Objectives

After completing this section, you should be able to

1. explain how dipole moments depend on both molecular shape and bond polarity.
2. predict whether a molecule will possess a dipole moment from the molecular formula or structure.
3. use the presence or absence of a dipole moment as an aid to deducing the structure of a given compound.

Key Terms

Make certain that you can define, and use in context, the key term below.

- dipole moment

Study Notes

You must be able to combine your knowledge of molecular shapes and bond polarities to determine whether or not a given compound will have a dipole moment. Conversely, the presence or absence of a dipole moment may also give an important clue to a compound’s structure. BCl\(_3\), for example, has no dipole moment, while NH\(_3\) does. This suggests that in BCl\(_3\) the chlorines around boron are in a trigonal planar arrangement, while the hydrogens around nitrogen in NH\(_3\) have a less symmetrical arrangement - trigonal pyramidal.

Remember that the $\ce{C-H}$ bond is assumed to be non-polar.

**Molecular Dipole Moments**

You previously learned how to calculate the dipole moments of simple diatomic molecules. In more complex molecules with more than one polar covalent bonds, the three-dimensional geometry and the compound’s symmetry determine whether the molecule has a net dipole moment.

Example \(\PageIndex{1}\): Polar Bonds vs. Polar Molecules

In a simple diatomic molecule like \(\ce{HCl}\), if the bond is polar, then the whole molecule is polar. What about more complicated molecules that have more than one bond?
Consider $CCl_4$, (left panel in figure above), which as a molecule is not polar - in the sense that it doesn't have an end (or a side) which is slightly negative and one which is slightly positive. The whole of the outside of the molecule is somewhat negative, but there is no overall separation of charge from top to bottom, or from left to right.

In contrast, $(CHCl_3)$ is a polar molecule (right panel in figure above). The hydrogen at the top of the molecule is less electronegative than carbon and so is slightly positive. This means that the molecule now has a slightly positive "top" and a slightly negative "bottom", and so is overall a polar molecule.

A polar molecule will need to be "lop-sided" in some way.

Mathematically, dipole moments are vectors; they possess both a magnitude and a direction. The dipole moment of a molecule is therefore the vector sum of the dipole moments of the individual bonds in the molecule. If the individual bond dipole moments cancel one another, there is no net dipole moment. Such is the case for CO$_2$, a linear molecule (Figure \(\PageIndex{1a}\)). Each C–O bond in CO$_2$ is polar, yet experiments show that the CO$_2$ molecule has no dipole moment. Because the two C–O bond dipoles in CO$_2$ are equal in magnitude and oriented at 180° to each other, they cancel. As a result, the CO$_2$ molecule has no net dipole moment even though it has a substantial separation of charge. In contrast, the H$_2$O molecule is not linear (Figure \(\PageIndex{1b}\)); it is bent in three-dimensional space, so the dipole moments do not cancel each other. Thus a molecule such as H$_2$O has a net dipole moment. We expect the concentration of negative charge to be on the oxygen, the more electronegative atom, and positive charge on the two hydrogens. This charge polarization allows H$_2$O to hydrogen-bond to other polarized or charged species, including other water molecules.

![Figure](left) $CCl_4$ (right) $CHCl_3$

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**Figure \(\PageIndex{1}\)** How Individual Bond Dipole Moments Are Added Together to Give an Overall Molecular Dipole Moment for Two Triatomic Molecules with Different Structures. (a) In CO$_2$, the C–O bond dipoles are equal in magnitude and oriented at 180° to each other, they cancel. As a result, the CO$_2$ molecule has no net dipole moment even though it has a substantial separation of charge. In contrast, the H$_2$O molecule is not linear; it is bent in three-dimensional space, so the dipole moments do not cancel each other. Thus a molecule such as H$_2$O has a net dipole moment. We expect the concentration of negative charge to be on the oxygen, the more electronegative atom, and positive charge on the two hydrogens. This charge polarization allows H$_2$O to hydrogen-bond to other polarized or charged species, including other water molecules.
magnitude but oriented in opposite directions (at 180°). Their vector sum is zero, so CO₂ therefore has no net dipole. (b) In H₂O, the O–H bond dipoles are also equal in magnitude, but they are oriented at 104.5° to each other. Hence the vector sum is not zero, and H₂O has a net dipole moment.

