

IB Chemistry
SL Internal Assessment

***Kinetics of the acid-catalyzed
iodination of propanone reaction***

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A: Introduction

Recently, MIT researchers announced a breakthrough contraceptive pill that would be taken monthly, rather than daily, to avoid unintended pregnancies (1). Once swallowed, the pill takes 4 weeks to fully dissolve, gradually releasing the contraceptive drug. The medical technology underlying this ingenious design is founded on chemical kinetics and rates of reaction. My interest in this topic was sparked by a simple in-class demonstration, the iodine clock reaction (2), which is based on the same fundamental kinetic principles. The investigation presented here considers the effect of temperature on the acid-catalyzed iodination of propanone (acetone) reaction, in addition to an examination of the kinetics associated with the reaction.

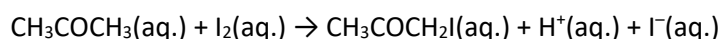
Research question

What is the effect of temperature ($^{\circ}\text{C}$) on the initial rate of reaction ($\text{mol dm}^{-3}\text{s}^{-1}$) of the iodination of propanone reaction?

Background research

The iodination of propanone and rate equation

Acid-catalyzed iodination of propanone is a spontaneous halogenation reaction between propanone and iodine in an acidic environment, forming colorless iodopropanone and hydrogen iodide as products. The reaction can be observed visually thanks to the gradual decolorization of the brown-colored iodine water converting into colorless iodopropanone and hydrogen iodide, expressed as follows (3):



The rate equation/Rate law

As with any non-reversible reaction, the initial rate of reaction should increase with concentration; this can be expressed by a rate law. Since the iodination of propanone is a reaction with three reactants—namely, acetone (Ac), sulphuric acid (H^+), and iodine (I_2)—the rate law may be expressed as shown below (3):

$$\text{rate} = k[\text{Ac}]^p[\text{H}^+]^q[\text{I}_2]^r$$

where k is the rate constant, a value unique to the reaction at any given temperature, and p , q , and r , are exponents representing each reactant's order of reaction. Additionally, the reactants are surrounded by square brackets to denote concentration, as required by the rate law.

Colorimetry

The Beer-Lambert law states that the absorption of a substance is proportional to its concentration (4), in the following expression:

$$A = \epsilon \times c \times l$$

where A is the absorbance, ϵ is the molar absorption coefficient, c is the concentration, and l is the optical path length. This law establishes a linear relationship between colorimeter absorbance readings and iodine concentration. A change in absorbance over time will therefore be proportional to a change in concentration over time—our rate. The iodination of propanone reaction is such that the reactants undergo a color change from brown (I_2) to colorless ($\text{CH}_3\text{COCH}_2\text{I}$). This decolorization can be observed thanks to a colorimeter with filters tailored to the absorption spectrum of aqueous iodine.

The rate of reaction must be taken where time $t=0$ by finding the tangent to the concentration vs. time graph (Figure 1), such that the reactants still have their starting concentrations. This is because the accumulation of products within the same reacting vessel will slow the reaction as it progresses, according to collision theory (3).

The Arrhenius equation

Having tested the effect of concentration of each reactant on the rate of reaction, the second part of the investigation will estimate the activation energy of the reaction by varying the temperature and

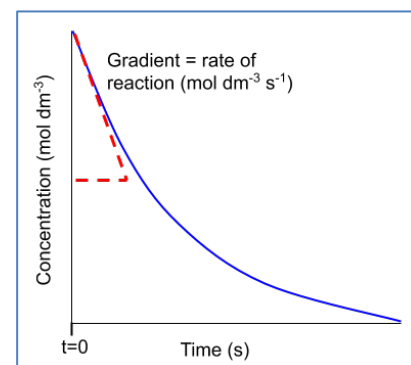


Figure 1. Graphically finding the rate of reaction

observing the effect on the rate of reaction. According to collision theory, one would expect that as the temperature is increased, the reactants experience more frequent collisions and a higher number of molecules will have the activation energy needed to react, as shown by the Maxwell-Boltzmann curves drawn below.

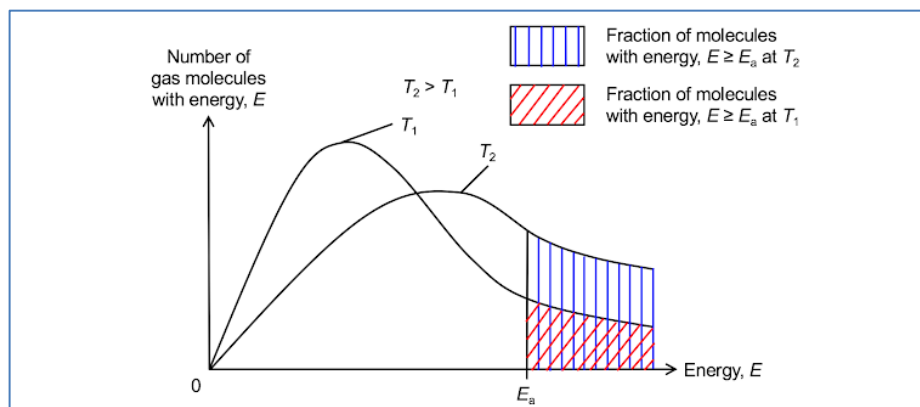


Figure 2. Maxwell-Boltzmann distributions of two temperatures (5)

Therefore, it follows that as the temperature increases, the rate of reaction should also increase. If the rate constant k is considered the “speed” inherent to the reaction, a higher temperature should mean a higher k --or speed--and hence a higher rate of reaction. This relationship can be modelled by the Arrhenius equation (6) (below), which shows that the rate constant is related to the temperature and activation energy, among other constants.

$$k = A \cdot e^{\frac{-E_a}{RT}}$$

Equation 1: The Arrhenius equation

The rate constant k is specific to the temperature at which the reaction was carried out, meaning that both k and T are variables in the expression. The Arrhenius equation can then be rearranged such that it can be plotted in terms of x (an expression of T) and y (an expression of k), as shown in Equation 2. Collecting a range of temperature trials and plotting $\frac{1}{T}$ on the x-axis and natural logarithm of k , $\ln k$ on the y-axis, should yield a gradient of $\left(\frac{-E_a}{R}\right)$, which can be multiplied by the negative of the gas constant R (-8.31) to return a value for the activation energy E_a .

$$k = A \cdot e^{\left(\frac{-E_a}{R \cdot T}\right)}$$

$$\ln k = \ln \left(A \cdot e^{\left(\frac{-E_a}{R \cdot T}\right)} \right)$$

$$\ln k = \ln A + \ln \left(e^{\left(\frac{-E_a}{R \cdot T}\right)} \right)$$

$$\ln k = \ln A + \frac{-E_a}{R \cdot T}$$

$$\ln k = \left(\frac{-E_a}{R} \right) \left(\frac{1}{T} \right) + \ln A$$

Equation 2: Rearranging the Arrhenius equation for plotting

Aim

The aim of this investigation is to experimentally determine the effect of temperature on the rate of reaction of the iodination of propanone reaction in acidic conditions. Furthermore, it aims to estimate a value for the activation energy of the reaction, and to compare the results to established literature.

This is an investigation in two parts: Part A involves systematically varying the concentration of the reactants to find an expression for the reaction’s rate equation with values for k and exponents for $[Ac]$, $[I_2]$, $[H^+]$. Part B will test one set of concentrations at a range of different temperatures, enabling plotting of the Arrhenius equation graphically to give an estimate of E_a , the reaction’s activation energy.

Hypothesis

According to kinetics theory, an increase in the temperature of a reaction would signify greater thermal heat energy, and hence more energetic and frequent collisions between reactants (7). This means that time for reaction to take place should decrease, and hence the rate of reaction should increase.

