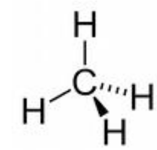
Molecular Models Lab



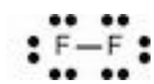
Objectives

1. Learn about the structures of covalent compounds and polyatomic ions.
2. Draw Lewis structures based on valence electrons and the octet rule.
3. Construct 3-dimensional models of molecules and ions with single, double, and triple bonds.
4. Use wedges and dotted lines to construct 3-dimensional drawings of molecules and ions.
5. Determine probable identities of molecules based on their 3-dimensional models.

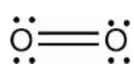
Background

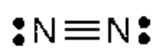
Covalent Bonding and Lewis Structures
Compounds and polyatomic ions that include nonmetals are held together by covalent bonds. These are different from ionic bonds, which involve positive and negative ions, where the positive ions are metals that have lost electrons and the negative ions are nonmetals that have gained electrons. Covalent bonds are formed between two nonmetals in compounds (e.g., CO_2 and NF_3) or ions (e.g., NO_3^- or SO_4^{2-}). In a covalent bond, both of the elements want to gain electrons to fill gaps in their outer ("valence") shells. Instead of transferring electrons and forming ions, they share electrons, allowing each atom to fill its valence shells with the shared electrons. Bonds typically involve pairs of electrons, forming molecular orbitals similar to atomic orbitals. A single bond is a single pair of shared electrons, a double bond is two shared pairs, and a triple bond is three.

Single bonds share two electrons between atoms. For example, the fluorine atom, with its seven valence electrons, needs only one more electron to fill its valence shell with an octet of electrons similar to that in the noble gas, neon. Two fluorine atoms, each with an unpaired electron in only one of its 2p-orbitals, can share those unpaired electrons, forming a single bond between them. The diagram below, for the F_2 molecule, is called a Lewis structure, named after Gilbert N. Lewis, who introduced this type of diagram in 1916. The Lewis structure shows all of the valence electrons within the molecule, and how the atoms are connected. Each line in the Lewis structure represents a bond containing two electrons.



Double bonds share four electrons and are represented with two lines (each line, again, representing two shared electrons) as shown below for the O_2 molecule. Triple bonds are represented with three lines, as shown below for the N_2 molecule.





Valence electrons, as mentioned above, are the electrons in the outer shell of an atom. Fluorine, with its electron configuration of $1s^2 2s^2 2p^5$, has seven valence electrons (i.e., the two 2s electrons and the five 2p electrons, all of which are in the n=2 shell, which is the highest occupied shell in the fluorine atom). Notice that the Lewis structure for the F_2 molecule has a total of 14 valence electrons, which is the sum of the valence electrons in the two fluorine atoms. This will be the case for all covalent molecules: the total valence electrons in the molecule will be equal to the sum of valence electrons from all atoms in the molecule. Check the diagrams for O_2 and N_2 to verify the previous statement.

The Octet Rule is general pattern observed in most covalent molecules. With very few exceptions (e.g., hydrogen and boron, and compounds with an odd number of total electrons), atoms in covalent compounds are surrounded by eight (an "octet") of electrons. This makes sense because by sharing valence electrons, they are filling up their outer ("valence") shell of electrons. If you look closely at electron configurations, the outer shell always consists only of "s" and "p" electrons, and when they are full, these subshells (s and p) have two and six electrons, respectively, for a total of eight. The eight valence electrons are found in all noble gas atoms, in common ions of many atoms (e.g., alkali metals, alkaline earth metals, and aluminum), and surrounding most atoms in covalent compounds.

Hydrogen is an exception. It is found with only one single bond (two electrons) attached to it. Note that the corresponding noble gas, helium, also has only two electrons and that its valence shell is complete with just the two. Boron is another exception; it is typically encountered with only three pairs (six electrons) around it in covalent compounds. Additional exceptions may be encountered in future chemistry courses, but not here.

A Lewis structure shows all valence electrons for a covalent molecule. It also shows which atoms are bonded to which other atoms, the type of bond, and the nonbonding pairs surrounding each atom. A Lewis structure is similar to what some books call a "structural formula" but also includes the nonbonding pairs as pairs of dots. A Lewis structure uses dashes for bonds (single, double, or triple) instead of using the dots for bonds. In summary, a Lewis structure has dashes for bonding pairs of electrons and dots for nonbonding electrons. Lewis structures may be used to represent the structures of covalent compounds or covalently-bound polyatomic ions, such as the nitrate ion or the ammonium ion.

A simple procedure for drawing Lewis structures is available in your textbook. Whatever the method of arriving at a correct Lewis structure, the resulting diagram must have the following two conditions:

- The number of valence electrons must match those from all of the atoms in the molecule or ion.
- Each atom must be surrounded by an octet of electrons. The electrons in an octet may be bonding electrons (single, double, or triple bonds) or nonbonding electrons (lone pairs). A line between atoms represents a pair of bonding electrons. Two dots on at atom represent a lone pair of nonbonding electrons. H and B are exceptions, as noted above.

