THE IODINATION OF ACETONE
Determining the Rate Constant and Activation Energy for a Chemical Reaction

The rate of a chemical reaction depends on several factors: the nature of the reaction, the concentrations of the reactants, the temperature, and the presence of a possible catalyst. In Part One of this experiment we will determine the rate law for a reaction by changing some of the above variables and measuring the rate of the reaction. During Part Two, we will explore the relation between the rate constant and temperature to discover the activation energy for this reaction.

In this experiment we will study the kinetics of the reaction between iodine and acetone:

\[
\text{H}_3\text{C}-\text{C}+\text{I}_2(\text{aq}) \rightarrow \text{H}_3\text{C}-\text{C}^{\text{I}} + \text{HI(\text{aq})}
\]

The rate of this reaction is found to depend on the concentration of the hydrogen ion (acid, HCl) as well as the concentrations of the reactants (acetone and iodine). The rate law for this reaction is

\[
\text{rate} = k[\text{acetone}]^m[H^+]^n[I_2]^p
\]

where \( k \) is the rate constant for the reaction and \( m, n, \) and \( p \) are the orders of the reaction with respect to acetone, hydrogen ions (acid), and iodine, respectively. Although orders of reaction can be any value, for this lab we will be looking only for integer values for the orders of reaction (0, 1, 2 are acceptable but not 0.5, 1.3, etc.)

The rate of the reaction can also be expressed as the change in the concentration of a reactant divided by the time interval:

\[
\text{rate} = -\frac{\Delta [I_2]}{\Delta t}
\]

The iodination of acetone is easily investigated because iodine (I\(_2\)) has a deep yellow/brown color. As the acetone is iodinated and the iodine converted to the iodide anion, this color will disappear, allowing the rate of the reaction to be easily monitored.

We can study the rate of this reaction by simply making I\(_2\) the limiting reactant in a large excess of acetone and H\(^+\) ion. By measuring the time required for the initial concentration of iodine (I\(_2\)) to be used up completely, the rate of the reaction can be determined by the equation

\[
\text{rate} = \frac{-\Delta [I_2]}{\Delta t} = \frac{t_{\text{final}} - t_{\text{initial}}}{t_{\text{final}} - t_{\text{initial}}} = \frac{0 - [I_2]_{\text{initial}}}{t_{\text{final}} - 0} = \frac{[I_2]_{\text{initial}}}{t_{\text{final}}}
\]

or simply as

\[
\text{rate} = \frac{[I_2]}{\text{time}}
\]
From the rate information we can determine the orders with respect to acetone (m), acid (n) and iodine (p) by varying the amounts of reactants and measuring the effect on the rate. Once the orders of reaction are known, we will be able to calculate the rate constant, k. In Part One of this experiment you will determine the rates of reactions, the orders of the reactants, and finally the rate constant at room temperature.

In the second part of this experiment you will study the rate of the reaction at different temperatures to find its activation energy, $E_a$. The temperature at which the reaction occurs influences the rate of the reaction. An increase in temperature increases the rate.

As with concentration, there is a quantitative relation between reaction rate and temperature, but here the relation is somewhat more complicated. This relation is based on the idea that to react, the reactant species must have a certain minimum amount of energy present (and the correct geometry, if appropriate) at the time the reactants collide in the reaction step.

This amount of energy, which is typically furnished by the kinetic energy of the species present, is called the activation energy ($E_a$, also known as the energy of activation) for the reaction. The formula (called the Arrhenius equation) relating the rate constant $k$ to absolute Kelvin temperature $T$ and $E_a$ is:

$$\ln k = -\frac{E_a}{RT} + \ln A$$

In this equation, $R$ is the gas constant (8.3145 J/mole K), and natural logarithms ($\ln$) need to be used (do not use base 10 logs!) The quantity $A$ is referred to as the collision frequency and $A$ can be used to determine the fraction of molecules present with sufficient energy and geometry to become products at a given instant in time.

By measuring $k$ at different temperatures, we can graphically determine the activation energy for a reaction. In Part Two of this experiment you will determine the effect of temperature on rate and calculate the activation energy for the reaction.

**DIRECTIONS:**

This lab will be completed as a worksheet - no formal typed lab report is required as long as your writing is legible and easy to read.

