 \times 6e^- + 4 \times 6e^- + 2e^- = 32e^-$</p>
<p>2. Write a plausible Lewis structure by drawing each atomic symbol, and connecting them with line bonds.</p>	<p>Placing the sulfur (least electronegative atom) in the center and radiating the oxygens symmetrically leads to one possible structure for H_2SO_4:</p> $\begin{array}{c} \text{O} \\ \\ \text{O}-\text{S}-\text{O} \\ \\ \text{O} \end{array}$
<p>3. Count the electrons in the line bonds and determine the remaining electrons to place in the structure.</p>	<p>Each line bond represents two shared e- for 8 e- placed in total. Twenty-four e- remain. Begin to place them on the terminal atoms:</p> $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ \text{:}\ddot{\text{O}}-\text{S}-\ddot{\text{O}}\text{:} \\ \text{:}\ddot{\text{O}}\text{:} \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$ <p>All 32 e- are placed, so we do not add more. Checking for octet, all atoms have 8 e- each.</p>
<p>4. Finally, to verify the correct Lewis structure, use a formal charge calculation on each atom.</p>	<p>Now that all atoms have eight e-, double-check that this is the <i>best</i> Lewis structure by using formal charge:</p> $\begin{aligned} O &= (6 \text{ val } e^-) - (6 \text{ lp } e^-) - \frac{1}{2}(2 \text{ bonding } e^-) = -1 \\ S &= (6 \text{ val } e^-) - (0 \text{ lp } e^-) - \frac{1}{2}(8 \text{ bonding } e^-) = +2 \end{aligned}$ <p>While the total of all the formal charges does equal the charge on the ion, the formal charges are too many and too large. We can try to share more e- to see if that helps:</p> $\begin{array}{c} \text{:}\ddot{\text{O}}\text{:} \\ \ominus \text{:}\ddot{\text{O}}=\text{S}=\ddot{\text{O}}\text{:}\ominus \\ \text{:}\ddot{\text{O}}\text{:} \\ \text{:}\ddot{\text{O}}\text{:} \end{array}$ $\begin{aligned} O &= (6 \text{ val } e^-) - (4 \text{ lp } e^-) - \frac{1}{2}(4 \text{ bonding } e^-) = 0 \\ O &= (6 \text{ val } e^-) - (6 \text{ lp } e^-) - \frac{1}{2}(2 \text{ bonding } e^-) = -1 \\ S &= (6 \text{ val } e^-) - (0 \text{ lp } e^-) - \frac{1}{2}(12 \text{ bonding } e^-) = 0 \end{aligned}$ <p>Now, the sulfur has an expanded octet, but the formal charges are smaller throughout the structure. Note the charges indicated on the structure.</p>



Molecular models can help with obtaining the correct Lewis structure since the bond positions for each atom are indicated. Additionally, models are important for showing the correct geometry or shape of a molecule.

Geometry can be predicted by Valence-Shell Electron-Pair Repulsion (VSEPR) Theory, based upon the idea that valence electrons in bonded atoms repel one another while being attracted to each nucleus. The theory defines an electron group – a lone pair, a single bond, a double bond, a triple bond, or a single electron (radical) – that creates a negative region in an area of space. The preferred shape is the one that maximizes the separation between these electrons. The mutual repulsions among electron groups lead to electron-group geometry that is the shape of the molecule.

Continuing with the example of carbon dioxide, the double bonds each represent one electron group for a total of two negative regions of space around the central atom. To separate these two electron groups by the maximum distance, they are spaced on opposite sides of the carbon atom – with a bond angle of 180° called a linear geometry (Figure 3).

