In this assignment you will be asked to determine the Lewis structures and the three-dimensional geometries of molecular species starting only with the molecular formulas. This time is to be used to help you perfect your skills at deducing Lewis structures and, most importantly, to help you become acquainted with various molecular geometries.

You will be asked to work with a list of molecular species. You are to do the following for each species, writing your answers on the worksheets provided:

1. Determine the number of valence electrons in the molecule (See your text, the notes, and/or the supplemental material provided in this handout)

2. Determine the Lewis structure of the molecule

3. Determine the geometry around each centralized atoms in the molecule from the Lewis structure

4. **OPTIONAL!!!!!!:** Draw an exact 3-D representation of the molecule using the wedge and dash technique described in the provided supplemental material.

Lewis structures and geometries will be studied in class over the next few weeks.

The following pages contain study supplemental material on the various topics involved in determining molecular structures. Your textbook, the class notes, and the class lectures also provide information on these topics. However, this handout will be used as the introduction to drawing Lewis structures and as the introduction for determining molecular geometry.

The supplements contain activities designed so that you can interact with them. The activities are divided into sections. Most of the sections as questions which you should answer by writing in the space provided. The sections are designed so that you can compare your answer with the correct answer before proceeding to the next section. Note: the answers are GIVEN to you. It would be completely useless and a source of later frustration if you simply copy the answers and call the assignment done.

Make an answer shield by using an additional blank piece of paper. Cover all the sections below what you are studying and answering at the present moment. When you have answered the questions, slide the answer shield down to expose the correct answer and compare it with your own. If it is the same, or you understand your mistake, proceed to the next section. If you do not understand your error, first check your notes, and then with your instructor. Note: ultimately only YOU will be asked to answer/draw Lewis structures. This assignment is designed to guide you through the material all by yourself with minimal interaction with others. So make sure that you understand the material covered!!

These supplements are designed so that you can study and refer back to just those topics that are giving you difficulty. These will be excellent study sheet for the final (both CH131 and CH133/ organic!)

Supplement #1: Definitions of Lewis structures

Determining the number of valence electrons

Determining Lewis structures

Supplement #2: Definitions on Molecular Geometries

The theory

Determining Molecular Geometries

Table of geometries

Supplement #3: Drawing 3-D structures

Supplement # 1: LEWIS STRUCTURES

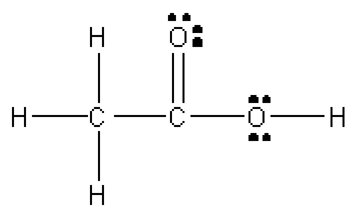
Definitions and Ideas

The distinguishing characteristic of a molecule of molecular ion is that its atoms are held together by what are called covalent bonds. In covalent bonding, two atoms are attracted to the same set of electrons. This mutual attraction to the same electrons keeps the atoms a set distance apart. The mutual attraction, in effect, bonds the atoms together. The two atoms are said to *share* the set of *bonding electrons*. The three principle types of covalent bonds are symbolized below using carbon atoms.

C - C	C = C	C ≡ C
single bond	double bond	triple bond
2 electrons shared	4 electrons shared	6 electrons shared

The only electrons that can become involved in covalent bonding are those in the outer energy shells (the highest n level) of the atom. The other electrons, those in the inner energy levels are simply buried too deeply in the atom to be affected by an outside nucleus. The outer shell electrons are called the *valence electrons*. In a molecule, or a molecular ion, some of these valence electrons will be shared in the covalent bonds. Other valence electrons, called *unshared pairs*, will be attracted to only one atom.

A Lewis structure is a line-and-dot picture that shows where the valence electrons are and what they are doing in a molecule. The Lewis structure for acetic acid (CH_3CO_2H), is shown below.



It shows, for example, that each hydrogen atom is held in place by a single bond and has no unshared valence electrons on it; that one oxygen has two pairs of unshared valence electrons and is sharing four other valence electrons with a carbon atom (in the double bond).

The first Lewis structure had to be determined by interpreting experimental data on the molecule. However, enough of this work has been done over time to enable us to predict Lewis structures with reasonable certainty. In other words, the principles used by nature to distribute valence electrons in molecules have been discovered.

