Determination of the Activation Enthalpy and Rate Expression for the Iodination of Propanone

First Name and Last Name

Class

Date

Introduction

In this internal assessment, I will investigate the rate of reaction, activation energy and the iodination of propanone in a chemical reaction. Almost all molecules possess a definite amount of energy that starts a reaction. Whenever the molecules collide, molecules' potential energy or kinetic energy is used to bend, stretch and break molecules bonds, and enhance chemical reactions. Svante Arrhenius first used the activation energy in 1889[1]. This concept of activation energy helps to understand the requirements of a chemical reaction. My interest in this topic was due to previous class demonstration where a reaction produced some energy. I learned that when a reaction starts, there is a certain amount of energy that is required to initiate a chemical reaction, thus in this exploration, I aim to use the process of iodination of propanone to the reaction rate and the activation energy.

Background

The rate equation or the rate law

The activation energy is the minimum amount of energy required to initiate molecules collisions by a reacting molecule to form a product. Ea represents activation energy, and it is measured in joules (J), kilocalories per mole (kcal/mol), or kilojoules per mole (kJ/mol). The activation energy is described by the Arrhenius equation as;

$$k = Ae^{\frac{-Ea}{R}}$$

where;

[1] López, Julio, Mònica Reig, Andriy Yaroshchuk, Edxon Licon, Oriol Gibert, and José Luis Cortina. "Experimental and theoretical study of nanofiltration of weak electrolytes: SO42–/HSO4–/H+ system." *Journal of membrane science* 550 (2018): 389-398.

A = is the frequency factor

k = is the rate law constant

R = is the universal gas constant, 8.314 J/mol•K

E = is the activation energy of the reaction

The rate law constant is determined by the rate of the reaction to be explored as the concentrations of the reactants are significantly changed. The variations of the concentrations of the reactants allows the orders of the reactions with respect to each reagent to be determined, deriving the rate law expression.

The iodination of propanone

The iodination of propanone is the best reaction to study due to the following reasons; the colour of iodine reactant is clear, and it is readily observable, making the change in iodine to be monitored (reaction between propanone and iodine forms a colourless iodopropanone and hydrogen iodide as products, as the brown-colored iodine water is converted into colorless iodopropanone and hydrogen iodide); has a fast rate of chemical reaction, enough to measure any change; and with respect to iodine, the reaction order is zero-order making the change in concentration be linear with time. The chemical equation of the reactants is expressed as follows;

CH3COCH3(aq.) + I2(aq.) → CH3COCH2I(aq.) + H+ (aq.) + I– (aq.)

Colorimetry refers to the scientific technique that states that the concentration of a solute is proportional to the absorbance, and is used to determine the concentration of colored compounds in solutions using Beer-Lambert law [2]. The law is expressed as,

$$A = \in \times c \times l$$

Where;

A = is the absorbance,

$\in$ = is the molar absorption coefficient,

C = is the concentration,

l = is the optical length.

Absorbance is the measure of the amount of light absorbed as the light passes through a particular substance or sample. The Beer-Lambert law when expressed graphically a linear relationship between colorimeter absorbance readings and iodine concentration is formed. Ideally, the change in absorbance on colorimeter over time will be proportional to a change in concentration over time (rate of reaction). During the chemical reaction in the iodination of propanone, the reactants undergo a color change from brown (iodine, I_2) to colorless iodopropanone (CH3COCH2I)[3]. The colorimeter has filters that help in observation when decolorization of occurs. The figure below shows how the rate of reaction is calculated;

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[2] Chi, Huynh Bui Linh, Dang Nguyen Nha Khanh, Ngo Thi Tuong Vy, Phan Xuan Hanh, Truong Nguyen Vu, Hoang Thuc Lam, and Nguyen Thi Kim Phuong. "Development of a low-cost colorimeter and its application for determination of environmental pollutants." *Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy* (2020): 119212.

[3] Sarda, Vijay, Bharat Inder Fozdar, and Sanjiv Kumar. "Unit-9 Chemical Kinetics." (2017).

