

Investigation of Solvent Polarity and dielectric constant effect on Alkaline Hydrolysis of Propyl Caprate in Aqueous Solvent of Acetone

Anil Kumar Singh

Department of Chemistry, Faculty of Engineering, Teerthanker Mahaveer University, Moradabad, 244001, Uttar Pradesh, India

Email: dr.anilkumarsingh2009@gmail.com

Received:
02/10/2025
Revised:
31/10/2025
Accepted:
08/11/2025
Published:
15/11/2025

ABSTRACT

The solvent effect of aquo-dipolar aprotic solvent system for the base catalyzed propyl caprate has been studied in water-acetone of various composition at different temperature range (20 to 400 C). With gradual Addition of organic co-solvent the rate has been decreasing which have been explain in term of initial and transition state. Solvation and desolvation are explained in term of iso activation energy and iso- dielectric activation energy. The influence of solvents on rate as well as on mechanism has been studies in relation to the idea of solvation. Wynne-jones and Eyring equation has been used to calculate the thermodynamic activation parameter. Iso-kinetic temperature has also been calculated.

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

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,2025),(Reichardt C,2003),(Seliverstov T. S.,2020),(Magda F Fathalla,2019),(Bano Arjuman,2017),(Younes Ghalandarzahi,2023),(Shashibata Kundo,2022) 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 behavior, 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 C₁₃H₂₆O₂. Its structure is linear as CH₃-(CH₂)₈-C(=O)-O-CH₂-CH₃. 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.

EXPERIMENTAL

Material and 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 (Vt) The V_∞ reading indicate the completion of of hydrolysis calculated after 24 hours in same procedure. Specific rate has been calculated which is kepted in Table-1

RESULTS AND 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 with mole%, as depicted in fig. 1, is slower as the temperature rises,

How to cite: Anil Kumar Singh, Investigation of Solvent Polarity and dielectric constant effect on Alkaline Hydrolysis of Propyl Caprate in Aqueous Solvent of Acetone. *Advances in Consumer Research*. 2025;2(5):1533–1537.

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's (Hughes E.D., 2035) idea. 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 Elsemongy (Elsemongy M. M., 2025), Singh & Jha (Singh, Lallan, 1981) and most recent report of Kumar (Kumar, 2025). 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 $k \times 10^3 (\text{dm}^3/\text{mole}/\text{mint})$

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

Table 2. Log k values with different mole %

Temp in OC	Mole%	3 + Log k				
		20OC	25OC	30OC	35OC	40OC
30%	9.56	1.684	2.011	2.339	2.644	2.949
40%	14.11	1.644	1.950	2.282	2.561	2.849
50%	19.77	1.603	1.941	2.203	2.469	2.757
60%	26.99	1.560	1.837	2.101	2.380	2.627
70%	36.45	1.522	1.780	2.050	2.267	2.528

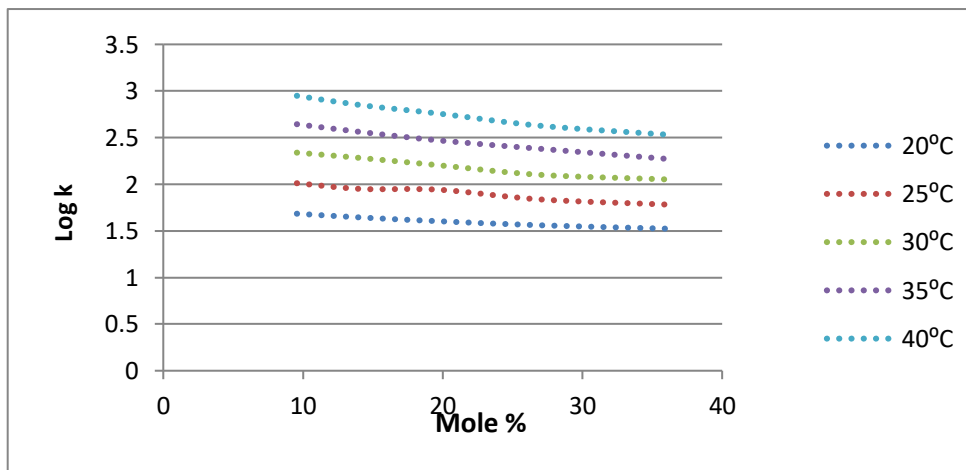


Fig. 1. plots of logk with mole %.

Effect of solvent on activation Energy (E_c) 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 $\log k$ against $103/T$), 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 ($\Delta H^\ddagger$) and entropy of activation ($\Delta S^\ddagger$) also decreases with increasing proportion of acetone (Elsemongy M. M., 1975) (Singh Lallan, 1984) (Sharma Sangita, 2013).

