# WATER

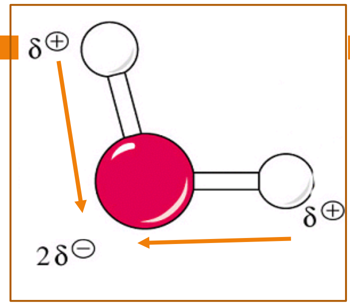
Course: Biochemistry I (BIOC 230)

Textbook:
**Principles of Biochemistry**, 5th Ed., by L. A. Moran and others. 2014, Pearson. . Chapter 2

## Why does the abundance of water allow life to exist on the planet earth?

## Properties of water

- The dipolar nature of the $H_2O$ molecule is shown in a ball-and-stick model




- Very polar, V-shaped
- Oxygen is highly electronegative
- H-bond donor and acceptor
- High boiling point, melting point, heat of vaporization, surface tension

## Hydrogen bonding

- H-bonds can occur between any electronegative atom and a hydrogen atom attached to another electronegative atom
- Hydrogen bonds are much weaker than typical covalent bond
- Orientation is important in H-bonding. H-bond is most stable when hydrogen atom and the electronegative atoms are aligned or nearly in line

**Hydrogen bonding in water**

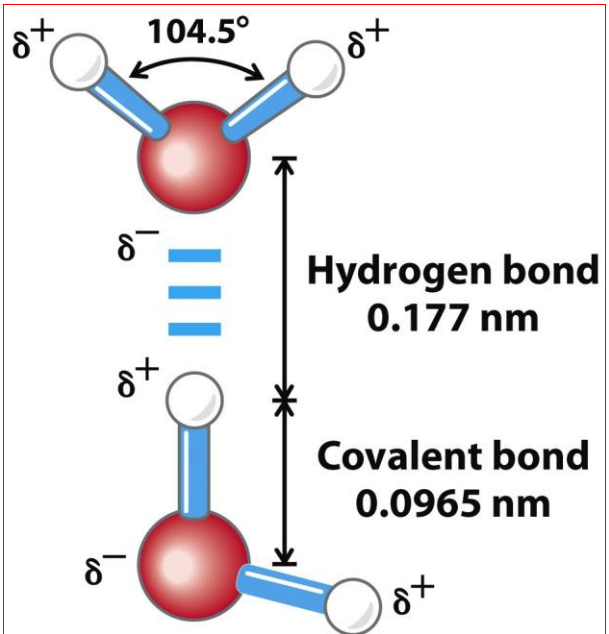



Figure 2-1b
*Lehninger Principles of Biochemistry, Fifth Edition*


Note: the atoms involved in the H-bond are aligned!!

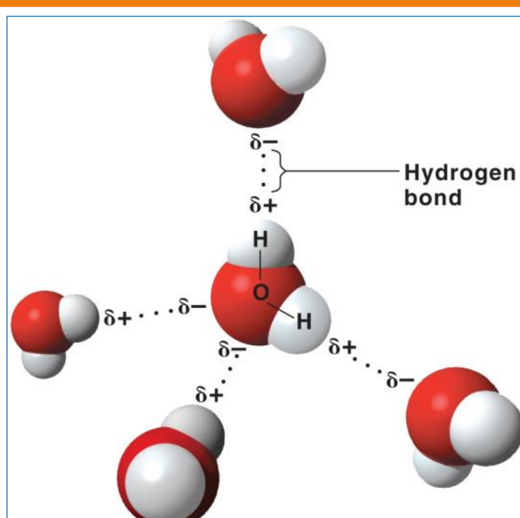
## H-bonding by a water molecule

- In ice form, each water molecule can form 4 H-bonds with surrounding water molecules>>> this gives ice an unusually high melting point
- The fluidity of liquid water compared to rigidity of ice is primarily a consequence of the irregular pattern of H-bonds in liquid water
- Average H-bond lifetime in water is ~10 picosecond ($10^{-11}$s)

# H-bonding by a water molecule

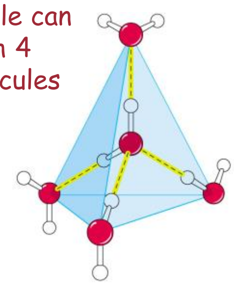
- The density of water increases as it cools until it reaches 1.000 gm/mL at 4°C (277K)
- Thus "**Gram**" is defined as the weight of **1 mL** of water at 4°C
- Water expands below 4°C, thus ice with its open lattice form is less dense than liquid water, ~0.924 gm/mL
- What are the consequences of this phenomenon? ice is less dense than water?

