INTRODUCTION INTO BIOCHEMISTRY

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قمة

QMA MEDICAL TEAM

1- Revision

2- Conjugate acid & base

- When an acid donate a proton, the new molecules is a proton acceptor so it a base, it's called base conjugate, and when a base accept a proton it becomes a proton donor, the new molecule is called conjugate acid
- strong acid is conjugated with a very weak base, that's why it's reaction is one way reaction
- strong base is conjugated with a very weak acid, that's why it's reaction is one way reaction
- weak acids and bases are two directional reactions because they have relative strong conjugates
- as a rule, the stronger the original molecule, the weaker the conjugate, and vise versa

3- Equilibrium constant

Acid/base solutions are at constant equilibrium.We can write equilibrium constant (Keq) for such reactions

$$K_a = \frac{[H_3O^+] \cdot [A^-]}{[HA]}$$

The value of the Ka indicates direction of reaction: (Higher Ka means stronger acid)

>1 means forward, <1 is backward

→ What is Pka

$$pK_a = -\log K_a$$

The values of Ka and pKa are inversely proportional

→ For base there is Kb

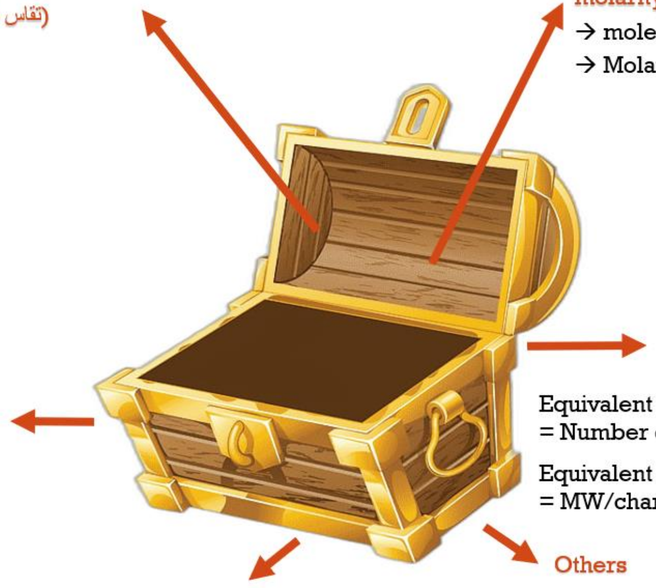
$$B + H_2O \rightleftharpoons BH^+ + OH^-$$

$$K_b = \frac{\boxed{[BH+][OH^-]}}{[B]}$$

Equal to each other!

H2O concentration is constant 55.5 M we cross it out for simplicity

4- Calculations



Concentration (تقاس بالمولات/ لتر)

molarity

→ moles = grams / MW

→ Molar solution = moles / volume

equivalence (Eq)

Equivalent (Eq of strong acid or base) = Number of H+ or OH – moles

Equivalent (Eq of ions) = MW/charge

normality (N)

Others

Titration

n.M1.V1=n.M2.V2

$$pK_a = -\log K_a$$

$$K_a = \frac{[B][H^+]}{[BH^+]}$$

$$K_b = \frac{[BH+][OH^-]}{[B]}$$

5- Ionization of water

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

$$K_{eq} = \frac{[H^\oplus][OH^\ominus]}{H_2O} \simeq 1.86 \times 10^{-16} M$$

$$K_{eq}(55.5\ M) = [H^\oplus][OH^\ominus]$$

$$K_w = [H^\oplus][OH^\ominus] = 1.0 \times 10^{-14}\ M^2$$

For pure water, there are equal concentrations of [H$^+$] and [OH$^-$], each with a value of 1 x 10^{-7} M.

Since Kw is a fixed value, the concentrations of [H$^+$] and [OH$^-$] are inversely changing.

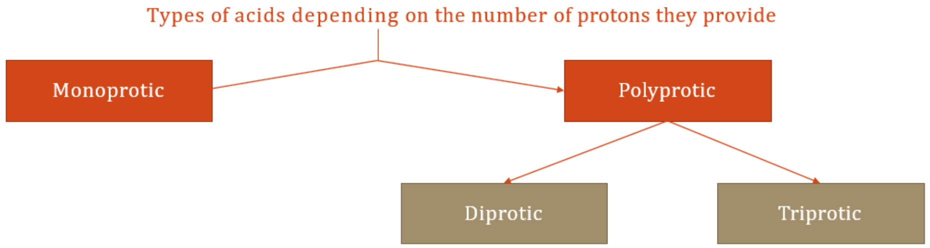
If the concentration of H$^+$ is high, then the concentration of OH- must be low, and vice versa. For example, if [H$^+$] = 10^{-2} M, then [OH$^-$] = 10^{-12} M

1- REVISION

	Bronsted- lorry
Acid	H+ donors
Base	H+ Acceptor

- Types of acids depending on the number of protons they contain:
  - Monoprotic acid (1 proton): HCl, HNO3, CH3COOH.
  - Polyprotic acids(more than 1 proton):

  A-Diprotic acid: H2SO4 / B-Triprotic acid: H3PO3



Types of acids depending on the number of protons they provide

Monoprotic

Polyprotic

Diprotic

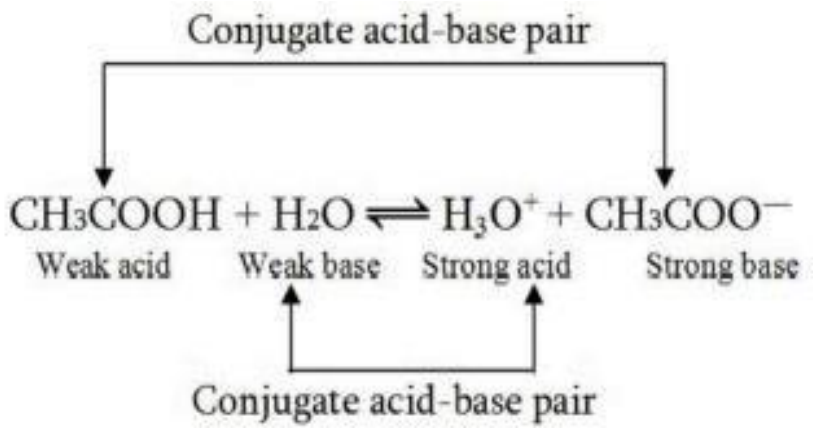
Triprotic

Acids differ in their ability to release protons/ Strong acids dissociate 100%/ Bases differ in their ability to accept protons/ Strong bases have strong affinity for protons /For multi-protic acids (H2 SO4 , H3PO4), each proton is donated at different strengths/ Rule The stronger the acid, the weaker the conjugate base.

