ACTIVATION ENERGY OF IODINATION OF ACETONE

Investigating the effect of temperature on the rate of iodination of Acetone, and hence determining the Activation energy of the reaction.
# 1 CONTENTS

Introduction: ................................................................. 2  
Research Question ........................................................... 5  
Hypothesis ........................................................................ 5  
Variables ........................................................................... 5  
  Independent Variable ......................................................... 5  
  Dependent Variable ............................................................ 6  
  Controlled Variable ............................................................ 6  
Apparatus ........................................................................... 8  
Pre Lab Preparations ............................................................. 9  
  HCl (1.0 mol dm$^{-3}$, 300 cm$^3$) ............................................. 9  
  Acetone (4 mol dm$^{-3}$, 300 cm$^3$) .......................................... 9  
  Iodine (0.005M, 300cm$^3$) .................................................. 10  
Procedure ........................................................................... 12  
  Setting up the apparatus ....................................................... 12  
  Investigation procedure ....................................................... 12  
  Safety Considerations ......................................................... 13  
Data Collection and Processing ............................................. 14  
  Qualitative Data ................................................................ 14  
  Raw Data ........................................................................ 14  
  Data Processing .................................................................. 14  
Conclusion and Evaluation .................................................. 22  
  Evaluation ....................................................................... 22  
  Error Evaluation ................................................................ 23  
Further Investigation ......................................................... 24  
Bibliography .......................................................................... 25
2 INTRODUCTION

According to Chemical Kinetics, the rate of reaction, that is how fast a reaction occurs, depends on the concentration of reactants, the temperature, the presence of catalysts, the surface area of the reactants, and the solvents\(^1\).

For any given reaction which is not reversible, the rate of reaction increases with the increase in temperature and concentration. To express the relation of rate of reaction with concentration of the reactants, the rate law is used. For a reaction:

\[
xA + yB \rightarrow zC
\]

The rate can be expressed by the following equation\(^2\):

\[
rate = k[A]^m[B]^n
\]

Where:
- \(k\) is the rate constant
- \([A]\) is the concentration of A in Moles per dm\(^3\)
- \([B]\) is the concentration of B in Moles per dm\(^3\)
- \(m\) and \(n\) are the order of the reaction.

As with the concentration, there is a relation between reaction rate and temperature. Temperature is the measure of the average kinetic energy of the molecules. The higher the Kinetic energy, the more the collisions taking place. While temperature affects the rate of the reaction, there is a certain minimum amount of energy required to initiate the reaction. This energy is called the Activation Energy.

Activation energy can be defined as the minimum energy requirement that must be met for a chemical reaction to occur\(^3\).

Figure 1.1 – Graph of Total energy in the system against the progress of the reaction, representing the activation energy\(^4\).

---

\(^1\) [http://chemwiki.ucdavis.edu/Physical_Chemistry/Kinetics/Factors_That_Affect_Reaction_Rates](http://chemwiki.ucdavis.edu/Physical_Chemistry/Kinetics/Factors_That_Affect_Reaction_Rates)  
\(^3\) [http://chemwiki.ucdavis.edu/Physical_Chemistry/Kinetics/Modeling_Reaction_Kinetics/Temperature_Dependence_of_Reaction_Rates/The_Arrhenius_Law/The_Arrhenius_Law%3A_Activation_Energies](http://chemwiki.ucdavis.edu/Physical_Chemistry/Kinetics/Modeling_Reaction_Kinetics/Temperature_Dependence_of_Reaction_Rates/The_Arrhenius_Law/The_Arrhenius_Law%3A_Activation_Energies)  
\(^4\) [http://courses.bio.indiana.edu/L104-Bonner/F13/imagesF13/L15/activation%20energy%20graph-01.jpg](http://courses.bio.indiana.edu/L104-Bonner/F13/imagesF13/L15/activation%20energy%20graph-01.jpg)
The equation relating the rate constant, \( k \), to the temperature at which the reaction occurs, \( T \), and the activation energy, \( E_a \), is\(^5\):

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

Where:

- \( k \) is the Rate Constant
- \( A \) is the frequency factor or the pre-exponential factor
- \( E_a \) is the Activation Energy at standard conditions
- \( R \) is the Universal Gas constant (8.314 joules mol\(^{-1}\) K\(^{-1}\))

This equation is known as the Arrhenius Equation. The equation can be rewritten as:

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

(2)

This way, we get a straight line \((y = mx + c)\) when we plot the graph of \( \ln(k) \) vs \( 1/T \). The slope of the equation will give us the activation energy.

Thus, by measuring \( k \) at different temperatures we can determine graphically the activation energy for a reaction, as shown below:

Figure 1.2 – An Arrhenius plot showing how Activation Energy is calculated. The graph is of the natural log of the Rate constant against the reciprocal value of the temperature of the reaction, in Kelvin\(^6\).

\[\text{An Arrhenius plot}\]

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

\[
slope = \frac{-E_a}{R}
\]

\[\text{1/T}\]

\[\ln k\]

\(^5\) http://www.chem1.com/acad/webtext/dynamics/dynamics-3.html

The reaction taking place in the experiment is:

Figure 1.2 – Reaction of Acetone with Iodine

\[
\begin{array}{c}
\text{C} & \text{O} \\
\text{CH}_3 & \text{CH}_3 \\
\end{array} + \text{I}_2(\text{aq}) + \text{H}^+ \rightarrow
\begin{array}{c}
\text{C} & \text{O} \\
\text{CH}_3 & \text{CH}_2\text{I} \\
\end{array} + \text{HI}(\text{aq})
\]


The rate of this reaction is expected to depend on the concentration of hydrogen ion in the solution, a catalyst, as well as the concentrations of the two reactants. By Equation 1, the rate law for this reaction is:

\[
\text{rate} = k[\text{acetone}]^m[\text{H}^+]^n[\text{I}_2]^p
\]  \hspace{1cm} (3)

