Investigating the Effect of Temperature on the Rate Constant in the Hydrolysis of Ethyl Acetate

1 Introduction

Hydrolysis is a chemical decomposition reaction involving a molecule of water breaking down the bonds of a compound. Typically, a titration would be performed for this investigation. However, I wanted to take an unconventional approach and examine whether the outcomes of my own methodology for ester hydrolysis would be as effective. Therefore, I will be exploring the effect of varying temperatures on the rate constant in the hydrolysis of ethyl acetate, as well as calculating the activation energy to verify the accuracy of this investigation.

2 Research Question

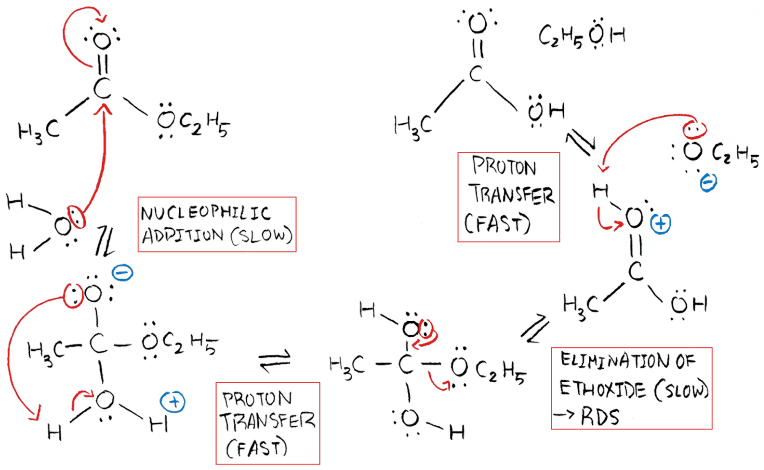
How does the rate constant in the hydrolysis of ethyl acetate vary with temperature at 30°C, 40°C, 50°C, 60°C, and 70°C?

3 Background Information

By mixing an ester with water, a reverse esterification reaction occurs: hydrolysis produces a carboxylic acid and an alcohol as indicated by the reaction below. Specifically, ethyl acetate (ethyl ethanoate) and water produce acetic acid (ethanoic acid) and ethanol:

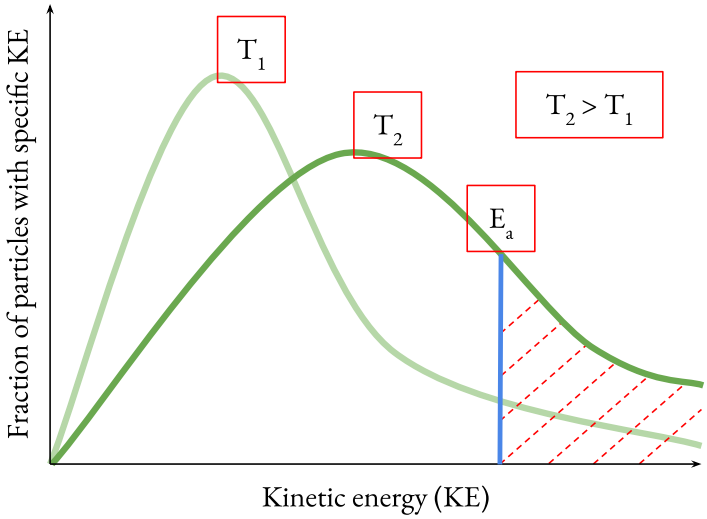
$$CH_3COOCH_2CH_{3(l)} + H_2O_{(l)} \rightleftharpoons CH_3COOH_{(aq)} + C_2H_5OH_{(aq)}$$

Figure 1: Mechanism of uncatalyzed ethyl acetate hydrolysis



The rate of hydrolysis of ethyl acetate is known to be second-order. For visualization, I drew the mechanism for the reaction[1] (see Figure 1). It begins with a nucleophilic addition to the carbonyl group's polarized π bond, forming a zwitterionic intermediate: it contains both positive and negative charges. Then, a proton transfer occurs, where the intermediate forms a neutral species. The positively charged O atom undergoes a proton dissociation via heterolysis, producing a coordinate covalent bond with the negatively charged O atom. Subsequently, the rate-determining step (RDS) involves breaking the C–O bond, which releases ethoxide as the leaving group, whilst a protonated carboxyl group remains. Lastly, a second proton transfer occurs from the protonated carboxyl group to the ethoxide group, which forms the products of acetic acid and ethanol.

Figure 2: Maxwell-Boltzmann distribution at different temperatures



Next, I drew a Maxwell-Boltzmann curve to help with my visualization and formulate my hypothesis concerning varying temperatures. The activation energy (E_a), which is the minimum amount of kinetic energy required to initiate a reaction, is seen in Figure 2. At higher temperatures, more particles have energy greater than E_a. As a result, a greater number of particles can react.

4 Hypothesis

Ergo, I predict that as temperature increases, the average kinetic energy of the reactant particles in the solution will increase proportionally. We can expect that the rate of hydrolysis and thus the rate constant will increase at higher temperatures.

5 Variables

5.1 Control Variables

Table 3: Control variables explained

Variables	Why is it controlled?	How is it controlled?
Volume of reactants	To isolate the effect of temperature on the rate constant, as volume can directly change the reaction rates.	Volumetric pipette to measure ethyl acetate. Graduated cylinder to measure water.
Concentration of reactants	To avoid altering the rates, similar to volume.	Diluting ethyl acetate with a set concentration of ethanol. The solution will be stirred thoroughly to avoid uneven concentrations.
Frequency of pH measurement	Constant intervals allow for consistent and comparable graphs.	pH is recorded by a pH probe every 10 seconds.
Height of pH probe	To avoid inconsistent and inaccurate measurements when too close to the beaker's inner walls.	Height of the pH probe will be held at the 50mL line on the beaker.

5.2 Independent Variable

Five trials with varying **temperatures** (T) in Celsius (°C): water will be set up between 30°C and 70°C, each at 10°C increments from each other. This range was chosen for small, consistent and observable changes between the measurements.

5.3 Dependent Variable

The rates of reaction (r) will be calculated by finding the slope of concentration versus time. Then, r will be used to find the dependent variable, **rate constants** (k) at each temperature. Because the reaction is second-order, the units for r are $moldm^{-3}s^{-1}$. Hence, the units for k can be derived:

$$k = \frac{r}{[A]^2} = \frac{moldm^{-3}s^{-1}}{(moldm^{-3})^2} = dm^3mol^{-1}s^{-1}$$

6 Methodology

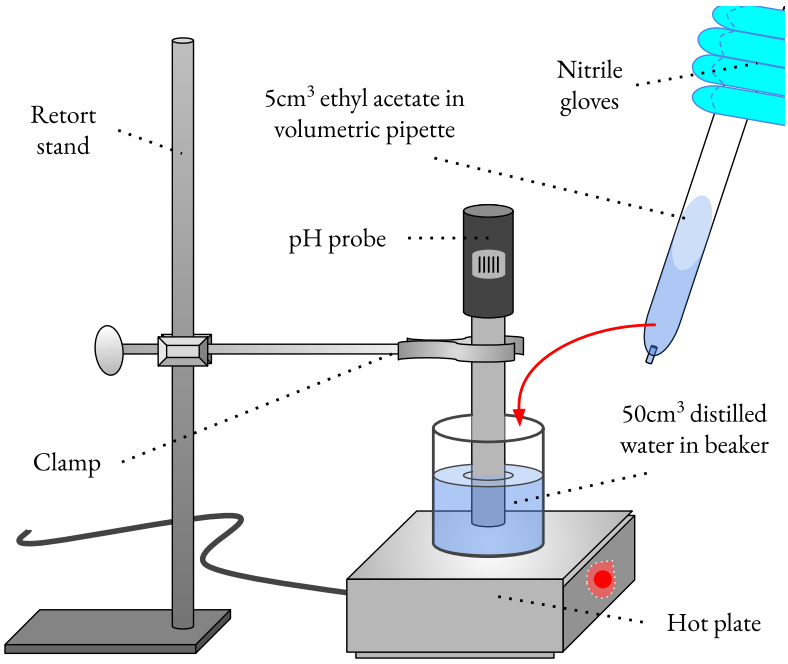
6.1 Preliminary Method Design

During the pre-trial, I realized that pure ethyl acetate was poorly soluble in water and had negligible pH changes. Accordingly, I used ethanol to dilute the esters, making them more miscible with water. I assumed that this is due to the hydroxyl group (–OH) in ethanol, allowing it to form hydrogen bonds with water, whereas ethyl acetate's ester group (–COO–) is less soluble. Hence, I chose ethanol, as it will also be a product of the reaction anyway. Subsequently, I drew the experiment setup to illustrate a simplified methodology (see Figure 4).