2- CONJUGATE ACID AND BASE

Rule:

The stronger the acid, the weaker the conjugate base.



$$CH_3COOH + H_2O \rightleftharpoons H_3O^+ + CH_3COO^-$$

Strong vs. weak acids

- **Strong** acids and bases have **one-way** reactions because their disassociation is very high, it's almost 100%.

$$HCl \rightarrow H^+ + Cl^-$$

$$NaOH \rightarrow Na^+ + OH^-$$

- **Weak** acids and bases do not ionize completely **(two-way reactions)**.

$$HC_2H_3O_2 \leftrightarrow H^+ + C_2H_3O_2^-$$

$$NH_3 + H_2O \leftrightarrow NH_4^+ + OH^-$$

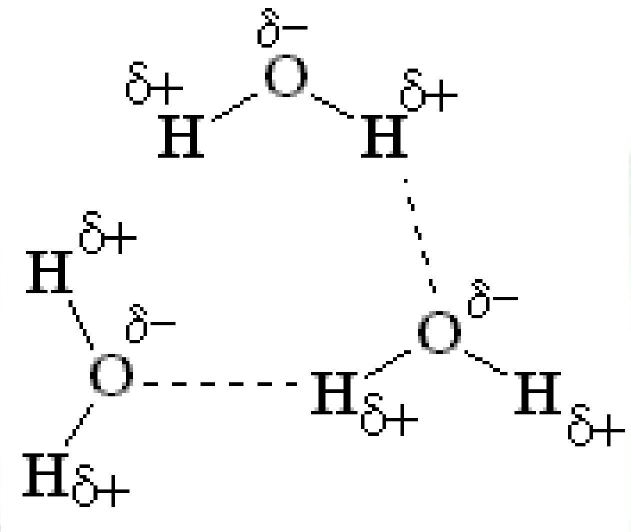
The double headed arrow indicates a two-way reaction.

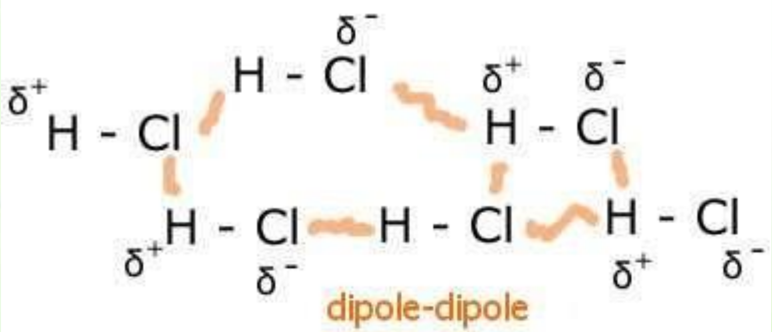
whether the acid is strong (has complete disassociation) or weak (partial disassociation), it donates its proton to the solution, and the newly formed proton-lacking molecule would be the conjugate base.

Generally, there's an opposite relationship between the acid or the base and its conjugate partner. Acids produce conjugate bases and bases produce conjugate acids. Strong acids produce weak conjugate bases and weak acids produce strong conjugate bases and the same principle applies to bases and their conjugate acids.

NOTE

Dipole-dipole interaction





dipole-dipole interaction

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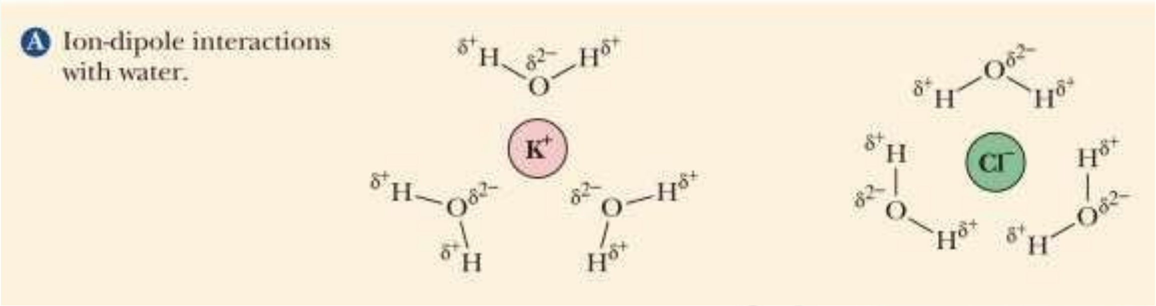
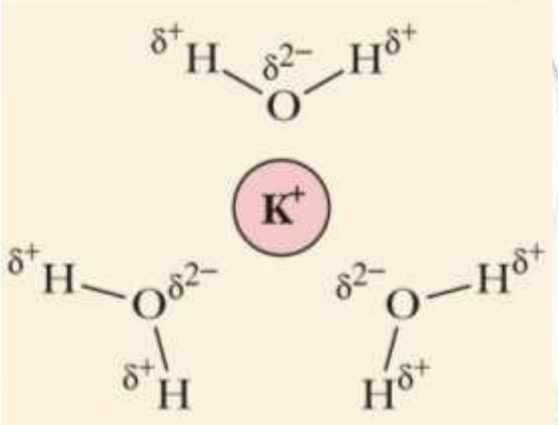
Dipole-charge interaction



A Ion-dipole interactions with water.



3- EQUILIBRIUM CONSTANT

ACID/BASE SOLUTIONS ARE AT CONSTANT EQUILIBRIUM.WE CAN WRITE EQUILIBRIUM CONSTANT (KEQ) FOR SUCH REACTIONS

$$HA \longleftrightarrow H^+ + A^-$$

$$K_a = \frac{[H_3O^+] \cdot [A^-]}{[HA]}$$

Note: $H_3O^+ = H^+$

The value of the Ka indicates direction of reaction:

a- When Ka is greater than 1 the product side is favored.

