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?

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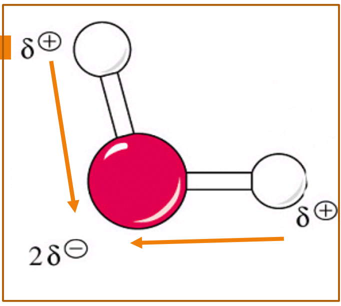
Properties of water



- 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

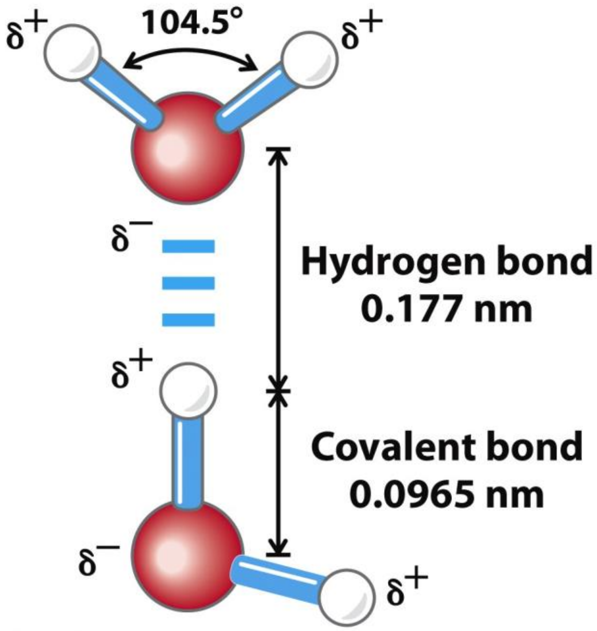


Figure 2-1b
Lehninger Principles of Biochemistry, Fifth Edition
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Note: the atoms involved in the H-bond are aligned!!

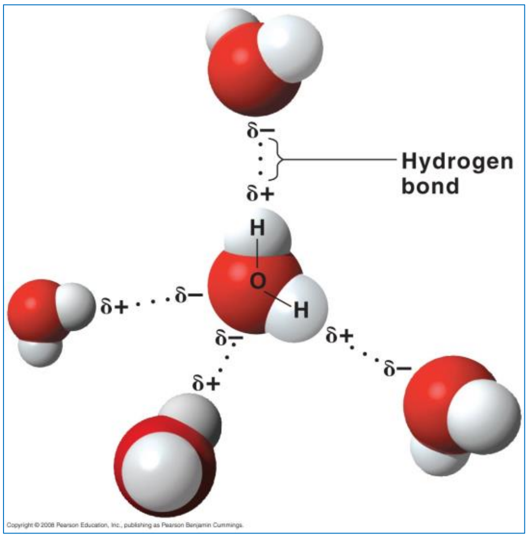
H-bonding by a water molecule

- 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



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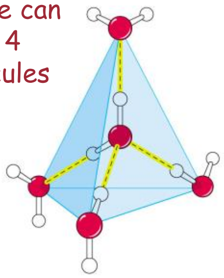
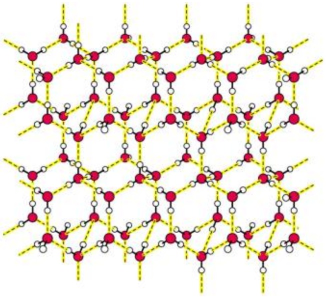
Hydrogen Bonding of Water

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?

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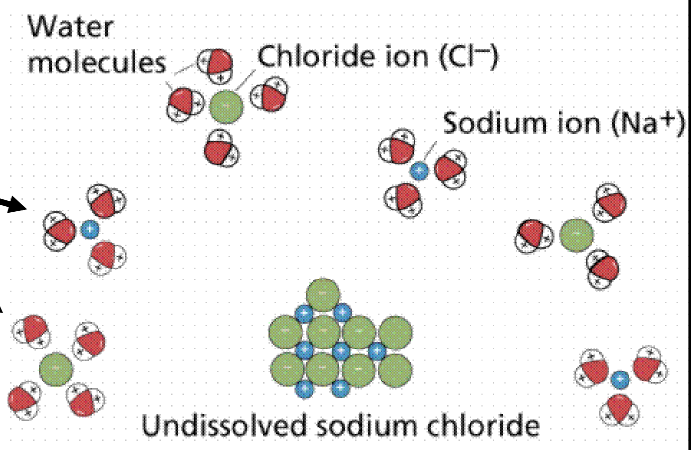
Water dissolves polar compounds

