Determination of reaction rate, order and molecularity of hydrolysis of ethyl acetate

(KINETICS OF ACID CATALYSED HYDROLYSIS OF ETHYL ACETATE)

Introduction:

Chemical reactions and reaction rate

Chemical kinetics is the part of physical chemistry that studies reaction rates. The reaction rate for a reactant or product in a particular reaction is intuitively defined as how fast a reaction takes place. Through the study of chemical kinetics, one can reasonably get an idea as to how to alter the reaction conditions and improve the reaction rate, which is necessary to increase the production of chemical products in the industry perspective. It will also help us to learn how to suppress or slow down unwanted side reactions.

For a generic reaction:

$$A + B \rightarrow C$$

the simple rate equation is of the form:

$$v = k c_A^a c_B^b$$

The concentration is usually in mol cm^{-3} and *k* is the reaction rate coefficient or rate constant. Although it is not really a constant, because it includes everything that affects reaction rate outside concentration: mainly temperature, ionic strength, surface area of the adsorbent or light irradiation (in the case of photochemical reactions).

The exponents a and b are called reaction orders and depend on the reaction mechanism. The stoichiometric coefficients and reaction orders are very often equal, but only in one step reactions.

Acid-Catalysed Hydrolysis of Methyl Esters

The hydrolysis of ester is catalyzed by either an acid or base. This can be achieved in a number of ways. The most common method is to use a Lewis acid or Bronsted acid to form a positively charged intermediate that is far more reactive and even mild nucleophiles such as water will react.

Expt. No.: **Date:**

Experiment	**Determination of Reaction Rate, Order and Molecularity of Hydrolysis of Ethyl Acetate**
Problem definition	Hydrolysis of ethyl acetate in acid medium to produce acetic acid and ethyl alcohol
Methodology	Following chemical kinetics of the reaction through acid-base titrimetric analysis
Solution	The formation of acetic acid in the hydrolysis of ethyl acetate will be followed by a titration with NaOH at different time intervals.
Student learning outcomes	Students will be able to calculate the rate constant of ester hydrolysis through (pseudo) first order kinetics.

Aim:

To determine the rate constant of the hydrolysis of ethyl acetate using an acid as a catalyst and to understand the order and molecularity of the reaction

Principle:

The hydrolysis of an ester occurs according to the equation:

$$CH_3COOC_2H_5 + H_2O \xrightarrow{H^+} CH_3COOH + C_2H_5OH$$

The following rate equation is applicable to the above reaction:

$$\text{Rate} \ \alpha \ [\text{Ester}]\,[H_2O]$$

Since $[H_2O]$ remains constant,

$$\text{Rate} = \frac{-dc}{dt} = k'_1\,[Ester]$$

where ‘c’ represents concentration of the ester at any time t; k'_1 is the specific velocity constant. As the reaction progresses, the accumulation of acetic acid increases. Drawing a known volume of the reaction mixture at known regular intervals of time and titrating it against standard sodium hydroxide solution will indicate the increase in acetic acid presence.

The acid hydrolysis of ester is a first-order bimolecular reaction, and the reaction follows pseudo first order kinetics. This is because the amount of water is in large excess so that its concentration does not change significantly to alter the reaction rate. The reaction goes practically to completion (the equilibrium shifts to the right) and the rate is first order with respect to the ester.

Requirements:

Reagents and solutions: Ethyl acetate, 0.5N HCl, 0.2N NaOH, Phenolphthalein indicator, Ice-cubes

Apparatus: Burette 50mL, Pipettes-5mL, 10mL, Conical flasks, Wash bottle Reaction bottle 250mL.

Procedure:

Exactly 100 mL of 0.5N-hydrochloric acid solution are taken in a 250 mL clean reaction bottle and exactly 5 mL of the ester is added to it. Zero time is noted when half the volume of ester solution in the pipette is transferred into the reaction bottle. After thorough mixing, immediately 10 mL of the solution is pipetted out into a clean conical flask containing ice-cubes. It is then titrated against 0.2 N sodium hydroxide solution from the burette using phenolphthalein indicator. The end-point is the first appearance of a pale permanent pink colour. The same volumes of the reaction mixture are withdrawn at regular intervals, say 10 minutes and is titrated against sodium hydroxide solution. The reaction is allowed to go to completion by keeping the reaction mixture over a hot water bath for about 90 minutes. The final reading is then noted.

Calculations:

Let V_0 be the volume of alkali used at zero time and $V_{t.}$ be the volume of alkali used after the time 't' seconds. Let V_∞ be the reading when the reaction is completed. Concentrations of the ester at various time intervals are expressed in terms of volume of NaOH solution.

a = initial concentration of ester = $(V_\alpha - V_o)$

(a-x) = concentration of ester at any time 't' = $(V_\alpha - V_O) - (V_t - V_o)$

= $(V_\alpha - V_o - V_t + Vo)$

= $(V_\alpha - V_t)$

The specific rate constant of the reactions is given by

$$k_1' = \frac{2.303}{t} \log \left(\frac{a}{a-x} \right)$$

$$k_1' = \frac{2.303}{t} \log \left(\frac{V_\alpha - V_o}{V_\alpha - V_t} \right)$$

$$k_1' = \text{Slope x } 2.303$$

The rate constant values are calculated at different time intervals which should nearly be the same. A graph is drawn between **log(V_α - V_t)** and time '**t**'. From the slope of the plot, the rate constant is calculated, and it is compared with the experimental value.

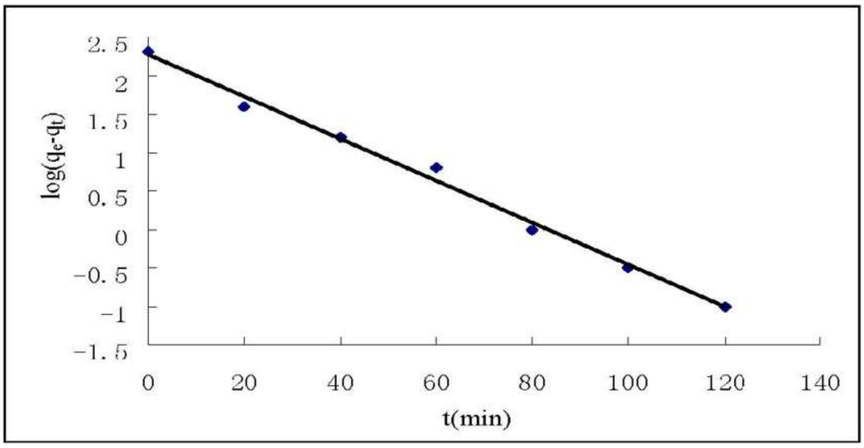

Table-1:

S. No.	Time min	Volume of NaOH mL	$(V_\infty - V_t)$ mL	$log\ (V_\infty - V_t)$	$K = \frac{2.303}{t}\log\frac{(V_\infty - V_0)}{(V_\infty - V_t)}$ min^{-1}
1	0				
2	10				
3	20				
4	30				
5	40				
6	∞				

Results:

The Rate Constant for the hydrolysis of an ester from

1. Calculated value =
2. Graphical value =
3. Molecularity of the reaction =
4. Order of the reaction =

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