Furthermore, if one considers the Maxwell-Boltzmann distributions shown earlier in Figure 2, a stretch toward the right (more energetic) side would cause more particles to surpass the required E_a threshold. Moreover, as it stretches further, the height of the curve increases as well, meaning that as the temperature increases, the rate at which the rate of reaction increases should increase as well – i.e., an exponential relationship between temperature and rate of reaction is expected.

With regard to the activation energy, its value cannot be deduced with any non-empirical method. There is no formal literature value for the activation energy of the iodination of propanone; however previous experimental studies have found values approximating 92kJmol^{-1} (8).

B: Methodology

Variables

Independent

In Part A, reactant concentrations were varied systematically to find the rate equation, as detailed in Table 4, which shows the required volume of each reactant. In Part B, the temperature of a run of reactant concentrations, detailed in Table 5, was varied from a minimum value of 25°C up to 60°C in 5 intervals ($25.0, 30.0, 40.0, 50.0, 60.0^\circ\text{C}$). This range was selected for its simplicity to reproduce in a lab setting using a standard hot water bath, representing a large enough temperature increment size that the uncertainty in water bath temperature ($\pm 0.5^\circ\text{C}$) was not a significant source of uncertainty. 25°C was selected rather than 20°C , due to the lab tap water temperature being limited at 22°C . Acetone has a boiling point of 54°C ; however, this was not an issue for the 60°C trial, because acetone was the one reactant not heated, lowering the overall solution temperature.

Dependent

Initial rate of reaction ($\text{mol dm}^{-3} \text{s}^{-1}$), as found from the gradient of the graph of the decolorization curve of the iodine-acetone-acid solution (see Appendices 4-7).

Table 1: Controlled & Uncontrolled Variables

Controlled		
Variable	Effect on data	How the variable is controlled
Reactant volumes / concentrations	As explained in the introduction, changing the concentration of acetone or sulphuric acid would have a directly proportional effect on the rate of reaction. Hence an unwanted deviation from the prescribed concentrations could result in aberrant rates of reaction.	Reactants were measured using precise $3\text{ml} \pm 0.1$ syringes.
Extent of solution mixing	Unmixed reactants via difference in densities means fewer reacting molecules per unit time, lower rate of reaction for trials that were not sufficiently mixed.	The cuvette with the heated solution was shaken firmly 4 times before starting logging.
Room temperature	Fluctuations in room temperature could affect the rate of cooling, by creating a larger temperature gradient between the solution and the air surrounding it.	Data was collected over a single continuous session in a lab setting, meaning that atmospheric variables did not change significantly in the space of just a few hours.

Table 1: Controlled & Uncontrolled Variables (continued)

Controlled		
Variable	Effect on data	How the variable is controlled
Temperature loss during data logging	Assuming that the water bath temperature is the exact temperature that the reactants will be at during data logging is incorrect, because there will be constant heat loss radiating into the surrounding environment.	A cuvette lid and colorimeter lid helped maintain a stable, insulated environment during data logging, in an effort to mitigate cooling from the external environment.
Time between initiating reaction and beginning of measurement	Given that the method requires that the reaction be initiated before insertion into colorimeter for logging (so that it can be shaken), there is a time delay and hence a reduction in the perceived initial rate of reaction.	The steps involving initiation, shaking and insertion into colorimeter will be performed swiftly and within 8 seconds, as displayed on a stopwatch.
Uncontrolled		
Overall temperature loss	Higher temperature runs in the 50°C and 60°C range will have a higher temperature gradient with the surrounding air than the room-temperature trials (25°C) and will therefore radiate heat at a greater rate than the low-temperature runs.	This will be monitored during the experiment, and an extension investigation could potentially account for this temperature loss.

Safety:

Chemical disposal / environmental considerations: (Table 2)

Note: For mixed chemicals (products from reaction): incinerate.

Ethical considerations:

There were no ethical considerations significant enough to impact the investigation.

Chemical hazards

Risks should be verified on PubChem (9). If any substances come into contact with skin, eyes, or mouth, they should be washed off immediately. Experimentation should be carried out in a well-ventilated area and with proper personal protective equipment (PPE) (glasses, lab coat) throughout (10).

Standard safety procedures are listed in Table 2, below.

Table 2: Chemical hazards

Chemical	Risk assessment	Recommended disposal / environmental considerations
Iodine solution (11)	Low hazard in concentrations below 1M (solution used was 0.05M).	Disposal at hazardous waste dump.
Sulphuric acid (12)	1M H ₂ SO ₄ is classified as an irritant by CLEAPSS, and should therefore be kept away from eyes, mouth, and skin. Spillage should be avoided by using stable test tube racks for storage.	Dilute with water, then neutralize with H ₂ O ₂ . Neutralization will be evident by temperature change. Can be washed down the sink afterwards.
Propanone solution (13)	Acetone is highly volatile and will produce ignitable fumes that are also irritants, so keep evaporation to a minimum by keeping container closed when possible and away from open flames. For this reason, propanone was not heated in the hot water bath but added separately later.	Must be disposed of as non-halogenated organic waste and taken to a hazardous waste dumping facility.
Iodopropanone (9)	Iodopropanone is one of the products of the reaction and a known irritant while aqueous and as fumes. Haloketones such as iodopropanone are lachrymators and should therefore be covered.	Once reactions have occurred the waste iodopropanone, hydrogen iodide, and excess reactants, should be decanted into a flask and covered/blocked to prevent species evaporation.

Method:

Table 3: Apparatus	
Materials	Chemicals
4 Cuvettes with lids (4cm ³)	50cm ³ 1M sulphuric acid (H ₂ SO ₄ aq.)
Colorimeter (±0.01% trans.)	50cm ³ ~0.05M iodine solution/iodine water (I ₂ aq.)
4x Glass beakers (100cm ³)	50cm ³ 1M propanone (acetone) solution (CH ₃ COCH ₃ aq.)
4x Luer-slip 3ml PFA* syringes (3cm ³ ±0.1)	50cm ³ distilled water (sub. deionized water) (H ₂ O)
4x Test tubes (25cm ³)	
Hot water bath (20-60 °C±1)	
Laptop/phone for colorimeter logging	

*Standard LDPE/HDPE syringes are subject to immediate degradation on exposure to acetone (14), so PFA/PTFE/FEP (Teflon) syringes (or an equivalent chemically inert plastic) are recommended instead.

Setup

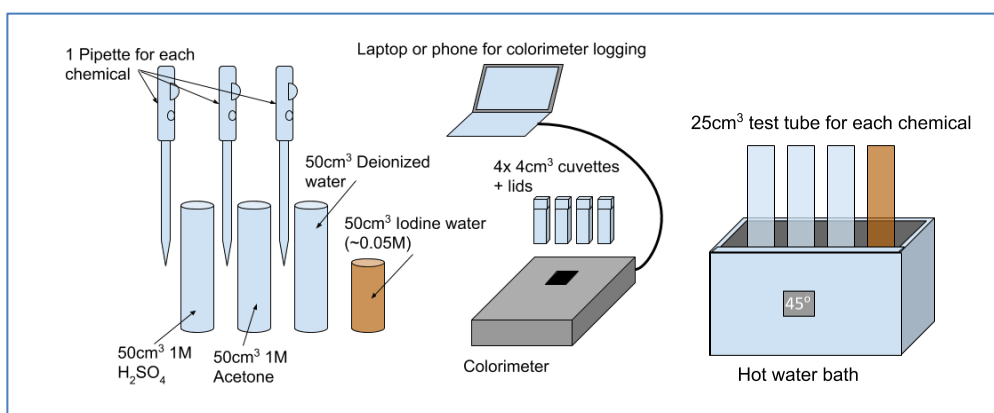


Figure 3. Material setup diagram created with Google Draw.

