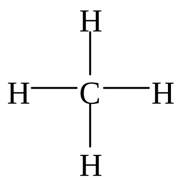
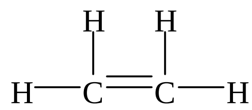
The Geometrical Structure of Molecules:

An Experiment Using Molecular Models

Many years ago it was observed that in many of its compounds the carbon atom formed four chemical linkages to other atoms. As early as 1870. graphic formulas of carbon compounds were drawn as shown:

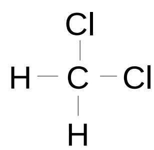


methane



ethylene

Although such drawings as these would imply that the atom-atom linkages, indicated by valence strokes, lie in a place, chemical evidence, particularly the existence of only one substance with the graphic formula:

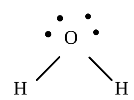


required that the linkages be directed toward the corners of a tetrahedron, at the center of which lay the carbon atom.

The concept of a tetrahedral carbon atom was developed and used extensively by organic chemists during the latter part of the nineteenth century. If carbon atoms are considered to be represented by a tetrahedron in the manner indicated, single carbon-carbon bonds arise when two such tetrahedra share a common corner, double bonds arise when the tetrahedra share an edge, and triple bonds arise when the tetrahedra share a face. Long before physical methods for confirmation were available, the model correctly predicted that ethylene, $H_2C{=}CH_2$, would be a planar molecule and that acetylene, $HC{\equiv}CH$, would be linear.

The physical significance of the chemical linkages between atoms, expressed by the lines or valence strokes in molecular structure diagrams, became evident soon after the discovery of the electron. In 1916, in a classic paper, G. N. Lewis suggested, on the basis of chemical evidence, that the single bonds in graphic formulas involve two electrons and that an atom tends to hold eight electrons in its outermost or valence shell.

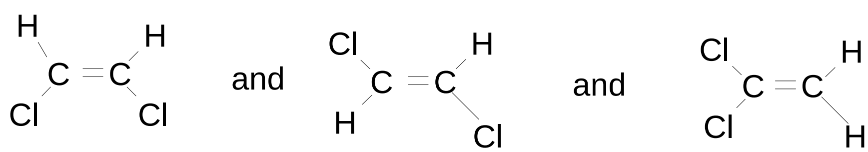
Lewis' proposal, that atoms generally have eight electrons in their outer shell, proved to be extremely useful and has come to be known as the octet rule. It can be applied to many atoms, but is particularly important in the treatment of covalent compounds of atoms in the second row of the Periodic Table. For compounds containing atoms such as carbon, oxygen, nitrogen, and fluorine, the eight valence electrons occur in pairs that occupy tetrahedral positions around the central atom core. Some of the electron pairs do not participate directly in chemical bonding and are called unshared or nonbonding pairs; however, the structures of compounds containing such unshared pairs reflect the tetrahedral arrangement of the four pairs of valence shell electrons. In the H_2O molecule, which obeys the octet rule, the four pairs of electrons around the central oxygen atom occupy essentially tetrahedral positions; there are two unshared nonbonding pairs and two bonding pairs which are shared by the O atom and the two H atoms. The H-O-H bond angle is nearly but not exactly tetrahedral since the properties of shared and unshared pairs of electrons are nearly but not exactly alike.



For some molecules with a given molecular formula, it is possible to satisfy the octet rule with different atomic arrangements. A simple example would be

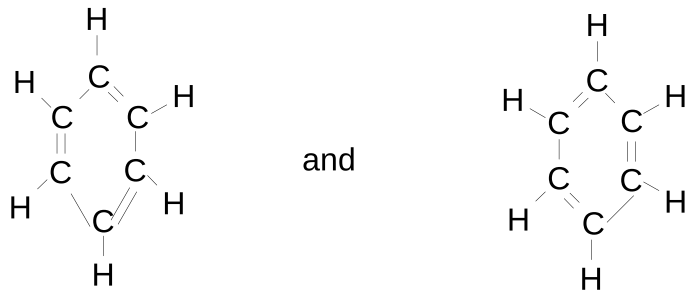
The two molecules are called isomers of each other, and the phenomenon is called isomerism. Although the molecular formulas of both substances are the same, C_2H_6O, their properties differ markedly because of their different atomic arrangements.

Isomerism is very common, particularly in organic chemistry, and when double bonds are present, isomerism can occur in very small molecules: For simplicity, in the following structures the three pairs of nonbonding electrons around each Cl atom have not been drawn in:



The first two isomers result from the fact that there is no rotation around a double bond, although such rotation does occur around single bonds. The third isomeric structure cannot be converted to either of the first two by rotation about the double bond.

With certain molecules, given the atomic arrangement, it is possible to satisfy the octet rule with more than one graphical formula. The classic example is benzene, whose molecular formula is C_6H_6:



These two structures are called resonance structures, and molecules such as benzene, which have two or more resonance structures, are said to exhibit resonance. The actual bonding in such molecules is thought to be an average of the bonding present in the resonance structures. The stability of molecules exhibiting resonance is found to be higher than that anticipated for any single resonance structure.