**Complete Part One and Part Two while in lab.** In Part One, you will perform a series of experiments which will examine the relationship between the concentration of reactants and the time for the iodination of acetone reaction. In Part Two, you will see the effect of temperature upon the reaction.

The remaining parts can be done outside of lab. **In Part Three**, you will use the data from Part One in order to find the rate of reactions, the orders of the reactants, and finally the value of $k$, the rate constant. **Part Four** uses the data from Part Two to examine the relationship between the rate constant $k$ and temperature in order to find the activation energy for the reaction.

Also note the special time and date that this lab will be due (typically during the 10th week recitation). This lab is worth 40 points total (20 points for Part 1 and Part 3, 20 points for Part 2 and Part 4).
For each trial listed below: measure out the appropriate quantities of **1.0 M HCl**, **4.0 M acetone** and **water** using a 10.00 mL graduated cylinder and place them in a 250 mL Erlenmeyer flask fitted with a rubber stopper. Now measure out the appropriate amount of **0.0050 M iodine** in a 10.00 mL graduated cylinder.

Start a timer (stopwatch) as you add the iodine to the 250 mL flask with the other chemicals. Swirl the stoppered flask (which helps to prevent acetone evaporation) **until the yellow color disappears**, then **halt the timer**. It may help to place the flask on a white piece of paper to help discern when the color disappears. Record the time elapsed in seconds.

Repeat this reaction mixture until two trials are within 20 seconds of each other.

Repeat this process for each of the four trials listed in the table below. Waste can be placed in the drain.

---

**Part One:** Changing Concentration to Find the Rate Constant - *Complete in the Lab*

For each mixture listed below, add all of the chemicals but iodine to a 250 mL Erlenmeyer flask. Add the iodine last, starting a stopwatch and measuring how long the reaction takes to turn the solution clear. Time should be recorded in seconds. **Repeat** each reaction mixture until **two** trials are within 20 seconds of each other.... repeat the trial again if the times vary too much.

<table>
<thead>
<tr>
<th>Trial #1:</th>
<th>HCl (mL)</th>
<th>Acetone (mL)</th>
<th>I₂ (mL)</th>
<th>Water (mL)</th>
<th>Total Volume (mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>10</td>
<td>25.00</td>
</tr>
</tbody>
</table>

Time in seconds for yellow color to disappear, first time: ___________________ seconds

Time in seconds for yellow color to disappear, second time: ___________________ seconds

Time in seconds for yellow color to disappear, third time (if necessary): ___________________ seconds

Time in seconds for yellow color to disappear, fourth time (if necessary): ___________________ seconds
Part One: Changing Concentration to Find the Rate Constant - continued

Trial #2:

<table>
<thead>
<tr>
<th>HCl (mL)</th>
<th>Acetone (mL)</th>
<th>I₂ (mL)</th>
<th>Water (mL)</th>
<th>Total Volume (mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5</td>
<td>10</td>
<td>5</td>
<td>25.00</td>
</tr>
</tbody>
</table>

Time in seconds for yellow color to disappear, first time: _______________ seconds
Time in seconds for yellow color to disappear, second time: _______________ seconds
Time in seconds for yellow color to disappear, third time (if necessary): _______________ seconds
Time in seconds for yellow color to disappear, fourth time (if necessary): _______________ seconds

Trial #3:

<table>
<thead>
<tr>
<th>HCl (mL)</th>
<th>Acetone (mL)</th>
<th>I₂ (mL)</th>
<th>Water (mL)</th>
<th>Total Volume (mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>10</td>
<td>5</td>
<td>5</td>
<td>25.00</td>
</tr>
</tbody>
</table>

Time in seconds for yellow color to disappear, first time: _______________ seconds
Time in seconds for yellow color to disappear, second time: _______________ seconds
Time in seconds for yellow color to disappear, third time (if necessary): _______________ seconds
Time in seconds for yellow color to disappear, fourth time (if necessary): _______________ seconds

Trial #4:

<table>
<thead>
<tr>
<th>HCl (mL)</th>
<th>Acetone (mL)</th>
<th>I₂ (mL)</th>
<th>Water (mL)</th>
<th>Total Volume (mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>10</td>
<td>5</td>
<td>5</td>
<td>5</td>
<td>25.00</td>
</tr>
</tbody>
</table>

Time in seconds for yellow color to disappear, first time: _______________ seconds
Time in seconds for yellow color to disappear, second time: _______________ seconds
Time in seconds for yellow color to disappear, third time (if necessary): _______________ seconds
Time in seconds for yellow color to disappear, fourth time (if necessary): _______________ seconds
Part Two: The Effect of Temperature on the Rate Constant - Complete in the Lab

We shall measure one of the reactions from Part One at different temperatures. You do not need to repeat these experiments twice (to be within 20 seconds of each other) as in Part One.