Table 4: Part A - Concentration trial volumes				
Run #	Volume of 1M acetone solution (cm ³) ±0.05	Volume of 1M sulphuric acid (cm ³) ±0.05	Volume of deionized water (cm ³) ±0.05	Volume of 0.05M iodine solution (cm ³) ±0.05
1	0.75	0.75	0.75	0.5
2	1.50	0.75	0.00	0.5
3	0.75	1.50	0.00	0.5
4	0.75	0.75	0.25	1

Table 5: Part B - Temperature trial volumes			
Vol. 1M acetone solution (cm ³) ±0.05	Vol. 1M H ₂ SO ₄ (cm ³) ±0.05	Vol. deionized water (cm ³) ±0.05	Vol. 0.05M iodine solution (cm ³) ±0.05
0.50	0.50	1.50	0.50

Pre-experiment

1. Set up data logging for the colorimeter through Bluetooth or laptop connection accessories, based on the device specifications.
2. Calibrate colorimeter. A blue filter (450-485 nm) should be applied because aqueous iodine has a peak absorbance wavelength of $\lambda_{max} = 464 \text{ nm}$ (10). Select transmittance for measurements.

Part B:

3. Pre-heat water bath to desired temperature in °C (25.0, 30.0, 40.0, 50.0, 60.0).
4. Fill 3x 25 cm³ test tubes with iodine, deionized H₂O, and H₂SO₄ respectively, indicating contents using a whiteboard marker, and place in test tube rack.
5. Immerse test tube rack in hot water bath and prevent spillage by verifying that the water level is less than half the height of the test tubes/rack.
6. Fill another test tube with acetone; store at room temperature on a test tube rack outside of the bath.

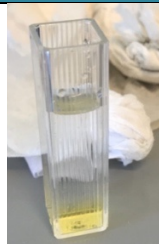
Trial Procedure

7. Using a syringe, transfer volumes of I₂, deionized water, and H₂SO₄ into a cuvette, with volumes given in Table 4 for Part A, Table 5 for Part B, and measuring from the bottom of the meniscus. A separate syringe should be used for each substance. The cuvette should be partially submerged in the water bath until ready to be used.
8. Measure the prescribed volume of acetone (Tables 4,5) in another syringe.
9. When ready to start the reaction, start the timer, dry the outside of the cuvette with a paper towel, pour the pre-measured acetone into the cuvette, cap with lid, and shake firmly 4 times. Place the capped cuvette in the colorimeter and start logging. If step 9 takes longer than 8 seconds, it must be repeated.
10. Repeat step 7-10 for each of the 5 trials of each of the 5 temperatures (25.0, 30.0, 40.0, 50.0, 60.0 °C), and the 4 concentration runs (standard, 2x propanone, 2x sulphuric acid, 2x iodine).
11. A buffer time of 5 minutes is required between increasing hot water bath temperature and using chemicals, to ensure that reactant temperature reflects that of the hot water bath.

C: Results and data

Qualitative data

Part A:

Run variant	Initial conditions	After reaction	 <p><i>Figure 4. Incomplete mixing after trial</i></p>
Standard	Reddish-brown solution	Colorless, transparent	
Double propanone	Reddish-brown solution, lighter than standard run	Colorless, transparent	
Double acid	Reddish-brown solution, lighter than standard run	Colorless, transparent	
Double iodine	Dark brown solution	Incomplete mixing was observed in some trials (Fig. 4). Acetone is less dense than water (0.784 g/ml), hence it had a tendency to remain at the top of cuvette even after shaking. Conversely, iodine is denser than water (4.94 g/ml); the acetone and iodine were separated in the solution, as is visible by the yellow tint of iodine at the bottom of the cuvette in Figure 4. This may have reduced the rate of reaction in some trials.	

Part B:

At temperatures above 30°C the reaction completed within less than 15 seconds of adding acetone, hence only a couple seconds of data collection were possible, contributing to uncertainties in the initial rate found from the decolorization graph.

Quantitative data

Raw data

Part A:

Table 7: Raw data of initial rate from decolorization graph and order of reaction				
Variation tested	Initial rate / mol dm ⁻³ s ⁻¹	Order of reaction		
		Calculated	Expected (15)	Percentage error (%)
Standard	0.0406	1.00	1x	N/A
Double propanone	0.0853	2.10	2x	0.05
Double acid	0.0835	2.06	2x	0.03
Double iodine	0.0401	0.99	1x	0.01

(Full decolorization graphs with initial rates are included in Appendix 4-7)

Part B:

Table 8: Raw data of initial rate at different temperatures						
Temp. (°C) ±0.5°C	Initial rate / mol cm ⁻³ s ⁻¹					
	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5	Average
60	12.6	6.80	1.46	16.0	6.11	8.596
50	7.75	6.12	15.2	12.4	6.62	9.616
40	6.36	12.8	7.31	13.2	0.832	8.103
30	2.44	4.62	2.94	1.64	3.46	3.021
25	2.76	2.40	1.28	2.33	2.38	2.229

(Bold indicates inconsistent results, red indicates outliers)

Processed data

Part B:

Table 9: Processed data of rate constant (k) values at different temperatures					
Temp. (°C) ±0.5	Average initial rate (mol dm ⁻³ s ⁻¹)	Rate constant k (mol ⁻¹ s ⁻¹)	Conc. of CH ₃ COCH ₃ aq. [Ac] (mol dm ⁻³) ±0.01	Conc. of H ₂ SO ₄ aq. [H ⁺] (mol dm ⁻³) ±0.01	Conc. of iodine aq. [I ₂] (mol dm ⁻³) ±0.01
60	0.01038	373680	0.167	0.167	0.008
50	0.009616	346190	0.167	0.167	0.008
40	0.009921	357147	0.167	0.167	0.008
30	0.003366	121185	0.167	0.167	0.008
25	0.002466	88785	0.167	0.167	0.008

Table 10: Processed data of 1/T and ln(k) for Arrhenius plot				
Temperature ±0.5°C			Rate constant k (mol ⁻¹ s ⁻¹)	ln(k)
Celsius (°C)	Kelvin (°K)	1 / Temperature (K ⁻¹)		
60.0	333	0.00300	373680	12.8311
50.0	323	0.00309	346190	12.7547
40.0	313	0.00319	357147	12.7859
30.0	303	0.00330	121185	11.7050
25.0	298	0.00336	88785	11.3939

D: Analysis & evaluation

Discussion of data patterns

Part A:

The raw data from the concentration trials is extremely close to literature values, displaying percentage errors of only 1% to 5%. Given that the rate appears to double with double the concentration of propanone

or sulfuric acid, they are assigned an exponent of 1 in the rate law. Meanwhile, doubling iodine concentration shows no increase in the rate of reaction, therefore giving it an exponent of 0 and hence removing it from the rate law entirely (because mathematically, anything to the power of 0 equals 1).

Using this rate law, the units of the rate constant k can be found:

$$\text{rate} = k[\text{Ac}]^1[\text{H}^+]^1[\text{I}_2]^0 \rightarrow \text{rate} = k[\text{Ac}]^1[\text{H}^+]^1$$

Another piece of information that can be found from this data is the units of k : The units Acetone and sulphuric acid (not iodine, due to its order of reaction = 0) are substituted to solve for k :

$$\text{mol dm}^{-3}\text{s}^{-1} = k \times \text{mol dm}^{-3} \times \text{mol dm}^{-3}$$

Where $\text{mol dm}^{-3} = M$: $M \text{ s}^{-1} = k \times M \times M$

$$\therefore k = \frac{M \text{ s}^{-1}}{M \times M} = M^{-1} \text{ s}^{-1} = \text{mol}^{-1} \text{ dm}^3 \text{ s}^{-1}$$

The units of k are therefore $\text{mol}^{-1} \text{ dm}^3 \text{ s}^{-1}$.

