* water

- our bodies contain 70% of water, many Biochemical Reactions they happen in water envir. & also water is the key player in many reactions

- involves in driving protein folding & enzyme catalitic analysis

- 2 covalent bond

oxygen have 2 unbond pairs of electrons & these 2 have strong negative charge that's why they repel each other pushing the 2H closer to each other

لهيك H2O بتصير linear

- water is polar

- Because of the difference in electronegativity between O & H
O : will have part − charge
H : " " " + "

- powerful solvent for ionic & polar compounds

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Polar
↓
electronegativity difference between atoms

Non polar
↓
electrons are shared equal

* Adhesion → water molecules stick to other subs.

* cohesion → " " each other
↳ contribute to the surface tension of water
(external forces) خاصية بتعمل للسائل لتقاوم

Non polar solvents can't dissolve polar compounds	Polar	Non polar
	↓	↓
	- Net dipole	- No net dipole
	- ↑ bp, ↑ MP	- ↓ bp, ↓ MP
	↑ surface tension	↓ surface tension
	↓ vapor pressure	↑ vapor pressure

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* Dipole moment allow water molecule to interact with each other by H-bond (dipole-dipole force)

* It take a higher temp. to convert liquid water into gas water & this means extensive network of molecular interaction - Intermolecule - between water molecule

• Each watermolecule in theory can make how many H-bond to other water molecules 4 (& this explains the high bp)

- 2 Types of chemical bonds

→ non covalent

→ covalent

* Typical bond stren. = 350 - 450 kJ/mol

Amount of energy needed to break a bond

* H-bond stren. = 20 kJ/mol

↳ weak bond

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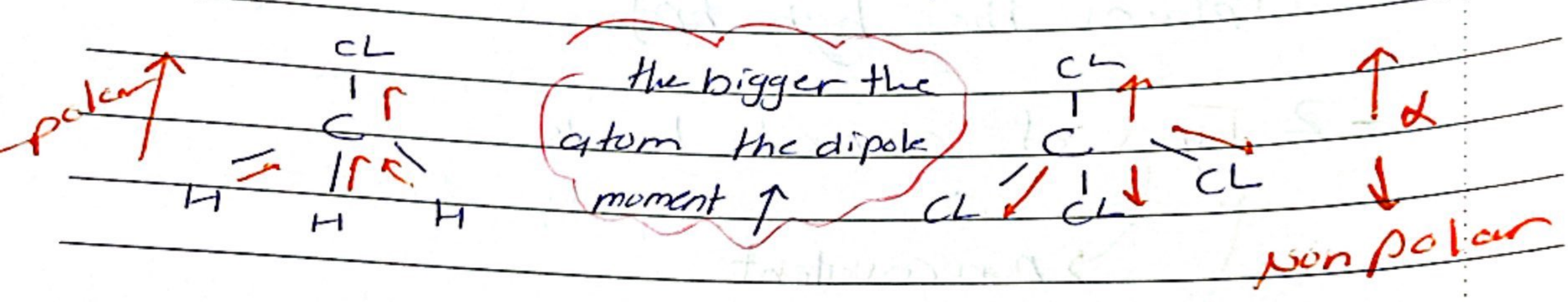
* Dipole moment

- Tell us on average where the electrons are in molecule (Measure of net polarity)

- imp. ability to dissolve solute, MP, bp, reactivity

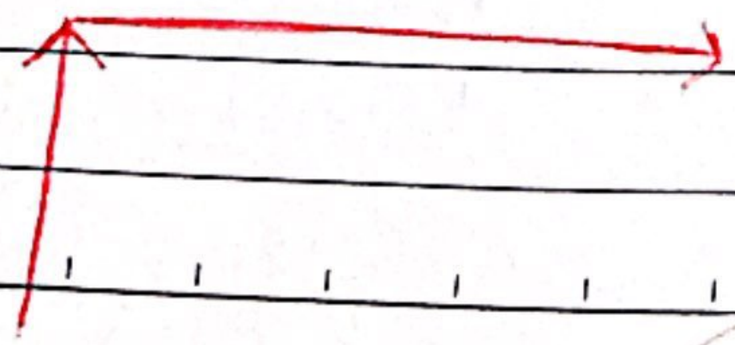
- Tell us the shape of molecule, H_2O if it was linear the 2 O-H bond dipols would cancel each other & the whole molecule would be non-polar
شكله خطي ما بيكون polar



$\delta^- C - H^{\delta+}$
2.5 2.1 electron.
← — | — →
non polar

$\delta^+ C - CL^{\delta-}$
2.5 3
— | — →
polar

* Electronegativity → A measure of the force of an atom's attraction for electrons it shares in a chemical bond with other atom



