Henderson Hassel balch Equation

The Henderson-Hassel balch equation is the equation commonly used in chemistry and biology to determine the pH of a solution.

- This equation shows a relationship between the pH or pOH of the solution, the pK_a or pK_b, and the concentration of the chemical species involved.

- This equation was developed independently by the American biological chemist L. J. Henderson and the Swedish physiologist K. A. Hassel balch to determine the pH of the bicarbonate buffer system in blood.

- This type of kinetic analysis has enabled us for nearly a century to relate theoretically the changes of the acidic intensity of dilute solutions to a quantity of acid or base added or subtracted.

- This equation can be considered as the backbone of acid-base physiology.

- This equation is commonly used to determine the amount of acid and conjugate base required to prepare a buffer of the desired pH.

Objectives of Henderson Hassel balch Equation

The principal objectives of the Henderson Hassel balch equation include the following:

1. To calculate the pH, pOH, $[H3O+]_{tot}$, $[OH-]_{tot}$, $[H3O+]_{water}$, and $[OH-]_{water}$ in a solution containing a strong acid (base) given the initial concentration of the acid (base).
2. To describe how a buffer solution (either acidic or basic) can resist significant changes in pH when small amounts of either acid or base are added to the buffer solution.
3. To describe how either an acidic or basic buffer solution is prepared.
4. To describe a "buffer solution".
5. To describe "buffer capacity".
6. To determine whether an aqueous solution of salt will be acidic, basic, or neutral given values of Ka and Kb for conjugate acid-base pairs.
7. To describe how the relative strengths of the conjugate acids or bases can be evaluated using the values of Kb and Ka for the bases and acids, respectively.

8. To determine the protonation state of different biomolecule functional groups in a pH seven buffer.

Derivation of Henderson Hasselbalch Equation For Acidic Buffer

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- According to the Bronsted-Lowry theory of acids and bases, an acid (HA) can donate a proton (H^+) while a base (B) can accept a proton.
- An acid after losing a proton forms a conjugate base ($A^–$), and the protonated base exists as conjugate acid (BH^+).
- The dissociation of acid is expressed in terms of the equilibrium equation as:

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

- This relationship can be described in terms of the equilibrium constant as:

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

Now, taking negative log on both sides of the equation gives:

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

OR

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

By definition,

$$-\log K_a = pK_a \text{ and } -\log[H^+] = pH$$

Thus,

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

This equation is then arranged to form the Henderson Hasselbalch equation as:

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

How is the buffer solution prepared using the Henderson-Hasselbalch equation?

The Henderson-Hasselbalch equation tells us how the pH of the buffer solution changes with the pK_a of a weak acid. The best buffer solution is prepared when we take an equal amount of salt and acid. The pH is controlled by the pK_a of the acid.

For example, for the buffer of acetic acid and sodium acetate, the pH will be:

$$[CH_3COOH] = [CH_3COONa]$$

$$pH = pK_a + \log [CH_3COONa] / [CH_3COOH]$$

$$pH = pK_a + \log (1)$$

$$pH = pK_a + 0$$

$$pH = pK_a$$

pK_a of the acid is 4.74. So the pH of this buffer is equal to the pK_a of the acid. Hence, the pH of the buffer is 4.74.

Solved Example

If [CH_3COOH] is equal to the 1.0 mole dm^{-3} and [CH_3COONa] is 0.1 mole dm^{-3} then find the pH of the buffer solution.

