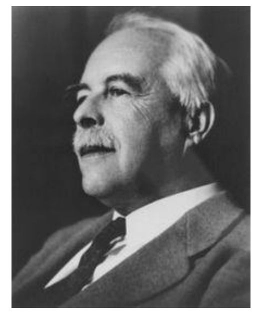
Lewis Structures & VSEPR Theory: Using PhET Simulation

A Dry Lab Activity

Learning Objectives:

- Gain practice drawing simple and complex Lewis Structures by-hand.
- Relate a compound's Lewis Structure to its Electron Geometry & Molecular Geometry via VSEPR Theory.
- View the geometries of a set of standard compounds using the "Molecule Shapes" PhET Simulation, and build molecular models of other compounds using the same simulation.

Background Information:



You can learn more about Gilbert Lewis here.

As you've learned in your General Chemistry lecture course, *molecular* compounds are made up of non-metallic atoms held together by *covalent bonds.* These bonds are formed by the sharing of electrons between the atoms. The scientist credited with the discovery of the covalent bond is Gilbert N. Lewis (1875-1946), a professor at UC Berkeley. A prolific scientist, Lewis' most profound contribution to the field of chemistry was the development of Lewis Theory. The four main ideas of Lewis Theory are:

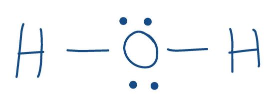
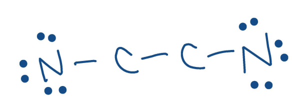
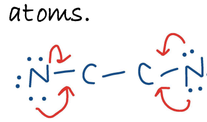
1. Electrons play a fundamental role in chemical bonding.
2. In some cases electrons are *transferred* from one atom to another (*ionic bonds*).
3. In other cases, one or more pairs of electrons are shared between atoms (*covalent bonds*).
4. Electrons are transferred or shared so that each atom in the molecule acquires a stable electron configuration. (Often an "octet" or 8 valence electrons.)

Lewis dot structures (aka *Lewis structures*) are a useful way to represent chemical compounds, because they keep track of and show the valence electrons involved in each bond. Pairs of bonding electrons are represented with lines (one line for each pair of e^-), while non-bonding pairs of electrons are shown as dots. In this lab activity, we will focus solely on **molecular compounds**, and their Lewis structures.

There are a few different methods of constructing Lewis structures, but they all arrive at the same conclusions. The method described here is similar to that taught in CHE101 lecture. We'll walk through the method here together – using water (H_2O) and cyanogen (C_2N_2) as examples. Water is a nice simple example, because only single bonds are required. C_2N_2 requires the use of multiple bonds, so it also provides a good example.

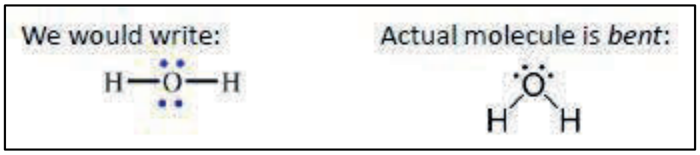
To Construct a Lewis Structure:

1. **Determine the total # of valence e^- in the compound.**
2. **Identify the central and terminal atoms.** The atom with the lowest electronegativity generally goes in the center, while the atoms with higher electronegativities appear in terminal positions. Hydrogens are ALWAYS terminal atoms. Carbons most often are central atoms.
3. **Write a plausible skeletal structure**, joining the atoms with single bonds first. Aim for symmetry in the structure. Count up the number of electrons used to form those bonds.
4. **For each bond, subtract 2 from the total # of valence e^-.** The result is the number of <u>remaining electrons</u>, that need to be accounted for.
5. **Place the <u>remaining electrons</u> onto the skeletal structure** – fill the octets of the *terminal atoms first*, then the central atom.
6. **If the central atom is left without an octet**, move lone pairs of electrons from the terminal atoms inward to form double or triple bonds as necessary.

H_2O	C_2N_2
$1(2) + 6 = 8\,e^-$	$4(2) + 5(2) = 18\,e^-$
H's are always terminal, so Oxygen must be central.	C is less electronegative, so the C's will go central and N's will be terminal. (Aim for symmetry when possible).
H — O — H 2 bonds formed = 4 e^-	N — C — C — N 4 bonds formed = 8 e^-
8 valence e^- - 4 bonding e^- = 4 e^- remaining	18 valence e^- - 6 bonding e^- = 12 e^- remaining
 8 e^- are accounted for in the proposed structure, so all is good!	 18 e^- are accounted for, but C's do not have full octets. (Each C has only 4 e^- around it.) So we move lone pairs of e^- in from the N-atoms.  And now 18 e^- are shown, and all atoms have an octet. :N≡C—C≡N:

For the purposes of this activity, which is meant to focus on simple Lewis Structures, we will not be worrying about calculating formal charge, or possible resonance structures.

