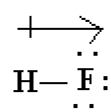
Predicting the Polarity of Molecules

Molecules come in various shapes and sizes. If it is a diatomic molecule, it is very simple and consists of only one bond. The predicting polarity of such molecules is discussed in the previous chapter under Bond Polarity section. However, as number of atoms in molecules increases, the complexity also increases. In such molecules, starting with tri-atomic molecules, the predicting the polarity depends upon two factors: (a) bond polarity, and (b) the shape of the molecule.

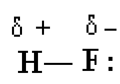
There are two ways to predict the molecularly polarities: (a) using VSEPR theory, and (b) using dipole moments. The first method is a theoretical prediction and the second method is an experimental determination. However, one can explain the dipole moments in terms of VSEPR theory.

Dipole Moments

Consider the simple example of hydrogen fluoride (HF), which is a covalent compound with one single polar bond. Since F has higher electronegativity compared to H, the electron density is shifted more towards fluorine. This shift in electron density is indicated by the arrow going from less electronegative atom (H) to more electronegative atom (F) and is placed above the Lewis structure that is shown below:



The + sign at the beginning of the arrow simply means that the H end of the molecule becomes positively charged. As a result of shift in electron density, there is a charge separation. This charge separation is not the entire charge separation but a partial, which is represented by the symbol δ(pronounced as "delta") and placed above atoms along with + and – signs.



Due to the partial charge separation, the HF molecule when placed in an electric field, will orient towards opposite charge; negative end towards positive electric field and positive end towards negative electric filed.

The dipole moment (μ, pronounced as "mu") is a quantitative measurement of either bond polarity or molecular polarity. It is defined as the product of the charge Q and the distance r between the charges, and the mathematical expression is written as,

$$\mu = Q \times r$$

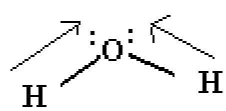
Here Q refers only to the magnitude of the charge but not to the sign. Dipole moments are commonly expressed in debye unit (D) after the well-known Dutch-American chemist and physicist Peter Debye. The Q is expressed in Coulomb (C) and distance in meter (m). Then the unit for μ is C x m. Therefore 1 D = 3.336 x 10^{-30} C x m.

Non-polar bonds or non-polar molecules do not have dipole moments and polar bonds or polar molecules have dipole moments. Thus the dipole moment is a tool to predict the polarity of a molecule and subsequently its shape:

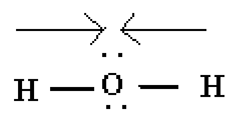
If $\mu = 0$, the bond or molecule is non-polar
If $\mu > 0$, the bond or molecule is polar.

For example O_2, N_2, Cl_2, CH_4, and CO_2 are non-polar molecules and hence have no dipole moments. On the other hand, H_2O, H_2S, and NH_3 are polar molecules and have appreciable dipole moments. The magnitude of the dipole moment depends on the magnitude of polarity that further translates into the degree of shift in electron density.

Let us see how the geometry (shape) of the molecule play a role in determining the polarity. Consider the water molecule (H_2O), which has the following Lewis structure:



bent molecule
has a dipole moment



linear molecule
(no dipole moment)

The bond polarities are shown by the arrows. Both OH bonds are the same and hence have the same strength. In the bent molecule (left structure), the bond polarities do not cancel each other and as a consequence it is a polar molecule with dipole moment. Suppose the water molecule is a linear type (right structure) instead of bent type. The both bond polarities acting in opposite directions with the same strength cancel each other resulting in non-polar nature with no dipole moment. In reality, the water molecule is a bent type of molecule with dipole moment of 1.87 D.

The geometry (shape) of water molecule plays an important role in our nature. In the winter time, the water on the surfaces of ponds and lakes freezes and turns into ice that floats on its underneath water. The ice on the surface also prevents further freezing of the body of water and keeps the temperature higher than the temperature on the surface. As a consequence, the aquatic life is sustained in the winter time. **This is how nature safeguards its assets.**

The ice floats on water because it has lower density than water. It has lower density because it has bent shape. As results, it packs fewer number of water molecules in a given volume. Now, suppose water molecules are linear as shown in the right structure. This will lead to higher density by packing more number of molecules in a given volume.

As a result, the ice would sink to the bottom of the ponds or lakes in the winter time thereby eradicating the aquatic life in the winter time. This has of course a devastating effect on the aquatic life in the winter.

Exercise

Which of the following molecules has the dipole moment?

(a) CH_4 , (b) HCN , (c) CH_2Cl_2, (d) NH_3, and (e) SO_2