As before, add all of the chemicals but iodine to a stoppered 250 mL Erlenmeyer flask. Using ice and/or a hot plate, get the solution to a desired temperature before adding the iodine. Record the temperature, then add the iodine to the Erlenmeyer, starting a stopwatch and measuring how long the reaction takes to turn the solution clear. Time should be recorded in seconds. The iodine does not need to be at the same temperature as the solution in the Erlenmeyer flask.

Record one trial at room temperature.
Record one trial at a temperature lower than room temperature, but above 15 degrees Celsius.
Record three trials at temperatures higher than room temperature, but under 60 degrees Celsius.
Temperature differences should be at least 5 degrees Celsius apart (i.e. spread out your temperatures!)

**Trial #5:**

<table>
<thead>
<tr>
<th>HCl (mL)</th>
<th>Acetone (mL)</th>
<th>I₂ (mL)</th>
<th>Water (mL)</th>
<th>Total Volume (mL)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>5</td>
<td>5</td>
<td>10</td>
<td>25.00</td>
</tr>
</tbody>
</table>

Temperature (°C): ________________  Time (seconds): ________________
Temperature (°C): ________________  Time (seconds): ________________
Temperature (°C): ________________  Time (seconds): ________________
Temperature (°C): ________________  Time (seconds): ________________
Temperature (°C): ________________  Time (seconds): ________________

Hint: As temperature increases, the reaction time should decrease. If you do not see this trend, repeat one or more experiments.

Get a stamp in your lab notebook before leaving!
Part Three: Determining the rate, orders of reaction, and rate constant

These steps can be done at home and do not need to be completed in the lab. Show your work for each step.

The ultimate goal of this section is to find the best value of the rate constant, $k$, for the iodination of acetone at room temperature. To get there, we need to first find the rates of each reaction, then the order of the reactants (acetone, HCl and iodine), and then finally, the rate constant $k$.

a. Find the average time in seconds for each Trial in Part One.

   *Example:* the first experiment took 230 seconds, the second experiment took 250 seconds.

   The *average time* would be: $(230 + 250) / 2 = 240$ seconds

Record your final values here:

   Average time in seconds for Trial 1: _________________ seconds
   Average time in seconds for Trial 2: _________________ seconds
   Average time in seconds for Trial 3: _________________ seconds
   Average time in seconds for Trial 4: _________________ seconds

Show an example of how you got these values here:
Part Three: Determining the rate, orders of reaction, and rate constant - continued

b. Find the concentration of each reactant (acetone, HCl and iodine) before the reaction started.

Your group took bulk reactants (which were, as a reminder: 1.0 M HCl, 4.0 M acetone, and 0.0050 M iodine) then placed them (with water) in an Erlenmeyer flask. The final volume was always 25.00 mL. Mixing chemicals dilutes the concentrations from the "bulk" value to a smaller value.

We can determine these diluted values using:  \( M_1V_1 = M_2V_2 \)

Example: Determine the concentration of iodine in trial #1.

Let \( M_1 = \) initial (undiluted) concentration of iodine (0.0050 M), \( V_1 = 5.00 \text{ mL} \) (of undiluted iodine added to the mixture), and \( V_2 = 25.00 \text{ mL} \) (the total volume of the diluted solution once HCl, acetone and water are added). Solving for \( M_2 \), the concentration of iodine in the diluted solution, one gets:

\[
M_2 = \frac{M_1V_1}{V_2} = \frac{0.0050 \text{ M} \times 5.00 \text{ mL}}{25.00 \text{ mL}} = 0.0010 \text{ M},
\]

which is the concentration of iodine used in the reaction in trial #1.

Example: Determine the concentration of iodine in trial #2.

