Experiment

Determination of equilibrium constant of the hydrolysis reaction of ethyl acetate with HCl

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Date: ………………. **Room Temperature: 28 ºC**

Objective

To determine the equilibrium constant of the hydrolysis reaction of ethyl acetate with HCl.

Requirements

(a) **Apparatus and Glassware:** Stoppered bottles, Burette, Pipettes, Beakers, Volumetric flask, Conical flask, etc.

(b) **Chemicals:**
- 0.5 M NaOH
- 0.3 M HCl
- Ethyl acetate
- Absolute ethanol
- Acetic acid
- Distilled Water
- Phenolphthalein indicator

1. Principle

The ester hydrolyses to give the acid and alcohol whereas an acid and an alcohol react to form back ester and water. At equilibrium, the two reactions proceed with equal rates. As the equilibrium state is reached very slowly, hydrochloric acid is used to catalyze the reaction and accelerate the equilibrium state to reach.

The equilibrium constant of the reaction

$$CH_3COOC_2H_5 + H_2O \rightleftharpoons CH_3COOH + C_2H_5OH$$

is given by:

$$K = \frac{C_{acid} \times C_{alcohol}}{C_{ester} \times C_{water}}$$

where *C*’s are the molar concentrations referred to the equilibrium state.

2. Solutions Preparation

2.1. 0.5 M NaOH in 1000 mL

$$w = \frac{\mathrm{M} \times \text{Molecular Weight} \times \text{Volume}}{1000}$$

$$w = \frac{0.5 \times 40 \times 1000}{1000} = 20.000 \text{ g}$$

Dissolve 20.000 g of NaOH in the 1000 mL volumetric flask with distilled water and make upto the mark with distilled water.

2.2. 3 M HCl in 100 mL

$$N_1V_1 = N_2V_2$$

$$11.2\ V_1 = 3 \times 100$$

$$V_1 = 26.78\ \text{mL}$$

Dilute 26.78 mL of concentrated HCl with distilled water in 100 mL volumetric flask.

3. Procedure

- Prepare the following mixtures in glass stoppered bottles numbered as 1 to 5.

Bottle No.	Volume of 3 M HCl mL	Volume of ethyl acetate mL	Volume of water mL	Volume of ethanol mL	Volume of acetic acid mL
1	5	0	5	0	0
2	5	5	0	0	0
3	5	4	1	0	0
4	5	4	0	1	0
5	5	4	0	0	1

- Stopper the bottles, shake and allow to stand for a couple of days so that equilibrium is established.
- Titrate the contents of each bottle with the standard sodium hydroxide solution using phenolphthalein as indicator.
- Also with the help of pipettes transfer 5 mL of 3 M HCl solution, 5 and 4 mL of ethyl acetate, 1 and 5 mL of water, 1 mL of ethanol, and 1 mL of acetic acid in separate accurately weighed weighing bottles. Weigh again weighing bottles with substance and determine the weights of each substance.

4. Observation Table

Titration of contents of each bottle with standard 0.5 M NaOH

S. No.	Bottle No.	Volume of 0.5 M NaOH used in mL
1	1	$V_1 =$ 36.0
2	2	$V_2 =$ 99.0
3	3	$V_3 =$ 98.5
4	4	$V_4 =$ 83.8
5	5	$V_5 =$ 118.1

5. Calculations

The initial weights of ester in bottles 2 to 5, water in bottle 3, absolute ethanol in bottle 4, and acetic acid in bottle 5 are known from the direct weighing.

- Weight of 5 mL 3 M HCl : 5.528 g
- Weight of 4 mL ethyl acetate: 3.695 g (0.042 mol)
- Weight of 5 mL ethyl acetate: 4.576 g (0.052 mol)
- Weight of 1 mL water : 0.931 g
- Weight of 5 mL water : 5.087 g
- Weight of 1 mL ethanol : 0.771 g (0.017 mol)
- Weight of 1 mL acetic acid : 1.043 g (0.017 mol)

Weight of HCl present in 5 mL of 3 M solution

$= 0.5 \times V_1 \times 36.46 \times 10^{-3}$ g

$= 0.5 \times 36 \times 36.46 \times 10^{-3}$ g = 0.655 g = 0.018 mol

Therefore, weight of water in 5 mL of 3 M HCl solution

= weight of solution – weight of HCl

= 5.528 – 0.6552 g = 4.8728 g = 0.271 mol

Hence, weight of water initially present in each bottle

= weight of water placed + weight of water in 5 mL of 3 M HCl.