* Intermolecular interaction responsible →
bp, Mp, high heat of vaibiration
high surface tension

- Inter → between molecules
→ In water their is a lot of
it - H-bond -

- Intra → between atoms

* In DNA base paining is based on
H-bonding
↳ - 2° structure & 3° structure of
protein

Electrostatic interaction
↓
H-bond

- certain type of p.sac., cellulose

* H-bond require 3 atoms
one of them should be H

donor لي فيها cov. bond بـ H بـ δ^- δ^+ لي وحدة مرتبطة
مثلا الي -O-

acceptor لي فيها par. (−) charge لي ثانية ايها
(O in another molecule)

* $A^0 = 10^{-10}$ → Measure distance between atoms
(Molecular interaction)

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* surface tension → allow small organisms to move across bodies of water

- play a leading role in the position rearrangement of cells & act in minimizing the exposed area of the aggregate & without it cells wouldn't have a shape

- Plays a part in our body's ability to transport these materials all through ourselves. The carbohydrates & proteins that our bodies use as food are metabolized & transported by water in the bloodstream

- water → imp. in dissolving essential vitamin & nutrients from food & delivering them to cells, imp. to flush out toxins

H-bond → F-H
O-H
N-H
H-bond لقدروا يعملوا

تأكدي من الرابطة C-H علاقة التجذر تكمل
par. - ort بأنها ما تقبل
δ^- δ^+

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* ↓ bond distance ↑ stren. bond

* strength of H bond depends on the type of H donor & acepter & on Directionality

* H-bond will be strong if all the atoms participate in H bond in the same line, It will be weaker if we don't have astraight line for the 3 atoms

* In 2° structure of protein we have interactions between H of the amino group -N- is the donor & -O- of carbonyl group

* Distance of H bond around = 1.8 A°
& distance of cov. bond = 1 A°, could be more

* β-sheets → parallel : lots stright H-bond
→ antiparallel : stright H-bond

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* water is self comp.

water tend to interact with each other, the extend of this interaction is more in ice water compair to liquid water

* scientist notice that in liquid water, water tend to form higher structures but these structures are very short led because there is cont. state of making & breaking bonds

& In liquid water, water molecules have freedom to move & also they have protons that are jumping between water molecules making new H-bond & breaking it

* In theory each H_2O molecule can make 4 H.b with other 4 water molecules liquid water & بس بالواقع هاد ما بحدث

- Each water molecule in liquid water make on average 2-3 H-bond

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- In ice H_2O molecule potentially 4 H-bonds
وهاد بسويه لما اتجمد بيي بدنلي expand

In order for each water molecule to make 4 H-bond with other 4 H bond water molecule must be pushed away from eachother which increases the valume of water

* In order to atoms to overlap it has to lose alot of energy
لهاد السبب انو cov. bond لا bond stre
require large amount of energy in order to break it

Note → Distance between atoms
هي بوضح لي بتعدلي شو نوع
bond عكس يكون

Ionic bonds are stronger than H-bond, sym. because here we have complete charges
part charge وهناك عندي

* Breaking bonds require an input energy
, Making cov. bond releases energy & that energy that is released is to make 2 atoms come closer together

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* van der waals sphere

Every atom has it, it's imaginary & it's like the boundry of an atom & depends on molecular weight & on electrons

Sphere overlap when we have co. bond (extensive in water)

No overlap, No bond

* High dielectric constant makes water a good solvent

Measure of the ability of solvent to seperate charges away from each other & keep them seperated

* لو عندي pack باكي 2 كيل seperation to the ions because of High dielectric, the ions will be sorru. by water molecules

will be making electrostatic interaction

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* water can weaken ioniz interaction between ions & can make H bonds to make it weaker
Because water tend to compete for interactions

* So in biological molecules like water for ex sometimes it must be removed in order for biological molecule to make a electrostatic interaction

هذا ← P.P لما يكونوا بشكلوا بنية على linear P.P
3D stru. ← P.P بسبب لازم يصيروا
Pol. ← un. هلأ بيرجع P.P مسطحة

water molecules must be removed away to allow strong bonding between atoms of a.a

* Interactions with other dipoles →

يعني مثلا عندي carboxyl Group لو عندي 2 منهم come together
dipole-dipole intera. ← بصير عندي

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* ليه Dipole ؟ لأنه
electronegativity difference
between O & C is very large

لو مثلا electrone بين H و C مش هالفرق
وهاني زي Methy Group كلها لا تعتبر
dipole أو إنها تعتبر ضعيفة بس لو
other group بتكون dipole وتعمل قريبة من
Methyl Group بتعمل induce وبتغير عندي
dipole