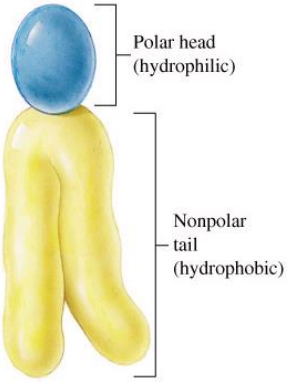
>> like dissolves like

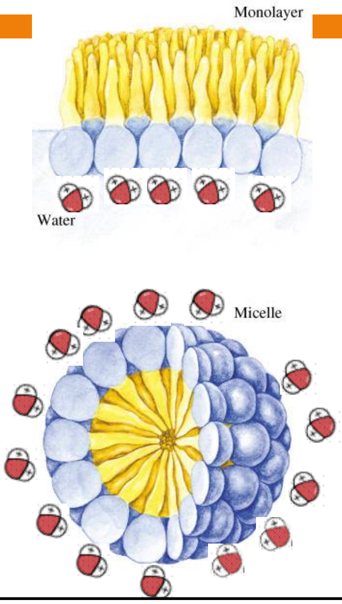
solvation shell
or
hydration shell



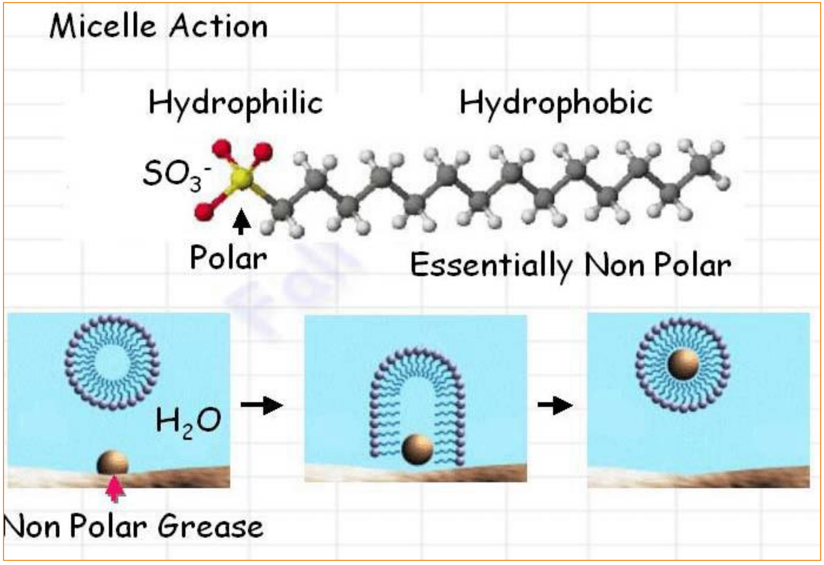
Non-polar substances are insoluble in water

Many lipids are amphipathic

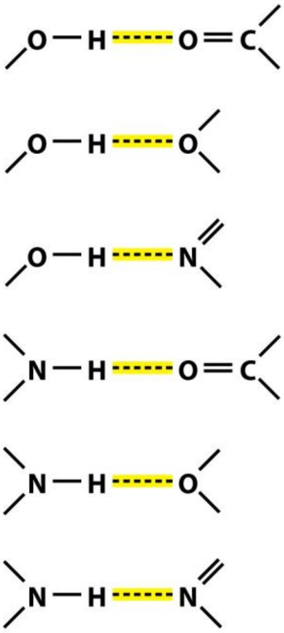




How detergents work?



Biological Hydrogen Bonds



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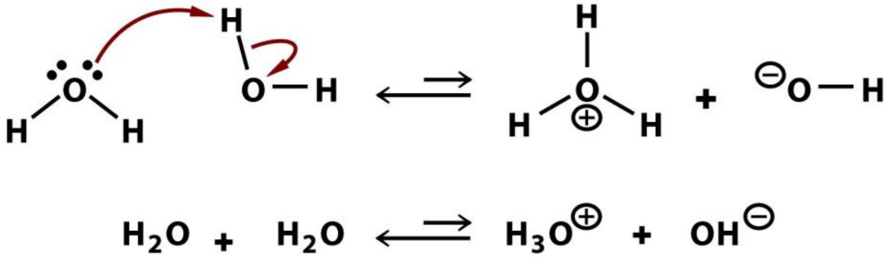
Ionization of Water

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



$$H_2O + H_2O \rightleftharpoons H_3O^{\oplus} + OH^{\ominus}$$

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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

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

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

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

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

$[H_2O] = 55.5\ M$

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)