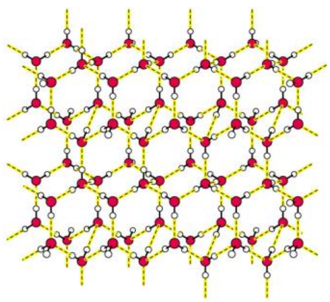
## Hydrogen Bonds between water molecules



# Hydrogen Bonding of Water

One $H_2O$ molecule can associate with 4 other $H_2O$ molecules





Crystal lattice of ice

**•Ice: 4 H-bonds per water molecule**

**•Water: 2.3 H-bonds per water molecule**

# Specific heat & heat of vaporization of water

- Water has high S.H. and high H.V.
- Specific heat (or heat capacity): amount of heat needed to raise the temperature of 1 gm of the substance by 1°C
- Consequence of high S.H: temperature fluctuations within cells are minimized
- Consequence of high H.V: perspiration is an effective mechanism for decreasing body temperature

## Water is an excellent solvent > the solvent of life

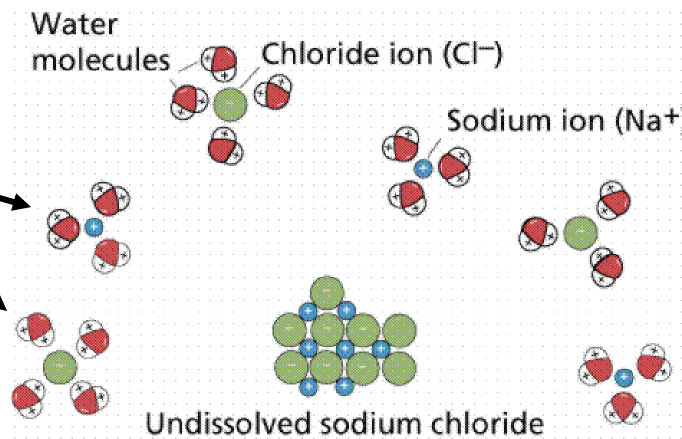
- Aqueous solution: water is the solvent
- Water is polar and thus dissolves ionic and non-ionic substances .> hydration shell
- Water do not dissolve non-polar compounds
- Water has intrinsic viscosity that doesn't greatly impede the movement of dissolved molecules
- Water molecules are small compared to other solvents and can associate with soluble particles to make them more soluble
- Contribute to osmotic pressure in cells

## Discussion!!

- Water is not a universal solvent. Is this an advantage or disadvantage?

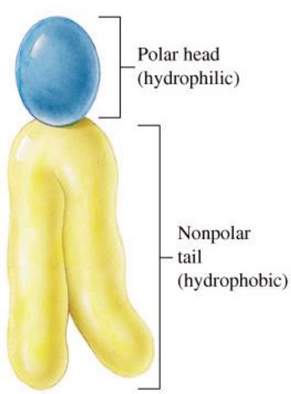
## Water dissolves polar compounds
*>> like dissolves like*