Where \(m\), \(n\), and \(p\), are the orders of the reaction with respect to acetone, hydrogen ion, and iodine, respectively, and \(k\) is the rate constant for the reaction. It has been found that the rate is independent of the concentration of iodine\(^8\). Thus, the values of \(m\), \(n\), \(p\) are found to be:\(^9\)

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>(m)</td>
<td>1</td>
</tr>
<tr>
<td>(n)</td>
<td>1</td>
</tr>
<tr>
<td>(p)</td>
<td>0</td>
</tr>
</tbody>
</table>

Table 1.1 – Values of ‘\(m\)’, ‘\(n\)’, ‘\(p\)’

The rate of this reaction can be expressed as the change in the concentration of iodine, \(\Delta[I_2]\), divided by the time interval, \(\Delta t\), required for the change\(^{10}\):

\[
\text{rate} = \frac{-\Delta[I_2]}{\Delta t}
\]  \hspace{1cm} (4)

The minus sign is present because during the reaction, there is a reduction in the concentration of iodine, and thus, the change is negative.

This reaction was selected because from research, it is considerably slow so that the time of the reaction can be calculated with ease. Another characteristic of this reaction would be that reaction mixture would have a distinct pale yellow colour which can be easily observed visually. In this experiment, the reaction will be conducted at different temperatures the time taken for iodine to completely react will be measured by observing the colour change. All further calculations will proceed as discussed further.

\(^7,6\) http://mhchem.org/222/pdfLabs222/KineticsPartI.pdf
\(^8\) It has been found that the rate of halogenation of acetone is independent of the concentration of halogen, except at very high acidities. http://www.tau.ac.il/~phchlab/experiments_new/kinetics/theory.html
3 RESEARCH QUESTION

Investigating the effect of temperature on the rate of iodination of Acetone, and hence determining the Activation energy of the reaction.

4 HYPOTHESIS

According to kinetics, increasing the temperature and providing heat energy increases the rate of reaction by speeding up the molecular collisions in a reaction. Thus, increasing the temperature in this reaction would reduce the time taken to complete the reaction. Not much can be concluded about the Activation Energy of the reaction, except the fact that it would be negative, as the slope of ln(k) vs. RT is a negative slope. Also, there is no literature value available of the Activation Energy of this particular reaction at Standard Conditions.

5 VARIABLES

5.1 INDEPENDENT VARIABLE

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>How it was measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature of the reaction mixture</td>
<td>°C ±0.05</td>
<td>This parameter was changed and controlled using a water bath. The decided temperature range was from 25°C to 45°C, at intervals of 5°C, the only reason being that 25°C was the room temperature, and reducing the temperature further would be difficult and would require a different apparatus; and increasing the temperature above 45°C would increase the rate of the reaction, which would make it difficult to measure the time accurately. The apparatus for the following was a water bath of heated water, in which the reaction container was dipped until the desired temperature was reached, and then adding the final reactant, Acetone, to the mixture. The temperature inside was continuously logged using the Pasco Spark Data Logger, and in the event of any decrease in temperature, the reaction container was briefly dipped in the water bath. During an event of an increase in temperature, the reaction container was dipped in another beaker of cool water in order to maintain the temperature. This method of maintaining a constant temperature is systematically not precise, but within the given limits of the lab apparatus, it was the only reasonable option. The detailed error analysis of the process is done further. The least count of the data logger and temperature probe was 0.1°C, making the error ±0.05°C</td>
</tr>
</tbody>
</table>
5.2 Dependent Variable

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>How it was measured</th>
</tr>
</thead>
<tbody>
<tr>
<td>Time of reaction</td>
<td>Seconds (s) ±0.005s</td>
<td>The time was measured using a stopwatch. The least count of the stopwatch is 0.01 seconds, and thus, the uncertainty is ±0.005 s. For each value of temperature, five similar trials were conducted. The time for each was noted down, and an average of the five values was considered to be the final time of the reaction. This way, any random errors in the experiment might be reduced.</td>
</tr>
</tbody>
</table>

5.3 Controlled Variable

<table>
<thead>
<tr>
<th>Variable</th>
<th>Unit</th>
<th>How it was controlled</th>
</tr>
</thead>
<tbody>
<tr>
<td>Concentration of the reactants</td>
<td>mol dm$^{-3}$</td>
<td>The concentration of the reactants in the reaction mixture was kept constant, as only the effect of temperature on the rate of reaction was of importance. Varying the concentration would also change the rate of the reaction. Therefore, the following constant concentrations were decided upon:</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Initial Concentrations (mol dm$^{-3}$)</th>
<th>HCl</th>
<th>Acetone</th>
<th>I$_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1</td>
<td>4</td>
<td>0.005</td>
</tr>
</tbody>
</table>

These values were maintained by making the reactants manually, with utmost care. For measuring the concentration, first, a solution of a known concentration was taken, or a solid form of the reactant was taken (wherever appropriate); to which appropriate amount of water was added in order to obtain the desired concentrations.

The solutions from which the reactants were made, are assumed to have no errors. The uncertainty in the produced concentrations is discussed further in Preparation of Reagents.

<table>
<thead>
<tr>
<th>Volume of each reactant</th>
<th>cm$^3$</th>
<th>Volume of each reactant in the reaction mixture was kept constant, to ensure that for each trial, the same amount of reactant is reacting with the other. This is essential in ensuring that temperature is the only factor causing a change in the rate. The volumes of the reactants were kept as follows:</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Table 3.2 – Volumes of the reactants used in the reaction.</th>
<th>HCl (cm$^3$)</th>
<th>Acetone (cm$^3$)</th>
<th>I$_2$ (cm$^3$)</th>
<th>Water (cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>20</td>
</tr>
</tbody>
</table>

Note: Water is not a reactant, but it varies the concentration of the other reactants, and hence, the amount of water was also constant.
These volumes were measured using a 10 cm\(^3\) measuring cylinder which has a least count of 0.1 cm\(^3\) and, and therefore, the uncertainty in each reactant is ±0.05 cm\(^3\) for HCl, ±0.05 cm\(^3\) for Acetone, ±0.05 cm\(^3\) for I\(_2\), and ±0.1 cm\(^3\) for water, as it was measured out twice.