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

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

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

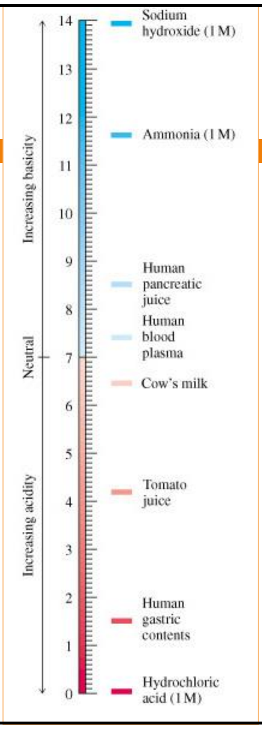
$$1.0 \times 10^{-14}\ M^2 = [H^+]\,[OH^-] = K_w$$

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

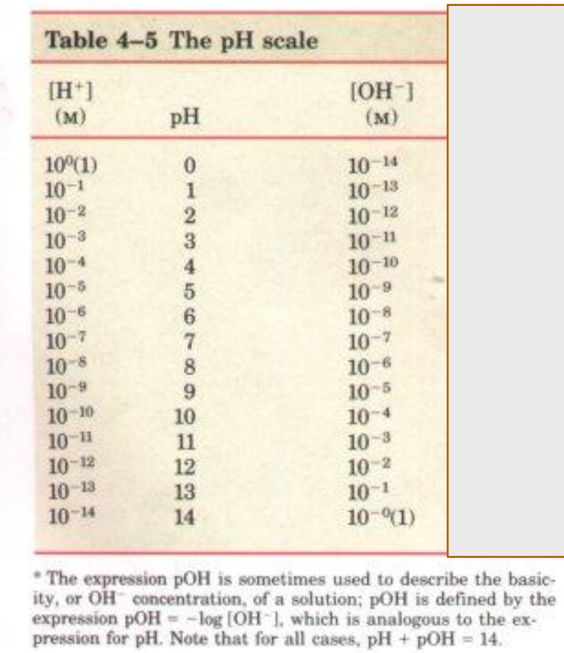


Table 4–5 The pH scale

$[H^+]$ (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.

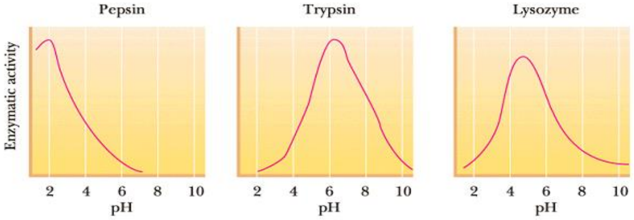
Calculation of pH of a solution?

- What is the pH of a solution of 0.01 M NaOH?
- 1.0×10^{-14} M^2 = $[H^+]$ $[OH^-]$
- [OH-]= 10^{-2}M >> [H+]=10^{-12}M
- pH= -log10^{-12} = 12

- What is the pH of a solution of 1M HCl?
- [OH-]= 10^{-14}M >> [H+]=1M
- pH= -log1 = 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)

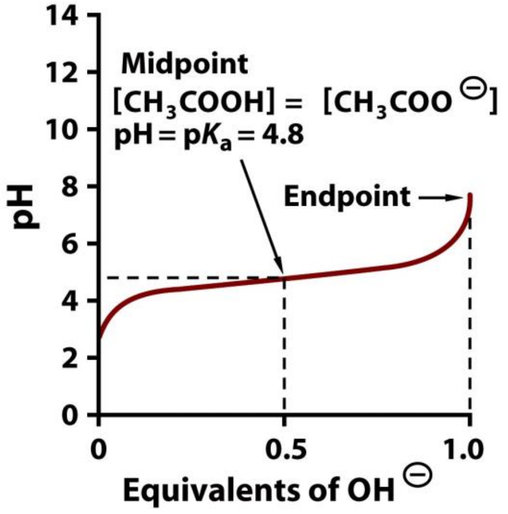
$$K_a = \frac{[H^+][A^-]}{[HA]}$$

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



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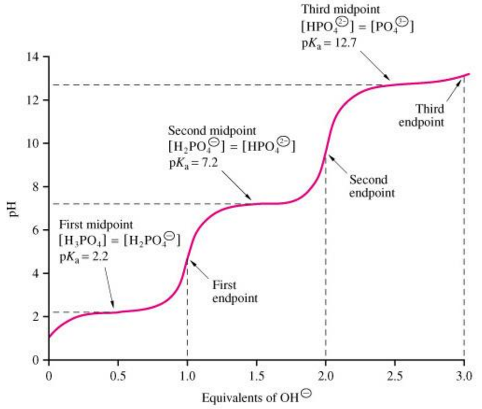
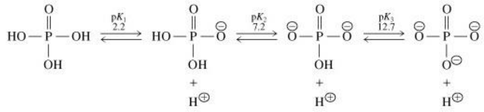
Phosphate has three ionizable H^+ and three pKas