Other examples of molecules with polar bonds are shown in Figure \(\PageIndex{2}\). In molecules like BCl₃ and CCl₄, that have only one type of bond and a molecular geometries that are highly symmetrical (trigonal planar and tetrahedral), the individual bond dipole moments completely cancel, and there is no net dipole moment. However, although a molecule like CHCl₃ has a tetrahedral geometry, the atoms bonded to carbon are not identical. Consequently, the bond dipole moments do not cancel one another, and the result is a molecule which has a dipole moment.

![Figure \(\PageIndex{2}\): Molecules with Polar Bonds. Individual bond dipole moments are indicated in red. Due to their different three-dimensional structures, some molecules with polar bonds have a net dipole moment (HCl, CH₂O, NH₃, and CHCl₃), indicated in purple, whereas others do not because the bond dipole moments cancel (BCl₃, CCl₄, PF₅, and SF₆).](image)

Molecules with asymmetrical charge distributions have a net dipole moment

Example \(\PageIndex{1}\)

Which molecule(s) has a net dipole moment?

a. H₂S  
b. NHF₂  
c. BF₃

**Given:** three chemical compounds

**Asked for:** net dipole moment

**Strategy:**

For each three-dimensional molecular geometry, predict whether the bond dipoles cancel. If they do not, then the molecule has a net dipole moment.

**Solution:**
a. The total number of electrons around the central atom, S, is eight, which gives four electron pairs. Two of these electron pairs are bonding pairs and two are lone pairs, so the molecular geometry of H₂S is bent. The bond dipoles cannot cancel one another, so the molecule has a net dipole moment.

\[ \text{H}_2\text{S} \]

b. Difluoroamine has a trigonal pyramidal molecular geometry. Because there is one hydrogen and two fluorines, and because of the lone pair of electrons on nitrogen, the molecule is not symmetrical, and the bond dipoles of NHF₂ cannot cancel one another. This means that NHF₂ has a net dipole moment. We expect polarization from the two fluorine atoms, the most electronegative atoms in the periodic table, to have a greater affect on the net dipole moment than polarization from the lone pair of electrons on nitrogen.

\[ \cdot \cdot \cdot ^{\text{N}} \cdot \text{H} \quad ^{\text{F}} \quad ^{\text{F}} \]

c. The molecular geometry of BF₃ is trigonal planar. Because all the B–F bonds are equal and the molecule is highly symmetrical, the dipoles cancel one another in three-dimensional space. Thus BF₃ has a net dipole moment of zero:

\[ \text{BF}_3 \]

Exercise 1

Which molecule(s) has a net dipole moment?

a. CH₃Cl
b. SO₃
c. XeO₃

Answer: CH₃Cl; XeO₃
Exercises

1. Determine whether each of the compounds listed below possesses a dipole moment. For the polar compounds, indicate the direction of the dipole moment.
   a. \( \text{O=C=O} \)
   b. \( \text{ICl} \)
   c. \( \text{SO}_2 \)
   d. \( \text{CH}_3\text{-O-CH}_3 \)
   e. \( \text{CH}_3\text{C(=O)CH}_3 \)

Answers:

1. a. carbon dioxide is nonpolar
   b. net dipole moment on iodine monochloride
   c. net dipole moment on sulfur dioxide
   d. net dipole moment on dimethyl ether
   e. net dipole moment on 2-propanone

Questions

Q2.2.1

The following molecule has no dipole moment in the molecule itself, explain.

\[
\begin{array}{c}
\text{HO} \\
\text{-} \\
\text{OH}
\end{array}
\]

Q2.2.2

Which of the following molecules has a net dipole?
Q2.2.3

Within reactions with carbonyls, such as a reduction reaction, the carbonyl is attacked from the carbon side and not the oxygen side. Using knowledge of electronegativity explain why this happens.

![Diagram of carbonyl and reduction reaction](image)

Solutions

S2.2.1

The hydroxyl groups are oriented opposite of one another and therefore the dipole moments would “cancel” one another out. Therefore having a zero net-dipole.

S2.2.2

1, 3, and 4 have a net dipoles.

S2.2.3

The oxygen is more electronegative than the carbon and therefore creates a dipole along the bond. This leads to having a partial positive charge on the carbon and the reduction can take place.
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