Solution: Since \( M_1 \) and \( V_2 \) are the same as in the previous example, we see that only \( V_1 \) has changed to 10.00 mL. Rearranging for \( M_2 \) as before:

\[
M_2 = \frac{M_1V_1}{V_2} = \frac{0.0050 \text{ M} \times 10.00 \text{ mL}}{25.00 \text{ mL}} = 0.0020 \text{ M},
\]

the concentration of iodine used in the reaction in trial #2.

i. Calculate the concentration of acetone (\( M_3 \)) used in Trial 1 - Trial 4.

The concentration of acetone was 4.0 M in the "bulk" solution (the "\( M_1 \)" value.)

The final volume (\( V_2 \)) is always 25.00 mL.

Trial 1, Trial 2 and Trial 4 used 5.00 mL of acetone from the bulk solution, but Trial 3 used 10.00 mL (your "\( V_1 \)" values)

<table>
<thead>
<tr>
<th>Volume acetone (mL)</th>
<th>Bulk Acetone (M)</th>
<th>Total Volume (mL)</th>
<th>acetone (M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td>5.00</td>
<td>4.0 M</td>
<td>25.00</td>
</tr>
<tr>
<td>Trial #2</td>
<td>5.00</td>
<td>4.0 M</td>
<td>25.00</td>
</tr>
<tr>
<td>Trial #3</td>
<td>10.00</td>
<td>4.0 M</td>
<td>25.00</td>
</tr>
<tr>
<td>Trial #4</td>
<td>5.00</td>
<td>4.0 M</td>
<td>25.00</td>
</tr>
</tbody>
</table>
ii. **Calculate the concentration of HCl (M$_2$) used in Trial 1 - Trial 4.**

The *concentration* of HCl was 1.0 M in the "bulk" solution (the "M$_1$" value.)
The final volume ($V_2$) is always 25.00 mL.
Trial 1, Trial 2 and Trial 3 used 5.00 mL of acetone from the bulk solution, but Trial 4 used 10.00 mL (your "$V_1" values)

<table>
<thead>
<tr>
<th>volume HCl (mL)</th>
<th>Bulk HCl (M)</th>
<th>Total Volume (mL)</th>
<th>HCl (M)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td>5.00</td>
<td>1.0 M</td>
<td>25.00</td>
</tr>
<tr>
<td>Trial #2</td>
<td>5.00</td>
<td>1.0 M</td>
<td>25.00</td>
</tr>
<tr>
<td>Trial #3</td>
<td>5.00</td>
<td>1.0 M</td>
<td>25.00</td>
</tr>
<tr>
<td>Trial #4</td>
<td>10.00</td>
<td>1.0 M</td>
<td>25.00</td>
</tr>
</tbody>
</table>

iii. **Complete the following table** showing the diluted concentrations of all reactants used in each trial. The I$_2$ concentrations have been completed for you (see the examples at the beginning of part b, above.)

<table>
<thead>
<tr>
<th>acetone (M)</th>
<th>HCl (M)</th>
<th>I$_2$ (M)</th>
</tr>
</thead>
<tbody>
<tr>
<td><em>step i, above</em></td>
<td><em>step ii, above</em></td>
<td>0.0010</td>
</tr>
<tr>
<td>Trial #1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Use this area to show relevant calculations and at least one example as to how you found a diluted concentration.
Part Three: Determining the rate, orders of reaction, and rate constant - continued

c. Find the rate of each trial

In this lab, rate is best described by: \( \text{rate} = \frac{[I_2]}{\text{average time in seconds}} \) (see first page of lab)

Find the rate for each reaction by using the calculated iodine concentration then dividing by the average time for that trial (Part Three, section a, above).

Example: Trial #1 required an average of 240 seconds to go to completion. Trial #2 required an average of 496 seconds to go to completion. Find the rate of reaction for both trial #1 and trial #2.

Solution: The rate of reaction is equal to the concentration of iodine divided by the average time elapsed for the reaction. (your values are in Part Three, section a.)