Weight of water in the

Bottle No. 1: 5.087 g + 4.873 g = 9.960 g = 0.553 mol

Bottle No. 2: 0 g + 4.873 g = 4.873 g = 0.271 mol

Bottle No. 3: 0.931 g + 4.873 g = 5.804 g = 0.322 mol

Bottle No. 4: 0 g + 4.873 g = 4.873 g = 0.271 mol

Bottle No. 5: 0 g + 4.873 g = 4.873 g = 0.271 mol

The amount of acetic acid formed due to hydrolysis of ester in the bottles 2 to 4 can be calculated by subtraction the titre of NaOH solution for bottle 1 from those for bottles 2 to 5 as following:

Bottle No. 2: $\dfrac{(V_2 - V_1) \times 0.5 \times 60}{1000} = \dfrac{(99 - 36) \times 0.5 \times 60}{1000} = 1.890\,\text{g} = 0.032\,\text{mol}$

Bottle No. 3: $\frac{(V_3 - V_1)\times 0.5\times 60}{1000} = \frac{(98.5-36)\times 0.5\times 60}{1000} = 1.875\text{ g} = 0.031\text{ mol}$

Bottle No. 4: $\frac{(V_4 - V_1)\times 0.5\times 60}{1000} = \frac{(83.8-36)\times 0.5\times 60}{1000} = 1.434\text{ g} = 0.024\text{ mol}$

Similarly, weight of acetic acid present in bottle 5

Bottle No. 5: $\frac{(V_5 - V_1)\times 0.5\times 60}{1000} = \frac{(118.1-36)\times 0.5\times 60}{1000} = 2.463\text{ g} = 0.041\text{ mol}$

Hence, weight of acetic acid formed in bottle 5

= 2.463 g – 1.043 g = 1.420 g = 0.024 mol

Number of moles of each substance in the initial mixture and then the final number at the equilibrium in bottles 2 to 5 can be calculated by knowing the chemical reaction taking place as that **for each mole acetic acid, 1 mole of ethanol is produced and 1 mole each of water and ester disappear**. Assuming the final volume of the resulting mixture to be 10 mL, the concentration (mol L^{-1}) of each substance at equilibrium can be calculated.

Then, *K* for the systems in bottles 2 to 5 can be calculated by using the equation:

$$K = \frac{C_{acid} \times C_{alcohol}}{C_{ester} \times C_{water}}$$

Bottle No.	State of reaction mixture	Number of moles of substance					$K = \frac{C_{acid} \times C_{alcohol}}{C_{ester} \times C_{water}}$
		C_{HCl}	C_{ester}	C_{water}	C_{acid}	$C_{alcohol}$	
2	Initial Mixture	0.018	0.052	0.271	0.000	0.000	
	At equilibrium	0.018	0.020	0.239	0.032	0.032	0.214
3	Initial Mixture	0.018	0.042	0.322	0.000	0.000	
	At equilibrium	0.018	0.011	0.291	0.031	0.031	0.300
4	Initial Mixture	0.018	0.042	0.271	0.000	0.017	
	At equilibrium	0.018	0.018	0.247	0.024	0.041	0.221
5	Initial Mixture	0.018	0.042	0.271	0.017	0.000	
	At equilibrium	0.018	0.018	0.247	0.041	0.024	0.221
						Average *K*	0.239

6. Results

The equilibrium constant *K* of the hydrolysis of ethyl acetate with HCl is found to be 0.239 under the experimental condition.

7. Precautions

(i) Weighing of substance should be done carefully.
(ii) Burette reading should be taken carefully.

8. Further Reading

(i) Study the theory and calculation of the equilibrium constant.

(ii) *Principle of Physical Chemistry*, B. R. Puri, L. R. Sharma, and Pathania, Vishal Publishing Co. Jalandhar.

(iii) *Advanced Practical Physical Chemistry*, J. B. Yadav, Krishna Prakashan Media (P) Ltd. Meerut.