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

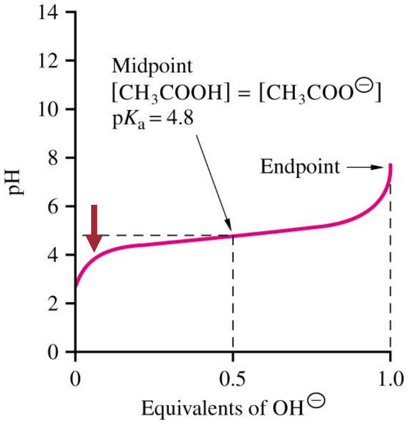
HA = weak acid

A^- = Conjugate base

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

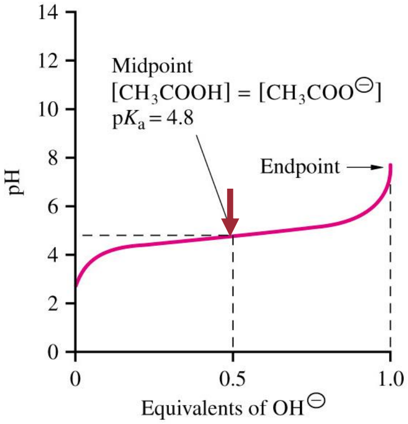
Case where 10% acetate ion 90% acetic acid

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



Case where 50% acetate ion 50% acetic acid

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



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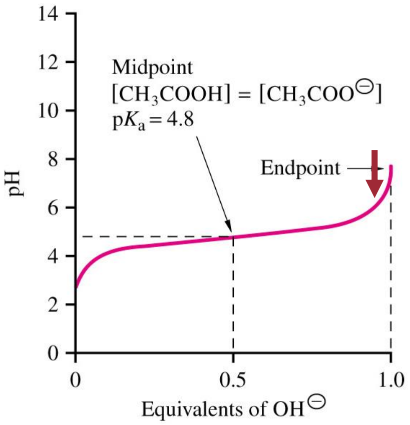
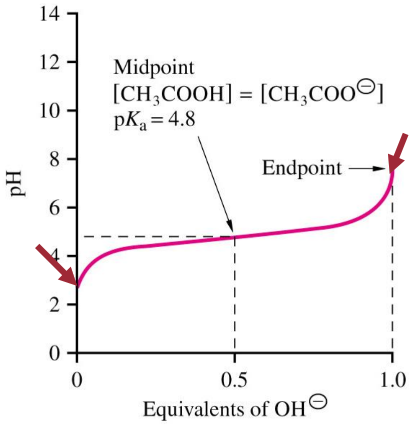
Case where 90% acetate ion 10% acetic acid

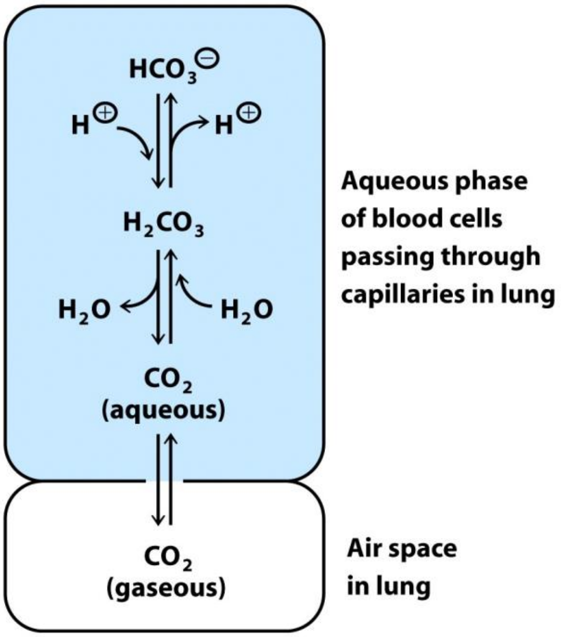
- $\mathrm{pH} = \mathrm{p}K_a + \log_{10} \frac{[0.9]}{[0.1]}$
- $\mathrm{pH} = 4.76 + 0.95$
- $\mathrm{pH} = 5.71$



Cases when buffering fails

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





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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

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