B- When Ka is less than 1 the reactants are favored

3- EQUILIBRIUM CONSTANT

What is pka ?

$$pK_a = -\log K_a$$

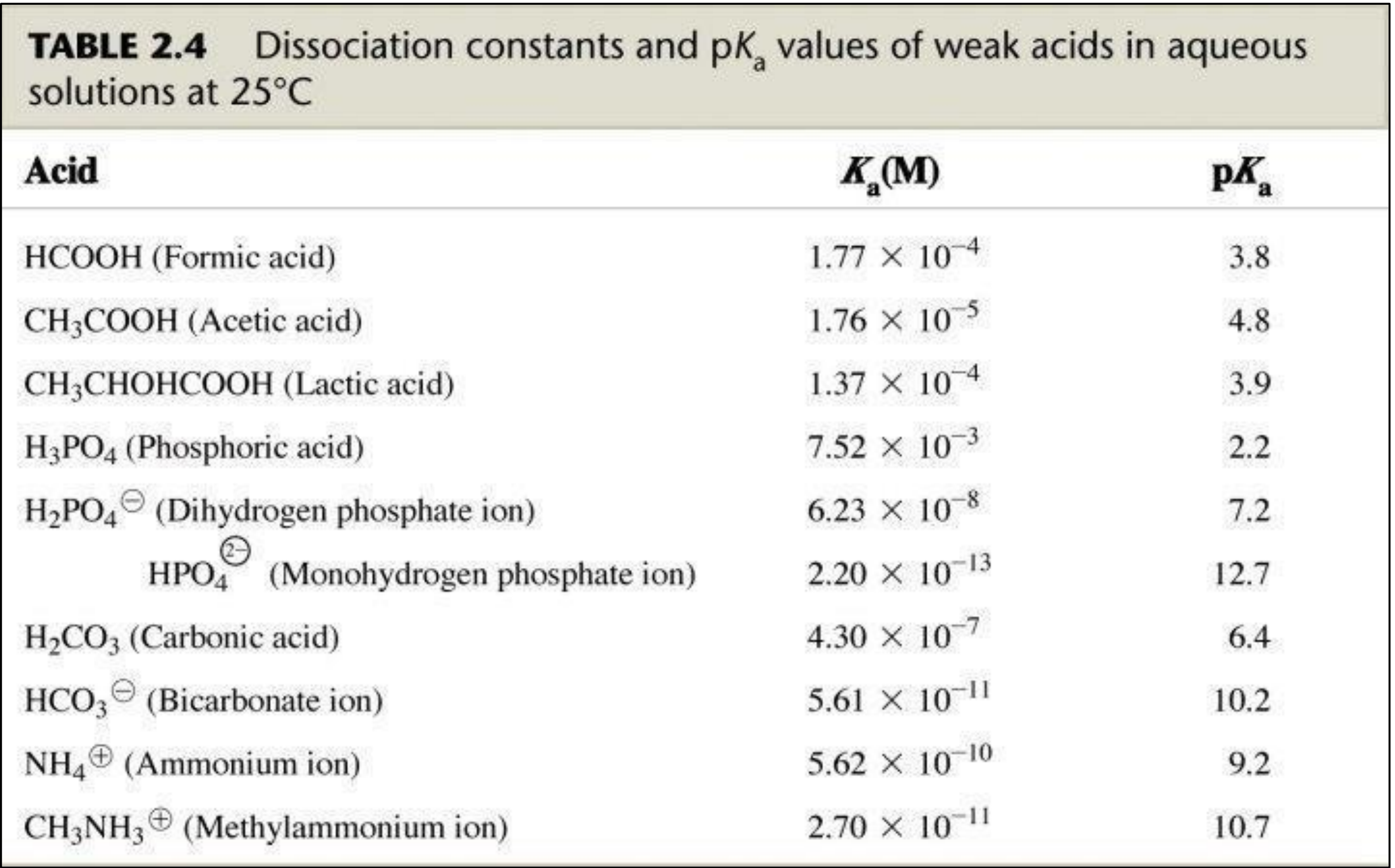


TABLE 2.4 Dissociation constants and pK_a values of weak acids in aqueous solutions at 25°C

Acid	K_a(M)	pK_a
HCOOH (Formic acid)	1.77×10^{-4}	3.8
CH_3COOH (Acetic acid)	1.76×10^{-5}	4.8
$CH_3CHOHCOOH$ (Lactic acid)	1.37×10^{-4}	3.9
H_3PO_4 (Phosphoric acid)	7.52×10^{-3}	2.2
$H_2PO_4^{\ominus}$ (Dihydrogen phosphate ion)	6.23×10^{-8}	7.2
$HPO_4^{2\ominus}$ (Monohydrogen phosphate ion)	2.20×10^{-13}	12.7
H_2CO_3 (Carbonic acid)	4.30×10^{-7}	6.4
$HCO_3^{\ominus}$ (Bicarbonate ion)	5.61×10^{-11}	10.2
$NH_4^{\oplus}$ (Ammonium ion)	5.62×10^{-10}	9.2
$CH_3NH_3^{\oplus}$ (Methylammonium ion)	2.70×10^{-11}	10.7

Notice how the values of Ka especially those of weaker acids contain negative powers that are difficult to deal with. So, to avoid this complexity it's better to convert those values into integers and that is by taking the negative log of these values and we end up with pKa values. the Ka values of strong acids are very high but their pKa values are the smallest. The values of Ka and pKa are inversely proportional. The higher the Ka the lower the pKa and vice versa.

Larger K_a means:
More dissociation
Smaller pK_a
Stronger acid

3- EQUILIBRIUM CONSTANT

BASE DISSOCIATION CONSTANT (K_B)

Reverse the reaction:

$$BH^+ \rightleftharpoons B + H^+ \qquad B + H_2O \rightleftharpoons BH^+ + OH^-$$

Equal to each other!

$$K_a = \frac{\boxed{[B][H^+]}}{[BH^+]}$$

$$K_b = \frac{\boxed{[BH+][OH^-]}}{[B]}$$

Equal to each other!