In this example, the first two times are 240 s and 496 s. Using the appropriate concentrations, we can calculate rate:

\[
\begin{align*}
\text{rate (trial #1)} &= \frac{[I_2]}{\text{average time in seconds}} = 0.0010 \text{ M} / 240 \text{ s} = 4.2 \times 10^{-6} \text{ M s}^{-1}. \\
\text{rate (trial #2)} &= \frac{[I_2]}{\text{average time in seconds}} = 0.0020 \text{ M} / 496 \text{ s} = 4.0 \times 10^{-6} \text{ M s}^{-1}.
\end{align*}
\]

Now, calculate your rate values by filling in the table below:

<table>
<thead>
<tr>
<th>I₂ (M)</th>
<th>average time (s)</th>
<th>rate (M s⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td>0.0010</td>
<td>_________</td>
</tr>
<tr>
<td>Trial #2</td>
<td>0.0020</td>
<td>_________</td>
</tr>
<tr>
<td>Trial #3</td>
<td>0.0010</td>
<td>_________</td>
</tr>
<tr>
<td>Trial #4</td>
<td>0.0010</td>
<td>_________</td>
</tr>
</tbody>
</table>

Use this space to show at least one example of how you calculated the rate of the reaction.
**Part Three:** Determining the rate, orders of reaction, and rate constant - *continued*

d. **Find the order** of the reaction with respect to each reactant \((m, n, \text{ and } p)\)

To find the order of each reactant, we need to localize the effect that each reactant had on the rate. This is expressed in a *rate order* which, for CH 222 and CH 223, can only be equal to zero, one or two (no fractions, negative numbers, etc.)

In this lab, it is safe to assume that water does not affect the rate, so we can ignore its contribution to any changes that the rate might exhibit.

Notice that trial 2 has twice as much iodine as trial 1. Any changes to the rates of trial 1 and trial 2 are a direct result of the iodine (HCl and acetone are constant), and we will use these trials to calculate \(p\), the reaction order for iodine.

Also notice that trial 3 has twice as much acetone as trial 1, so any changes to the rates of trials 3 and 1 will be the result of acetone only (HCl and iodine are constant), and we will use these trials to calculate \(m\), the reaction order for acetone.

Lastly, notice that trial 4 has twice as much HCl as trial 1, yet acetone and iodine concentrations remain constant; we will use these trials to calculate \(n\), the reaction order for HCl.

*Example:* Find the order of reaction with respect to iodine \((p)\) if these values are used:

\[
\text{rate (trial #1)} = \frac{[I_2]}{\text{average time in seconds}} = 0.0010 \text{ M} / 240 \text{ s} = 4.2 \times 10^{-6} \text{ M s}^{-1}.
\]

\[
\text{rate (trial #2)} = \frac{[I_2]}{\text{average time in seconds}} = 0.0020 \text{ M} / 496 \text{ s} = 4.0 \times 10^{-6} \text{ M s}^{-1}.
\]

*Solution:* Notice how in trial #2 we doubled the concentration of \([I_2]\) while leaving the other reactants' concentrations (HCl, acetone) unchanged. An effect upon the rate of the reaction will reflect the influence of the iodine only, and this will allow us to determine \(p\).

In these sample calculations, doubling the concentration of iodine (to 0.0020 M from 0.0010 M) spawned a negligible change in the rate \((4.0 \times 10^{-6} \text{ M s}^{-1} \text{ versus } 4.2 \times 10^{-6} \text{ M s}^{-1})\). Because we are only concerned with whole integer values of rate orders, this implies a *zero order reactant*, and \(p = 0\).

A more formal approach to determining \(p\) would be as follows: divide the expression for rate 2 by the expression for rate 1; this results in the following:

\[
\frac{\text{rate 2}}{\text{rate 1}} = \frac{k[\text{acetone}]^m[HCl]^n[I_2]^p}{k[\text{acetone}]^m[HCl]^n[I_2]^p}
\]

The values of \(k\), [acetone] and [HCl] remain constant between trial 1 and trial 2 (only \([I_2]\) changes), so the expression reduces to
\[
\frac{\text{rate } 2}{\text{rate } 1} = \frac{4.0 \times 10^{-6}}{4.2 \times 10^{-6}} = \frac{[0.0020]^p}{[0.0010]^p} = 2^p
\]

**Part Three:** Determining the rate, orders of reaction, and rate constant - *continued*

\[0.95 = (2)^p\]

Taking the logarithm of both sides leads to

\[\log 0.95 = \log 2^p = p \log 2\]

and solving for \(p\):

\[p = \frac{\log 0.95}{\log 2} = -0.074 \approx 0\]

Therefore, the order with respect to iodine equals **zero**, or \(p = 0\).

*Now, find the order of each reactant* by filling in the tables below. *Note: rate* values from Part 3 section c; *concentration* (M) values from Part 3, section b, subsection iii. Show your work on the following page. *Remember* that m, n and p can be **0, 1, or 2 only**! Round your answers as necessary!