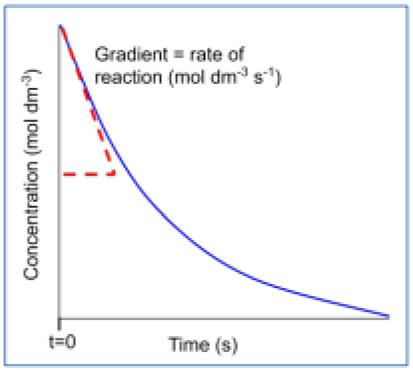


Figure 1. Graphically finding the rate of reaction

The rate of the reaction is calculated when the reaction is starting by finding the gradient to the concentration against time $t_{0.}$ Finding the gradient at time t_0 is necessary as the accumulation of products within the reacting vessel eventually slows down the rate of the reaction as it progresses.

Aim

The aim of this project is to experimentally determine the activation energy of the reaction, effects of concentration of a reactant on the rate of reaction and the iodination of propanone in acidic conditions.

Hypothesis

The increase of concentration of reactants increases the rate of reaction of propanone in acidic conditions. This means that when the concentration of a reactant increases, the rate of chemical reaction will also increase, resulting in the formation of new products within a short time.

Variables

Table 1: Controlled and uncontrolled variables

Controlled	
Variables	**How will they be changed/measured/controlled**
Reactants Volumes/Concentrations	The change in the concentration of propanone or sulphuric acid would affect the rate of the chemical reaction. When the concentration is high, the rate of chemical reaction will increase proportionally and result in aberrant reactions. For a controlled experiment, reactant was measured using syringes of 3ml with an error rate of ±0.1.
Room temperature	The experiment process was conducted on a stable, cool room temperature which created a temperature gradient between the solution and the air surrounding. The significance of experimenting on a cool lab setting enhanced the experiment so that fluctuations on temperatures was not great.
Temperature loss	During data logging, the water temperature was exact, meaning no heat loss into the surrounding environment. Temperature loss was controlled by using a cuvette lid and colorimeter by maintaining a stable insulated

	environment during data logging and it helped in the mitigation of heat loss to the external environment.
The time between initiating a reaction and beginning of the measurement	This method requires that the reaction be initiated before insertion into the colorimeter for logging (it needs shaking), leading to time delay and hence a reduction in the anticipated initial rate of reaction. This is controlled by performing the following steps within 8 seconds as recorded on a stopwatch; initiation, shaking and insertion into colorimeter.
Uncontrolled	
Overall temperature loss	Conducting the experiment when temperatures are high such as 50^{o}C and 60^{o} C range will lead to higher temperature gradients with the surrounding air than room temperature of 25^{o} C. It will, therefore emit heat at a greater rate than the low-temperature experiment. The temperature loss will be monitored during the experiment, and any potential temperature loss will be accounted for.

Safety

Environmental considerations / Chemical disposal;

The product of the reaction (iodopropanone), irritates the eyes. The mixture should also be disposed as soon as the measurements have been recorded by flushing down with lots of water.

Ethical issues:

There were no ethical considerations significant enough to accounted.

Chemical hazards:

During experiment, if any substances come into contact with the skin, mouth or eyes, they should be thoroughly washed off immediately. Also, the experiment should be carried out in a well-ventilated room and with safety wears such as glasses, lab coat and gloves.

Table 2: Chemical hazards

Chemical	**Risk assessment/disposal/environmental considerations**
Iodine solution	The concentration below 1M is less hazard. The solution that was used was 0.02M. The product should be disposed of at the hazardous waste dump.
Sulphuric acid	Sulphuric acid is highly corrosive and it should be kept away from the mouth, eyes, and skin. Spillage should also be avoided by using stable test tube racks for storage during the experiment. Sulphuric acid can be washed down the sink using water.

Propanone solution	Propanone is highly volatile, produces ignitable fumes that are irritants. The container should be kept closed and away from open flames. It should be dump in a hazardous waste facility after the experiment.
Iodopropanone	Iodopropanone is a product of the reaction, and it is irritant in aqueous form and as fumes. The holding containers should be covered. After the reaction, the waste products, iodopropanone, and hydrogen iodide should be spilt into a flask and covered to prevent evaporation.

Method:

Table 3: Materials

Materials	**Chemicals**
- A data logger with colorimeter accessories - Computer - Micro-tip plastic pipette - 5cm^3 graduated pipette - Cuvette	- 1M sulfuric acid - 1M propanone solution - 0.02M iodine solution

- Deionized water	

Experimental Procedures

Part A: Colorimeter Calibrations

1. Set up the interface box and using the software manual, connect it to the computer. Calibrate the colorimeter as described on the device specifications. The blue filter should be used for the experiment.