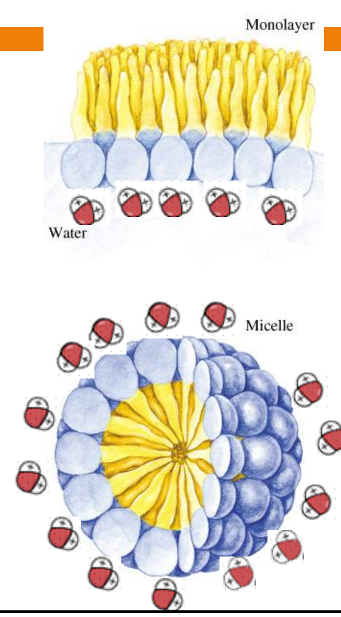
solvation shell
or
hydration shell



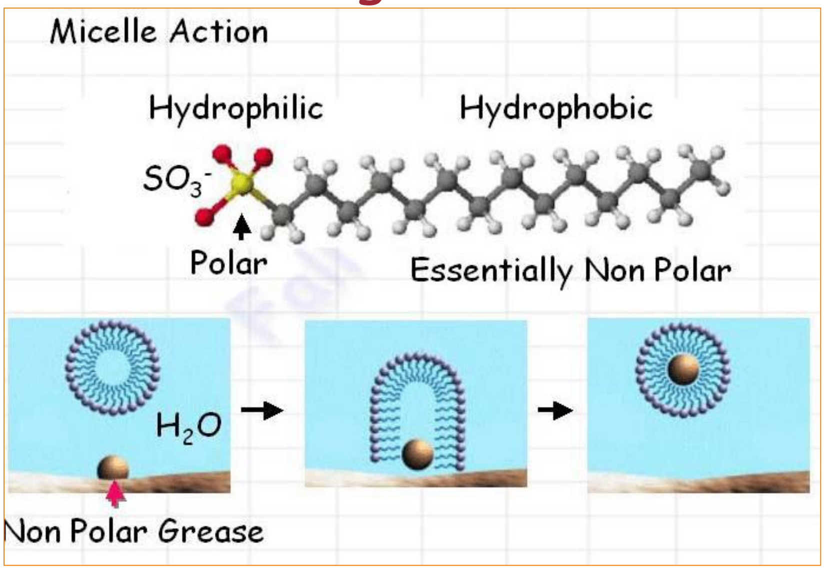

## Non-polar substances are insoluble in water

Many lipids are amphipathic



# How detergents work?




## Biological Hydrogen Bonds

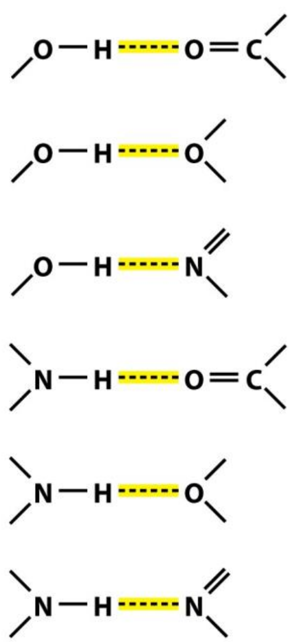
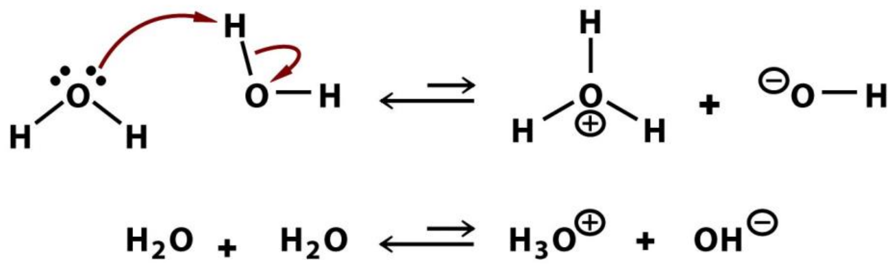



Figure 2-10b Principles of Biochemistry, 4/e

# Ionization of Water

One of the most important properties of water is its slightly tendency to ionize.




Unnumbered figure pg 38 Principles of Biochemistry, 4/e
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Hydronium ion

Hydroxide ion

# BrØnsted-Lowry concept of acids and bases

- Acid: proton donor
- Base: proton acceptor or hyroxide ion donor

## Ionization of Water

$$H_20 + H_20 \rightleftharpoons H_3O^+ + OH^-$$

$$H_20 \rightleftharpoons H^+ + OH^-$$

$$K_{eq} = \frac{[H^+]\,[OH^-]}{[H_2O]}$$

$K_{eq}$=1.8 X $10^{-16}$M

$[H_2O]$ = 55.5 M

**NOW! What is the conc of H+ and OH-???**

How to calculate the conc of water= (1000 gm is the weight of 1 liter)/ 18gm is the mass of 1 mole