Part B:

The rate of reaction ($\text{mol dm}^{-3}\text{s}^{-1}$) can be plotted against the temperature of the solution as shown below in Figure 5. An exponential relationship was expected, as discussed in the introduction. When the outlier (indicated in red) is included, the correlation observed is only of moderate strength ($0.6 < R^2 < 0.8$) (16). Without the outlier, the correlation becomes much stronger ($R^2 = 0.96$). While uncertainty in the temperature remains at a constant $\pm 0.5^\circ\text{C}$, the rate of reaction is subject to extremely high range values from 40°C to 60°C (76%, 47%, 85% of the average). Given the large error bars, all five points can fit on the best-fit exponential graph, however they could also theoretically fit a linear relationship – so much so that an exponential relationship is not evidently present at first glance without computer-generated curves of best fit. The low number of data points ($n=5$) also requires that this plot be observed with some degree of skepticism.

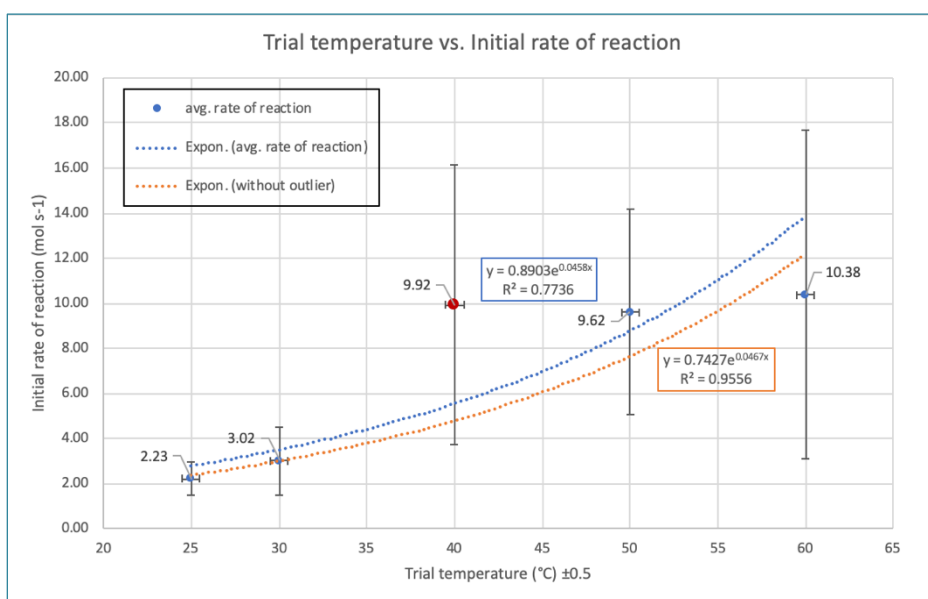


Figure 5. Graph of Trial temperature vs. Initial rate of reaction

Figure 6 (below) displays an Arrhenius plot of $-\ln(k)$ against the reciprocal of the temperature. The largest error bars on this graph are clearly visible on the ~ 0.00320 outlier, closely followed by the 0.00300 data point—the third and first highest temperatures trials respectively. Two trendlines are plotted: one with the outlier included, the other without. Interestingly, removing the outlier appears to have little effect on the gradient of the trendline (changing from 4602.7 to 4643.5 $\Delta = 40.8$), but greatly increases the strength of the observed correlation, moving from the strong $R^2 = 0.8$ to very strong $R^2 = 0.96$. It is also worth noting that the horizontal error bars increase with $1/T$, meaning that more uncertainty in measured temperature is present around the $25^\circ/30^\circ\text{C}$ range.

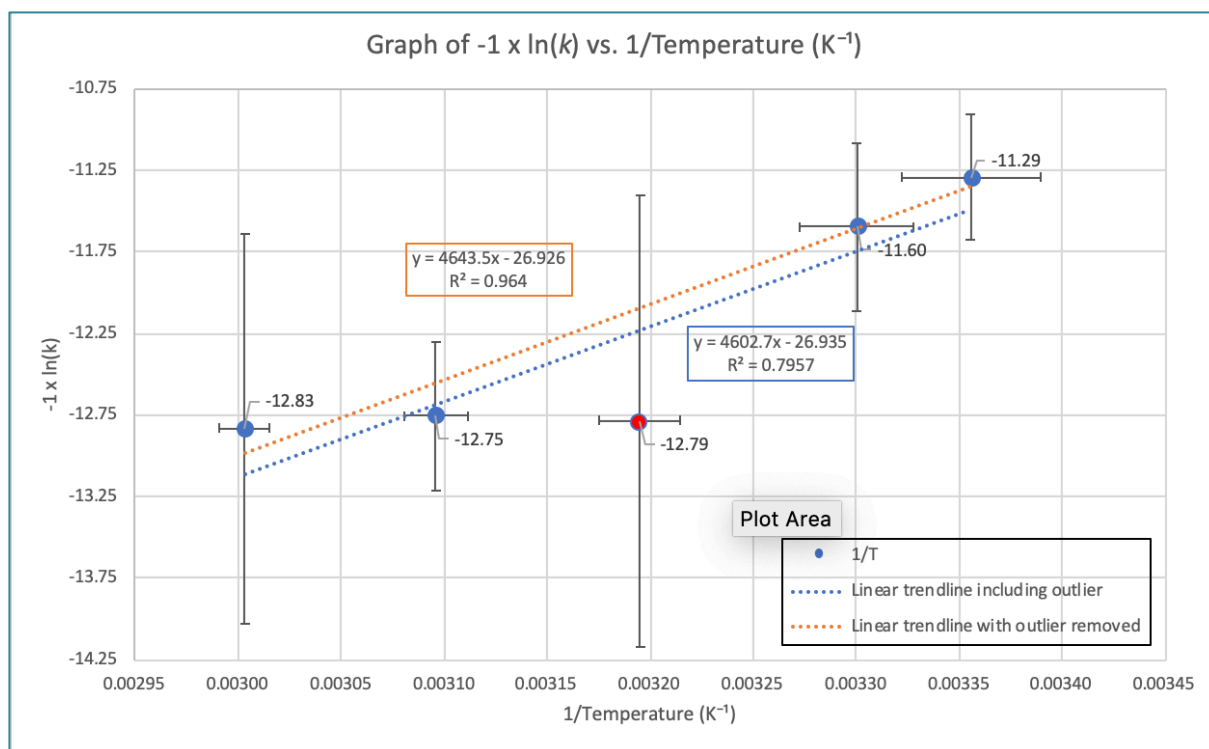


Figure 6. Graph of $-\ln(k)$ vs. $1/\text{Temperature (K}^{-1}\text{)}$

Using the gradient of the trendline with the outlier removed (4643.5), an expression for the estimated activation energy of the reaction can be found (as discussed in the introduction) by multiplying by 8.31 (the gas constant R). This returns a value of 38'587 Joules per mol (38.6 kJ mol^{-1}). This differs considerably from values found in past studies for the activation energy of the iodination of propanone reaction (8) at 92 kJ mol^{-1} , incurring a percentage error of 58.1%. This is only roughly a third of what was expected per the hypothesis and literature, suggesting errors in the methodology; uncertainties are quantified in the *impact of uncertainties* section below.