Part B: Chemical reactions

2. Calibrate colorimeter. Choose the option for transmittance and a time interval of 10 minutes.

3. Using a clean graduated pipette, transfer 0.75 cm^3 of 1M propanone, and 0.75 cm^3 1M sulphuric acid into a clean cuvette. Add 1.50 cm^3 of deionized water.

4. Uncap the cuvette, start the timer, and quickly add 30 drops of 0.02 M iodine solution using a micro-tip plastic pipette. Cap the cuvette, shake well four times, lower it into the cell compartment of the colorimeter. If this step takes longer than 8 seconds, repeat.

5. Stop recording when the transmittance signal flattens.

6. Measure the initial rate of decrease in absorbance according to the software manual. Save the data file.

7. Repeat steps (3) to (6) for the 4 concentration runs, (standard, 2x sulphuric acid, 2x propanone, 2x iodine).

Qualitative Data

Part A:

Table 4: Qualitative analysis of the process

Qualitative observations		
Run Variant	**Initial condition**	**After reaction**
Standard run	Reddish-brown solution	Transparent, colorless
Double propanone	The reddish-brown solution, but lighter than the standard run	Transparent, colorless
Double acid	Reddish-brown solution, but lighter than the standard run	Transparent, colorless
Double iodine	Dark brown solution	An incomplete mixing was observed at the top of water since it is less dense than water, thus reducing the chemical reaction rate.

Results and Data

Raw Data

Table 5: Raw data of the initial rate from the decolorization graph and order of the reaction

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	0.4	0.24
60	0.58	0.35	0.34	0.22
80	0.51	0.3	0.3	0.2
100	0.48	0.24	0.25	0.19
120	0.47	0.17	0.21	0.17
140	0.43	0.1	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	0.01	0.09
220	0.35	0	0	0.09
240	0.33	0	0	0.09
260	0.3	0	0	0.09
280	0.27	0	0	0
300	0.22	0	0	0

Determination of the Activation Energy:

Calculating the rate of chemical reactions, results and discussion:

Table 6: The concentrations and volumes used in the four experiments

Run	Vol. of 1M Propanone / cm^3	Vol. of 1M sulfuric acid / cm^3	Vol. of deionized water / cm^3	No. of drops of 0.02M I_2(aq)	No. 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

The initial concentrations of all reagent were calculated using the volumes and the stock concentrations listed in table 11. During calculation, the reaction rate was obtained as the change in concentration of iodine over reaction time.

Table 7: Processed data for absorbance and time for experiment 1 for a standard run.

Experiment 1	
Time(seconds)	**Experiment 1**
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

The initial concentration of iodine (I_2), run 1;

[Propanone] initial = $\frac{[propanone]initial(volume\ of\ propanone)stock}{(Volume\ of\ water)}$

= Number of moles of iodine / the initial volume of water

=0.02 mol dm^{-3} * 0.003dm^3 / (3.003 * 10^{-3}) dm^3

= 1.99 * 10^{-2} mol dm^{-3}

The initial concentration of propanone (CH_3COCH_3) run 1;

= Number of moles of propanone / the initial volume of water

=1.0 mol dm^3 * 0.75dm^3 / (3.003) dm^3

= 0.25 mol dm^{-3}

The initial concentration of sulphuric acid (H^+) in run 1;

