7.2: Molecular Dipoles

Electrostatic potential maps are useful because they clearly show the electron distribution around covalent bonds within molecules. They must be calculated, however, using sophisticated computer programs, and then rendered in color for visualization. Because of this, the polarization of covalent bonds is typically shown using a special arrow (a dipole arrow) to indicate the direction in which the bond is polarized. A **dipole arrow** is crossed at the beginning (as in a plus sign) and points in the direction of the greatest electron density. Thus for hydrogen fluoride, the electronegativities are 2.20 and 3.98 for the hydrogen and fluorine, respectively. We would predict that the H—F bond would be polarized with the greatest electron density towards the fluorine.

A molecule such as water, with two covalent bonds, will have *two* local dipoles, each oriented along the covalent bonds, as shown below. Because water is asymmetric (it has a bend structure) both of these local dipoles point in the same direction, generating a **molecular dipole**, in which the entire molecule has a charge imbalance, with the "oxygen end" being anionic and the "hydrogen end" being cationic.

Molecules with local dipoles do not necessarily possess a molecular dipole. Consider the molecule boron trihydride (BH_3). The BH_3 molecule is planar with all three hydrogens spaced evenly surrounding the boron (trigonal planar). The electronegativities of boron and hydrogen are 2.04 and 2.20, respectively. The bonds in BH_3 will therefore be somewhat polarized, with the local dipoles oriented towards the hydrogen atoms, as shown below. But because the molecule is *symmetrical*, the three dipole arrows cancel and, as a *molecule*, BH_3 has no net molecular dipole.

? Exercise 7.2.1

For each of the molecules of NH_3 and CO_2 indicate whether a molecular dipole exists. If a dipole does exist, use a dipole arrow to indicate the direction of the molecular dipole.