Investigating the Effects of Concentration on the Rate of Reaction

First and Last Name

Class

Date

Personal engagement

A metal will erode faster in acidic environment than in non-acidic environment. The rate of reaction increases as the concentration, temperature and catalyst increases. I was interested to know how concentration of reactants will affect the rate of reaction and how the values I will obtain varies with theoretical values and hence answering my research question "To determine the activation enthalpy and rate expression for the iodination of propanone"

Theoretical Background

For a chemical reaction to occur, several factors do affect the rate of this reaction. The factors include the concentration of the reacting agents, temperature, and the presence of a catalyst[1]. Iodation of propanone is a halogenation reaction between propanone and Iodine, where an acid is used as a catalyst. A chemical reaction between propanone and Iodine in acidic environment forms a colourless solution iodopropanone and hydrogen iodide. In this experiment, the concentration of propanone, sulphuric acid and Iodine will vary and the reaction rate of each will be calculated and comparison will be made.

The presence of sulphuric acid catalyses the reaction rate by adding the hydrogen Ions to the solution, thus increasing the reaction rate. By increasing the concentration of reactants, the reaction rate also increases; this is because there are many reacting ions, thus increasing the reaction rate. When the concentration is high, it reaches a point where increasing the

[1] Bhavsar, Kalpesh V., and Ganapati D. Yadav. "Synthesis of geranyl acetate by transesterification of geraniol with ethyl acetate over Candida antarctica lipase as catalyst in solvent-free system." *Flavour and Fragrance Journal* 34, no. 4 (2019): 288-293.

concentration has little or no effect on the reaction and thus the reaction stops. The following equation can show the reaction rate.

$$\text{Rate} = \frac{-\Delta[I\ 2\ ]}{\Delta t}$$

The reaction rate increases with an increase in concentration, and the reaction rate depreciates with a decrease in the concentration of reactants. The presence of an acid as a catalyst also increases reaction rate[2]. The reaction between Iodine and propanone results in colourless products (iodopropanone and hydrogen iodide) and the chemical equation can be shown using a chemical equation below.

CH3COCH3 (aq.) + I_2(aq.) → CH3COCH2I(aq.) + H+ (aq.) + I– (aq.).

As the reaction continues, Iodine's colour brown starts to disappear, forming a colourless liquid (iodopropanone and hydrogen iodide).

There will be four elements used (Propanone, sulphuric acid, deionized water, and iodine solution). The concentration of sulphuric acid, propanone, and Iodine will vary. This will help to determine how the concentration of sulphuric acid, propanone, and Iodine will affect the reaction rate. Iodine is considered ideal in this experiment because of its distinct brown colour. When the Iodine reacts with propanone. The reaction rate will be recorded by colorimeter, and the data will be saved on a computer. The concentration of propanone

[2] Easter, Quinn T., and Suzanne A. Blum. "Kinetics of the Same Reaction Monitored over Nine Orders of Magnitude in Concentration: When Are Unique Subensemble and Single-Turnover Reactivity Displayed?." *Angewandte Chemie* 130, no. 37 (2018): 12203-12208.

sulphuric acid and Iodine will also be changed, and the reaction rate will also be recorded. Based on these results, I will compare and contrast these results, which will help calculate how the concentration of reactants affects the rate of a reaction.

This experiment aims to investigate how concentration affects the rate of a chemical reaction for the iodation of propanone using acid as a catalyst. The next aim is to calculate the activation enthalpy for this reaction and contrast the results to what has been learned in theory.

Colorimetry

Colorimetry is a method used to calculate the concentration of compounds that are coloured in a given solution. According to Beer-Lambert's law, the absorption rate of a substance is directly proportional to the concentration of the reactant[3]. The absorption rate can be shown by the following equation below.