= Number of moles of sulphuric acid / the initial volume of water

=1.0 mol dm^3 * 0.75dm^3 / (3.003) dm^3

= 0.25 mol dm^{-3}

The rate of reaction $= \frac{\text{change in iodine(I2)}}{\text{Time taken}}$

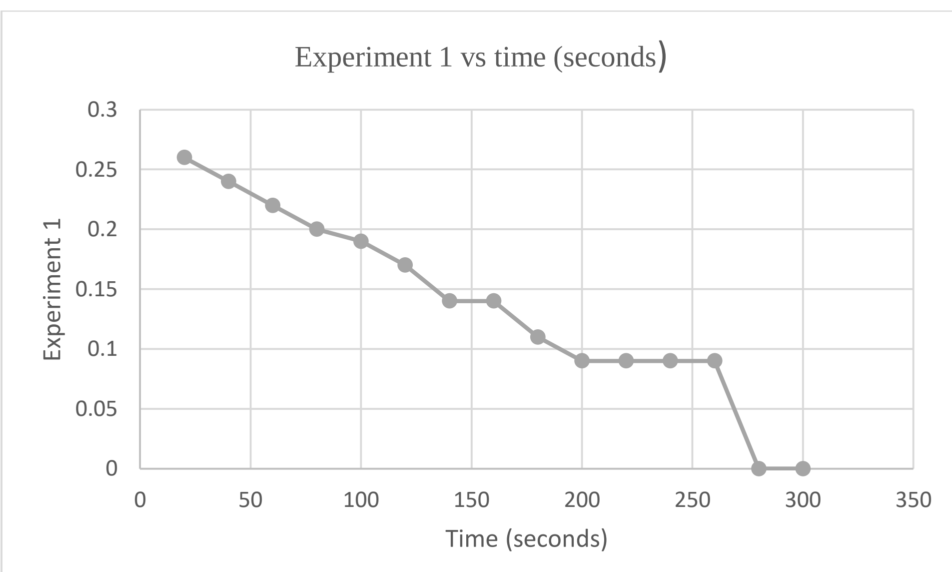
$$= \frac{1.99 * 10-2 \text{ mol dm}-3-0}{0.61-0.27} = 5.85 * 10^{-2} \text{ mol dm}^{-3} \text{ s}^{-1}$$

Therefore, k $= \frac{\text{rate}}{\text{(propanone)(sulpuric acid)}}$

$$= \frac{5.58 * 10-2 \text{ mol dm}-3 \text{ s}-1}{0.25 \text{ mol dm}-3 * 0.25 \text{ mol dm}-3}$$

$$= 9.36 * 10^{-1} \text{ dm}^3 \text{ s}^{-1}$$

Fig 1: The graph of absorbance vs. time for experiment 1

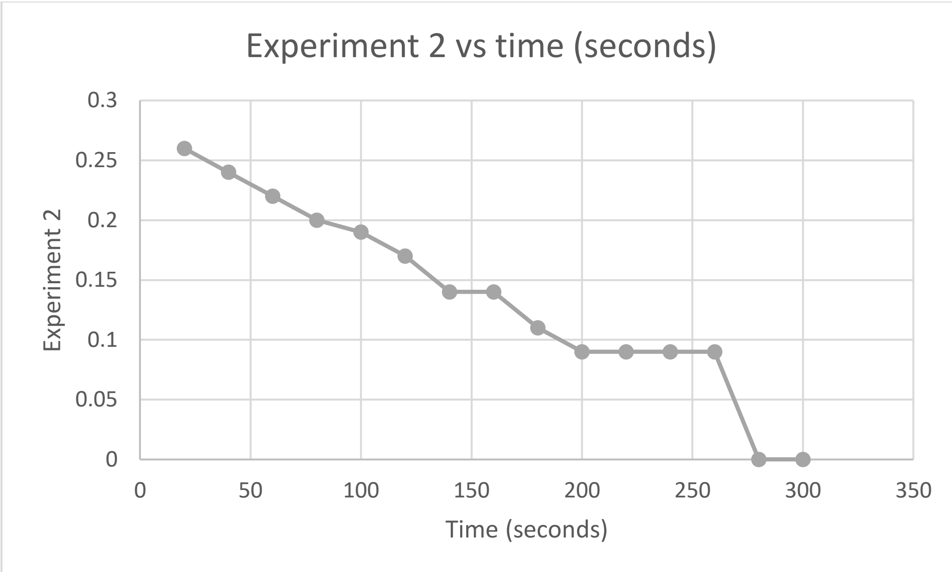


From the graph, the rate of reaction is high (absorbance) when reactants mix and fall down as the reaction continues.