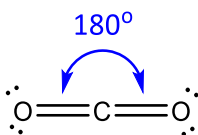


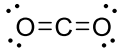
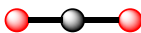
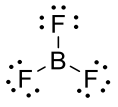
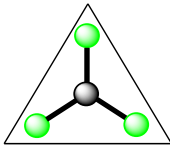
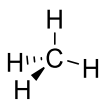
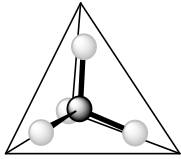
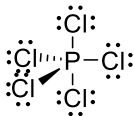
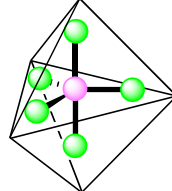
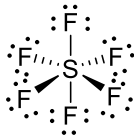
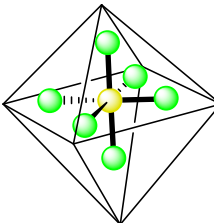
Figure 3. Electron-group Geometry of Carbon Dioxide.

There are five basic shapes that electron groups will adopt thanks to their mutual repulsions: linear, trigonal planar, tetrahedral, trigonal bipyramidal, and octahedral (Table 1). Remembering the polyhedral shapes from which they are named will be helpful in identifying the geometry. Note the use of wedges and dashes to create perspective. A wedge projects toward the viewer while a dash projects back into the page (Figure 4).³

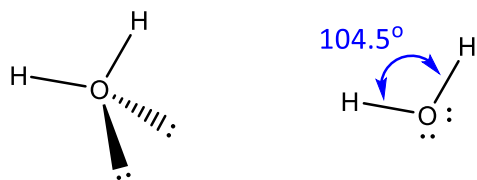


Figure 4. Wedge and dash perspective lines.

Table 1. Valence Shell Electron Pair Repulsion Geometries.

Formula	Bonding groups	Lone pairs	Electron-Group Geometry	Bond angles
CO ₂	2	0	linear  	180°
BF ₃	3	0	trigonal planar  	120°
CH ₄	4	0	tetrahedral  	109.5°
PCl ₅	5	0	trigonal bipyramidal  	120°/90°
SF ₆	6	0	octahedral  	90°/90°

You may be familiar with deviations from the five basic geometries of VSEPR Theory already. For example, water has a bond angle of 104.5° despite having four electron groups, two lone pairs and two single bonds, for which a tetrahedral geometry would be predicted (Figure 5). This decreased bond angle occurs because lone pairs have greater repulsion, being more dispersed, than bonding pairs that are localized between two nuclei.



Tetrahedral electron-geometry, with 109.5° bond angles, is predicted for water with four e- groups, however the actual molecular bond angle is smaller.

Figure 5. Electron-Group vs. Molecular Geometry of Water.

We can use modern simulation software to visualize actual geometries. [University of Colorado's PhET Interactive Simulation](#) demonstrates the bond angle differences between the model (theoretical) and real molecular geometry (Figure 6). While the electron-group geometry is still called tetrahedral, the molecular geometry is called bent since visualizing only the atoms leads to a bent line.