$A= \varepsilon X c X l$

Where;

A is the absorbance (The total amount of light passing through a solution)

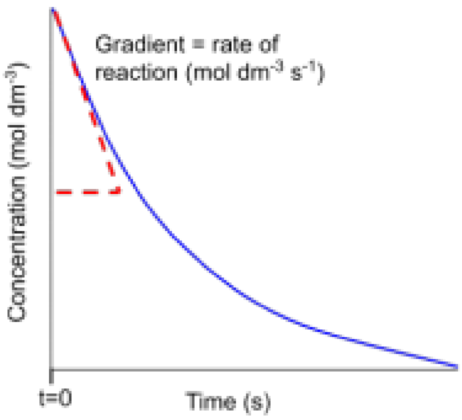
ε is the coefficient of absorption

c represents concentration

l optical length

[3] Fernandes, Godfree P., and Ganapati D. Yadav. "Selective glycerolysis of urea to glycerol carbonate using combustion synthesized magnesium oxide as catalyst." *Catalysis Today* 309 (2018): 153-160.

As the concentration of a reactant colour rises, more optical radiation will be absorbed; hence the rate of absorption rises. This law establishes a directly proportional relationship between absorption readings and calorimeter readings. In this experiment, the iodation of propanone where the reaction involves colour change, from the brown colour of Iodine (I_2) to colourless solution (iodopropanone and hydrogen iodide CH3COCH2I(aq.)) and this decolourization can be observed by colorimeter. The reaction rate can be taken at the time (t=0) and by finding the curve's gradient (concentration against time), as shown in the figure below.



Hypothesis

According to Beer-Lambert's law, the reaction rate is directly proportional to the concentration of reacting elements. As the concentration rises, the rate of reaction will also increase. As the concentration of Iodine reduces, the brown colour also reduces and hence the use of colorimetry. Regarding activation enthalpy, the values cannot be predicted with any method as there is no constant value for empirical enthalpy. As the rate of concentration increases, I predict that the rate of reaction will increase up to a certain level where an increase in concentration will not affect the rate of reaction.

Variables

Variable	Effect on data	How the variables will be controlled
Reactant volumes and concentrations	Changing the concentration of propanone or a catalyst (Sulphuric acid) will directly affect the reaction rate. A small deviation from the given concentrations will have advanced effects on the reaction rate, affecting the results.	Measurement of reactants was done using 5cm^3 graduated pipettes.
The expanse of mixing solutions	The purpose of mixing reactants is to make sure there are maximum reacting molecules per unit time, thus increasing the reaction rate; unmixed reactants, therefore, mean fewer reacting molecules hence the lower reaction rate.	Uncap cuvette is inverted upside down several times to make sure the reactants have mixed properly.

Methodology

Materials

Apparatus	Quantity	Uncertainty
Micro-tip plastic pipettes	4	±0.5cm^3
5cm^3 graduated pipettes	3	±0.5cm^3
Computer	1	-
Colorimeter with data logger	1	±0.01% trans
1 M sulphuric acid (H2SO4 aq.)	50cm^3	±0.5cm^3
1 M propanone solution (CH3COCH3 aq.)	150cm^3	±0.5cm^3
0.02 m iodine solution (I_2 aq.)	100cm^3	±0.5cm^3
Deionised water (H2O)	150cm^3	±0.5cm^3

Procedure

Part A: Evaluation for the colorimeter

1. Open the interface box of the colorimeter, set it up and connect it to the computer. Set the colorimeter according to the manual that accompanies the data logger. A blue filter will be used in this experiment.

Part B: Kinetic runs

2. Start the colorimeter with graphical display, open the option for transmittance, and set the time interval to 10 minutes.
3. Transfer 0.75cm^3 of 1 M propanone and 0.75 cm^3 of 1M sulphuric acid (H2SO4 aq.) using a clean graduated pipette. Add 1.50 cm^3 of deionized water and cup the cuvette and mix the solution by inverting the cuvette upside down four times.
4. Remove the cap, add 30 drops of 0.02 M iodine solution using a micro-tip plastic pipette. Cap the cuvette and lower it into the cell compartment of the colorimeter and immediately start recording.
5. When the transmittance signal flattens, stop recording the results.
6. According to the calorimeter manual, measure the initial rate of decrease in absorbance by converting the OY axis to absorption scale. Save this data.
7. According to
8. the following table, repeat the steps above (3) to (6) with other experiments.