<table>
<thead>
<tr>
<th>Total volume of the reaction mixture</th>
<th>cm(^3)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>The total volume of the reaction mixture was kept constant at 50 cm(^3). The reactants were added in fixed amounts like mentioned above, into the main reaction container.</td>
</tr>
</tbody>
</table>
Table 5.1 – Apparatus used in the investigation

<table>
<thead>
<tr>
<th>Apparatus</th>
<th>Capacity</th>
<th>Uncertainty</th>
<th>Quantity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Glass beakers</td>
<td>50 cm³</td>
<td>-</td>
<td>4</td>
</tr>
<tr>
<td>Glass beaker</td>
<td>500 cm³</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Conical flask</td>
<td>200 cm³</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Measuring cylinder</td>
<td>10 cm³</td>
<td>± 0.1 cm³</td>
<td>4</td>
</tr>
<tr>
<td>Measuring cylinder</td>
<td>50 cm³</td>
<td>± 0.5 cm³</td>
<td>1</td>
</tr>
<tr>
<td>Measuring cylinder</td>
<td>500 cm³</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Bunsen Burner</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Tripod Stand</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Wire Mesh</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Label stickers</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Stopwatch</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Magnetic stirrer</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>White paper sheet</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Airtight bottles</td>
<td>&gt;300 cm³</td>
<td>-</td>
<td>2</td>
</tr>
<tr>
<td>Dropper</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Glass rod</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Digital balance</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Pasco Spark Data Logger</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
<tr>
<td>Spark Temperature probe (DS18B20)</td>
<td>-</td>
<td>-</td>
<td>1</td>
</tr>
</tbody>
</table>
7 PRE LAB PREPARATIONS

7.1.1 HCl (1.0 mol dm$^{-3}$, 300 cm$^{3}$)

**Preparation**
1. Concentrated HCl of 12.0 mol dm$^{-3}$ concentration was used as initial solution.
2. Using equation
   
   \[ M_1 V_1 = M_2 V_2 \]
   
   \[ M_1 = 12 \text{ mol dm}^{-3} \]
   \[ M_2 = 1.0 \text{ mol dm}^{-3} \]
   \[ V_2 = 0.3 \text{ dm}^{3} \]

   \[ V_1 = \frac{1 \times 0.3}{12} = 0.025 \text{ dm}^{3} = 25 \text{ cm}^{3} \]

3. Take 25 cm$^{3}$ of 5.0 M HCl in a 50 cm$^{3}$ measuring cylinder
4. Pour the HCl in a 500 cm$^{3}$ measuring cylinder and add distilled water to it until the whole solution becomes 300 cm$^{3}$. (Distilled water amount added should be (300-25) cm$^{3} = 275$ cm$^{3}$
5. Add the solution in the beaker and stir it using a clean and dry glass rod
6. Using an aluminium foil, cover the beaker, in order to avoid evaporation of HCl

**Uncertainty**
The error in measuring volume in Step 4 is ±0.5 cm$^{3}$, as the least count of the measuring cylinder is 1 cm$^{3}$. The error in measuring volume of water in step 5 is ±2.5 cm$^{3}$, as the least count of the 500 cm$^{3}$ measuring cylinder is 5 cm$^{3}$.

Therefore, the total error in measuring the volume is

\[ ±(0.5 + 2.5)\text{cm}^3 = ±2.5\text{cm}^3 = ± 0.003 \text{ dm}^3 \]

Thus, the concentration is 1.0 ± 0.003 M

7.1.2 Acetone (4 mol dm$^{3}$, 300 cm$^{3}$)

**Calculations**

\[ M_r \text{ of Acetone} = 58.08 \text{ g mol}^{-1} \]

<table>
<thead>
<tr>
<th>Mass of Acetone (g)</th>
<th>Volume of Acetone Solution (dm$^{3}$)</th>
<th>Concentration (mol dm$^{3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>58.08</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>58.08 x 4 = 232.23</td>
<td>1</td>
<td>1 x 4 = 4</td>
</tr>
<tr>
<td>232.23 x 0.3</td>
<td>1 x 0.3</td>
<td>4</td>
</tr>
<tr>
<td>69.669</td>
<td>0.3</td>
<td>4</td>
</tr>
</tbody>
</table>

Therefore, the required mass of Acetone in grams is 69.669 grams.

Density of Acetone (STP) = 0.790 g cm$^{-3}$

Volume = \[ \frac{\text{Mass}}{\text{Density}} = \frac{69.669}{0.790} = 88.1886 \approx 88.2 \text{ cm}^3 \]
**Preparation**

1. Measure 88 cm$^3$ Acetone in a 100 cm$^3$ measuring cylinder
2. Pour the Acetone into a 500 cm$^3$ measuring cylinder
3. Add distilled water to the 500 cm$^3$ measuring cylinder until the solution becomes 300 cm$^3$ in total. (Amount of distilled water added should be about (300-88) cm$^3 = 212$ cm$^3$)
4. Pour out the contents of the 500 cm$^3$ measuring cylinder into a clean, airtight chemical container.

**Uncertainty**

The uncertainty in step 1 is ±0.5 cm$^3$ as the least count of the measuring cylinder is 1.0 cm$^3$. The uncertainty in step 4 is ±2.5 cm$^3$ as the least count of the measuring cylinder is 5.0 cm$^3$.