* weakest → london , caused because
movement of electrons

* orientation is very imp.
وتعتمد على interaction

attractive Repulsion

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* Water is very good solvent for molecules

- هاذا كيف بنو

subs. soluble in water this means water molecules surround this subs & make interactions

* some subs. like ions, polar molecules like Glucose are soluble in water because they have functional Groups can interact with water molecules, they can form H-bond with water molecules (Alcohol Group in Glucose)

* non polar subs. not soluble in water, they are surrouded by water molecules, water molecules prefair to interact with each other rather than interact with molecule made of H-C bond

لو ضفت NaCl
للماء
$\Delta G = -$
لأنها spon.

* dissolve solid NaCl in water, the first thing must happen →

! → Dissraption of ionic bond between Na & CL

$\Delta H = +$, $\Delta S = +$ (2atoms together now they are seperated more freedom

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2 → Dissraption of H-bond between water molecules

$\Delta H = +$ $\Delta S = -$ → More ordered around ions

because in order for water molecule to start forming a hydration shell or interacting with ions they must be released from H-bonding with other water molecules

3 → Hydration - إضافة

ΔH_{hyd} → large Negative (New interactions are stronger than interactions between water molecules)

ΔS_{hyd} → $\pm$

4 → Net effect

ΔH_{net} → $+$

ΔS_{net} → $+$

Ionic bond
(average 86 kJ/mol)
Very strong bond
compair to
Hydrogen
bond

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* whenever we want to describe a process thermo. we have to Dissect this process & take to considiration the change in enthalpy & entropy for solutes & solvent molecule & for any new structures that might form

Hydration shell ونسميه

Means that water molecules are making / surr. solute molecule

$\Delta G = -9.6$ kJ/mol

وبالنهاية ΔH_{net}, ΔS_{net} موجبات

we could say that this process is spon. & driven by ΔS not ΔH

* very impo. effect in water hydrophobic effect

مهم

Major factors for driving protein folding

- So whenever you dissolve nonpolar subs. like oil in water the hydrophobic affect will kick in

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* If you mix water with oil & even if you shake it for 1 hour, after stop shaking, eveincelly all molecules will start intregating, clustring together, not because they like to interact together

But because they hate water (to minimize contact with water)

Table 2.2 shows how ΔG ΔS ΔH they change whenever we take nonpolar molecule & transfeet from water into a non polar solvet

Nonpolar ← Methane in water مثلا عندي

ΔH, ΔS → + , ΔG → − لوصف إنو وهاي العملية

intropycly driven why?

Introphy large because the increase of randomless of water molecules

Why مش

* when a nonpolar solute is mixed with water, water molecules will start surrounding nonpolar solute & they can't interact with nonpolar solute, they will start interacting with each other & their will be several layers of watershells

لـ ولا وحدة تتعامل H-bonding مع
تبعي solute

- H_2O arround polar solute → hydration shell
- " " nonpolar " → clathrate

فرق بين هول shells اللي

Hyd. → water make interaction, H_2O can come & go (freedom) can be replaced for water

Cla. → water can't make interaction

رهيك شو فقط
او نزلنا آخاج
ينزعه معي

oil in water, i will have 2 types of water

Free water
↑ΔS

water that make shell arornd non-polar or what we call it interfacial, ↓ΔS, can't move, can't be replaced with other water molecule

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* لو بلشنا نحط بالمي وضفنا بدين زيت
some water molecule will lose it's freedom

So to maximize the ΔS of water even after the addition of nonpolar solute, the nonpolar solute tend to come together, reducing the amount of ice water

ΔS_{H_2O} ΔS_{H_2O+oil}

ΔS is large in water itself

* هيك هنا صار نستخدم البينا لفظ over solvents
هنا مع نضيف other solvent هلأ صار عندي 2 phases
water phase, nonpolar solvent phase
و الزيت بدو
migrate to non-polar

- مثال آخر ← لو عندي
nonpolar subs. called cyclohexane & it's in the vapor form & then we transfer this vapor cyclo. into a pure liquid cyclohexane

من غاز لسائل قلت عندي fre. (−) ← ΔS
ΔH ← (−) , ΔG ← (−) 2 kcal/mol
ولو طبيت pure بالحوض
ΔH (±) , ΔS (−)
ΔG (+) 6 kcal/mol

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* some reactions driven by ΔS or ΔH

* protein folding is driven by ↑ΔS of H_2O

* understanding ΔS, ΔH contribution to a process very impo. it allows us to understand how enzymes catalyse reaction, how enzymes bind to it's substrate, enzymes lower activation energy