Run	The volume of 1M Propanone (cm^3)	The volume of 1M Sulphuric acid (cm^3)	The volume of deionized water (cm^3)	Number of drops of 0.02 M Iodine solution I_2 (aq)	Number of drops of deionized water

1	0.75	0.75	1.50	30	-
2	1.50	0.75	0.75	30	-
3	0.75	1.50	0.75	30	-
4	0.75	0.75	1.50	15	15

Risk assessment

Avoid skin contact with these chemicals. Sulphuric acid is corrosive to the skin, and coming into contact with this chemical is very dangerous. Sulphuric acid can cause the eye, nose, and throat to irritate; hence protective gloves, masks, and eye-protective equipment must be worn at all times. Propanone is a highly flammable gas and hence has the potential of exploding. If the acids come into contact with your skin, dilute the acid using distilled water to avoid burning the acid's skin.

Environmental concerns

Sulphuric acid and propanone are highly flammable elements, and hence their disposal should be done with great care to avoid these elements coming into contact with the environment.

Results

Run	**Physical conditions before experiment**	**Physical conditions After an experiment**
Standard	-Reddish-brown solution	Colourless
Double Propanone	The reddish-brown solution, but is lighter in colour than the standard run	Colourless
Double Iodine	Dark brown solution	Ununiformed mixing was observed even after mixing the solution. This is because propanone is less dense than water; hence it normally floats on top even after mixing and shaking.

The table below shows the data obtained from this experiment.

	Absorbance			
Time (Seconds)	**Experiment 1**	**Experiment 2**	**Experiment 3**	**Experiment 4**
20	0.61	0.54	0.45	0.26
40	0.61	0.41	0.40	0.24
60	0.58	0.35	0.34	0.22
80	0.51	0.30	0.30	0.2

100	0.48	0.24	0.25	0.19
120	0.47	0.17	0.21	0.17
140	0.43	0.10	0.15	0.14
160	0.41	0.06	0.08	0.14
180	0.39	0.06	0.04	0.11
200	0.36	0.00	0.01	0.09
220	0.35	0.0	0.00	0.09
240	0.33	0.0	0.00	0.09
260	0.30	0.0	0.00	0.09
280	0.27	0.0	0.00	0.00
300	0.22	0.0	0.00	0.00

Sample calculations and processed data

The data obtained in this experiment is very close to theoretical data. The reaction rate tends to double as the concentration of propanone increases; it has also been noted that the rate of reaction also increases as the concentration of sulfuric acid increases, but there is no effect when the concentration of Iodine is increased. Sulphuric acid and propanone theoretically have been assigned the exponent 1 using the rate law. The following equation can explain the rate law

Rate= $k[CH3COCH2I]^1[H^+]\ [I_2]^0$

Where k is the constant and the square brackets [] indicates propanone, sulphuric acid, and Iodine concentration. Iodine has been assigned exponent value 0, and hence it is removed entirely from the rate law equation. Using the rate law, the constant rate k can be found can be calculated. To find each reactant's concentration in this experiment (Propanone, sulphuric acid, and Iodine).

To calculate the concentration of Iodine used in Experiment 1 using this formula.

M1V1 = M2V2 where;

M1- Undiluted concentration of Iodine

V1-Volume of Iodine used.

M2- Diluted concentration of Iodine

The V2-Total volume of the product

M1V1 = M2V2

$(0.02M*3\ mL)=(M_2*\ 6mL)$

$0.6=M_2 * 6$

$M_2=0.01M$

Concentration of iodine used in Experiment 2

M1V1 = M2V2

$(0.02M*3\ mL)=(M_2*\ 6mL)$

$0.6=M_2 * 6$

$M_2=0.01M$

Concentration of iodine used in Experiment 3

M1V1 = M2V2

$(0.02M*3\ mL)=(M_2*\ 6mL)$

$0.6=M_2 * 6$

$M_2=0.01M$

Concentration of iodine used in Experiment 4

M1V1 = M2V2

$(0.02M*3\ mL)=(M_2* 6mL)$

$0.6=M_2 *6$

$M_2=0.01M$

Using this information, the concentration of Experiment (Run) 2,3 and 4 can be calculated and filled in the table below

Run	The volume of 1M Propanone (cm^3)	The volume of 1M Sulphuric acid (cm^3)	The volume of deionized water (cm^3)	Number of drops of 0.02 M Iodine solution I_2 (aq)	Concentration Of Iodine
1	0.75	0.75	1.50	30	0.01 M
2	1.50	0.75	0.75	30	0.01M
3	0.75	1.50	0.75	30	0.01M
4	0.75	0.75	1.50	15	0.133M

Graphs

To represent the above data, I have come up with the following line graphs showing the absorbance rate against time in four runs that were carried out in this experiment.

