3.8: Polarity of molecules

The polarity of an atom

The negative charge of electrons balances the positive charge of protons in an atom. The electrons symmetrically distributed around the nucleus leave no negative or positive end. The atoms are nonpolar. Fig. 3.8.1 illustrates the polarity of a hydrogen atom with color codes.

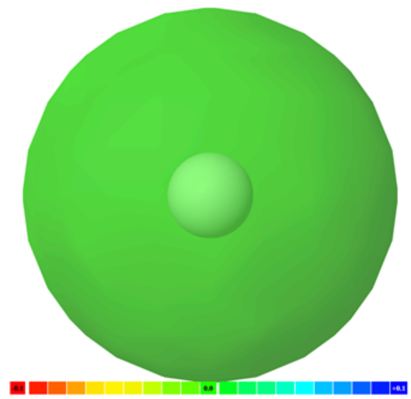

Figure 3.8.1: Electrostatic potential map of hydrogen atom, shown nonpolar by green color code. Source: drawn using free software https://chemagic.org/molecules/amini.html

The polarity of a covalent bond

When atoms of one element combine to make a covalent bond, e.g., H-H and F-F, the positive and negative charges are still symmetrical, and the bond is **nonpolar**, i.e., no negative end separated from a positive end. However, when atoms of different elements combine to make a covalent bond, the more electronegative atom attracts the bonding electron pair towards itself stronger than the other atom. The separation of positive and negative charges happens as the electrons shift more towards the electronegative atom. The bond becomes **polar** with a partially positive (δ+) end on the electropositive atom and a partially negative (δ-) end on the electronegative atom. For example, fluorine is more electronegative than hydrogen. Consequently, fluorine pulls the bonding electron pair towards itself in the H-F molecule, creating a partial negative charge (δ-) on fluorine and a partial positive charge (δ+) on hydrogen. The H-F bond is polar. Fig. 3.8.2 illustrates the polarity in H-F with color codes.

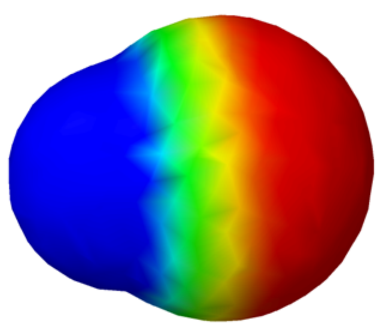

Figure 3.8.2: H-F molecule showing δ+ end in blue, δ- end in red and neutral part in green. Source: drawn using free software http://molview.org/?cid=14917

Bond polarity is a vector that has a magnitude and direction and can be represented by an arrow, like other vectors, as shown in Fig. 3.8.3 for the case of a water molecule.

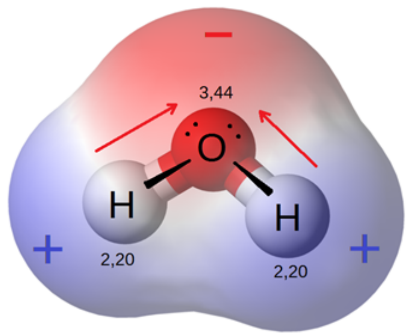

Figure 3.8.3: The water molecule is made up of oxygen and hydrogen, with respective electronegativities of 3.44 and 2.20. The electronegativity difference polarizes each H–O bond, shifting its electrons towards the oxygen (illustrated by red arrows). These effects add as vectors to make the overall molecule polar. Source: Riccardo Rovinetti / CC BY-SA (https://creativecommons.org/licenses/by-sa/3.0)

A bond is categorized as a nonpolar covalent, polar covalent, or an ionic bond based on the following convention: nonpolar covalent if the electronegative difference of the bonded atom is less than 0.5, a polar covalent if the electronegativity difference is between 0.5 to 1.9, and an ionic if the electronegativity difference is more than 1.9.

The polarity of a Molecule

The molecules fall into the following categories concerning molecular polarity.

