PHMD 221

ادل محاضرة اونلاين.

ندرس الحموض م لقواعد لان
اغلب الادوية تكون اما حمض او قاعدة.
لذلك هي علم مهم

Acid-base equilibria
Asynchronous lecture

Dr. Ghaith Al-Zarieni

1- How drug behaves.
- Acid & base in drugs,
* affect how format the medication
2- * affect physical - chemical properties
3- * ionization profile.

Arrhenius theory

An acid is any substance that ionizes (partially or completely) in water to give hydrogen ions (which associate with the solvent to give hydronium ions, H_3O^+):

$$HA + H_2O \rightleftharpoons H_3O^+ + A^-$$

A base ionizes in water to give hydroxide ions. Weak (partially ionized) bases generally ionize as follows:

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

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Theory of solvent systems-solvent cations and anions

First noticed by Franklin then Germann, working with liquid $COCl_2$ as a solvent. This theory recognizes the ionization of a solvent to give a cation and an anion; for example, $2H_2O \rightleftharpoons H_3O^+ + OH^-$ or $2NH_3 \rightleftharpoons NH_4^+ + NH_2^-$

An acid is defined as a solute that yields the characteristic cation of the solvent while a base is a solute that yields the characteristic anion of the solvent

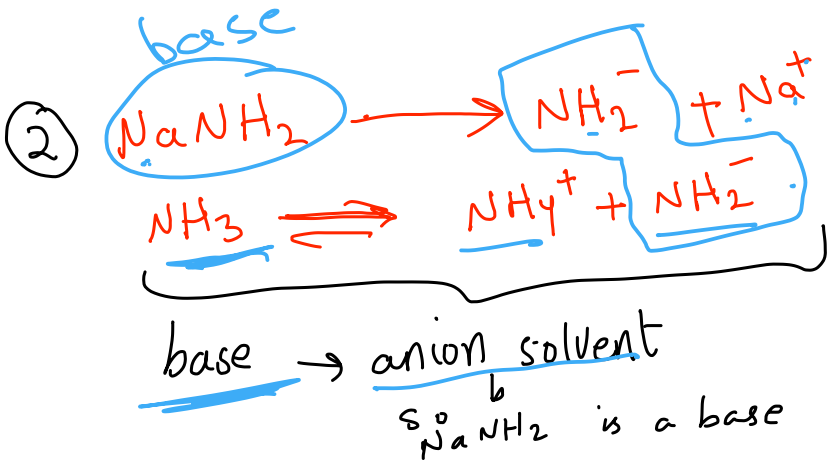
NH_4Cl is a strong acid in liquid ammonia