Figure 1: Processed Data for time against Absorbance rate for experiment 1.

Time (Seconds)	**Absorbance**
20	0.61
40	0.61
60	0.58
80	0.51
100	0.48
120	0.47
140	0.43
160	0.41
180	0.39
200	0.36
220	0.35
240	0.33
260	0.3
280	0.27
300	0.22
Average time (160)	

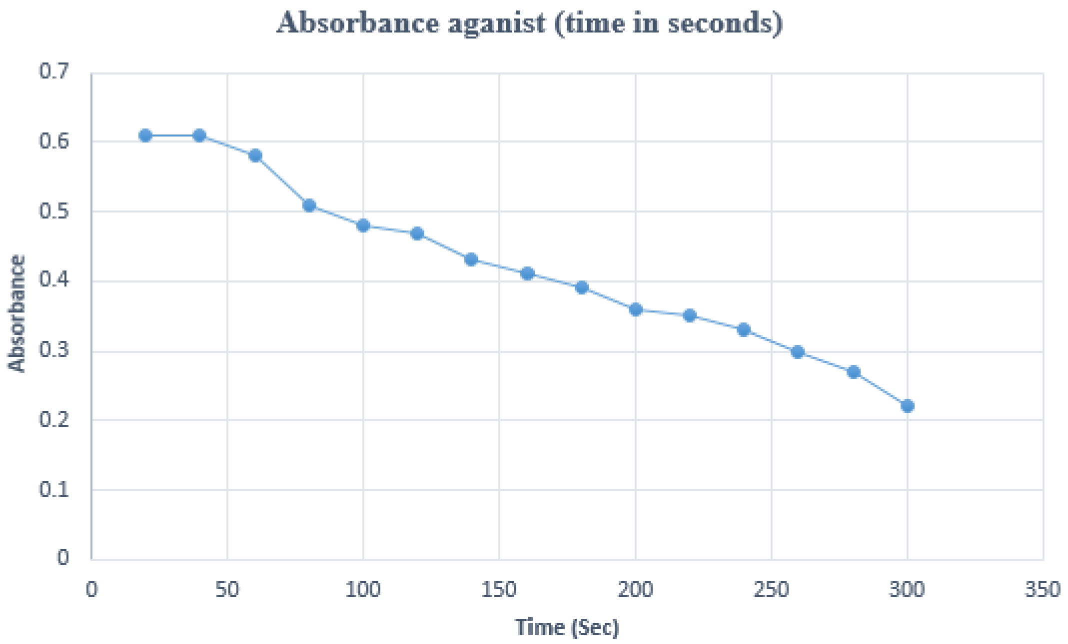
The rate of reaction in this experiment can be calculated using the formula below

Rate = $[I_2]$ / (average time in seconds) where $[I_2]$ is the concentration of Iodine.

$=\frac{0.01M}{160\ s}$

$=6.25*10^{-4}\ Ms^{-1}$

Graph 1: Absorbance against time



According to the graph above, the rate of reaction is directly proportional to concentration. The reaction continues to decrease as time increases this is because as the reaction continues, the amount of molecules in the solution reduces, thus slowing down the reaction. The Absorbance rate is high at the beginning of the reaction, and as the reaction continues, the absorbance rate reduces with time.

Figure 2: Processed Data for time against the Absorbance rate for experiment 2 (Increasing propanone concentration).

