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Experiment 08

TITLE: Determination of Partition coefficient of acetic acid between n-butyl alcohol and water.

OBJECTIVE: To determine the partition coefficient of acetic acid between n-butyl alcohol and water.

THEORY/PRINCIPLES: In dilute solution at constant temperature a solute which exists in the same molecular species in two immiscible solvents will distribute itself between the two solvents in accordance with the PARTITION LAW.

The partition coefficient = k

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

where C_1 = concentration of acetic acid in water

C_2 = concentration of acetic acid in n-butyl alcohol

k is an equilibrium constant known as the partition coefficient. It is independent of the amount of solute taken, as well as the volume of solvent used.

k is the ratio of concentrations, and not the ratio of masses of solute.

The partition coefficient (k) is constant providing:

1) Temperature constant
2) Solvents are immiscible and do not react with each other.
3) The solute does not react, associate or dissociate in the solvents.

PROCEDURE:

1) Approximately 200 mL of distilled water was boiled in a beaker for ten minutes.
2) The CO_2 free water was poured into a flask, and the flask was stoppered lightly and cooled
3) About 70 mL of 2M acetic acid was placed in a 200 mL glass stoppered bottle and 50 mL of n-butyl alcohol was added to it.
4) The bottle was stoppered and its contents were shaken for at least a minute
5) The liquid layers were allowed to separate and the temperature of the mixture was recorded.
6) The pipette was rinsed by sucking up a little of the solution and then discarding it.
7) A 25 mL pipette was inserted into the flask and 25 mL aliquot of the upper alcohol layer was carefully withdrawn.
8) The solution was pipetted into a second glass stoppered bottle and approximately an equal volume of boiled distilled water was added.
9) The bottle was shaken thoroughly in order for acid to be transferred to the water layer
10) About 3 drops of phenolphthalein indicator was added to the contents of the bottle.
11) A clean, dry burette was filled with 1.0 M NaOH
12) The bottle was stoppered and the contents were titrated with 1.0 M NaOH, while being vigorously shaken. The titration was continued until a first permanent pink colour was observed.
13) The results obtained were recorded.
14) Another 25 mL pipette was rinsed with solution by pipetting a small volume of the lower aqueous layer and then discarding it.
15) 25 mL aliquot of the lower aqueous layer of the first bottle was pipetted into a flask
16) About 3 drops of phenolphthalein indicator was added to the solution in the flask.

17) The burette was refilled with NaOH
18) The contents of the flask was titrated with the NaOH and the results were recorded
19) About 25 mL of the fresh butanol and boiled distilled water was added to the original mixture which contained 50 mL n-butyl alcohol.
20) The procedure above (steps 1 through 18) was repeated for the new solution.

OBSERVATIONS:

When the phenolphthalein indicator was added to the solution in the flask it remained clear. On titration with the NaOH the solution changed colour from clear to a light pink colour.

RESULTS:

Temperature of mixture = 25^{o} C

1) *25 mL of water + 25 mL of upper layer – Titration with NaOH*

   Final Volume (mL) = 32.5 mL

   Initial Volume (mL) = 0.00 mL

   Volume used (mL) = 32.5 mL

2) *25 mL of lower layer – Titration with NaOH*

   Final Volume (mL) = 27.00 mL

   Initial Volume (mL) = 0.00 mL

   Volume used (mL) = 27.00 mL

Given Sample 2:

25 mL of upper layer + water

Final volume = 18.40 mL

Initial volume = 0.00 mL

Volume used = 18.40 mL

25mL of lower layer

Final Volume (mL) = 15.70 mL

Initial volume = 0.00 mL

Volume used = 15.70 mL

Table 1: Result of concentration and partition coefficicnet vlaues for water and alcohol

Alcohol Layer		Water Layer		Alkali for titration (mL)		$k = C_1/C_2$
Sample Removed (mL)	Fresh Alcohol added (mL)	Sample Removed (mL)	Water added (mL)	Water	Alcohol	
				C_1	C_2	
25	-	25	-	1.08	1.30	0.831
-	25	-	25			
25	-	25	-	0.628	0.736	0.853

DISCUSSION:

The values obtained for the partition coefficient, k were 0.831 and 0.853 respectively, a difference of 0.022. The small difference in values could be attributed to an experimental error/s, as well as the abnormal distribution of the acetic acid between the two solvents.