6.2 Apparatus and Materials

- $10cm^3$ of 99.9% ethyl acetate
- $90cm^3$ of 99.5% ethanol
- $1000cm^3$ of distilled water
- $2 \times 100cm^3$ glass beaker
- $10cm^3$ volumetric pipette ($\pm 0.02cm^3$)[2]
- $100cm^3$ graduated cylinder ($\pm 0.5cm^3$)[3]
- Thermometer ($\pm 0.5°C$)[4]
- pH probe (± 0.01)[5]
- Phone ($\pm 0.5s$)[6]
- Glass stirring rod
- Manual pipette filler
- Hot plate
- Retort stand and clamps

Figure 4: Simplified setup of laboratory experiment



6.3 Preparation of Reactants

Moles are calculated for each reactant to ensure that ethyl acetate is the limiting reagent.

Table 5: Stoichiometric quantities and uncertainties for reactants[7]

Reactant	Volume	Density	Mass	Molar Mass	Moles
Ethyl acetate	$5 \pm 0.02cm^3$	$0.902gcm^{-3}$	$4.51 \pm 0.02g$	$88.11gmol^{-1}$	$0.05 \pm 2.2 \times 10^{-4}$mol or $\pm 0.44\%$
Distilled water	$50 \pm 0.02cm^3$	$1.000gcm^{-3}$	$50 \pm 0.02g$	$18.02gmol^{-1}$	$2.77 \pm 1.1 \times 10^{-3}$mol or $\pm 0.0004\%$

6.4 Procedure

1. Add 10cm^3 of ethyl acetate into a beaker of 90cm^3 of ethanol and stir until bubbles subside
2. Measure **50cm^3** of distilled water in a graduated cylinder
3. Transfer the distilled water into a beaker and place it onto the hot plate
4. Use the hot plate and the thermometer to adjust the temperature of the water to the target value
5. Measure **5cm^3** of diluted ethyl acetate with the volumetric pipette and add the reactant to the water
6. Insert the pH probe in the solution as soon as the ester is added
7. Use the phone and immediately start recording a video for 60 seconds
8. Stir at a constant rate until 60 seconds have passed
9. Dispose of the solution in a waste disposal container
10. Watch the videotape and record the initial pH and the pH every 10 seconds
11. Repeat steps 2 to 10 for the remaining trials

6.5 Safety, Environmental and Ethical Considerations

Table 6: Risk Assessment

Items	Hazards	How severe?	How likely?	Precautions or actions in case of an accident
99.9% ethyl acetate[8]	CHEMICAL HAZARD	High severity: flammable and irritates (skin, eyes, nose and throat)	Moderately likely: spillage Unlikely: fire	Add ethyl acetate into water or ethanol, never the opposite. Wear a lab coat, nitrile gloves and safety goggles. Wipe up spillages promptly. If on the skin, wash contaminated areas with soap and water. If in the eye, flush for at least 15 minutes.
99.5% ethanol[9]	CHEMICAL HAZARD	High severity: flammable and irritates (skin, eyes, nose and throat)	Moderately likely: spillage Unlikely: fire	Refer to the "precautions or actions in case of an accident" for ethyl acetate.
Hot plate	PHYSICAL HAZARD	Relatively severe: burns, electric shock and fire	Plausible: skin burns Unlikely: electric shock and fire	Check the device for damage before use. If burned, run cold water on the affected area immediately for at least 20 minutes. Call for emergency assistance in case of electrical shock.
Hot water	PHYSICAL HAZARD	Moderate severity: burns	Plausible: skin burns	Do not touch water directly. Refer to the "actions in case of an accident" for the hot plate.
Glass beakers	PHYSICAL HAZARD	Moderate severity: cuts and bleeding	Plausible: broken glass	When transporting glass, handle it with care. If glass breaks, do not touch it directly. If skin is cut, wash the wound with soap and warm water.

It is essential to pour all products into a waste container to be disposed of safely later. Then, residual amounts of excess ethyl acetate and ethanol should be rinsed thoroughly with enough tap water to minimize environmental damage and potentially harming aquatic life. If unsure about any precautions or actions about an incident, notify the lab supervisor. This experiment has no relevant ethical considerations.

7 Quantitative Data

Qualitative observations include bubbles that initially form, however, the stirring will ensure the solution is consistently mixed; otherwise, visual elements are insignificant to the data collection. As displayed on the pH probe, it will be rounded to two decimal places. Since the δpH is ± 0.01, the mean δpH will be rounded to 1s.f. for consistency (see Appendix A).

Sample calculation for the mean pH uncertainty at T = 30°C and t = 0s

$$\delta\text{pH} = \frac{max - min}{2} = \frac{7.58 - 7.43}{2} = \pm 0.08$$

7.1 Raw Data

Recordings began when ethyl acetate and water were mixed. pH was measured every 10s (from t = 0s to 60s), repeated three times for each temperature, to calculate mean pH per time, to later find the rate of reaction.

Table 7: Raw data from experiment

Temperature (T / °C)	Trial #	pH ± 0.01 (t = 0s)	pH ± 0.01 (t = 10s)	pH ± 0.01 (t = 20s)	pH ± 0.01 (t = 30s)	pH ± 0.01 (t = 40s)	pH ± 0.01 (t = 50s)	pH ± 0.01 (t = 60s)
30	1	7.46	7.44	7.33	7.20	7.08	6.86	6.85
	2	7.58	7.51	7.39	7.22	7.11	6.91	6.90
	3	7.43	7.40	7.32	7.15	7.02	6.88	6.85
	Mean:	7.49 ± 0.08	7.45 ± 0.06	7.35 ± 0.04	7.19 ± 0.04	7.07 ± 0.05	6.88 ± 0.03	6.87 ± 0.03
40	1	7.48	7.41	7.24	7.11	7.05	6.96	6.95
	2	7.45	7.35	7.27	7.13	6.99	6.99	6.97
	3	7.51	7.36	7.28	7.15	7.01	6.94	6.95
	Mean:	7.48 ± 0.03	7.37 ± 0.03	7.26 ± 0.02	7.13 ± 0.02	7.01 ± 0.03	6.96 ± 0.03	6.96 ± 0.01
50	1	7.42	7.23	7.08	6.97	6.97	7.01	7.08
	2	7.51	7.31	7.09	6.99	6.99	7.04	7.10
	3	7.49	7.30	7.11	6.99	6.95	6.95	6.97
	Mean:	7.47 ± 0.05	7.28 ± 0.04	7.09 ± 0.02	6.98 ± 0.01	6.97 ± 0.02	7.00 ± 0.05	7.05 ± 0.07
60	1	7.47	7.13	6.98	6.92	6.97	7.02	7.11
	2	7.48	7.20	7.09	7.07	7.03	7.07	7.10
	3	7.52	7.13	7.04	7.00	7.05	7.12	7.16
	Mean:	7.49 ± 0.03	7.15 ± 0.04	7.04 ± 0.06	7.00 ± 0.08	7.02 ± 0.04	7.07 ± 0.05	7.12 ± 0.03
70	1	7.47	7.01	6.98	7.08	7.17	7.24	7.26
	2	7.55	7.06	7.02	7.10	7.12	7.17	7.25
	3	7.45	7.01	6.99	7.12	7.14	7.24	7.27
	Mean:	7.49 ± 0.03	7.03 ± 0.03	6.99 ± 0.02	7.10 ± 0.02	7.14 ± 0.03	7.22 ± 0.04	7.26 ± 0.01

7.2 Data Processing

7.2.1 Determining Concentrations

The concentration of mean pH values can be determined with the formula: $c = 10^{-pH}$ for each trial. The changes in concentration is based on acetic acid ($c[CH_3COOH]$), which contributes to the H^+ ions produced from the dissociation of the formed species. Correspondingly, the uncertainty must be calculated using the following formula for exponential uncertainties of concentrations:[10]

$$\frac{\delta c}{c} = \ln 10 \times \delta pH.$$

To keep consistent with the experimental uncertainties, δc will also be rounded to 1s.f. after the decimal place (see Appendix B). Forthwith, these calculations allow for a concentration versus time graph to determine the reaction rates at each temperature in Section 7.2.2.