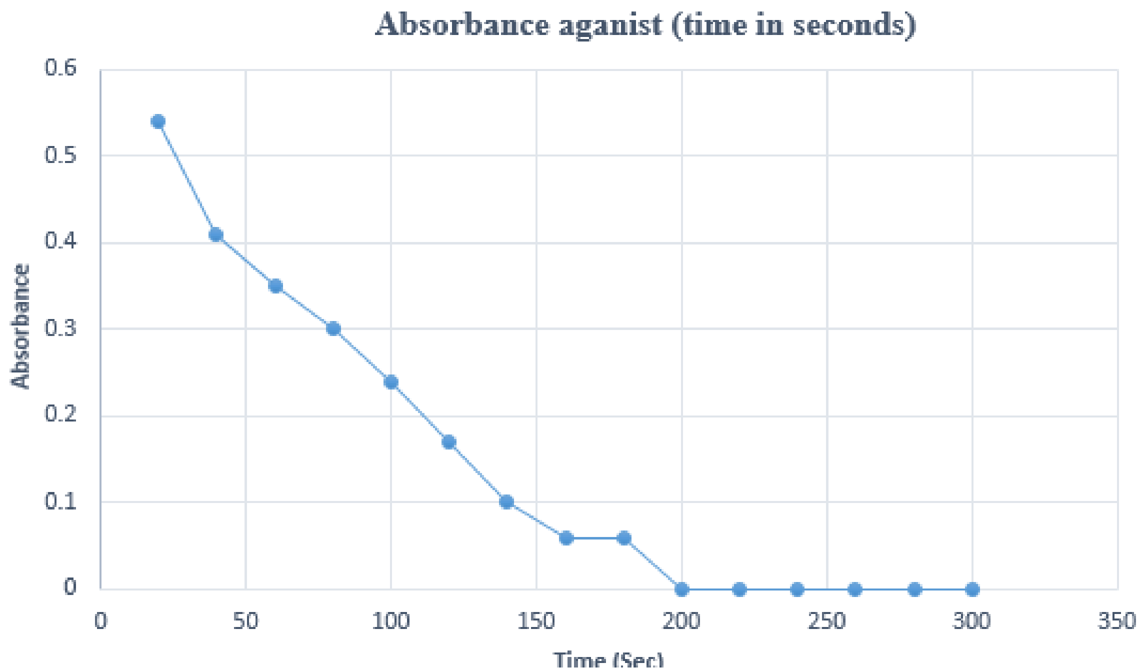
Time (Seconds)	**Absorbance**
20	0.54
40	0.41
60	0.35
80	0.3
100	0.24
120	0.17
140	0.1
160	0.06
180	0.06
200	0
220	0
240	0
260	0
280	0
300	0
Average time(100)	

Rate = $[I_2]$ / (average time in seconds) where $[I_2]$ is the concentration of Iodine.

$=\frac{0.01\text{M}}{100\text{ s}}$

$=1.0*10^{-4}\ \text{Ms}^{-1}$

Graph 2: Absorbance against time



From the graph above, increasing the propanone concentration and keeping other elements (sulphuric acid and Iodine) constant increases the reaction rate. The reaction rate stops at (180 seconds). As the reaction occurs, the reacting molecules reduce, and the reaction rate reduces with time.

Figure 3: Processed Data for time against Absorbance rate for experiment 3 (Increasing sulphuric acid concentration).

