Experiment no: 02 **Date of Experiment:18/06/2021**

Name: SOHOM SAHA

Section: C Stream: CSE Roll No: 17(10900120045)

Date of Submission: 26/05/2021

Determination of the Partition Coefficient of Acetic Acid Between n-Butanol and Water

Theory:

According to Nernst distribution law, when a solute, soluble in each of two immiscible solvent, is shaken with a mixture of two such solvent to attain equilibrium, the solute distributes itself in both of the solvent and the ratio of concentration of the solute in the two solvent is a constant at a constant temperature. For this law to be held, the solvent pair as well as the solute must be non-reactive towards themselves and there must not be any association or dissociation of the solute in any of the solvent. This ratio is called distribution coefficient of the solute in those two solvent. The equilibrium is known as heterogeneous equilibrium since it involves a heterogeneous phase of two immiscible solvents.

When acetic acid is added in a heterogeneous mixture of water and n-butanol with vigorous shaking, acetic acid distributes itself in those two solvents following Nernst distribution law, constituting a heterogeneous equilibrium.

$$\text{AcOH(water)} \rightleftharpoons \text{AcOH(n-butanol)}$$

If the concentration of acetic acid is C_1 and C_2 respectively in n-butanol and water, then according to Nernst distribution law

$$K_d = \frac{C_1}{C_2}$$

Where K_d is the distribution coefficient of acetic acid in n-butanol and water.

K_d is determined by simple acid-base titration. Suppose V_1 mL of S (N) NaOH is required to neutralize V mL of n-butanol solution of acetic acid (organic layer). Then, $C_1 = \frac{V_1 S}{V}$. Suppose V_2 mL of S (N) NaOH is required to neutralize V mL of aqueous solution of acetic acid (aqueous layer). Then, $C_1 = \frac{V_2 S}{V}$

Then,

$$K_d = \frac{V_1 S/V}{V_2 S/V}$$

Or, $$K_d = \frac{V_1}{V_2}$$

Thus, from the ratio of the volume of NaOH required in two titration, K_d can be obtained.

Apparatus Required :

1) Standard Joint Stoppered Bottle(250 ml)-2
2) Funel-1
3) Beaker(100ml)-2
4) Pipette(10 ml)-1
5) Burette(50 ml)-1
6) Separating Funnel(250 ml)-1

Chemicals Required :

1) N-Butanol,
2) Acetic Acid [CH_3COOH]
3) NaOH solution
4) Phenolphathalein Indicator

Procedure:

1) **Preparation of solutions**

Take two bottles I and II which contains –

Bottle I: 40ml n-Butanol and 60ml water and 1 to 2 ml acetic acid

Bottle II: 30ml n-Butanol and 70 ml water and 1 to 2 ml acetic acid

2) **Attainment of distribution**

Shake the bottles vigorously after every 3 to 4 minutes for 20 minutes durations. And after each time of shaking, open the lid of the 2 bottles to release the pressure. Then wait for 5 min. and pour the entire solution into a separating funnel. Allow the mixture to separate two clear layers where the upper layer is the organic layer and the lower layer is aqueous layer.

3) **Titration**

Step I

The aqueous layer was collected in a clean and dry 100 ml beaker. 5ml of the solution was pipette out in to conical flask. About 10 ml of distilled water was added and the resulting solution was titrated with supplied ~0.2 (N) NaOH using phenolphthalein indicator. At end point color of the solution is light pink.

Step II

The organic layer was collected into a clean and dry 100ml beaker. 5ml of the organic layer was pipette out into a conical flask. About 10 ml of distilled water was added and the resulting solution was titrated with supplied ~ 0.2 (N) NaOH using phenolphthalein indicators. During titration the solution was shaken vigorously. At the end point color of the solution is light pink.

The process of Step -1 &Step -2 is done for the two bottles. And at least two readings are taken for each titration.

(1) Recording of room temperature

Initial temperature	Final temperature	Mean temperature
31	**31**	**31**

(2) Titration data for acetic acid in aqueous and organic layer:

Bottle No.	Volume of Solution taken	Titration of organic layer				Titration of aqueous layer			
		Initial Burette reading (mL)	Final Burette reading (mL)	Volume required (mL)	Mean volume (mL)	Initial Burette reading (mL)	Final Burette reading (mL)	Volume required (mL)	Mean volume (mL)
I (4:6)	5	2.4	5.4	3	3	0	2.4	2.4	2.4
	5	2.4	5.4	3		0	2.4	2.4	
II (3:7)	5	8.2	11.8	3.6	3.6	5.4	8.2	2.8	2.8
	5	8.2	11.8	3.6		5.4	8.2	2.8	

Calculation:

For Bottle I, $K_{d_1} = \frac{org.}{aq.} = 1.25$

For Bottle II, $K_{d_2} = \frac{org.}{aq.} = 1.29$

Therefore, average $K_d = \frac{(K_{d1}+K_{d2})}{2} = 1.27$ at 31°C.

Conclusion:

The average distribution coefficient (K_d) of acetic acid in n-butanol and water is 1.27 at 31°C.

Discussion:

1) The distribution coefficient or partition coefficient of a solute between two immiscible solvents depends on the nature of the solvent, solubility of the solute as well as on the temperature.
2) Prior to the experiment all the apparatus should be well cleaned with distilled water to wash the impurities out.
3) If there is any chemical reaction, association or dissociation of the solute in any of the solvents, the concentration terms will change and the overall calculation will be erratic.
4) If the solutions are not shaken properly, a particular solvent might contain higher amount of solute compared to other and proper distribution of solute is not achieved or partition coefficient cannot be found out.
5) Higher amount of indicator should not be used; otherwise estimation of concentration of solute in the two phases will be erratic.
6) Since solubility of acetic acid is greater in n-butanol than in water, K_d is greater than1. If any other solute is used, which is more soluble in water, K_d will be less than 1.