EX most enzymes that operate in our cells operate in aquoes envir. which mean that the enzyme will be surrounded by water molecule, the substrate that must bind to the enzyme so that the enzyme can convert this substrate into product also will be surr. by water molecule (& this sub. might be anonpolar)

- This process is driven by the increase of ΔS & their is an ΔH contribut

Most Biochemical reactions happen in water

Because when the sub. bind to the enzyme, the water molecules will have freedom, but also when it's bind to enzyme their will be new molecular interaction forming

وهاد كيدي .spon

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* Osmosis → movement of water across semipermeable membrane

لو عندي solution عندي
polar subs. dissolved in water

حطيت solution في celendar وحطيت celendar في beaker فيه H_2O وغطيت celendar عندي semipermeable membrane (غشاء شبه كامل)

* هذا هي بتصير بالجسم بس حركة الماء من برا لجوا
لازم نعرف بدنو لازم نطلع على con. تبع free water

high → low

* bound water molecule → can't move across the membrane because it bind to a sub.

$[F.H_2O]_{in} < [F.H_2O]_{out}$

* osmotic pressure

amount of force → press. that could be applied to bring back the level of water in celendar to original state

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* Dialysis تعتمد على osmosis

* water can behave as acid & bases
sub. can donate — accept proton

* water can autoionized
can be converted to ions, this happens when H_2O molecules becomes acid & other H_2O molecule become base

* بالحي في cont. state ~~Protein jumping~~ من جزيئات الماء يهيد
Reactions that happen in aquoses envir & rely on transfer proton in water, these are one of the quickest reactions that could happen & this is why the majority of chemical reactions happen in water

* we will see that converting a substrate into a product using an enzyme it might envolves several reactions happening inside the enzyme & some of these reactions might require the help of water or require that water behave as acid or base

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* The auto ionization of water can be expressed by the equilibrium const.

$$K_{eq} = \frac{[H_3O^+][OH^-]}{2H_2O}$$

Give us idea about products to reactants

تركيز عالي بالي variable
ليتر ثابت

1L H_2O ب 1000 g
MM H_2O 18

55.5 Molar

$K_w = 1 \times 10^{-14}$ at 25°

$= [OH^-][H_3O^+]$

hydroxyl ion

* Most water molecules don't ionize only fracianal water molecules

كيف صرفت ؟ من التركيز

* pH → indicates level of acidity (con. of protons)

- Sørensen → expressed conc. of proton in easier way

بدل ما استخدم ارقام صغيرة

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

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*henderson hasselbalch equation

$$pH = pka + \log \frac{[A^-]}{[HA]}$$

This equation relate con. of acid & it's conjegute base with pH

ka → acid desociatic constant

تضعيف weak strong ← $ka = \frac{[H^+][A^-]}{[HA]}$

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

This equation imp.
لتحضير Buffer او في ايجاد
ration for acid or base

— Very small ka value means, i will have more con. of [HA] which make the acid weak

- Smaller ka value ↑ pka

- ↓ Pka, strongest the acid easily loss it's proton which mean ↑ proton ↑ ka

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* $k_a = \frac{\text{Con. of prod.}}{\text{" " react.}} = k_{eq} = K_D = \frac{1}{k_a}$

* Each acid have a certain k_a value

could convert to pka

بتعطيني فكرة عن
how strong the acid

- لما أضاف acid مع الماء
some acid molecule will lose it's proton & a conj. base will start appearing
لحظة ما بتوصل equilibrium
$[A^-] = [HA]$
$pH = pk_a$
بدأ لوغاريتم تبعي هيلوي !

* acetic acid → acetate

لما تخسر بروتون هاز أغير طريقة حاسبها

predominate
يعني ↑con.

$pH < pk_a \rightarrow [HA] > [A^-]$
$pH > pk_a \rightarrow [A^-] > [HA]$

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* some acids like acetic acid can donate 1 proton, some acids can donate 2

- Monoprotic acid → donate 1 proton & 1 pka
- Diprotic " → " 2 " " 2 "
- Triprotic " → " 3 " " 3 "

• Titration exp. allows us to gain a lot of inf. ex allows us to determine pka

- نضيف strong base بالتدريج مش مرة واحدة

* In order to determine equivalents you need to know con. of weak acid & strong base

كل ما زدت بـ OH ، pH بتزداد

- OH that i will add must be neutralized? what does that mean?