Time (Seconds)	**Absorbance**
20	0.45
40	0.4
60	0.34
80	0.3
100	0.25

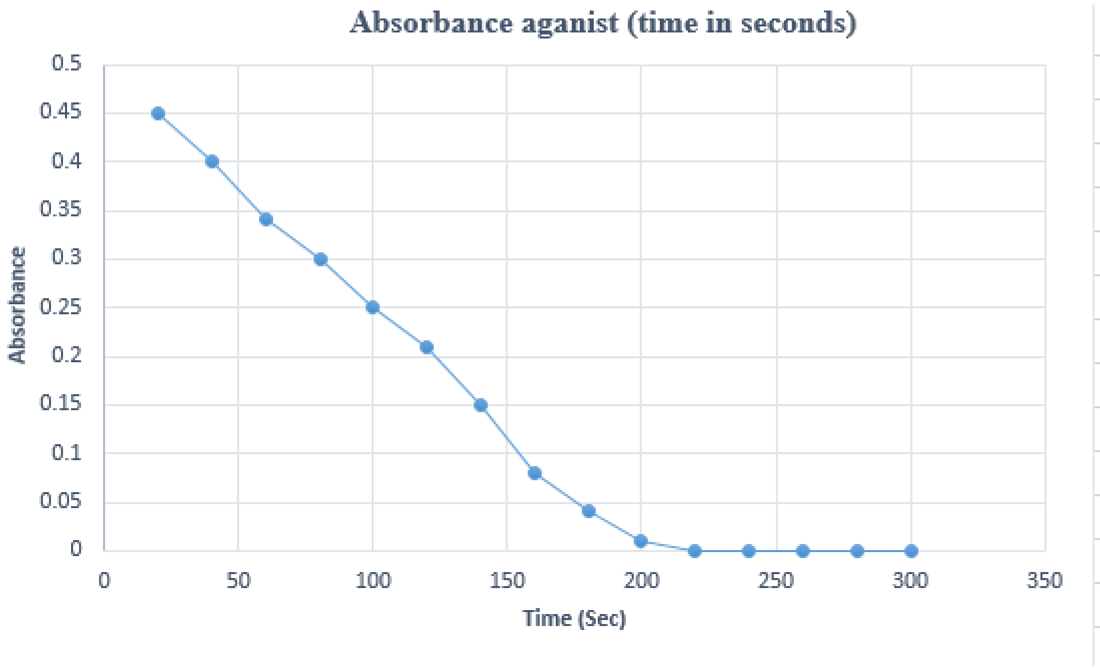
120	0.21
140	0.15
160	0.08
180	0.04
200	0.01
220	0
240	0
260	0
280	0
300	0
Average Time(120)	

Rate = $[I_2]$ / (average time in seconds) where $[I_2]$ is the concentration of Iodine.

$=\frac{0.01\text{M}}{120\text{ s}}$

$=8.33*10^{-5}$ Ms^{-1}

Graph 3: Absorbance against time



From the graph above, increasing the concentration of sulphuric acid, which acts as a catalyst in this experiment increases the hydrogen Ions in the reaction and thus increasing the rate of reaction. The absorbance rate is high at the start and decreases as time increases. The reaction stops at time 200 seconds.

Figure 4: Processed Data for time against Absorbance rate for experiment 4 (Increasing the concentration of Iodine).

Time (Seconds)	**Absorbance**
20	0.26
40	0.24
60	0.22
80	0.2

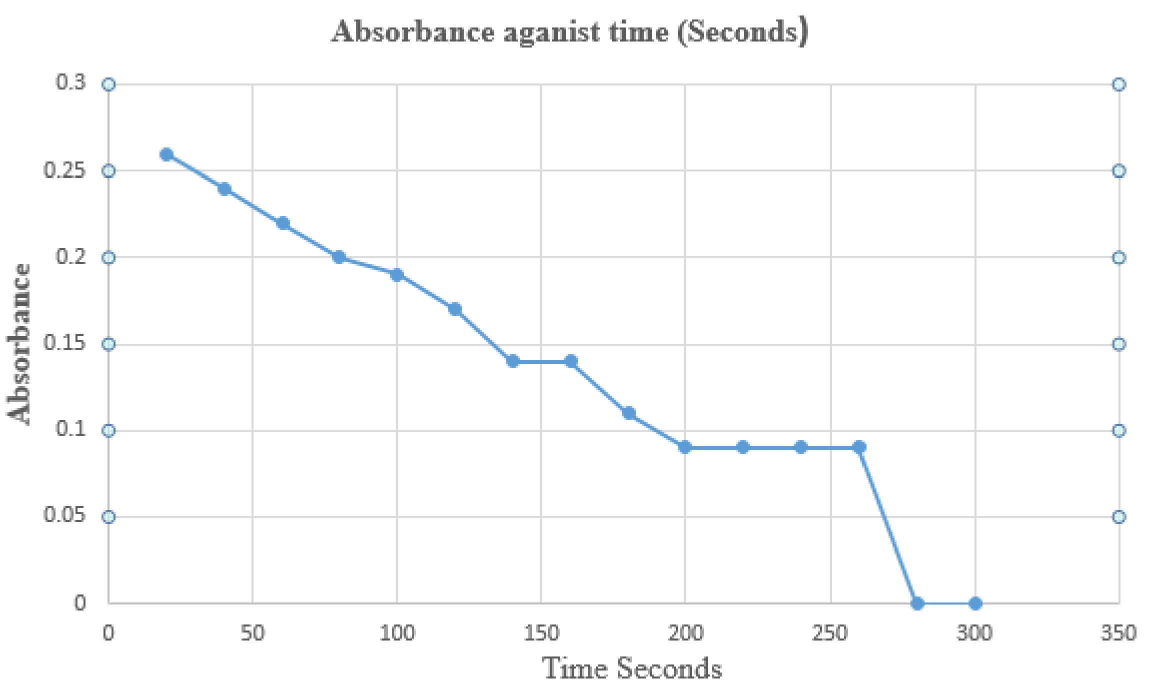
100	0.19
120	0.17
140	0.14
160	0.14
180	0.11
200	0.09
220	0.09
240	0.09
260	0.09
280	0
300	0
Average time(140 s)	