The molecule is nonpolar if there is no polar bond in it, e.g., H-H, F-F, and CH_4 are nonpolar molecules. Fig. 3.8.4 illustrates CH_4 molecules with green color electron clouds that represent a nonpolar molecule.

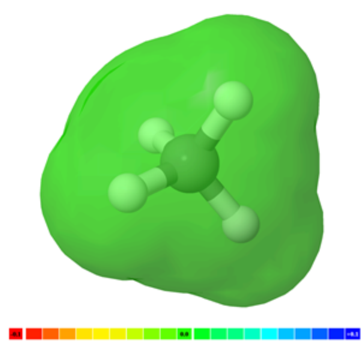

Figure 3.8.4: Methane (CH_4) with no polar bond is nonpolar. Source: drawn using free software https://chemagic.org/molecules/amini.html

If there is only one polar bond in a molecule, then the molecule is polar, e.g., the H-F molecule shown in Fig. 3.8.2.

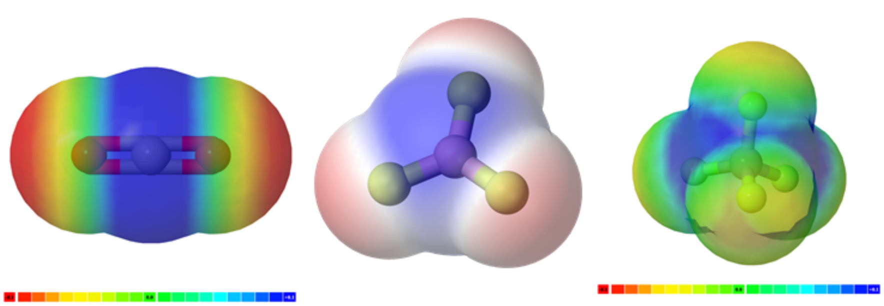

Figure 3.8.5: Examples of symmetric molecules with all polar bonds but the molecule as a whole is nonpolar. The examples are (from left to right) carbon dioxide CO_2, boron trifluoride BF_3, and carbon tetrafluoride CF_4.

If there is more than one polar bond in a molecule, the molecule may be polar or may be nonpolar, depending on the symmetry of the molecule: a) Polarity vector of individual bonds cancel out in symmetric molecules making the molecule nonpolar. For example, symmetric molecules, like CO_2, BF_3, and CCl_4, are nonpolar, although each bond in them is polar. Fig. 3.8.5 illustrates the symmetric molecules that have polar bonds, but the polarity of bonds cancels each other, making the molecule nonpolar. b) If a molecule has polar bonds and it is not symmetric, the polarity vectors do not cancel out, and the molecule is polar. Examples of polar molecules include $CHCl_3$, NH_3, and H_2O, as illustrated in Fig. 3.8.6.

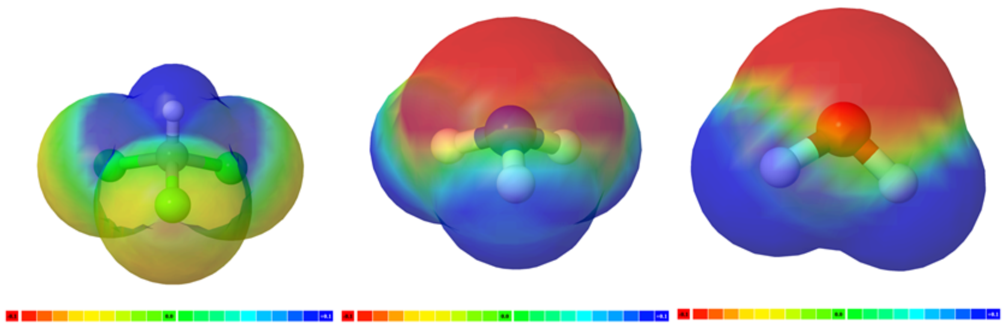

Figure 3.8.6: Non-symmetric molecules with polar bonds are polar molecules with a net δ+ end in red color and δ- ends in blue color. The examples are (from left to right) chloroform ($CHCl_3$), ammonia (NH_3), and water (H_2O).