H2O concentration is constant 55.5 M we cross it out for simplicity

Similarly, Equilibrium constant for base dissociation Kb is equal to the concentration of the hydroxyl ion multiplied by the concentration of the conjugate acid over the concentration of the base. (Again, if there is water then it will be added to the denominator .However, since H2O concentration is constant 55.5 M we cross it out for simplicity)

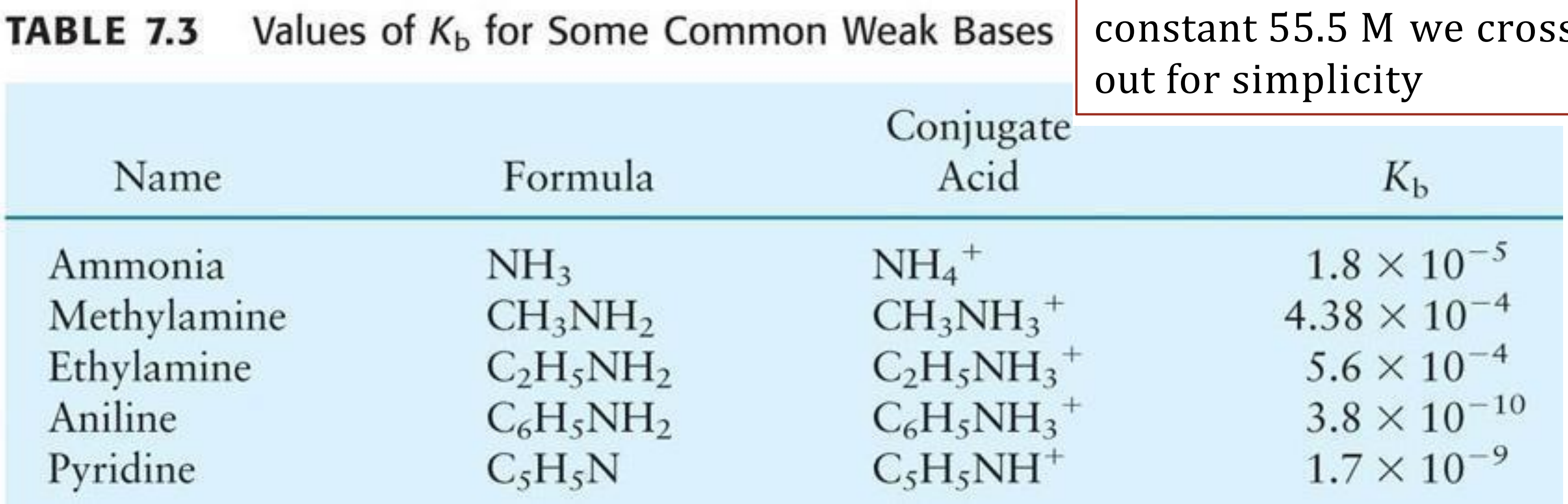
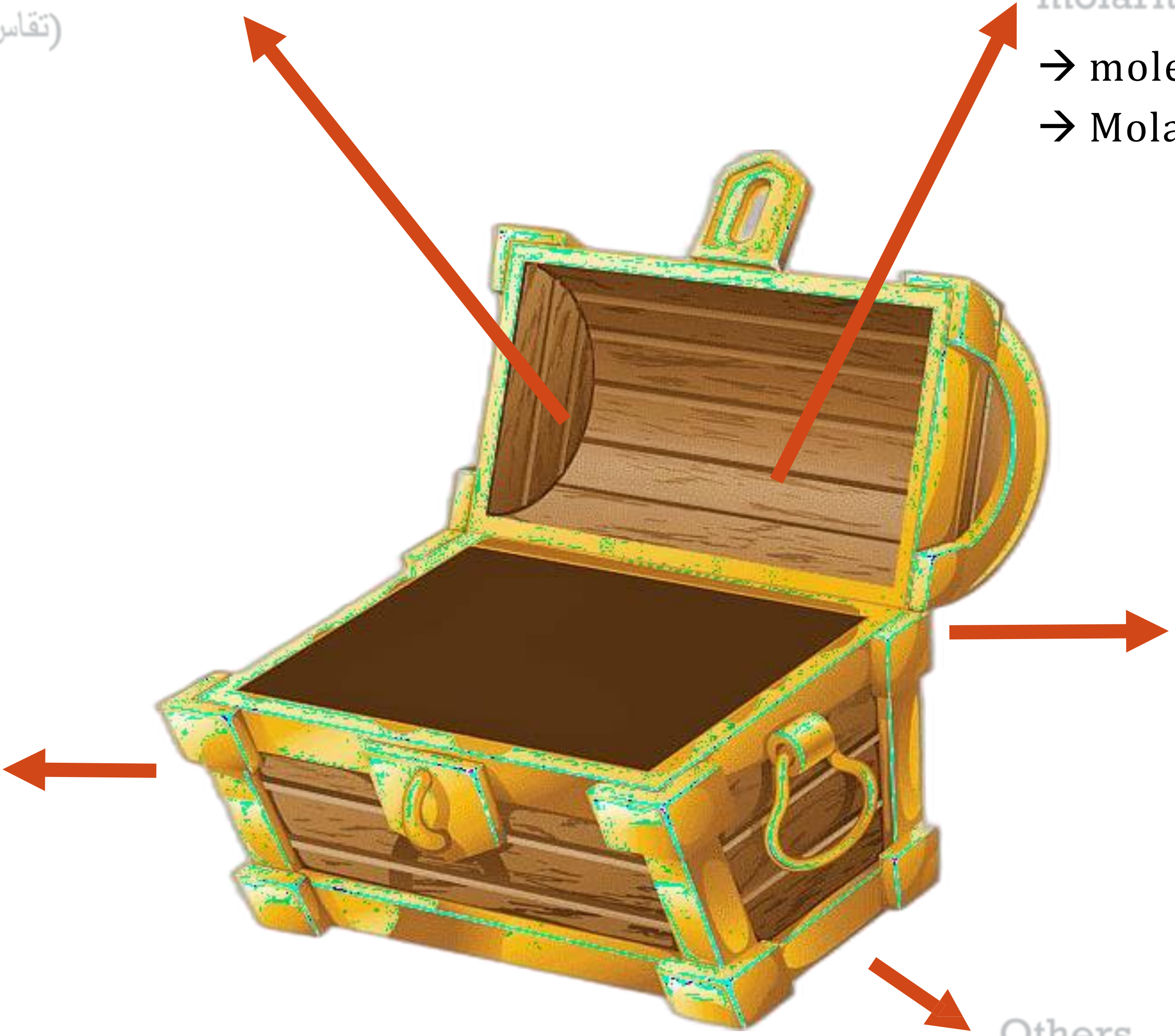