EXERCISES:

1) Solution containing 70 mL of 2M acetic acid and 50 mL of n-butyl alcohol.

   - Upper Layer – C_2

     1.0 M NaOH was used

     1000 mL contains 1.0 moles NaOH

     32.5 mL contains $\frac{1}{1000} \times 32.5 = 0.0325$ moles NaOH

     $NaOH + CH_3COOH \rightarrow CH_3COO^-Na^+ + H_2O$

     1 mole NaOH reacts with 1 mole CH_3COOH

     0.0325 moles NaOH reacts with 0.0325 moles CH_3COOH

     25 mL contains 0.0325 moles CH_3COOH

     1000 mL contains $\frac{0.0325}{25} \times 1000 = 1.3$ moles CH_3COOH

     therefore, C_2 concentration = 1.3 mol L^{-1}

- Lower Layer – C_1

  1.0 M NaOH was used

  1000 mL contains 1.0 moles NaOH

  27 mL contains $\frac{1.0}{1000} \times \frac{27}{1} = 0.027$ moles NaOH

  By the partition law acid must distribute itself equally between two phases,

  $NaOH + CH_3COOH \rightarrow CH_3COO^-Na^+ + H_2O$

  therefore, ratio is 1:1

  1 mole NaOH reacts with 1 mole CH_3COOH

  0.027 moles NaOH reacts with 0.027 moles of CH_3COOH

  25 mL contains 0.027 moles CH_3COOH

  1000 mL contains $\frac{0.027}{25} \times 1000 = 1.08$ moles

  therefore, C_1 concentration is 1.08 mol L^{-1}

  k = partition coefficient = $\frac{C_1}{C_2} = \frac{1.08}{1.3}$ = **0.831**

2) Solution #2 – Containing the remainder of solution 1 (70 mL acetic acid and 50 mL n – butyl alcohol), plus n-butanol (25 mL) and water.

- Upper Layer : C_2

  1.0 M NaOH was used

  1000 mL cointains 1.0 moles NaOH

  18.4 mL contains $\frac{1}{1000} \times \frac{18.4}{1}$ = 0.0184 moles NaOH

  $NaOH + CH_3COOH \rightarrow CH_3COO^-Na^+ + H_2O$

  1 mole NaOH reacts with 1 mole CH_3COOH

  0.0184 moles NaOH reacts with 0.0184 moles CH_3COOH

  25 mL contains 0.0184 moles CH_3COOH

  Therefore, C_2 concentration = 0.736 mol L^{-1}

- <u>Lower Layer:</u> C_1

  1.0 M NaOH was used

  1000 mL cointains 1.0 moles NaOH

  15.7 mL contains $\frac{1}{1000} \times 15.7$ = 0.0157 moles NaOH

By partition law, acid must distribute itself evenly between the two phases.

$NaOH + CH_3COOH \rightarrow CH_3COO^-Na^+ + H_2O$

therefore, ratio is 1:1

1 mole NaOH reacts with 1 mole CH_3COOH

0.0157 moles NaOH reacts with 0.0157 moles of CH_3COOH

25 mL contains 0.0157 moles of CH_3COOH

1000 mL contains $\frac{0.0157}{25} \times 1000 = 0.628$ moles CH_3COOH

therefore, C_1 = 0.628 mol L^{-1}

k = partition coefficient = $\frac{C_1}{C_2} = \frac{0.628}{0.736}$ = **<u>0.853</u>**