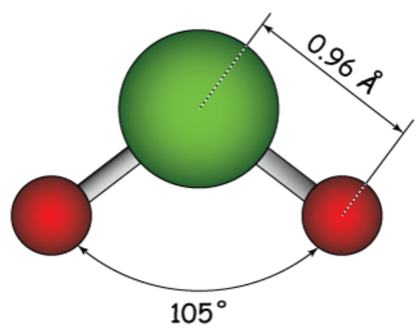
THE WATER MOLECULE

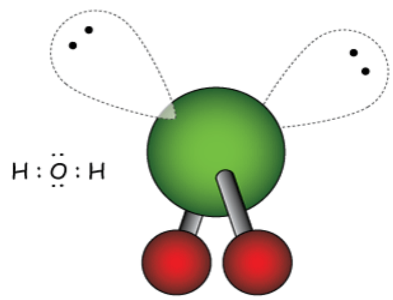
Water (H_2O) is a nonlinear covalently-bonded triatomic molecule with some interesting properties that arise from its electronic structure.

The basic geometry of the water molecule gives rise to big differences in its properties when compared with other triatomic molecules.

The average structure of the water molecule is shown on the right.



It's important to remember that any such structure is an average over a constantly **translating**, **rotating** and **vibrating** molecule. Molecules never stop (cannot stop) moving. The two most important features of water are (1) that the molecule is bent, with the angle between the Hydrogen atoms approximately 105˚ (as you will see below, the consequences of this fact are immense), and (2) it is composed of a highly electronegative (electron-withdrawing) atom and two H atoms, which are not electronegative and bring only one electron to the bond.



Lone pairs

Oxygen has six outer-shell electrons, two of which it shares in molecular orbitals with the H atoms so that it has a full octet. The other two reside in p-like orbitals in a roughly tetrahedral configuration, as VSEPR theory would predict.

These lone pairs, the fact that water is a bent molecule, and the fact that oxygen withdraws some of the electron density from the hydrogens, make water quite **polar**. Water has a **negative** end and a **positive** end. We refer to these as "δ+" and "δ-" ("delta-plus" & "delta-minus") ends.

This charge separation leads to a fairly large **dipole moment** for water, $\mu = 1.8$ D. The dipole moment is a measure of the degree of separation of charge in a molecule.

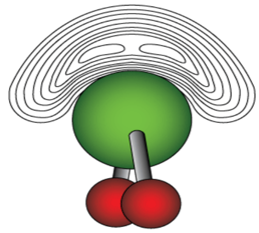
The linear molecule CO_2, O=C=O, has no dipole moment because its charge distribution is symmetric; while each oxygen carries slightly more charge than the central carbon, they are symmetrically located around the carbon, so there's no "+ end" and no "- end".

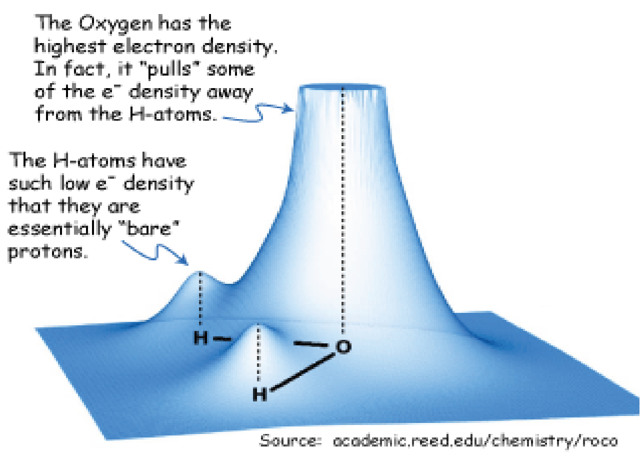
The importance of the polarity of water cannot be overstated. It leads to all kinds of effects that determine the outcome of reactions and the structure of large molecules and assemblies of large molecules.

We ought to pause here to note that the lone-pair p-like orbital picture above is a bit idealized. When calculations are performed to map the **electron density** of the H_2O electrons not involved in bonding, we really get a picture more like the one on the right.

This **contour map** is meant to show that there are two regions of high electron density (the two small closed curves), and that the density decreases as we move away. Think of this map just like a contour map of mountains. The outer rings represent the lowest electron density, the inner ones the "mountain tops".

The region of negative charge is really a little closer to the oxygen atom than the first lone-pair illustration above would lead one to believe.





Here's another view of the electron density of water. It shows that most of the electrons are drawn close to the **electronegative** oxygen atom, leaving very little to the hydrogens. The hydrogens are nearly "bare" in water.

This is partly what leads water to be so polar: "unshielded" protons on one side, and a region of negative charge on the other. The molecule is **electrically neutral**, but the *distribution* of its charges is uneven. Think about a battery. It's charge-neutral because it has a negative end and a positive end, but it has two **poles**, + and -.

Source: http://www.drcruzan.com/Water.html