## Chapter 2 - 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.
pH - 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
Properties of water
- Polarity
- Hydrogen bonding potential
- Specific heat, heat of vaporization
- Nucleophilic
- Ionization
- Water is an ideal biological solvent

It is the unique combination of properties of water that make it the perfect solvent for biological systems. We will discuss each of these properties in more detail.

Water is close to a tetrahedral shape with the unshared electrons on the two $\mathrm{sp}^{3}$-hybridized orbital are in two corners and the hydrogen in others

Compared to a tetrahedron, $\mathrm{CH}_{4}\left(109^{\circ}\right)$ or $\mathrm{NH}_{3}$ the bond angle is smaller (109.5 and $107^{\circ}$ vs. $104.5^{\circ}$ )


## Water has hydrogen bonding potential

-H-bonds are non-covalent, weak interactions
$\cdot \mathrm{H}_{2} \mathrm{O}$ is both a Hydrogen donor and acceptor -One $\mathrm{H}_{2} \mathrm{O}$ can form up to four H -bonds

## What Are the Properties of Water?

A comparison of ice and water, in terms of H -bonds and Motion

- Ice: 4 H bonds per water molecule
- Water: 2.3 H bonds per water molecule
- Ice: H-bond lifetime - about 10 microsec
- Water: H-bond lifetime - about 10 psec
- $\quad(10 \mathrm{psec}=0.00000000001 \mathrm{sec})$

The Solvent Properties of Water Derive from Its Polar Nature - Water has a high dielectric constant - Ions are always hydrated in water and carry around a "hydration shell" -Water forms H bonds with polar solutes


## The Solvent Properties of Water Derive from Its Polar Nature

What makes this molecule important? solvent ability - easily disrupts ionic compounds - dielectric constant (D) is high (measure of the ability to keep ions apart)

- 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 ...

High specific heat...

High heat of vaporization...
Water is nucleophilic
Water participates in many chemical reactions
-it is electron rich
-it is a weak nucleophile
-it is present in high concentration


Acid \& Base and pH pH - pouvoir hydrogene (the power of hydrogen)
Water undergoes ionization

Water ionizes to form the hydronium (hydroxyl) ion and hydroxide ions
Water can act as both an acid and base
The equilibrium constant for the ionization of water is:

The concentration of pure water

- 1 liter $=1000 \mathrm{~g} \mathrm{MW}$ of water is 10.015
- the final concentration of water is 55 M and $\mathrm{H}+$ concentration is about $1.8 \times 10$
- Very little water actually dissociates
- So Keq is very small - not easily measured or easy to use

Instead a different constant is used where the denominator is ignored

$$
\mathrm{K}_{\mathrm{w}}=1.0 \times 10^{-14}
$$

pH is a measure of the proton concentration of a solution
when $\left[\mathrm{H}^{+}\right]=\left[\mathrm{OH}^{-}\right]$the solution is when $\left[\mathrm{H}^{+}\right]>[\mathrm{OH}]$ the solution is when $\left[\mathrm{H}^{+}\right]<\left[\mathrm{OH}^{-}\right]$the solution is

Note the relationship! A change in 1 pH units is a ten fold change in hydrogen ion concentration

The extent of ionization of a weak acid is a function of its acid dissociation constant oKa
Bronsted and Lowry acid and bases

> - acid donates protons
-bases accepts protons
Strong acids dissociate nearly fully
Weak acids only partially dissociate

Consider a weak acid, HA The acid dissociation constant is given by:

$$
\mathrm{HA} \rightleftarrows \mathrm{H}+\mathrm{A}
$$

Acids with $\mathrm{Ka}<1$ are considered weak acids $\qquad$ Ka for acetic acid is $1.76 \times 10^{-5} \rightarrow$ difficult to work with so instead use log scale:

$$
\mathrm{pK}_{\mathrm{a}}=-\log \mathrm{K}_{\mathrm{a}}
$$

So the pK of acetic acid is $=-\log 1.76 \times 10=4.75$
The pH is a measure of acidity and the pKa is a measure of acid strength

What Are Buffers, and What Do They Do?
Buffers are solutions that resist changes in pH as acid and base are added

Most buffers consist of a weak acid and its conjugate base
Note how the plot of pH versus base added is flat near the $\mathrm{p} K_{\mathrm{a}}$


Buffers can only be used reliably within a pH unit of their $\mathrm{p} K_{\mathrm{a}}$

The Henderson-Hasselbalch Equation<br>Know this! You'll use it constantly.

For any acid HA , the relationship between the $\mathrm{pK}_{\mathrm{a}}$, the concentrations existing at equilibrium and the solution pH is given by: $\quad H A \leftrightarrows H^{+}+A^{-}$

The relationship between pH and pKa is described by the Henderson-Hasselbalch equation

What is the H-H Equation Used For?
This is used to determine the concentration of acid and base at a given pH . It is Also used to determine the pH of a known solution. These concepts are used to calculate buffer strength and understand the pH of a biological solution.

Remember that buffers are mixtures of weak acids and their conjugate bases that resist pH by shifting the equilibrium between the acid and base in response to the pH of a solution.

Case 1) when the concentration of base equals the acid.

Case 2) when the pH is above or below 1 pH unit of the pKa

Calculate the pH of a mixture of $\mathbf{2 5 0 ~ m M}$ acetic acid and 100 mM Na acetate. The pKa of acetic acid is 4.75 . Start with the HH equation

What is the ratio of lactic acid to lactate in a buffer at pH of 5.00 .

- The pKa of lactic acid is 3.86 ?

What is the concentration of base and acid you need to add to make a 50 mM solution of lactate buffer at pH 4.0? The MW of Lactic acid is 91 amu and sodium lactate is 102 amu .

This is for you to take home try and we will calculate an answer with Dr Provost -!