TABLE 7.3 Values of K_b for Some Common Weak Bases

Name	Formula	Conjugate Acid	K_b
Ammonia	NH_3	NH_4^+	1.8×10^{-5}
Methylamine	CH_3NH_2	$CH_3NH_3^+$	4.38×10^{-4}
Ethylamine	$C_2H_5NH_2$	$C_2H_5NH_3^+$	5.6×10^{-4}
Aniline	$C_6H_5NH_2$	$C_6H_5NH_3^+$	3.8×10^{-10}
Pyridine	C_5H_5N	$C_5H_5NH^+$	1.7×10^{-9}

4- CALCULATIONS

Concentration (تقاس بالمولات/لتر)



molarity

→ moles = grams / MW

→ Molar solution = moles / volume

equivalence (Eq)

normality (N)

Others

$$pK_a = -\log K_a$$

$$K_a = \frac{[B][H^+]}{[BH^+]} \qquad K_b = \frac{[BH+][OH^-]}{[B]}$$

MOLARITY OF SOLUTIONS

- Moles of a solution are the amount in grams in relation to its molecular weight (MW or a.m.u.).

$$\text{moles} = \text{grams} / \text{MW}$$

- A molar solution is where the number of grams equal to its molecular weight (moles) in 1 liter of solution.

$$\text{M} = \text{moles} / \text{volume (L)}$$

- Since (mol = grams / MW), you can calculate the grams of a chemical you need to dissolve in a known volume (L) of water to obtain a certain concentration (M) using the following formula:

$$\boxed{\text{grams} = \text{M} \times \text{volume (L)} \times \text{MW}}$$

Concentration (تقاس بالمولات/لتر)

molarity

→ moles = grams / MW

→ Molar solution = moles / volume

equivalence (Eq)

normality (N)

Others $pK_a = -\log K_a$

$K_a = \frac{[B][H^+]}{[BH^+]}$ $K_b = \frac{[BH+][OH^-]}{[B]}$

- How many grams do you need to make 5M NaCl solution in 100 ml (MW 58.4)?

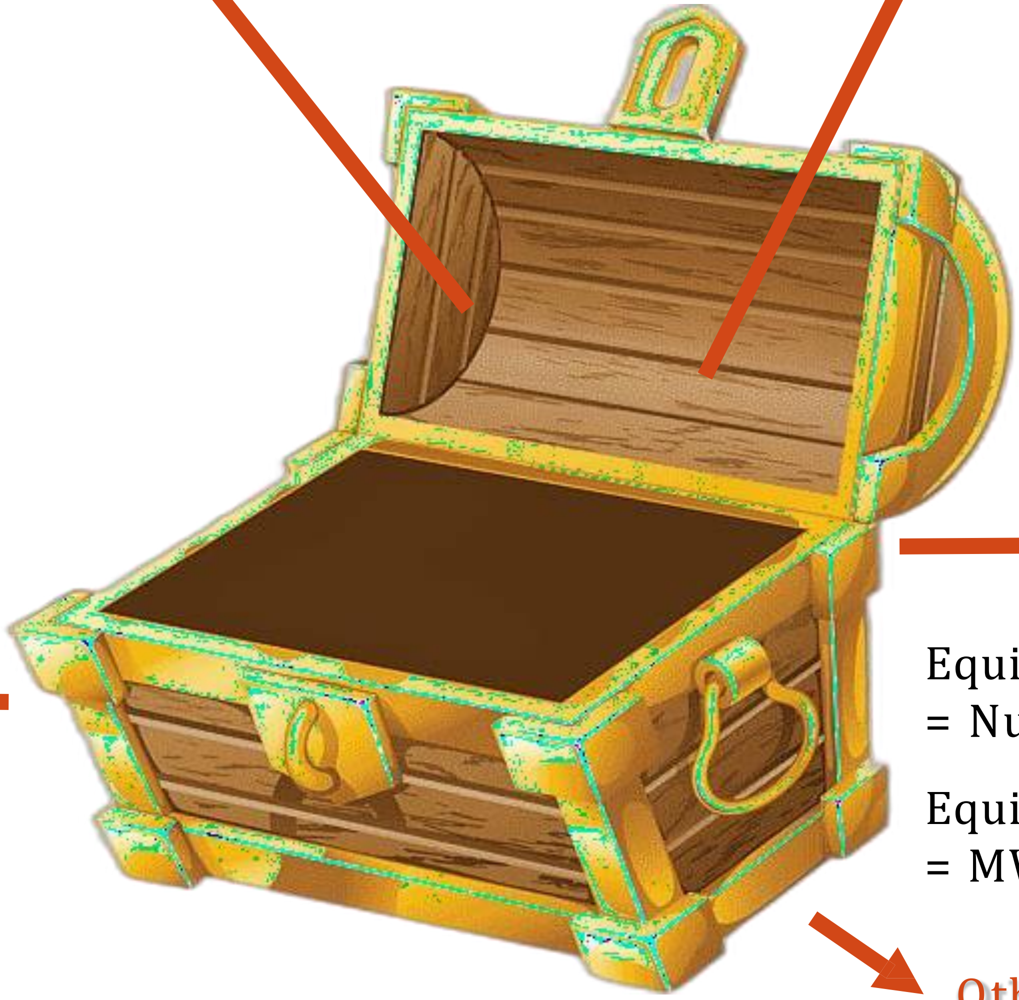
$g = MW \times L \times M$

$58.4 \times 0.1 \times 5$

$= 29,2$

- How many moles are in 100 ml that contains 5M NaCl (MW 58.4)?