Rate = $[I_2]$ / (average time in seconds) where $[I_2]$ is the concentration of Iodine.

$=\frac{0.01\text{M}}{160\text{ s}}$

$=6.25*10^{-4}\ Ms^{-1}$

Graph 4: Absorbance against time



From the graph above, by increasing the concentration of Iodine, the reaction rate increases. At the start of the experiment, the absorbance rate is very high, and the reaction rate reduces as time increases and eventually stops at time 260 seconds.

Conclusion

The following table shows the rate of reaction. To determine how the rate of reaction is affected by concentration, comparison will be done using the standard run as the reference point of this experiment.

Run	The volume of 1M Propanone (cm^3)	The volume of 1M Sulphuric acid (cm^3)	The volume of deionized water (cm^3)	Number of drops of 0.02 M Iodine solution I_2 (aq)	Rate of reaction
1	0.75	0.75	1.50	30	$6.25*10^{-4}$ Ms^{-1}
2	1.50	0.75	0.75	30	$1.0*10^{-4}$ Ms^{-1}
3	0.75	1.50	0.75	30	$8.33*10^{-4}$ Ms^{-1}
4	0.75	0.75	1.50	15	$6.25*10^{-4}$ Ms^{-1}

In the first experiment (Standard run), as the rate of reaction increases, the concentration of sulphuric acid, propanone and Iodine also increases, as indicated by graph 1. By doubling the concentration of sulphuric acid the rate of reaction also increases.

Rate = $\frac{\text{rate of double sulphuric acid}}{\text{rate of standard run}}$

= $\frac{8.33*10-4}{6.25*10-4}$

=1.328

By doubling the concentration of propanone the rate of reaction increases as shown by the calculation below;

Rate = $\frac{\text{Rate of standard run}}{\text{rate of Doubele propanone}}$

= $\frac{6.25*10-4}{1.0*10-4}$

=0.16

By doubling the concentration of Iodine it has no effect on the rate of reaction; hence it can be deduced that increasing the concentration of Iodine has no effect on the rate of reaction.

Rate = $\frac{\text{Rate of standard run}}{\text{rate of Doubele Iodine}}$

= $\frac{6.25*10-4}{6.25*10-4}$

=1

In conclusion the rate of reaction is affected by the concentration of the reactants. In this experiment it can concluded that the rate of reaction is highest when the concentration of sulphuric acid (catalyst) has been doubled. The rate of reaction is moderate when the concentration of propanone is doubled and there is no change when the concentration of Iodine is doubled.

The hypothesis stated that as the concentration of reactants increases the rate of reaction also increases. This experiment supports and proves this prediction. Despite the errors that might have occurred, which indicates that a directly proportional (linear) relationship could fit the ranges. This results answers the research question that the rate of iodinasation of propanone is directly proportional to the concentration of elements.

Evaluation

Limitation	Effect on investigation	How can it be improved
Independent variable The use of sulphuric acid, propanone and Iodine	The independent variables used in this experiment proved to be very effective in answering the research question as it shows rate of reactions affected by	The rate of reaction is affected by concentration and temperature. It can be very interesting to compare both concentration and temperature and how each

	concentrations. Despite this success this success these variables only provided one factor that affects the rate of reaction.	affects the rate of reaction and based on their results, calculate the deviations of these factors.