



Kinetic and Solvent Polarity Investigation of Alkaline Hydrolysis of Propyl Caprate in Aqueous Solvent of Acetone

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KEYWORDS

Activation energy, Propyl caprate, Dielectric constant, water-acetone, solvent effect, Hydrolysis

ABSTRACT:

Introduction: The rate of a chemical reaction is significantly influenced not only by the nature of the reactants and products but also by the solvent medium in which the reaction takes place. This phenomenon is known as the kinetic solvent effect. Solvents affect reaction kinetics through several factors such as polarity, dielectric constant, solvation ability, hydrogen bonding, and viscosity. These interactions can stabilize or destabilize the transition state relative to the reactants, thereby either accelerating or retarding the reaction

Objectives: The objective of the research is to determine the medicinal potential of propyl caprate ester. This compound is used in cosmetics and personal care industry as emollient which help to soften and moisture the skin. It is also used in pharmaceutical, serving as recipient to improve the stability and bioavailability of active ingredients

Methods: The chemical used are Merck grade and acetone are purified by standard procedure. The ester has been taken and thermo stated for 30 minutes in a conical flask. In a few minutes, 0.5 ml of ester that had been withdrawn and added to organic solvent Now 10 ml of aliquot was withdrawn and put into a flask in which N/10 HCl has been placed already. Now titrate the solution by adding N/10 NaOH from the burette using phenolphthalein as indicator. Similarly again pipette out 5ml of reaction mixture after 5 minutes and repeated the procedure. Repeat the above procedure by withdrawing 5ml of reaction mixture after 15,30,45,60 minute

Results: On the basis of find the different physical and chemical properties of this ester. Specific rate, activation energy and different thermodynamic parameters are reported.

Conclusions: The hydrolysis of the propyl caprate in water- acetone has been carried out at different composition and different temperature. With increase of solvent fraction, the rate has been found to be decrease which is possibly due to dielectric values and also due to polarity of less polar solvent of the reaction media

1. Introduction

The rate of a chemical reaction is significantly influenced not only by the nature of the reactants and products but also by the solvent medium in which the reaction takes place. This phenomenon is known as the kinetic solvent effect. Solvents affect reaction kinetics through several factors such as polarity, dielectric constant, solvation ability, hydrogen bonding, and viscosity. These interactions can stabilize or destabilize the transition state relative to the reactants, thereby either accelerating or retarding the reaction. In many studies Alaa.omer,¹ Reichardt C,² Seliverstove T. S.³, Magda F Fathalla⁴, Bano Arjuman⁵, Younes Ghalandarzehi⁶, Shashibata Kundo⁷ has been published in field of kinetics reaction of ester hydrolysis for the

calculation of specific rate, mechanism and other physical properties but no satisfactory result has been found particularly propyl caprate ester in aqueous mixture of acetone. The solvent effect has been very closely related to solvent solute interaction which is become more complex when it is mixed with water in compare to pure solvent. Binary solvents are used because they allow fine-tuning of physicochemical properties like polarity, dielectric constant, and hydrogen-bonding ability. Such mixtures often exhibit non-ideal behaviour, leading to unique solvent-solute interactions that cannot be explained simply as the sum of the properties of the two pure solvents. In this report the solvent effect for the hydrolysis of propyl caprate has been noticed. The molecular formula of propyl



caprate is $C_{13}H_{16}O_2$. Its structure is linear as $CH_3-(CH_2)_8-C(=O)-O-CH_2-CH_3$. Acetone itself does not readily react with ester under neutral aqueous condition but in water, ester linkage in propyl caprate can undergoes hydrolysis. In basic medium (specification), giving deconate salt and propanol. Propyl caprate has unique properties hence it is used for various applications. This compound is used in cosmetics and personal care industry as emollient which help to soften and moisture the skin. It is also used in pharmaceutical, serving as recipient to improve the stability and bioavailability of active ingredients.

2. Objectives

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3. Methods

The chemical used are Merck grade and acetone are purified by standard procedure. The ester has been taken and thermo stated for 30 minutes in a conical flask. In a few minutes, 0.5 ml of ester that had been withdrawn and added to organic solvent Now 10 ml of aliquot was withdrawn and put into a flask in which N/10 HCl has been placed already. Now titrate the solution by adding N/10 NaOH from the burette using phenolphthalein as indicator. Similarly again pipette out 5ml of reaction mixture after 5 minutes and repeated the procedure. Repeat the above procedure by withdrawing 5ml of reaction mixture after 15,30,45,60 minute. This give the values of different timing (V_t) The V_∞ reading indicate the completion of of hydrolysis calculated after 24 hours in same procedure. Specific rate has been calculated which is kept in Table-1

4. Results

On the basis of experimental result it has been found that the specific rate of the reaction decreases with increase of temperature. Iso-composition activation energy and dielectric activation energy has been calculated on the basis of Arrhenius plots which show polarity of solvent at initial and transition state.