Concentration (تقاس بالمولات/ لتر)



molarity

→ moles = grams / MW

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equivalence (Eq)

Equivalent (Eq of strong acid or base)
= Number of H+ or OH – moles

Equivalent (Eq of ions)
= MW/charge

normality (N)

Others

$$pK_a = -\log K_a \qquad K_a = \frac{[B][H^+]}{[BH^+]} \qquad K_b = \frac{[BH+][OH^-]}{[B]}$$

EQUIVALENTS

- When it comes to acids, bases and ions, it is useful to think of them as equivalents.
- An equivalent is the amount of moles of hydrogen ions that an acid can donate .
  - or a base can accept.
- A 1 g-Eq of any ion is defined as the molar mass of the ion divided by the ionic charge.

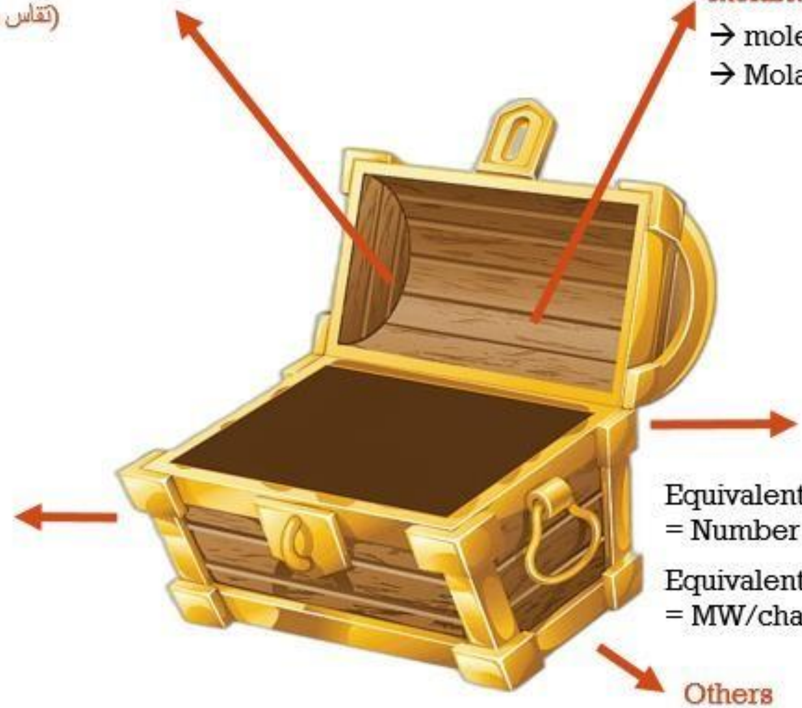
EXAMPLES

- For acids:
- 1 mole HCl = 1 mole $[H^+]$ = 1 equivalent
- 1 mole H_2SO_4 = 2 moles $[H^+]$ = 2 equivalents
  - 1 eq of H_2SO_4 = ½ mol (because 1 mole gives two H^+ ions)

Remember: One equivalent of any acid neutralizes one equivalent of any base.

- For ions:
- One equivalent of Na^+ = 23.1 g
- One equivalent of Cl^- = 35.5 g
- One equivalent of Mg^{2+} = (24.3)/2 = 12.15 g

Concentration (تقاس بالمولات/ لتر)



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equivalence (Eq)

Equivalent (Eq of strong acid or base) = Number of H+ or OH – moles

Equivalent (Eq of ions) = MW/charge

normality (N)

Others

$$1\ Eq = \frac{MW}{|C|}$$

$$pK_a = -\log K_a \qquad K_a = \frac{[B][H^+]}{[BH^+]} \qquad K_b = \frac{[BH+][OH^-]}{[B]}$$

- Calculate milligrams of Ca+2 in blood if total concentration of Ca+2 is 5 mEq/L.

$$1\ Eq \rightarrow \frac{40.08}{2} = 20$$

$$1\ Eq \rightarrow 20\ g$$

$$0.005\ Eq \rightarrow ??$$

$$20 \times 0.005 \times 10^3$$

$$\boxed{= 100\ mg}$$

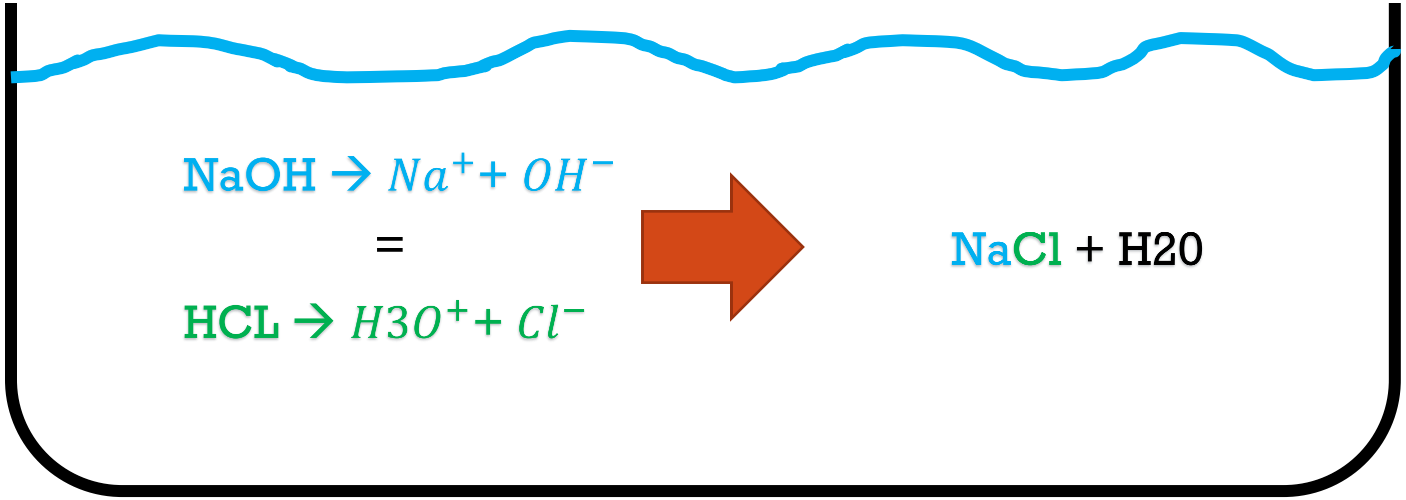
- 1 mol HCl = 1 mol [H+] = 1 equivalent
- 1 mol H2 SO4 = 2 mol [H+] = 2 equivalents
- One equivalent of Na+ = 23.1 g
- One equivalent of Cl- = 35.5 g
- One equivalent of Mg+2 = (24.3)/2 = 12.15 g