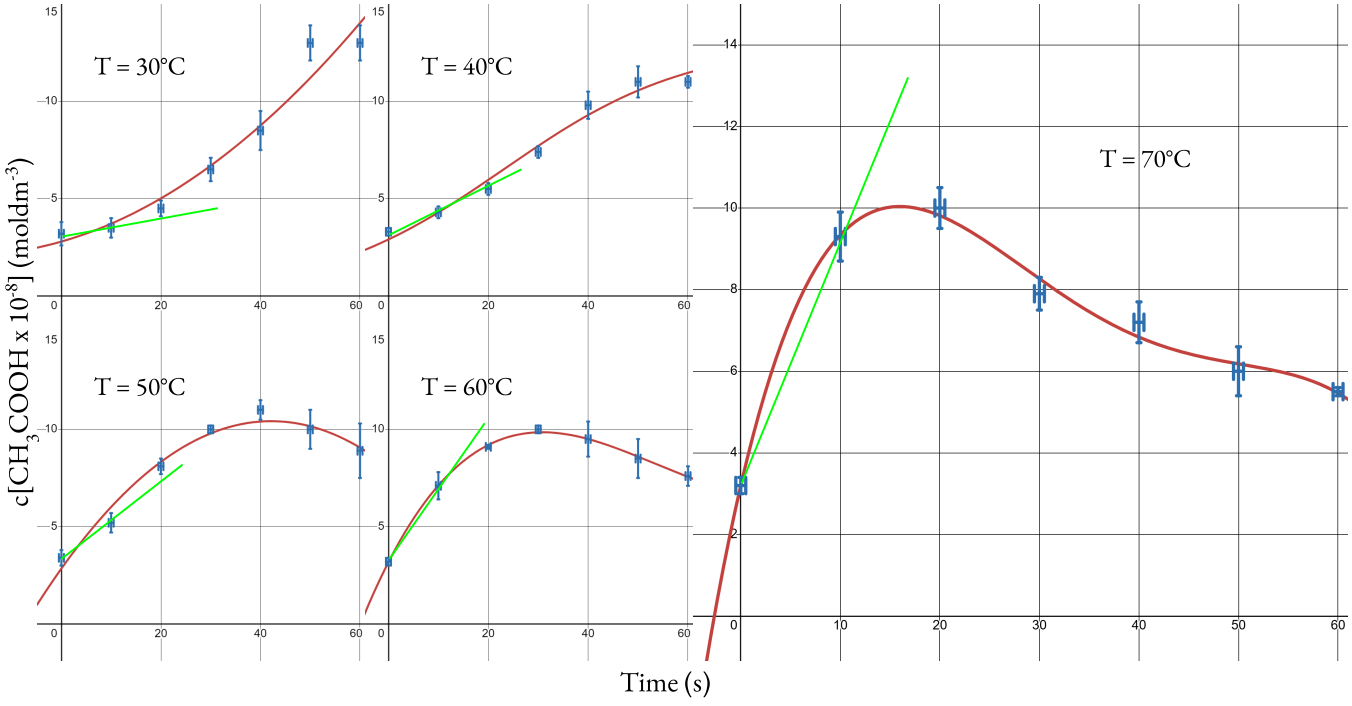
Sample calculation for concentration at T = 30°C and t = 0s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.08 \times 10^{-7.49} = \pm 6.0 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-7.49 \pm 0.08} \approx (3.2 \pm 0.6) \times 10^{-8} \text{moldm}^{-3}$$

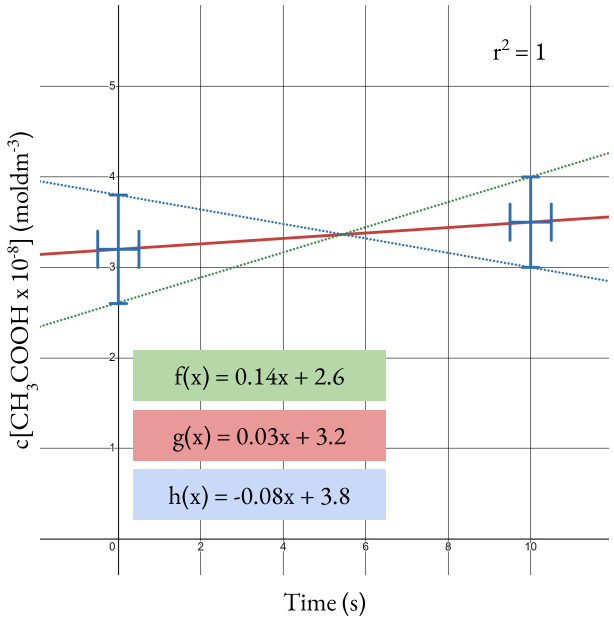
7.2.2 Determining Initial Rates of Reaction

Figure 8: Concentration versus time graphs at each temperature ($R^2 > 0.95$)



The graphs above have highly accurate regressions ($R^2 > 0.95$), however, they have different degree polynomial trend lines (e.g. quadratic, cubic, or quartic) with non-linear and varying slopes (discussed in Section 8). Hence, before calculating the rate constant (k), I simply decided to find the slope (m) between the already found concentrations with the least uncertainties, at 0s and 10s (see the green lines in Figure 8) to approximate the initial rate (r). Through this linearization, I can also graph[11] the gradients' uncertainties (δr) (see Figure 9). Calculations done in Sections 7.2.2 and 7.2.3 will be rounded to four decimal places to keep precise values for steps in Section 7.3.

Figure 9: Sample zoomed-in graph for initial rate of reaction at T = 30°C



Sample calculation for initial rate at T = 30°C

$$r = \frac{\Delta c}{\Delta t} = m_{g(x)}$$

$$= \frac{3.5\times10^{-8} - 3.2\times10^{-8}}{10-0}$$

$$= 3 \times 10^{-10}\text{moldm}^{-3}\text{s}^{-1}$$

$$\delta r = \frac{m_{max(f(x))} - m_{min(h(x))}}{2}$$

$$= \frac{1.4\times10^{-9} - (-8\times10^{-10})}{2}$$

$$= \pm\, 1.1 \times 10^{-9}\text{moldm}^{-3}\text{s}^{-1}$$

or

$$= \frac{Absolute\ uncertainty}{Gradient\ of\ g(x)} \times 100$$

$$= \frac{1.1\times10^{-9}}{3\times10^{-10}} \times 100$$

$$\approx \pm\, 366.6667\%$$

7.2.3 Determining Rate Constants

Previously, the moles were calculated for each reactant as well as the initial rate in Section 6.3 and 7.2.2 respectively. Accordingly, I can calculate the rate constant. In Table 10, instead of using absolute uncertainties, I will take the percentage uncertainties to efficiently calculate the uncertainties in Section 7.3.

Sample calculation for rate constant at T = 30°C

$$r = k[CH_3COOCH_2CH_3][H_2O]$$

$$[CH_3COOCH_2CH_3] = \frac{0.05mol \pm 0.44\%}{0.005dm^3 \pm 0.4\%} = 10\text{moldm}^{-3} \pm 0.84\%$$

$$[H_2O] = \frac{2.77mol \pm 0.0004\%}{0.05dm^3 \pm 0.0004\%} = 55.4\text{moldm}^{-3} \pm 0.0008\%$$

$$k = \frac{r}{[CH_3COOCH_2CH_3][H_2O]} = \frac{3\times10^{-10}moldm^{-3}s^{-1} \pm 366.6667\%}{(10moldm^{-3} \pm 0.84\%)(55.4moldm^{-3} \pm 0.0008\%)} \approx 5.4152 \times 10^{-13}\text{dm}^3\text{mol}^{-1}\text{s}^{-1} \pm 367.5075\%$$

Table 10: Calculated values for initial rate of reaction and rate constant (see Appendix C)

T ± 0.5 (°C)	**$r \times 10^{-9}$ ($moldm^{-3}s^{-1}$)**	**δr ($moldm^{-3}s^{-1}$)**	**$k \times 10^{-12}$ ($dm^3mol^{-1}s^{-1}$)**	**δk ($dm^3mol^{-1}s^{-1}$)**
30	0.3 ± 1.1	± 366.6667%	0.5415 ± 1.9901	± 367.5075%
40	1 ± 0.5	± 50%	1.8051 ± 0.9177	± 50.8408%
50	1.8 ± 0.9	± 50%	3.2491 ± 1.6519	± 50.8408%
60	3.9 ± 0.9	± 23.0769%	7.0397 ± 1.6837	± 23.9177%
70	6.1 ± 0.8	± 13.1148%	11.0108 ± 1.5366	± 13.9556%

7.3 Calculating Activation Energy

Thus far, the processed values are difficult to compare with literature values from other studies. Consequently, I must calculate the activation energy to verify the accuracy of my data relative to a well-studied literature E_a. To achieve this, I must calculate the absolute temperature converted from Celcius to Kelvin as well as the natural logarithm[12] for k. Values will be rounded to four decimal places to keep consistent with previous calculations and generate precise points for the following graph. Absolute uncertainties were calculated to draw the individual error bars on the Arrhenius graph to find E_a.

