

## Water and pH

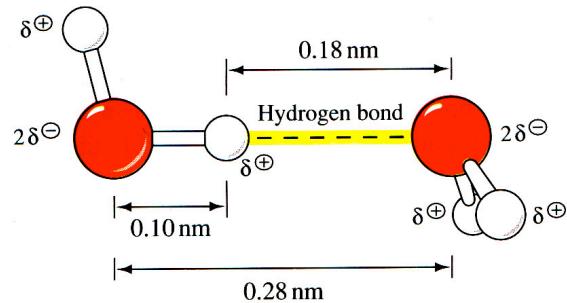
Water - one of the most important molecules in life.

- 70% of the bodies mass is water
- 2/3 of total body water is intracellular (55-66% body weight of men and 10% less for women)
- The rest is interstitial fluid of which 25% is in the blood plasma.
- The body tightly controls both the volume and pH of water.
- The bicarbonate system is crucial for blood maintenance
  - changes of pH greater than 0.1 are dangerous and can lead to coma – diabetics

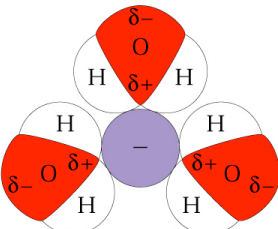
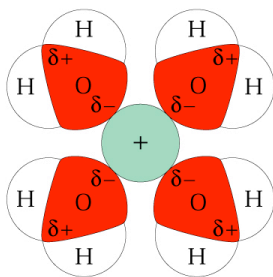
Important Properties of water

Water has hydrogen bonding potential

- H-bonds are non-covalent, weak interactions
- H<sub>2</sub>O is both a Hydrogen donor and acceptor
- One H<sub>2</sub>O can form up to four H-bonds



Water is an ideal biological solvent



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- Water is close to a tetrahedral shape with the unshared electrons on the two sp<sup>3</sup>-hybridized orbital are in two corners and the hydrogen in others
- Compared to a tetrahedron, CH<sub>4</sub> (109°) or NH<sub>3</sub> the bond angle is smaller (109.5° and 107° vs. 104.5°)
- Due to the bent shape of the molecule, there is an uneven distribution of electrons. It is a polar molecule, a dipole or two guys named -ski?

What makes this molecule important?

- solvent ability - easily disrupts ionic compounds
  - dielectric constant (D) is high (measure of the ability to keep ions apart)

$$F = \frac{K q_1 q_2}{D r^2}$$

Coulombs Law - The force of attraction between two charged pairs

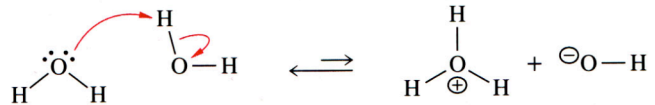
- large electronegativity creates a strong ionic type bond (dipole).
- Liquid water has a higher density than solid water (ice). Is this normal? Think of why this is important?
- orderliness - solvating shells
  - ability to take place in many hydrogen bonds (up to 4 at a time)
  - Strong nucleophile

- Specific heat and heat of vaporization is high for water due to extensive H bonding

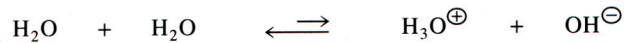
**Water and H-Bonds**

High specific heat

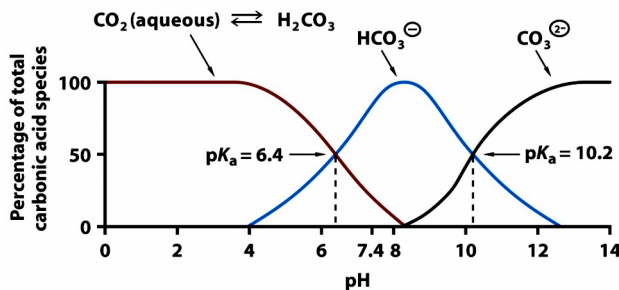
High Heat of vaporization



Water is nucleophilic



Water weakly ionizes



Water reacts with CO<sub>2</sub> to form an important blood buffer  
 We breath in and out gaseous CO<sub>2</sub>  
 In the blood, CO<sub>2</sub> reacts with water to form the buffering compound H<sub>2</sub>CO<sub>3</sub>  
 Primary buffering compounds at physiological pH is H<sub>2</sub>CO<sub>3</sub> and HCO<sub>3</sub><sup>-</sup>

### Noncovalent bonds:

The major noncovalent interactions in cells are electrostatic (ionic), hydrophobic, hydrogen bonds, and van der Waals. London forces are minimal unless tight association occurs

