4.5 Molecular Polarity

You have learned that different atoms can have different tendencies to attract bonding pairs of electrons. When 2 atoms with sufficiently different electronegativities combine, a dipole forms: one end of the bond is negative, and the other end is positive.

Figure 1 shows what happens when a balloon charged with static electricity is placed near a stream of running tap water. As gravity pulls the water vertically down, the water bends. What causes this effect?

Figure 1 When you place an electrostatically charged balloon near a stream of water, the water stream bends toward the balloon.

Polar and Non-polar Polyatomic Molecules

You have learned that diatomic molecules, such as hydrogen fluoride, are polar when their atoms have sufficiently different electronegativities. Polyatomic molecules (molecules with more than 2 atoms) can also exhibit polar behaviour. Water molecules are an example of this. Each water molecule is composed of 1 oxygen atom and 2 hydrogen atoms. Since an oxygen atom has a greater electronegativity than a hydrogen atom, each H–O bond is polar (has a bond dipole). **Figure 2** shows the charge distribution in a water molecule.

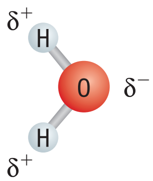


Figure 2 Representation of the charge distribution in a water molecule, using a ball-and-stick model

The polarity of the individual water molecules causes the bending of the stream of running tap water in Figure 1. The static charge on the balloon is a negatively charged electric field. As shown in **Figure 3**, the dipoles in the water molecules become oriented toward this electric field, causing the entire stream of water to be pulled toward the charged balloon.

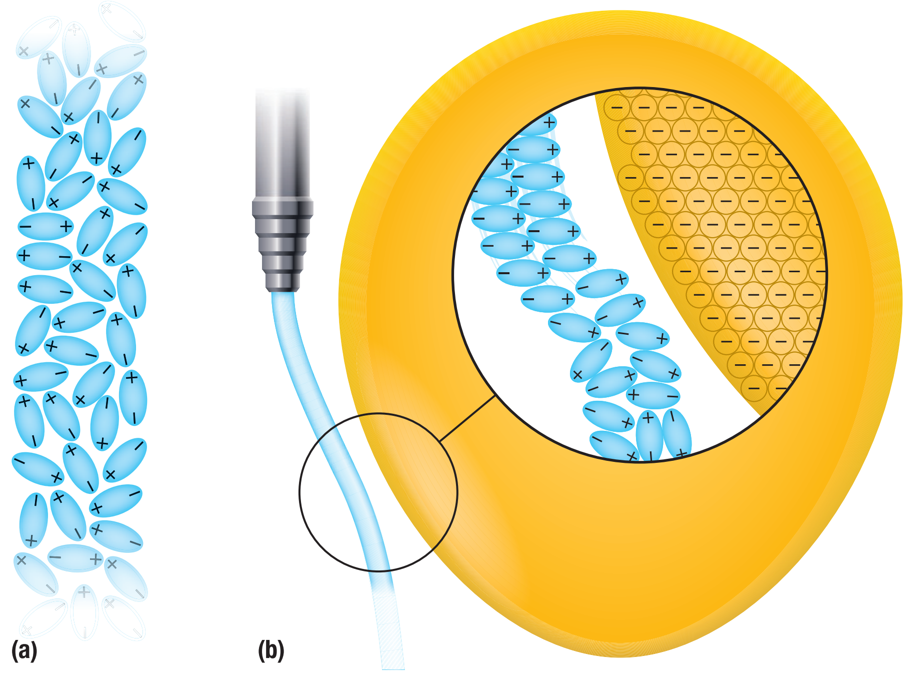


Figure 3 (a) In the absence of an electric field, the dipoles in water molecules are randomly oriented. (b) When a negatively charged balloon is placed next to the stream of water molecules, the dipoles cause the water molecules to move so that their positive poles align closer to the balloon.

Since an oxygen atom is more electronegative than a hydrogen atom, the negative ends of both bond dipoles in a water molecule point in the direction of the oxygen atom (**Figure 4**). Water has two lone pairs of electrons on the oxygen atom that give it a bent or V-shaped three-dimensional structure. As a result, the bond dipoles add together to give the water molecule a net dipole, represented by the red arrow in Figure 4. Therefore, water molecules are strongly polar. Molecules that have net dipoles are **polar molecules**.

polar molecule a molecule that has a net dipole

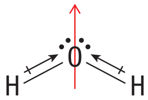


Figure 4 Water has a net negative dipole in the direction of the oxygen atom.