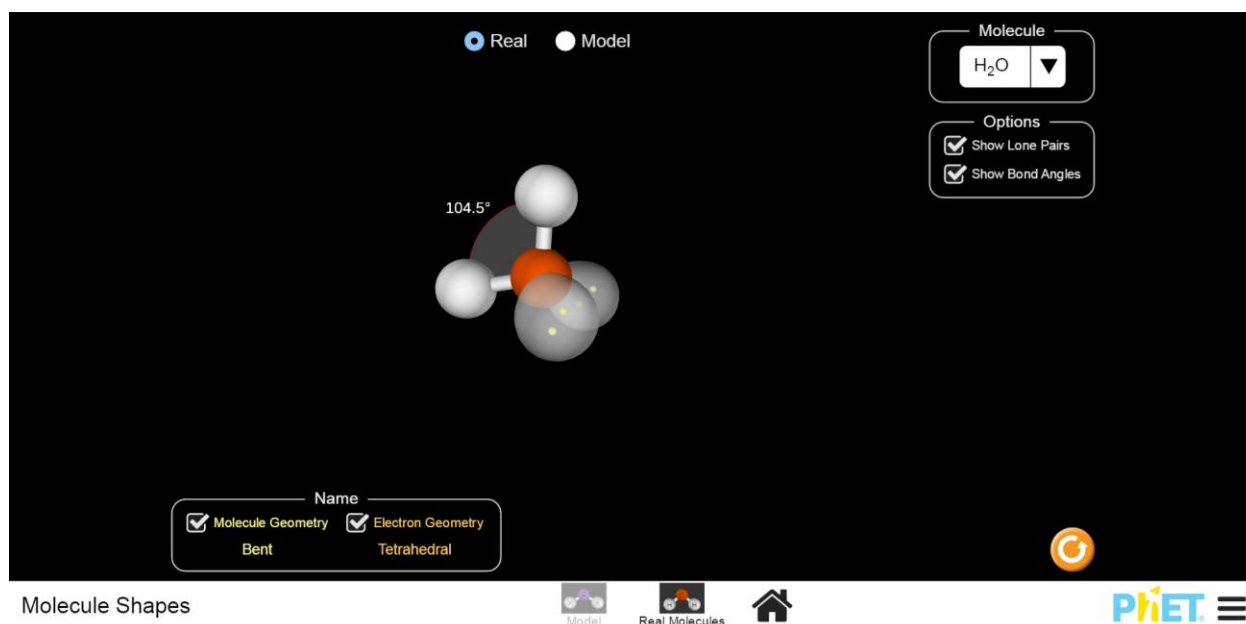


Figure 6. [University of Colorado PhET Interactive Simulation](#) Demonstrates the Real Shape of Water.⁴

In pre-lab question #1, you are asked to use the PhET Simulation to fill in a table showing how lone pairs affect geometries. *Complete the table now to create a comprehensive illustration of all the molecular geometries.*

Understanding Lewis structures and molecular geometry is important because it allows chemists to predict properties and reactivity of molecules. To complete this understanding, we need to add the concept of bond polarity. While electrons are shared in covalent bonds, they might not be shared evenly. To determine where the electron density lies between two atoms in a bond, we need to review the periodic trend of electronegativity. Atoms have greater electronegativity, the ability to attract bonding electrons to themselves, in the upper right of the periodic table (Figure 7). Atoms at the top of a group are small enough for electrons to experience a stronger attractive force from the protons

in the positive nucleus. Atoms on the right side of a period have more protons to create attraction for the electrons than atoms on the left side of a period.

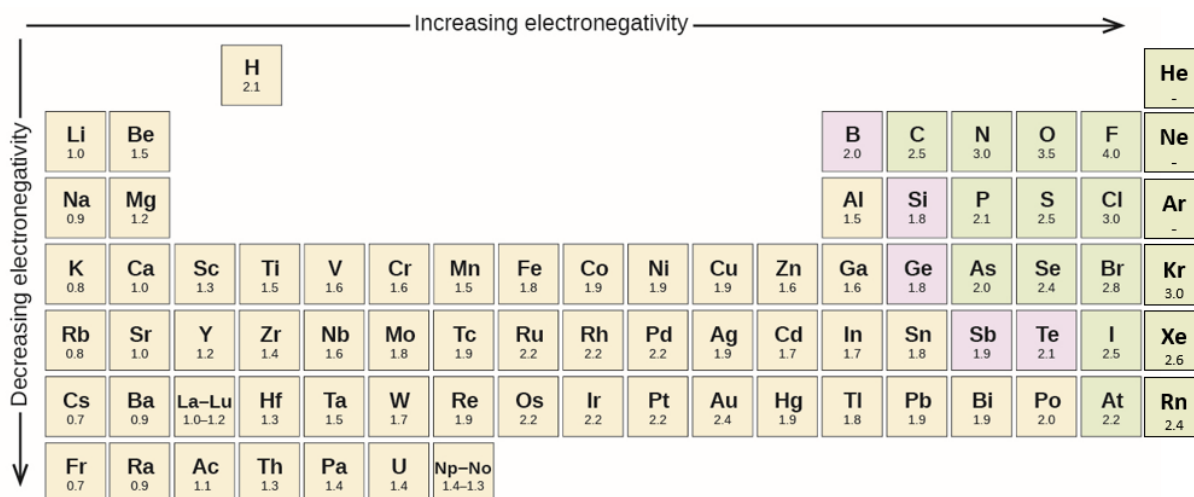


Figure 7. Electronegativity Values Calculated by Linus Pauling Demonstrate Increasing Electronegativity to the Upper Right of the Periodic Table.⁵