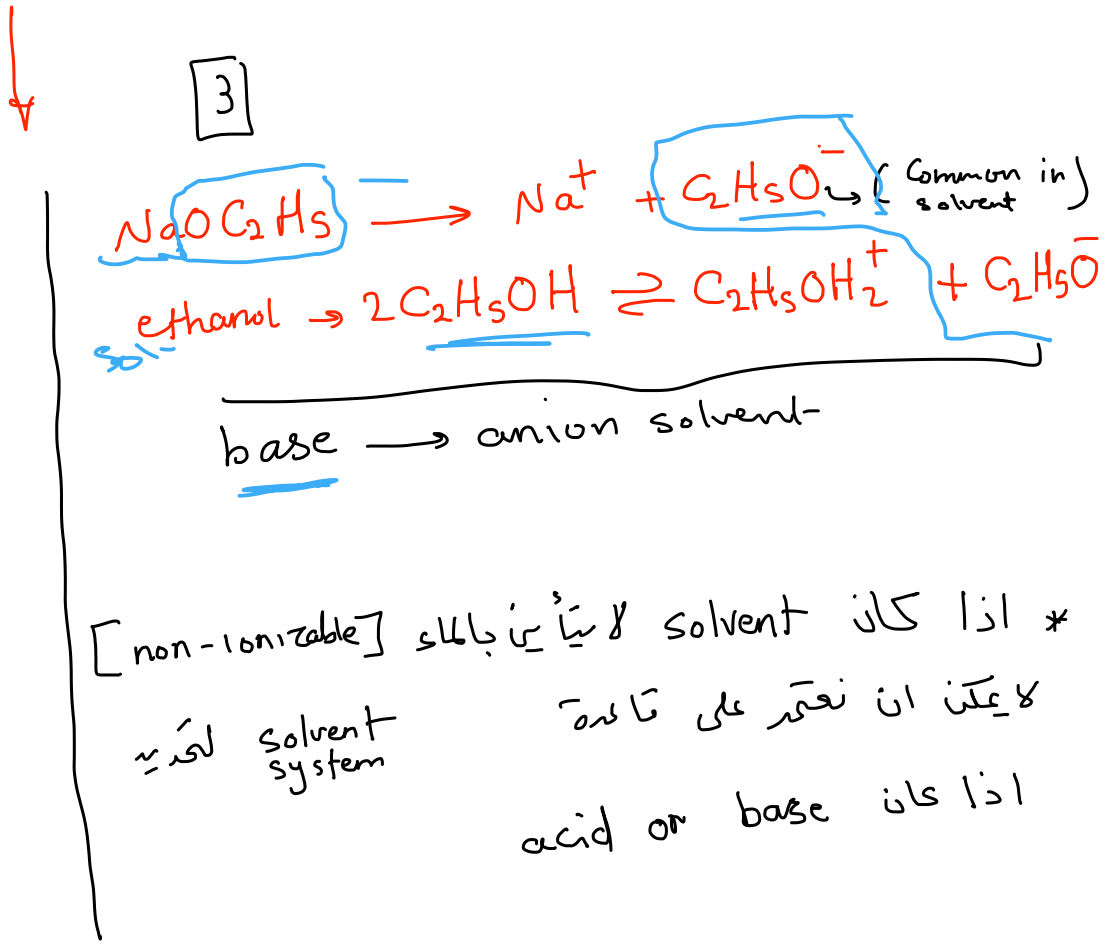
$NaNH_2$ is a strong base in liquid ammonia

$NaOC_2H_5$ is a strong base in ethanol ($2C_2H_5OH \rightleftharpoons C_2H_5OH_2^+ + C_2H_5O^-$)

The theory of solvent system is suitable for ionizable solvents, but it is not applicable to acid-base reactions in non-ionizable solvents such as benzene or dioxane







* اذا كان solvent لا يتأين بالماء [non-ionizable]
لا يمكن ان نعتمد على قاعدة solvent system لتحديد
اذا كان acid or base

Bronsted-Lowry theory

Acid: any substance that can donate a proton

Base: any substance that can accept a proton

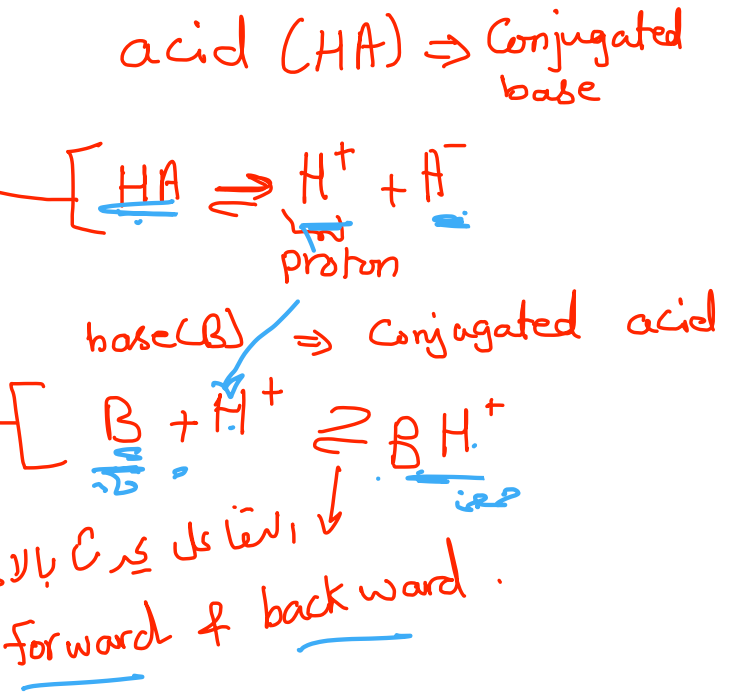
Acid 1+ Base 2 ⇌ Acid 2 + Base 1

half reaction: Acid 1 = H + Base 1 (conjugate pairs)