However, not every molecule that has polar covalent bonds is a polar molecule. A **non-polar molecule** is a molecule with no net dipole. Some non-polar molecules have polar bonds but do not have a net dipole, due to the arrangement of atoms in a molecule. This happens when the sum of the individual bond dipoles is zero. For example, a carbon dioxide molecule is linear, with the negative charge distribution on the oxygen atoms and the positive charge distribution on the central carbon atom (**Figure 5**). However, since the polarities of these bonds are equal and opposite, they cancel each other out.

non-polar molecule a molecule that has only non-polar bonds, or a bond dipole sum of zero

Investigation 4.5.1

Testing for Polar Molecules (page 256)
Now that you know the polarity of a molecule affects its behaviour when it is near differently charged objects, perform Investigation 4.5.1 to examine the effect of charge on different substances.

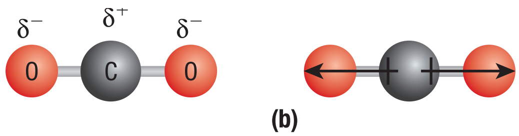
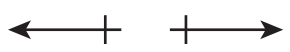
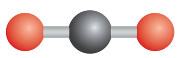
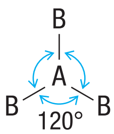
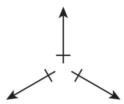
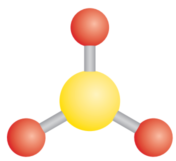
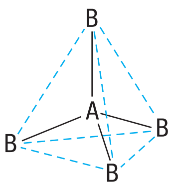
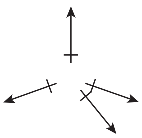
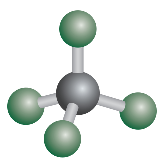


Figure 5 (a) The structure of and charge distribution in carbon dioxide. Oxygen is more electronegative than carbon. (b) The opposing bond polarities of carbon dioxide cancel each other out, and the carbon dioxide molecule has no net dipole.

To predict whether a specific molecule is polar or non-polar, you must consider two characteristics: the types of bonds in the molecule (polar or non-polar) and the geometric shape of the molecule. **Table 1** lists some common molecular structures that give rise to non-polar molecules. WEB LINK

Table 1 Types of Molecular Structures with Polar Bonds but No Net Dipole

Type	General example	Cancellation of polar bonds	Specific example	Ball-and-stick model
linear molecules with 2 identical bonds	B—A—B		CO_2	
planar molecules with 3 identical bonds			SO_3	
tetrahedral molecules with 4 identical bonds (109.5° apart)			CCl_4	

Tutorial 1 Predicting the Polarity of Molecules

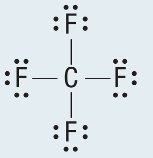
In this Tutorial, you will determine the net dipole of a molecule. If the sum of the dipoles in the molecule is zero, the molecule is non-polar. If the sum is non-zero, the molecule is polar. Since you only want to know whether the molecular dipole is zero, you can use symmetry arguments.

Sample Problem 1: Predicting the Polarity of Tetrafluoromethane

Predict whether tetrafluoromethane, CF_4, is a polar or a non-polar molecule.

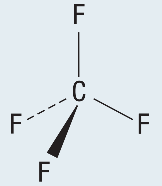
Solution

Step 1. Draw the simplified Lewis structure of tetrafluoromethane.



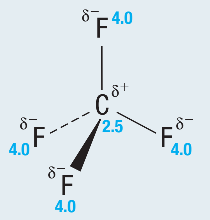
Step 2. Use the VSEPR theory to predict the three-dimensional structure, then draw a diagram.

Since carbon is the central atom and it is bonded to 4 fluorine atoms, you would expect a molecule of tetrafluoromethane to have a tetrahedral shape.



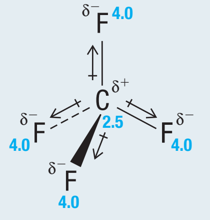
Step 3. Identify the electronegativity of each atom, and determine the partial charges in the molecule.

The carbon atom is less electronegative than the surrounding fluorine atoms, so it accumulates a partial positive charge from each bond with fluorine. Each fluorine atom acquires a partial negative charge.



Step 4. Draw the bond dipoles, and determine whether the molecule has a net dipole.

In this tetrahedral shape, all of the atoms bonded to the central carbon atom are identical and all the directions are equivalent. Therefore, the four bond dipoles cancel each other. The overall net dipole is zero, so tetrafluoromethane is a non-polar molecule.

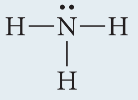


Sample Problem 2: Predicting the Polarity of Ammonia

Predict whether ammonia, NH_3, is a polar or a non-polar molecule.

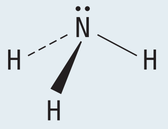
Solution

Step 1. Draw the simplified Lewis structure of ammonia.



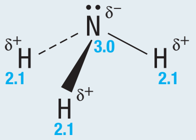
Step 2. Use VSEPR theory to predict the three-dimensional structure, then draw a diagram.

