1 Introduction

When learning about catalysis, I was particularly intrigued by the specific subset of acid catalysts. Acid catalysts are often regarded as the most important area of catalysis in industry. More specifically, these acids allow for the protonation of a double bonded oxygen group in various carbonyls, including ketones such as acetone [4]. As acetone is a major organic solvent which sees its own applications in industry and personal life, this combination of acid catalysis and organic chemistry is particularly relevant. A common iteration of this mechanism results from the use of iodine (a frequently found halogen in organic chemistry) due to its strong color [6]. Thus, I was drawn to investigating the reaction between acetone and iodine in the presence of a hydrochloric acid catalyst and determining the activation energy (E_a) by looking for the loss of color in the reaction solution.

1.1 Research Question

How does varying temperature affect the rate of reaction between iodine and acetone solution in the presence of a hydrochloric acid catalyst?

This question will be answered through empirical theory and experimentation, and the resulting data will also facilitate the calculation of the activation energy of this general reaction.

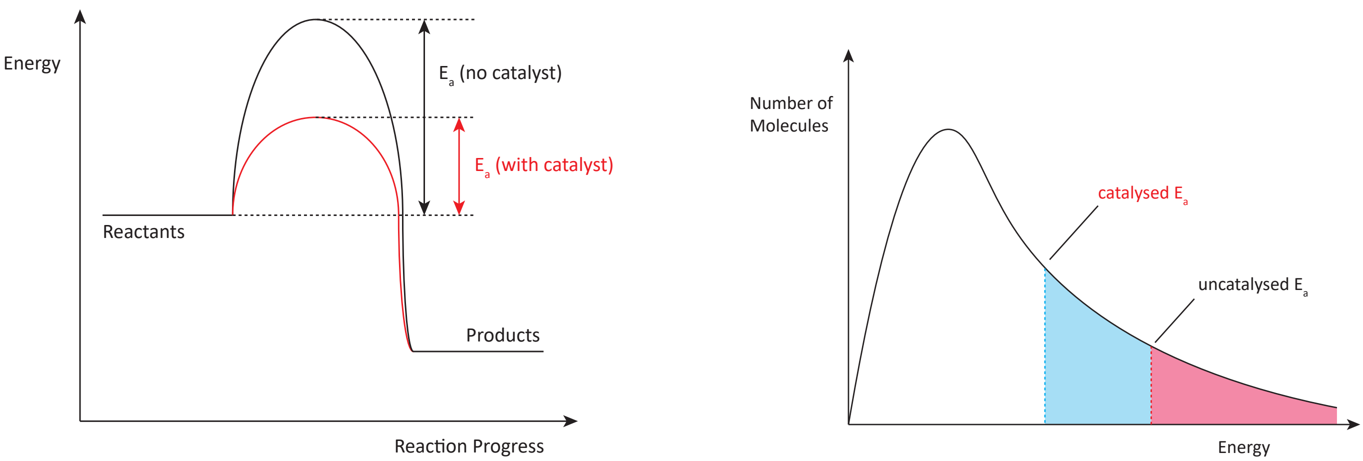
2 Background

The stoichiometric reaction being studied in this investigation can be depicted as:

$$CH_3COCH_{3(aq)} + I_{2(aq)} \xrightarrow{HCl} CH_3COCH_2I_{(aq)} + HI_{(aq)}$$

As the iodine is the limiting reagent, it is fully consumed to produce iodoacetone and hydrogen iodide so its brownish-red color slowly disappears from the reactant solution, allowing for the identification of the completion of the reaction [15, 12]. To determine the activation energy of this reaction, the time taken for completion was measured at various temperatures and the Arrhenius equation was then used. However, as the Arrhenius equation is dependent on the rate constant (k), it was first necessary to determine the rate law of the overall reaction.

Additionally, because of the slow nature of this reaction, the HCl catalyst was used to provide an alternative pathway with a lower E_a. This allowed for a quicker rate, rendering the reaction feasible for the purpose of this investigation. The basic premise behind the significance of catalysts on lowering the E_a and increasing the rate through kinetics can be seen in Fig. 1.



(a) The catalyst provides an alternative pathway for the reaction with a lower E_a

(b) The Maxwell Boltzmann Distribution shows how more molecules can then react as a larger proportion of molecules have sufficient energy ($> E_a$) [17].

Figure 1: Catalyst Function

2.1 Rate Law and Reaction Mechanism

Most reactions involving complex molecules/ions and catalysts rarely occur in a single step identical to the overall reaction, but instead can be further dissolved into multiple steps. This series of reactions is known as a reaction mechanism and plays an instrumental role in determining the rate of a reaction. Of these multiple steps, the slowest is referred to as the rate-determining step as it essentially dictates the rate of the overall reaction [14]. Multiple mechanisms are possible for this reaction (and thus have been proposed), but based on empirical evidence and the rate determined in this experiment, the most likely mechanism is shown in Table 1.

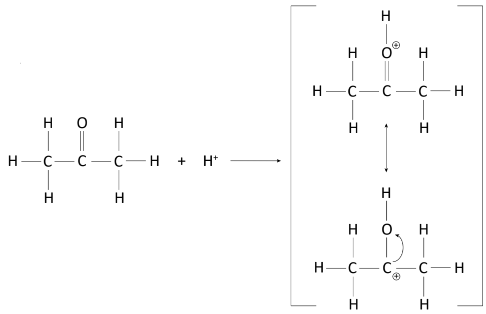
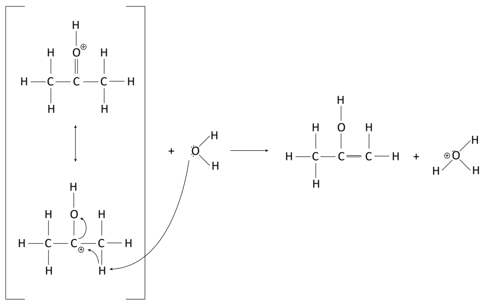
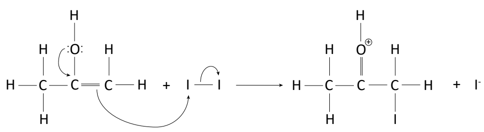
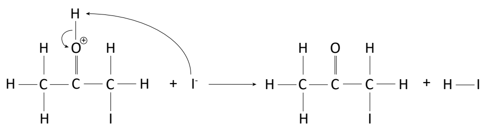
Structural Depiction	Description
	Firstly, protonization of the carbonyl oxygen in acetone occurs as the acid donates its hydrogen ion. This process happens readily, as the highly polar double bond between carbon and oxygen makes the oxygen acquire a high partial negative charge (δ^{-}). But, as the oxygen must donate both electrons for the electron pair (behave as a nucleophile), it acquires a positive charge. However, this structure is resonance stabilized, as if the more electronegative oxygen atom takes both electrons in its bond with carbon, the carbon will be left with the positive charge.
	Due to this polarization of the double bond, the α-carbon also becomes more acidic, allowing for easier deprotonation. Thus, as the water molecule approaches, the highly electronegative oxygen with multiple lone pairs attracts a hydrogen molecule from the α-carbon and behaves as a nucleophile. This produces hydronium ion (giving us back the acid catalyst) and the α-carbon can form a double bond with the carbocation, resulting in an electrically neutral enol. These two steps together are referred to as enolization.
	1 of the iodine atoms then behaves as an electrophile (as it is highly electronegative) and the enol becomes a nucleophile, facilitating a S_N2 attack and the heterolytical cleavage of the halogen molecule. The π-bond between the carbon atoms provides the electron pair for the positive iodine, and the oxygen is able to donate its lone pair, creating a dative bond to counteract the resulting positive charge on the carbon atom. This results in the halogenation of the α-carbon and leaves a single iodine ion.
	Due to the resulting positive charge on the oxygen atom, the functional group becomes prime for deprotonization and facilitates the transfer of the hydrogen ion to the highly negative iodine ion. This leaves a double bond between the oxygen and carbon, providing a stable octet configuration for all species involved.