Base 2 + proton = Acid 2

e.g. $HOAc + NH_3 \rightleftharpoons NH_4^+ + OAc^-$

e.g. $NH_4^+ + H_2O \rightleftharpoons H_3O^+ + NH_3$



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التعريف العام

Lewis theory

An acid: is a substance that can accept an electron pair
A base: is a substance that can donate an electron pair

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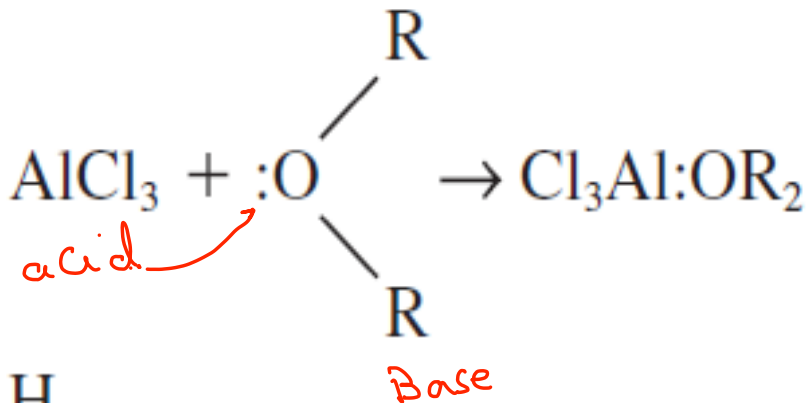
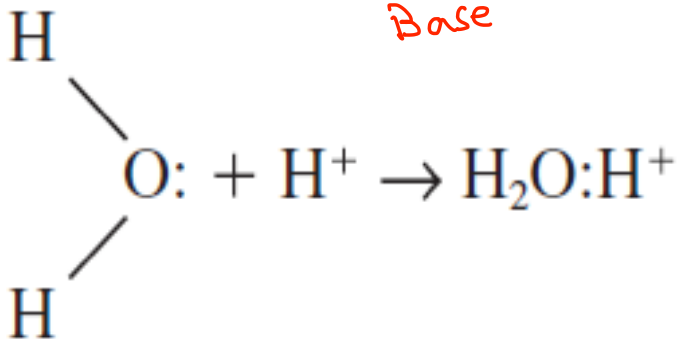
$$H^+ \text{ (solvated)} + :NH_3 \rightarrow H:NH_3^+$$





$$H^+ + :OH^- \rightarrow H:OH$$

Acids and bases in water

* solvent ليس بالضرورة يكون water

In water, acids and bases will dissolve, ionize, dissociate. The amount of ionization depends on the strength

Strong acids completely ionize in water:

* الحموض القويه تتأين كلياً ويكون تفاعل باتجاه واحد اي لايوجد اتزان

$HCl + H_2O \rightarrow H_3O^+ + Cl^-$

لاحظ

goes in one direction [one narrow] → in this case no equilibrium.

Ka of this reaction is = ∞

$\frac{0}{0} = \infty$

weak acids

partially dissociation

For acetic acid $HOAc + H_2O \rightleftharpoons H_3O^+ + OAc^-$

two narrow
two direction

* الحموض الضعيفه تتأين جزئياً وتكون التفاعل باتجاهين امامي وعكسي ويكون هناك اتزان.

[weak acid or weak base]

↓

there is equilibrium

↓

we express it by equilibrium

$$Ka = \frac{[H_3O^+]^1[OAc^-]^1}{[HOAc]^1}$$; $[H_2O] = 1$ in diluted solutions

$$Ka = \frac{[\text{Conc of Product}]}{[\quad]} = \frac{\text{تركيز النواتج}}{\text{تركيز المتفاعلات}}$$

[فقط للحمض والقاعدة الضعيف]

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[conc. of reactant]

constant Ka.

