PH - Pouvoir Hydrogene (the Power of Hydrogen)

Trivia time: Why was the concept of pH developed?

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 = 1000g MW of water is 10.015
- the final concentration of water is 55M and H+ concentration is about 1.8×10^{-9}
- 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

$$K_W = 1.0 \text{ X } 10^{-14}$$

pH is a measure of the acidity and basicity of a solution

when $[H^+] = [OH^-]$ the solution is neutral and pH is 7
when $[H^+] > [OH^-]$ the solution is acidic and pH is less than 7
when $[H^+] < [OH^-]$ the solution is basic and pH is more than 7

a change in 1 pH units is = a ten fold change in hydrogen ion concentration

<u>The extent of ionization of a weak acid is a function of its acid dissociation constant pKa</u>

Bronsted and Lowry acid and bases
- acid donates protons
- bases accepts protons

Strong acids dissociate nearly fully

Weak acids only partially dissociate

Acids with Ka < 1 are considered weak acids

Ka for acetic acid is 1.76×10^{-5} -> difficult to work with so instead use log scale:

$$pK_a = -\log K_a$$

So the pKa of acetic acid is = $-\log 1.76 \times 10^{-5} = 4.75$

The pH is a measure of acidity and the pKa is a measure of acid strength

Dissociation constants and pKa values

Chemical	Ka (M)	pKa
Formic acid	1.77×10^{-4}	3.8
Carbonic acid	4.30×10^{-7}	6.4
Bicarbonate	5.61×10^{-11}	10.2
Ammonium	5.62×10^{-10}	9.2

pKa of a weak acid is determined experimentally by titration.

- pKa is when the concentration of acid and base is equal (is that then equal to pH 7?) in a titration.
- There is a point in a titration of a weak acid where the change in pH is very little. This is the buffer action of the acid.
- Many acids have more than one ionizable group (polyprotic)

The relationship between pH and pKa FOR A WEAK ACID 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 weak acids 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.

$$pH = pKa + Log \frac{[A^-]}{[HA]}$$

$$= pKa + Log \frac{[x]}{[x]}$$

$$pH = pKa$$

When pH = pKa 50% of the acid is dissociated

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

$$5.00 = 4.00 + Log \frac{[A^-]}{[HA]}$$

$$1.00 = Log \frac{[A^-]}{[HA]}$$

$$10.0 = \frac{[A^-]}{[HA]}$$

Then 90% of the buffer is in the conjugate base for
If pH is 2 units different then 99% of buffer is in the conjugate base form
What does this mean about the buffering ability if more acid or base is added?

Calculate the pH of a mixture of 250 mM acetic acid and 100 mM Na acetate
The pKa of acetic acid is 4.75.

What is the ratio of lactic acid to lactate in a buffer at pH of 5. The pKa of lactic acid is 3.86?

What is the concentration 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.