Sample calculation for $\frac{1}{T}$ *and lnk at* $T = 30°C$

$$\frac{1}{T} = \frac{1}{(30 \pm 0.5) + 273.15} \approx 0.003299 K^{-1}$$

$$\delta\frac{1}{T} = \left(\frac{0.5}{30} \times 0.003299\right) \pm 5.4978 \times 10^{-5} K^{-1}$$

$$\ln k = \ln((0.54152 \pm 1.9901) \times 10^{-12} dm^3 mol^{-1} s^{-1}) \approx -28.2444$$

$$\delta \ln k = \frac{\delta k}{k} = \frac{1.9901 dm^3 mol^{-1} s^{-1}}{0.54152 dm^3 mol^{-1} s^{-1}} \approx \pm 3.6751$$

Table 11: Calculated values for lnk and $\frac{1}{T}$ (see Appendix D)

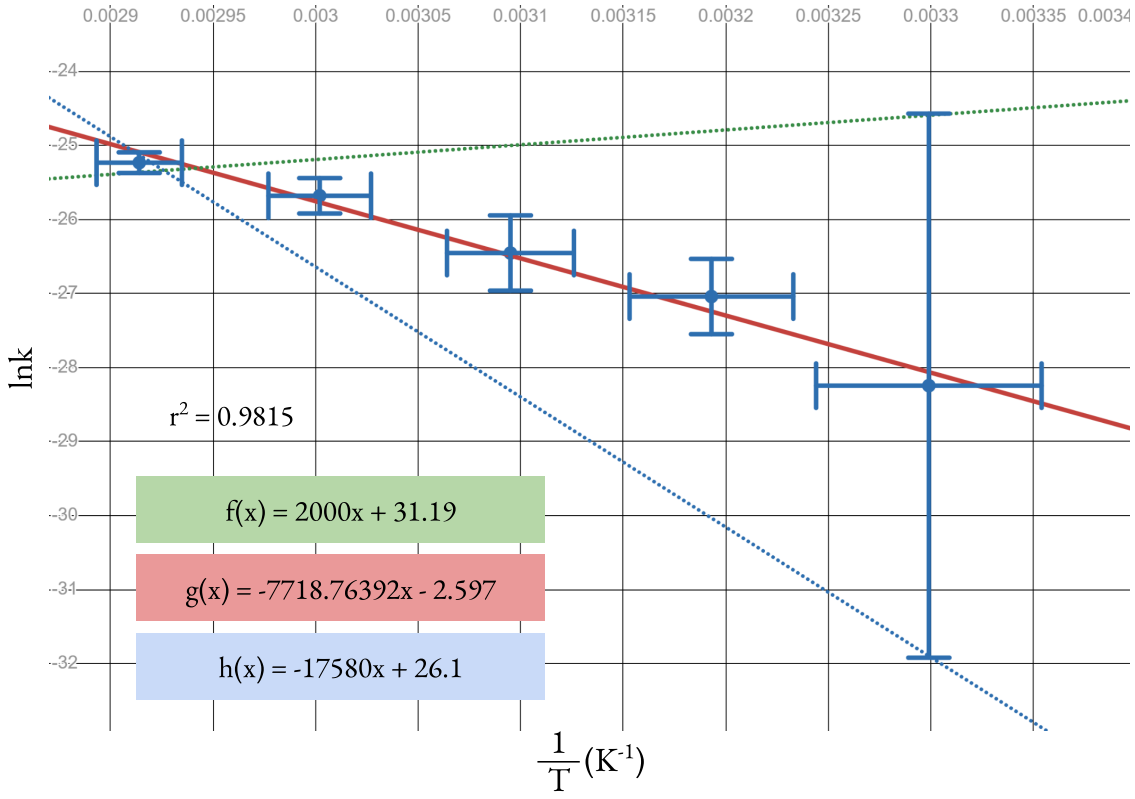
T ± 0.5 (°C)	**$\frac{1}{T}$ (K^{-1})**	**$\delta\frac{1}{T} \times 10^{-5}$ (K^{-1})**	**lnk**	**δlnk**
30	0.003299	± 5.4978	-28.2444	± 3.6751
40	0.003193	± 3.9917	-27.0404	± 0.5084
50	0.003095	± 3.095	-26.4526	± 0.5084
60	0.003002	± 2.5014	-25.6795	± 0.2392
70	0.002914	± 2.0816	-25.2321	± 0.1396

Algebraically, we know $k = Ae^{\frac{-E_a}{RT}}$ from the Arrhenius equation. Subsequently,

$$\ln k = \frac{-E_a}{R} \times \frac{1}{T} + \ln A \leftrightarrow \frac{d(\ln k)}{d(\frac{1}{T})} = \frac{-E_a}{R}$$

The differentiation shows a linear equation in the form y = mx + b. When plotting lnk (y-axis) and $\frac{1}{T}$ (x-axis), the gradient (m) is $\frac{-E_a}{R}$. Then, after graphing the values from Table 11, I can isolate for E_a (see Figure 12).

Figure 12: Arrhenius graph between lnk and $\frac{1}{T}$



As stated, $m = \frac{-E_a}{R} \leftrightarrow E_a = -mR$; values will be rounded to 3s.f. to effectively compare with the literature value and maintain accuracy when performing uncertainty calculations.

Calculation for activation energy

$E_a = -(-7718.76392\text{K} \times 8.31\text{Jmol}^{-1}\text{K}^{-1}) \approx 64100\text{Jmol}^{-1} \approx 64.1\text{kJmol}^{-1}$

Maximum gradient: $E_a = -2000\text{K} \times 8.31\text{Jmol}^{-1}\text{K}^{-1} \approx -16600\text{Jmol}^{-1} \approx -16.6\text{kJmol}^{-1}$

Minimum gradient: $-(-17580\text{K} \times 8.31\text{Jmol}^{-1}\text{K}^{-1}) \approx 146000\text{Jmol}^{-1} \approx 14.6\text{kJmol}^{-1}$

Calculation for activation energy uncertainties

$$\text{Absolute uncertainty} = \frac{E_{a_{max}} - E_{a_{min}}}{2} = \frac{14.6-(-16.6)}{2} = \pm 15.6\ \text{kJmol}^{-1}$$

$$\text{Percentage uncertainty} = \frac{15.6}{64.1} \times 100 = \pm 24.3\%$$

$$\text{Percent error (literature } E_a = 48.3\text{kJmol}^{-1})^{[13]} = \frac{|experimental - accepted|}{accepted} \times 100 = \frac{|64.1-48.3|}{48.3} \times 100 = 32.7\%$$

8 Conclusion

How does the rate constant in the hydrolysis of ethyl acetate vary with temperature at 30°C, 40°C, 50°C, 60°C, and 70°C? The conducted investigation allowed me to answer this research question. Analyzing the data, I can demonstrate my initial hypothesis: the rate constant of ethyl acetate hydrolysis increases with temperature. For instance, at 30°C, the rate constant was about $5.4152 \times 10^{-13} dm^3 mol^{-1} s^{-1}$ whilst at 40°C, it increased to $1.8051 \times 10^{-12} dm^3 mol^{-1} s^{-1}$ and so on, clearly illustrating this trend. Next, the accuracy of my findings was justified using the experimental activation energy ($64.1 kJmol^{-1}$) and its literature value ($48.3 kJmol^{-1}$), which came to a percentage error of 32.7%. Although this is considered relatively high, it confirms that my experimental data provides a reasonable approximation of the temperature and rate constant trend. Nevertheless, in future iterations, it would be beneficial to refine my methodology to reduce this error (discussed in Section 9.2).

Before determining the rate constant, the initial rate had to be calculated from the concentration and time graphs. There, at higher temperatures, the slope becomes steeper during the first 10 seconds, which supports my hypothesis that the rate of hydrolysis increases with temperature: the reaction reaches equilibrium faster. However, increasing heat introduced an issue in the data collection resulting in non-linear regression models, particularly at 70°C, where the concentration reaches a maximum after 10s, but then falls. This outcome could be because the activation energy is higher compared to one with a catalyst, meaning the forward reaction is weaker. Also, the reaction is exothermic; when temperature increases, equilibrium shifts to reactants, which increases the probability of a reverse reaction. Despite this, it was essential to focus on the first 10 seconds where the initial rate allowed me to find the rate constant of each temperature to answer the research question.

My findings are further solidified in the Arrhenius graph. It illustrated a linear regression model with an r^2 near 1 (0.9815), marking a strong correlation. However, visually, there were some significant error bars. Namely, the percentage uncertainty of the rate constant at 30°C was over 367%, along with other apparent uncertainties that were lower, but still contributed to the large overall uncertainty of 24.3% in the E_a, which reinforces the lack of precision in the experiment. Ergo, while we can notice that this investigation lacks precision, my findings are relatively accurate and altogether confirm a positive trend between rate constant and temperature.

9 Evaluation

9.1 Strengths

My investigation provided a clear trend with no outliers. I was also able to collect data from multiple trials to calculate the mean, rather than relying on one value, minimizing random errors. Additionally, the control variables were effectively regulated, which allowed me to focus exclusively on temperature and pH changes. This decreased the chances for external factors, reducing possible random and systematic errors. Altogether, an obvious conclusion was reached without the need for advanced equipment or additional resources to perform my methodology.