Therefore, the total uncertainty in volume = ±(0.5 + 2.5) cm$^3 = ±3.0$ cm$^3 = 0.003$ dm$^3$

Therefore, the uncertainty in Concentration is 4 ± 0.003 mol dm$^{-3}$

---

**7.1.3 Iodine (0.005M, 300cm$^3$)**

**Calculations**

Molar Mass of I$_2$ = 253.81

Concentration required = 0.005 mol dm$^3$

Mass = Moles × Molar Mass

Mass = 0.005 × 253.81 = 1.269 grams

Therefore, 1.269 grams of I$_2$ will yield 1 dm$^3$ of 0.005M solution.

Thus, for 200cm$^3$ of solution:

$$\left(1.269 \text{ grams} \times \frac{200 \text{ cm}^3}{1000 \text{ cm}^3}\right) = 0.2538 = 0.254 \text{ grams}$$

**Preparation**

1. Measure 300cm$^3$ concentrated Potassium Iodide (KI) in a washed and dry 500cm$^3$ measuring cylinder, and pour it in a clean beaker.
2. Measure 0.254 grams of Iodine granules on a digital balance as accurately as possible
3. Take the Iodine granules and add it to the KI solution
4. With a glass rod, stir the solution until the granules are not visible. If the Iodine is taking a long time to dissolve, crush the pellets with the glass rod and put the beaker over a magnetic stirrer, and start the process.
5. After a few minutes, the granules should disappear and should impart a dark maroon colour to the solution.
6. Cover the beaker with a plastic or aluminium foil to prevent any impurities from falling in.
Uncertainty

The uncertainty in measuring volume in the first step is ±2.5 cm$^3$, as the least count of a 500 cm$^3$ measuring cylinder is 5 cm$^3$.

The uncertainty in measuring the mass in Step 2 is ±0.0005g as the least count of the digital balance is 0.001g.

Thus, the total uncertainty in Moles is ±0.0005 mol because moles is nothing but the mass divided by the molar mass.

The uncertainty in volume is ±2.5cm$^3$ that is ±0.0025dm$^3$.

Therefore, the Total Percentage uncertainty:

\[
\frac{2.5}{300} \times 100 + \frac{0.0005}{0.005} \times 100 = 10.008\%
\]

Therefore, the absolute uncertainty is

\[
\frac{10.008}{100} \times 0.005 \text{ mol dm}^{-3} \approx 0.0005 \text{ mol dm}^{-3}
\]

The final concentration of I$_2$ solution is 0.005 ± 0.0005 M.
8 Procedure

8.1 Setting up the apparatus

1. Take the individual beakers of the reagents and label them according to their contents.
2. Place them in a line, and in front of each one of them, for the sake of convenience, place a 10cm³ measuring cylinder which is cleaned and dry.
3. Fill a 500cm³ beaker with approximately 300cm³ distilled water and place it next to the beakers with its own 10cm³ measuring cylinder.
4. Besides the chemicals, place a 1000 cm³ glass beaker filled with approximately 400 cm³ of water, on a wire mesh over a tripod stand.
5. Place a Bunsen burner under the stand.
6. Take a dry and cleaned 200 cm³ conical flask, which will be our reaction container, and place the temperature probe inside such that the tip touches the base of the conical flask. Lead the remaining wire out of the flask.
7. Keep a cork ready next to the flask as on adding the reactants, the cork will have to be fastened on the flask.
8. Place a piece of white paper next to the setup, which will be used to compare the colour.

8.2 Investigation procedure

<table>
<thead>
<tr>
<th>Trial</th>
<th>Volumes of reactants</th>
<th>Total Volume (cm³)</th>
<th>Temperature (°C) ± 0.05°C</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>HCl (cm³)</td>
<td>± 0.1 cm³</td>
<td>Acetone (cm³)</td>
</tr>
<tr>
<td>1</td>
<td>10</td>
<td></td>
<td>10</td>
</tr>
<tr>
<td>2</td>
<td>10</td>
<td></td>
<td>10</td>
</tr>
<tr>
<td>3</td>
<td>10</td>
<td></td>
<td>10</td>
</tr>
<tr>
<td>4</td>
<td>10</td>
<td></td>
<td>10</td>
</tr>
<tr>
<td>5</td>
<td>10</td>
<td></td>
<td>10</td>
</tr>
</tbody>
</table>

1. Switch on the Bunsen burner
2. Set up a new experiment on the data logger and start logging the temperature
3. Measure and add 10 cm³ of HCl in the reaction container.
4. Add 20 cm³ of water after measuring it in the measuring cylinder, into the reaction container.
5. To this, add 10 cm³ of iodine solution.
6. Make sure the temperature probe inside is dipped in the liquid.
7. Fasten the reaction container with the cork.
8. Using a test tube holder, dip the flask in the water bath.
9. Keep the container in the water until the temperature required is reached. You will have to keep an eye on the data logger simultaneously.
10. When the temperature required is reached, quickly remove the flask from the water bath and let the temperature come to the required amount.
11. When the required temperature is attained, uncork the flask, add 10 cm³ of Acetone to it, and then cork it again as fast as you can. Start the stopwatch simultaneously.
12. There should be a small drop in the temperature, and to heat up the reaction again, dip the container in the water bath for a short time, until the temperature required is reached.
13. Remove the container from the water bath again, and keep swirling it with your hand until the colour of the contents becomes transparent. Use the white sheet of paper to compare the colour.

14. If there is a drop in the temperature, dip it in the water bath again for a short time, to reach the desired temperature. Under rare circumstances, if there is cooling required, pour some cold water over the flask to maintain the temperature.

15. At the point the solution becomes transparent, stop the stopwatch.

16. Record the time in a table.

17. Clean the reaction container properly and dry it with a cloth, and prepare it for the next run.

Repeat Steps 3 to 17 five times for each trial, recording your results in a table given below.