Table 1: Proposed Mechanism

As ketones (specifically acetone) are extremely weak bases, the slowest step in this mechanism would be theorized as the initial one, where the acetone must acquire the donated proton from the acid catalyst. This process is slow even in the presence of a catalyst due to it not being enegetically favorable. Based on this empirical understanding (and the later confirmation via experimentation), this step is the rate-determining step [7]. As the speed of this step is dependent on the concentration of acetone and acid (not the halogen) which both have coefficients of 1, the overall rate law can be theorized as: $rate = k[CH_3COCH_3][HCl]$.

Although a catalyst is utilized for this reaction, it is still generally slow to complete at lower temperatures, making it difficult to perform many trials at lower temperatures.

2.2 Experimental Determination of Rate Law

Although the empirical determination of the rate law can be suggested through the proposed mechanism above, it is still difficult to be fully confident in a rate law without experimental determination. Fortunately, this process is relatively straightforward and relies on basic mathematical principles. The general rate for any reaction can be expressed as a product of powers of the concentrations of all reactants and/or catalysts involved. Thus, for the iodination of acetone, the rate law must be:

$$rate = k[CH_3COCH_3]^p[HCl]^q[I_2]^r$$

where p, q, r are integers greater than or equal to 0. Additionally, k is a constant for the reaction at a fixed temperature. Thus, by altering the concentration of individual reactants while keeping the remaining concentrations the same, different rates can be calculated and the results can be divided to determine the orders (p, q, r). For example, if we double the concentration of acetone while leaving the remaining concentrations untouched, we would have the result:

$$\frac{rate_2}{rate_1} = \frac{k[CH_3COCH_3]^p 2^p [HCl]^q [I_2]^r}{k[CH_3COCH_3]^p [HCl]^q [I_2]^r} = 2^p$$

Then, by taking the logarithm (base 2) of both sides:

$$p = \log_2 \left(\frac{rate_2}{rate_1} \right)$$

This process can then be performed for the remaining reactants, allowing for the simple calculation of p, q, r and the final determination/confirmation of the overall rate law [1].

2.3 Determination of Activation Energy

As mentioned previously, to determine the activation energy of a specific reaction, you must have the value of the rate constant k, which is temperature dependent. By finding/confirming the rate law of $rate = k[CH_3COCH_3][HCl]$, this process becomes straightforward. Because iodine is a limiting reactant, and acetone and acid are used in large excess quantities (keeping their concentration relatively stable), the rate is theorized to remain largely linear for the duration of the reaction [15]. Through this apparatus, the rate can then be defined as $\frac{\Delta[I_2]}{t}$, or the change in concentration of iodine over time. As the loss of color indicates reaction completion (and the total depletion of iodine), this simplifies to $\frac{[I_{2(initial)}]}{t}$. Then, through substitution and rearranging of the above rate equation, we see:

$$k = \frac{[I_{2(initial)}]}{t[CH_3COCH_3][HCl]}$$

This result allows us to experimentally determine the rate constant for various trials of this reaction. After calculating this rate constant at multiple temperatures, the Arrhenius Equation facilitates the determination of activation energy. The Arrhenius Equation highlights the dependence of the rate constant on the absolute temperature as [8]:

$$k = Ae^{\frac{-E_a}{RT}}$$

where A is the steric constant for each chemical reaction, T is the absolute temperature (in Kelvin), and R is the universal gas constant ($8.31 \frac{J}{K \cdot mol}$). Taking the natural log of this entire equation results in the following relationship:

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

Thus, a linear relationship exists between the natural logarithm of the rate constant ($\ln k$) and the inverse of the temperature($\frac{1}{T}$) with the gradient being $\frac{-E_a}{R}$. As R is a known constant, a plot of the graph between these two variables can be used to find the slope of the line and thus the activation energy (E_a).

3 Hypothesis

Increasing the temperature of the reaction between iodine solution and acetone in the presence of hydrocholoric acid catalyst will directly increase the rate of the reaction.

As discussed earlier, the increase in temperature with the addition of a catalyst allows for a larger proportion of molecules to have sufficient energy greater than the activation energy and induces more frequent successful collisions, resulting in a quicker rate [9]. The exact activation energy will be determined by the experiment and the hypothesis can then simultaneously be confirmed or rejected.

4 Variables

4.1 Rate Law Experiment

Independent Variable: Concentration of reactants ($\frac{mol}{dm^3}$)

It has empirically been confirmed that the rate of a reaction is solely dependent on the rate constant (which is constant at a fixed temperature) and the concentrations of the reactants (and catalysts in the case of specific mechanisms). Thus, to find the rate law for this specific iodination of acetone reaction, a baseline was provided through the initial configuration and then each set of trials manipulated the concentration of a certain reactant (HCl, $Acetone$, or I_2) for the purpose of comparison. This allowed for the determination of the order of each reactant in the rate law through simple proportions. To make this process easy, the baseline configuration used 5 mL of each reactant/catalyst, and the manipulated trials doubled these volumes for each reactant to 10 mL. The total volume was held constant through the addition of water, so this doubling in volume of the reactant meant a direct doubling of that reactant's concentration, and thus the effect on the rate could easily be identified. As the rate law is crucial to the determination of the activation energy in the second part of this investigation, the choice of independent variable is justified.

Dependent Variable: Time taken for solution to lose its color (s)

By using the time for the completion of the reaction (once the iodine color has disappeared) and the initial concentration of iodine, the rate of the reaction can be determined for each chosen configuration of reactants. These rates can then be compared to the baseline provided by the initial configuration for the experiment to identify how the changing of concentrations of each reactant impacts the overall rate. By doing this for each reactant, the rate law for the total reaction can be empirically confirmed/found, allowing us to determine the rate constant in the activation energy experiment. Additionally, as time is also the dependent variable for the activation energy experiment, the trials for the first configuration can then be utilized further. Thus, the time taken for the reaction to lose its color is relevant to the overall investigation.

