CHM 130LL: Molecular Models

In this lab, you will study covalently bonded molecules—i.e., molecules where nonmetal atoms are held together because they share one or more pairs of electrons. In this experiment, you will:

- draw Lewis dot structures for simple molecules
- use Lewis dot structures to make three-dimensional models of molecules
- learn how the electrons around a central atom determine a molecule's shape
- use the polarity of individual bonds and the three-dimensional shape of a molecule to determine if the molecule is polar or nonpolar
- use the "like dissolves like" rule to determine if two compounds are soluble or miscible based on the polarity of each compound

You will work in pairs and use a set of molecular models to build models of all the molecules to be explored. When all your models are built, **show your instructor for his/her initial** on the front page of the report.

I. Guidelines for Drawing Lewis dot structures

1. Add up the total number of valence electrons for all the atoms in the molecule. Remember that the number of valence electrons is equal to the Group Number (from the Periodic Table) for all the Group A elements.
2. Write the element symbol for the central atom (usually it is underlined).
3. Write the element symbols for all the outer atoms around the central atom, then draw a straight line to connect each outer atom to the central atom via single bonds.
4. Distribute the rest of the valence electrons in pairs, making sure that each H has 2 electrons total (or one pair) and all other atoms have an "octet".
5. If there are not enough electrons for each atom in the molecule to have an octet (except H has only 2 electrons total) then you will need to consider using a double bond between 2 atoms. If this doesn't allow all atoms (except H with 2) to have an octet, then consider a triple bond.

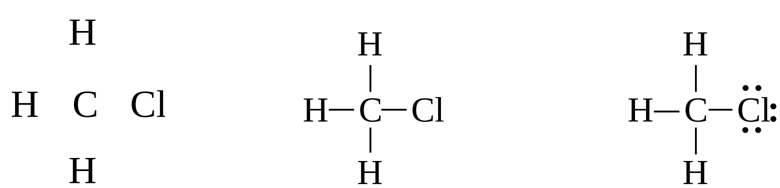
Example: Draw the *Lewis dot structure* for $\underline{C}H_3Cl$.

1. Calculate the total number of valence electrons for all atoms in the compound:

$$\text{valence } e^- \text{ for C} + 3\,(\text{valence } e^- \text{ for H}) + \text{valence } e^- \text{ for Cl} = 4 + 3(1) + 7 = 14\ e^-$$

2. The central atom is C since it is underlined. (See figure labeled Step 3 below.)
3. Next, we connect all the atoms with single bonds. (See figure labeled Step 4 below.)
4. The C atom has an octet, and each H atom has a pair of electrons. The last three pairs are put around the Cl, so it also has an octet. Thus, the Lewis electron-dot structure for CH_3Cl is shown below:

Step 3 **Step 4** **Step 5 – final structure**



The most common type of molecular models are those using balls and sticks. ***Each ball represents an atom***, and ***each stick represents a bond of 2 electrons*** between two atoms. The convention is to use different colored balls to represent different elements. Below are the most commonly used colors for a few elements and the rationale for each color:

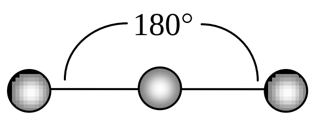
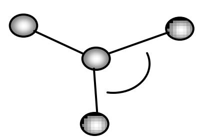
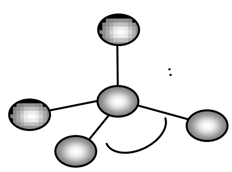
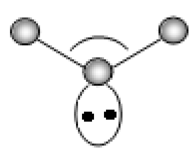
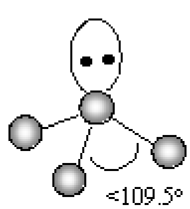
carbon = black (color of coal)
nitrogen = blue (color of the sky since nitrogen makes up 78% of air)
oxygen = red (since fire is red and requires oxygen)
hydrogen = white (color of clouds since hydrogen is the lightest element)

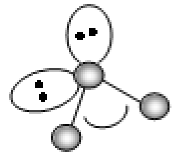
Although single bonds are actually longer than double bonds and triple bonds, use the short grey sticks for the single bonds and the longer sticks to make the multiple bonds. Note: you will need to use 2 long grey sticks to form double bonds and 3 grey sticks for triple bonds. The long grey sticks will bend so that you can attach more than 1 stick between 2 atoms.