5. Discussion

Rate constant:

The solvent effect plays a important role in controlling the rate of a chemical reaction. The medium in which a reaction takes place can stabilize or destabilize reactants, transition states, or intermediates, and this directly influences the rate constant. According to the calculated rate constant result shown in Table 1, the rate constant values in the solvolysis reaction of propyl caprate decrease as the amount of acetone in the reaction media

Increases. The degree of rate depletion

Table 2. Log k values with different mole %

mole%, as depicted in fig. 1, is slower as the temperature rises, according to a plot of the logk values against the mole% of organic co-solvent. However, the depletion of rate is possibly due to decrease in dielectric constant values of the reaction media or polarity of less polar solvent

The two depletion factors mentioned above are both oppressive and in good agreement with Hughes and Ingold's⁸idea. This theory states that when there is concentration or contraction of charges on the transition state, an increase in the dielectric constant values of the reaction medium causes the rate to increase; when there is diffusion or destruction of charges on the transition state, the rate decreases. In this report the rate of reaction has been found to be decreases with increase proportion of solvent (acetone) which is good agreement with earlier report of Elsemongy⁹, Singh. Lallan¹⁰ and most recent report of Kumar¹¹. However, the partial dielectric constant effect and the salvation change occurring in the reaction media are the causes of the decrease in the rate constant values.

TABLE 1. Specific rate constant k $\times 10^3$ (dm)³/mole/mint]

Temp in °C	% of Acetone				
	30%	40%	50%	60%	70%
20°C	48.30	44.05	40.08	36.30	33.26
25°C	102.56	89.12	87.29	68.70	60.25
30°C	218.27	191.42	159.58	126.18	112.20
35°C	440.55	363.91	294.44	239.88	184.92
40°C	889.20	706.31	571.47	423.64	337.28



Table 2. Log k values with different mole %

Temp in °C	Mole %	3 + Log k				
		20 ^o C	25 ^o C	30 ^o C	35 ^o C	40 ^o C
30%	9.56	1.68 4	2.01 1	2.33 9	2.64 4	2.94 9
40%	14.11	1.64 4	1.95 0	2.28 2	2.56 1	2.84 9
50%	19.77	1.60 3	1.94 1	2.20 3	2.46 9	2.75 7
60%	26.99	1.56 0	1.83 7	2.10 1	2.38 0	2.62 7
70%	36.45	1.52 2	1.78 0	2.05 0	2.26 7	2.52 8

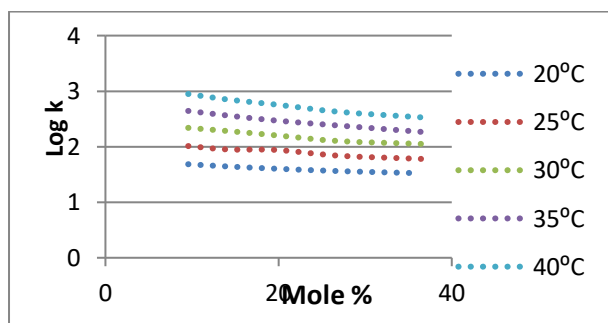


Fig. 1. plots of log k with mole %.

Effect of solvent on activation Energy (Ec)

and rate of reaction:

Water is a highly polar protic solvent ($D \approx 80$ at 25 °C). It stabilizes charged or polar transition states more than non polar solvents. As a result, the activation energy (E_c) decreases if the reaction involves formation of polar/ionic intermediates or transition states. By the observation of data mention in Table-4 (which has been calculated with plots of logk against $10^3/T$), it has been found that the iso composition activation energy goes on decreasing from 113.25 to 92.95 kJ/mole with increasing proportion of acetone from 30 to 70% (v/v) The depletion of activation energy infer that transition state is solvated and initial state is desolvated. This fact is also supported because the values of enthalpy of activation (ΔH^*) and entropy of activation (ΔS^*) also decreases with increasing proportion of acetone (Elsomony M. M⁹, Singh Lallan¹², Sharma Sangita¹³