Unique Control Variable: Temperature (K)

Because the temperature impacts the rate constant (k), it was crucial to maintain a constant temperature for the determination of the rate formula. As the premise of finding the rate law relies on the resultant rate proportions of changing concentrations, a change in k would introduce a confounding variable and render the results inconclusive. A room temperature of 294.8 K was taken as this constant temperature for all trials conducted as part of the rate law experiment and it was ensured that all reactants were at this fixed temperature prior to the initialization of the reaction through constant temperature checks via thermometer.

4.2 Activation Energy Experiment

Independent Variable: Temperature (K)

As mentioned in the background, the rate constant varies depending on temperature, and the calculation of multiple rate constants at known temperatures can be used to find the activation energy through the Arrhenius equation. The linear relationship between the inverse of the temperature and the natural logarithm of the rate constant allows for simple graphing and gradient calculation which can then be used to find the activation energy, indicating the relevance to the investigation. Because specific temperatures are not required and instead a variety of temperatures are crucial, temperatures in the ranges of $283 - 285$, $293 - 298$ (room temperature in the above experiment), $303 - 308$, and $313 - 318$ K were used to conduct trials and were manipulated through the use of heated or ice-filled water baths. I refrained from adding higher temperatures for fear of partial evaporation of the reactants, as this would impact concentrations, and lead to erroneous calculations with regards to the rate of reaction and rate constant.

Dependent Variable: Time taken for solution to lose its color (s)

This is an easily observable characteristic of the reaction which allows for the determination of the completion of the reaction and thus leads to a straightforward process for quantifying the rate of the reaction (as discussed previously). All times were calculated in seconds (s) for consistency and to maintain the appropriate rates for k for a second order reaction ($\frac{dm^3}{mol \cdot s}$). Because the rate constant can then be used to determine the activation energy of the reaction, this choice of a dependent variable is entirely relevant to the investigation and allows for the answering of the initial research question.

Unique Control Variable: Volumes of reactants (cm^3)

All trials utilized for this experiment had identical volumes of each reactant and identical total volumes leading to the same concentration of each reactant for all trials. These volumes were chosen to make iodine the limiting reactant and provide large excess of HCl and $Acetone$, so as to ensure that all iodine was used up after the reactions completion and prevent large fluctuations in the concentration of the other reactants which could also impact the rate. This was necessary as the experiment was designed to investigate the change of the rate due to temperature alone, and thus the control variable was necessary.

4.3 Universal Controls

Pressure

Large fluctuations in pressure can impact the rate of evaporation of the reactants involved in the experiment which would affect the concentrations and induce erroneous rate calculations. Pressure changes have also been found to impact the kinetics of molecules with regards to aqueous reactants which could have introducing confounding causes for the change in the rate constant with varying temperatures. To control for pressure, all experiments were carried out in a controlled environment and a uniform laboratory at a fixed altitude.

Purity/Molarity of Reactants

As the molarity of the reactants was used to determine their respective concentrations, it was crucial that these molarities were accurately measured and maintained for the duration of all trials. To control, all reactants were properly diluted prior to the beginning of the experiment and sufficient quantities were produced so as to allow for consistent utilization for all trials. The diluted solutions were stored safely to prevent any external contamination or evaporation.

Physical Manipulation of Reaction

Swirling of the reaction mixture is crucial for ensuring that the reactants evenly mix throughout and helps faciliate more frequent collisisons between particles (thereby increasing the rate of the reaction). To ensure that discrepancies in swirling did not account for the various results, all trials were given 30 seconds of swiriling and then allowed to sit to completion. This attempted to control the confounding variable and let the reaction occur naturally after all reactants were adequately mixed.

5 Methodology

5.1 Apparatus

Chemicals	Glassware	Miscellaneous
• 120 cm^3 $1M$ HCl • 120 cm^3 $4M$ $Acetone$ • 120 cm^3 $.005M$ I_2 solution • 165 cm^3 Distilled H_2O	• 100 mL Earlenmeyer Flask • 1000 mL Beaker • 10 mL Graduated Cylinder • Test Tube(s)	• Ice • Thermometer • Ring Stand • Poly Water Bath • $2x$ Beaker Clamp • Water Source

Table 2: Materials

5.2 Experimental Procedure

5.2.1 Rate Law Determination

1. Prepare a water bath at room temperature in a 1000 mL beaker.
2. Clamp a 100 mL earlenmeyer flask and a separate test tube into the water bath.
3. Measure out the appropriate amounts of HCl, $Acetone$, and H_2O (as listed in Table 3) into the 10 mL graduated cylinder and add these substances to the clamped earlenmeyer flask.
4. Measure out the appropriate amount of I_2 (as listed in Table 3) into the 10 mL graduated cylinder and pour into the clamped test tube.
5. Ensure that the the reactants in the test tube and flask are fully immersed in the water bath and allow 5 minutes for temperature equilibrium to be reached.
6. Record the water bath temperature after this period is complete. Attempt to maintain this temperature for all trials to limit potential confounding results for rate law determination.
7. Remove the test tube containing the iodine solution and immediately add its contents to the flask containing HCl, $Acetone$, and H_2O, starting a timer after the addition.
8. Swirl the reaction mixture by gently swirling the ring for 30 s and then allow the solution to sit.
9. When the iodine color (brownish-red) has completely disappeared, stop the timer and record the total reaction time (as the reaction is complete).
10. Clean the glassware thoroughly and dry (it is not necessary to clean the test tube as it will always contain iodine solution with a constant concentration).
11. Repeat steps 2-10 two more times for configuration #1 in Table 3.

12. Repeat steps 2-11 for all remaining configurations in Table 3.
13. Thoroughly clean all glassware and dispose of any leftover products/substances safely.

5.2.2 Activation Energy Determination

1. Prepare a water bath at temperature within the range listed in Table 4 either in the Pro Water Bath (for high temperatures) or in a 1000 mL beaker with ice (for the low temperature).
2. Clamp a 100 mL earlenmeyer flask and a separate test tube into the water bath.
3. Measure out the appropriate amounts of HCl, $Acetone$, and H_2O (as listed in Table 4) into the 10 mL graduated cylinder and add these substances to the clamped earlenmeyer flask.
4. Measure out the appropriate amount of I_2 (as listed in Table 4) into the 10 mL graduated cylinder and pour into the clamped test tube.
5. Extra care should be taken to measure out exact volumes of the reactants, as they must be controlled for accurate determination of temperature-dependence on the rate constant.
6. Ensure that the the reactants in the test tube and flask are fully immersed in the water bath and allow 5 minutes for temperature equilibrium to be reached.
7. Record the water bath temperature after this period is complete.
8. Remove the test tube containing the iodine solution and immediately add its contents to the flask containing HCl, $Acetone$, and H_2O, starting a timer after the addition.
9. Swirl the reaction mixture by gently swirling the ring for 30 s and then allow the solution to sit.
10. When the iodine color (brownish-red) has completely disappeared, stop the timer and record the total reaction time (as the reaction is complete).
11. Clean the glassware thoroughly and dry (it is not necessary to clean the test tube as it will always contain iodine solution with a constant concentration).
12. Repeat steps 2-11 two more times for temperature #1 in Table 4.
13. Repeat steps 2-12 for all remaining temperature ranges in Table 4.
14. Thoroughly clean all glassware and dispose of any leftover products/substances safely.