K_w

4H 2O 4H 2O

$$2H_2O \rightleftharpoons H_3O^+ + OH^-$$

weak electrolyte

$$Kw = \frac{[H_3O^+][OH^-]}{[H_2O]^2}$$ نواتج / متفاعلات = Keq

$$Kw = [H_3O^+][OH^-] = 1 * 10^{-14}$$ → by experimental

$$[H_3O^+] = [OH^-] = 1 * 10^{-7}\ M \text{ for pure water}$$

water is

weak acid, weak base, weak water

@ same time

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pH scale

On a wide range of conc. for H^+ & OH^- from 1 M or more, 10 M or less a log scale is used to express the range:

$P = -\log[H^+]$

$P \equiv -\log$

$PK_w = -\log[K_w]$

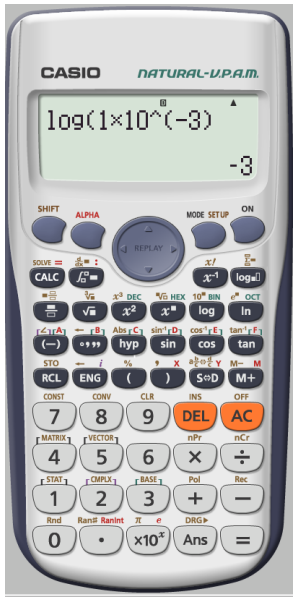
$P_{Ka} = -\log[Ka]$

$P_{OH} = -\log[OH]$

$pH = -\log[H^+]$

(-) sign is used because most of the conc. encountered are less than 1M, and so this gives a +ve number.

$-\log Kw = -\log[H^+][OH^-]$.....$pKw = pH + pOH$



T_{10} $\log_{10}$

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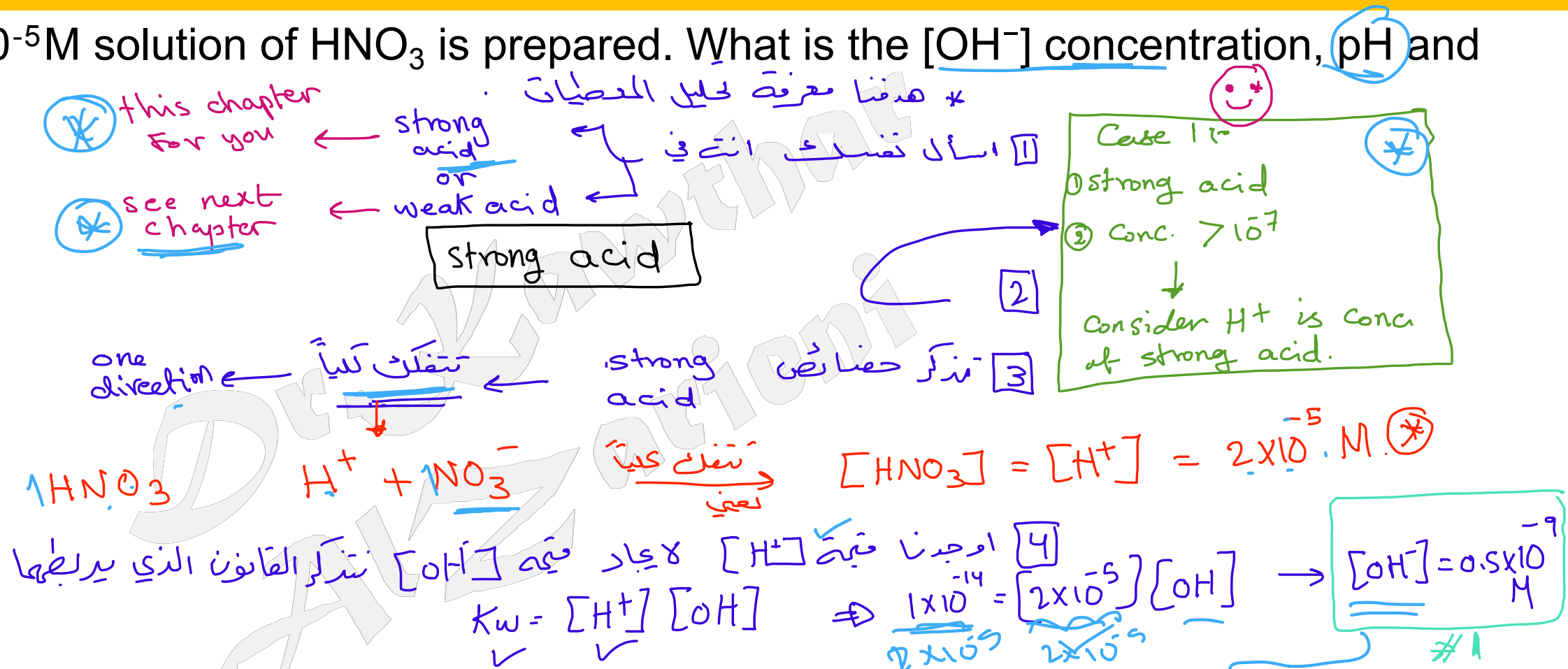
Question 1

