Introduction pH, Buffers and Chemical Bonds





Acids, Bases and pH

- Acid: a substance that can release hydrogen ions (protons/H⁺).
- Base: a substance that can accept hydrogen ions.
- **PH:** the concentration of hydrogen ions, it determines the acidity of the solution.
- The pH of a solution is the negative base 10 logarithm of its hydrogen ion concentration
 pH = log₁₀ [H+]
- The relationship between pH and hydrogen ion concentration is inverse.

H	[- [H ⁺]	рΗ	[H+] (n	nol/I)
0	(10^{0})	1.0	1	10-1	\uparrow
2	(10^{-2})	0.01	2	10-2	
3	(10^{-3})	0.001	3	10 ⁻³	Increasing
4	(10^{-4})	0.0001	4	10-4	acidity
5	(10^{-5})	0.00001	5	10 ⁻⁵	
6	(10^{-6})	0.000001	6	10 ⁻⁶	
7	(10^{-7})	0.0000001	7	10-7	Neutral
8	(10^{-8})	0.00000001	8	10 - 8	
9	(10^{-9})	0.00000001	9	10- ⁹	
0	(10^{-10})	0.0000000001	10	10-10	Increasing
1	(10^{-11})	0.00000000001	11	10-11	alkalinity
2	(10^{-12})	0.000000000001	12	10-12	
3	(10^{-13})	0.0000000000001	13	10-13	
4	(10^{-14})	0.00000000000001	14	10-14	\mathbf{V}



Acids, Bases and pH Cont.

Example 1: what is the pH of a solution whose hydrogen ion concentration is 3.2 X 10⁻⁴ mol/L?

pH = -log [H⁺]
= -log (3.2 X 10⁻⁴)
pH = 3.5

H	[H ⁺]		рΗ	[H+] (n	nol/I)
0	(10^{0})	1.0	1	10-1	\uparrow
2	(10^{-2})	0.01	2	10 ⁻²	
3	(10^{-3})	0.001	3	10- ³	Increasing
4	(10^{-4})	0.0001	4	10-4	acidity
5	(10^{-5})	0.00001	5	10-5	
6	(10^{-6})	0.000001	6	10-6	
7	(10^{-7})	0.0000001	7	10-7	Neutral
8	(10^{-8})	0.00000001	8	10 - 8	
9	(10^{-9})	0.000000001	9	10- ⁹	
0	(10^{-10})	0.0000000001	10	10-10	Increasing
1	(10^{-11})	0.00000000001	11	10-11	alkalinity
2	(10^{-12})	0.000000000001	12	10-12	
3	(10^{-13})	0.0000000000001	13	10-13	
4	(10^{-14})	0.000000000000001	14	10-14	Ψ



Dissociation constant Ka

Dissociation constant (Ka): the tendency of any acid (HA) to lose a proton and form its conjugate base (A⁻).

$$Ka = \frac{[A^-]}{|HA|}$$

$$HA = \frac{A^-}{Conjugate} + H^+$$

$$Acid = \frac{A^-}{Base} + H^+$$

The stronger the acid, the greater its tendency to lose its proton.

- The acid (proton donor) dissociates into a hydrogen ion (H⁺) and an anionic component (A⁻), called the conjugate base (or salt).
- **Strong acids**: are acids that dissociate completely in solution like HCl. \circ HCl \rightarrow Cl⁻+ H⁺
- ♦ Weak acids: are acids that dissociate only to a limited extent like H2CO3. \odot H2CO3 → HCO3⁻+ H⁺



рКа

✤pKa = $-\log Ka$

PKa is the pH at which 50% dissociation occurs (concentration of the acid = concentration of the conjugate base).

- PKa value is easier to work with and remember than Ka value.
- The stronger the tendency of an acid to dissociate the higher is the Ka and the lower is its pKa (the relationship between any value and its P value is inverse).





Buffers

- A buffer is a solution that resists pH changes when acids or bases are added to the solution.
- Buffer solutions consist of a weak acid (undissociated acid) and its conjugate base (the form of the acid having lost its proton).

HA Acid

- ☆A buffer works because added acids (H⁺) are neutralized by the conjugate base (A⁻) which is converted to the acid (HA).
- Added bases are neutralized by the acid (HA), which is converted to the conjugate base (A⁻).
- Two factors determine the effectiveness of a buffer:
 - 1. Its pKa relative to the pH of the solution.
 - 2. Its concentration.



 $+ H^{+}$

Handerson-Hasselbalch Equation

Henderson-Hasselbalch adjusted equation describes the relationship between the acid and its conjugate base with pH and pKa.

 \circ pH = pKa + $\log \frac{A^{-}}{HA}$

- The most effective buffers (maximum buffering capacity) is when pH=pKa meaning it has equal concentrations of acid [HA] and its conjugate base [A⁻] (50% of both forms HA & A⁻ present in solution). the buffer can then respond equally to both acid and base if added to the solution.
- At pH = pKa ± 1 the buffer capacity falls to 33% of the maximum value.
 Therefore the buffer is effective one point up or down the pH pKa value.



Buffer Systems in The Body

- The buffer systems functioning in blood plasma include plasma proteins, phosphate, and bicarbonate and carbonic acid buffers.
- Protein buffer systems work predominantly inside cells.
- It takes only seconds for the chemical buffers in the blood to make adjustments to pH.
- The respiratory tract can adjust the blood pH upward in minutes by exhaling CO2 from the body.
- The renal system can also adjust blood pH through the excretion of hydrogen ions (H⁺)and the conservation of bicarbonate, but this process takes hours to days to have an effect.



Chemical Bonds

The attractive forces that hold atoms together in compounds.