Table 3: Rate Law Experiment

Volumes (mL)				
HCl	$Acetone$	I_2	H_2O	Total
5	5	5	10	25
5	5	10	5	25
5	10	5	5	25
10	5	5	5	25

Table 4: Activation Energy Experiment

Temperature (°C)	Volumes (mL)				
	HCl	$Acetone$	I_2	H_2O	Total
10 – 15	5	5	5	10	25
30 – 35	5	5	10	5	25
40 – 45	5	10	5	5	25

Table 5: Experimental Configurations

5.3 Risk Assessment

(a) **Experimental Safety**

(i) Acetone is highly flammable and can cause moderate irritation on repeated exposure to skin. Hydrochloric acid is corrosive and can lead to severe damage to both the eyes and skin in the case of direct contact. Strong iodine solution is partially corrosive and can cause blistering or necrosis of the skin on direct contact [10, 11, 12]. To counteract these potential concerns, an apron and goggles were worn for the duration of the experiment. All materials were kept at a moderate distance from the body and spills were immediately cleaned.

(ii) Glassware is relatively fragile and any potential breakage can be harmful to those in the lab, both through glass shards and substance spillage. To remedy, extreme caution is used at all times in the lab, especially when handling glassware. In the case that glass did break, the teacher would immediately assist in disposing of any pieces prior to the resumption of the experiment.

(iii) Hot water or glassware can cause sudden reactions and burns of the skin. As water was heated and glassware (with various chemicals) were placed in the water baths, tongs were used at all times to handle warm glass. The water was never directly touched and the water bath was kept closed when not in use.

(b) **Environmental Concerns**

All materials were properly stored and disposed of based on lab best practices and teacher advice to prevent any potential environmental contamination. No limited resources were used nor were any harmful byproducts produced.

(c) **Ethical Concerns**

Materials were measured out in small quantities to minimize the potential wastage of any chemicals. No live organisms were employed, so limited ethical concerns were present.

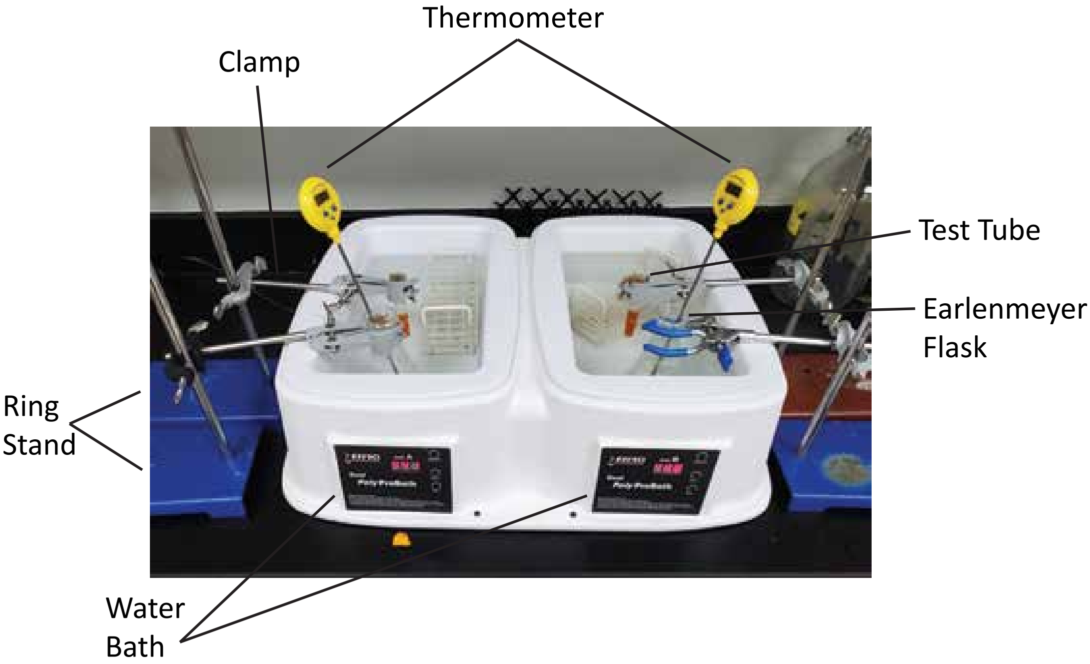


Figure 2: Labelled image depicting the visual setup of the experiment being conducted for two different temperatures.

6 Results

6.1 Raw Data

Setup	Volumes ($\pm.05mL$)					Time ($\pm.05s$)		
	HCl	$Acetone$	I_2	H_2O	Total	#1	#2	#3
#1	5	5	5	10	25	342	354	331
#2	5	5	10	5	25	621	682	634
#3	5	10	5	5	25	161	183	164
#4	10	5	5	5	25	152	165	153

Table 6: Rate Law Experiment (all trials performed at 294.8 K)

Temperature ($\pm.05K$)	Time ($\pm.05s$)		
	#1	#2	#3
287.1	734	725	756
294.8	342	354	331
306.8	134	142	115
317.5	37	42	46

Table 7: Activation Energy Experiment (all trials carried out with volume setup #1 in Table 6)

Table 8: Raw Data

6.2 Qualitative Data

- The iodine solution had a distinctive brownish-red color, similar to that of rust on iron metal.
- A noticeable loss in color could be observed within the first 30 seconds of the reaction, even for trials that took over 10 minutes to come to full completion.
- No observable immediate signs of a vigorous reaction could be observed (outside of the color loss) immediately after the addition of iodine to the remainder of the reactants.
- The acetone had a relatively pungent odor similar to that of nail polish remover.
- The iodine solution seemed to be particularly viscous, especially as opposed to the remainder of the reactants.