Nitrogen is the central atom that is bonded to 3 hydrogen atoms. There is 1 lone pair of electrons on the nitrogen atom. The three-dimensional structure of ammonia is therefore trigonal pyramidal.



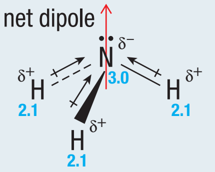
Step 3. Identify the electronegativity of each atom, and determine the partial charges in the molecule.

The nitrogen atom is more electronegative than the hydrogen atoms, so it has a partial negative charge from each bond. Each hydrogen atom acquires a partial positive charge.



Step 4. Draw the bond dipoles, and determine whether the molecule has a net dipole.

In a trigonal pyramidal shape, all of the atoms bonded to nitrogen are identical, but the bond dipoles do not cancel each other out. Therefore, the ammonia molecule has a net dipole. Ammonia is a polar molecule with a net dipole pointing in the direction of the lone pair of electrons on the nitrogen atom.



Practice

1. Predict the polarity of each of the following molecules. Include a three-dimensional structure for each molecule. If the molecule is polar, indicate the direction of the net dipole. T/I C
   (a) NF_3 [ans: polar]
   (b) CBr_4 [ans: non-polar]
   (c) SF_2 [ans: polar]
2. Predict the polarity of each the following molecules or ions: T/I C
   (a) PO_3^{3-} [ans: polar]
   (b) NH_4^+ [ans: non-polar]
   (c) B_2H_6 [ans: non-polar]
   (d) CH_3CH_2OH [ans: polar]

3. Some substances have bonds that we predict to be polar, but the molecule turns out to be non-polar. K/U T/I C
   (a) Write the formula of one such substance.
   (b) Draw the Lewis structure of the molecule, and show calculations to support the polarity of the bond.
   (c) Draw a diagram illustrating the structure of the molecule, and show why the molecule is non-polar.

You have seen that bond polarity, molecular shape, and the distribution of atoms all influence the polarity of a molecule. **Figure 6** is a flow chart that you can use to help you predict whether a molecule is polar or non-polar.