Table 3. Values logk at different temperature

Temperature in OC	103/T	3 + Logk				
		30%	40%	50%	60%	70%
20OC	3.413	1.684	2.011	2.339	2.644	2.949
25OC	3.356	1.644	1.950	2.282	2.561	2.849
30OC	3.300	1.603	1.941	2.203	2.469	2.757
35OC	3.247	1.560	1.837	2.101	2.380	2.627
40OC	3.195	1.522	1.780	2.050	2.267	2.528

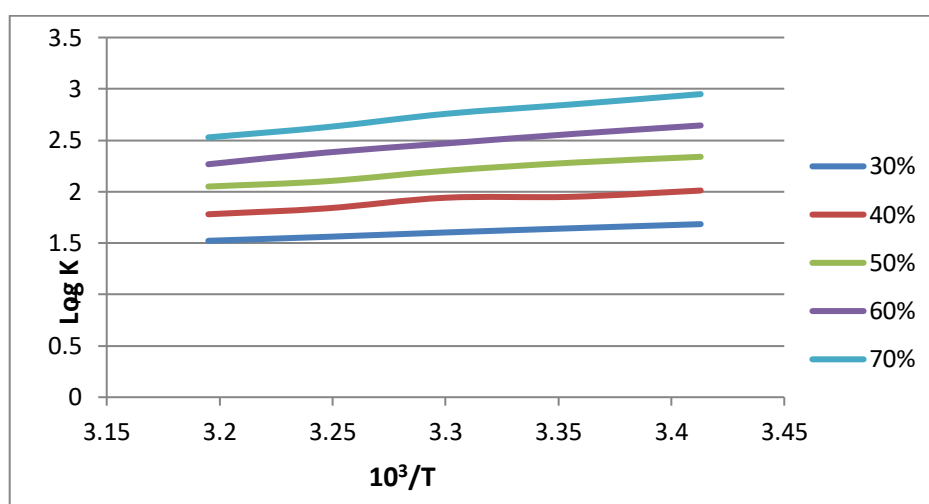


Fig. 2. plots of log k with 103/T

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

% of Ec	30%	40%	50%	60%	70%
Eexp in KJ/mole	113.25	110.88	102.77	99.44	92.95

Table 5. the values logkD at Constant D

Temperature in OC	103/T	D=40	D=45	D=50	D=55	D=60
20OC	3.412	1.531	1.560	1.590	1.635	1.660
25OC	3.355	1.815	1.860	1.905	1.950	1.990
30OC	3.300	2.055	2.120	2.180	2.245	2.310
35OC	3.247	2.319	2.400	2.480	2.570	2.660
40OC	3.195	2.575	2.675	2.775	2.875	2.970

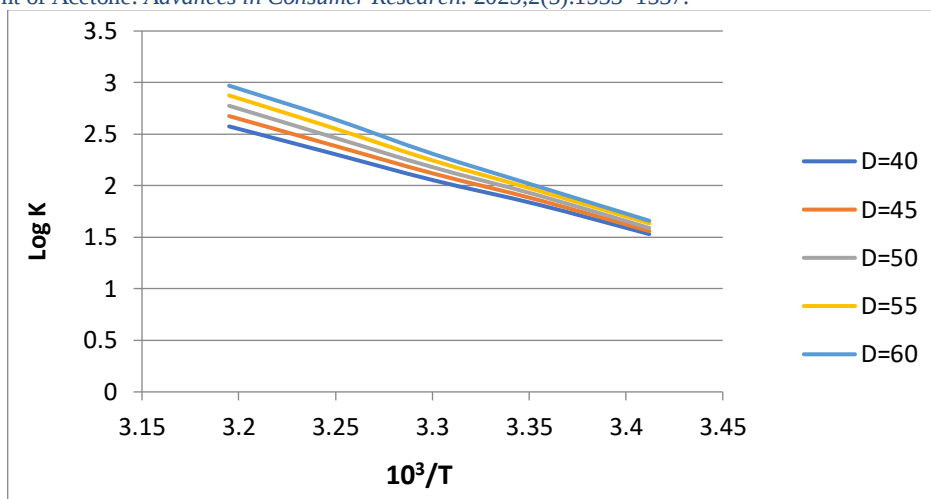


Fig 3. Plot of log kd with 103/T

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 Arrhenious plot $\log k_D$ against D and summerised in Table-6, it has been observed that there is enhancement of (ED) values with increasing D which good agreemet of earlier views of (Elsemongy M. M,2075) and Wolfoard(Wolfod . R.K, 1964),(AKLOF G, 1932). A group of researchers. (Elsemongy M. M,2075),(Varma. D. K,2023),(Namaishanker Sudhansu,2020), also support this view.(Singh Anil Kr,2021),(Rai H. C,2018)

Table: 6. Dielectrric activation energy(ed) at constnt d

Dielectric constant(D)	D=40	D=45	D=50	D=55	D=60
ED 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 solvetion 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.