As you can see, Lewis structures are only a 2-dimensional representation of the bonding and lone pairs within a molecule. They do not demonstrate the *true shape* of a molecule. For example, the structure for water we drew above looks linear, but the true molecular shape of water is actually bent:



So scientists use another model to predict molecular shapes, called the **Valence-Shell Electron-Pair Repulsion Theory**, or **VSEPR** for short. This bonding model focuses on pairs of electrons in the valence shell of the central atom, and the fact that electron pairs repel each other (either bonded OR lone pairs of electrons). The model uses the number of **electron groups** (sometimes called *electron domains*) to predict the shape that these groups will take around the central atom. The best arrangement of the given number of electron groups is the one that minimizes the repulsions among them.

At this point in your General Chemistry 1 (CHE101) course, you may not have fully discussed VSEPR theory yet. **THIS IS OK!!** We are going to use today's activity for you to explore VSEPR and molecular shapes through a computer simulation program. This program is open-sourced via a website, and provides a *great* introduction to how molecules really look, and how their shapes come to be.

To be successful in today's activity, there are a few key VSEPR terms that you should be familiar with:

Electron Groups: an electron group can be a single bond, double bond, triple bond, or lone pair of electrons – each of which counts as 1 group. To get the total number of electron groups on a central atom, just add up how many of these groups are present. You'll see in our water example, that the central oxygen has 4 total electron groups (2 single bonds, and 2 lone pairs).

Non-Bonding Pairs: This is just another name for lone pairs. So water has two non-bonding pairs of electrons.

Electron Geometry: The shape of the distribution of electron groups.

Molecular Geometry: The shape of the distribution of only the nuclei (atoms) around the central atom (not including the nonbonding pairs).

The electron geometry and molecular geometry will only be the same if there are no nonbonding pairs.

Equipment Required

- Laptop computer with internet access.
- Website: https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html
- *Optional* - second electronic device (such as a smartphone) to take pictures of work.

Activity Instructions

This activity is to be completed during your scheduled lab period. **You will be submitting two things:**
1) Paper worksheet to your instructor (you'll work on this with your partner, following the instructions)
2) LabFlow Report (you'll enter this into LabFlow before leaving the lab room – or up to 24 hours after your lab period ends)

You may work with a partner on the activity, but you must each turn in an individual worksheet to your Instructor AND submit the report to LabFlow.

Part A: Real Molecules

1. You may detach the last 3 pages from the rest of the packet while you work. Make sure to fill in the heading with your full name, section day/time, section code, and Instructor's name.
2. In Table 1: Real Molecules, fill in the following columns for each compound (*H_2O is worked for you as an example):*
    a. **Total Valence e-**: Just like you've learned in lecture, add up the valence electrons contributed by each atom in the molecule. Use the periodic table on the back of your lab book for assistance if you need it.
    b. **Can Central Atom Expand its Octet**: enter "yes" or "no". Remember that any element in period (row) 3 or below on the periodic table has the capability of expanding its valence shell to hold more than an octet of electrons. (Answering "yes" doesn't mean that the central atom *will definitely* display an expanded octet in this compound, it only means that it *can if it needs to*.)
    c. **Lewis Structure**: Draw the Lewis dot structure of the given molecule, using the procedure outlined in the Background Information (or your own tried-and-true method of drawing structures learned in lecture).
    d. **# Electron Groups & # Non-Bonding Pairs:** record the number of electron groups and non-bonding pairs on the central atom. Remember that a single bond, double bond, triple bond, or lone pair ALL count as ONE electron group. The # of non-bonding pairs is the number of "lone pairs" of electrons on the *central atom*.

