Lecture 4
pH Calculations

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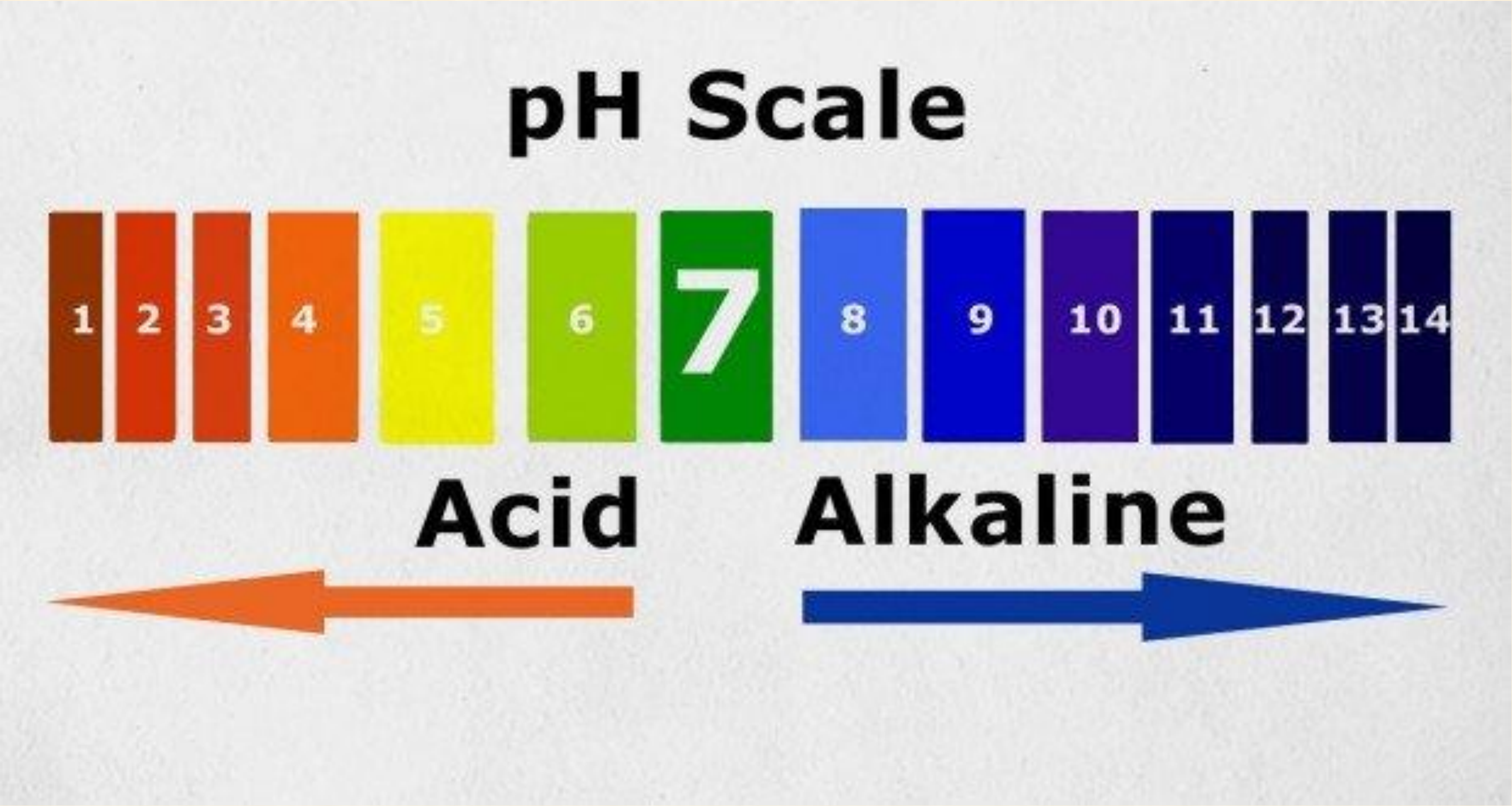

What is pH?

$$pH = -\log_{10} [H^+_{(aq)}]$$

where $[H^+]$ is the concentration of hydrogen ions in mol dm^{-3}

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to convert pH into
hydrogen ion concentration

$$[H^+(aq)] = \text{antilog}(-pH)$$

IONIC PRODUCT OF WATER $K_w = [H^+(aq)][OH^-(aq)]$ $mol^2\ dm^{-6}$

$= 1 \times 10^{-14}$ $mol^2\ dm^{-6}$ (at 25°C)