Once the symmetry of a species has been determined, it is possible to predict its polarity, that is, whether the molecule will contain a region of positive charge and a region of negative charge, and thus have a dipole moment. Covalent bonds between different kinds of atoms in molecules are typically polar; all heteronuclear diatomic molecules are polar. In some molecules the polarity from one bond may be canceled by that arising from others, so that the overall molecular polarity may vanish. Carbon dioxide, CO_2, which is linear, is a nonpolar molecule; methane, CH_4, which is tetrahedral, is also nonpolar. On the other hand, the related molecules of lower symmetry, COS and CH_3Cl, do not have complete cancellation of bond polarities and are therefore polar.

In this experiment, assuming that all atoms present in the species studied obey the octet rule, you will assemble models of some simple molecules and ions. On the basis of the models you will be able to draw the geometrical structure of the species and predict the polarity of the species.

EXPERIMENTAL PROCEDURE:

There are many different styles of molecular models. Your instructor will illustrate the use of your model kit. In this experiment we will only deal with atoms that obey the octet rule; i.e., all atoms will have 4 electron pairs around it, except for H which will have 1 electron pair. Our approach in this experiment will be to use the models to help us visualize in 3 dimensions the shapes of various molecules and ions, a common application that chemists use.

For each molecule or ion, draw a Lewis structure using the rules you have been taught in lecture or following the rules in your textbook.

Make a molecular model of this species, by counting the number of electron pairs around the central atom or atoms, and using the appropriate model piece for that central atom. Then connect all the terminal atoms to the central atoms, using the appropriate connectors to represent single or multiple bonds. In most kits, single bonds are represented by inflexible sticks and multiple bonds are represented by flexible tubing or springs.

Holding the model in front of you, draw a sketch of the model, in perspective, using bold lines to indicate atoms coming out towards you, dotted lines to indicate atoms going away from you and normal lines to indicate atoms in the same plane as the central atom. Describe, in words, the geometrical shape of the molecule. Also, predict, based on the symmetry of your models, whether the species is polar or not. If your instructor wishes, he may also ask you to determine whether there are other isomers that could be constructed for each species. If your instructor wishes, he may ask you to predict whether resonance forms are possible for each species. Your instructor will help you with these steps.

PART A:

Using the above procedure, construct and report on models of the molecules and ions listed here and on the data sheet. Your instructor may assign others for you to try. It is recommended that this part be done together in class and each model discussed so that the procedure becomes clear for everyone.

CH_4	CH_2Cl_2	CH_4O	H_2O
H_3O^+	C_2H_4	$C_2H_2Br_2$	C_2H_2
HF	NH_3	H_2O_2	N_2
SO_3	SO_2	SO_4^{-2}	CO_2

PART B:

Assuming that stability requires that each atom obey the octet rule, predict the stability of the following species:

PCl_3 NH_2 OH CO

PART C:

When you have completed Parts A and B, see your laboratory instructor, who will check your results and assign you a set of unknown species. Working by yourself, use the procedure in this experiment to construct models for each species, and report on the geometry, bonding and polarity of the unknown species, on the basis of the model you constructed.

Geometrical Structures of Molecules Using Molecular Models

Name ____ **Section** _________

DATA SHEET:

Part A:

Species	Lewis Structure	Bonding Sketch	Geometry	Polarity
CH_4				
CH_2Cl_2				
CH_4O				
H_2O				
H_3O^+				
C_2H_4				
$C_2H_2Br_2$				

C_2H_2				
HF				
NH_3				
H_2O_2				
N_2				
SO_3				
SO_2				
SO_4^{-2}				
CO_2				

Lab #9

Name ____ **Section** ___________

Part B:

Stability predicted for PCl_3 _______ NH_2 _______ OH _______ CO _______

Part C: Unknowns

Species	Lewis Structure	Bonding Sketch	Geometry	Polarity

Lab #9

Prestudy

A

The Geometrical Structure of Molecules

Name _______________________________________Section _______________

1.(3 points) Draw the Lewis dot diagram for HBr

2.(3 points) How many bonding electrons are present in the sulfate ion?

3.(4 points) Using the VSEPR approach, draw the geometrical structure of SO_3.

4. Considering the geometry of SO_3, determine whether it is polar or nonpolar.

Lab #9

Prestudy

B

The Geometrical Structure of Molecules

Name ____________________________ Section ______ Date ________

1.(3 points) Draw the Lewis dot diagram for HCl.

2.(3 points) How many bonding electrons are present in the perchlorate ion?

3.(4 points) Using the VSEPR approach, determine the geometrical structure of SiO_2.

2. Considering the geometry of SiO_2, determine whether it is polar or nonpolar.