## Ionization of Water (cont'd)

$$K_{eq} = \frac{[H^+]\,[OH^-]}{[H_2O]}$$

$$[H_2O]\,K_{eq} = [H^+]\,[OH^-]$$

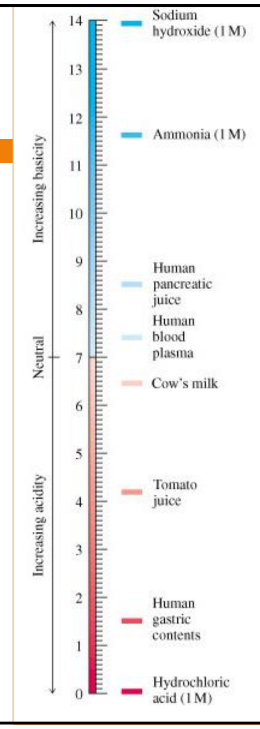
$$(1.8 \times 10^{-16} M)(55.5\ M) = [H^+]\,[OH^-]$$

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

If $[H^+]=[OH^-]$ then $[H^+] = 1.0 \times 10^{-7}$ M

$K_w$ (=[H+] [OH-]): the ion-product **constant** of water.

## pH Scale




- ✓ Devised by Sorenson (1902)
- ✓ [H+] can range from 1M (pH=0) and 1 X $10^{-14}$M (pH=14)
- ✓ using a log scale simplifies notation
- ✓ pH = -log [$H^+$]
- ✓ Neutral pH = 7.0

## Measurement of pH

- pH is measured using a pH meter
- Normal pH of blood is 7.4, which is frequently referred to as "physiological pH"
- In diabetes, blood pH is low>> acidosis
- pH>7.4>> alkalosis, results from prolonged vomiting or hyperventilation

**Table 4–5 The pH scale**

| $[H^+]$ (M) | pH | $[OH^-]$ (M) |
|---|---|---|
| $10^0$(1) | 0 | $10^{-14}$ |
| $10^{-1}$ | 1 | $10^{-13}$ |
| $10^{-2}$ | 2 | $10^{-12}$ |
| $10^{-3}$ | 3 | $10^{-11}$ |
| $10^{-4}$ | 4 | $10^{-10}$ |
| $10^{-5}$ | 5 | $10^{-9}$ |
| $10^{-6}$ | 6 | $10^{-8}$ |
| $10^{-7}$ | 7 | $10^{-7}$ |
| $10^{-8}$ | 8 | $10^{-6}$ |
| $10^{-9}$ | 9 | $10^{-5}$ |
| $10^{-10}$ | 10 | $10^{-4}$ |
| $10^{-11}$ | 11 | $10^{-3}$ |
| $10^{-12}$ | 12 | $10^{-2}$ |
| $10^{-13}$ | 13 | $10^{-1}$ |
| $10^{-14}$ | 14 | $10^{-0}$(1) |

* The expression pOH is sometimes used to describe the basicity, or $OH^-$ concentration, of a solution; pOH is defined by the expression pOH = $-\log [OH^-]$, which is analogous to the expression for pH. Note that for all cases, pH + pOH = 14.

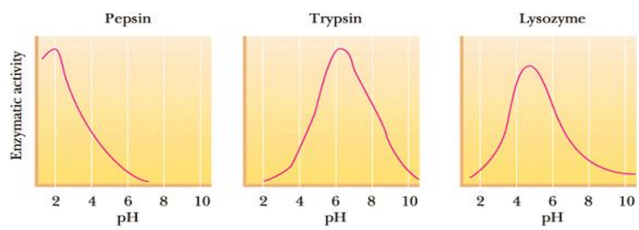
# Calculation of pH of a solution?

- What is the pH of a solution of 0.01 M NaOH?
- $1.0 \times 10^{-14}\ M^2 = [H^+]\,[OH^-]$
- $[OH^-] = 10^{-2}M$ >> $[H^+] = 10^{-12}M$
- pH= $-\log 10^{-12} = 12$

- What is the pH of a solution of 1M HCl?
- $[OH^-] = 10^{-14}M$ >> $[H^+] = 1M$
- pH= $-\log 1 = 0$

## Weak Acids and Bases Equilibria

- Strong acids / bases – disassociate completely
- Weak acids / bases – disassociate only partially
- Enzyme activity is sensitive to pH
- Weak acids/bases play important role in protein structure/function




## Acid/conjugate base pairs

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

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

HA = acid ( donates $H^+$)(Bronsted Acid)

$A^-$ = Conjugate base (accepts $H^+$)(Bronsted Base)