OH that i will add will interact with H^+ to produce H_2O

عا بني تركيز H^+ رح يقل ورح يكون في حاجة لـ More [HA] to lose proton

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- لما نزيد OH تركيز conj. base يزيد وتركيز acid يقل

* الـ equivalents بـ

We have certain number of moles of [HA]
one equ. mean we add same number of moles of [HA] as OH

100 [HA] $\xrightarrow{1\ equ.}$ 100 [OH^-]
$\xrightarrow{0.5\ equ.}$ 50 [OH^-]

لاحظ بالحالة نوصلها
Relative abun. will be
50 : 50
$[A^-] = [HA]$
$pH = pka = 4.76$

* كيف بـ exp. أعرف إنه [OH] لازم أضيف عشان أوصل 0.5 equ. ؟

From number of moles of our weak acid

$M = \frac{n}{V} \rightarrow n = 0.1\ mol$

فلازم أضيف 0.1 من OH

$1L = 10^3$

* For all mon. $\rightarrow$ 0.5 equ. $pH = pka$

* لو ضليت أضيف OH ستريح يصير ؟ رح يظل الخط
لسبب لما بدو يبطل في H^+ لأنه unutilized
So I will have pure OH in our solution

* Products more stable than the reactants, the reaction will happen spon.

- which more stable (H_3PO_4 / $H_2PO_4^-$)?

لما تخسر بروتون بصير قاعدة أقل stable أكثر إذا
صار بصير قاعدة less stable (اعتمادا على قيم pKa)

والشحنة السالبة تعني صارلي proton قاعدة عندي
More negative charge
وهاد بخلي
Molecule less stable

More negative → less stable

* Buffers → pH تقاوم التغير بـ
وضعيفة
weak acid & it's con. base

بس بالأخير ما بتقدر تقاوم
إذا ضليت أضيف رح يصير collapse

can keep only pH around certain point
as long as pH = ± kpa value of the weak acid

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* بقدر نقدم Buffer لـ PCR

Dpn poly. can work in pH around 8, during PCR while poly. synthesized new strands some protons might be released & these protons will lower pH of PCR reac if there is no buffer

لو في Buffer بيقتنص protons وخلي pH around 8

* We have a buffering system in our blood pH = 7.4, inside our cells pH = 7

ليه كتابة Buffer؟ شو بصير لو pH تبع blood بزيد أو نقل؟

Everything inside the blood عكس تخرب وبروتينز عكس يصيروا denaturation

* Best buffer region
acid = conj. base

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* Imagine a base generated during your exp. it will decrease con. [HA] & ↑ con. of [A⁻]
↑pH very smallely لوضلية أضيف
وغرفة ما نقطة ما

Ratio 10% [HA] : 90% [A⁻]

beyond this point any OH⁻ added we will have sharp increase in pH

هاد بجدن لما اطلع بر الـ Buffer region

* خاصر بحكي لضيف buffer system مصنوع من weak acid
وهاد weak فيه
Pka value = pH of my exp.

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Non-covalent interaction

1) Electrostatic interactions

by coulombs law

calculate bond stre

energy of interaction

$$U = \frac{kq_1q_2}{Dr}$$

distance between the center of 2 atoms

- **q** is the charges
- **r** is the radius,
- **k** equals $8.99 \times 10^9 Jm/C^2$ con.
- **D** is the dielectric constant, a shielding of charge.

D = 1 in a vacuum
D = 2-3 in grease
D = 80 in water

Dielectric effect	D
hexane	1.9
benzene	2.3
diethyl ether	4.3
$CHCl_3$	5.1
acetone	21.4