<table>
<thead>
<tr>
<th>Trial No.</th>
<th>Temperature (°C) ± 0.005</th>
<th>Time Taken (s) ±0.005s</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial 1</td>
<td>25</td>
<td>T₁</td>
</tr>
<tr>
<td>Trial 2</td>
<td>30</td>
<td>T₂</td>
</tr>
<tr>
<td>Trial 3</td>
<td>35</td>
<td>T₃</td>
</tr>
<tr>
<td>Trial 4</td>
<td>40</td>
<td>T₄</td>
</tr>
<tr>
<td>Trial 5</td>
<td>45</td>
<td>T₅</td>
</tr>
</tbody>
</table>

**Table 7.2 – Observation Table to record the results.**

8.3 **Safety Considerations**

- Handle HCl with care, especially concentrated HCl, while making the reactant.
- Do not touch iodine pellets directly with your hand. Use a spatula.
- Do not try to inhale over iodine solution or Acetone, as both form vapours, though iodine takes time.
- While the experiment is going on, wear a lab coat, safety goggles, and gloves at all times.
- Do not touch the Bunsen burner, tripod stand, or the wire mesh at any time in the experiment, as they are extremely hot.
- Always dip the reaction container gently in the water bath to avoid splashes.
- Conduct the experiment under adult supervision.
9 DATA COLLECTION AND PROCESSING

9.1 QUALITATIVE DATA
On adding Iodine to the reaction mixture, the solution turns pale yellow. After the addition of Acetone, the solution slowly starts to lose the colour and becomes colourless. This is a considerably slow reaction and requires patience. The time taken to turn colourless starts decreasing as the temperature increases.

9.2 RAW DATA
The following table illustrates the readings obtained on conducting the investigation.

<table>
<thead>
<tr>
<th>Trial No.</th>
<th>Temperature (°C) ± 0.005</th>
<th>Time Taken (s) ±0.005s</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>T1</td>
<td>T2</td>
</tr>
<tr>
<td>1</td>
<td>25</td>
<td>174.90</td>
</tr>
<tr>
<td>2</td>
<td>30</td>
<td>102.32</td>
</tr>
<tr>
<td>3</td>
<td>35</td>
<td>61.88</td>
</tr>
<tr>
<td>4</td>
<td>40</td>
<td>36.60</td>
</tr>
<tr>
<td>5</td>
<td>45</td>
<td>25.5</td>
</tr>
</tbody>
</table>

9.3 DATA PROCESSING
Of the readings shown in Table 6.1, an average of the values was taken for each of the trials.

Trial 1:

\[
\frac{174.9 + 175.38 + 172.46 + 175.27 + 176.15}{5} = 174.832 \approx 174.83 \text{ s}
\]

Uncertainty:
The uncertainty of this average value can be calculated by calculating the standard deviation in the values.

The standard deviation in values is given by the formula\(^{11}\):

\[
\sigma = \sqrt{\frac{\sum_{i=1}^{n}(x_i - x_{avg})^2}{n}}
\]

Therefore,

\[
\sigma = \sqrt{\frac{(174.9 - 174.83)^2 + (175.38 - 174.83)^2 + (172.46 - 174.83)^2 + (175.27 - 174.83)^2 + (176.15 - 174.83)^2}{5}}
\]

\[
\sigma = \pm 1.40 \text{ s}
\]

Similarly, the process was repeated for the other trials. The results are shown below.

---

\(^{11}\) [https://www.mathsisfun.com/data/standard-deviation-formulas.html]
Table 8.3.1 – Average of the readings for each trial

<table>
<thead>
<tr>
<th>Trial</th>
<th>$T_{\text{avg}}$ (s)</th>
<th>Standard Deviation (s)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>174.83 ± 1.40</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>101.88 ± 1.48</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>60.83 ± 1.45</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>36.83 ± 0.76</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>25.29 ± 1.09</td>
<td></td>
</tr>
</tbody>
</table>

Next, the actual concentration of each reagent in the reaction mixture was calculated.

**Sample calculation for Trial 1:**

HCl Initial Concentration ($M_1$) = 1 ± 0.003 mol dm$^{-3}$

HCl Initial Volume ($V_1$) = 10 ± 0.1 cm$^3$

Total Volume ($V_2$) = 50 ± (0.1+0.1+0.1+0.1) cm$^3$ = 50 ± 0.4 cm$^3$

Therefore, HCl Final Concentration ($M_2$) = $M_1V_1/V_2$

$$(1 ± 0.003 \text{ mol dm}^{-3}) \times (10 ± 0.1 \text{ mL}) \over (50 ± 0.4 \text{ mL}) = (1 ± 0.3\%) \times (10 ± 1\%) = 0.2 ± 1.1\%$$

= 0.2 ± 0.0022 mol dm$^{-3}$

Similarly, the final concentration, which is the concentration of each reactant in the reaction mixture was calculated similarly. The results are shown in the table below.

Table 8.3.2 – Initial Volumes, Initial Concentrations, Final Volumes, and Final Concentrations of all the reactants. Note: The Final Volume is same as the Total Volume.

<table>
<thead>
<tr>
<th>Initial Volumes (cm$^3$)</th>
<th>HCl (± 0.1 cm$^3$)</th>
<th>Acetone (± 0.1 cm$^3$)</th>
<th>I$_2$ (± 0.1 cm$^3$)</th>
<th>Water (± 0.1 cm$^3$)</th>
<th>Total Volume (± 0.4 cm$^3$)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>10</td>
<td>10</td>
<td>10</td>
<td>20</td>
<td>25</td>
</tr>
</tbody>
</table>

Initial Concentrations (M)

<table>
<thead>
<tr>
<th>HCl (± 0.003 mol dm$^{-3}$)</th>
<th>Acetone (± 0.003 mol dm$^{-3}$)</th>
<th>I$_2$ (± 0.0005 mol dm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1.000</td>
<td>4.000</td>
<td>0.005</td>
</tr>
</tbody>
</table>

Final Concentrations (M)

<table>
<thead>
<tr>
<th>HCl (± 0.0022 mol dm$^{-3}$)</th>
<th>Acetone (± 0.015 mol dm$^{-3}$)</th>
<th>I$_2$ (± 0.0001 mol dm$^{-3}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.200</td>
<td>0.800</td>
<td>0.001</td>
</tr>
</tbody>
</table>

The next step is to find inverse of the Temperature, as the Arrhenius plot requires the value of $T^{-1}$ to be on the x-axis. To find this, we first need to convert the temperature from Celsius scale to Kelvin. For this, the value 273 has to be added to the Celsius reading.