A 2.0×10^{-5}M solution of HNO_3 is prepared. What is the $[OH^-]$ concentration, pH and pOH?



Question 1

A 2.0×10^{-5} M solution of HNO_3 is prepared. What is the $[OH^-]$ concentration, pH and pOH?

$Kw = 1 \times 10^{-4} = [H^+][OH^-]$

$[H^+] = 2 \times 10^{-5}$ M

$[OH^-] = Kw/[H^+] = 1 \times 10^{-14}/2 \times 10^{-5} = 0.5 \times 10^{-9}$

$[OH^-] = 5 \times 10^{-10}$ M

$pOH = - \log 5 \times 10^{-10} = 9.3$

or

$pH = - \log[H^+] = - \log 2 \times 10^{-5} = 4.7$

$pH = 5 - \log 2 = 5 - 0.3 = 4.7$

$pOH = 14 - 4.7 = 9.3$

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Question 2

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

Calculate the pH and pOH of NaOH solution of a 9×10^{-3} M.

[NaOH] = $[OH^-]$, because NaOH is a strong base and completely ionized

1:1

$NaOH \rightarrow Na + OH^-$

$9\times10^{-3} = [OH^-]$

pOH

$14 = pH + pOH$ تذكر

$7 > pH$ حموض

$7 < pH$ قواعد

$[OH^-] = 9\times10^{-3}$ ← 1 قاعدة قوية ← نتأين كلياً

2 من تركيز $[OH^-]$ نستطيع إيجاد pOH

$pOH = -\log[OH^-] = -\log[9\times10^{-3}]$

$pOH = 2.05$

$pH = 14 - pOH \Rightarrow pH = 11.95$

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Question 2

Calculate the pH and pOH of NaOH solution of a 9×10^{-3} M.