Table 8: Processed data for absorbance and time when concentration of propanone is increased (experiment 2)

Experiment 2	
Time(seconds)	Experiment 2
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

Fig 2: The graph of absorbance against time



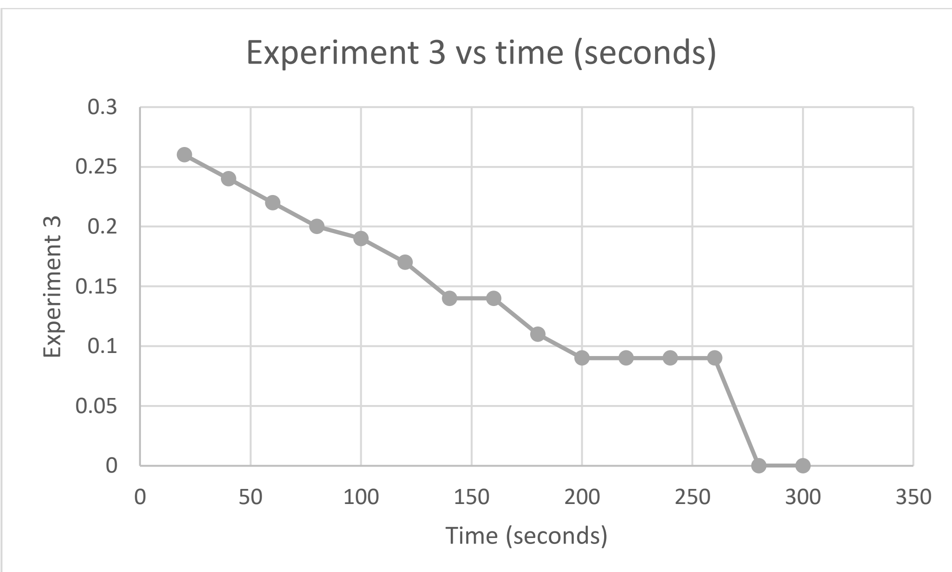
the graph shows that as the concentration of propanone increases, the rate of reaction increases and takes 20-180 seconds to complete.

Table 9: Processed data for absorbance and time as concentration of sulphuric acid is increased (experiment 3)

Experiment 3	
Time(seconds)	Experiment 3
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

Fig 3: The graph of absorbance against time

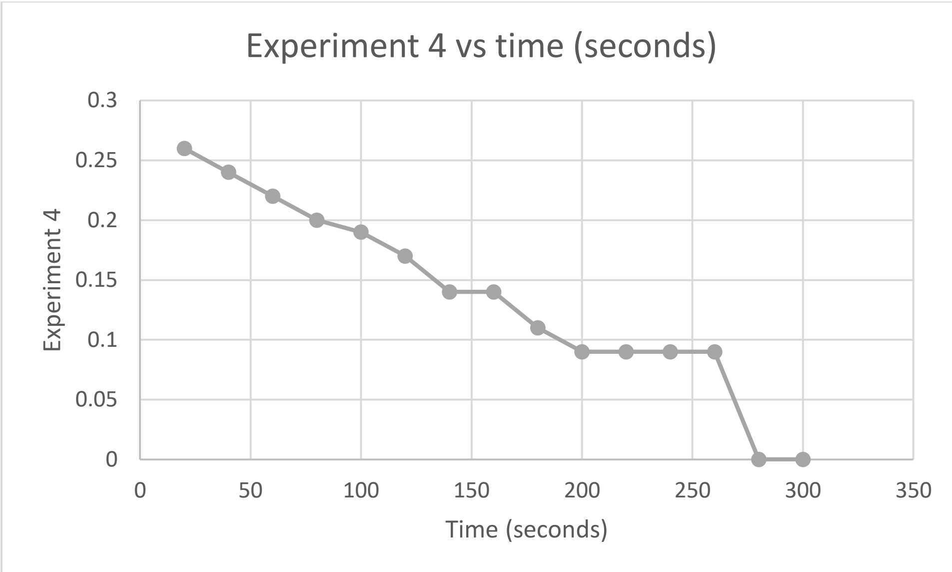


When the concentration of sulphuric acid is increased, the rate of reaction increases and the whole chemical reaction takes 20-200 seconds.

Table 10: Processed data for absorbance and time when concentration of iodine is increased (experiment 4)

Experiment 4	
Time(seconds)	Experiment 4
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

Fig 4: The graph of absorbance against time



From the graph, increasing the concentration of iodine does not increase the rate of reaction.