- Chemically, bonding occurs when an atom gives up electrons, accepts electrons, or shares electrons with another atom.
- A stable compound occurs when the total energy of the combination has lower energy than the separated atoms.



Ionic Bonding

- In ionic bonding, electrons are completely transferred from one atom to another.
- The oppositely charged ions are attracted to each other by electrostatic forces, which are the basis of the ionic bond.
- Ionic compounds share many features in common including:
 - I. Ionic bonds form between metals and non-metals.
 - II. In naming simple ionic compounds, the metal is always first, the non-metal second (for example sodium chloride).
 - III. Ionic compounds dissolve easily in water and other polar solvents.
 - IV. In solution, ionic compounds easily conduct electricity.
 - V. Ionic compounds tend to form crystalline solids with high melting temperatures.





Covalent Bonding

- Results from sharing one or more electron pairs between two atoms.
- Covalent bonding occurs because the atoms in the compound have a similar tendency for electrons (generally to gain electrons).
- The elements involved will share electrons in an effort to fill their valence shells.





Electron from hydrogenElectron from carbon



Polar Covalent Bonding

- A polar bond is formed when electrons are unequally shared between two atoms.
- It occurs because one atom has a stronger affinity for electrons than the other (yet not enough to pull the electrons away completely and form an ion).
- In a polar covalent bond, the bonding electrons will spend a greater amount of time around the atom that has the stronger affinity for electrons.



Polar bond in water molecule The large oxygen atom has a stronger affinity for electrons than the small hydrogen atoms.



Electronegativity

- Electronegativity: is the ability of an atom to attract electrons towards itself in a covalent bond.
- If the electronegativity difference between two atoms is < 0.5 it will be essentially non-polar.
- If the difference is between 0.5 and 2 it is polar.
- If the difference is > 2.0 it is often considered to be ionic.

Electronegativity of selected elements

Ρ	2.1	К	0.8
Н	2.1	Na	0.9
С	2.5	Са	1.0
Ν	3.0	Mg	1.2
0	3.5	Cl	3.0
F	4.0		



Hydrogen Bond

- Hydrogen bond is the attractive interaction of a hydrogen atom with an electronegative atom (like nitrogen, oxygen or fluorine).
- The partial positive region of hydrogen is attracted to the partial negative region of another molecule.
- The hydrogen must be covalently bonded to another electronegative atom to create the bond.
- The hydrogen bond is stronger than a van der Waals interaction, but weaker than covalent and ionic bonds.





Non Polar Covalent Bonding

- Hydrophobic Interactions
- Nonpolar groups do not form hydrogen bonds with water (they are insoluble in water).
- Hydrophobic substances are "excluded" from aqueous solution, this drive these molecules to cluster together (e.g. oil droplets in water).
- No affinity between nonpolar substances except van der Waals forces that promote the weak bonding of nonpolar substances.



Van Der Waals Forces

- Van der Waals forces are weak attractive forces between electrically neutral atoms or molecules.
- They are much weaker than the ionic bond or the covalent bond.
- These forces may develop because the rapid shifting of electrons within molecules causes some parts of the molecule to become momentarily charged (either positively or negatively). For this reason, weak, transient forces of attraction can develop between particles that are actually neutral. The magnitude of the forces is dependent on the distance between neighboring molecules.



MCQ 1

Which one of these can make a polar covalent bond:

- a. P&H
- b. K & Na
- c. Cl & H
- d. Mg & Ca
- e. P&C

Electronegativity of selected elements

Ρ	2.1	К	0.8
Н	2.1	Na	0.9
С	2.5	Ca	1.0
Ν	3.0	Mg	1.2
0	3.5	Cl	3.0
F	4.0		



MCQ 2, 3

A solution with pH = 5 is than another solution with pH = 7:

- a. 10 times more basic
- b. 1000 times more basic
- c. 10 times more acidic
- d. 2 times more basic
- e. 100 times more acidic

The concentration of acid is 0.35 and the conjugate base is 0.35 and the pH is 4.6. Calculate the pKa:



MCQ 4, 5

Regarding the Henderson-Hasselbalch equation, which statement is accurate?

- a. pH is less than pKa
- b. Shows that pH is equal to pKa in all conditions
- c. pH is more than pKa
- d. Relates pH, pKa, acid concentration, and conjugate base concentration

The best buffer occurs when:

- a. pKa = 1
- b. pH = 7
- c. pKa > pH
- d. pH = 7.4
- e. Conjugate base concentration = weak acid concentration



MCQ 6, 7

- Suppose that the acid (CH3COOH) has a pKa = 7.76 was placed in a solution that has a pH=4.25, the dominant form of this acid in the solution will be?
 - a. CH3COA
 - b. CH3CO0-
 - c. CH3CH+
 - d. CH3COOH
 - e. CH3COOH2

Regarding pH, pKa and Ka, choose the correct answer?

- a. Question 29Answera. No relation between strength of acid and Ka
- b. The higher the pH the stronger the acid
- c. At pH lower than pKa more dissociation to acids
- d. The higher the pKa the stronger the acid
- e. For acids, at pH higher than pKa more base than acid



MCQ 8, 9

The stronger the acid,...... (choose the correct answer)?

- a. The higher the pH
- b. The higher the Ka
- c. The higher the OH concentration
- d. The higher the pKa
- e. The lower the Ka and pKa

Which one of the following solutions has a stronger acidity?

- a. pH = 8
- b. H = 107
- c. pH=6
- d. pH = 10
- e. pH = 9



MCQ Answer Key

Q	Answer	Q	Answer
1	С	6	d
2	е	7	е
3	4.6	8	b
4	d	9	С
5	е		