6.3 Calculations

6.3.1 Rate Law Experiment

Rationale	Sample Calculation
Firstly, for each volumetric configuration, we must calculate the average time for the three unique trials performed, using the simple arithmetic mean formula: $$\bar{t} = \frac{1}{n}\sum_{i=1}^{n} t_i$$ where n represents the number of trials (3).	Example for Setup #1: $$\bar{t} = \frac{(342 \pm .05) + (354 \pm .05) + (331 \pm .05)}{3} = \frac{(1027 \pm .15)}{3} = (342.0 \pm 0.5)\,\mathrm{s}$$
Then, we must calculate the concentrations of each reactant based on the total volume and their specific volume using the mole-constant dilution formula: $$M_1V_1 = M_2V_2 \; or \; M_2 = \frac{M_1V_1}{V_2}$$ where M_1 is the initial molarity of the reactant, V_1 is the initial volume of the reactant, and V_2 is the total volume ($25mL$). We can additionally calculate potential discrepancies for the largest percent uncertainty and then propagate this error for the remaining results.	Example for Setup #1: $$[I_2] = \frac{0.005\,\mathrm{mol\,dm^{-3}} \times (5.0 \pm 0.5)\,\mathrm{mL}}{(25.0 \pm 0.2)\,\mathrm{mL}} = \frac{(.025 + .00025)}{(25 \pm .2)} = \frac{(.025 + 1\%)}{(25 \pm .8\%)} = .001 \pm 1.8\% = (0.001\,00 \pm 0.000\,18)\,\mathrm{mol\,dm^{-3}}$$ Through an identical process, the final concentrations of $[HCl]$ and $[Acetone]$ can also be determined. Because $[I_2]$ has the smallest quantity, it has the largest percent error of 1.8%, which is carried over for all final concentrations.
Using the two above steps, we can then determine the rate for each individual configuration using the previously discussed equation: $$rate = \frac{[I_2]}{\bar{t}}$$ The same propagation approach is utilized, but the uncertainties are largely irrelevant for the purpose of rate calculation which is predicated on approximation already.	Example for Setup #1: $$rate = \frac{(0.001\,00 \pm 0.000\,18)\,\mathrm{mol\,dm^{-3}}}{(342.0 \pm 0.5)\,\mathrm{s}} = \frac{.001 \pm 1.8\%}{342 \pm .01\%} = 2.92 \times 10^{-6} \pm 1.81\% = 2.92 \times 10^{-6}\,\mathrm{mol\,dm^{-3}\,s^{-1}}$$
After determining the rates for all trials, we can compare the rates for configurations 2 – 4 to the baseline provided by 1 to determine the rate law. As in each of the last 3 trials, the concentration of one reactant was changed while maintaining the total volume, the concentration of that reactant is doubled for that specific trial. Thus, we can calculate our order m by the formula: $$m = \log_2\left(\frac{rate_i}{rate_1}\right)$$ where $rate_i$ is the rate for the given setup and $rate_1$ is the rate for configuration #1. The result must be approximated, as m must be a whole integer >= 0.	Example for Setup #4 (compared to the baseline of Setup #1): $$m = \log_2\left(\frac{6.37 \times 10^{-6}}{2.92 \times 10^{-6}}\right) = \log_2 2.18 = 1.12 \approx \mathbf{1}$$ Thus, the concentration of HCl is first order with respect to the overall reaction based on this determination. The remaining orders are also calculated in the same manner.

Table 9: Rate Law Calculations

Using this process for all trials, the order of HCl, $Acetone$, and I_2 are found to be 1, 1, and 0 respectively. This confirms the theorized rate law of $rate = k[HCl][CH_3COCH_3]$ and is further supported by the published literature on this subject [2]. Through this knowledge, we can now determine the activation energy.

6.3.2 Activation Energy Experiment

<table>
<tr><td>Rationale</td><td>Sample Calculation</td></tr>
<tr><td colspan="2">The first three steps–calculating the average (mean) time for each temperature, determining diluted concentrations, and finding the rate using those two values–are identical for this section as well, and are thus not included to limit redundancy.</td></tr>
<tr><td>After these three steps, we must determine the value of the rate constant k, which we can do by utilizing the rate law. As $rate = k[HCl][Acetone]$, we can rearrange to get:

$$k = \frac{rate}{[HCl][Acetone]}$$

Furthermore, the concentrations of HCl and $Acetone$ are consistent for all temperatures as identical volumes were chosen to ease calculations and limit confounding variables.</td><td>Example for 294.8 K:

$$\begin{aligned} k &= \frac{(2.92 \times 10^{-6} \pm 1.9\%)}{(.2 \pm 1.8\%) \times (.8 \pm 1.8\%)} \\ &= 1.83 \times 10^{-5} \pm 5.5\% \\ &= (1.83 \pm 0.10) \times 10^{-5}\ \mathrm{dm^3\ mol^{-1}\ s^{-1}} \end{aligned}$$</td></tr>
<tr><td>After determining k at each temperature, we will create an Arrhenius graph to determine the activation energy. Taking the natural logarithm of the Arrhenius equation results in:

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

Thus, a linear relationship exists between $\ln k$ and $\frac{1}{T}$, so these values must be determined (along with their uncertainties) for the purpose of graphing.</td><td>Example for 294.8 K:

$$\begin{aligned} \frac{1}{T} &= \frac{1}{(294.80 \pm 0.05)\ \mathrm{K}} = \frac{1}{(294.8 \pm .017\%)} \\ &= .00339 \pm .017\% = (3.3900 \pm 0.0058) \times 10^{-3}\ \mathrm{K^{-1}} \end{aligned}$$

$$\begin{aligned} \ln k &= \ln\left((1.83 \pm 0.10) \times 10^{-5}\right) = \ln\left(1.83 \times 10^{-5}\right) + \frac{.10}{1.83} \\ &= -10.91 \pm .05 \end{aligned}$$</td></tr>
</table>

Table 10: Activation Energy Calculations

This process is again carried out for all four temperatures, providing the necessary values for graphing purposes.

6.4 Processed Data

Setup	Avg. Time (±0.5 s)	Rate ($\mathrm{mol\,dm^{-3}\,s^{-1}}$)
#1	342	$(2.920 \pm 0.053) \times 10^{-6}$
#2	646	$(3.100 \pm 0.056) \times 10^{-6}$
#3	169	$(5.920 \pm 0.107) \times 10^{-6}$
#4	157	$(6.370 \pm 0.115) \times 10^{-6}$

Table 11: Rate Law Experiment (all trials performed at 294.8 K)

Temperature	k ($\mathrm{dm^3\,mol^{-1}\,s^{-1}}$)	$\frac{1}{T}$ (±.17%) ($\mathrm{K^{-1}}$)	$\ln k$ (±.055)
287.1	$(8.47 \pm 0.47) \times 10^{-6}$	3.48×10^{-3}	−11.68
294.8	$(1.83 \pm 0.10) \times 10^{-5}$	3.39×10^{-3}	−10.91
306.8	$(4.81 \pm 0.26) \times 10^{-5}$	3.26×10^{-3}	−9.94
317.5	$(1.49 \pm 0.08) \times 10^{-4}$	3.15×10^{-3}	−8.81

Table 12: Activation Energy Experiment (all trials carried out with volume setup #1 in Table 6)

As determined already, the rates in the Rate Law Experiment were sufficient for calculating/deriving the rate law of the overall reaction. However, to calculate the activation energy, the values of $\ln k$ and $\frac{1}{T}$ were plotted and a linear regression was utilized to calculate a line of best fit (to allow for the determination of the gradient between the 2 variables). The table, including data points and uncertainties, are depicted in Fig. 3. The initial best fit line (for the entire dataset) had a very high correlation coefficient (R^2) of around 99%, indicating a good fit, however this value was partially misleading. By significantly overshooting the data point at 294.8 K, the regression was able to overcome its slightly lower predictions at the other three temperatures. In fact, this line of best fit was completely outside of the range of uncertainty for the data point at 287.1 K. By removing the outlier at 294.8 K, a new trend line was produced with a R^2 of 99.5% and a much better ability to account for the actual data points. However, both lines seemed to generate similar gradients, thus minimizing the overall impact of the improved regression.