Solution:

$$pH = 4.74 + \log 0.1/1$$

$$= 4.74 + \log 1/10$$

$$= 4.74 + \log 10^{-1}$$

$$‘= 4.74 – 1$$

$$pH = 3.74$$

Henderson-Hasselbalch equation for basic buffers

The basic buffer has also the Henderson equation. However, this equation is used to find the pH of the basic buffer solution. Let us take the weak base and its salt of strong acid. The dissociation of a weak base is as follows:

$$NH_3 + H_2O \rightleftharpoons NH_4^+ + OH^–$$

$$K_b = [\ NH_4^+][OH^–] / [NH_3]$$

Similarly, by taking the log, multiplying it with a negative sign, and rearranging we get,

$$pOH = pK_b + \log [salt] / [base]$$

where,

- K_b is the base dissociation constant

Equation

- The Henderson Hasselbalch equation can be expressed in two ways:
  - $pH = pK_a + \log \frac{[conjugate\ base]}{[weak\ acid]}$ (for weak acid)
  - $pOH = pK_b + \log \frac{[conjugate\ acid]}{[weak\ base]}$ (for weak base)

where pK_a= dissociation constant of acid
pK_b= dissociation constant of base

Applications of Henderson Hasselbalch Equation

Calculating the pH of a solution using pK_a

- This equation can be used to determine the pH of different solutions in different chemical equations as well as in biological systems like enzymes and proteins.

Calculating the ionized and unionized concentrations of chemicals.

- One of the most potent applications of the Henderson Hasselbalch equation is the ability to determine the concentrations of ionized and unionized chemicals.
- Generally, the amount of ionized and unionized species is detected using some spectroscopic technique, and thus, this equation is useful in the condition where spectroscopic studies are not feasible.
- The knowledge of the concentration of ionized and unionized chemicals is essential in fields like organic chemistry, analytical chemistry, and pharmaceuticals sciences.

Calculating pK_a of a molecule using pH

- Determining the pK_a of a molecule is important as the pK_a is an essential characteristic of the chemistry of the structure of the molecule.
- Henderson Hasselbalch equation can be used to determine the pK_a when the ratio of ionized and unionized forms and the pH of the solution is known.

Determination of solubility

- It has been observed that the Henderson Hasselbalch equation is important in determining the pH dependency of solubility.
- Based on the pH of a solution, the solubility of the solution can be determined, and there is also a close relationship between pH and solubility of various components in a solution.

Calculating the isoelectric point of protein

- This equation can also be used in determining the isoelectric point of different proteins (pH at which proteins neither lose or accept protons).

Limitations

- The most critical assumption of this equation is that the concentration of acid and its conjugate base will remain the same during the equilibrium.
- The significance of hydrolysis of water and its effect on the pH of the overall solution is neglected.
- Similarly, the hydrolysis of the base and dissociation of acid is also neglected.
- The assumption made in the equation might fail while dealing with strong acids or bases.

Question and Answers

What is the Henderson-Hasselback equation? Give example.

Henderson hasselbalch equation is the mathematical derivation that relates pH with the acid dissociation constants and the concentrations of the conjugate base. For example, if a buffer solution of pH 1 is needed, by using this equation we can determine the amount of required acid and conjugate base.

What is the importance of the Henderson-Hasselbalch equation?

It is of great importance in the pharmaceuticals and chemical industry for the preparation of buffer solutions.

What is meant by buffer solution?

A buffer solution is a complex solution based on the principle of the common ion effect. When this solution is added to the medium, it helps to retain the pH upon the addition of a small amount of acid or base.

What is a basic buffer solution?

A basic buffer solution has a pH from 7 to 14 in the basic region. For example, ammonia buffer has a pH of 10. It is added to maintain the specific pH to some extent.

What is the Henderson Hasselbalch constant?

In this equation pKa is the -log of the acid dissociation constant.

What do you mean by buffer capacity?

The buffer capacity is the tendency of the buffer solution to which it can resist the pH.

What is the relationship between pKa and pH?

Both depend upon the ratio of concentrations of conjugate base and acid.

Why is the Henderson Hasselbalch equation only used for weak acids?

It cannot be applied to strong acids because the acid dissociation constant ka for strong acids is very high.

How to find the ratio using the Henderson Hasselbalch equation?

The ratio can found out by inserting the values of the acid dissociation constant and required pH. Then rearrange the equation to make a ratio subject. Finally, the anti-log is taken on both sides to calculate the ratio of salt and acid to be used.