Note: When it comes to acids, bases and ions, it is useful to think of them as equivalents/ One equivalent of any acid neutralizes one equivalent of any base

TITRATION

→ Titration: To neutralize a solution where it's nor acidic nor basic

n X V1 X M1 = n X V2 X M2



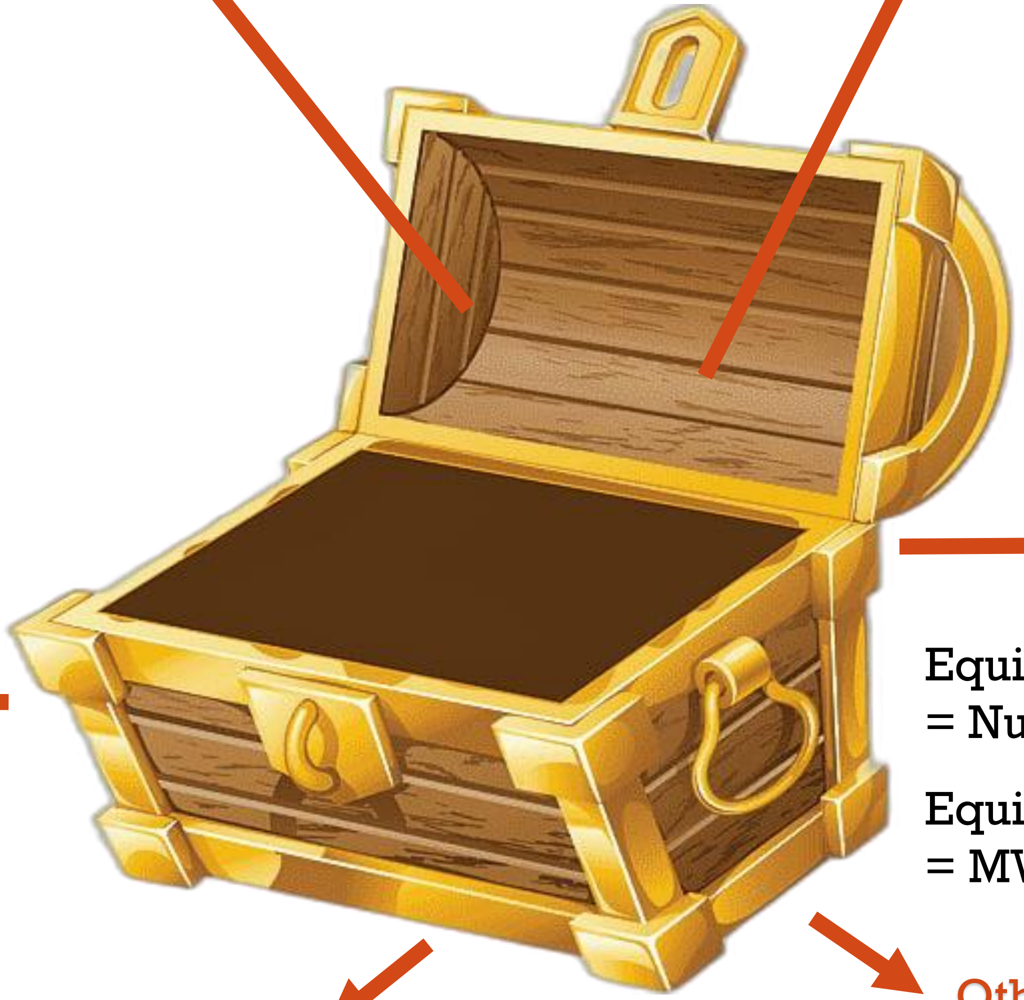
NaOH → $Na^{+} + OH^{-}$

=

HCL → $H3O^{+} + Cl^{-}$

NaCl + H20

Concentration (تقاس بالمولات /لتر)



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Equivalent (Eq of strong acid or base)
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Equivalent (Eq of ions)
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normality (N)

Titration
n.M1.V1=n.M2.V2

Others

$$pK_a = -\log K_a \qquad K_a = \frac{[B][H^+]}{[BH^+]} \qquad K_b = \frac{[BH+][OH^-]}{[B]}$$

MOLARITY AND EQUIVALENTS

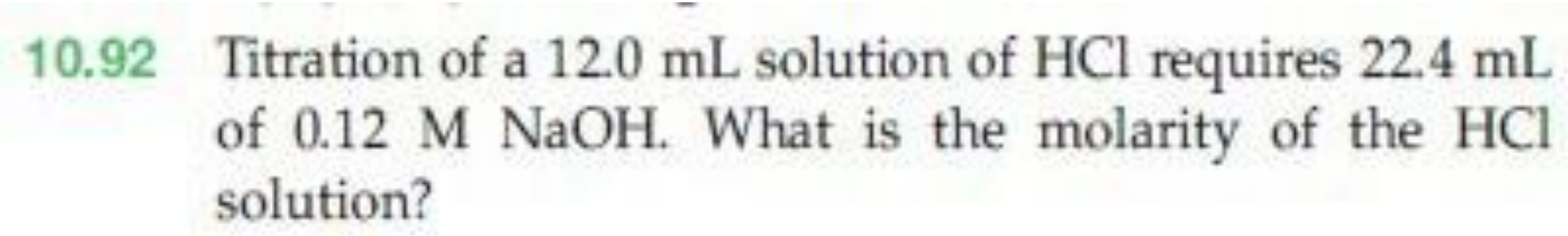
Equivalents = n x M x volume (L)

One equivalent of any acid neutralizes one equivalent of a base.