REFERENCES

1. Alaa.Omer, Faraha.rabh.Shawkyelshazly, Magdaf. Fathalla, Kinetic and mechanism for the reaction of 5-Nitroisatin with Mor pholine in water-methanol and water-Acetoneitrile mixed solvent” J of Solution chemistry 54, 2025,pp263-285, DOI: 10.1007/s10953-024-01410-7
2. Reichardt C. Solvent and Solvent Effects in Organic Chemistry, 3rd edn, ,Wiley-VCH, Weinheim..(2003). DOI:10.1002/3527601791
3. Seliverstove T. S., M.A. Kushner& L. G. Matusevich,. Kinetics and mechanism of hydrolysis of Benzyl Ether bond in aqueous- organic media.Russian J of Physical Chemistry A., , Vol-94, 2020,pp310-316
4. Magda F Fathalla,Yassir R. Elmarassi.The reaction of 2-chloroquinoxaline with piperidine in DMSO- H2O and DMF- H2O mixture. Kinetic and solvent effect Journal of solution chemistry.. Vol. 48: 2019.pp1287-1308.
5. Bano Arjuman, AK Singh, A kinetics study of dipolar protic solvent in alkaline hydrolysis of ethyl Nicotinate in water-ethanol media- A Solvent effect Journal of Ultra Chemistry, 13(6), 2017,pp145-150.
<http://dx.doi.org/10.22147/juc/130603>
6. Kundo Younes, Ghalandarzehi, Halime Kord-Tamndani, Effect of solvents on kinetics and mechanistic investigation of highly substituted piperidines: Spectrometric Approach Asian Journal of Green Chemistry. 7, 2023,pp70-84,
7. Shashibata, Manish Kumar Rai, Ramsingh Kurrey, Joyce. Rai Kinetic study of solvent effect on the hydrolysis of mono 3,5dimethylaniline phosphate Rai Journal of Ravishanker University, vol- 35,issue-2, 2022.pp
8. Hughes E.D., C.K Ingold. Structure and mechanism of organic chemistry Journal of the Chemical Society (Resumed). 1935 pp244-255.
9. Elsemongy M. M., Abu Elamayaan M. S. and Moussa. M.N.H., Kinetic of hydrolysis of Acetone

- How to cite: Anil Kumar Singh, Investigation of Solvent Polarity and dielectric constant effect on Alkaline Hydrolysis of Propyl Caprate in Aqueous Solvent of Acetone. *Advances in Consumer Research*. 2025;2(5):1533–1537.
- in dioxane-water mixture. *Z. Physik. Chem*(New Folge,95, 1975)p251,
 10. Singh. Lallan, Gupta AK . RT Singh, Indian Chem. Soc. 58, 1981,pp966-969,
 11. Kumar Dr. Rajesh, Solvent effect on specific rate constant by the addition of ZnO- nanoparticles in alkali catalyzed hydrolysis of ethylnicotinate International Journal of Latest Technology in Engineering Management &Applied Science. vol 14(4), 2025, pp745-749.
 12. Singh Lallan, Gupta AK . Singh RT , Varma D.K., Jha RC . Effect of DMSO on kinetics behaviour of alkaline Catalysed hydrolysis of methyl salicylate J. Reaction Kinetic Catalyst &letters. Vol-24 ,No1-2,. 1984,Pp161-165.
 13. Sharma Sangita Jayesh Ramani, JasminBhalodia and Bjal Vyas,. Kinetic study of specific base catalysed hydrolysis of Ethyl Acrylate in water-Ethanol binary system” Russian Journal of physical chemistry A. Vol-87, NO-3, 2013, PP730-736,
 14. Varma. D. K. ,Rajesh Kumar, Parhalad Kumar,Vivek Kumar and Shalini Kumari, International Journal of Current Science.Vol-issue-2,2023,pp930-937
 15. Namaishanker Sudhansu, Kinetic studies of the solvent effect of aquo- DMSO solvent systems on the extensive thermodynamic properties of acid catalysed solvolysis of higher mathanoate Schlor Research Journal of Interdisciplinary Studies.vol6/612020,pp,14348-14355
 16. .Wolfod . R.K, “Kinetic of acid hydrolysis of acetal in dimethyl sulfoxide-water solvents at 150,250 and 350”J of physical chemistry. 68, 1964,pp3392-3398.
 17. AKLOF G., Dielectric Constants Of Some Organic Solvent-Water Mixtures At Various Temperatur J. Am. Chem. Soc 54 11:, 1932,pp4125–4139,
 18. . Singh Anil Kr., Kinetics Investigation of Solvent polarity on Reaction Rate for Solvolysis of Ethyl Caprylate Ester in Binary Solvent System. In Proceedings of 10th International conference on system modeling and advance in research trend.(IEEE) 10-11DEC, 2021,pp676-679,
 19. . Rai H. C ., PriyankaPria, Kumari Sweetiand Savita. Solvent effect Alkali catalysed hydrolysis of ethyl picolinate in aquo-acetone. Journal of Emerging Technologies Innovative Research (JETIR) VOL. 5, Issue 7, 2018, pp1139-1141