For example, for 25°C, its conversion to Kelvin would be (25 + 273) K = 298 K
This was done for all the temperatures used in the experiment. The results are shown in the table below:

<table>
<thead>
<tr>
<th>Table 8.3.4 – Temperatures in Kelvin from Celsius scale</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (°C)</td>
</tr>
<tr>
<td>------------------</td>
</tr>
<tr>
<td>25 ± 0.05</td>
</tr>
<tr>
<td>30 ± 0.05</td>
</tr>
<tr>
<td>35 ± 0.05</td>
</tr>
<tr>
<td>40 ± 0.05</td>
</tr>
<tr>
<td>45 ± 0.05</td>
</tr>
</tbody>
</table>

To find \( T^{-1} \), we need to find the inverse of all the Kelvin values.

For example, for the value of 298 K, the inverse would be \( \frac{1}{298} \approx 0.003355705 \)

The Uncertainty of these inverse values would have the same percentage uncertainty. Therefore:

**Percentage uncertainty of Trial 1:**

\[
\frac{0.05}{298} \times 100 = 0.01677\% \approx 0.017\%
\]

Since the uncertainty is almost negligible in the temperature readings, it has been ignored throughout.

Similarly, the inverse value for all Temperature values were found:

<table>
<thead>
<tr>
<th>Table 8.3.5 – Inverse of the Temperature values in Kelvin</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temperature (K)</td>
</tr>
<tr>
<td>-----------------</td>
</tr>
<tr>
<td>298 ± 0.05</td>
</tr>
<tr>
<td>303 ± 0.05</td>
</tr>
<tr>
<td>308 ± 0.05</td>
</tr>
<tr>
<td>313 ± 0.05</td>
</tr>
<tr>
<td>318 ± 0.05</td>
</tr>
</tbody>
</table>

The next step is to calculate the rate of the reaction. As we know, the rate of the reaction can be expressed as the change in concentration of the reactant, divided by the time taken for reaction. In this investigation, we are looking at the rate of reaction with respect to Iodine, as we are sure that the Iodine is reacting completely from the Qualitative data observation. Thus, we know that the rate of change of concentration of Iodine is same as the Final Concentration of Iodine for a trial (Table 7.2) because all of the Iodine is reacting. Therefore, the equation becomes:

\[
rate = \frac{\Delta [I_2]}{t_{avg}}
\]

**Sample Calculation of Rate for Trial 1:**

\[
\left( \frac{0.001}{174.83} \right) = 5.71978 \times 10^{-6} \text{ mol dm}^{-3}\text{s}^{-1}
\]

Similarly, the rate of reaction of each trial was calculated.
For calculating the uncertainty in rate, the percentage uncertainties in the concentration of Iodine and time are added.

Uncertainty in \([I_2]\) = 10.008% (From Pre-Lab Preparation of Iodine)

Uncertainty in Time = \(\frac{140}{174.83} \times 100 = 0.8\%\) (From Table 7.1)

Total Percentage Uncertainty = (10.008 + 0.8)% = 10.808%

The process was carried on for all the readings.

The results are shown in the table below.

<table>
<thead>
<tr>
<th>Trial</th>
<th>Temperature (˚C)</th>
<th>Rate (mol dm(^{-3}) s(^{-1}))</th>
<th>Percentage Uncertainty (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>25</td>
<td>5.71978 x 10(^{-6})</td>
<td>10.808</td>
</tr>
<tr>
<td>2</td>
<td>30</td>
<td>9.81528 x 10(^{-6})</td>
<td>11.461</td>
</tr>
<tr>
<td>3</td>
<td>35</td>
<td>1.64387 x 10(^{-6})</td>
<td>12.392</td>
</tr>
<tr>
<td>4</td>
<td>40</td>
<td>2.71518 x 10(^{-5})</td>
<td>12.072</td>
</tr>
<tr>
<td>5</td>
<td>45</td>
<td>3.95351 x 10(^{-5})</td>
<td>14.318</td>
</tr>
</tbody>
</table>

The graph of Rate of the Reaction vs. Temperature is shown below:

Figure 8.3.1 – The Graph of Rate of Reaction against the Temperature. This graph is discussed in the Conclusion and Evaluation section. The points marked in red are also discussed later.
The next step is calculating the rate constant \( (k) \), as the y-axis of the Arrhenius plot is natural log of \( k \). To calculate \( k \), we need to know the Rate of the reaction, the concentrations of the reactants of non-zero order, and the orders of the reaction. The order of reaction of the reactants were found in another experiment. The orders are summarized in the table below:

Table 8.3.7 – Values of ‘\( m \)’, ‘\( n \)’, ‘\( p \)’, where ‘\( m \)’ is the order of Acetone, ‘\( n \)’ is the order of H\(^+\) ion, and ‘\( p \)’ is the order of I\(_2\).

<table>
<thead>
<tr>
<th>Variable</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>( m )</td>
<td>1</td>
</tr>
<tr>
<td>( n )</td>
<td>1</td>
</tr>
<tr>
<td>( p )</td>
<td>0</td>
</tr>
</tbody>
</table>

Now that we know the order of the reactions with respect to all the reactants, we can calculate the rate constant \( (k) \), using the rate law.