To determine the uncertainty of the coefficients in the regression, the statistical premise of 95% confidence intervals was employed. Using the $\frac{1}{T}$ as the x variable and the $\ln k$ as the y, the following procedure was used for the regression of $y = \beta x + \alpha$ [5].

$$S_x = \sum x_i = 13.28$$
$$S_y = \sum y_i = -41.34$$
$$S_{xx} = \sum x_i^2 = 44.15$$
$$S_{yy} = \sum y_i^2 = 431.87$$
$$S_{xy} = \sum x_i y_i = -137.79$$

$$\hat{\beta} = \frac{nS_{xy} - S_x S_y}{nS_{xx} - S_x^2} = -8.54$$
$$\hat{\alpha} = \frac{1}{n}S_y - \hat{\beta}\frac{1}{n}S_x = 18.02$$
$$s_\epsilon^2 = \frac{1}{n(n-2)}\left[nS_{yy} - S_y^2 - \hat{\beta}^2(nS_{xx} - S_x^2)\right] = .01005$$
$$s_{\hat{\beta}}^2 = \frac{ns_\epsilon^2}{nS_{xx} - S_x^2} = .160$$
$$\beta \in [\hat{\beta} \mp t_2^* s_{\hat{\beta}}] = \mathbf{-8.54 \pm 1.72}$$

Thus, the gradient (β) is -8.54 ± 1.72, which can be equated to the slope of the relationship in the Arrhenius equation ($\frac{-E_a}{R}$) to determine the activation energy (using the universal gas constant R). The factor of 10^3 is also reincorporated, as the inverse temperature values had been normalized by factoring out 10^{-3} for improved graphing:

$$E_a = (-8.54 \pm 1.72)\,\mathrm{K}^{-1} \times -8.3145\,\mathrm{J\,mol^{-1}\,K^{-1}} \times 10^3 = (-8.54 \pm 20.1\%) \times -8.3145 \times 10^3 = 71005.83 \pm 20.1\% = (71.01 \pm 14.27)\,\mathrm{kJ\,mol^{-1}}$$

Using the literature value of 86.60 kJ mol^{-1}, the percent error can also be determined:

$$\textit{Total Percent Error} = \left|\frac{\textit{Literature Value - Experimental Value}}{\textit{Literature Value}}\right| \times 100 = \left|\frac{\textit{86.60 - 71.01}}{\textit{86.60}}\right| \times 100 = 18.0\%$$

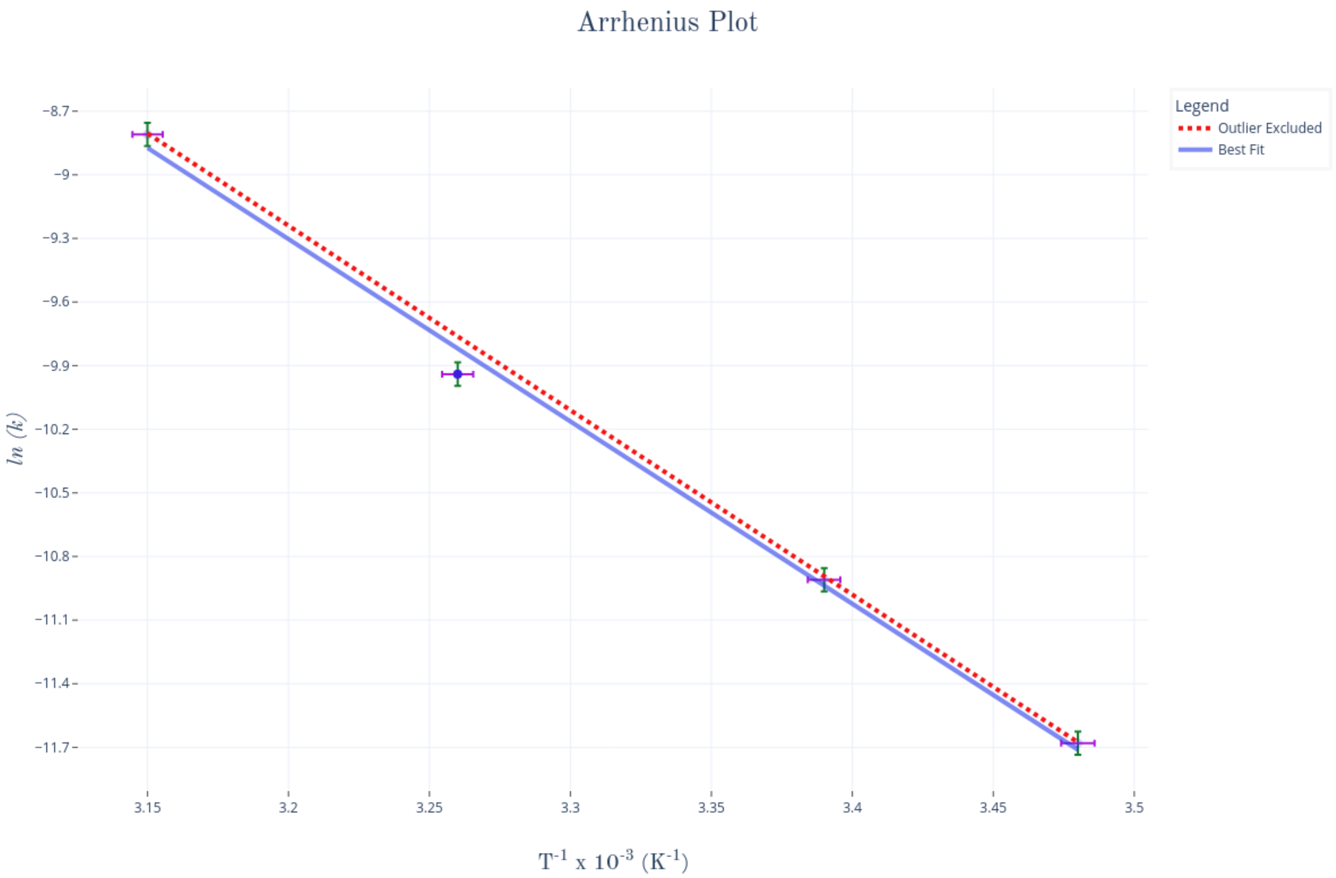


Figure 3: Arrhenius plot of $\ln k$ versus $\frac{1}{T}$ (scaled by 10^3), including a best fit line for the general data and an improved trendline with the outlier removed. The blue regression had a final equation of $y = -8.54x + 18.02$, while the red (outlier removed) regression had a final equation of $y = -8.73x + 18.61$.