Once a Lewis structure has been drawn with appropriate molecular geometry, the difference in electronegativity of atoms can be shown to further illustrate the electron density in the molecule. The difference in electronegativity in a bond can be shown two ways: with a cross-base arrow pointing toward the more electronegative atom or with delta plus ($\delta+$) or delta minus ($\delta-$) indicating the charge density (Figure 8).



Figure 8. A Cross-base Arrow or Delta Plus/Minus Symbols Represent Bond Polarity in Hydrogen Chloride.

As electronegativity differences increase between two atoms in a bond, the bond polarity increases until the bond becomes ionic. Nonpolar defines a bond where electrons are shared relatively equally. Polar defines a bond with one electronegative atom that pulls more electron density to itself. Ionic bonds occur most often between a metal and non-metal due to the propensity of the metal to give up electrons to the non-metal, evidenced by the very large electronegativity difference between the atoms in the bond.

Finally, bond polarity combined with geometry defines the polarity of the whole molecule. For example, in carbon dioxide, the individual bonds are polar, however the pull of electrons from each oxygen cancels the other since it is a linear geometry; and the whole molecule is non-polar (Figure 9). In contrast, water has a dipole since an area of charge density can be demonstrated on the oxygen.

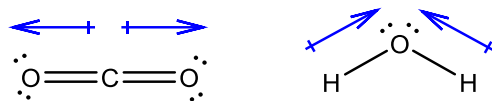


Figure 9. Opposing Polar Bonds in the Nonpolar Carbon Dioxide Molecule and Polar Bonds in Polar Water.

Lastly, we work to define the bond structure, geometry, and polarity in order to predict the physical and chemical properties of the molecule. Dissolution, or dissolving solute into solvent, is an important physical property. The principle of “like dissolves like” is used to predict if a compound will dissolve in a solvent. If two molecules have the same or “like” polarity, they will dissolve together. A polar molecule such as H_2SO_4 will dissolve in a polar molecular such as water. A non-polar compound will dissolve in a non-polar solvent. Polar and non-polar molecules will not dissolve together; for example, in salad dressing, oil and water separate (Figure 10).

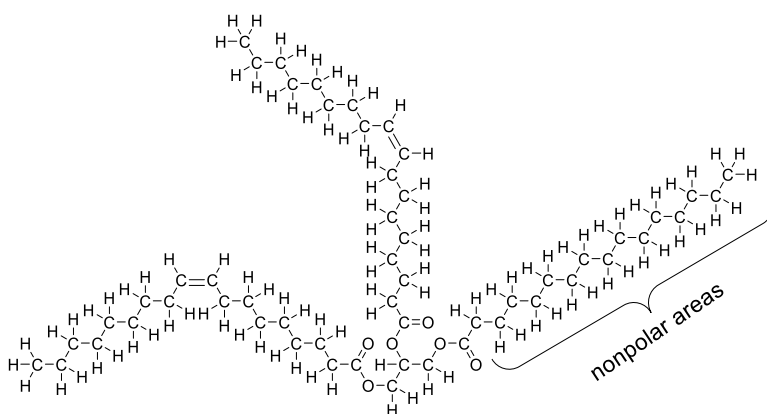


Figure 10. An Example of a Triglyceride, a Molecule Found in Olive Oil, with Large Nonpolar Areas Made of Carbon-to-Carbon and Carbon-to-Hydrogen Bonds That Make It Insoluble with Water.