Table 3. Values logk at different temperature

Temperature in °C	10 ³ /T	3 + Logk				
		30%	40%	50%	60%	70%
20°C	3.413	1.684	2.011	2.339	2.644	2.949
25°C	3.356	1.644	1.950	2.282	2.561	2.849
30°C	3.300	1.603	1.941	2.203	2.469	2.757
35°C	3.247	1.560	1.837	2.101	2.380	2.627
40°C	3.195	1.522	1.780	2.050	2.267	2.528

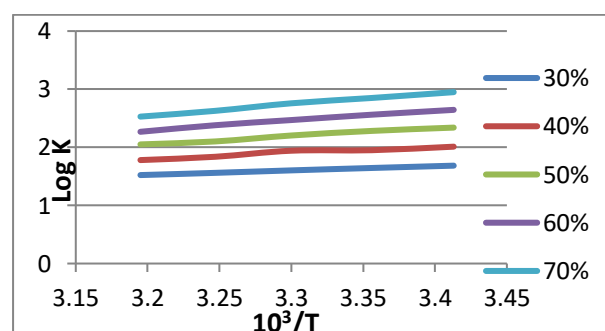
Fig. 2. plots of log k with $10^3/T$

Table 4. Values of Energy of activation at different solvent composition.

% of E_c	30%	40%	50%	60%	70%
E_{exp} in KJ/mole	113.25	110.88	102.77	99.44	92.95

Table 5. the values logk_D at Constant D

Temperat ure in °C	10 ³ / T	D=4 0	D=4 5	D=5 0	D=5 5	D=6 0
20°C	3.41 2	1.53 1	1.56 0	1.59 0	1.63 5	1.66 0
25°C	3.35 5	1.81 5	1.86 0	1.90 5	1.95 0	1.99 0
30°C	3.30 0	2.05 5	2.12 0	2.18 0	2.24 5	2.31 0
35°C	3.24 7	2.31 9	2.40 0	2.48 0	2.57 0	2.66 0
40°C	3.19	2.57	2.67	2.77	2.87	2.97



	5	5	5	5	5	0
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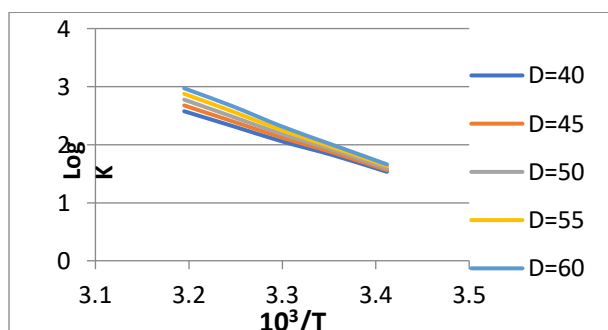


Fig 3. Plot of $\log k_d$ with $10^3/T$

Rate of reaction and dielectric Effect:

The reaction rate of many reactions is strongly influenced by the dielectric constant (D) of the solvent. The dielectric constant is a measure of how well a solvent can stabilize charges or dipoles. Its effect on rate depends on the nature of the reaction—particularly the type of transition state formed. With view of minimise the dielectric effect, the iso-dielectric constant energy has been evaluated with the slope of Arrhenius plot $\log k_D$ against D and summerised in Table-6, it has been observed that there is enhancement of (E_D) values with increasing D which good agreemet of earlier views of Elsemongy M. M⁹ and Wolfoard(Wolfod . R.K¹⁶, AKLOF G¹⁷. A group of researchers. Elsemongy M. M⁹. Varma. D. K¹⁴. Namaishanker Sudhansu¹⁵ also support this view.(Singh Anil Kr¹⁸, Rai H. C, 2018¹⁹

TABLE: 6. DIELECTRIC ACTIVATION ENERGY(E_D) AT CONSTSNT D

Dielectric constant(D)	D=40	D=45	D=50	D=55	D=60
E_D in kJ/mole	93.31	94.86	101.83	104.97	111.17

Conclusions

The hydrolysis of the propyl caprate in water- acetone has been carried out at different composition and different temperature. With increase of solvent fraction, the rate has been found to be decrease which is possibly due to dielectric values and also due to polarity of less polar solvent of the reaction media. The isocomposition activation energy and dielectric activation energy has been calculated by Arrhenious

plots which shows solvation and desolvation effect of initial and transition state Thermo dynamic activation parameter has been also been calculated to undesand the clear mechanism of the reaction.

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