6.5 Analysis

Overall, there do not appear to be any serious/obvious anomalies for all data collected in this experiment. The general trend line depicted in the linear regression of Fig. 3 is consistent with the scientific theory of the Arrhenius Equation and the linear relationship between the natural log of the rate constant and the inverse of the temperature of the reaction. The data collected for the trial at 294.8 K did appear to be an anomaly based on this statistical regression, however it was used to accurately determine the rate law for the overall stoichiometric reaction and its elimination did not result in a significantly larger correlation coefficient, indicating that it may not be as large of a structural deviation as initially thought. One possible explanation for this, however, may be that there were major fluctuations in room temperature at the time of the experiment, leading to a consistent change in proportions for all data calculated during thos trials. This explanation would account for the correct rate law being empirically derived from data at this temperature, and would also explain the reason for its status as an apparent outlier in the multi-temperature regression. The high R^2 value also suggests a strong statistical significance of the determined results, further providing support to the initial claims and lending credibility to the design and implementation of the experiment in its entirety. The uncertainties of the results were generally low for the majority of measurements, including those for temperature and volume, however the error for the final regression (and thus the activation energy) did become large due to a limited dataset size. This large error indicates systematic errors in the premise of the experiment, which will be further analyzed.

7 Evaluation

7.1 Error Evaluation

As with any laboratory experiment, it is crucial to both identify and evaluate errors related to equipment and experimental design. The large percentage error calculated above also emphasizes the need for a thorough analysis of potential sources of error throughout the experiment, and thus they are discussed below. It is obviously imperative to recognize that many of these errors are a result of the constraints of utilizing a school laboratory with limited access to equipment and controlled environments, however, finding potential room for improvement can still help in the description of obtained results and create further extensions for future work.

7.1.1 Equipment

Equipment	Absolute Uncertainty	Smallest Measurement	Percentage Uncertainty	Significance/Improvement
Electric Timer (to determine time of reaction)	±0.05 s	37 s	.14%	This is a very low percent error (< .5%) and lends credibility to the results of the overall investigation. It is highly unlikely that human error with regards to the starting and stopping of the electric timer was a much larger contributor to overall issues with the final results, as opposed to the equipment itself. Thus, no material improvement is required for the purpose of time determinations.
10 mL Graduated Cylinder (to measure out reactants)	±0.05 mL	5 mL	1%	This is a moderate percent error, as it is still relatively low for the purpose and scope of the general investigation, but is quickly compounded. Because the volumes are used in a multitude of locations during the calculations (and there may be potential issues with the initial molarity), an improvement to the volumetric measuring process could drastically reduce overall experimental error. To achieve this beneficial result, a more precise measuring tool (such as a 1 mL syringe) could have been used.
Thermometer (to determine temperature of water baths)	±0.05 K	287.71 K	.01%	This is an extremely low percent error (< .1%) and strengthens the overall results, especially of the determination of the rate constant. The overall impact of this temperature fluctuation on the final result is very minimal and no equipment improvements are required for temperature determination. Controlling the temperature for the duration of the experiment was instead a more potent and potentially harmful issue for the results and study as a whole.

Table 13: Equipment Error Evaluation

7.1.2 Experimental Design

Cause/Description	Impact on Results	Potential Alleviation
Limited Temperature Range (with a potential outlier)	Due to time and some feasibility constraints, only 4 unique temperatures were chosen at which to run trials for the final activation energy experiment. These temperatures were relatively close magnitude-wise, indicating limited issues with intermediate temperature trends, however extreme temperatures were neglected on both ends of the spectrum. This could have caused serious drifts in the gradient calculation through the linear regression process. Additionally, 1 of the 4 temperatures appeared to provide outlier data, which was not thoroughly investigated nor confirmed.	Obviously, more temperatures could have been used for testing purposes to assess whether extremely high or low temperatures cause serious deviations in the rate of the overall reaction. This would have also assisted in limiting the uncertainty with regards to the linear regression. It is, however, important to consider that at these extreme temperatures the reactant mixtures (containing water) could begin to boil or freeze, further introducing a confounding variable into the experiment.
Determination of completion of reaction (Random)	As iodine provides a strong color to the reactant mixture, a lack of color was relied for determining when the reaction had finished. This leads to potential variance with regards to the "specific" instance at which the reaction was truly finished and limits the consistency between trials. This issue is especially pertinent for quick trials (such as those at high temperatures), as the change is relatively rapid, and any hesitations or lack of sureness can have a serious impact on the final results.	To remedy this, a spectrophotometer can be used to accurately measure wavelength absorbance of the reactant mixture during the duration of the reaction. This would ensure a consistent reading and limit human error with regards to the determination of completion. Due to issues with maintaining temperature equilibrium and the lack of resources, the device was not used for this investigation.
Inadequate Temperature Control (Random)	The impact of temperature on the rate constant inherently relies on maintaining a constant temperature for all reactants for the entirety of the reaction. However, because of the need for manual swirling while the reactants were in the water bath in addition to the open environment of the laboratory, it was difficult to accurately maintain the isolated temperature consistently.	To ease the swirling process, an external magnetic stirring device could have been utilized to provide both more uniform mixing and limit the time spent outside the bath by the reactants. Ideally, a closed environment could be used to minimize external temperature fluctuations, however this was outside of the potential scope of this investigation.
Unaccounted change in concentrations of acid and acetone (Systematic)	The rate law determined for the reaction is $2nd$ order and depends on the concentration of HCl and $Acetone$. To determine the rate, the assumption was made that the concentrations of these two reactants/catalysts remained constant, but there were obviously minor reductions for the concentration of both. This means that the simplification used to calculate the rate was not entirely accurate, as the rate did not stay even for the duration of the reaction.	Some more complex mathematical techniques have been used in previous literature to attempt to better account for variations in the rate of the reaction over time, but they are largely out of the scope of this investigation. Overall, it has been found that ensuring $[HCl]$ and $[Acetone]$ significantly outweigh $[I_2]$ can minimize the error introduced by this issue, so it probably had limited impact on the final results.