By combining Lewis Theory, VSEPR Theory, and electronegativity, we can gain a comprehensive illustration of molecular structure. So now, what are your thoughts about the John Ellis Water Machines? Do you think that it is possible to change the natural bond angle of water?

As we have seen, it takes a combination of concepts and several steps to come to an overall picture of a molecule. In this experiment, you will be asked to use ball-and-stick molecular models or the PhET Simulation software to draw Lewis structures, molecular geometries, and then define bond and molecular polarity and solubility.

Experimental Procedure

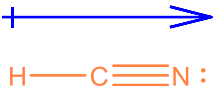
1. Follow your instructor’s directions. Use either the ball-and-stick models or modeling software to help draw accurate Lewis structures and VSEPR geometries, both molecular and electron-geometries. Then, examine the bond polarity and how that affects molecular polarity. Decide if the compound is more likely to dissolve in hexanes, C_6H_{14} a non-polar molecule, or water, H_2O a polar molecule.
2. Draw the tables in your lab notebook, and fill in as required, following the example.

Experiment 11: Molecular Modeling Data

Name: _____ Date: _____

Lab Partner: _____ Section: _____

1)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
HCN	10	$\text{H}-\text{C}\equiv\text{N}:$ <p style="text-align: center;">√ octets √ formal charges (Include formal charges other than 0.)</p>	Molecular Geometry: Linear Electron-Group Geo.: linear
Bond Polarity (ΔEN)		Molecule Polarity	
$\Delta\text{EN}(\text{H}-\text{C}) = 2.1 - 2.5 = 0.4$ $\Delta\text{EN}(\text{C}-\text{N}) = 2.5 - 3.0 = 0.5$		 <p style="text-align: center;">$\text{H}-\text{C}\equiv\text{N}:$</p>	
		More soluble in hexane or water?	
		water	

2)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
OCl^- <i>(hypochlorite, oxidizing agent in bleach)</i>		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	
		More soluble in hexane or water?	

3)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
NOCl <i>(nitrosyl chloride, found in 'aqua regia' to dissolve gold)</i>		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

4)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
SOCl ₂ <i>(thionyl chloride, used in chemical synthesis)</i>		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

5)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
N_2 (nitrogen, 78% of air)			Molecular Geometry: Electron-Group Geo.:
		(Include formal charges other than 0.)	
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

6)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
XeO_3			Molecular Geometry: Electron-Group Geo.:
		(Include formal charges other than 0.)	
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

7)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
I_3^-		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

8)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
SiF_4		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

9)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
PH ₃		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

10)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
BF ₄ ⁻		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

11)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
SbCl_6^-		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

12)

Formula	Total Valence Electrons	Rough Lewis Structure	Molecular Geometry/ Electron-Group Geometry
TeF_4		(Include formal charges other than 0.)	Molecular Geometry: Electron-Group Geo.:
Bond Polarity (ΔEN)		Molecule Polarity	More soluble in hexane or water?

Clean up/Disposal

- If you are using ball-and-stick models, please disassemble them at the end of the lab period and return to the proper box.
- If you are using a computer, please shut it down, and return to its storage location.

Post-lab

When a molecule has resonance forms, the most stable forms contribute most strongly to the actual structure of the molecule. Stability of resonance structures can be predicted by the following rules:

- a) Molecules where all atoms have an octet are more stable.
 - b) If a molecule has a charge, the more stable structure will have a negative charge on a more electronegative atom, or a positive charge on a less electronegative atom.
 - c) Molecules with charges separated by smaller distance are more stable than those with larger charge separation.
1. Draw correct Lewis structures for NO_2F . If there is a difference in stability, rank the resonance forms from most (1) to least stable (2).
 2. Draw correct Lewis structures for SO_3^{2-} . If there is a difference in stability, rank the resonance forms from most (1) to least stable (3).
 3. Draw correct Lewis structures for N_3^- . If there is a difference in stability, rank the resonance forms from most (1) to least stable (3).
 4. Include your Experimental Data Tables with your lab report.