9.2 Weaknesses and Improvements

Table 13: Errors, their significance and improvements

Errors	Significance	Improvements
Methodology	After retrieving the raw data, I was able to calculate the initial rate for each temperature but had no visual confirmation if my methodology was properly executed. Moreover, the initial rates had significant percentage uncertainties and **random errors**, with large error bars and high variability on the Arrhenius plot.	Visually, a titration with acid-base indicators would make the reaction easier to understand, as the reactants could be mixed intentionally at a slower pace. Although this may cause **human error** in perceiving colour changes, a titration would reduce **random errors** by capturing more precise volume changes with a burette.
Measuring pH	My raw data for pH values at 0s were slightly different in every trial. The initial pH should have been the exact same as I am mixing the same concentrations of each reactant. This presents **human error** from possibly not stirring uniformly, reading the pH probe incorrectly, or recording the video at the wrong time. Furthermore, it resulted in **random errors** as seen in the high levels of uncertainty (e.g. δk at T = 30°C was over 300%). The incorrect calibration of the pH probe could have placed consistent deviations in my findings: **systematic error**.	A magnetic stirrer could electronically prevent uneven concentrations in the solution and maintain consistent reaction conditions for every trial. Similarly, instead of a pH probe, an electronic pH meter could gather data without needing to manually input data on a spreadsheet, reducing **human error**. This device can also increase the sample size; computers process much more data efficiently, which would reduce **random errors**. A buffer solution calibration before each trial would help correct the **systematic error**.
Measuring volume	There may be a **parallax error** when reading the meniscus of the liquids inside volume-measuring instruments. Reading the values from too high or low may vary, where the refraction of light in liquids changes slightly from different angles. A **systematic error** arises as the measurements may be displaced from true values.	Ensure measurements were taken consistently at eye level. Or, to eliminate this type of **human error**, use an instrument (e.g. digital burette) to automate readings and dispense the same volume of reactants every trial rather than doing it manually.
Temperature control	The sole use of a hot plate may have been inadequate to control temperature, leading to small fluctuations in the conditions between trials. Moreover, during the heating process, some reactants may have lost volume, through evaporation, causing a source of **systematic error**.	A laboratory water bath would help maintain constant temperatures. Next, I used a beaker because a pH probe could not fit into an Erlenmeyer flask. However, a pH meter could have fit through a narrower neck, preventing heat loss, particularly at higher temperatures.
Sample size	To find k values, I needed initial rates, which are most accurately found by the slope of a straight line near t = 0s. We saw that the concentration versus time graphs were non-linear, so to minimize uncertainty, I used pH values at 0s and 10s to form the linear regressions. However, merely two points were unreliable, which resulted in a misleadingly perfect correlation ($r^2 = 1$). Also, on a larger scale, using strictly five different temperatures and the limited three trials increased **random errors**.	Record the pH more frequently in a smaller time frame (between the 0s and 10s interval), to reduce **random errors** and increase precision in the initial rate calculation. Similarly, to increase the sample size, I can add more trials along with a broader range of temperatures to decrease the variability in the data, and reinforce if my final findings are in fact true, even after drastic changes in temperature conditions.
Apparatus not dried	After every trial, apparatuses were rinsed with tap water, which may have left contaminants and water droplets. This causes a **systematic error** as the concentration of reactants, initial rate, and k could have been affected.	A clean paper towel should have been used to clean and dry the instruments before every trial, to ensure there is no excess water or substances left inside, eliminating the possibility for a **systematic error**.

9.3 Extensions

My investigation could be further developed through a similar hydrolysis of other compounds including methyl acetate and pentyl acetate, which belong to the same family of esters. If time permits, the data retrieved from this would allow me to compare how varying lengths of a carbon chain, structural, and functional components may affect the rate constant and activation energy as well. Additionally, while keeping the same methodology, an idea to extend the study is not only to vary temperature but also to vary the concentration of ethyl acetate rather than keeping it constant. This way, I will be able to figure out the most efficient and economical method to derive the rate constant, and for future iterations, it will allow trials to be done with less time and equipment needed.

10 References

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11 Appendix A

Mean pH uncertainty calculations rounded to 1s.f. as performed in Section 7:

T = 30℃ and t = 0s

$$\delta pH = \frac{max - min}{2} = \frac{7.58 - 7.43}{2} = \pm 0.08$$

T = 30℃ and t = 10s

$$\delta pH = \frac{max - min}{2} = \frac{7.51 - 7.40}{2} = \pm 0.06$$

T = 30℃ and t = 20s

$$\delta pH = \frac{max - min}{2} = \frac{7.39 - 7.32}{2} = \pm 0.04$$

T = 30℃ and t = 30s

$$\delta pH = \frac{max - min}{2} = \frac{7.22 - 7.15}{2} = \pm 0.04$$

T = 30℃ and t = 40s

$$\delta pH = \frac{max - min}{2} = \frac{7.11 - 7.02}{2} = \pm 0.05$$

T = 30℃ and t = 50s

$$\delta pH = \frac{max - min}{2} = \frac{6.91 - 6.86}{2} = \pm 0.03$$

T = 30℃ and t = 60s

$$\delta pH = \frac{max - min}{2} = \frac{6.90 - 6.85}{2} = \pm 0.03$$

T = 40℃ and t = 0s

$$\delta pH = \frac{max - min}{2} = \frac{7.51 - 7.45}{2} = \pm 0.03$$

T = 40℃ and t = 10s

$$\delta pH = \frac{max - min}{2} = \frac{7.41 - 7.35}{2} = \pm 0.03$$

T = 40℃ and t = 20s

$$\delta pH = \frac{max - min}{2} = \frac{7.28 - 7.24}{2} = \pm 0.02$$

T = 40℃ and t = 30s

$$\delta pH = \frac{max - min}{2} = \frac{7.15 - 7.11}{2} = \pm 0.02$$

T = 40℃ and t = 40s

$$\delta pH = \frac{max - min}{2} = \frac{7.05 - 6.99}{2} = \pm 0.03$$

T = 40℃ and t = 50s

$$\delta pH = \frac{max - min}{2} = \frac{6.99 - 6.94}{2} = \pm 0.03$$

T = 40℃ and t = 60s

$$\delta pH = \frac{max - min}{2} = \frac{6.97 - 6.95}{2} = \pm 0.01$$

T = 50℃ and t = 0s

$$\delta pH = \frac{max - min}{2} = \frac{7.51 - 7.42}{2} = \pm 0.05$$

T = 50℃ and t = 10s

$$\delta pH = \frac{max - min}{2} = \frac{7.31 - 7.23}{2} = \pm 0.04$$

T = 50℃ and t = 20s

$$\delta pH = \frac{max - min}{2} = \frac{7.11 - 7.08}{2} = \pm 0.02$$

T = 50℃ and t = 30s

$$\delta pH = \frac{max - min}{2} = \frac{6.99 - 6.97}{2} = \pm 0.01$$

T = 50℃ and t = 40s

$$\delta pH = \frac{max - min}{2} = \frac{6.99 - 6.95}{2} = \pm 0.02$$

T = 50℃ and t = 50s

$$\delta pH = \frac{max - min}{2} = \frac{7.04 - 6.95}{2} = \pm 0.05$$

T = 50℃ and t = 60s

$$\delta pH = \frac{max - min}{2} = \frac{7.10 - 6.97}{2} = \pm 0.07$$

T = 60℃ and t = 0s

$$\delta pH = \frac{max - min}{2} = \frac{7.52 - 6.47}{2} = \pm 0.03$$

T = 60℃ and t = 10s

$$\delta pH = \frac{max - min}{2} = \frac{7.20 - 7.13}{2} = \pm 0.04$$

T = 60℃ and t = 20s

$$\delta pH = \frac{max - min}{2} = \frac{7.09 - 6.98}{2} = \pm 0.06$$

T = 60℃ and t = 30s

$$\delta pH = \frac{max - min}{2} = \frac{7.07 - 6.92}{2} = \pm 0.08$$

T = 60℃ and t = 40s

$$\delta pH = \frac{max - min}{2} = \frac{7.05 - 6.97}{2} = \pm 0.04$$

T = 60℃ and t = 50s

$$\delta pH = \frac{max - min}{2} = \frac{7.12 - 7.02}{2} = \pm 0.05$$

T = 60℃ and t = 60s

$$\delta pH = \frac{max - min}{2} = \frac{7.16 - 7.10}{2} = \pm 0.03$$

T = 70℃ and t = 0s

$$\delta pH = \frac{max - min}{2} = \frac{7.55 - 7.45}{2} = \pm 0.05$$

T = 70℃ and t = 10s

$$\delta pH = \frac{max - min}{2} = \frac{7.06 - 7.01}{2} = \pm 0.03$$

T = 70℃ and t = 20s

$$\delta pH = \frac{max - min}{2} = \frac{7.02 - 7.98}{2} = \pm 0.02$$

T = 70℃ and t = 30s

$$\delta pH = \frac{max - min}{2} = \frac{7.12 - 7.08}{2} = \pm 0.02$$

T = 70℃ and t = 40s

$$\delta pH = \frac{max - min}{2} = \frac{7.17 - 7.12}{2} = \pm 0.03$$

T = 70℃ and t = 50s

$$\delta pH = \frac{max - min}{2} = \frac{7.24 - 7.17}{2} = \pm 0.04$$

T = 70℃ and t = 60s

$$\delta pH = \frac{max - min}{2} = \frac{7.27 - 7.25}{2} = \pm 0.01$$

12 Appendix B

Concentration with uncertainties rounded to 1s.f. after the decimal place as performed in Section 7.2:

T = 30℃ and t = 0s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.08 \times 10^{-7.49}$$
$$\delta c = \pm 6.0 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.49 \pm 0.08} = (3.2 \pm 0.6) \times 10^{-8} \text{moldm}^{-3}$$

T = 40℃ and t = 0s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.48}$$
$$\delta c = \pm 2.3 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.48 \pm 0.03} = (3.3 \pm 0.2) \times 10^{-8} \text{moldm}^{-3}$$

T = 30℃ and t = 10s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.06 \times 10^{-7.45}$$
$$\delta c = \pm 4.9 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.45 \pm 0.06} = (3.5 \pm 0.5) \times 10^{-8} \text{moldm}^{-3}$$