Autoionization of H_2O

$$H_2O + H_2O \rightleftharpoons H_3O^+ + OH^-$$

Pairs 1 2 2 1

acid | base | acid | base

$$H_2O + H_2O \rightleftharpoons H_3O^+ + OH^-$$

1 # 2

acid | base | Conjugate acid of H_2O #2 | Conjugate base of H_2O #1

$$H_2O + H_2O \rightleftharpoons H_3O^+ + OH^-$$

Conjugate acid of OH^- | Conjugate base of H_3O^+ | acid | base

<u>Amphoterism</u> - an ion or molecule can act as an acid or base depending upon the reaction conditions

Calculating pH - weak acids

A weak acid is one which only partially dissociates in aqueous solution

A weak acid, HA, dissociates as follows $$HA_{(aq)} \rightleftharpoons H^+_{(aq)} + A^-_{(aq)} \quad (1)$$

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Applying the Equilibrium Law $$K_a = \frac{[H^+_{(aq)}]\,[A^-_{(aq)}]}{[HA_{(aq)}]} \quad \text{mol dm}^{-3} \qquad (2)$$

The ions are formed in equal amounts, so $$[H^+_{(aq)}] = [A^-_{(aq)}]$$

therefore $$K_a = \frac{[H^+_{(aq)}]^2}{[HA_{(aq)}]} \qquad (3)$$

Rearranging (3) gives $$[H^+_{(aq)}]^2 = [HA_{(aq)}]\,K_a$$

therefore $$[H^+_{(aq)}] = \sqrt{[HA_{(aq)}]\,K_a}$$

$$pH = -\log\,[H^+_{(aq)}]$$

Calculating pH - weak acids

Calculate the pH of a weak acid HX of concentration 0.1M ($K_a = 4 \times 10^{-5}$ mol dm^{-3})

HX dissociates as follows $\quad HX_{(aq)} \rightleftharpoons H^+_{(aq)} + X^-_{(aq)}$

Dissociation constant for a weak acid

$$K_a = \frac{[H^+_{(aq)}]\,[X^-_{(aq)}]}{[HX_{(aq)}]} \text{ mol dm}^{-3}$$

Substitute for X^- as ions are formed in equal amounts and the rearrange equation

$$[H^+_{(aq)}] = \sqrt{[HX_{(aq)}]\,K_a} \text{ mol dm}^{-3}$$

ASSUMPTION
HA is a weak acid so it will not have dissociated very much. You can assume that its equilibrium concentration is approximately that of the original concentration

$$[H^+_{(aq)}] = \sqrt{0.1 \times 4 \times 10^{-5}} \text{ mol dm}^{-3}$$

$$= \sqrt{4.00 \times 10^{-6}} \text{ mol dm}^{-3}$$

$$= 2.00 \times 10^{-3} \text{ mol dm}^{-3}$$

ANSWER $\quad pH = -\log [H^+_{(aq)}] = 2.699$

Format for solving problems of weak acids using an equilibrium table

$$HA(aq) \rightleftharpoons H^+(aq) + A^-(aq)$$

	$HA(aq)$	$H^+(aq)$	$A^-(aq)$
Initial concentration (M):			
Change in concentration (M):			
Equilibrium concentration (M):			

- Fill in initial concentrations
- Determine concentration changes in terms of *x*
- Determine equilibrium concentrations in terms of initial concentrations (C_i) and *x*
- Substitute into the K_a expression and solve for x

Percent Ionization

- Another way to measure the strength of an acid is to determine the percentage of acid molecules that ionize when dissolved in water; this is called the **percent ionization**.
  - The higher the percent ionization, the stronger the acid.

$$\text{Percent Ionization} = \frac{\text{molarity of ionized acid}}{\text{initial molarity of acid}} \times 100\%$$

- Because $[\text{ionized acid}]_{equil} = [H_3O^+]_{equil}$

$$\text{Percent Ionization} = \frac{[H_3O^+]_{equil}}{[HA]_{init}} \times 100\%$$

Problem: (a) Calculate pH and (b) the fraction of CH_3CO_2H ionized at equilibrium. The concentration of CH_3CO_2H is 1 M (initial, or total). The K_a for acetic acid is 1.8×10^{-5}

Estimate major species in solution **CH_3CO_2H** (a weak acid) and **H_2O.**

$$CH_3CO_2H \rightleftharpoons H^+ + CH_3CO_2^- \qquad K_a = 1.8 \times 10^{-5}$$

$$H_2O \rightleftharpoons H^+ + OH^- \qquad K_w = 1.0 \times 10^{-14}$$

Problem: (a) Calculate pH and (b) the fraction of CH_3CO_2H ionized at equilibrium.

$$CH_3CO_2H \rightleftharpoons H^+ + CH_3CO_2^-$$

	CH_3CO_2H	H^+	$CH_3CO_2^-$
Initial	**1.0M**	**~ 0**	**0**
Equilibrium	**1.0 – x**	**x**	**x**