The Arrhenius pre-exponential constant A can also be found from this graph, as the y-intercept as seen in the equation below, where $\ln A$ takes the role of c in the equation of a line $y = m \cdot x + c$.

$$\ln k = \left(\frac{-E_a}{R}\right)\left(\frac{1}{T}\right) + \ln A$$

However, because $-\ln k$ was plotted on the y-axis, $\ln A$ will equal the negative of the y-intercept instead (+25.873). Hence, $A = e^{25.873} = 172,385,657,748 = 1.72 \times 10^{11}$

Now, all the variables associated with the Arrhenius equation of the reaction are known. The equation can be expressed back in its standard form:

$$k = A \times e^{\left(\frac{-E_a}{R \cdot T}\right)} \rightarrow k = 7.4 \times 10^{10} \times e^{\left(\frac{-35.7}{8.31 \times T}\right)}$$

Impact of uncertainties

Table 11: Apparatus uncertainty	
Type of apparatus	Uncertainty absolute value
Hot water bath temperature	$\pm 0.5^\circ\text{C}$
Colorimeter	$\pm 0.1\%$ Transmittance
Syringe readings	$\pm 0.1\text{ cm}^3$
Thermometer	$\pm 0.5^\circ\text{C}$

Uncertainties in the initial rates

A significant deal of the uncertainty originated from the data found for the initial rates of reaction.

Table 12: Uncertainties in the initial rates											
Temp. (°C)	Initial rate (mol dm ⁻³ s ⁻¹)										
	Trials					Average		Range (w/ outliers)		Standard dev. (w/ outliers)	
	Trial 1	Trial 2	Trial 3	Trial 4	Trial 5	w/ outliers	w/o outliers	abs	%	abs	%
60	12.6	6.80	1.46	16.0	6.11	8.596	10.380	7.275	0.846	5.730	0.667
50	7.75	6.12	15.2	12.4	6.62	9.616	9.616	4.551	0.473	3.989	0.415
40	6.36	12.8	7.31	13.2	0.83	8.103	9.921	6.193	0.764	5.118	0.632
30	2.44	4.62	2.94	1.64	3.46	3.021	3.021	1.492	0.494	1.120	0.371
25	2.76	2.40	1.28	2.33	2.38	2.229	2.229	0.741	0.332	0.557	0.250

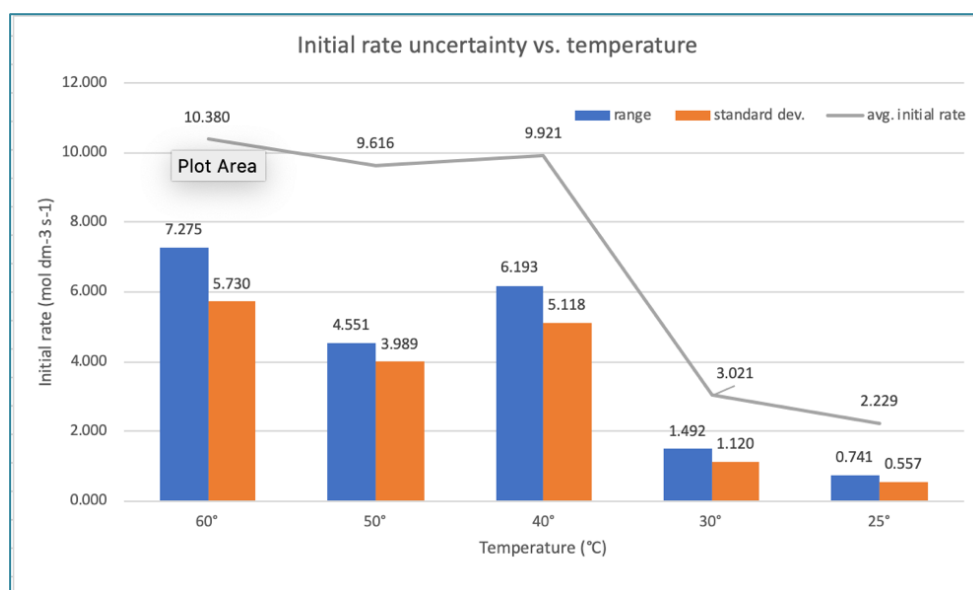


Figure 7. Graph of Initial Rate of Uncertainty vs Temperature

As can be seen in Figure 7, the uncertainties represented by the range and standard deviation comprise a large proportion of the average initial rate. The range for the 60°C trial in Table 12 is 84% of the average rate, and the standard deviation being 66% shows that the values are not just made unreliable by a few isolated outliers, but by systematic discrepancies in the data. A strange trend is visible in the raw initial rate data, where it would appear that half of the data points in the 50°C and 60°C trials occupy the 5-6 Ms⁻¹ range, and the others a 12-16 Ms⁻¹ range.

Percentage error

Assuming the aforementioned literature value for the activation energy of the iodination of propanone of 92kJmol⁻¹, the percentage error with and without the 40°C outlier can be found as such:

$$\frac{|Theoretical - Experimental|}{Theoretical} \times 100 = \% \text{ error}$$

$$\text{Including outlier: } \frac{|92 - 38.24|}{92} \times 100 = 58.43\%$$

$$\text{Without outlier: } \frac{|92 - 38.59|}{92} \times 100 = 58.04\%$$

That both percentage uncertainties yield a value of 58% (varying by 0.40%), suggests that a large systematic/methodological error is responsible.

Evaluation

Data limitations and improvements

Random errors

Parallax error

Given that such small volumes of chemicals were being used, the electrostatic force caused the polar liquids to form a curved meniscus. When misread, reactant volumes could be incorrectly added. The use of an air-displacement single-channel pipette for volumetric measurements could eliminate this limitation.

Systematic errors

Time delay between reaction start time and colorimeter logging / Too short reaction times for high-temperature trials

A significant drawback associated with the colorimeter method is that a cuvette is required. Due to the cuvette's small size (4 cm³), neither a magnetic stirrer nor a stirring rod is a viable option. Instead, the cuvette needs to be shaken, with a lid on. This is a time-consuming process, considering that the total reaction time for the 60°C trials was ~15s.

The simplest way to reduce this error would have been to increase the volume of iodine and reduce the concentration of H₂SO₄ and acetone. Given that the order of reaction of iodine is 0, this should have no impact on the reaction constant *k*, while lengthening the overall reaction time, minimizing the effect of having few data points from which to estimate the rate of reaction.

A second option would be to shift the temperature range down by 10-20°C and reduce its scope, such that the lowest trials require cooling instead of heating, provided by refrigeration or an ice bath, and the highest temperature trials are only around 20-30°C. As seen in figures 5 and 6, the 25°C and 30°C trials were the most precise by far.

Temperature loss

The temperature appeared to have significantly decreased in high-temperature trials due to the temperature gradient between the solution and room temperature. Also, the addition of room-temperature acetone solution would have reduced the temperature, but by an unknown amount. This led to incorrect estimations of the temperature at which the reaction was carried out.

This could be mitigated using several different approaches: Reactants could be heated a certain number of degrees above the target temperature, this additional margin having been found empirically by measuring the temperature before and after the addition of acetone. This additional temperature could also compensate for the temperature lost through radiation. Another, more palliative method, could be to use a range of temperatures closer to the 'equilibrium' ambient temperature, hence decreasing the temperature gradient and therefore reduce the heat energy radiated into the environment. Lastly, an extension is proposed in Appendix 4 that describes a possible technique for rectifying the temperature value, through the use of a 'cooling coefficient'.

Reactant evaporation

During the temperature trials all of the reactants except acetone were kept at hot temperatures for hours on end. For volatile substances like acetone, even room temperature is enough for significant evaporation in that period; the same applies to the H₂SO₄ and iodine water.

The error caused by this evaporative process could have been mitigated by the aforementioned reduction in temperature range, in addition to the usage of stopper on the tops of the test tubes. This would have the added benefit of lowering the human risk factor of both noxious fumes and spillage.

