

### Water

the solvent for virtually all of biochemistry, ~70% of the mass within each cell is water

**Carbon** has **four electrons** in the **outer shell** - these hybridise into 4 sp<sup>3</sup> hybrid orbitals as tetrahedron. If symmetrical, the angle is **109.28 degrees**.

WATER AS A SOLVENT (substances such as household sugar **dissolve in water**, means that their molecules **separate** from each other, each becoming **surrounded** by water molecules.)

When a substance dissolves in a liquid, the mixture is termed a **solution**.

The dissolved substance is the **solute**, and the liquid that does the dissolving is the **solvent**.

**Water is an excellent solvent for many substances** because of its **polar bonds**.

Covalent bond	<b>Inside a molecule</b>
Hydrogen bond	<b>between molecules</b>
Polar bonds (H <sub>2</sub> O)	<b>uneven charge</b>
Non-polar bonds (O <sub>2</sub> )	<b>even charge</b>

### Henderson-Hasselbalch equation

$$\text{pH} = \text{pK}_a + \log \frac{[\text{conjugate base}]}{[\text{weak acid}]} \text{ (for weak acid)}$$

$$\text{pOH} = \text{pK}_b + \log \frac{[\text{conjugate acid}]}{[\text{weak base}]} \text{ (for weak base)}$$

### pH (potential hydrogen)

The **acidity of a solution** is defined by the **concentration of H<sup>+</sup> ions** it possesses.

pH scale      $\text{pH} = -\log_{10}[\text{H}^+]$

pure water      $[\text{H}^+] = 10^{-7}$  moles/liter  
pH (7)

**acids**            substance, **proton (H<sup>+</sup>) donors**

**bases**            substance, **proton acceptors (such as OH<sup>-</sup>)**

Water can act as both a weak acid and a weak base.

### pH (potential hydrogen) (cont)

Acids in an aqueous environment     proton moves from one molecule to the other

pH is a measure of **acidity (<7)** or **alkalinity (>7)**.

**Higher amounts** of protons in a solution     results in a lower pH (acidic)

**Lower amount** of protons     results in a higher pH (basic, or alkali)

**Different Enzymes** have different **optimal pH** according to their environment.

The **strength of an acid** is measured by its **dissociation constant, K<sub>a</sub>**. The **larger** the **K<sub>a</sub>** the more it **dissociates** and the **stronger** the **acid**.

The **pH** of a solution of a **weak acid** and its **conjugate base** is related to the **concentration of the acid and base** and the **pK<sub>a</sub>** by the Henderson-Hasselbalch equation.

When **ph < pK<sub>a</sub>**, the **weak acid predominates**. When **pH > pK<sub>a</sub>**, the **conjugate base predominates**.

### Buffers

A solution which pH **resists** change upon addition of either small amounts of strong acid or strong base are added.

(consist of a **weak acid and its conjugate base**)

**BUFFER CAPACITY** - is related to the concentrations of the weak acid and its conjugate base,

The greater the concentration of the weak acid and its conjugate base, the greater the buffer capacity.

H<sub>2</sub>PO<sub>4</sub><sup>-</sup> / HPO<sub>4</sub><sup>2-</sup> is the principal buffer in cells, H<sub>2</sub>CO<sub>3</sub> / HCO<sub>3</sub><sup>-</sup> is an important buffer in blood.

Buffers work because the concentration of the weak acid and base are kept in the narrow window of the titration curve.

### Biological Buffer Systems

Maintenance of intracellular pH is vital to all cells:

1. Enzyme-catalyzed reactions have optimal pH,
2. Solubility of polar molecules depends on H-bond donors and acceptors,
3. Equilibrium between CO<sub>2</sub> gas and dissolved HCO<sub>3</sub><sup>-</sup> depends on pH.

Buffer systems in vivo are mainly based on:

1. Phosphate, concentration in millimolar range,
2. Bicarbonate, important for blood plasma,
3. Histidine, efficient buffer at neutral pH.

Buffer systems in vitro are often based on sulfonic acids of cyclic amines:

HEPES, PIPES, CHES.