Table 12: Average reaction rates for each set of conditions

	Concentration of Propanone	Concentration of sulphuric acid	Concentration of Iodine(I_2)	Rate of reaction
Standard run	0.25	0.25	$1.99 * 10^{-2}$ mol dm^{-3}	$5.85 * 10^{-2}$ mol dm^{-3} s^{-1}
Double propanone	0.5	0.25	$1.99 * 10^{-2}$ mol dm^{-3}	$1.17 * 10^{-1}$ mol dm^{3} s^{1}
Double sulphuric acid	0.25	0.5	$1.99 * 10^{-2}$ mol dm^{-3}	$1.17 * 10^{-1}$ mol dm^{3} s^{1}

Double iodine	0.25	0.25	3.98 * 10^{-2} mol dm^{-3}	5.85 * 10^{-2} mol dm^{-3} s^{-1}

$Rate_0$ = k $[propanone]_0$ $[sulphuric\ acid]_0$

5.85 * 10^{-2} mol dm^{-3} s^{-1} = k (0.25M) (0.25M)

k =9.36 * 10^{-1} mol dm^3 s^1

the rate of the reaction for double propanone

r = 9.36 * 10^{-1} mol dm^3 s^1 (0.5) (0.25)

r =1.17 mol dm^3 s^1

the rate of the reaction for double sulphuric acid

r = 9.36 * 10^{-1} mol dm^3 s^1 (0.5) (0.25)

r =1.17 mol dm^3 s^1

the rate of the reaction for double iodine

r = 9.36 * 10^{-1} mol dm^3 s^1 (0.25) (0.25)

r =1.17 mol dm^3 s^1

When comparing the standard run to the doubled propanone, the reaction rate doubled when the initial concentration of propanone doubled, hence the reaction is first order with respect to propanone.

$$=\frac{\text{Rate1}}{\text{Rate 2}}$$

$$= \frac{5.85 * 10-2 \text{ mol dm}-3 \text{ s}-1}{1.17* 10-1 \text{ mol dm3 s1}} = 0.5$$

When comparing the standard run to the doubled sulphuric acid, the reaction rate doubled when the initial concentration of sulphuric acid doubled, hence the reaction is first order with respect to sulphuric acid.

$$=\frac{\text{Rate1}}{\text{Rate 2}}$$

$$= \frac{5.85 * 10-2 \text{ mol dm}-3 \text{ s}-1}{1.17* 10-1 \text{ mol dm3 s1}} = 0.5$$

When comparing the standard run to the double iodine, the reaction rate remained constant when iodine's initial concentration doubled; hence, the reaction is zero-order to iodine.

$$=\frac{\text{Rate1}}{\text{Rate 2}}$$

$$= \frac{5.85 * 10-2 \text{ mol dm}-3 \text{ s}-1}{15.85 * 10-2 \text{ mol dm}-3 \text{ s}-1} = 1.0$$

Impact of uncertainties:

Table 13: Significant errors of certain materials

Uncertainties

Colorimeter	+/- 0.1% absorbance
Syringe readings	+/-0.1cm^3

Evaluation:

Systematic errors

There is a time delay between colorimeter logging and reaction start time. The reaction starts within a short time that hinders initial readings of colorimeter. This error can be reduced by increasing the volume of iodine and reducing the concentration of propanone and sulphuric acid.

Extensions:

When a chemical reaction starts, there is an activation energy that is required for the molecules to start reacting. The reaction process is high at this point, and it is reduced as new products are formed, and the rate of reaction reduces consequently. The rate of chemical reaction is determined by the concentration of the reactants. When the concentration of a reactant is increased, the rate of chemical reaction increases. I found this investigation interesting, and I would like to take other investigations in the future since I wondered how iodized medical pills react with body enzymes when injected or swallowed in the body. Conducting this experiment in future would allow me to get an insight into how pills are broken down without any health implication.

Conclusion:

The hypothesis stated that as the concentration of reactants increases, the reaction rate would also increase. From the experiment results and findings, this investigation strongly supports the prediction. During the iodination of propanone, the increase of the reactants' concentrations increased the reaction rate; hence, the reaction is first order concerning both sulphuric acid and propanone concentrations zero-order to iodine concentration.

The iodination of propanone was observed as the brown color of iodine water disappeared to form a colorless product. The disappearance of brown color was proof that a chemical reaction has taken place, and new products have been formed. It was concluded that there is an activation energy that initiates a chemical process during a chemical reaction.