Molecular Geometry. Once you have a Lewis structure, you can now determine the geometry of the electron groups around the central atom. The "central atom" is basically the atom of interest. It's the atom you're looking at, to see how other atoms are arranged around it. The geometry is important in determining the properties and reactivity of chemical compounds. In many compounds, there are many "central" atoms. In fact, any atom that has more than one other atom attached to it can be called a "central" atom. It's not always the center of the molecule, it's just the center of attention when you're considering the molecular geometry.

Electron Groups. When considering the geometry (shape) of atoms around a central atom, it's necessary to consider all of the groups of electrons around that atom. Because electrons are all negatively charged, they repel each other, so the groups of electrons tend to stay as far away from each other as possible. This concept it often called "valence shell electron pair repulsion" or VSEPR theory. For our purposes, an "Electron Group" is any single bond, double bond, triple bond, or nonbonding pair of electrons. Double and triple bonds are considered to be individual electron groups because they represent four or six electrons all being shared by a single atom bonded to the central atom. Single bond and lone pairs are also individual electron groups. There is an important distinction between the electron groups surrounding a central atom (which arrange themselves in specific geometries depending on their number) and the atoms surrounding a central atom. Only the atoms are considered when defining the geometry of the molecule.

Procedure for Drawing Lewis Structures
- Calculate the sum of valence electrons in the molecule (the total valence electrons from each atom).
  - For negative ions, add one electron for each negative charge.
  - For positive ions, subtract one electron for each positive charge.
- Draw a temporary structure, a first try.
  - Least electronegative atom goes in the middle.
  - (Hydrogen never goes in the middle.)
  - Unless told otherwise, assume all other atoms are bound to the central atom.
  - Put a single bond between each pair of bonded atoms. (A single bond is a single dash.)
  - Make an octet of electrons (using dot pairs for nonbonding "lone pairs") around each atom.
- Count the electrons in the temporary structure.
- Compare the number of electrons in the temporary to the total number of available valence electrons.
  - If the temporary structure does not have enough electrons, add electron pairs to the central atom. In this case, the octet rule may be violated for the central atom.
  - If the temporary structure has too many electrons, then you need to make double or triple bonds to correct the total. Remember to keep following the octet rule.
- Check the number of electrons and the octet rule again.

Procedure for Determining Electron Group Geometries and Molecular Geometries

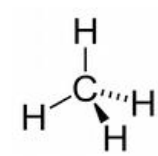
Once you have a Lewis structure, the central atom geometry may be determined.
- Count the number of electron groups around the central atom. An "electron group" is a single bond, a double bond, a triple bond, or a nonbonding pair.
- The geometry of the electron groups should minimize electron group repulsions. See the table below for a list of Electron Group Geometries for central atoms surrounded by 2, 3, or 4 electron groups.
- The molecular geometry is the arrangement of atoms in space, not including the lone pairs. (The lone pairs take up space, but are not included when describing the molecular geometry.) See the table below for a list of molecular geometries for various numbers of electron groups and atoms surrounding a central atom.

You can probably memorize the table, but the purpose of this lab is to encourage you to make models of various molecules, so that you will be able to visualize the common structures around central atoms in covalently bonded molecules and ions. By the end of today's lab period, you should be able to construct Lewis structures for covalent molecules and ions based on their chemical formulas, and to envision molecular shapes based simply on their Lewis structures. You will also practice drawing 3-dimensional diagrams of simple molecules that show their geometries from perspective viewpoints.

Number of electron groups	Geometry of electron groups	Number of bonding pairs	Number of lone pairs	Molecular Geometry
2	Linear (180º)	2	0	Linear
3	Trigonal Planar (120º)	3	0	Trigonal planar
		2	1	Bent (120º)
4	Tetrahedral (109º)	4	0	Tetrahedral
		3	1	Trigonal pyramidal
		2	2	Bent (109º)

Procedure for Drawing 3-Dimensional Structures

A 3-dimensional structure shows what a molecule looks like, with the correct bond angles and a 3-dimensional perspective, if necessary. If a molecule or ion is planar, it can be drawn with straight lines for bonds (using single lines for any bonds). The lone pairs need not be shown in a 3-D structure. If a molecule is not planar, the idea is to use as many regular lines as possible, then use wedges to represent bonds that are protruding out in front of the page and dotted lines for bonds that are pointing back behind the page, as shown in the diagram to the right for the CH_4 molecule, which has a tetrahedral molecular geometry.

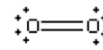


Procedure

In the <u>data table</u>: Work from ***right to left*** for each molecule or ion. That is, start with the valence electron calculation, the draw the Lewis structure, then determine the name of the molecular geometry and draw your 3-dimensional structure.

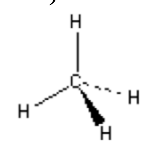
- **Valence Electrons column**: Show your <u>calculation</u> for the number of valence electrons. For example, the calculation for H_2O would be (2)(1)+(1)(6)=8.

- **Lewis Structure column**: Draw the <u>Lewis dot structure</u> here (see above, i.e., include the nonbonding pairs in your structure). Use lines for bonds and dots for lone pairs. See examples for O_2 and carbon monoxide.