Methodological error

In this investigation, the gradient of the transmittance vs. time graph was erroneously assumed to be equal to the rate of reaction. This was not an issue for Part A, given that the order of reaction was just the ratio between (in this case) transmittance change over time. It had more serious ramifications for Part B, however, where the value found for *k* was many orders of magnitude from the value that was expected.

Unfortunately, this error only came to light at the end of the writeup process, so a calibration curve could not be calculated, nor better data collected.

Conclusion

The hypothesis stated that as the temperature at which the reaction was carried out increases, the initial rate of reaction will increase exponentially. The trend in the findings of this investigation strongly supports this prediction, despite error bars indicating that, theoretically, a linear relationship could fit within the ranges. This allows for the research question to be answered with moderate certainty: the temperature at which the acid-catalyzed iodination of propanone reaction is carried out will be exponentially correlated with the initial rate of the reaction.

From the Arrhenius plot in Figure 6, the calculated value for the activation energy of the reaction without outliers is 38.6 kJmol^{-1} . This is approximately a third of literature values (92 kJmol^{-1}); therefore, the percentage error was quite large at 58%. This discrepancy was explained through the uncertainty in the data collected—range, standard deviation, and propagation of instrumental errors—and analyzing sources of error in the methodology that may have contributed to the low activation energy value found.

Extensions

Given the set of advantages and disadvantages of finding the rate of reaction using a colorimeter, it may be worthwhile to compare results with other methods, observing where uncertainty is most present such that a better combined approach may be formulated. For instance, a time-based trial system such as the one detailed by Meyer (8) has the potential to produce more reliable (accurate) results, given that it is not limited to the small volumes of the cuvettes, hence reducing both the volumetric uncertainty and the error due to temperature loss. Furthermore, a time-based trial system could allow for precise temperature measurement throughout the reaction period, such that better estimates of $1/T$ can be formulated and hence more realistic estimations of activation energy. In addition, the methodology carried out in this investigation could be applied to other similar iodination reactions, such as the iodination of ethanol, where the Beer-Lambert law can be applied as the solution turns from brown to colorless.

Works Cited

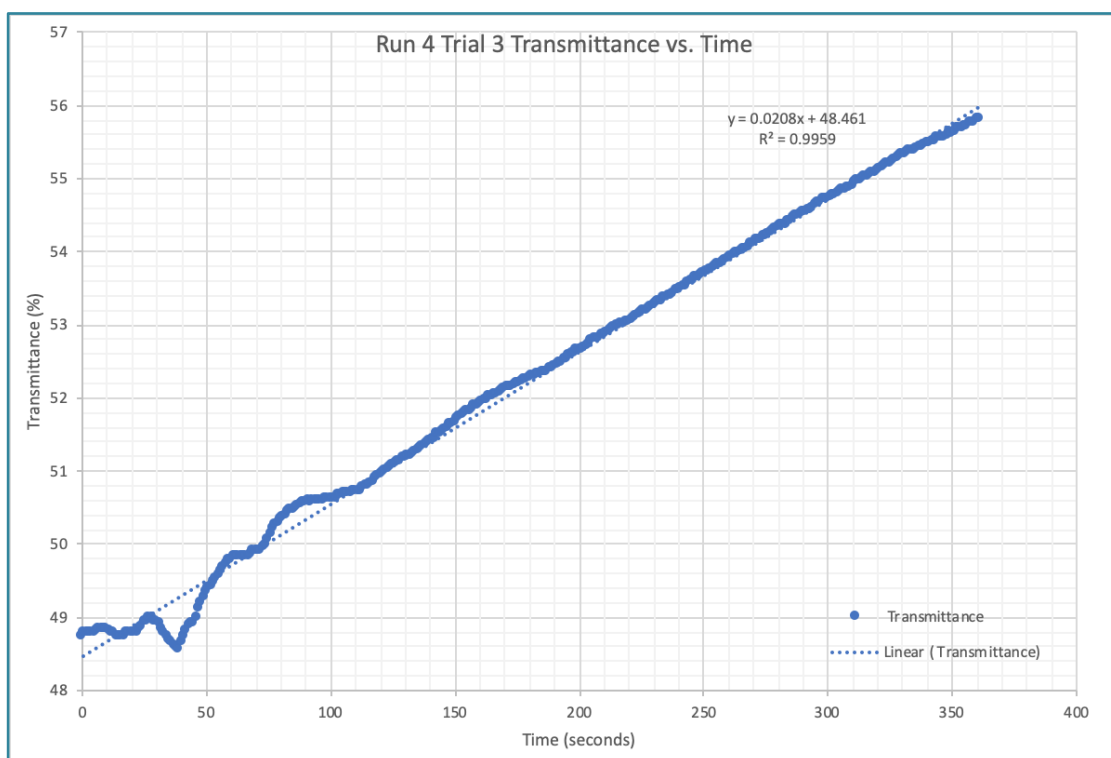
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F: Appendices

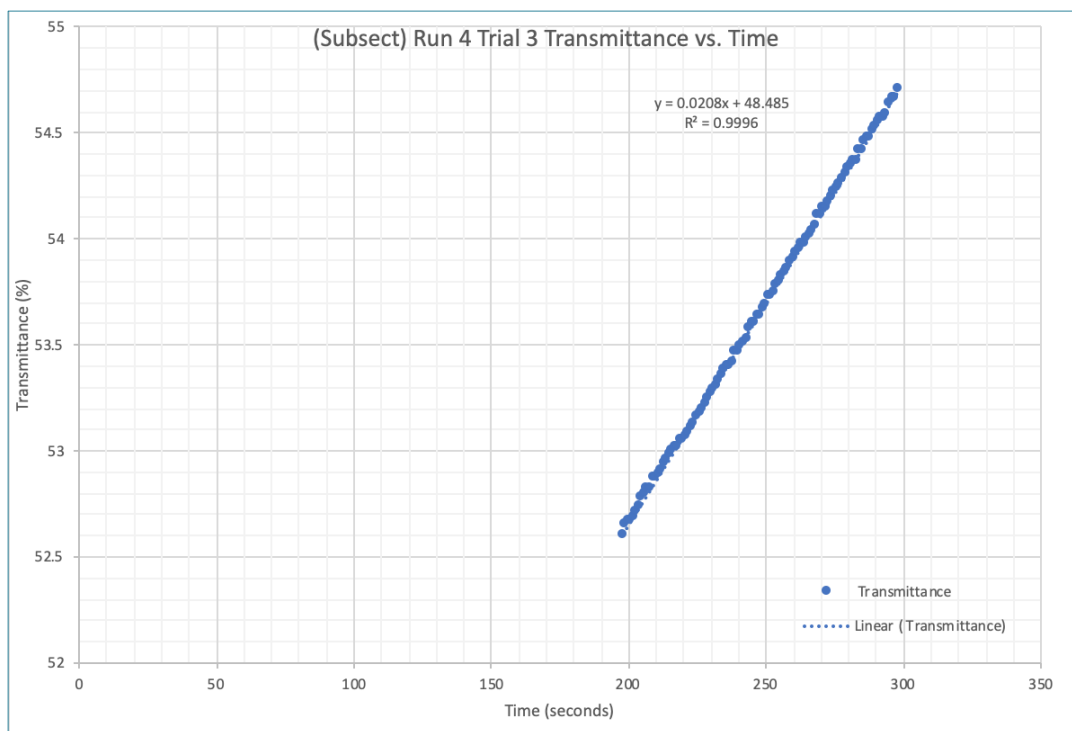
1. Example initial rate calculations

Timestamp	Transmittan	Absorbance	Colour
0	48.73	0.313	Green
1	48.78	0.312	Green
2	48.78	0.312	Green
3	48.78	0.312	Green
4	48.78	0.312	Green
5	48.8	0.312	Green
6	48.82	0.312	Green
7	48.84	0.312	Green
8	48.84	0.312	Green
9	48.84	0.312	Green
10	48.84	0.312	Green