Based on the equation above, since *x* eq of an acid is neutralized by the same *x* eq of a base, then (n x M x vol) of an acid is neutralized by (n x M x vol) of a base.

This is done in a process known as Titration.

Titration is the slow addition of one solution of a known concentration to a known volume of another solution of unknown concentration until the reaction reaches neutralization.9



10.92 Titration of a 12.0 mL solution of HCl requires 22.4 mL of 0.12 M NaOH. What is the molarity of the HCl solution?

- Note that each one produces 1 mole of H^+ or OH^-, so 1M of HCl is equal to 1M of NaOH, so 1M HCl produces 1M of H^+, which is neutralized by 1M NaOH, which produces 1M OH^-

Eq of acid = Eq of base

N x M1 x Vol1 = n x M2 x Vol2

1 x 0.12 x 22.4 = 1 x M2 x 12

M2 = (0.12 x 22.4) / 12

M2 = 0.224 M

10.93 What volume of 0.085 M HNO_3 is required to titrate 15.0 mL of 0.12 M $Ba(OH)_2$ solution?

- Note that 1 mole of HNO_3 produces 1 mole of H^+, but 1 mole of $Ba(OH)_2$ produces 2 moles of OH^-. In other words, the n is different.
- Also, remember that **Equivalents = n x M x volume (L), where n is the number of charges or the number of H + (or OH-) the acid or base can produce or accept.**
- Titration means that we an acid to a base slowly. At one point during titration, the acid and the base neutralize or cancel each other. In other words, “to titrate” means “to neutralize”. At the point of neutralization, the concentration of H+ is equal to the concentration of OH-. The best way to calculate how much acid is needed to neutralize a base (or the opposite) is to calculate the equivalents.

Eq of acid = Eq of base

N x M1 x Vol1 = n x M2 x Vol2

1 x 0.085 x Vol = 2 x 0.12 x 15

Vol = (2 x 0.12 x 15) / 1 x 0.085

Vol = 42.35 mL

5- IONIZATION OF WATER

5- IONIZATION OF WATER

- Water dissociates into hydronium (H_3O^+) and hydroxyl (OH^-) ions.
- For simplicity, we refer to H_3O^+ as H^+ and write the reaction equilibrium as:

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

- The equilibrium constant Keq of the dissociation of water is:

$$K_{eq} = \frac{[H^{\oplus}]\,[OH^{\ominus}]}{H_2O}$$

- The equilibrium constant for water ionization under standard conditions is 1.8×10^{-16} M.

KW

- Since there are 55.6 moles of water in 1 liter, the product of the hydrogen and hydroxide ion concentrations results in a value of 1 x 10^{-14} for:

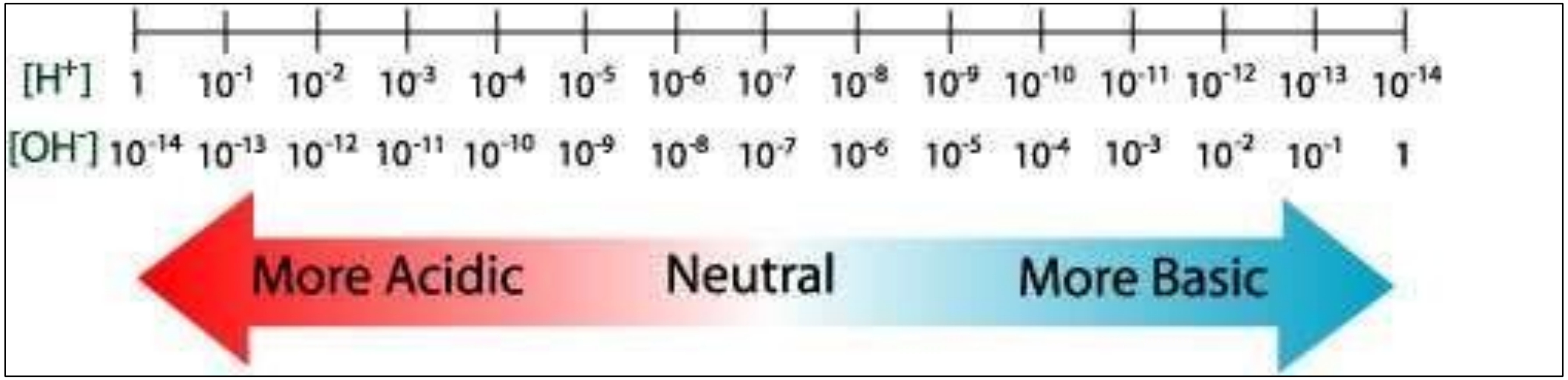
$$K_{eq}\,(55.5\ \mathrm{M}) = [\mathrm{H}^{\oplus}]\,[\mathrm{OH}^{\ominus}]$$

- This constant, Kw, is called the ion product for water

$$K_w = [\mathrm{H}^{\oplus}]\,[\mathrm{OH}^{\ominus}] = 1.0 \times 10^{-14}\ \mathrm{M}^2$$

$[H^+]$ AND $[OH^-]$

- For pure water, there are equal concentrations of $[H^+]$ and $[OH^-]$, each with a value of 1×10^{-7} M.
- Since Kw is a fixed value, the concentrations of $[H^+]$ and $[OH^-]$ are inversely changing.
- If the concentration of H^+ is high, then the concentration of OH- must be low, and vice versa. For example, if $[H^+] = 10^{-2}$ M, then $[OH^-] = 10^{-12}$ M



$[H^+]$	1	10^{-1}	10^{-2}	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}	10^{-9}	10^{-10}	10^{-11}	10^{-12}	10^{-13}	10^{-14}
$[OH^-]$	10^{-14}	10^{-13}	10^{-12}	10^{-11}	10^{-10}	10^{-9}	10^{-8}	10^{-7}	10^{-6}	10^{-5}	10^{-4}	10^{-3}	10^{-2}	10^{-1}	1