University of Wisconsin
Chemistry 116
Introduction to Molecular Structures by Building Models*

Anyone who has even the slightest interest in chemistry is interested in how substances appear, e.g. color, texture, odor, and physical form, and how they interact with other substances in chemical reactions or the formation of solutions. To consider yourself a *chemist*, and yes you are a chemist when you take a chemistry course at UW, you really want to understand how the "macroscopic" appearance, reactivity, and solubility of the substance results from the "microscopic" behavior of the atoms or molecules which make up the substance. Where an ordinary person sees a few milliliters of water in a cup, a *chemist* "sees" about a septillion little water molecules moving and interacting in a way that keeps them mostly in the cup. The chemist also "sees" the 1 in 10,000 water molecules that have escaped the bulk liquid to make up the water vapor above the liquid in the cup.

Water has several unique properties, it is a liquid at temperatures where most molecules its size are gases, the solid form is less dense than the liquid form (ice floats !!), and it's a wonderful solvent. These properties can be attributed to the specific structure and bonding of the water molecule. The structure and bonding in the molecule govern the interactions the molecule has with other atoms and molecules, and ultimately determine the physical and chemical properties of the bulk material.

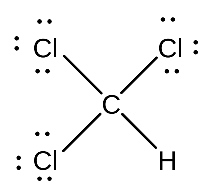
In this activity, you will construct molecular models of a variety of compounds. From the models, you will predict the polarity of the molecule, identify important interactions the molecule could have with other molecules, identify locations on the molecule where it could be charged, identify locations of reactivity, and justify the compounds solubility in different types of solvents. An added benefit is that you will become familiar with a variety of ways that chemical formulas can be written to help describe molecular structure.

Preparation for the Activity

Before you come to lab to do the activity, remind yourself how to draw Lewis Diagrams for simple molecules. Refer to Section 3.8 in your textbook (*Principles of Modern Chemistry 6th Ed*, Oxtoby, Gillis, Campion). Also read about hybridization in section 6.4.2 of the text. Finally, view the campy intermolecular forces video located at http://www.youtube.com/watch?v=p-t1McO4-Bw

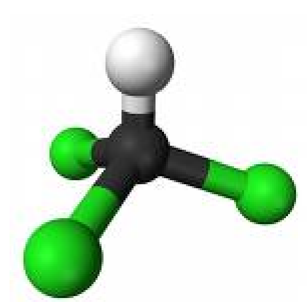
Example Molecule As an example, we will use chloroform to illustrate the process of predicting the molecular structure and drawing conclusion from the geometry and bonding of the molecule. Chloroform has the formula $CHCl_3$. Chloroform is a volatile liquid found in most chemical laboratories because of its use as a general solvent. It is also commonly used in the extraction process for isolating alkaloids from plant materials. Common alkaloids are caffeine, nicotine, cocaine and morphine. Chloroform was used as one of the original anesthetics in the late 19th century and today is used to make the refrigerant CHF_2Cl (R-22).

Draw the Lewis Structure



Identify the electron pair geometry and hybridization *There are 4 bonding pairs of electrons around the central carbon atom. There are 3 lone pairs and 1 bonding pair around each chlorine atom, and 1 bonding pair around the hydrogen atom. Each C-Cl bond is described as an overlap between an sp^3 hybrid orbital from C with an sp^3 hybrid orbital from Cl. The 4 electron pairs around the carbon and each Cl atom will orient into a tetrahedral shape to minimize electron repulsions. The C-H bond is described as an overlap of the sp^3 hybrid from C and the 1s orbital from the H.*

Predict the geometry and build the molecule *The geometry of the molecule is determined by the arrangement of the bonding electron pairs around the C atom, so the geometry is also tetrahedral with bond angles near 109.5^o A slight distortion from pure tetrahedral occurs because of the unequal sizes of H and Cl*



Identify the polar bonds and predict the polarity of the molecule *The C-Cl bonds are polar due to the high electronegativity of Cl. The C-H bond is only slightly polar because the electronegativity difference between C and H is small. Because of the arrangement of the 3 C-Cl polar bonds, the molecule is also polar with the Cl atoms being partially negative and the H atom being partially positive.*

Identify the important intermolecular forces and justify physical properties
All molecules have some degree of polarizability and therefore can attract each other via dispersion forces. The large electron clouds around the Cl atoms will be fairly polarizable. The molecule is polar so dipole-dipole forces should also be present. Chloroform is a liquid at room temperature because of the strengths of these intermolecular forces; however, it is still reasonably volatile. The solubility is a little harder to understand. Since chloroform is polar, you would expect some solubility in water, but the solubility turns out to be pretty low, only 0.8 g/100mL. On the other hand, chloroform is completely soluble in hexane and other organic solvents.

Identify parts of the molecule that justify its chemical properties *The C-Cl and C-H bonds are in general not very reactive. This is part of why chloroform is a good solvent. Also when C-H bonds in hydrocarbons are replaced with C-Cl or C-F bonds, the hydrocarbon becomes less flammable. Good refrigerants are not flammable.*

Activity For each of the following molecules:

- Draw the Lewis structure.
- Identify the electron pair geometry and hybridization.
- Predict the geometry and bond angles.
- Build the molecule.
- Draw a 3-D sketch.
- Predict the polarity of the molecule.
- Identify important intermolecular forces and justify some physical and chemical properties of the molecule.

water[1]	hydrogen sulfide	carbon dioxide	methyl ethyl ketone
isopropanol	cyclohexane	benzene	napthalene[2]
acetic acid	methyl amine	alanine	polyethylene[3]

[1] Work with your neighbors to build an H-bonded network.
[2] Couple your benzene ring with a friend's benzene.
[3] Start with the ethylene molecule and combine with multiple neighbors

Also choose one of the following “interesting molecules”.

cocaine	caffeine	Methyl cyanoacrylate	Ethylene glycol
VX agent	aspirin	TNT	adreniline
acetylcholine	GABA	*trans*-retinal	putrescine

Lab Report Hand in your written descriptions of the structure, bonding, and properties of all of the molecules that you built. Be sure your descriptions follow good scientific writing by being “precise and concise”.

* L Buchanan, J. Laaser and R. McClain, January 2009.