Controlling Ideas for Predicting Lewis Structures

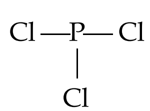
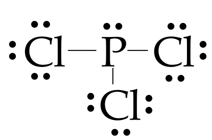
There are many methods used to deduce Lewis structures. The method used on the remaining parts of this supplement may differ slightly from the one given in your textbook. Whatever method is used, the following principles are controlling the work.

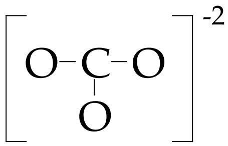
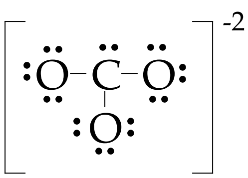
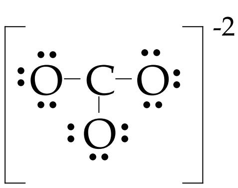
1. Number of valence electrons: the Lewis structure picture must show just the number of valence electrons used in the actual molecule or molecular ion
2. Octet (duet) rule: each atom in the molecule will usually have 8 valence electrons on it (octet rule). This counts *all* the valence electrons the atom is sharing as well as its own unshared pairs. Hydrogen atoms will only have 2 valence electrons (duet rule) each. The octet rule is not always followed, but it is an excellent place to start. Aluminum and boron prefer to have only 3 pairs (6 electrons total) around them.

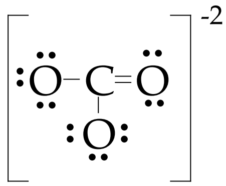
Note: The method for deducing Lewis structures given in the remainder of this supplement only works well with covalent compounds containing the main group elements.

The Number of Valence Electrons

	A. Generate the electron configuration for each different atom in a $HCCl_3$ atom H = C = Cl =
a. H = $1s^1$ C = $1s^2 2s^2 2p^2$ Cl = $1s^2 2s^2 2p^6 3s^2 3p^5$	B. The number of valence electrons an atom has can be determined in several ways. Once is to generate the electron configuration of the atom and then count the number of electrons in the highest n level (this will be the outermost s and p orbital electrons) Determine the number of valence electrons for each atom in the $HCCl_3$ molecule H = C = Cl =
b. H = 1 C = 4 Cl = 7	C. The total number of valence electrons in a neutral molecule can be determined by summing the number of valence electrons for each atom in the molecule. If the species is a molecular ion, one must go one step further to account for the charge. Add the extra electrons to the total number of valence electrons if the charged species is an anion (negative ion) or subtract the electrons from the total number of valence electrons if the charged species is a cation (positive ion). Determine the total number of valence electrons in an $HCCl_3$ molecule. Remember that there are 3 Chlorine atoms! # valence electrons ________________________________
c. # valence e^{-1} = 26 1H x 1 = 1 1 C x 4 = 4 3Cl x 7 = <u>21</u> 26	D. Thus, 26 electrons must be shown in the Lewis structure of $HCCl_3$ For other examples of calculating the # of valence electrons, see the three other Lewis structure examples that follow.

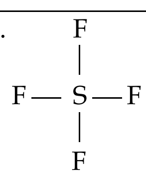
	A. You are to determine the Lewis structure for PCl_3, given only its molecular formula and the fact that there are no Cl-Cl bonds. What does the last fact tell you?
a. This tells me that the P is the central atom and that there are only P-Cl bonds in the molecule	B. Determine the number of valence electrons in a PCl_3 molecule # valence electrons _______________________
b. # valence e^- = 26 1 P x 5 = 5 3Cl x 7 = <u>21</u> 26	C. We will ignore this number for a moment and just guess at a possible Lewis structure. Recalling the answer for A above, connect the atoms with single bonds
c. 	D. Now add unshared electron *pairs* to each atom until each is surrounded by 8 electrons (shared and unshared (lone pairs)). If a hydrogen atom were present, remember that the hydrogen would only be surrounded by 2 electrons.
d. 	E. This is our first guess at the Lewis structure and must be checked for the number of electrons. How many electrons are shown in the picture?
e. 26 e^- 10 unshared pairs 3 bonding pairs = 13 pairs = 26 e^-	F. This number is exactly what we calculated that nature uses in the molecule (the number of valence electrons) Since our first guess Lewis structure contains the correct number of electrons and since each has atom has an octet, this is a correct Lewis structure for PCl_3.