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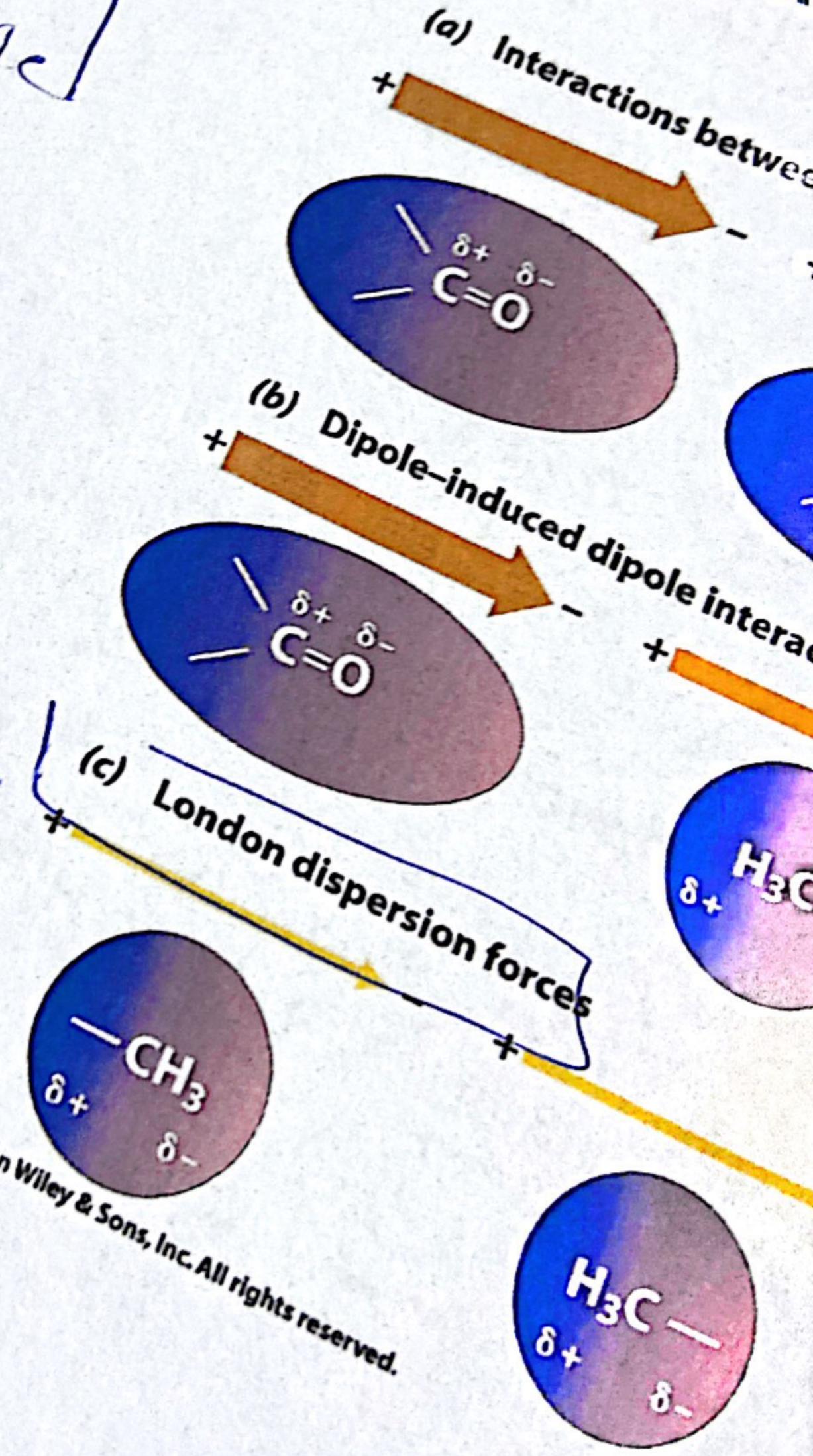
ion-dipole
dipole-dipole
london -dipole

2)

van der Waa



subtype of
van der waals
& it's a non polar

Figure 2-5

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ratio between acetic acid acetate (HA & A⁻)