Using the data received from the colorimeter (above), the transmittance is plotted against the timestamp to produce the following graph:

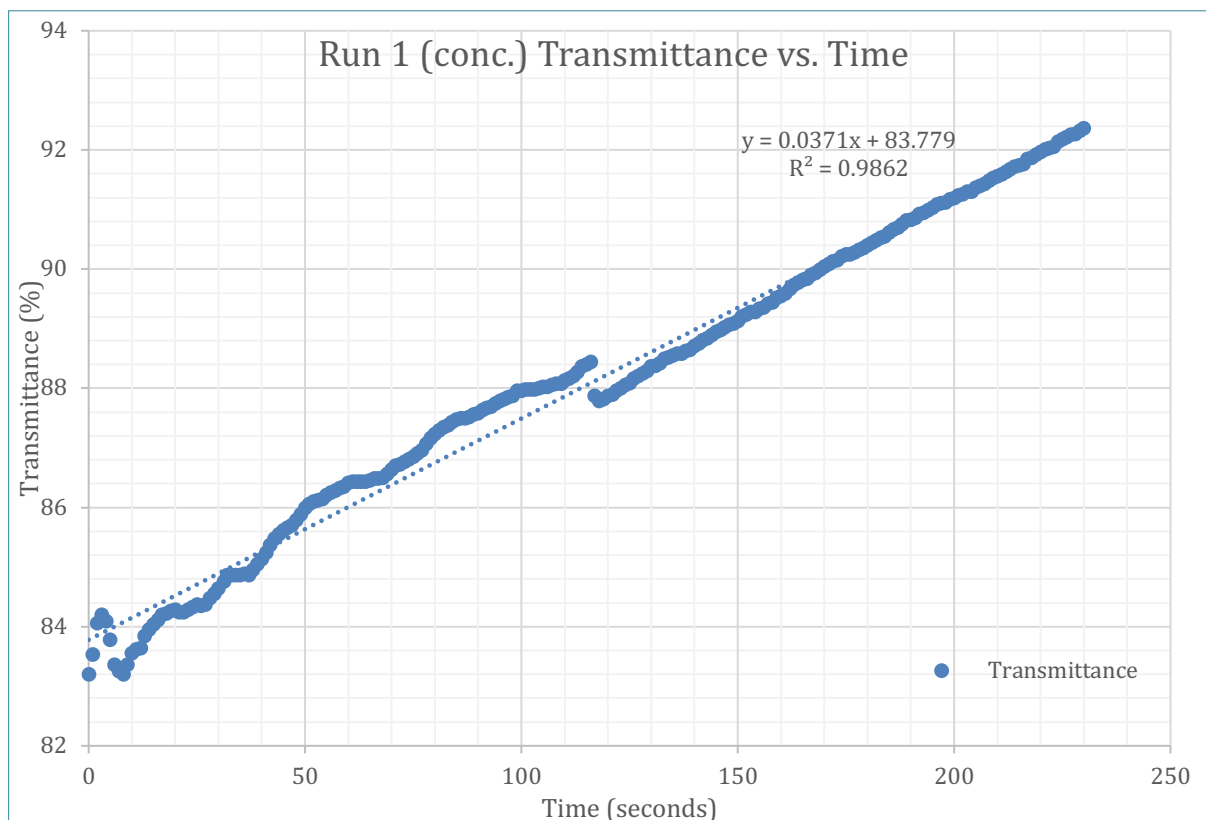


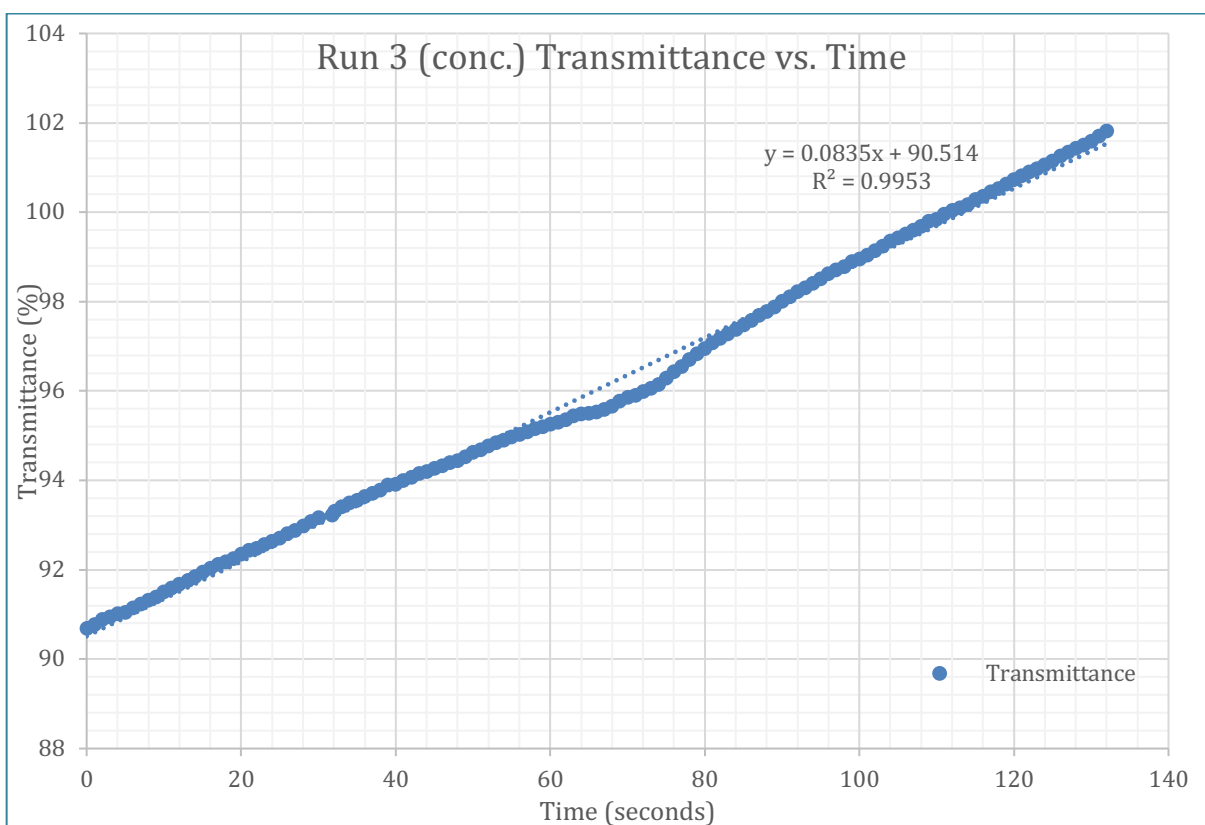
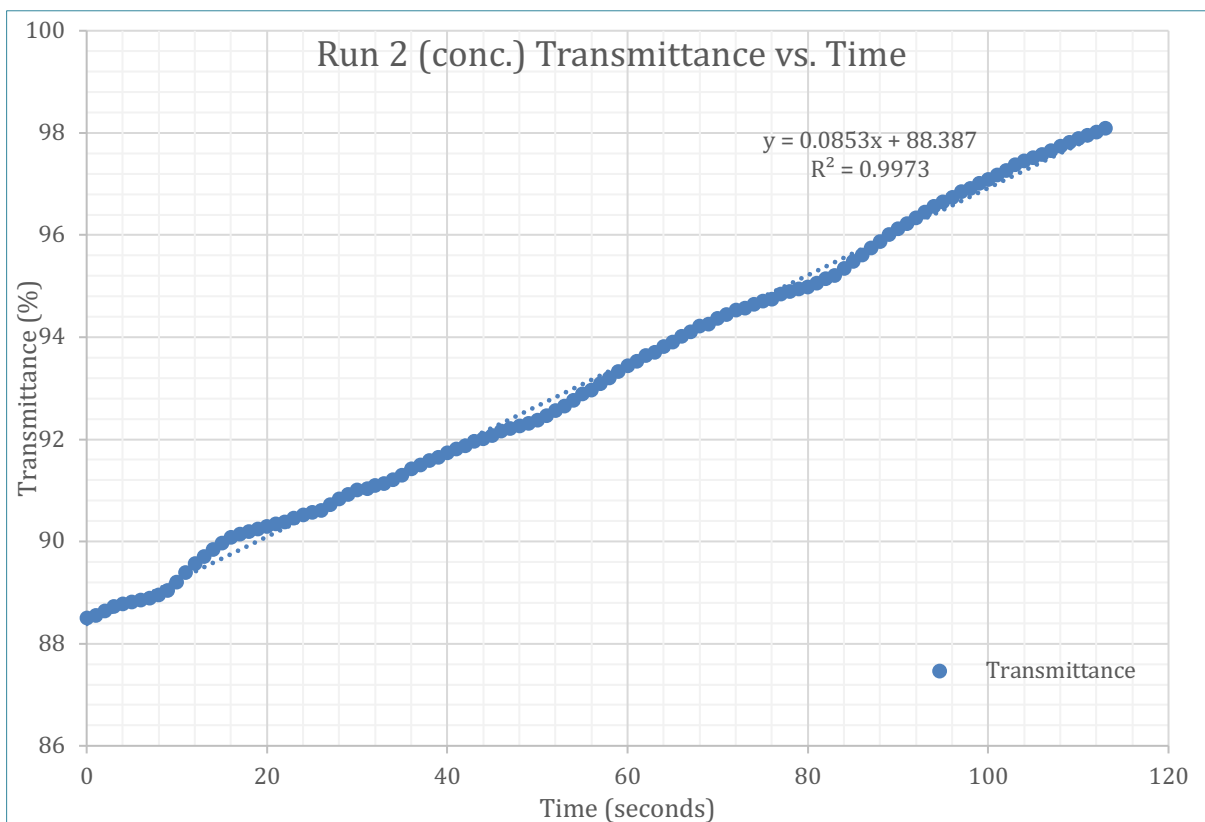
This graph has significant deviations at the beginning (until ~200) due to the colorimeter being turned on before the sample was fully inserted into the chamber. Therefore when calculating the rate of reaction, a subset is taken that doesn't include the visible errors at the beginning, and ends before the curvature at the end (around 320s), due to the necessity of finding the *initial* rate.