3. Now open the PhET simulation website on your laptop: https://phet.colorado.edu/sims/html/molecule-shapes/latest/molecule-shapes_en.html
   Double-click on "Real Molecules". In the drop-down menu on the right, select XeF_2. Make sure to check the boxes for "show lone pairs" under options. At the bottom, check the boxes for "molecule geometry" and "electron geometry". You can click and drag on the model to rotate it. Now fill in the rest of the headings in Table 1: Real Molecules for XeF_2:
   e. **Electron Geometry & Molecular Geometry:** record the geometries that are displayed at the bottom of the model screen.
   f. **Sketch:** sketch the molecule with the molecular geometry shown on the PhET simulation. Use lines, dashes, and wedges as appropriate.

   Repeat for all of the other molecules in Table 1.

Part B: Model Building

Now you'll be working through the Lewis Structure and building a model of it in the PhET Simulation.

1. In the simulation, click on the House Icon at the bottom then double-click on "Model". Click on "Remove All" on the right-hand side.
2. Choose TWO of the molecules listed below. In Table 2: Building Models , write the molecular formulas for the two compounds in the appropriate spot.
3. Complete the first four columns just as you did in Part A.
4. Now in the PhET simulation, build a model of the compound. Use the icons on the right-hand side to add single bonds, double bonds, triple bonds, or lone pairs to the central atom. (Notice that the atoms are just generic ones – you cannot select specific elements. This is ok! It gives you the general idea.)
5. Once your model is complete, record the Electron Geometry & Molecular Geometry, and Bond Angle.
6. Sketch your model in the last box.
7. Finally, take a picture of the model with your smartphone (or capture a screenshot on the device you're using for the PhET Simulation), and **save it**. You'll upload this image to LabFlow later!

Compounds to Choose From:
IF_5
H_2CO
HCN
NCl_3
CS_2
NO_3^-

Write-Up/Submission

Make sure Tables 1 & 2 are completely filled in. And make sure you've saved the pictures of your models from Part B!

Now log into Labflow. Open the Report Tile for the Lewis Structures module. **(DO THIS WHILE YOU'RE STILL IN THE LAB, IF POSSIBLE. If you have run out of time or do not have a device to access Labflow, you can complete the report up to 24 hours past your lab time.)**

You'll be asked if you're doing the report virtually or in-person. Choose "in-person" if you performed the activity in the lab. Choose "virtually" if you were absent/remote.

In-person students will be prompted for a passcode – this is a number that will be provided by your instructor on the board. Type in the number and continue. If you chose "virtually" above, a passcode will be provided to you.

Now use the tables you constructed to complete the report. You'll only be asked to provide the information from the grayed-out headings in the tables for each molecule.

For Part B, you'll be asked to upload the two images of the PhET models that you built.

In-Person Students: Before you leave, submit your worksheet to your Instructor. They will initial it and give you a score for Participation at the top before you leave. This participation score will be added manually into your Report grade later.

Absent/Virtual Students: You'll need to scan or take pictures of your completed lab pages, and submit them to LabFlow at the end of your report for full credit.

LEWIS STRUCTURES & VSEPR:WITH PhET SIMULATION **Instructor Initials & Participation (+5): _________**

Name:		Person #:
Instructor:	Section Code:	Section Day/Time:

TABLE 1: Real Molecules

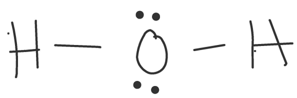
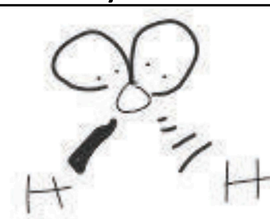
Molecular Formula	Total Valence e-	Can Central Atom Expand its Octet?	Lewis Structure	# e^- groups / #NB pairs	Electron Geometry / Molecular Geometry	Sketch of Molecular Geometry
H_2O *(worked example)*	*8*	*No*		*4*	*Tetrahedral*	
				2	*Bent*	
XeF_2						
BF_3						
ClF_3						
NH_3						

TABLE 1: Real Molecules – Continued Name: ______________________

Molecular Formula	Total Valence e-	Can CA Expand its Octet?	Lewis Structure	# e^- groups / #NB pairs	Electron Geometry / Molecular Geometry	Sketch of Molecular Geometry
CH_4						
SF_4						
XeF_4						
BrF_5						
PCl_5						
SF_6						

TABLE 2: Model Building Name: ________________________

Chosen Molecular Formula	Total Valence e-	Can CA Expand its Octet?	Lewis Structure	# e^- groups	Electron Geometry	Bond Angle(s)	Sketch of Molecular Geometry from Model Built in PhET
				#NB pairs	Molecular Geometry		