Titratio

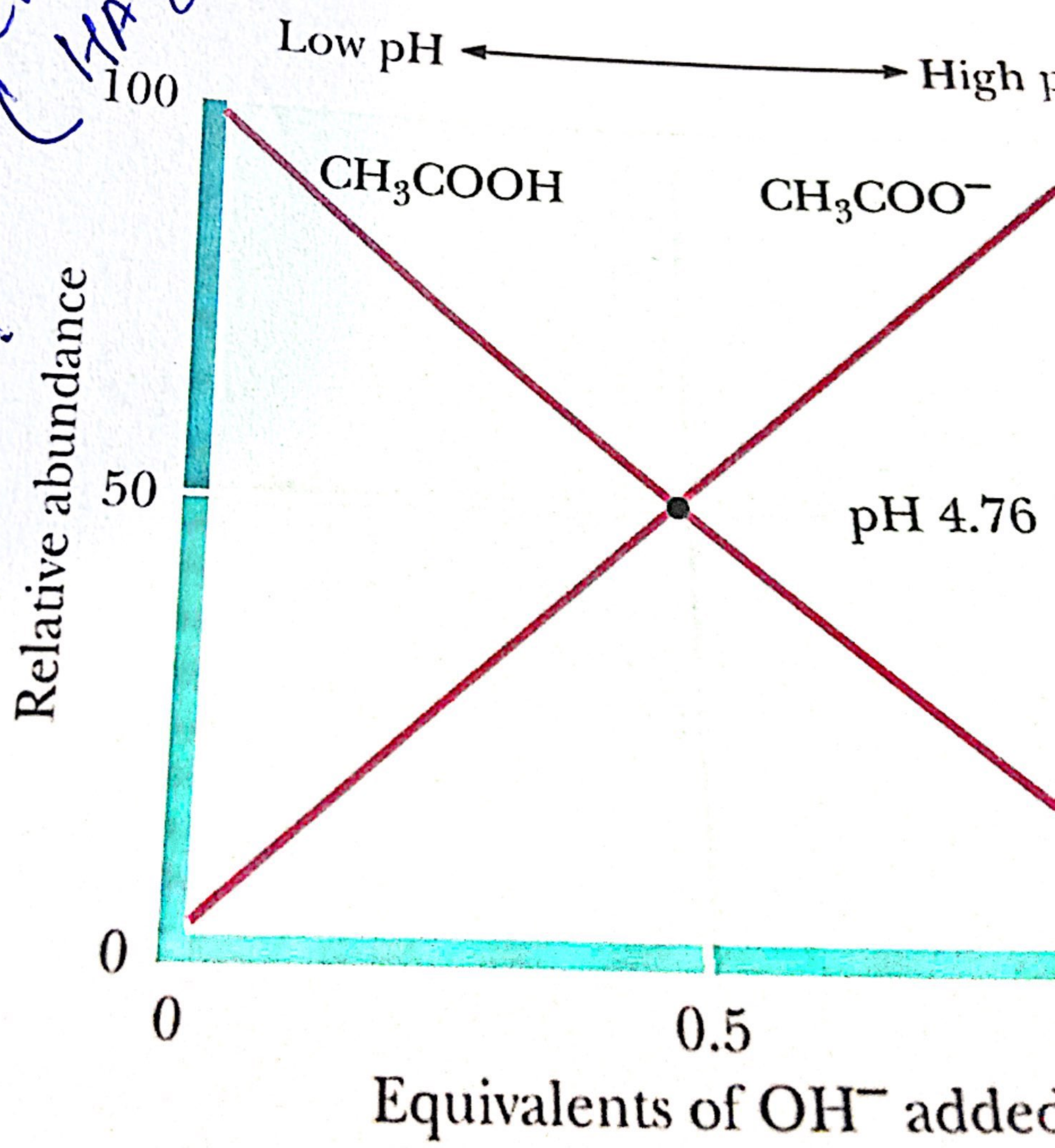

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Table 2.7

pH Values and Base/Acid Ratios for Buffers

If the pH equals	The ratio of base form/acid form equals
$pK_a - 3$	1/1000
$pK_a - 2$	1/100
$pK_a - 1$	1/10
pK_a	1/1
$pK_a + 1$	10/1
$pK_a + 2$	100/1
$pK_a + 3$	1000/1