T = 40℃ and t = 10s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.37}$$
$$\delta c = \pm 2.9 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.37 \pm 0.03} = (4.3 \pm 0.3) \times 10^{-8} \text{moldm}^{-3}$$

T = 30℃ and t = 20s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.04 \times 10^{-7.35}$$
$$\delta c = \pm 4.1 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.35 \pm 0.04} = (4.5 \pm 0.4) \times 10^{-8} \text{moldm}^{-3}$$

T = 40℃ and t = 20s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.02 \times 10^{-7.26}$$
$$\delta c = \pm 2.5 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.26 \pm 0.02} = (5.5 \pm 0.3) \times 10^{-8} \text{moldm}^{-3}$$

T = 30℃ and t = 30s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.04 \times 10^{-7.19}$$
$$\delta c = \pm 5.9 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.19 \pm 0.04} = (6.5 \pm 0.6) \times 10^{-8} \text{moldm}^{-3}$$

T = 40℃ and t = 30s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.02 \times 10^{-7.13}$$
$$\delta c = \pm 3.4 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.13 \pm 0.02} = (7.4 \pm 0.3) \times 10^{-8} \text{moldm}^{-3}$$

T = 30℃ and t = 40s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.05 \times 10^{-7.07}$$
$$\delta c = \pm 9.8 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.07 \pm 0.05} = (8.5 \pm 1.0) \times 10^{-8} \text{moldm}^{-3}$$

T = 40℃ and t = 40s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.01}$$
$$\delta c = \pm 6.8 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-7.01 \pm 0.03} = (9.8 \pm 0.7) \times 10^{-8} \text{moldm}^{-3}$$

T = 30℃ and t = 50s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-6.88}$$
$$\delta c = \pm 9.1 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-6.88 \pm 0.05} = (1.3 \pm 0.09) \times 10^{-7} \text{moldm}^{-3}$$

T = 40℃ and t = 50s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-6.96}$$
$$\delta c = \pm 7.6 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-6.96 \pm 0.03} = (1.1 \pm 0.08) \times 10^{-7} \text{moldm}^{-3}$$

T = 30℃ and t = 60s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-6.87}$$
$$\delta c = \pm 9.3 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-6.87 \pm 0.03} = (1.3 \pm 0.09) \times 10^{-7} \text{moldm}^{-3}$$

T = 40℃ and t = 60s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.01 \times 10^{-6.96}$$
$$\delta c = \pm 2.5 \times 10^{-9} \text{moldm}^{-3}$$
$$c = 10^{-pH} = 10^{-6.96 \pm 0.01} = (1.1 \pm 0.03) \times 10^{-7} \text{moldm}^{-3}$$

T = 50℃ and t = 0s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.05 \times 10^{-7.47}$$

$$\delta c = \pm 3.9 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.47 \pm 0.05} = (3.4 \pm 0.4) \times 10^{-8} moldm^{-3}$$

T = 50℃ and t = 10s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.04 \times 10^{-7.28}$$

$$\delta c = \pm 4.8 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.28 \pm 0.04} = (5.2 \pm 0.5) \times 10^{-8} moldm^{-3}$$

T = 50℃ and t = 20s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.02 \times 10^{-7.09}$$

$$\delta c = \pm 3.7 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.09 \pm 0.02} = (8.1 \pm 0.4) \times 10^{-8} moldm^{-3}$$

T = 50℃ and t = 30s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.01 \times 10^{-6.98}$$

$$\delta c = \pm 2.4 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-6.98 \pm 0.01} = (1.0 \pm 0.02) \times 10^{-7} moldm^{-3}$$

T = 50℃ and t = 40s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.02 \times 10^{-6.97}$$

$$\delta c = \pm 4.9 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-6.97 \pm 0.02} = (1.1 \pm 0.05) \times 10^{-7} moldm^{-3}$$

T = 50℃ and t = 50s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.05 \times 10^{-7.00}$$

$$\delta c = \pm 1.2 \times 10^{-8} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.00 \pm 0.05} = (1.0 \pm 0.1) \times 10^{-7} moldm^{-3}$$

T = 50℃ and t = 60s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.07 \times 10^{-7.05}$$

$$\delta c = \pm 1.4 \times 10^{-8} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.05 \pm 0.07} = (8.9 \pm 1.4) \times 10^{-8} moldm^{-3}$$

T = 60℃ and t = 0s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.49}$$

$$\delta c = \pm 2.2 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.49 \pm 0.03} = (3.2 \pm 0.2) \times 10^{-8} moldm^{-3}$$

T = 60℃ and t = 10s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.04 \times 10^{-7.15}$$

$$\delta c = \pm 6.5 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.15 \pm 0.04} = (7.1 \pm 0.7) \times 10^{-8} moldm^{-3}$$

T = 60℃ and t = 20s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.06 \times 10^{-7.04}$$

$$\delta c = \pm 1.3 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.04 \pm 0.06} = (9.1 \pm 0.1) \times 10^{-8} moldm^{-3}$$

T = 60℃ and t = 30s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.08 \times 10^{-7.00}$$

$$\delta c = \pm 1.8 \times 10^{-8} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.00 \pm 0.08} = (1.0 \pm 0.2) \times 10^{-7} moldm^{-3}$$

T = 60℃ and t = 40s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.04 \times 10^{-7.02}$$

$$\delta c = \pm 8.8 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.02 \pm 0.04} = (9.5 \pm 0.9) \times 10^{-8} moldm^{-3}$$

T = 60℃ and t = 50s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.05 \times 10^{-7.07}$$

$$\delta c = \pm 9.8 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.07 \pm 0.05} = (8.5 \pm 1.0) \times 10^{-8} moldm^{-3}$$

T = 60℃ and t = 60s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.12}$$

$$\delta c = \pm 5.2 \times 10^{-9} moldm^{-3}$$

$$c = 10^{-pH} = 10^{-7.12 \pm 0.03} = (7.6 \pm 0.5) \times 10^{-8} moldm^{-3}$$

T = 70℃ and t = 0s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.49}$$

$$\delta c = \pm 2.2 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-7.49 \pm 0.03} = (3.2 \pm 0.2) \times 10^{-8} \text{moldm}^{-3}$$

T = 70℃ and t = 10s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.03}$$

$$\delta c = \pm 6.4 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-7.03 \pm 0.03} = (9.3 \pm 0.6) \times 10^{-8} \text{moldm}^{-3}$$

T = 70℃ and t = 20s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.02 \times 10^{-6.99}$$

$$\delta c = \pm 4.7 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-6.99 \pm 0.02} = (1.0 \pm 0.05) \times 10^{-7} \text{moldm}^{-3}$$

T = 70℃ and t = 30s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.02 \times 10^{-7.10}$$

$$\delta c = \pm 3.7 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-7.10 \pm 0.02} = (7.9 \pm 0.4) \times 10^{-8} \text{moldm}^{-3}$$

T = 70℃ and t = 40s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.03 \times 10^{-7.14}$$

$$\delta c = \pm 5.0 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-7.14 \pm 0.03} = (7.2 \pm 0.5) \times 10^{-8} \text{moldm}^{-3}$$

T = 70℃ and t = 50s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.04 \times 10^{-7.22}$$

$$\delta c = \pm 5.5 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-7.22 \pm 0.04} = (6.0 \pm 0.6) \times 10^{-8} \text{moldm}^{-3}$$

T = 70℃ and t = 60s

$$\delta c = \ln 10 \times \delta pH \times c = \ln 10 \times 0.01 \times 10^{-7.26}$$

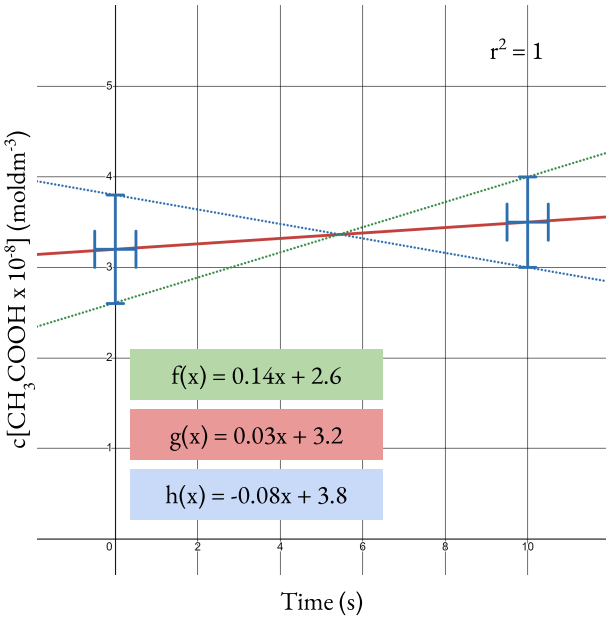
$$\delta c = \pm 1.3 \times 10^{-9} \text{moldm}^{-3}$$

$$c = 10^{-pH} = 10^{-7.26 \pm 0.01} = (5.5 \pm 0.1) \times 10^{-8} \text{moldm}^{-3}$$

13 Appendix C

Initial rate of reaction and rate constant with uncertainties rounded to four decimal places as performed in Section 7.2.2 and 7.2.3:

