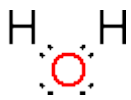


# Water Molecule Structure: Introduction

Water is a tiny molecule with the molecular formula  $H_2O$ , consisting of two light hydrogen atoms attached to each 16-fold heavier oxygen atom. Each hydrogen atom has a nucleus consisting of a single positively-charged proton surrounded by a 'cloud' of a single negatively-charged electron and the oxygen atom has a nucleus consisting of a eight positively-charged protons and eight uncharged neutrons surrounded by a 'cloud' of a eight negatively-charged electrons. On forming the molecule, the ten electrons pair up into five 'orbitals', one pair closely associated with the oxygen atom, two pairs associated with the oxygen atom as 'outer' electrons and two pairs forming each of the two identical O-H covalent bonds.

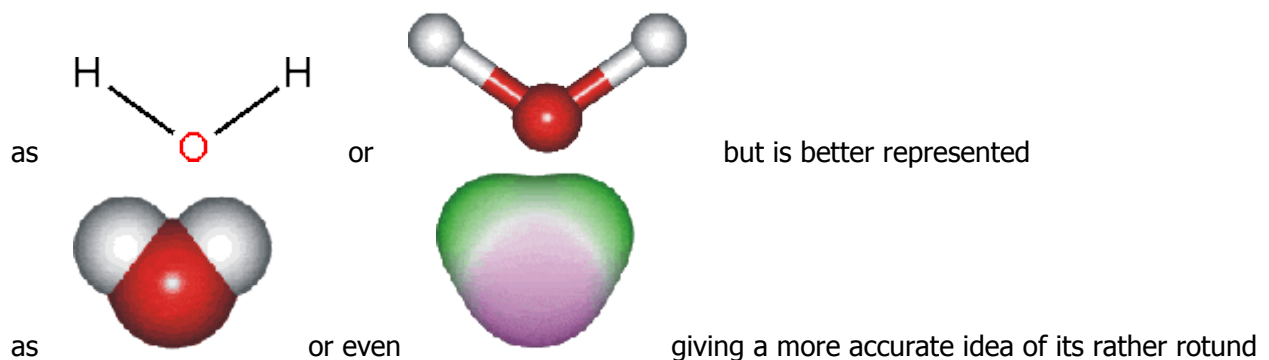
The eight outer electrons are often shown as the pairs of dots in  where the pairs of electrons between the O and H atoms represent the O-H covalent bonds and the other two pairs of electrons represent the so-called 'lone pairs'. These electron pairs form electron 'clouds' that are spread out around the oxygen nucleus as they repel each other. This is the reason for water's bent structure.

The eight positive charges in the oxygen nucleus attract all these electrons strongly relative to the single positive charges on each of the hydrogen atoms. This leaves the hydrogen atoms partially denuded of electrons, and hence partially positively charged, and the oxygen atom partially negatively charged, that is,  $\overset{\delta+}{H}-\overset{\delta-}{O}-\overset{\delta+}{H}$ .

Due to the presence of these charges and the bent nature of the molecule, the center of the positive charge (half way between the two hydrogen atoms) does not coincide with the center of the negative charge (on the oxygen atom). In liquid water, this gives a molecular dipole moment from the center of negative charge to the center of positive charge, equivalent to a unit negative charge (that is, one electron) separated from a unit positive charge by 0.061 nm. The presence of this dipole moment in all water molecules causes its polar nature.

Water is much smaller than almost all other molecules. For example, it has a smaller volume, and is much lighter, than the four other common atmospheric molecules, oxygen ( $O_2$ ), nitrogen ( $N_2$ ), argon (Ar) and carbon dioxide ( $CO_2$ ). As a result, both liquid and solid water (ice) have high densities of molecules. One liter of water at room temperature (25 °C) weighs almost a kilogram (997 g) and contains about 33 million million million million molecules.

The molecule is V-shaped. It is often shown



shape and also indicating the charge (pink showing negatively charged surface and green showing positively charged surface).

In liquid water, the mean O-H length is about 0.097 nm, the mean H-O-H angle is about  $106^\circ$  and the mean negative charge on the oxygen atom is about 70% of that of an electron with each hydrogen atom positively charged sharing the neutralizing charge. Individual water molecules will have different values for these parameters dependent on their energy and surroundings. The opposite charges on the oxygen and hydrogen atoms causes different water molecules to attract each other. This attraction is particularly strong when the O-H bond from one water molecule points directly at a nearby oxygen atom in another water molecule, that is, when the three atoms O-H O are in a straight line. This is called 'hydrogen bonding' as the hydrogen atoms appear to hold on to both O atoms. This attraction between neighboring water molecules, together with the high density of molecules due to their small size, produces a great cohesive effect within liquid water that is responsible for water's liquid nature at ambient temperatures.

Heavy water ( $D_2O$ ) has similar, but not identical, properties to  $H_2O$ . The deuterium atom (D) is a stable isotope of hydrogen that has a neutron alongside the proton in its nucleus, almost doubling its atomic mass.

Source:<http://www1.lsbu.ac.uk/water/mol-easy.html>