**For I\(_2\) (p):**

<table>
<thead>
<tr>
<th>I(_2) (M)</th>
<th>rate (M s(^{-1}))</th>
<th>My value of p is:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td>0.0010</td>
<td></td>
</tr>
<tr>
<td>Trial #2</td>
<td>0.0020</td>
<td></td>
</tr>
</tbody>
</table>

**For acetone (m):**

<table>
<thead>
<tr>
<th>acetone (M)</th>
<th>rate (M s(^{-1}))</th>
<th>My value of m is:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

**For HCl (n):**

<table>
<thead>
<tr>
<th>HCl (M)</th>
<th>rate (M s(^{-1}))</th>
<th>My value of n is:</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #4</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Part Three: Determining the rate, orders of reaction, and rate constant - continued

Use this space to show how you got each of the orders of reaction (m, n and p):

e. **Find the value of k, the rate constant** for the iodination of acetone reaction.

You now have all the necessary information to calculate the rate constant, k, for each trial. For this reaction,

\[
\text{rate} = k \text{[acetone]}^m \text{[HCl]}^n \text{[I}_2\text{]}^p
\]

Rate values appear in Part 3 section c
[acetone], [HCl] and [I2] are the concentrations for each trial (Part 3, section b, subsection iii)
m, n and p are the orders of reaction (Part 3, section d)

*Example:* Find the value of k for trial #1 if the rate = \(4.2 \times 10^{-6}\) M s\(^{-1}\) and assuming that the order with respect to acetone (m) and HCl (n) is two and the order with respect to I\(_2\) (p) is zero.

*Solution:* In trial #1, the diluted concentration of acetone is 0.80 M, the HCl is 0.20 M and I\(_2\) is 0.0010 M. Using the given values, we can calculate k from the following equation:

\[
\text{rate} = k \text{[acetone]}^m \text{[HCl]}^n \text{[I}_2\text{]}^p
\]

\[
4.2 \times 10^{-6} = k[0.80]^2[0.20]^2[0.0010]^0
\]

\[
k = \frac{4.2 \times 10^{-6}}{[0.80]^2[0.20]^2}
\]

and solving for k we get a value of \(k = 1.6 \times 10^{-4}\) M\(^{-1}\) s\(^{-1}\)
**Part Three:** Determining the rate, orders of reaction, and rate constant - continued

Now **find the rate constant \( k \) for each trial** by completing the table:

My value of \( m = \) __________ (these can be found in Part 3, section d)

My value of \( n = \) __________

My value of \( p = \) __________

<table>
<thead>
<tr>
<th>acetone (M)</th>
<th>HCl (M)</th>
<th>( I_2 ) (M)</th>
<th>rate (M s(^{-1}))</th>
<th>value of ( k )</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td>_______</td>
<td>_______</td>
<td>0.0010</td>
<td>_______</td>
</tr>
<tr>
<td>Trial #2</td>
<td>_______</td>
<td>_______</td>
<td>0.0020</td>
<td>_______</td>
</tr>
<tr>
<td>Trial #3</td>
<td>_______</td>
<td>_______</td>
<td>0.0010</td>
<td>_______</td>
</tr>
<tr>
<td>Trial #4</td>
<td>_______</td>
<td>_______</td>
<td>0.0010</td>
<td>_______</td>
</tr>
</tbody>
</table>

*Concentrations in Part 3, section b, subsection iii  
Rate values in Part 3 section c*

Average value of \( k \): ______________________

parts per thousand of your four \( k \) values: ______________________

Use this space to show **a sample calculation for \( k \)** and also relevant parts per thousand calculations:
Part Four: Determining the Activation Energy for the iodination of acetone reaction

In Part Two, above, you determined the time elapsed for a given set of concentrations as the temperature was altered. We shall use that information and the information gathered from Part Three to determine the energy of activation and collision frequency for the iodination of acetone reaction using the Arrhenius equation.

a. **Find the inverse Kelvin temperature** for each value in Trial #5.

Convert your temperatures from °C to K, then take the inverse of your Kelvin temperatures.

*Example:* Convert 37.5 °C to an inverse Kelvin temperature.