[NaOH] = [OH^-], because NaOH is a strong base and completely ionized

[OH^-] = 9×10^{-3} M

pOH = - log 9×10^{-3} = 2.05

pH = 14 - pOH = 14 - 2.05 = 11.95

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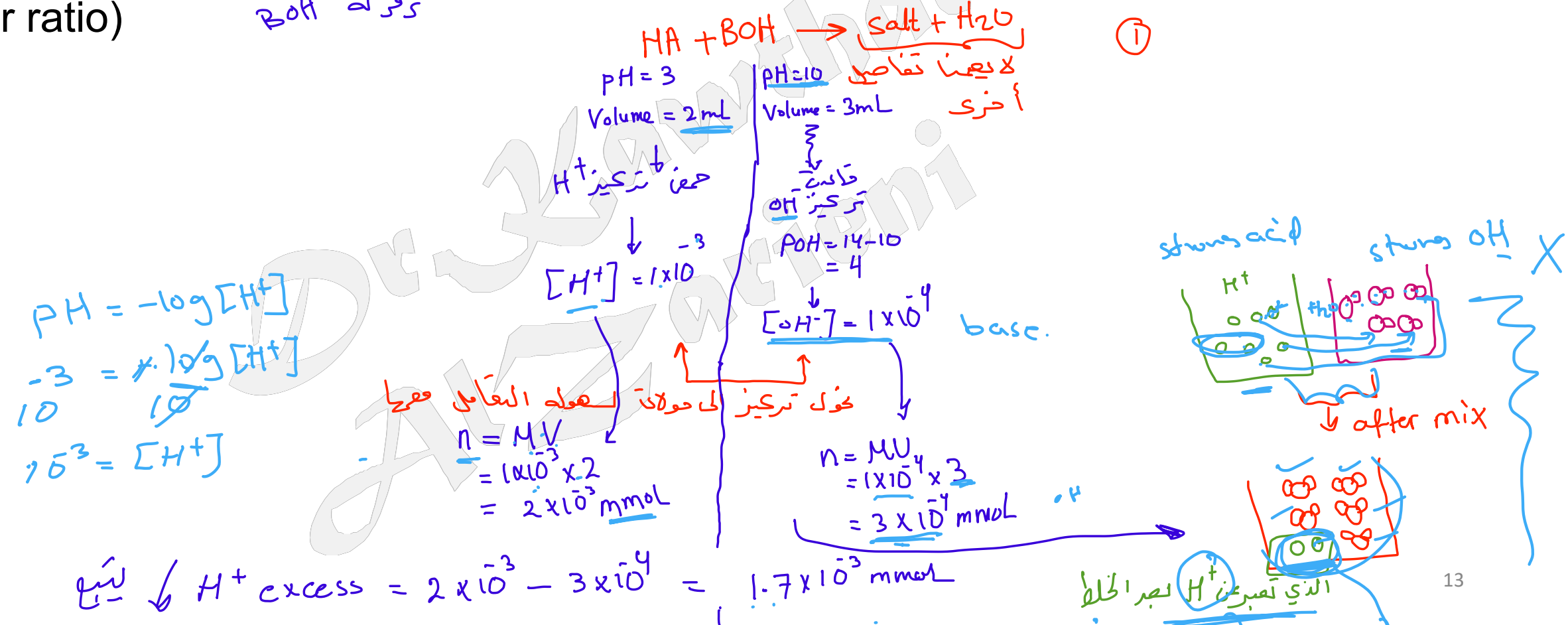
Question 3

strong acid + strong base → salt + water

Calculate the pH of a solution prepared by mixing 2.0 mL of a strong acid solution of pH 3.0 and 3.0 mL of a strong base of pH 10.0? (assume the acid and base react in 1:1 molar ratio)



Solution of question 3

For the acid solution: $[H^+] = 1 \times 10^{-3}M$ (pH=3)

For the base solution: pH + pOH = 14 2+3

تابع الحل

* تذكر ما يميز الخلط ان الحجم بعد الخلط يساوي مجموع حجمي قبل الخلط.

pOH = 14 – pH =14-10 = 4

mmol of $[H^+] = M \times V = 1 \times 10^{-3} \times 2 = 2\times10^{-3}$

mmol of $[OH^-] = M \times V = 1 \times 10^{-4} \times 3 = 3 \times 10^{-4}$

There is an excess of acid = $(2 \times 10^{-3}) - (3 \times 10^{-4})$

1.7×10^{-3} mmol of H^+ in (2+3) mL

$[H^+] = (1.7 \times 10^{-3} /5) = 3.4 \times 10^{-4}M$

pH = 4- log 3.4 = 4- 0.531 = 3.468

$[H^+] = \frac{1.7\times10^{-3}}{5} = 3.4\times10^{-4}M$

(2+3)

تركيز

* $pH = -\log[3.4\times10^{-4}]$

$= 3.468.$

نستنتج أن

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Notes

When $[H^+]=[OH^-]$ the solution is natural

If $[H^+] > [OH^-]$ the solution is acidic → excess number of H^+ moles

If $[H^+] < [OH^-]$ the solution is Alkaline → excess number of OH^- moles.