II. Molecular Shapes

To determine the shape of a molecule you must first draw the Lewis dot structure. Then you assign a generic ABE formula to the molecule where A is the center atom, B is any atom bonded to the center atom, and E is a lone pair on the center atom. Then you look up that generic ABE formula in the table below to find the shape.

CHM 130 Table of Molecular Shapes and Bond Angles

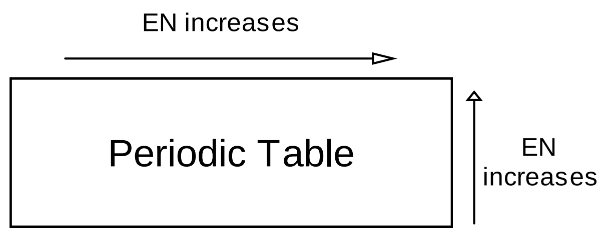
General formula	MOLECULAR GEOMETRY	NAME of SHAPE	Bond Angles
AB_2		linear	180˚
AB_3		trigonal planar	120˚
AB_4		tetrahedral	109.5˚
AB_2E		bent	<120˚
AB_3E		trigonal pyramid	<109.5˚

AB_2E_2		**bent**	**$<109.5^\circ$**

III. Polarity of Individual Bonds

Electronegativity is the ability of an atom in a chemical bond to attract bonded electrons to itself.

Trends for Electronegativity (EN)
Fluorine (F) is the most electronegative element in the Periodic Table. In general, the closer an element is to fluorine, the more electronegative it is. The exception is hydrogen, (H), which has an electro-negativity value between boron (B) and carbon (C). For example, when comparing whether Cl or P is closer to F on the Periodic Table, Cl is closer, so Cl must be more electronegative than P.



Exception: H's EN is between B and C

When two atoms share electrons in a covalent bond, they will not share equally if one atom is more electronegative than the other. The "tug of war" for the electrons shared results in the atom with the higher electronegativity pulling the electrons more strongly towards itself, and thus, forming the **negative (electron rich) end** of the bond. Since electrons spend less time around the other atom, that atom becomes the **positive (electron deficient) end** of the bond. Thus, one end of the bond is partially negative, and the other end is partially positive, so the bond has two poles (like the positive and negative ends of a magnet). This separation of charges is called a **dipole**, and bonds with a dipole are ***polar covalent bonds***.

In the example below, very electronegative F pulls the bonding electrons away from the less electronegative H. We show this using ***delta (δ) notation***, where the more electronegative atoms gets the δ^- and the less electronegative atom gets the δ^+. We also use an arrow to indicate the dipole (pointing from the positive H end to the negative F end) in HF molecule, as shown below:

$$\overset{\delta^+}{\mathrm{H}}—\overset{\delta^-}{\mathrm{F}}$$
$$\longmapsto$$

where δ means "partial,"
so each atom has a partial charge

In general, the greater the **difference** in electronegativity values, the more polar the bond.

In some molecules, two atoms have equal electronegativities, so they share the bonding electrons equally in what is called a **nonpolar covalent bond**. For example, the electrons in the H–H bond in H_2 are shared equally by the H atoms, so this a nonpolar covalent bond.

Note: Since the electronegativity values for C and H are very close, the *C-H bond is considered to be nonpolar.* Use this generalization when making your predictions.

IV. Polarity of Molecules

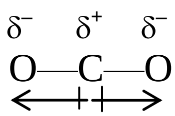
Molecular polarity depends on both the polarity of the individual bonds and on the geometry around the central atom. A **polar molecule** has an overall dipole (a partial positive end and partial negative end). However, in some molecules with polar covalent bonds, the dipoles cancel out one another, so the molecule has no overall (or net) dipole. Molecules with no net dipole are **nonpolar molecules**. Nonpolar molecules are typically symmetrical, and the center of the δ+ and δ- charge coincides.