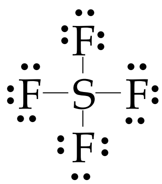
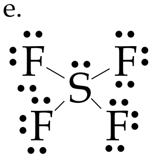
	A. You are to determine the Lewis structure for the molecular ion CO_3^{-2} (no O-O bonds) Determine the number of valence electrons in one CO_3^{-2} ion # valence electrons ________________________
a. # valence e^- = 24 1 C x 4 = 4 3 O x 6 = <u>18</u> 24	B. The species is charged because it has 2 more electrons than those contributed by neutral atoms Recalling that there are no O-O bonds, draw a picture connecting the appropriate atoms with single bonds
b. 	C. Now add the unshared electron pairs until each non-hydrogen atom is surrounded by a total of 8 electrons (octet)
c. 	D. Count the number of electrons in this first guess picture. How does this number compare to the calculated number of valence electrons that you determined above?
d. 26 e^- shown. This is 2 electrons too many, since it was previously determined that there are only 24 valence e^-.	E. Two electrons must be removed from the first guess picture. Remove then as an unshared pair from the central atom; i.e. the carbon atom
e. 	F. This structure has the required 24 valence electrons but now the central carbon atom does not have an octet. The central carbon atom is surrounded by 6 electrons instead of 8. This problem is solved by turning an unshared pair of electrons on one of the oxygen atoms into a complete bonded pair between the C and O atoms. That is, we will use the unshared pair of electrons from an oxygen to create a double bond:

	Redraw the Lewis structure using this idea:
f. 	G. This Lewis structure contains the required 24 electrons and each atom has an octet. This is a correct Lewis structure.

<u>In general, whenever your first guess picture contains too many electrons, the correct Lewis structure will contain double or triple bonds</u>. These multiple bonds occur most often between C, N, O, P, S, Se atoms. These six multiple bonders are easy to recall because they form a triangle on the periodic table.

For a molecule where the multiple bond can be located in two or more positions is best represented by a series of Lewis structures that is given the term *resonance*. We will do more of this at a later time.

	A. You are to determine the Lewis structure for SF_4 (no F-F bonds) Determine the number of valence electrons in one SF_4 molecule # valence electrons ______________________
a. # valence e^- = 34 1 S x 6 = 6 4 F x 7 = 28 34	B. Recalling that there are no F-F bonds, draw a picture connecting the appropriate atoms with single bonds:
b. 	C. Now add the unshared electron pairs until each non-hydrogen atom is surrounded by a total of 8 electrons (octet)

c. 	D. Count the number of electrons in this first guess picture. How does this number compare to the calculated number of valence electrons?
d. 32 e^- are shown and this is 2 valence electrons too little given the calculated number of valence electrons. The structure should have 34 valence electrons	E. Two electrons must be added to our first guess picture. There is no way to do this without giving one of the atoms more than 8 electrons. However, this is indeed what nature is doing, in this case, the octet rule is NOT upheld. Place two electrons, in the form of an unshared pair, on the central atom – in this case, the sulfur atom
e. 	F. This Lewis structure contains the required 34 electrons. Although the octet rule is not upheld, this is so for only one atom. Thus, it is a correct and valid Lewis structure.

<u>**In general, whenever your first guess picture contains too few electrons the octet rule will have to be broken on the central atom. The central atom in these cases MUST be in the third or higher period (row!) on the periodic table. Such orbitals have the 3s, 3p, and even though it is empty, they have the 3d orbital available that will accept the extra electrons. NOTE: atoms in the first and second row will never violate the octet rule!**</u>

Note: multiple bonds cannot help in too few electron cases.

Supplement #2: GEOMETRIES OF MOLECULES

Definitions and Ideas

This page contains all the essential ideas needed to determine the geometry of molecules. However, few students are able to understand these ideas from this page alone. Understanding will come from doing the exercises in the remainder of the supplement. Use this page to get some initial feeling for the ideas now. Use it later as a quick reference on definitions.

The Lewis structure of a molecule indicates which atoms are bonded to which and where all the valence electrons are in the molecule. A Lewis structure does not show the geometric arrangement of the atoms in a molecule. However, the Lewis structure is the starting point for determining molecular structures.