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More on strong acids and bases

Acid base
0 7 14
nn.



What is the pH of a $1*10^{-9}$ M HCl ? $= -\log [H^+]$ equal conc. strong acid

pH = 9 $-\log[H^+]$ [pH for acid < 7] whats happened ???

domain

If the concentration of an acid or base is much less than 10^{-7} *M*, then its contribution to the acidity or basicity will be negligible compared with the contribution from water. The pH of a 10^{-8} *M* sodium hydroxide solution would therefore not differ significantly from 7

If the concentration of the acid or base is around 10^{-7} *M*, then its contribution is not negligible and neither is that from water; hence the sum of the two contributions must be taken

water acid & bas

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Case 1 ☞ strong acid with higher conc. at 10^{-7} [Discussed in slide 10] ☺

[neglect the $[H^+]$ which comes from water, consider $[H^+]$ is concentration of strong acid]

Case 2 ☞ if you have conc. of strong acid $< 10^{-7}$ M,

neglect the concentration of strong acid & only takes conc of $[H^+]$ which coming from water

$pH = pOH = 7$

(6)

[Calculate pH & pOH for strong acid.

(d) 1.2×10^{-7} M

$< 10^{-7}$

↓

water is domai

$pH = pOH = 7$]

Case 3 :- Conc very close of 10^{-7} ⇝ take both

sum of the two contributions must be taken. [Next example)

☺

Example

Calculate the pH & pOH of a solution of 1.0×10^{-7} M HCl

① strong acid

② case 3
conc. around 10^{-7}

③ take both distribution → water, acid

Equilibria:

$[HCl] = [H^+] = 1\times10^{-7}$

$HCl \rightleftharpoons H^+ + Cl^-$ strong

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

$[H^+][OH^-] = 1.0 \times 10^{-14}$

$[H^+]\ H_2O$ diss. $= [OH^-]H_2O$ diss. $= x$

$\underbrace{[H^+]}_{x}\underbrace{[OH^-]}_{x} = 1\times10^{-14}$

$H^+_{total} = H^+_{(water)} + H^+_{acid}$

اضافة لـ H^+

$1\times10^{-14} = [x + 1\times10^{-7}][x]$

$0 = x^2 + 1\times10^{-7}x$

اجعلها معادلة تربيعية

$0 = x^2 + 1\times10^{-7}x - 1\times10^{-14}$

$x = 6.2\times10^{-8}$ M

[باستخدام الآلة الحاسبة]

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Solution

Since the hydrogen ions from the ionization of water are not negligible compared to the HCl added

$[H^+] = C_{HCl} + [H^+]\ H_2O$ diss.

Then,

$([H^+]_{HCl} + x)(x) = 1.0 \times 10^{-14}\ (1.00 \times 10^{-7} + x)(x) = 1.0 \times 10^{-14}$

$x^2 + 1.00 * 10^{-7}x - 1.0 * 10^{-14} = 0$

Using the quadratic equation $x = 6.2 \times 10^{-8} M$

تابع الكل.

H^+ tot = H^+ water + H^+ acid

$= 6.2 \times 10^{-8} + 1.0 \times 10^{-7}$

$H^+ = 1.62 \times 10^{-7}$

$pH = -\log 1.62 \times 10^{-7}$

$= 6.79$

$pOH = 14 - 6.79 = 7.21$.

$\times 1 \times 10^{-7}$ M

that mean dissociation H^+ comes From water Lower H^+ comes from < H^+ comes from pure water.