*Solution:* 37.5 °C = 310.7 K. To find the inverse, calculate $(310.7 \text{ K})^{-1} = 3.219 \times 10^{-3} \text{ K}^{-1}$

Complete the table below. The first column (Temperature (°C)) comes from your data collected in Part Two, Trial #5, while in lab.

<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Temperature (K)</th>
<th>Temperature $^{-1}$ (K$^{-1}$)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Temp #1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temp #2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temp #3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temp #4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Temp #5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Use this space to show a sample calculation for getting from Temperature (°C) to an inverse Kelvin temperature:
Part Four: Determining the Activation Energy for the iodination of acetone reaction - continued

In Part Two, above, you determined the time elapsed for a given set of concentrations as the temperature was altered. We shall use that information and the information gathered from Part Three to determine the energy of activation and collision frequency for the iodination of acetone reaction using the Arrhenius equation.

b. Find the rate for each temperature value in Trial #5.

Recall from earlier (Part 3 section c) that, for this experiment: rate = [I₂]/(average time in seconds)

Use this equation to find the rate of reaction (in M s⁻¹) for each temperature. Time values come from Part 2 - Trial #5:

<table>
<thead>
<tr>
<th>I₂ (M)</th>
<th>time (s)</th>
<th>rate (M s⁻¹)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1 0.0010</td>
<td>__________</td>
<td>__________</td>
</tr>
<tr>
<td>Trial #2 0.0010</td>
<td>__________</td>
<td>__________</td>
</tr>
<tr>
<td>Trial #3 0.0010</td>
<td>__________</td>
<td>__________</td>
</tr>
<tr>
<td>Trial #4 0.0010</td>
<td>__________</td>
<td>__________</td>
</tr>
<tr>
<td>Trial #5 0.0010</td>
<td>__________</td>
<td>__________</td>
</tr>
</tbody>
</table>

Use this space to show at least one example of how you calculated the rate of the reaction.
Part Four: Determining the Activation Energy for the iodination of acetone reaction - continued

c. **Find the value of the rate constant, k,** for each temperature value in Trial #5.

We will use the process developed in Part Three to help us find the values of k for each temperature.

i. First, we need the **diluted concentrations:** *(these can be found in Part 3, section b)*

   Concentration (M) of **acetone** when 5.00 mL was used: _______________

   Concentration (M) of **HCl** when 5.00 mL was used: _______________

   Concentration (M) of **I₂** when 5.00 mL was used: _______________

ii. Next, we need the reaction orders for each reactant: *(these can be found in Part 3, section d)*

   My value of m (acetone) = __________

   My value of n (HCl) = __________

   My value of p (I₂) = __________

iii. Now the technique used in Part 3, section 3, to find the value of k and ln k.

Use the **rates from Part 4 section b** and the values for concentration and order, above, to find k. The only variable that will change is the rate; the orders and concentrations remain constant. Take the **natural log (ln) of each k** value as well (i.e. ln (2.6 * 10⁻⁵) = -10.6)

<table>
<thead>
<tr>
<th>rate (M s⁻¹)</th>
<th>k</th>
<th>ln k</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #2</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #4</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Trial #5</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Show a sample calculation for these steps on the next page.
Part Four: Determining the Activation Energy for the iodination of acetone reaction - continued

Use this space to show at least one example of how you calculated the rate constant $k$ and $\ln k$.

d. Create a graph of $\ln k$ versus inverse Kelvin temperature values

You will be creating a graph of $\ln k$ versus inverse temperature in order to find the energy of activation.

First, collect your inverse temperature (the x-axis) and $\ln k$ values (the y-axis) here. Inverse Kelvin temperature values come from Part Four, section a. $\ln k$ values come from Part Four, section c, subsection iii.

<table>
<thead>
<tr>
<th>Temperature$^{-1}$ (K$^{-1}$)</th>
<th>$\ln k$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Trial #1</td>
<td>_______</td>
</tr>
<tr>
<td>Trial #2</td>
<td>_______</td>
</tr>
<tr>
<td>Trial #3</td>
<td>_______</td>
</tr>
<tr>
<td>Trial #4</td>
<td>_______</td>
</tr>
<tr>
<td>Trial #5</td>
<td>_______</td>
</tr>
</tbody>
</table>

Using Excel or a similar program, create a graph of your $\ln k$ values versus the inverse Kelvin temperature values. Make the graph at least as big as half a sheet of paper, and be sure to include unit labels ($\ln k$ for the y-axis and (Temperature)$^{-1}$ for the x-axis.