Graph for initial rate of reaction, concentration versus time graph at T = 30°C



Initial rate at T = 30°C

$$r = \frac{\Delta c}{\Delta t} = m_{g(x)}$$

$$= \frac{3.5\times10^{-8} - 3.2\times10^{-8}}{10-0}$$

$$= 3 \times 10^{-10}\text{moldm}^{-3}\text{s}^{-1}$$

$$\delta r = \frac{m_{max(f(x))} - m_{min(h(x))}}{2}$$

$$= \frac{1.4\times10^{-9} - (-8\times10^{-10})}{2}$$

$$= \pm\ 1.1 \times 10^{-9}\text{moldm}^{-3}\text{s}^{-1}$$

or

$$= \frac{Absolute\ uncertainty}{Gradient\ of\ g(x)} \times 100$$

$$= \frac{1.1\times10^{-9}}{3\times10^{-10}} \times 100$$

$$\approx \pm\ 366.6667\%$$

Rate constant at T = 30°C

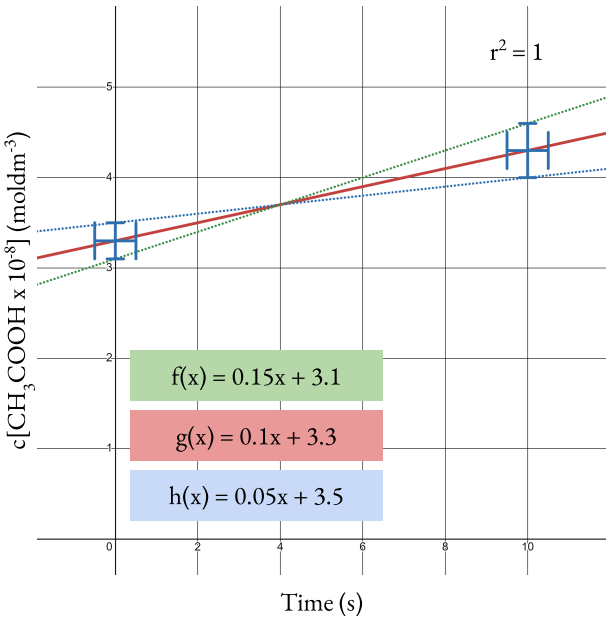
$$r = k[CH_3COOCH_2CH_3][H_2O]$$

$$[CH_3COOCH_2CH_3] = \frac{0.05mol \pm 0.44\%}{0.005dm^3 \pm 0.4\%} = 10\text{moldm}^{-3} \pm 0.84\%$$

$$[H_2O] = \frac{2.77mol \pm 0.0004\%}{0.05dm^3 \pm 0.0004\%} = 55.4\text{moldm}^{-3} \pm 0.0008\%$$

$$k = \frac{r}{[CH_3COOCH_2CH_3][H_2O]} = \frac{3\times10^{-10}moldm^{-3}s^{-1} \pm 366.6667\%}{(10moldm^{-3} \pm 0.84\%)(55.4moldm^{-3} \pm 0.0008\%)} \approx 5.4152 \times 10^{-13}\text{dm}^3\text{mol}^{-1}\text{s}^{-1} \pm 367.5075\%$$

Graph for initial rate of reaction, concentration versus time graph at T = 40°C



Initial rate at T = 40°C

$$r = \frac{\Delta c}{\Delta t} = m_{g(x)}$$

$$= \frac{4.3\times10^{-8} - 3.3\times10^{-8}}{10-0}$$

$$= 1 \times 10^{-9}\text{moldm}^{-3}\text{s}^{-1}$$

$$\delta r = \frac{m_{max(f(x))} - m_{min(h(x))}}{2}$$

$$= \frac{1.5\times10^{-9} - 5\times10^{-10}}{2}$$

$$= \pm 5 \times 10^{-10}\text{moldm}^{-3}\text{s}^{-1}$$

or

$$= \frac{Absolute\ uncertainty}{Gradient\ of\ g(x)} \times 100$$

$$= \frac{5\times10^{-10}}{1\times10^{-9}} \times 100$$

$$\approx \pm 50\%$$

Rate constant at T = 40°C

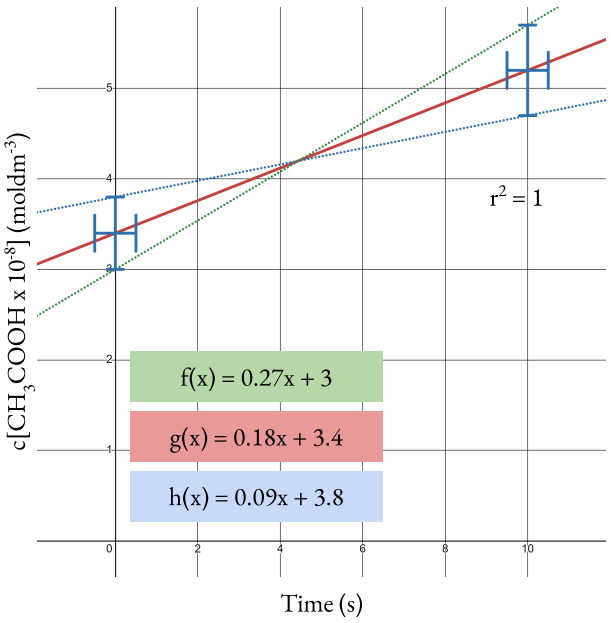
$$r = k[CH_3COOCH_2CH_3][H_2O]$$

$$[CH_3COOCH_2CH_3] = \frac{0.05mol \pm 0.44\%}{0.005dm^3 \pm 0.4\%} = 10\text{moldm}^{-3} \pm 0.84\%$$

$$[H_2O] = \frac{2.77mol \pm 0.0004\%}{0.05dm^3 \pm 0.0004\%} = 55.4\text{moldm}^{-3} \pm 0.0008\%$$

$$k = \frac{r}{[CH_3COOCH_2CH_3][H_2O]} = \frac{1\times10^{-9}moldm^{-3}s^{-1} \pm 50\%}{(10moldm^{-3} \pm 0.84\%)(55.4moldm^{-3} \pm 0.0008\%)} \approx 1.8051 \times 10^{-12}\text{dm}^3\text{mol}^{-1}\text{s}^{-1} \pm 50.8408\%$$

Graph for initial rate of reaction, concentration versus time graph at T = 50°C



Initial rate at T = 50°C

$$r = \frac{\Delta c}{\Delta t} = m_{g(x)}$$

$$= \frac{5.2\times10^{-8} - 3.4\times10^{-8}}{10-0}$$

$$= 1.8 \times 10^{-9}\text{moldm}^{-3}\text{s}^{-1}$$

$$\delta r = \frac{m_{max(f(x))} - m_{min(h(x))}}{2}$$

$$= \frac{2.7\times10^{-9} - 9\times10^{-10}}{2}$$

$$= \pm\, 9 \times 10^{-10}\text{moldm}^{-3}\text{s}^{-1}$$

or

$$= \frac{Absolute\ uncertainty}{Gradient\ of\ g(x)} \times 100$$

$$= \frac{9\times10^{-10}}{1.8\times10^{-9}} \times 100$$

$$\approx \pm\, 50\%$$

Rate constant at T = 50°C

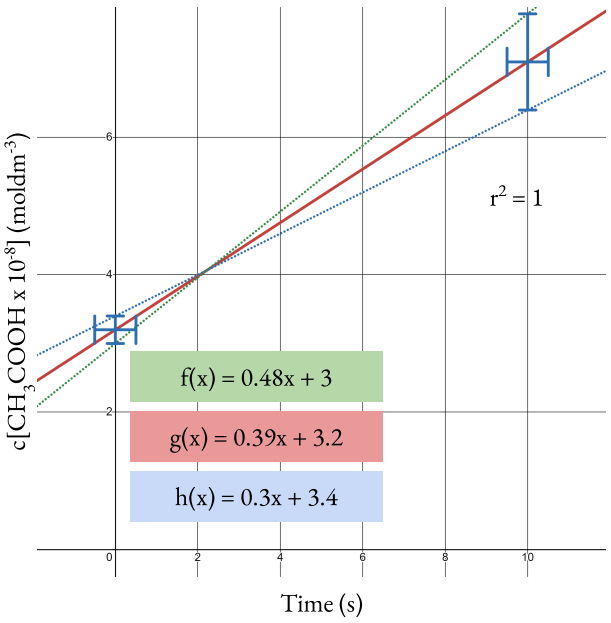
$$r = k[CH_3COOCH_2CH_3][H_2O]$$

$$[CH_3COOCH_2CH_3] = \frac{0.05mol \pm 0.44\%}{0.005dm^3 \pm 0.4\%} = 10\text{moldm}^{-3} \pm 0.84\%$$

$$[H_2O] = \frac{2.77mol \pm 0.0004\%}{0.05dm^3 \pm 0.0004\%} = 55.4\text{moldm}^{-3} \pm 0.0008\%$$

$$k = \frac{r}{[CH_3COOCH_2CH_3][H_2O]} = \frac{1.8\times10^{-9}moldm^{-3}s^{-1} \pm 50\%}{(10moldm^{-3} \pm 0.84\%)(55.4moldm^{-3} \pm 0.0008\%)} \approx 3.2491 \times 10^{-12}\text{dm}^3\text{mol}^{-1}\text{s}^{-1} \pm 50.8408\%$$