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Solution cont…

Therefore, the total H^+ concentration = $(1.00 * 10^{-7} + 6.2 * 10^{-8}) = 1.62 \times 10^{-7}$ M

pH = - log 1.62×10^{-7} = 6.79

pOH = 14.00 −6.79 = 7.21

Or

Since $[OH]^- = x$

pOH = $-\log(6.2 \times 10^{-8}) = 7.21$

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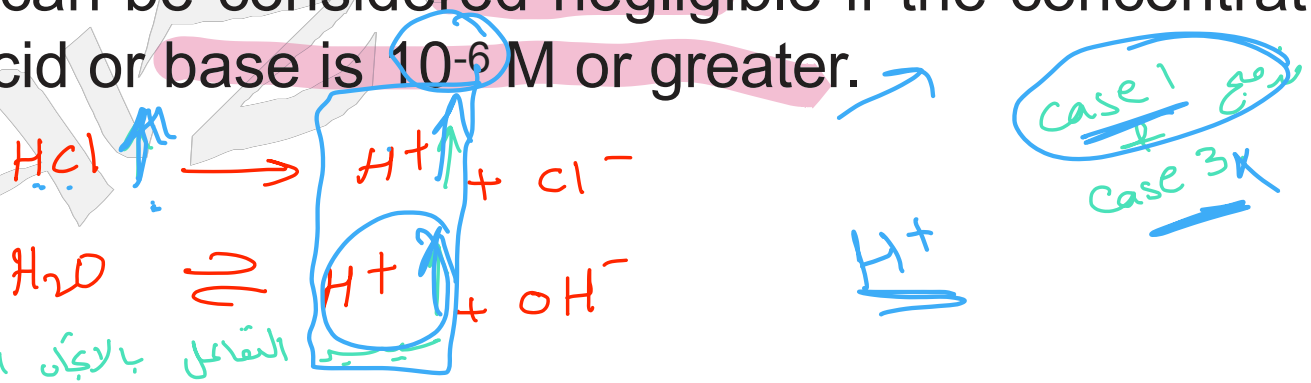
Notes

- Note that, owing to the presence of the added H^+, the ionization of water is suppressed by the common ion effect (Le Chˆatelier's principle)

قمع/تلغى

- We usually neglect the contribution of water to the acidity in the presence of an acid since its ionization is suppressed in the presence of the acid

- At higher acid (or base) concentrations, the suppression is even greater and the contribution from the water becomes negligible. The contribution from the autoionization of water can be considered negligible if the concentration of protons or hydroxyl ions from an acid or base is 10^{-6} M or greater.



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

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

سيسير التفاعل بالاتجاه العكس فيقلل تركيز H^+

H^+

case 1 مهم

case 3 ✗

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pH at elevated temperature: Blood pH

$pKw = pH + pOH = 14$ at 25 C° $Kw = 1.0\times10^{-14}$

تأثير التراكيز بالحرارة.

$[H^+]$ is temperature dependent, and Kw at 100 C°

is $Kw = 5.5\times10^{-13} = [H^+][OH^-]$, $[H^+] = [OH^-] = \sqrt{5.5\times10^{-13}} = 7.4\times10^{-7}$ $pH = -\log 7.4\times10^{-7} = 6.13$

$\sqrt{x^2}$

$[H^+] = \quad = 7\times10^{-7}$

$pKw = -\log 5.5\times10^{-13} = 12.26$ at 100 C°

experim

كم تحديدها

Not all measurements or interpretations are done at room Temperature (25 C°)

For example, the pH of the body (at 37 C°)is (7.35-7.45) and this is a slightly alkaline relative to neutral H_2O

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At 37 C°

$-\log[2.5\times10^{-14}]$

At 37 C° $K_w = 2.5 \times 10^{-14}$ pKw = 13.6

pH = pOH of a neutral solution at 37 C°

= (13.6/2) = 6.8 instead of 7

not significant

A difference of 0.2 pH units due to the difference in temperature from 25 C° to 37

A change of 0.3 pH units in the body is extreme

The hydrochloric acid concentration in the stomach is about 0.1 to 0.02 M. Since pH = −log[H⁺], the pH at 0.02 M would be 1.7. It will be the same regardless of the temperature since the hydrogen ion concentration is the same, and the same pH would be measured at either temperature

pH = 1.7

But the pOH would be 14.0 −1.7 = 12.3 at 25C° it is 13.6 −1.7 = 11.9 at 37C°

Temp. affect the ionization of water in the body & chang pH neutrality

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