The ideas used to determine geometries from Lewis structures are called the Valence Shell Electron Pair Repulsion Theory (abbreviated VSEPR theory). The ideas are as follows. The sets of valence electrons on each atom are free to move around, but not away from, the atom (much like a dog on a short leash can move around its handler). Since each set of valence electrons is negatively charged, the individual sets repel one another. This repulsion forces the individual sets to place themselves around the atom so that they are as far away from one another as possible. Thus, the sets of electrons occupy a fixed geometry around the atom. Any other atom sharing the electron sets (i.e. bonded atoms) will also occupy this fixed geometry.

The individual sets of valence electrons that can move away form each other are often called independent regions of electron density. For geometry purposes each of the following is considered one independent region of electron density.

.. each unshared pair counts as 1 region

— each single bond counts as 1 region

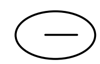
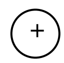
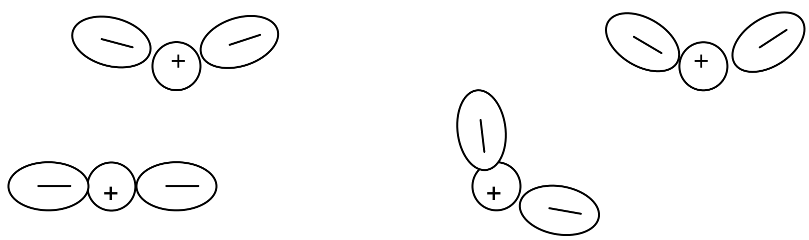
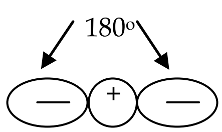
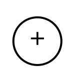
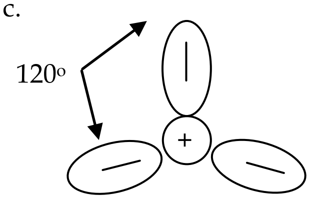
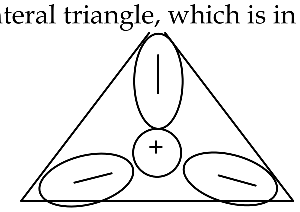
= each double bond counts as 1 region

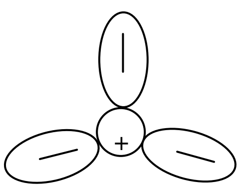
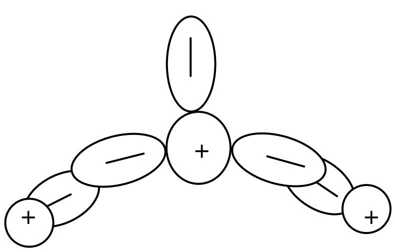
≡ each triple bond counts as 1 region

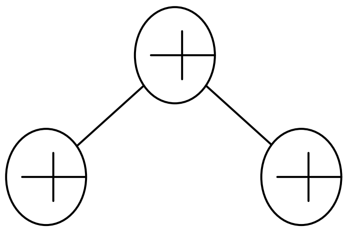
Therefore you see that all electron density regions count as 1!

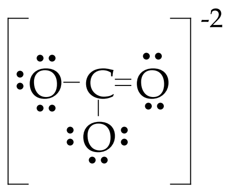
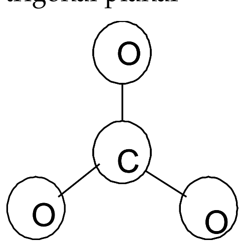
The geometry of a molecule is determined from the number of such regions on each centrally located atom (sometimes there is one central atom, sometimes there are multiple atoms that we can determine respective geometries for). A central atom is one which has two or more other atoms bonded to it. A given number of regions on a central atom will assume the fixed geometry given in the table on the following pages. Bonded atoms "tag along" with the electron regions of the central atom, taking the same position in space as the electron region that they are sharing. The molecular geometry describes the positions the bonded atoms take around the central atom. The molecular geometry also takes into account lone pair electrons and shows that they take up space and help to determine the overall shape of the molecule. If the central atom has all of its electron regions used in bonding, the electron and molecular geometries are the same. If the central atom has unshared pairs of electrons, then the molecular geometry and electron geometry will not be the same, but will be based off of one another. In essence, the molecular geometry will be a "daughter" or "offspring" of the electron geometry as shown in the following tables.