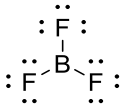
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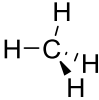

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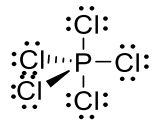
Pre-lab 11

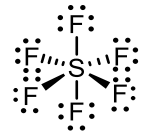
Point your web browser to University of Colorado's PhET Interactive Simulations, and double-click 'Real Molecules' and select water from the drop-down list. Select the radio button 'Show Bond Angles', name 'Molecule Geometry' and 'Electron Geometry'. Using the Molecule Shapes PhET, fill in the table below to create a study tool of molecular geometries of molecules with lone pairs. They can be considered subgroups of electron-group geometries. (Note: you can rotate the molecule by right-mouse clicking on it to get different perspectives of each molecule.)

Include: a) a drawing of the molecule with correct perspective (use wedges and dashes if necessary), b) the name of the molecular geometry and the electron-group geometry, and c) the bond angles around the central atom.

Formula	Bonding groups	Lone pairs	Molecular Geometry/ Electron-Group Geometry	Bond angles
CO ₂	2	0	Molecular Geometry: linear Electron-Group Geo.: linear :O=C=O:	180°
BF ₃	3	0	Molecular Geometry: trigonal planar Electron-Group Geo.: trigonal planar 	120°
SO ₂	2	1	Molecular Geometry: Electron-Group Geo.:	

Formula	Bonding groups	Lone pairs	Molecular Geometry/ Electron-Group Geometry	Bond angles
CH ₄	4	0	Molecular Geometry: tetrahedral Electron-Group Geo.: tetrahedral 	109.5°
NH ₃	3	1	Molecular Geometry: Electron-Group Geo.:	
H ₂ O	2	2	Molecular Geometry: bent Electron-Group Geo.: tetrahedral 	104.5°

Formula	Bonding groups	Lone pairs	Molecular Geometry/ Electron-Group Geometry	Bond angles
PCl ₅	5	0	Molecular Geometry: trigonal bipyramidal Electron-Group Geo.: trigonal bipyramidal 	120°/90°
SF ₄	4	1	Molecular Geometry: Electron-Group Geo.:	
ClF ₃	3	2	Molecular Geometry: Electron-Group Geo.:	
XeF ₂	2	3	Molecular Geometry: Electron-Group Geo.:	

Formula	Bonding groups	Lone pairs	Molecular Geometry/ Electron-Group Geometry	Bond angles
SF ₆	6	0	Molecular Geometry: octahedral Electron-Group Geo.: octahedral 	90°
BrF ₅	5	1	Molecular Geometry: Electron-Group Geo.:	
XeF ₄	4	2	Molecular Geometry: Electron-Group Geo.:	

References

1. John Ellis Water®. John Ellis Water Machines. <http://johnellis.com/> (accessed March 15, 2017).
2. Image used under a [Creative Commons Attribution License \(by 4.0\)](#) from OpenStax, Chemistry. OpenStax CNX. Mar 10, 2017 <http://cnx.org/contents/85abf193-2bd2-4908-8563-90b8a7ac8df6@9.422>. Download for free at <http://cnx.org/contents/85abf193-2bd2-4908-8563-90b8a7ac8df6@9.422>.
3. This tutorial helps to illustrate VSEPR Theory molecular shapes:
https://florida.pbslearningmedia.org/asset/lsp07_int_molecularshp/.
4. Image used under a [Creative Commons Attribution License \(by 4.0\)](#). PhET Interactive Simulations, University of Colorado Boulder, February 28, 2017. <https://phet.colorado.edu>.
5. Image used under a [Creative Commons Attribution License \(by 4.0\)](#) from OpenStax, Chemistry. OpenStax CNX. Mar 10, 2017 <http://cnx.org/contents/85abf193-2bd2-4908-8563-90b8a7ac8df6@9.422>. Download for free at <http://cnx.org/contents/85abf193-2bd2-4908-8563-90b8a7ac8df6@9.422>.