For a molecule to be polar, two requirements must be met:

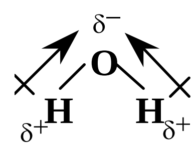
1. The molecules must contain polar covalent bonds (i.e. dipoles).
2. The shape of the molecule must be such that the dipoles in the molecules do not cancel one another, like a "tug of war" with two equally matched teams.

   Note: The three-dimensional shape of the molecule NOT the two-dimensional Lewis dot structures determines if dipoles in the molecules will cancel.

For example, consider the following molecules: CO_2 and H_2O. In CO_2, each C–O bond is polar with oxygen at the partial negative end (indicated with δ^-) and carbon at the partial positive end (indicated with δ^+). In H_2O, each O–H bond is polar with oxygen at the partial negative end (indicated with δ^-) and hydrogen at the partial positive end (indicated with δ^+). The dipoles for each molecule are shown as arrows. Because the CO_2 molecule is linear, its dipoles pull in exactly opposite directions to cancel each other, making the overall molecule nonpolar.



CO_2 is a linear molecule
with two polar bonds that cancel. Thus,
CO_2 is a *nonpolar molecule*.



Water is a bent molecule
with two polar bonds that do not cancel each other out. Thus, **water is a *polar molecule*.**

However, the water molecule, **H_2O**, **is bent**. The oxygen end of the molecule is partially negative (indicated with δ^-) and the hydrogen ends are partially positive (indicated with δ^+), but the angle prevents the dipoles from canceling each other out. Thus, **H_2O is a polar molecule.**

Use the following guidelines and your models to predict whether the molecules are polar or nonpolar.

A molecule with polar bonds is <u>polar</u> if the polar bonds do not cancel with each other.

V. Polarity and Physical Properties

Finally, the polarity of a molecule will determine its physical properties. The **"like dissolves like" rule** states that polar molecules will only dissolve in or mix with other polar molecules, and nonpolar molecules will only dissolve in or mix with other nonpolar molecules. Polar molecules never mix with or dissolve in nonpolar molecules. For example, Italian dressing contains oil and vinegar. Since oil is nonpolar and vinegar is polar, the two will never mix and always form two separate layers.

CHM 130LL: Molecular Models

Name: ________________________

Partner: ________________________

Instructor Initial __________

Section Number: ___________________

I. Lewis Dot Structures and Molecular Models

Indicate the number of valence electrons for each of the following atoms:

H ______ C ______ Br ______ O ______ P ______ Mg _________

Part A: Molecules with Five Atoms

Draw Lewis dot structures for the molecules below:
(Note: Central atoms are underlined.)

$\underline{C}H_4$	$\underline{C}H_3Cl$	$\underline{C}Cl_4$
# e^- = ____________________ Shape: ___________________ Polar bonds? Yes or No or both Polar molecule? Yes or No	# e^- = ____________________ Shape: ___________________ Polar bonds? Yes or No or both Polar molecule? Yes or No	# e^- = ____________________ Shape: ___________________ Polar bonds? Yes or No or both Polar molecule? Yes or No

Use the molecular modeling kits to ***make models of each of the molecules***.
Use the colors designated below for atoms of each element:

carbon=black hydrogen=white chlorine=green

Use the *short grey sticks for single bonds*. *The longer bonds are for double bonds.*

Question: The grey sticks in your models represent a covalent bond (a shared pair of electrons) holding atoms together. Given that electrons are negatively charged, why are these three molecules three-dimensional with 109.5˚ bond angles (a shape called "tetrahedral") rather than being flat with 90˚ bond angles? *(Hint: think about what happens when electrons get close to one another)*

Answer:

Part B: Diatomic Molecules

Draw the Lewis dot structure for the **HCl** molecule on the right:

Next, make a model of the HCl molecule.

HCl
e^- = ____________________ Shape: ____________________ Polar bonds? Yes or No Polar molecule? Yes or No

Part C: Molecules with Three Atoms

Draw Lewis dot structures for the molecules below:
(Note: Central atoms are underlined.)