Graph for initial rate of reaction, concentration versus time graph at T = 60°C



Initial rate at T = 60°C

$$r = \frac{\Delta c}{\Delta t} = m_{g(x)}$$

$$= \frac{7.1\times10^{-8} - 3.2\times10^{-8}}{10-0}$$

$$= 3.9 \times 10^{-9}\text{moldm}^{-3}\text{s}^{-1}$$

$$\delta r = \frac{m_{max(f(x))} - m_{min(h(x))}}{2}$$

$$= \frac{4.8\times10^{-9} - 3\times10^{-9}}{2}$$

$$= \pm 9 \times 10^{-10}\text{moldm}^{-3}\text{s}^{-1}$$

or

$$= \frac{Absolute\ uncertainty}{Gradient\ of\ g(x)} \times 100$$

$$= \frac{9\times10^{-10}}{3.9\times10^{-9}} \times 100$$

$$\approx \pm 23.0769\%$$

Rate constant at T = 60°C

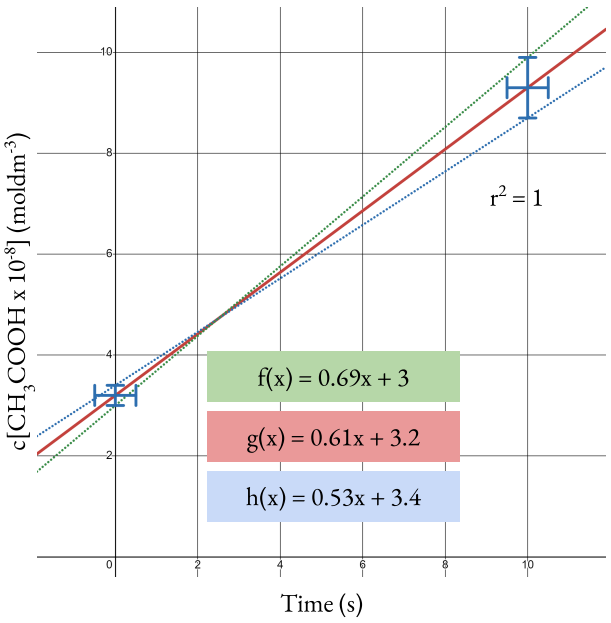
$$r = k[CH_3COOCH_2CH_3][H_2O]$$

$$[CH_3COOCH_2CH_3] = \frac{0.05mol \pm 0.44\%}{0.005dm^3 \pm 0.4\%} = 10\text{moldm}^{-3} \pm 0.84\%$$

$$[H_2O] = \frac{2.77mol \pm 0.0004\%}{0.05dm^3 \pm 0.0004\%} = 55.4\text{moldm}^{-3} \pm 0.0008\%$$

$$k = \frac{r}{[CH_3COOCH_2CH_3][H_2O]} = \frac{3.9\times10^{-9}moldm^{-3}s^{-1} \pm 23.0769\%}{(10moldm^{-3} \pm 0.84\%)(55.4moldm^{-3} \pm 0.0008\%)} \approx 7.0397 \times 10^{-12}\text{dm}^3\text{mol}^{-1}\text{s}^{-1} \pm 23.9177\%$$

Graph for initial rate of reaction, concentration versus time graph at T = 70°C



Initial rate at T = 70°C

$$r = \frac{\Delta c}{\Delta t} = m_{g(x)}$$

$$= \frac{9.3\times10^{-8} - 3.2\times10^{-8}}{10-0}$$

$$= 6.1 \times 10^{-9}\text{moldm}^{-3}\text{s}^{-1}$$

$$\delta r = \frac{m_{max(f(x))} - m_{min(h(x))}}{2}$$

$$= \frac{6.9\times10^{-9} - 5.3\times10^{-9}}{2}$$

$$= \pm 8 \times 10^{-10}\text{moldm}^{-3}\text{s}^{-1}$$

or

$$= \frac{Absolute\ uncertainty}{Gradient\ of\ g(x)} \times 100$$

$$= \frac{8\times10^{-10}}{6.1\times10^{-9}} \times 100$$

$$\approx \pm 13.1148\%$$

Rate constant at T = 70°C

$$r = k[CH_3COOCH_2CH_3][H_2O]$$

$$[CH_3COOCH_2CH_3] = \frac{0.05mol \pm 0.44\%}{0.005dm^3 \pm 0.4\%} = 10\text{moldm}^{-3} \pm 0.84\%$$

$$[H_2O] = \frac{2.77mol \pm 0.0004\%}{0.05dm^3 \pm 0.0004\%} = 55.4\text{moldm}^{-3} \pm 0.0008\%$$

$$k = \frac{r}{[CH_3COOCH_2CH_3][H_2O]} = \frac{6.1\times10^{-9}moldm^{-3}s^{-1} \pm 13.1148\%}{(10moldm^{-3} \pm 0.84\%)(55.4moldm^{-3} \pm 0.0008\%)} \approx 1.1011 \times 10^{-11}\text{dm}^3\text{mol}^{-1}\text{s}^{-1} \pm 13.9556\%$$

14 Appendix D

Natural logarithm for the rate constant and reciprocal for absolute temperature uncertainties rounded to four decimal places as performed in Section 7.3:

$$T = 30℃$$

$$\frac{1}{T} = \frac{1}{(30\pm0.5)+273.15} \approx 0.003299\text{K}^{-1}$$

$$\delta\frac{1}{T} = (\frac{0.5}{30} \times 0.003299) \pm 5.4978 \times 10^{-5}\text{K}^{-1}$$

$$\ln k = \ln((0.54152 \pm 1.9901) \times 10^{-12}\text{dm}^3\text{mol}^{-1}\text{s}^{-1}) \approx -28.2444$$

$$\delta\ln k = \frac{\delta k}{k} = \frac{1.9901 dm^3 mol^{-1} s^{-1}}{0.54152 dm^3 mol^{-1} s^{-1}} \approx \pm 3.6751$$

$$T = 40℃$$

$$\frac{1}{T} = \frac{1}{(40\pm0.5)+273.15} \approx 0.003193\text{K}^{-1}$$

$$\delta\frac{1}{T} = (\frac{0.5}{40} \times 0.003193) \pm 3.9917 \times 10^{-5}\text{K}^{-1}$$

$$\ln k = \ln((1.8051 \pm 0.9177) \times 10^{-12}\text{dm}^3\text{mol}^{-1}\text{s}^{-1}) \approx -27.0404$$

$$\delta\ln k = \frac{\delta k}{k} = \frac{0.9177 dm^3 mol^{-1} s^{-1}}{1.8051 dm^3 mol^{-1} s^{-1}} \approx \pm 0.5084$$

$$T = 50℃$$

$$\frac{1}{T} = \frac{1}{(50\pm0.5)+273.15} \approx 0.003095\text{K}^{-1}$$

$$\delta\frac{1}{T} = (\frac{0.5}{50} \times 0.003095) \pm 3.095 \times 10^{-5}\text{K}^{-1}$$

$$\ln k = \ln((3.2491 \pm 1.6519) \times 10^{-12}\text{dm}^3\text{mol}^{-1}\text{s}^{-1}) \approx -26.4526$$

$$\delta\ln k = \frac{\delta k}{k} = \frac{1.6519 dm^3 mol^{-1} s^{-1}}{3.2491 dm^3 mol^{-1} s^{-1}} \approx \pm 0.5084$$

$$T = 60℃$$

$$\frac{1}{T} = \frac{1}{(60\pm0.5)+273.15} \approx 0.003002\text{K}^{-1}$$

$$\delta\frac{1}{T} = (\frac{0.5}{60} \times 0.003002) \pm 2.5014 \times 10^{-5}\text{K}^{-1}$$

$$\ln k = \ln((7.0397 \pm 1.6837) \times 10^{-12}\text{dm}^3\text{mol}^{-1}\text{s}^{-1}) \approx -25.6795$$

$$\delta\ln k = \frac{\delta k}{k} = \frac{1.6837 dm^3 mol^{-1} s^{-1}}{7.0397 dm^3 mol^{-1} s^{-1}} \approx \pm 0.2392$$

$$T = 70℃$$

$$\frac{1}{T} = \frac{1}{(70 \pm 0.5) + 273.15} \approx 0.002914 \mathrm{K}^{-1}$$

$$\delta\frac{1}{T} = \left(\frac{0.5}{70} \times 0.002914\right) \pm 2.0816 \times 10^{-5} \mathrm{K}^{-1}$$

$$\ln k = \ln((11.0108 \pm 1.5366) \times 10^{-12} \mathrm{dm}^3\mathrm{mol}^{-1}\mathrm{s}^{-1}) \approx -25.2321$$

$$\delta \ln k = \frac{\delta k}{k} = \frac{1.5366 dm^3 mol^{-1} s^{-1}}{11.0108 dm^3 mol^{-1} s^{-1}} \approx \pm 0.1396$$