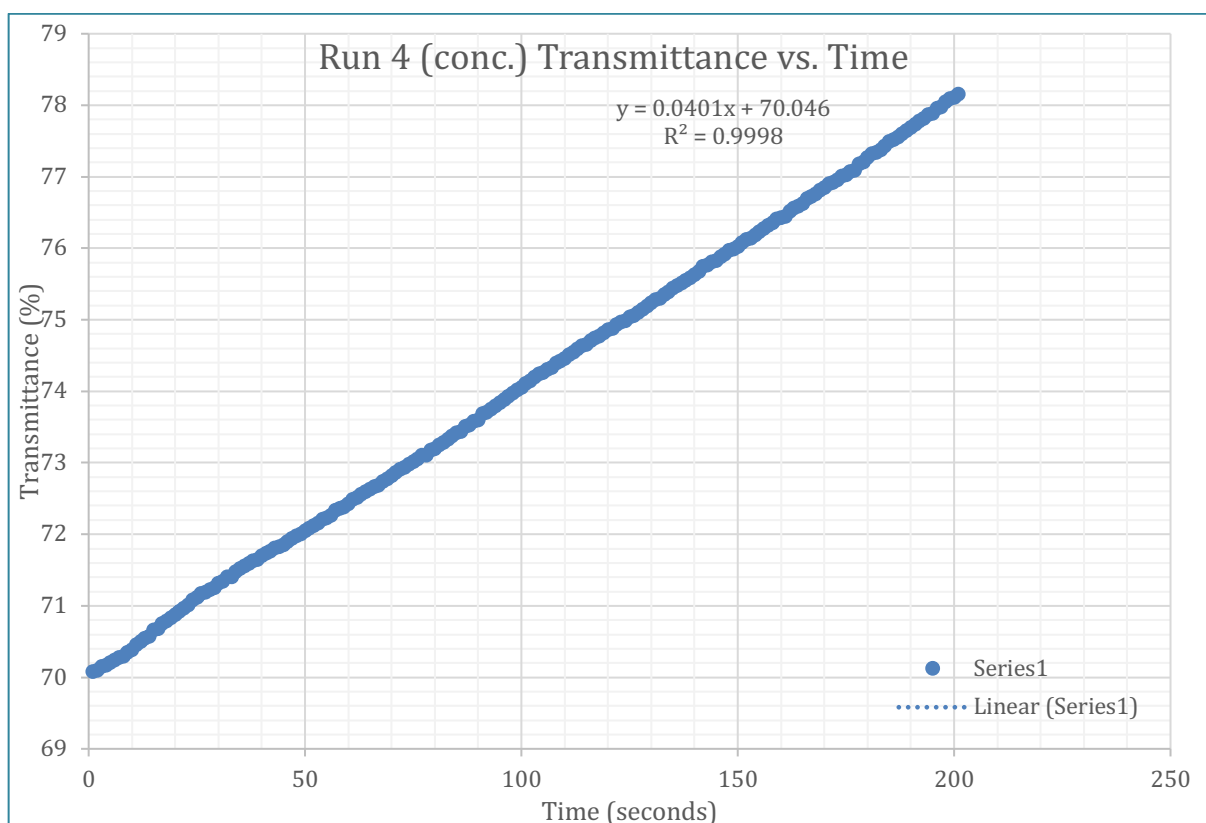


The gradient of the graph, 0.0208, is the initial rate of the reaction for this run and trial.

2. Decolorization graphs for concentration trials:







3. Accounting for the effect of radiating temperature

One can consider the effect that the error caused by high-temperature trials radiating heat may have had on value found for the activation energy E_a . Assuming that all temperature trials will tend towards restoring thermal equilibrium with their environment (the laboratory), it follows that trials for which the temperature already approximates room temperature (22°C), e.g. the 25° trial, will cool at a slower rate.

Therefore, future variations of the colorimeter method could apply a cooling coefficient $K_{cooling}$ to the temperature trial value, for more accurate estimation of the actual temperature at which the reaction takes place. Here, an improved value (T_{new}) is found as the old value minus the delta between the old temperature value and room temperature ($T_{equilibrium}$), times a cooling coefficient $K_{cooling}$.

$$T_{new} = T_{old} - K_{cooling} \times |T_{old} - T_{equilibrium}|$$

Taking an example cooling coefficient of 10% ($K=0.10$), the high-temperature values will experience a larger decline in temperatures, hence yielding temperature values across trials that are closer together. This also means that $1/T$ will experience a similar clustering effect. This will reduce the difference between temperature values, therefore yielding a lower change in x ($1/T$) for the same change in y ($\ln(k)$); this means that the gradient of the plot will increase, and thereby reach a larger (if not more realistic) value for E_a .

However, this technique was applied to this investigation because sufficient data was not collected for finding such a cooling coefficient. This technique could be included in the data processing of future investigations.