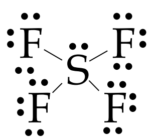
<u>VSEPR theory</u>

	A. The determination of molecular geometries is based on the idea that independent regions of electron density (negative charge) repel each other while they are simultaneously attracted to regions of positive charge. Consequently, these regions of electron density will arrange themselves to be as far apart as possible while they are simultaneously attracted to a nucleus
	B. If an atom has two independent regions of electron density  arranged about a nucleus  Which of the following represents the best arrangement 
b. 	C. In this arrangement they are simultaneously close to the positive charge and far from each other. This arrangement is called linear. Show how three independent regions of electron density can arrange themselves around a nucleus and all be equally far away from one another. 
c. 	D. This arrangement is called trigonal plane (or triangular plane). The three areas of electron density are arranged so that imaginary lines drawn between them define an equilateral triangle, which is in a single plane. 

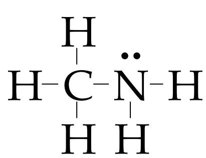
	E. If an atom has 4, 5, or 6 independent regions of electron density arranged around its nucleus, the regions achieve maximum separation with three dimensional arrangements. These are called tetrahedral, trigonal bipyramidal (or trigonal bipyramidal) and octahedral arrangements, respectively. These arrangements are pictured in the table provided and models will be displayed in class. Study these until you can properly visualize them in your mind. You need to be able to identify the geometry of a molecule after you draw its Lewis structure.
	F. Let us consider again an atom that has three regions of electron density. What geometry will these regions take around the nucleus? Name the geometry and draw it.
f. 	G. This is called the electron geometry of this atom, because it is the arrangement of the regions of electron density. Assume that the other two nuclei are bonded to the one pictured; that is, that two of the electron regions are being shared. Draw a picture showing where the two nuclei will attach themselves. If the electron regions are being shared (as in a covalent bond, then you must draw a picture of overlapping electron regions!
g. 	H. In this case, it does not really matter which two of the three electron densities that you chose. The resulting picture is identical any way you draw it. The positions are thus said to be equivalent. Redraw the picture ignoring the electron densities. Instead of drawing the bubbles, fill in with lines, showing the bonds. Draw the structure with the same geometry as you have previously. Name this arrangement.

h.  bent or angular	I. This is called the molecular geometry because it gives the arrangements of atoms (nuclei) around the central atom (nucleus). The molecular geometry will be the same as the electron geometry only if all the electron regions are shared (bonded to) other atoms. If one or more of the electron regions on the central atom is unshared, the molecular geometry will differ from the electron geometry. However, the molecular geometry is caused by the electron geometry. Thus it is determined to be the daughter of the electron geometry. In the present case, the atoms are in a bent geometry (not linear) because the invisible unshared electron region is pushing down (repelling) the two shared regions.

	A. You are to determine the molecular geometry of CO_3^{-2} (no O-O bonds) Determine the Lewis structure of the molecular ion:
a. 	B. Which is the central atom? Central atom = ___________________
b. the C atom	C. How many independent regions of electron density are on this central atom? # regions = _________________________
c. 3 regions	D. Note that the double bond counts as only one region because the 4 electrons in the double bond must stay together. How will the 3 regions arrange themselves around the carbon atom? What is the <u>electron geometry</u>? Electron geometry = ________________________________
d. trigonal planar	E. How many of the three regions are used in bonding to other atoms? # bonded regions = _____________________________
e. all 3	F. What will the arrangement of oxygen atoms around the carbon? What is the <u>molecular geometry</u>? Molecular geometry = _______________________________
f. trigonal planar 	G. The molecular geometry is identical to the electron geometry because all the electron regions on the central atom are shared and are used in bonding (that is, there are no lone pairs on the central carbon atom which we used to determine the geometry)

