Introduction

The polarity of a substance is related to many of its important properties - boiling/melting point, what the substance will dissolve in, etc. Since experimentation is always costly and sometimes dangerous, we would like to determine the polarity of a molecule **without doing experiments**.

Polar bonds?

At first glance, it seems obvious what makes a polar molecule: **polar bonds**. Polar bonds are only a **part** of the requirement, though. For a whole **molecule** to be polar, it must have electron density unevenly distributed **across the molecule**.

Examples

A good example molecule to study is carbon tetrachloride (CCl_4). A three dimensional structure for carbon tetrachloride would look like this.:

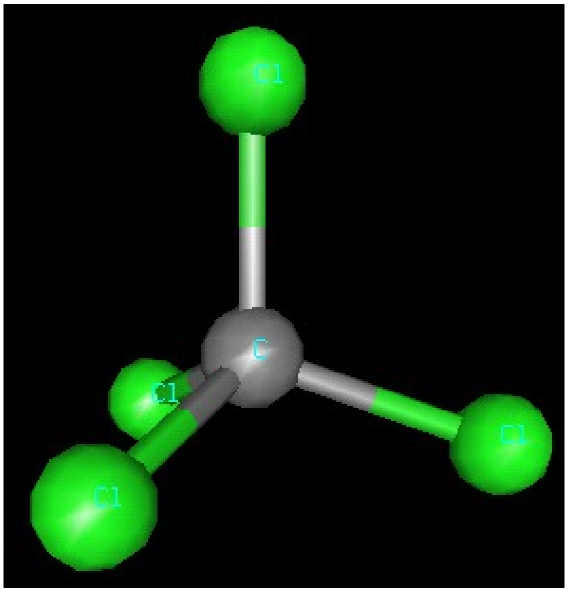

Illustration 1: Carbon tetrachloride, a tetrahedral molecule

- This is a **ball-and-stick** model of CCl_4. The gray ball is a carbon atom and the green balls are chlorine atoms.
- Carbon tetrachloride is tetrahedral - four things are around the carbon and all four are atoms.
- Carbon-chloride bonds are polar. Look at the electronegativity difference between the two atoms.

We know that the carbon-chlorine bonds are all polar bonds. There is a significant electronegativity difference between carbon and chlorine. So, the chlorine atoms tend to pull electrons towards themselves. **However**, the four chlorine atoms are all equally spaced around the carbon. Carbon tetrachloride is symmetric, and the chlorine atoms are effectively pulling against each other. Carbon tetrachloride, then, is **not a polar molecule** because there's no **net** difference in electron density across the molecule.

Let's look at another example - the water molecule.

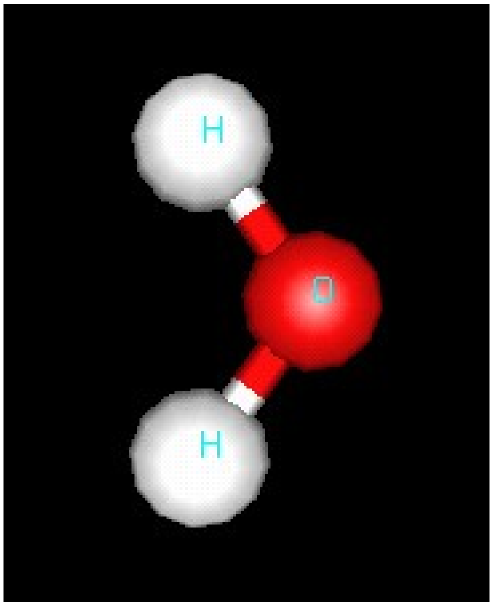

Illustration 2: The bent water molecule

- The water molecule is bent - it has four things around the oxygen atom, but only two are other atoms.
- Oxygen-hydrogen bonds are polar, since oxygen is much more electronegative than hydrogen.

We know that the hydrogen-oxygen bonds are polar bonds. There is a significant electronegativity difference between hydrogen and oxygen. So, the oxygen atom tends to pull electrons towards itself. Since this molecule is **not** symmetrical, one side of the molecule (the oxygen side) takes on a slight negative charge. The side with the two hydrogen atoms takes on a slight positive charge. Water, then, is **a polar molecule**.

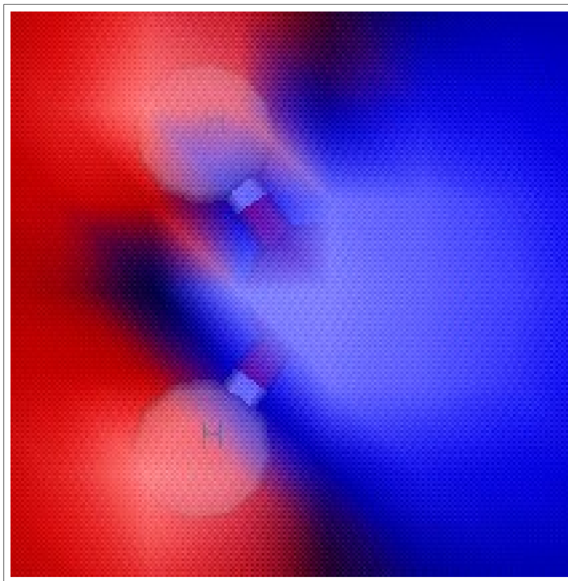

Illustration 3: Electron density around the water molecule

- This is the same picture as Illustration 2, but with areas of higher electron density highlighted in blue and lower electron density highlighted in red.
- You can clearly see that one side of the molecule is electron-deficient, while the other side is electron-rich.

Shape is important! If we'd mistakenly thought water was a linear molecule, we might have concluded water was nonpolar.

If we tried to mix water and carbon tetrachloride, we'd find that they would not mix. Polar molecules like water tend to associate with others of their kind than with nonpolar molecules like carbon tetrachloride.

<u>What makes a polar molecule?</u>

So what makes a polar molecule?
1. At least one **polar bond must be present**. (For reference, carbon-hydrogen bonds are considered nonpolar, since carbon and hydrogen are similar in electronegativity.)
2. If there are multiple polar bonds, they **must not be arranged symmetrically**.

Some molecules are more polar than others, just as some bonds are more polar than others. The polarity of a molecule can be measured, and the **dipole moment** is often tabulated for polar molecules. The **dipole moment** is a quantitative measure of the polarity of a molecule, expressed in Debye (D) units. The larger the **dipole moment**, the more polar the molecule.

A molecule that is nonpolar will have a **zero dipole moment**.

<u>Summary</u>

We have learned how to tell if a molecule is polar based on the nature of the bonds in the molecule **and** the shape of the molecule. In the future, we will use this information to estimate important properties of materials.