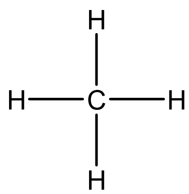
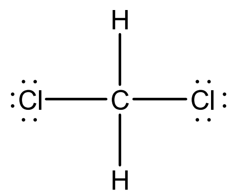
Experiment #12: MOLECULAR MODELS

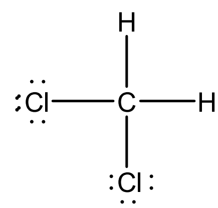
An aspect of chemistry, which traditionally proves to be difficult to many students, is the visualization of compounds, ions, and molecules in three dimensional space. In lecture you have seen how the octet rule can be used to draw "Lewis dot structures," which are often useful in predicting how groups of atoms will combine to form molecules or complex ions. You have also learned to predict the geometry of a molecule from its dot structure, and from the geometry to predict whether or not the molecule will have a net dipole moment. As with most topics that prove to be difficult, all it takes is a bit of practice. In this experiment you will construct three-dimensional models of various molecules and ions, and use these models to predict some molecular properties. The following Lewis dot structures can be used to illustrate the usefulness of three-dimensional models:



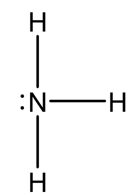
(1)



(2)

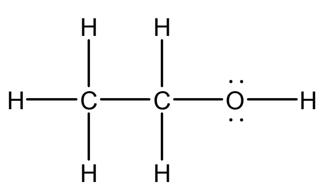


(3)

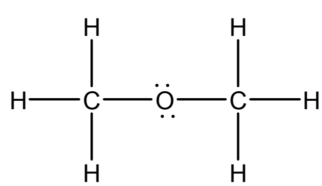


(4)

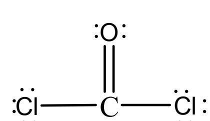
From VSEPR theory, structures 1-3 are all predicted to be tetrahedral, with 109° bond angles. Structure 4 is predicted to be trigonal pyramidal (for the molecular geometry), with bond angles close to 109°. When you construct models of structures 1-3 you will find that the square appearance of the two-dimensional sketches shown here is not a very good representation of the actual 3-dimensional structures. In fact, you will find that structures 2 and 3 are actually the same molecule, but viewed from different angles. You will also find that this molecule has a net dipole moment, despite its apparent symmetry as viewed from the angle of structure 2. Finally, you will note that structure 4 also has a net dipole moment. In more complex situations, it may be possible to draw more than one Lewis dot structure which follows the octet rule. Consider the four structures shown below:



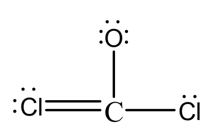
(5)



(6)



(7)



(8)

In determining which of two alternative dot structures is more stable, it is useful to consider the concept of "formal charge." The formal charge on an atom in a molecule is defined as follows:

Formal Charge = (# valence e^- on free atom) – (# e^- assigned to the atom in the molecule)

The number of electrons assigned to the atom **in the molecule** is calculated by adding all non-bonding electrons plus half the bonding (shared) electrons found around the atom.

$$FC = V - \left(\frac{B}{2} + L \right)$$

V = # of valence electrons on free atom

B = # of electrons participating in bonding

L = # of lone pair electrons on the atom in the molecule

None of the atoms in structures 5 or 6 has a formal charge, so these two structures are predicted to be stable. In this case, structures 5 and 6 are said to be "isomers," both with the molecular formula C_2H_6O. (Structure 5 is ethyl alcohol and structure 6 is dimethyl ether.) None of the atoms in structure 7 has a formal charge, but in structure 8 the oxygen atom has a –1 formal charge and the double-bonded chlorine atom has a +1 formal charge. In most cases, structures without formal charges are more stable, so we predict that $COCl_2$ (phosgene) has the bonding predicted by structure 7.

EXPERIMENTAL PROCEDURE

Please work in pairs during the first part of this experiment. Each student should check out a molecular model kit from the Service Center. For each molecular formula in the first part of the experiment, the following set of steps should be followed:

(1) Draw a Lewis dot structure for the formula. Use formal charge to reject unstable possibilities. Note that carbon must always have four bonds in order to have a formal charge of zero. If the only stable dot structure has one or more formal charges, indicate these charges in your dot structure.

(2) Choose appropriate parts from the kit to represent the necessary atoms, bonds, and non-bonding pairs:

H atom = small sphere

C atom = black 4-hole

O atom = blue 4-hole

Other atoms = red and green 4-hole

Single bond to H atom = short straight stick

Single bond to other atoms = long straight sticks

Double bond = two curved sticks

Triple bond = three curved sticks

Non-bonding pair = short straight stick

Expanded Octet Atoms:

10 e- valence = black 5-hole

12 e- valence = gray with 6 square faces

(3) Construct a three-dimensional model corresponding to your dot structure. Use your model to answer the questions concerning geometry and polarity. In the second part of the experiment, each student will be given a list of "unknown" molecules. Working independently, please complete all the steps above for each of the molecules on your list.

Part I . Known Molecules. Name: ________________________ Section: _________

Formula	Lewis Dot Structure	Molecular Geometry, Bond Angles, Central Atom Hybridization	Polarity? (yes or no)
H_2O			
C_2H_2			
N_2F_2			
$C_2H_2Cl_2$			
NO_2^-			
NO_3^-			

Instructor date and sign: ___________________________

Formula	Lewis Dot Structure	Molecular Geometry, Bond Angles, Central Atom Hybridization	Polarity? (yes or no)
SF_4			
XeF_4			
XeF_2			
FNO_2			
NH_2^-			
PF_5			

Part II. UNKNOWNS.

Formula	Lewis Dot Structure	Molecular Geometry, Bond Angles, Central Atom Hybridization	Polarity? (yes or no)

PART III. Additional Properties

Among the known molecules (part I), which ones have

a) stable isomers? Draw structures of all isomers.

b) resonance forms? (Draw structures to justify your answers.)