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

$K_a$ & $pK_a$ value describe tendency to loose $H^+$

$$pK_a = -\log K_a$$

large $K_a$ = stronger acid
small $K_a$ = weaker acid

# pKa values determined by titration

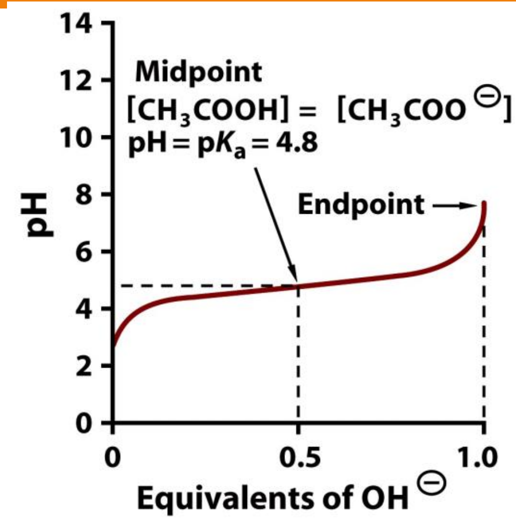
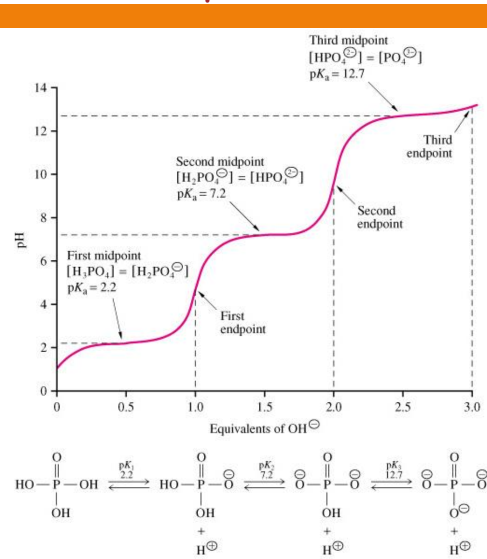



Figure 2-16 Principles of Biochemistry, 4/e


# Phosphate has three ionizable $H^+$ and three pKas



## Buffers

- Buffers are aqueous systems that resist changes in pH when small amounts of a strong acid or base are added.
- A buffered system consist of a weak acid and its conjugate base.
- The most effective buffering occurs at the region of minimum slope on a titration curve

  (i.e. around the pKa).
- Buffers are effective at pHs that are within +/-1 pH unit of the pKa

## Henderson-Hasselbach Equation

1) $K_a = \frac{[H^+][A^-]}{[HA]}$

2) $[H^+] = K_a \frac{[HA]}{[A^-]}$

3) $-\log[H^+] = -\log K_a - \log \frac{[HA]}{[A^-]}$

4) $-\log[H^+] = -\log K_a + \log \frac{[A^-]}{[HA]}$

5) $pH = pK_a + \log \frac{[A^-]}{[HA]}$

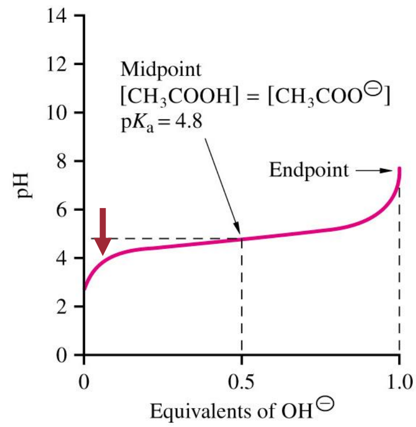
HA = weak acid

$A^-$ = Conjugate base

* H-H equation describes the relationship between pH, pKa and buffer concentration

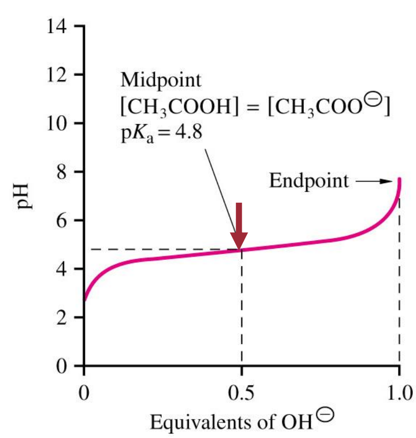
## Case where 10% acetate ion 90% acetic acid