Staple the graph to the end of this lab report packet.
Part Four: Determining the Activation Energy for the iodination of acetone reaction - continued

e. **Find the energy of activation** for the iodination of acetone using the data in Trial #5.

The data points on the graph from the last section should correspond roughly to a straight line with a negative slope. This is the behavior predicted by the Arrhenius equation:

\[
\ln k = -\frac{E_a}{RT} + \ln A
\]

where \(\ln k\) is the y-axis, \((\text{Temperature in Kelvin})^{-1}\) is the x-axis, \(-E_a/R\) is the slope, \(R = 8.3145 \text{ J K}^{-1} \text{ mol}^{-1}\) (the "energy" gas constant), \(E_a\) is the energy of activation, and \(A\) is the collision frequency.

Perform a linear regression analysis using your calculator or graphing program (inverse Kelvin temperatures will be your x-axis, \(\ln k\) values will be your y-axis.) Record the values that you collected here:

Slope = ___________  
y-intercept = ___________  
correlation coefficient \((r)\) = ___________

The energy of activation, \(E_a\), can be determined from the slope. From the value of the slope determined through linear regression, **calculate the activation energy**.

\[
\text{Energy of activation} = -R \times \text{slope} = ___________
\]

The collision frequency, \(A\), can be determined from the y-intercept. From the value of the y-intercept determined through linear regression, **calculate the collision frequency**.

\[
\text{Collision frequency} = e^{\text{y-int}} = ___________
\]

*Note that \(e\) is the anti natural logarithm.*

e. **You are done!** Finish the postlab questions (which will be similar to the work you have just completed) and you are good to go!
POSTLAB QUESTIONS:

1. In a reaction involving the iodination of acetone, the following reaction mixture was used: 5.00 mL 4.0 M acetone, 5.00 mL 1.0 M HCl, 5.00 mL 0.0050 M I$_2$, and 10.0 mL water.
   
a. What was the molarity of the acetone in the reaction mixture? (Recall that $M_1V_1 = M_2V_2$)

b. The color of the above reaction mixture disappeared in 250 seconds. What was the rate of the reaction? (Hint: First determine the initial concentration of the iodine, then use the equation for rate from the lab.)

2. A second reaction mixture was made: 10.00 mL acetone, 5.00 mL HCl, 5.00 mL I$_2$, and 5.00 mL of H$_2$O.
   
a. What was the molarity of the acetone in this reaction mixture?

b. The iodine color disappeared in 120 seconds. What was the rate of the reaction?

c. Determine the order of the reaction (m) with respect to acetone using the information from question 1 and 2. (Round off the value of m to the nearest integer)

3. A third reaction mixture is made: 10.00 mL acetone, 5.00 mL HCl, 10.00 mL I$_2$. If the reaction is zero order with respect to iodine, how long will it take for the iodine color to disappear? (*Hint: rate = [I$_2$]/time, use the rate from question 2c and the new [I$_2$] to solve for the time elapsed.*)
POSTLAB QUESTIONS: *Continued*

4. The following reaction

\[ 2 \text{N}_2\text{O}_5(g) \rightarrow 4 \text{NO}_2(g) + \text{O}_2(g) \]

was studied at several temperatures, and the following values of \( k \) were obtained:

<table>
<thead>
<tr>
<th>( k \ (\text{s}^{-1}) )</th>
<th>( T \ (\degree\text{C}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2.0*10^{-5}</td>
<td>20.0</td>
</tr>
<tr>
<td>7.3*10^{-5}</td>
<td>30.0</td>
</tr>
<tr>
<td>2.7*10^{-4}</td>
<td>40.0</td>
</tr>
<tr>
<td>9.1*10^{-4}</td>
<td>50.0</td>
</tr>
<tr>
<td>2.9*10^{-3}</td>
<td>60.0</td>
</tr>
</tbody>
</table>

Using linear regression and the techniques developed in this lab, calculate the **activation energy** and **collision frequency** for this reaction. Include a graph of ln \( k \) versus \( (T)^{-1} \). *Hint:* make sure you use inverse Kelvin temperatures!

Slope = ___________ y-intercept = ___________ correlation coefficient (r) = ___________

Energy of activation = _____________

Collision frequency = _____________