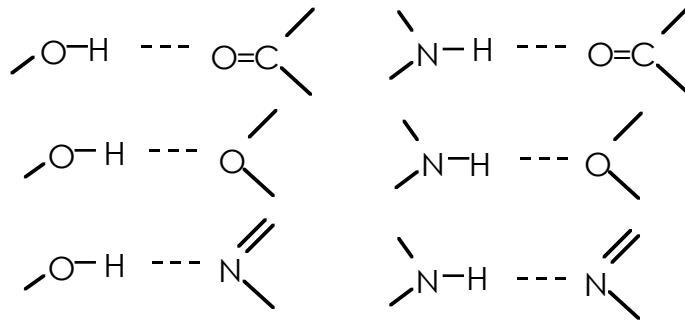
Most covalent bonds are 8 to 10 times stronger yet the overall shape and effectiveness of large molecules are due to the much weaker non-covalent bonds.

### Ionic Bonds or salt bridges... into the 21st century?

- Simple magnetic attraction
- The force of attraction (F) depends on distance and relative shielding
- Water and salts weaken bond
- Strongest single noncovalent bond

### Hydrogen bonds

- result from the interactions of strong covalent bonds between hydrogen and a highly electronegative atom (N and O)
- strongest bonds are when the arrangement is linear.
- The hydrogen is "shared" by a the covalently bonded atom and another electronegative atom
- You must be able to identify the donor and acceptor



### Van der Waals

- Next to London dispersion forces, these are the weakest of the nonionic bonds but are important due to the large number of van der Waal interactions in a protein
- These bonds originate from very small dipole moments generated in atoms as electrons move around the nucleus.
- These are small ionic, dipolar interactions
- The energy of the attraction is related to the distance between nuclei

### Hydrophobic interactions

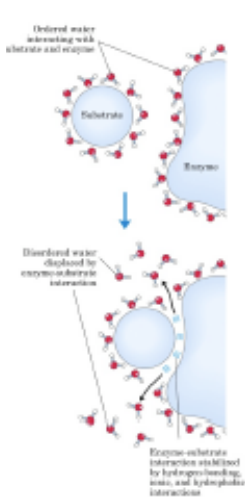
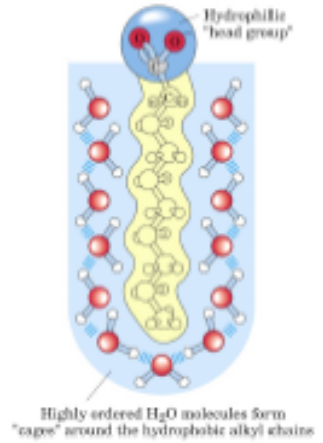
- the association of relatively nonpolar molecular groups in an aqueous environment.
- Driven by the order of water entropy
  - the lack of interactions with apolar molecules with decreases the randomness of the order of water. ( an increase in entropy)

Water forms cage-like structure around hydrocarbons forming shells of highly ordered water  
 Shell formation is due to water forming hydrogen bonds with each other  
 Aggregation of hydrophobic molecules reduces total surface area and results in less order (increase in entropy)

**Why are non-polar molecules insoluble in water?**

A:

Water molecules surrounding a hydrophobic molecule are ordered but cannot make hydrogen bonds or ionic interactions to the non-polar molecule.



This reduces the entropy (disorder) of water and is thermodynamically unfavorable and is called the hydrophobic effect.

Molecular associations are often accompanied by the release of water molecules that are ordered at the molecular surface. Release of ordered molecules is entropically favorable.

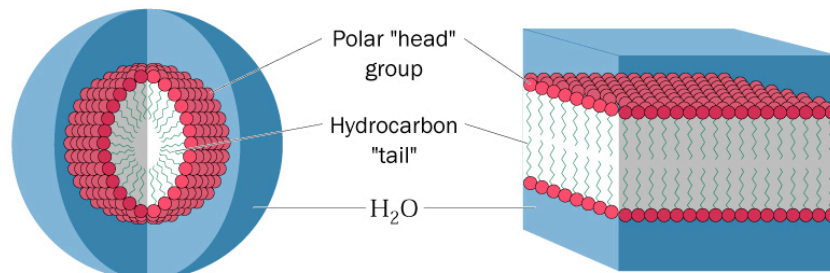
Minimization of the hydrophobic portions of the molecule permits the water max degrees of freedom (a minimization of entropy increase)

Thus nonpolar molecules aggregation is not due to attraction to other hydrophobic compounds, but due to inability to interact with water

- Very important in maintaining protein structure  
 - hydrophobic portions of proteins are solvated by "hiding" inside the molecule away from the water.
- Driving force for the formation of amipathic lipid bilayers, membranes

(a) Micelle

(b) Bilayer



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