- $pH = pK_a + \log_{10} \frac{[0.1]}{[0.9]}$
- $pH = 4.76 + (-0.95)$
- $pH = 3.81$



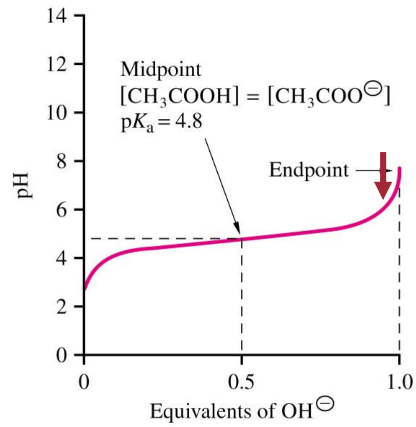

## Case where 50% acetate ion 50% acetic acid

- $pH = pK_a + \log_{10} \frac{[0.5]}{[0.5]}$
- $pH = 4.76 + 0$
- $pH = 4.76 = pK_a$



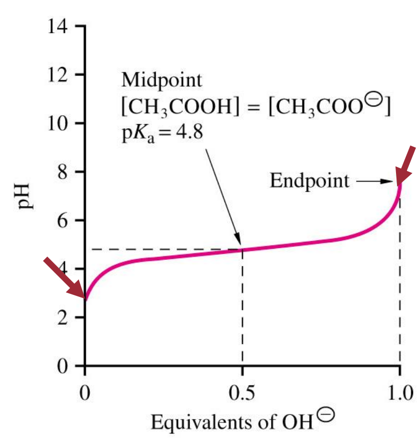
## Case where 90% acetate ion 10% acetic acid

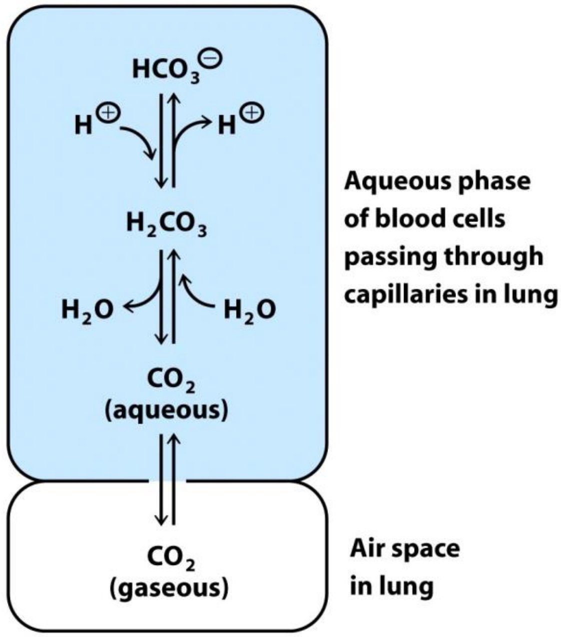
- $pH = pK_a + \log_{10} \frac{[0.9]}{[0.1]}$
- $pH = 4.76 + 0.95$
- $pH = 5.71$




## Cases when buffering fails

- $pH = pK_a + \log_{10} \frac{[0.99]}{[0.01]}$
- $pH = 4.76 + 2.00$
- $pH = 6.76$
- $pH = pK_a + \log_{10} \frac{[0.01]}{[0.99]}$
- $pH = 4.76 - 2.00$
- $pH = 2.76$



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## Class activity!

1. Which of the following functional groups is NOT a polar group?
   A. Hydroxyl group (-OH)
   B. Carboxy group (-COOH)
   C. Sulfhydryl group (-SH)
   D. Methyl group (-$CH_3$)
2. Which one of the above groups is ionized (charged) at physiological pH?
3. Which of the above groups can be a hydrogen bond donor or acceptor?

## Class activity!

1. A weak acid has a pKa of 6.5. If it is used as a buffer, the buffer capacity of this buffer is:
   A. 5-8
   B. 5.5-7.5
   C. 4.5-8.5
2. The optimum pH of an enzyme is 8. You want prepare a buffer solution for this enzyme, then the best buffer will be
   A. Buffer A, pKa=4.8
   B. Buffer B, pKa=9.5
   C. Buffer C, pKa=7.8

## End