**Sample calculation for Trial 1:**

\[
Rate_1 = k[Aacetone]^1[H^+]^1[I_2]^0
\]

\[
(5.71978 \times 10^{-6}) = k(0.8)^1(0.2)^1(0.001)^0
\]

\[
k = \frac{(5.71978 \times 10^{-6})}{((0.8)(0.2))}
\]

\[
k = 3.57486 \times 10^{-5} \text{ mol}^{-1} \text{ dm}^3 \text{ s}^{-1}
\]

**Uncertainty in Rate Constant:**

\[
k = \frac{(5.71978 \times 10^{-6} \pm 10.808\%)}{(0.8 \pm 1.875\%)(0.2 \pm 1.100\%)}
\]

\[
\Delta k = 10.808 + 1.875 + 1.100 = 13.783\%
\]

\[
\therefore k = 3.57486 \times 10^{-5} \pm 13.783\% \text{ mol}^{-1} \text{ dm}^3 \text{ s}^{-1}
\]

Similarly, the calculations were repeated for all the trials. The results are displayed in the table below.

**Table 8.3.8 – Values of rate constant (k) for each trial**

<table>
<thead>
<tr>
<th>Trial</th>
<th>( K ) (mol(^{-1}) dm(^3) s(^{-1}))</th>
<th>Percentage Uncertainty (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>3.5749 \times 10^{-5}</td>
<td>± 13.783</td>
</tr>
<tr>
<td>2</td>
<td>6.1345 \times 10^{-5}</td>
<td>± 14.436</td>
</tr>
<tr>
<td>3</td>
<td>1.0274 \times 10^{-4}</td>
<td>± 15.367</td>
</tr>
<tr>
<td>4</td>
<td>1.6970 \times 10^{-4}</td>
<td>± 15.047</td>
</tr>
<tr>
<td>5</td>
<td>2.4709 \times 10^{-4}</td>
<td>± 17.293</td>
</tr>
</tbody>
</table>
Now we need to find the values of natural log of \( k \).

**Sample Calculation for Trial 1:**

\[
\ln(3.5749 \times 10^{-5}) = -10.238999
\]

The absolute uncertainty in a natural log (logarithms to base \( e \), usually written as \( \ln \) or \( \log_{e} \)) is equal to a ratio of the quantity uncertainty and to the quantity\(^{12}\).

Therefore:

\[
\ln(k \pm \Delta k) = \ln(k) \pm \frac{\Delta k}{k}, \text{ where } \frac{\Delta k}{k} \text{ is nothing but the } \frac{\text{Uncertainty of } k}{100}
\]

Thus, Percentage uncertainty for \( \ln(k) \) is \( \left( \frac{\text{Uncertainty of } k}{100} \right) \div \ln(k) \times 100 \)

For Trial 1, the percentage uncertainty in \( \ln(k) \) is \( \left( \frac{13.783}{100} \right) \div (-10.238999) \times 100 = \pm 1.346\%

This calculation was done for all the trials. The results are given below:

<table>
<thead>
<tr>
<th>Trial</th>
<th>( \ln(k) )</th>
<th>Percentage uncertainty (%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>-10.2389999</td>
<td>± 1.346</td>
</tr>
<tr>
<td>2</td>
<td>-9.6989891</td>
<td>± 1.488</td>
</tr>
<tr>
<td>3</td>
<td>-9.1832898</td>
<td>± 1.673</td>
</tr>
<tr>
<td>4</td>
<td>-8.6814865</td>
<td>± 1.733</td>
</tr>
<tr>
<td>5</td>
<td>-8.3057410</td>
<td>± 2.082</td>
</tr>
</tbody>
</table>

\( ^{12} \) [http://phys114115lab.capuphysics.ca/App%20A%20-%20uncertainties/Print%20AppendixA.htm](http://phys114115lab.capuphysics.ca/App%20A%20-%20uncertainties/Print%20AppendixA.htm)
The activation energy is given by the slope of the graph of $\ln(k) = -\frac{E_a}{R} \left(\frac{1}{T}\right) + \ln(A)$. The plot is shown below:

![Arrhenius plot](image)

Figure 8.3.2 – Arrhenius plot of Iodination of Acetone.

The slope of the graph is -9265.1, which is equal to $\frac{E_a}{R}$.

$$-9265.1 = \frac{E_a}{R}$$

$$E_a = -9265.1 \times R$$

$$R = 8.3144621 \text{ } J \text{ } K^{-1} \text{ } mol^{-1}$$

Hence,

$$E_a = -9265.1 \times 8.3144621$$

$$E_a = -77034.3228 \text{ } J \text{ } mol^{-1}$$

$$E_a = -77.034 \text{ } kJ \text{ } mol^{-1}$$

The uncertainty in the slope can be calculated by the average of the worst fit lines. One of the worst fit slopes can be calculated by considering the lowest value possible of the smallest $y$ value and the highest value possible of the greatest $y$ value, and then calculating the slope of the line joining the two points.

**Least possible $y$ value**

$$-10.238999 - \left(\frac{1.346}{100} \times 10.238999\right) = -10.376816 \text{ } \text{ Corresponding } x = 0.003355705$$

**Greatest possible $y$ value**

$$-8.3057410 + \left(\frac{2.082}{100} \times 8.3057410\right) = -8.132816 \text{ } \text{ Corresponding } x = 0.003144654$$
\[ \text{Slope} = \frac{(y_2 - y_1)}{(x_2 - x_1)} \]

\[ \text{Slope} = \frac{-10.376816 - (-8.132816)}{0.003355705 - 0.003144654} \approx -1063.5 \]

For the second worst fit slope, we consider the highest value possible of the least y value and the lowest value possible of the greatest y value.