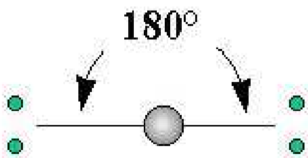
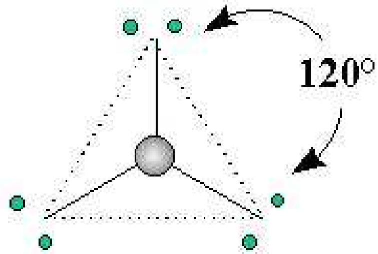
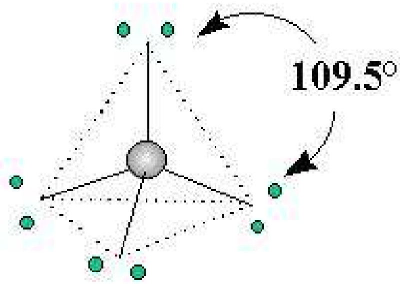
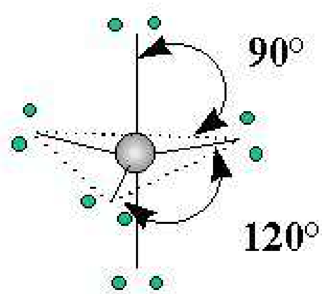
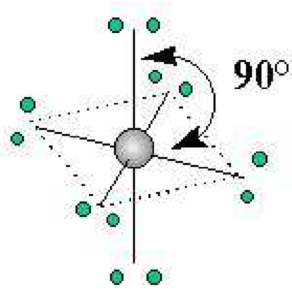
	A. You are to determine the molecular geometry of SF_4 (no F-F bonds) Determine the Lewis structure of the molecule.
a. 	B. Which is the central atom in the molecule? Central atom = ______________________________
b. the S atom	C. How many independent regions of electron density are on this central atom? # regions = ____________________________
c. 5 regions 1 unshared pair + 4 single bonds	D. According to the tables, how will these 5 regions arrange themselves around the S atom? Electron geometry = _____________________________
d. trigonal bipyramidal	E. To properly see this geometry you should inspect the model on display or build your own. The geometry has 3 regions in a triangular plane (t regions). The other two are directly above and below the triangle, forming the apex (a regions) of two pyramids How many of the 5 regions are used in bonding? # bonded regions = _________________________
e. 4	F. Since not all regions are used in bonding, the molecule geometry will NOT be the same as the electron geometry but will be some derivative of it. We must determine where the unshared pair will be located in the electron geometry. Refer to the figure in E above. If the unshared pair is located in one of the apex (a) positions, the molecular geometry would be a single triangular pyramid. If the unshared pair is located in one of the triangle (t) positions, a seesaw molecular geometry is obtained.

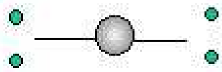
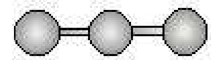
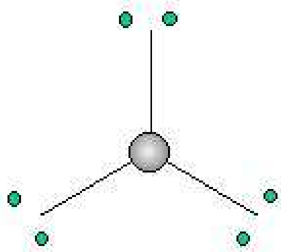
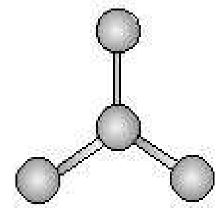
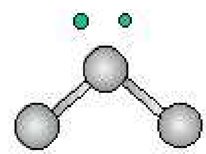
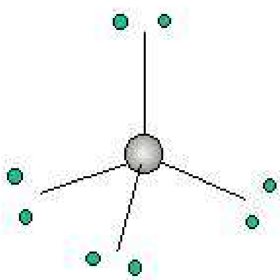
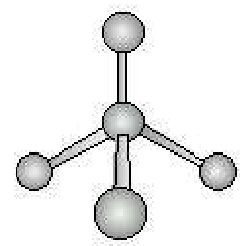
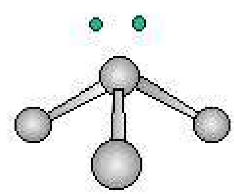
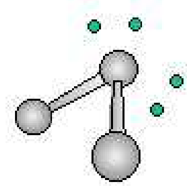
	G. According to the table, which molecular geometry is actually found in nature? Molecular geometry = ________________________
g. see saw	