  For many of the molecules, the first element listed in the formula is typically the least electronegative element (most "metallic character") in the compound and is found in the middle of the structure, with the other elements attached to it. See below for additional guidance.

- **Molecular Geometry column**: Write the <u>name of the molecular geometry</u> for each atom with two or more other atoms attached to it (each "central atom). There may be more than one of these 'central' atoms, so do both or all of them, and make sure you let me know which atoms are which. (Your choices are "linear", "bent 109º", "bent 120º", "trigonal planar", "trigonal pyramidal", or "tetrahedral".)



- **3-D Structure column**: No change, except that I would like you to use wedges and dotted lines, as we do in the lecture class, to show the 3-dimensional structure. An example for CH_4 is shown above.

- For the "**unknowns**," we will have some models in the lab. Use what you've learned about the geometries, bonds, and lone pairs around various elements to determine what molecules the unknown molecular models represent. It is possible that more than one answer exists for each model, but you only need to come up with one of those answers.

Additional information: A few of the compounds in this lab are a little more complex than the simple ("everything attached to the central atom") type of molecule. Remember a hydrogen atom can only be connected to one other atom, so it never goes in the middle. For clarification, I've described the more complex structures here:

HOCl: Connected as shown in the formula.
H_2O_2: Two oxygen atoms connected to each other; with one hydrogen atom on each side.
N_2H_4: Nitrogen atoms are connected to each other, with two H's on each side.
NH_2OH: Two H's and O are connected to the nitrogen, with the other H connected to the O.
C_2H_4: Carbons are connected to each other, with two H's on each side.
CH_3OH: Oxygen and three hydrogens attached to carbon; other hydrogen attached to oxygen.
HCOOH: One H and two O's connected to carbon, with other H connected to one O atom.
C_2H_3Cl: Carbon atoms connected to each other, with two other atoms connected to each C.
C_2H_2: Carbons connected to each other, with one H on each.
HOCN: Connected as shown in the formula.
CH_2O: Carbon in middle, everything else attached directly to it.

That's it. Have fun making your models.

Pre-lab Assignment

1. Write the electron configurations and identify the number of valence electrons for each of the following elements.

   Oxygen

   Sulfur

   Nitrogen

   Phosphorus

   Hydrogen

   Fluorine

2. Write the name of the molecular geometry for each of the following molecules.

   a. A molecule with a central atom surrounded by two singly-bonded atoms and two lone pairs.

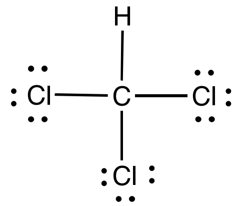
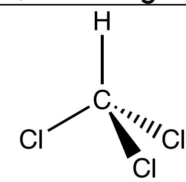
   b. A molecule surrounded by three atoms and one lone pair.

   c. A molecule surrounded by three atoms and no lone pairs.

   d. A molecule with a central atom surrounded by two doubly-bonded atoms.

   e. A molecule that contains only two atoms.

DATA TABLE

Formula	Total Valence Electrons	Lewis Dot Structure	Electron Group Geometry	Molecular Geometry	3-D Structure (Bond Angles)
$CHCl_3$	4+1+3(7)= 26		Tetrahedral	Tetrahedral	 (109.5º)
H_2					
Cl_2					
Br_2					
HCl					
HBr					
CH_4					

*Specify geometry and bond angles around _each_ central atom, if there is more than one.

DATA TABLE

Formula	Total Valence Electrons	Lewis Dot Structure	Electron Group Geometry	Molecular Geometry* & Bond Angles*	3-D Structure
CH_2Cl_2					
HOCl #					
H_2O_2 #					
NH_3					
N_2H_4 #					
NH_2OH #					
HOCN #					

* Specify geometry and bond angles around *each* central atom, if there is more than one.
# See additional information on page 4

DATA TABLE

Formula	Total Valence Electrons	Lewis Dot Structure	Electron Group Geometry	Molecular Geometry* & Bond Angles*	3-D Structure (Bond Angles*)
O_2					
C_2H_4 #					
CH_3OH #					
HCOOH #					
C_2H_3Cl #					
C_2H_2 #					
CH_2O #					

* Specify geometry and bond angles around *each* central atom, if there is more than one.
# See additional information on page 4

DATA TABLE

Chemical Formula	Total Valence Electrons	Lewis Dot Structure	Electron Group Geometry	Molecular Geometry* & Bond Angles*	3-D Structure (Bond Angles*)
N_2					
CO_2					
CN^-					
H_3O^+					
NO_2^-					
SO_2					
O_3					

* Specify geometry and bond angles around *each* central atom, if there is more than one.
# See additional information on page 4

Unknown Molecules

	3-D Structure	Molecular Geometry* (Bond Angles*)	Proposed Lewis Dot Structure	Chemical Formula	Total Valence Electrons
#1					
#2					
#3					
#4					
#5					

*Specify geometry and bond angles around *each* central atom, if there is more than one.