Table 14: Experimental Design Error Evaluation

7.1.3 Summary

As demonstrated by Table 13, there were limited equipment based errors for the majority of this experiment. Both of the primary tools used for measurement had uncertainties less than 1%, indicating that higher precision would not have drastically improved confidence or accuracy of the final results. It is important to note that the use of this equipment led to random error, as the determination of when to start and stop the timer was subject to the experimenter and varied between trials. Table 14 highlights both systematic and random errors associated with the actual design of the experiment itself. The lack of temperatures at which trials were conducted is the first major example of a systematic error, as this contributed to the final linear regression and drastically increased the uncertainty of the coefficients. Because the statistical approach of confidence intervals is inherently predicated on the degrees of freedom in the experiment (which approximately relates to the total data points), a lack of temperature ranges was a major inhibiter in producing more definite results. The lack of accountability in the change in concentration of the non-iodine reactants also provided another source of systematic error that could have been remedied to more accurately determine the rate of reaction. Prior literature has suggested that the concentrations of these reactants both undergo somewhat material fluctuations and can have large impacts on the rate of the otherwise slow iodination of acetone. The random errors of inadequate temperature control and a subjective mechanism for determining the completion of the reaction were also present, but would have required more complicated equipment and procedures to effectively control, which suggests that their alleviation is outside of the scope of this investigation. Overall, the investigation had a multitude of strengths and weaknesses in both the equipment utilized and the experimental procedure designed, which were partially discussed above and will be further analyzed in the subsequent comparison to documented scientific literature.

7.2 Comparison to Scientific Literature

The percent error of the result generated through this experiment ($(71.01 \pm 14.27)\,\mathrm{kJ\,mol^{-1}}$) and the accepted literature value from multiple papers ($86.60\,\mathrm{kJ\,mol^{-1}}$) was calculated to be 18% in the results section. This error is larger than the 12% uncertainty of the calculated result, indicating a serious systematic error in the methodology of this experiment. Therefore, it is worth comparing the procedure detailed throughout this paper and those employed by the various literature to analyze potential areas for improvement and justifications for the variation in the final result. The first approach was detailed by Rice and Kilpatrick [13] in which small quantities of the reaction mixture were drawn from the total reaction and passed through sodium bicarbonate and thiosulfate solution. The large concentrations of HCl and $Acetone$ (as compared to $[I_2]$) was similar to that employed here, but the repeated usage of sodium bicarbonate and thiosulfate solution and the subsequent liberation of iodine was used to determine the rate of disappearance of iodine (or the overall rate of reaction of the iodination of acetone). This method allowed for more frequent assessments of the rate of the iodination reaction and provided more datapoints to ensure that the change in concentration of the non-iodine reactants was not affecting the rate. However, repeatedly opening the reactant solution to draw these samples out may have caused a similar issue to the presented investigation in which the temperature fluctuated. Overall, this procedure was unique in its lack of reliance on the light-absorbance of iodine solution, and was thus able to produce results with very limited uncertainty. In fact, the focus of the investigation was to minimize potential errors in the apparatus. Much of the difficulty in thoroughly comparing this investigation to Rice and Kilpatrick [13] is the large divide in equipment access and time constraints.

Bell and Yates [3] also proposed a very similar experiment to Rice and Kilpatrick [13] by using titration techniques to repeatedly determine the rate of removal of I_2 from the reactant mixture, however they incorporated a buffer solution via the addition of potassium iodate to maintain the relative pH value of the overall solution. This helped introduce the discovery that this reaction between iodine and acetone is highly reversible in strongly acidic solutions. It is important to recognize that HCl simply behaves as a catalyst in this reaction, it is not an active reactant, and thus it lowers the activation energy of both the forward and backward reaction. Both of the reactions are exceedingly slow in the absence of a catalyst (especially as compared to the general halogenation of many organic compounds), however the introduction of an acid catalyst allows for a more feasible reaction in both directions. At moderately acidic pH values for the reaction mixture, this allows for an eventual equilibrium shifted distinctively to the right. However, for more concentrated acidic solutions ($> 0.05\,\mathrm{mol\,dm^{-3}}$), the backwards reaction becomes more feasible, shifting the equilibrium towards the left and preventing the complete halogenation of the reaction. This result is particularly influential for the investigation presented here, as the production of reactants in the reverse reaction would have artifically inflated the total duration of the reaction and produced incorrect calculations for the rate of consumption of I_2 solution. The introducation of buffer solutions, as used by Bell and Yates [3], can prevent large fluctuations in the pH of the solution mixture, especially after the intermediate production of enols (which are slightly acidic themselves). This result also indicates an "optimal" concentration of H^+ ions at which the equilibrium constant is maximum and the time required for equilibrium to be reached is minimum, which would be worth further investigation via the use of various acidic concentrations.

A more traditional approach to the study of this reaction is also described by Albery and Robinson [2], where the absorbance of iodine and the change in absorbance of the reaction mixture is measured with the help of a spectrophotometer to determine the rate of the reaction at various points. This procedure was able to generate highly consistent (and accurate) results with limited trials through the use of a differential method for activation energy calculations. Although the mathematical premise of the investigation falls outside of the scope of this research, the introduction of absorbance data could facilitate an easier mechanism for calculating the activation energy and provide a more relevant baseline for comparison with the linear regression. The use of a spectrophotomer does require constant transfer of small quantities of the reaction mixture from the temperature-stable vessel to the external machine. To minimize heat loss to the surroundings, Albery and Robinson [2] were able to use thermostatted pipettes which would most likely not have been feasible for this experiment.

7.3 Extensions

Many of the potential methodological extensions/improvements to this investigation were discussed in the comparison to external literature, however, there are other relevant extensions that could provide important information for industrial and theoretical purposes. Comparing various acidic catalysts and alternative halogens for this type of reaction could assist in determining optimal techniques for mass production of enols and improving the ability to rationalize the differences in proposed mechanisms for enolization in acidic-solutions. It would also be intriguing to compare this investigation to the same reaction with a basic catalyst. These experiments could provide an ability to investigate different potential products and the direct impact of the pH of the reactant mixture on the rate and mechanism of the general iodination of acetone [16].

8 Conclusion

Although the calculated value for the activation energy of the iodination of acetone reaction ($(71.01 \pm 14.27)\,\mathrm{kJ\,mol^{-1}}$) had a percent error of over 18% as compared to the widely accepted literature value of $86.60\,\mathrm{kJ\,mol^{-1}}$, the trends determined through the course of the experiment and the evaluation of the potential limitations support the general process and seem to confirm the initial hypothesis and the empirical theory upon which it was proposed. Furthermore, the investigation clearly focused on analyzing the initial research question–**How does varying temperature affect the rate of reaction between iodine and acetone solution in the presence of a hydrochloric acid catalyst?**–as it allowed for the determination of the rate at multiple temperatures. The linear regression calculated through proper stastical methods also lends credibility on the determination of the activation energy and the result could have been improved through remediation of the most glaring errors described above.

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