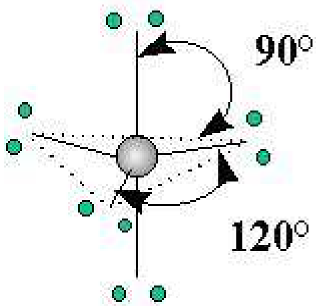
	A. You are to determine the molecular geometry of a methylamine molecule, CH_3NH_2 Determine the Lewis structure of the molecule (the H atom bonding is indicated by the formula, and remember, H can only form one bond, a consequence of the duet rule!)
a. 	B. Which is (are) the central atom(s) in the molecule? Central atom(s) = ________________________________
b. both the C and the N atoms can be thought of as central atoms	C. In cases where there is more than one central atom, the total geometry depends on the geometry around each central atom. How many independent regions of electron density are on each central atom? # regions: C = _______________ N = _________________
c. C = 4 N = 4	D. Note that the bond between the C and N is counted twice, as a region belonging to each atom. How will the regions around each atom arrange themselves? Electron geometries: C = _____________________________ N = _____________________________

d.
C = tetrahedral
N = tetrahedral
	E. How many of the regions around each central atom are used in bonding?
	
	# bonded regions: C = _______________
	N = _______________

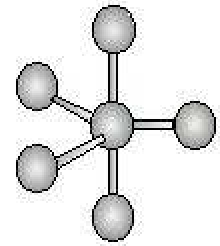
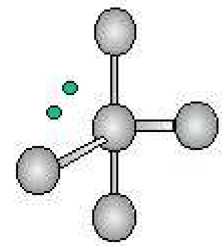
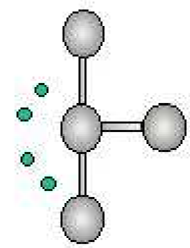
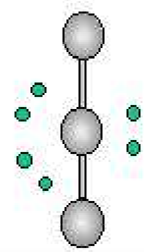
e. C = 4 N = 3	F. According to the table of electron geometries, what will be the arrangement of atoms around each central atom? Molecular geometries: C = ____________________ N = ____________________
f. C = tetrahedral N = trigonal pyramidal	

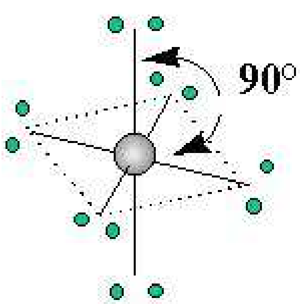
Number of electron pairs	Arrangement of electron pairs	Electron-pair geometry	Predicted bond angles
2		Linear	180°
3		Trigonal planar	120°
4		Tetrahedral	109.5°
5		Trigonal bipyramid	90° 120°
6		Octahedral	90°

Total Electron Pairs	Electron Pair Geometry	Bonding Pairs	Nonbonding Pairs	Molecular Geometry
2	 Linear	2	0	 Linear
3	 Trigonal planar	3	0	 Trigonal planar
		2	1	 Bent
4	 Tetrahedral	4	0	 Tetrahedral
		3	1	 Trigonal pyramidal
		2	2	 Bent

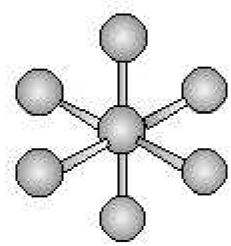
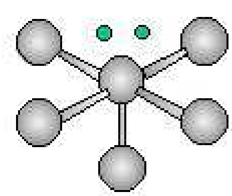
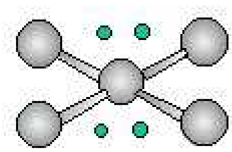


Trigonal Bipyramidal

B.P.	N.B.P.		
5	0	**Trigonal Bipyramidal**	
4	1	**Seesaw**	
3	2	**T-shaped**	
2	3	**Linear**	



Octahedral

B.P.	N.B.P.		
6	0	**Octahedral**	
5	1	**Square Pyramidal**	
4	2	**Square Planar**	

Supplement #3: 3-D DRAWING

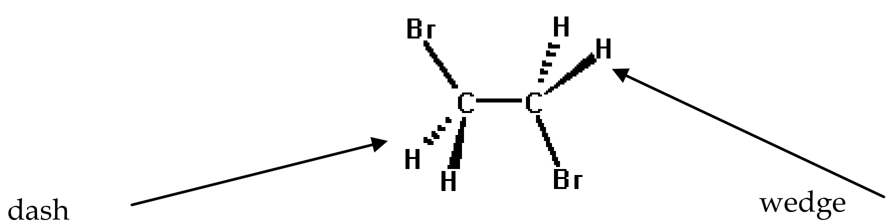
Often it is necessary to try and represent three-dimensional molecular geometries in drawings. The following instructions are intended to illustrate a method for drawing 3-D geometries. The important consideration is to obtain realistic drawings that represent the geometry of the molecule.