Highest value of least y value

\[ -10.238999 + \left( \frac{1.346}{100} \times 10.238999 \right) = -10.101182 \quad \text{Corresponding} \ x = 0.00355705 \]

Lowest value of greatest y value

\[ -8.3057410 - \left( \frac{2.082}{100} \times 8.3057410 \right) = -8.378667 \quad \text{Corresponding} \ x = 0.003144654 \]

\[ \text{Slope} = \frac{-10.101182 - (-8.378667)}{0.003355705 - 0.003144654} \approx -816.6 \]

The difference between the actual slope and the worst slopes is as follows:

\[ | -926.5 - (-1063.5) | = 1367.4 \]

\[ | -926.5 - (-816.6) | = 1103.5 \]

Taking the average of the differences gives us the average uncertainty in the slope.

\[ \frac{1367.4 + 1103.5}{2} = 1235.45 \approx \pm 1235.5 \]

Therefore, the percentage uncertainty in the slope is

\[ \frac{1235.5}{926.1} \times 100 = 13.33\% \]

The uncertainty in slope is equal to the uncertainty in the value of Activation Energy because ‘R’ is a constant.

Thus, the Activation Energy of the reaction of Iodination of Acetone is \(-77.034 \pm 13.33\%\) kJ mol\(^{-1}\)
10 CONCLUSION AND EVALUATION

10.1 EVALUATION

From the Graph in Figure 8.3.1, which is a graph of the rate of reaction against temperature, we can see that according to this graph, there is an exponential increase in the rate with the increase in temperature. All the values are within the limits of uncertainty, which is increases with the increase in temperature. This is because these values depend on the standard deviation in the measurements of time, which stays the same even when the magnitude of time decreases. Thus, the overall percentage error increases.

The two points marked in red, just touch the trend line with their error bars. The reason for this is that as the temperature increases, it is difficult to control it using the apparatus set up. When the temperature becomes greater than 40, the rate of cooling and heating both increases due to the increase in difference with the room temperature. Therefore, it is difficult to keep the temperature constant while at lower temperatures, it is not that difficult.

This type of graph also suggests that the reaction follows a general trend seen in most other reactions, the temperature having a positive and exponential effect on the rate.

The hypothesis during the start of the reaction was that the rate of reaction would increase with the increase in temperature. This hypothesis is now proven correct by the experiment. This is also supported by the Boltzmann curve. Increasing the temperature would result in more number of molecules having enough energy to overcome the activation energy barrier.

Figure 10.1.1 – Effect of increasing temperature on the Boltzmann curve. As the temperature increases, more number of molecules can overcome the Activation energy barrier and react.¹³

From the graph in Figure 8.3.2, which is the Arrhenius plot, we can see that all of the points lie on the trend line. The trend followed by the line is the trend that should be followed for any Arrhenius plot – a reducing, linear relation.

¹³ Image source: Pearson Baccalaureate: Higher Level Chemistry for the IB Diploma (Print)
10.2 Error Evaluation
To render our result in the investigation correct for the activation energy of this reaction, we have no standard literature value available for comparison. The table below shows the different possible sources of errors and the effect they could have on the experiment.

<table>
<thead>
<tr>
<th>Source of Error</th>
<th>Type of Error</th>
<th>Effect on the Investigation</th>
<th>Possible Improvements</th>
</tr>
</thead>
<tbody>
<tr>
<td>Keeping the temperature constant</td>
<td>Systematic</td>
<td>The temperature of the reaction mixture was kept constant using heating in a water bath with a Bunsen burner. Whenever the temperature increased, the container was removed from the water bath and whenever the temperature decreased, it was re-immersed. This way, the temperature was not constant throughout a trial. This was a very inefficient way of maintaining a steady temperature, with clear visibility of the contents inside, but with the given limits of apparatus available in the lab, this was the most logical method.</td>
<td>A hot plate with a controlled heating feature can be used. If this is not possible, the experiment can be repeated more number of times and then the values can be averaged. This way, we can get a fairly accurate value.</td>
</tr>
<tr>
<td>Presence of water in the beakers</td>
<td>Systematic</td>
<td>While making solutions of different concentrations or conducting the reaction, the containers may have some remaining water drops in them due to a previous wash. This way, there might be small variations in the concentration, or presence of impurities in the reaction which could have an effect in the rate.</td>
<td>The beakers or the other containers can be washed and dried by a dry cloth which would absorb the water. Also, acetone can be used to wash the beaker, as acetone would then evaporate from the beaker, leaving it completely dry.</td>
</tr>
<tr>
<td>Variation in pressure</td>
<td>Systematic</td>
<td>The pressure in the reaction container during the experiment could vary each time, because the container was closed with a cork, to prevent evaporation of acetone. Consequently, the pressure might have also changed in the container, causing a change in the rate of reaction.</td>
<td>Using larger container, change in pressure is minimum.</td>
</tr>
</tbody>
</table>
Watching colour change | Systematic | The colour change was identified visually. This may have some error in terms of timely identification. Due to external light, it was difficult to identify the colour change. This might have caused an error in the reading of the time. | A light sensor apparatus can be made, which uses the principle of colorimeter. Electronically viewing the colours would decrease the chances of error.

## 11 Further Investigation

The investigation can be taken further by finding the Activation energy of different compounds when reacted with Iodine, for example, the Iodination of Ethanol. This way, the Activation Energy of different organic compounds when reacted with Iodine can be compared. Furthermore, other Arrhenius parameters for this reaction can also be studied, like the frequency factor. The frequency factor of the reaction can be calculated from the y-intercept of the Arrhenius plot. The Frequency Factor of different reactions can also be studied and compared. From this analysis, we can get to know how readily a reaction takes place in contrast with others. A reaction with high Frequency Factor would have a lesser Activation energy requirement, and vice versa. Along with this, the results of the same experiment could be compared by using different methods. For instance, spectrometry can be used to observe the rate of change of concentration of the reactants, and then determine the Activation Energy.
12 BIBLIOGRAPHY

MHChem

Clark University
http://web.clark.edu/amixon/142_pm/w10kinetics.pdf

ChemWiki
http://chemwiki.ucdavis.edu/Physical_Chemistry/Kinetics/Modeling_Reaction_Kinetics/Temperature_Dependence_of_Reaction_Rates/The_Arrhenius_Law/The_Arrhenius_Law%3A_Activation_Energies

Dr. Paul J. McElligott

Charleston Country School District