outside buffering region

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ratio 1:1

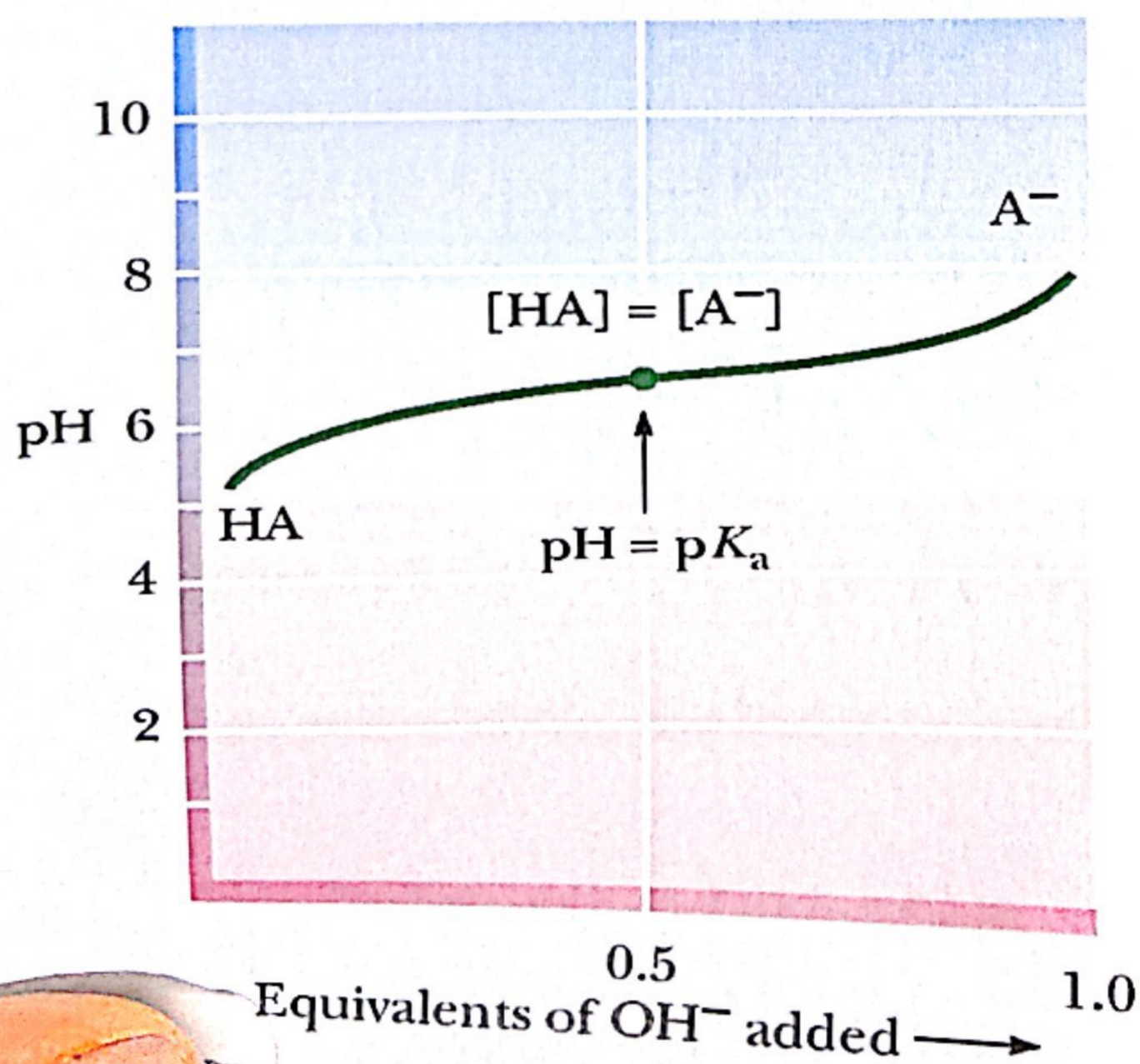
pKa = pH

ratio 10:1

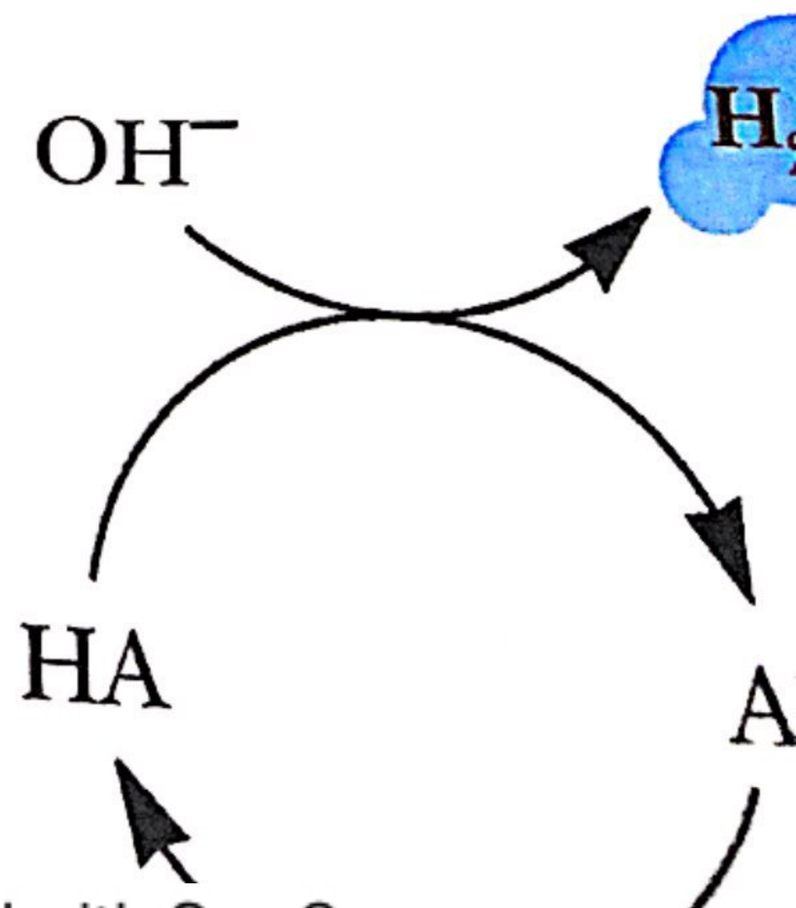
$pH = pKa + \log \frac{1}{10}$

$pH = pKa - 1$

* كيف عالم تغير نسبة من
1:1 لـ 1000 : 1 ؟
بزيد H^+



Buffer action:



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