In order to keep the situation simple, atoms in a molecule will be represented simply by their symbol. The bond attaching atoms will be represented by lines connecting the atoms. For example, HCl can be represented as:

H —— Cl

Molecules with geometries that are in one plane can be represented on paper quite easily. The difficulty arises with some of the molecules that are based on the tetrahedron, trigonal bipyramidal, and onctahedron. Some of these are 3-D and therefore require perspective drawings.

A technique for suggesting perspective is to use the wedge and dash method. Bonds which are meant to be shown coming out of the plane of the paper _toward_ the reader are shown with the solid wedge, and those going out of the plane of the paper, _away_ from the reader are shown as a dashed wedge. Atoms that lie in the plane of the paper and go neither towards nor away from the reader are drawn with the straight flat line

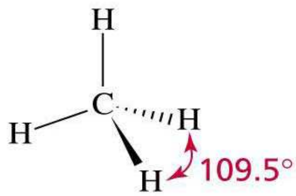


In the figure above, the Br are in the plane of the paper and are drawn with the straight lines that we are used to. The hydrogens in the molecule, however, appear to come out of the paper towards the reader (wedge) and appear to go away from the reader (dash).

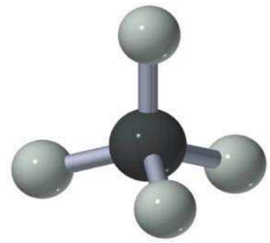
Consider the methane molecule: CH_4. The molecule is tetrahedral in nature. It is not a flat square. Therefore drawing it as a flat molecule is not an accurate representation of the actual molecule.

```
    H
    |
H — C — H
    |
    H
```

If the line, wedge, and dash technique is applied to methane, the actual depiction of methane is created:



perspective formula of methane



ball-and-stick model of methane

Name: ____

$SiCl_4$ (no Cl-Cl bonds)

valence electrons ______________________

Lewis structure:

Molecular geometry = ____________________

3-D drawing: (optional)

PCl_3 (no Cl-Cl bonds)

valence electrons ______________________

Lewis structure:

Molecular geometry = ____________________

3-D drawing: (optional)

NO_3^{-1} (no O-O bonds) # valence electrons ______________________

Lewis structure: Molecular geometry = ___________________

3-D drawing: (optional)

SF_6 (no F-F bonds) # valence electrons ______________________

Lewis structure: Molecular geometry = ___________________

3-D drawing: (optional)

PCl_5 (no Cl-Cl bonds) # valence electrons ______________________

Lewis structure: Molecular geometry = ___________________

3-D drawing: (optional)

IF_3 (no F-F bonds) # valence electrons ______________________

Lewis structure: Molecular geometry = ___________________

3-D drawing: (optional)

XeF_5^{+1} (no F-F bonds)

\# valence electrons ______________________

Lewis structure:

Molecular geometry = ___________________

3-D drawing: (optional)

SO_4^{-2} (no O-O bonds)

\# valence electrons ______________________

Lewis structure:

Molecular geometry = ___________________

3-D drawing: (optional)

C_4H_8O

valence electrons ________________________

Lewis structure:

Molecular geometry = ____________________

3-D drawing: (optional)

C_5H_{12}

valence electrons ________________________

Lewis structure:

Molecular geometry = ____________________

3-D drawing: (optional)

Examples of work to be done during the in-class activity periods:

(note: only the molecular formulas are given, you will be determining the number of valence electrons, the Lewis structure, the geometry and give the 3-D drawing)

NH_3 # valence electrons __________8_____________

Lewis structure: Molecular geometry = trigonal pyramidal

3-D drawing: (optinal)

$CH_3CH_2CH_3$ # valence electrons __________20____________

Lewis structure: Molecular geometry = tetrahedral around each C

3-D drawing: (optional)