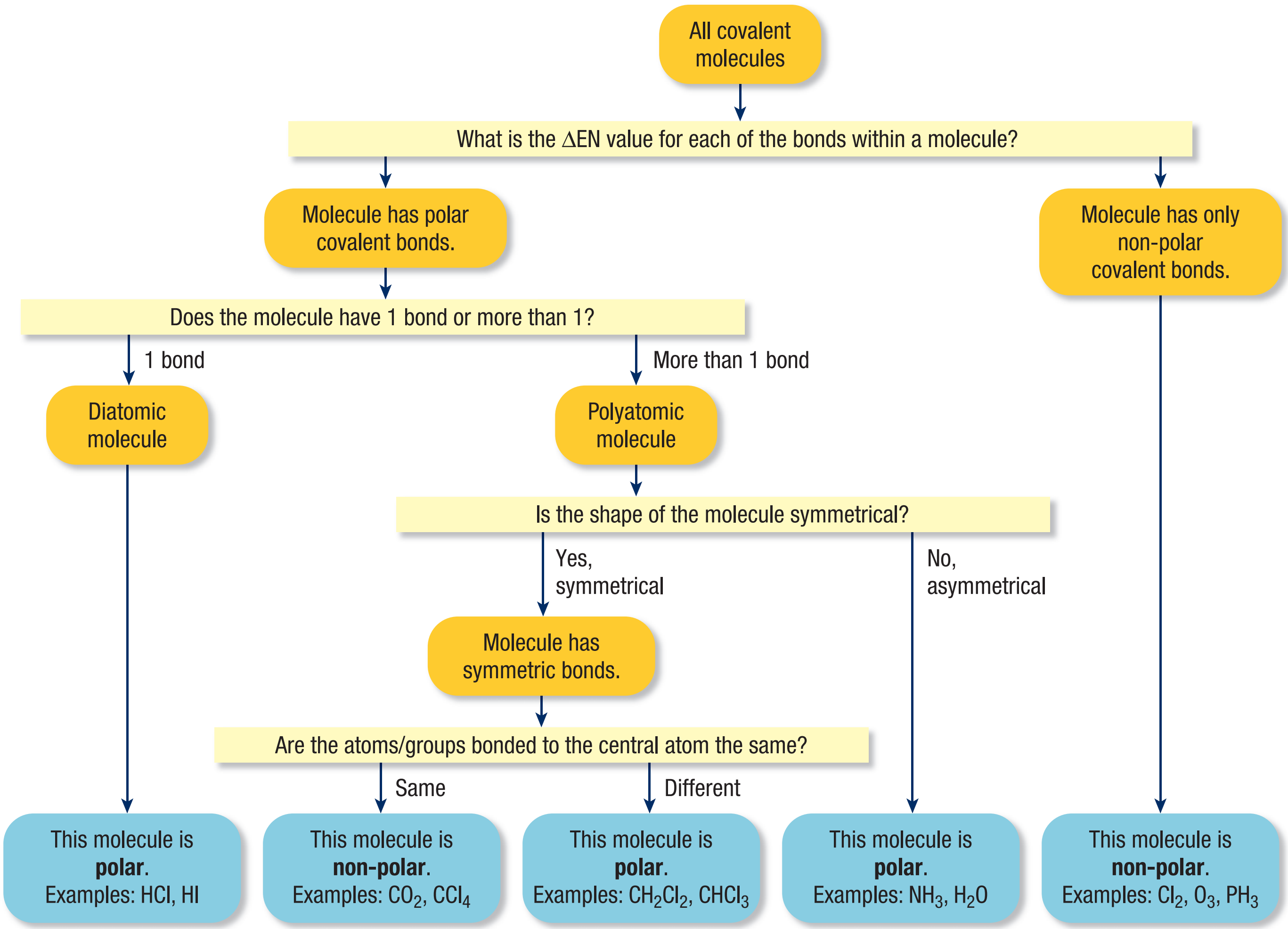


Figure 6 Flow chart to determine whether a molecule is polar or non-polar

4.5 Review

Summary

- The polarity of a molecule depends on both the direction and polarity of its bonds.
- When the sum of the bond dipoles is non-zero, the molecule is polar.
- The bond dipoles for molecules with symmetrically arranged atoms add up to zero and the molecules are non-polar.
- The polarity of a molecule can be predicted based on bond polarity, molecular shape, and the distribution of atoms.

Questions

1. Use the VSEPR theory to explain why a molecule of diboron tetrafluoride, B_2F_4, is non-polar. K/U
2. Use the VSEPR theory to explain why a molecule of methanol, CH_3OH, is polar. K/U
3. Explain why phosphorus trihydride, PH_3, is a non-polar molecule, while phosphorus trifluoride, PF_3, is a polar molecule. K/U
4. Use partial charges to represent the dipole in the bonds of the following molecules: K/U C
   (a) F–B in BF_3
   (b) N–Cl in NCl_3
   (c) H–C in C_4H_{10}
   (d) C–C in C_4H_{10}
5. Predict whether each of the following molecules is polar or non-polar: T/I C
   (a) OCl_2
   (b) BeH_2
   (c) SiF_4
   (d) SO_2
   (e) SO_3
   (f) CHF_3
   (g) CCl_2F_2
6. For each of the following molecules, draw the simplified Lewis structures and predict whether each molecule is polar or non-polar: T/I C
   (a) HOCN
   (b) CF_3Cl
   (c) H_2CO
7. Draw a three-dimensional diagram for each of the following molecules, and determine whether each molecule is polar or non-polar. Indicate any polarity on your diagram. T/I C
   (a) PCl_3
   (b) ClF_3
   (c) $XeCl_4$
   (d) H_2S
   (e) FCN
8. (a) The molecule dichlorofluoromethane, $CHFCl_2$, is used as a refrigerant. Tetrafluoromethane, CF_4, was also considered as a possible refrigerant. Draw the three-dimensional structures of $CHFCl_2$ and CF_4. Predict the polarities of both molecules.
   (b) Explain the difference between the two molecules. What causes the difference?
   (c) What physical properties would be different due to the different polarities of these molecules? Which of these properties could be important to the use of each gas as a refrigerant? K/U T/I C A
9. When a crystal of sodium chloride dissolves in water, the positive ends of the water dipole align with the negative chloride ions, and the negative ends of the water dipole align with the positive sodium ions. Draw a series of diagrams that illustrate this process. T/I C
10. Both water and carbon dioxide are important greenhouse gases because they can absorb infrared energy from sunlight, convert it into thermal energy, and release energy into the atmosphere. To absorb infrared energy, a molecule must have a vibrating dipole whose vibrational frequency matches the frequency of the infrared energy. Water has a strong dipole, so infrared energy vibrations cause its dipole to vibrate. Research the role of water and carbon dioxide as greenhouse gases to find answers to the following questions: K/U T/I A
    (a) While water absorbs infrared light some 80 times more efficiently than carbon dioxide, carbon dioxide absorbs enough to be a legitimate source of concern for climate change. However, given that carbon dioxide has no net dipole, how can it absorb infrared light at all?
    (b) When scientists discuss the greenhouse effect, carbon dioxide is the gas that is held responsible, even though there are other greenhouse gases such as water vapour. Why do you think this is?

WEB LINK