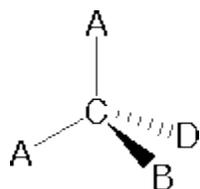# The Shape of Molecules

The three dimensional shape or **configuration** of a molecule is an important characteristic. This shape is dependent on the preferred spatial orientation of covalent bonds to atoms having two or more bonding partners. Three dimensional configurations are best viewed with the aid of models. In order to represent such configurations on a two-dimensional surface (paper, blackboard or screen), we often use **perspective drawings** in which the direction of a bond is specified by the line connecting the bonded atoms. In most cases the focus of configuration is a carbon atom so the lines specifying bond directions will originate there. As defined in the diagram on the right, a simple straight line represents a bond lying approximately in the surface plane. The two bonds to substituent **A** in the structure on the left are of this kind. A wedge shaped bond is directed in front of this plane (thick end toward the viewer), as shown by the bond to substituent **B**; and a hatched bond is directed in back of the plane (away from the viewer), as shown by the bond to substituent **D**. Some texts and other sources may use a dashed bond in the same manner as we have defined the hatched bond, but this can be confusing because the dashed bond is often used to represent a partial bond (i.e. a covalent bond that is partially formed or partially broken). The following examples make use of this notation, and also illustrate the importance of including non-bonding valence shell electron pairs (colored blue) when viewing such configurations .
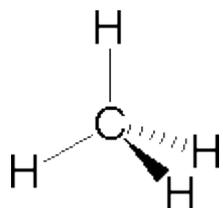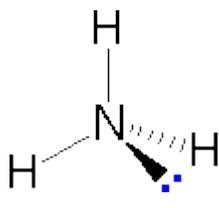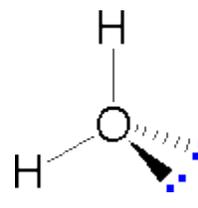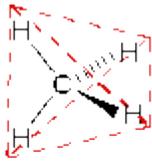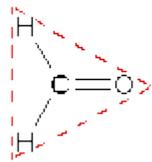
Methane   Ammonia   Water

Bonding configurations are readily predicted by valence-shell electron-pair repulsion theory, commonly referred to as **VSEPR** in most introductory chemistry texts. This simple model is based on the fact that electrons repel each other, and that it is reasonable to expect that the bonds and non-bonding valence electron pairs associated with a given atom will prefer to be as far apart as possible. The bonding configurations of carbon are easy to remember, since there are only three categories.

| Configuration	Bonding Partners	Bond Angles	Example
Tetrahedral	4	109.5°	
Trigonal	3	120°	
Linear	2	180°	
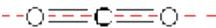
In the three examples shown above, the central atom (carbon) does not have any non-bonding valence electrons; consequently the configuration may be estimated from the number of bonding partners alone. For molecules of water and ammonia, however, the non-bonding electrons must be included in the calculation. In each case there are four regions of electron density associated with the valence shell so that a tetrahedral bond angle is expected. The measured bond angles of these compounds (H_2O 104.5° & NH_3 107.3°) show that they are closer to being tetrahedral than trigonal or linear. Of course, it is the configuration of atoms (not electrons) that defines the the shape of a molecule, and in this sense ammonia is said to be pyramidal (not tetrahedral). The compound boron trifluoride, BF_3, does not have non-bonding valence electrons and the configuration of its atoms is trigonal. Nice treatments of VSEPR theory have been provided by Oxford and Purdue . Click on the university name to visit their site.

The best way to study the three-dimensional shapes of molecules is by using molecular models. Many kinds of model kits are available to students and professional chemists. Some of the useful features of physical models can be approximated by the model viewing applet **Jmol**. This powerful visualization tool allows the user to move a molecular stucture in any way desired. Atom distances and angles are easily determined. To measure a distance, double-click on two atoms. To measure a bond angle, do a double-click, single-click, double-click on three atoms. To measure a torsion angle, do a double-click, single-click, single-click, double-click on four atoms. A pop-up menu of commands may be accessed by the right button on a PC or a control-click on a Mac while the cursor is inside the display frame.
You may examine several Jmol models of compounds discussed above by .

One way in which the shapes of molecules manifest themselves experimentally is through molecular dipole moments. A molecule which has one or more polar covalent bonds may have a dipole moment as a result of the accumulated bond dipoles. In the case of water, we know that the O-H covalent bond is polar, due to the different electronegativities of hydrogen and oxygen. Since there are two O-H bonds in water, their bond dipoles will interact and may result in a molecular dipole which can be measured. The following diagram shows four possible orientations of the O-H bonds.
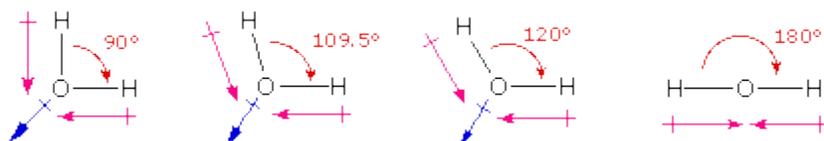
The bond dipoles are colored magenta and the resulting molecular dipole is colored blue. In the linear configuration (bond angle 180º) the bond dipoles cancel, and the molecular dipole is zero. For other bond angles (120 to 90º) the molecular dipole would vary in size, being largest for the 90º configuration. In a similar manner the configurations of methane (CH_4) and carbon dioxide (CO_2) may be deduced from their zero molecular dipole moments. Since the bond dipoles have canceled, the configurations of these molecules must be tetrahedral (or square-planar) and linear respectively. The case of methane provides insight to other arguments that have been used to confirm its tetrahedral configuration. For purposes of discussion we shall consider three other configurations for CH_4, square-planar, square-pyramidal and triangular-pyramidal. Models of these possibilities may be examined by .

Substitution of one hydrogen by a chlorine atom gives a CH_3Cl compound. Since the tetrahedral, square-planar and square-pyramidal configurations have structurally equivalent hydrogen atoms, they would each give a single substitution product. However, in the trigonal-pyramidal configuration one hydrogen (the apex) is structurally different from the other three (the pyramid base). Substitution in this case should give two different CH_3Cl compounds if all the hydrogens react. In the case of disubstitution, the tetrahedral configuration of methane would lead to a single CH_2Cl_2 product, but the other configurations would give two different CH_2Cl_2 compounds. These substitution possibilities are shown in the above insert.