$H_2\underline{O}$	$\underline{C}O_2$
# e^- = ____________________ Shape: ____________________ Polar bonds? Yes or No or both Polar molecule? Yes or No	# e^- = ____________________ Shape: ____________________ Polar bonds? Yes or No or both Polar molecule? Yes or No
$\underline{S}O_2$ # e^- = ____________________ Shape: ____________________ Polar bonds? Yes or No or both Polar molecule? Yes or No	$H\underline{C}N$ # e^- = ____________________ Shape: ____________________ Polar bonds? Yes or No or both Polar molecule? Yes or No

Make models of each molecule above using the colors designated below:

carbon=black sulfur = black oxygen=red hydrogen=white nitrogen=blue

Use the *short grey sticks for single bonds* and the *long flexible grey sticks* for *double and triple bonds*. (Note: In reality, single bonds are longer than double or triple bonds.)

Fill in the table below:

Molecule	**# of lone pairs on central atom**	**linear or bent?** (Circle one)
H_2O		linear bent
SO_2		linear bent
CO_2		linear bent
HCN		linear bent

Question: Based on your answers in the table above and the molecules' Lewis dot structures, explain why some of the molecules are bent while others are linear?

Answer:

Part D: Molecules with Four Atoms

Draw Lewis dot structures for the molecules below:
(Note: Central atoms are underlined.)

formaldehyde, <u>C</u>H_2O	ammonia, <u>N</u>H_3
$\#\ e^- =$ ______________________ Shape: ____________________ Polar bonds? Yes or No or both Polar molecule? Yes or N	$\#\ e^- =$ ______________________ Shape: ____________________ Polar bonds? Yes or No or both Polar molecule? Yes or No

Make models of each molecule above using the colors designated below:

carbon=black oxygen=red hydrogen=white nitrogen=blue

Use the *short grey sticks for single bonds* and the *long flexible grey sticks* for *double and triple bonds*.

Refer to your models for NH_3 and CH_2O to fill in the table below:

Note: A molecule is "planar" if the centers of all the atoms sit in one plane. (A "plane" is flat like a piece of paper)

Molecule	**# of lone pairs on central atom**	**planar or nonplanar?** (Circle one)
NH_3		planar nonplanar
CH_2O		planar nonplanar

Question: Given the type of electrons around its central atom, what prevents the H atoms in the NH_3 molecule from being in the same plane as the N atom?

Answer:

II. Polarity of Individual Bonds

For all the ***polar covalent bonds*** below, indicate the less electronegative atom (positive end) with a δ^+ and the more electronegative atom (negative end) with a δ^-, then draw an arrow from the less electronegative to the more electronegative atom. Do not draw delta charges or dipole arrow for nonpolar bonds.

H–Cl C–O O–H N–H C–Cl C–H

III. Polarity and Physical Properties

The polarity of a molecule determines its physical properties, like solubility and miscibility. **Solubility** indicates whether a solid will dissolve in a liquid. For example, table sugar is ***soluble*** in water since it dissolves in water, but silver metal is ***insoluble*** in water since it does not dissolve in water. **Miscibility** refers to whether two liquids will mix. For example, rum and Coke are ***miscible*** because they mix, but oil and vinegar are ***immiscible*** because they do not mix. Now chemicals will mix if they have the same polarity. For example two nonpolar chemicals can mix, and two polar chemicals can mix. But a nonpolar chemical will never mix with a polar chemical. This is called "like dissolves like."

Fill in the blanks using these terms: *soluble, insoluble, miscible, immiscible.*

a. If a solid dissolves in a liquid, it is ________________.

b. If two liquids do not mix, they are ________________.

c. If two liquids mix, they are ________________.

d. If a solid does not dissolve in a liquid, it is ________________.

Refer to your answers on page 8 and the discussion on "like dissolves like" on the bottom of page 4 to answer the following questions:

1. Water molecules are ________. polar nonpolar

2. CCl_4 molecules are ________. polar nonpolar

3. Given that CCl_4 is a liquid at room temperature, CCl_4 and water are _________.

   (Circle one) soluble insoluble miscible immiscible

4. Explain your answer to question 3 above based on polarity and "like dissolves like".

5. A student noticed that iodine solid, I_2*(s)*,
   is insoluble in water; thus, iodine must be ________. polar nonpolar

6. Thus, iodine, I_2*(s)*, must be _______________ in CCl_4.

   (Circle one) soluble insoluble miscible immiscible

7. Explain your answer to question 6 based on polarity and "like dissolves like".