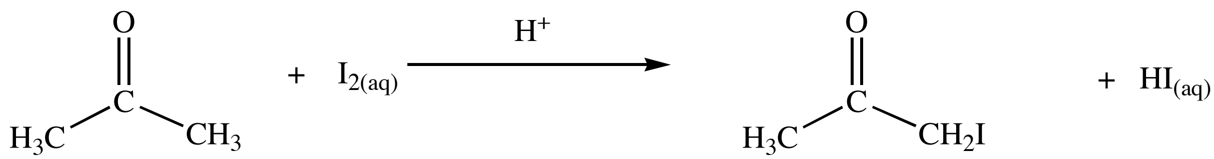
THE IODINATION OF ACETONE

Part One: Determining the Rate 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 this experiment we will first 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:



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

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

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:

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

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

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

or simply as

$$rate = \frac{[I_2]}{time}$$

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.

Procedure: *Finding the rate, orders of reaction and rate constant, k at room temperature*

For each experiment 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 125 mL flask. Making sure not to spill any on your hands or clothes, measure out the appropriate amount of **0.0050 M iodine** in a 10.00 mL flask (***Note:*** use these concentration values in this lab regardless of what the stockroom lists as the actual concentration.) Start the stopwatch as you add the iodine to the 125 mL flask. Swirl the flask (which helps to prevent acetone evaporation) until the yellow color disappears, then halt the stopwatch. 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 of the same experiment are within 20 seconds of each other. Determine the **average time elapsed in seconds** for this experiment.

Repeat this process for each of the four experiments listed in the table below.

Experiment	**HCl (mL)**	**Acetone (mL)**	**I_2 (mL)**	**Water (mL)**	**Total Volume (mL)**
1	5	5	5	10	25.00
2	5	5	10	5	25.00
3	5	10	5	5	25.00
4	10	5	5	5	25.00

Calculations:

1. Determine the concentration of **each reactant** (acetone, HCl and iodine) in **each reaction mixture**.

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

Solution: Using the relation $\mathbf{M_1V_1 = M_2V_2}$ let $\mathbf{M_1}$ = initial (undiluted) concentration of iodine (0.0050 M), $\mathbf{V_1}$ = 5.00 mL (of undiluted iodine added to the mixture), and $\mathbf{V_2}$ = 25.00 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:

$\mathbf{M_2}$ = 0.0050 M * 5.00 mL / 25.00 mL = **0.0010 M**, which is the concentration of iodine used in the reaction in experiment #1.

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

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

$\mathbf{M_2}$ = 0.0050 M * 10.00 mL / 25.00 mL = **0.0020 M**, the concentration of iodine used in the reaction in experiment #2.

2. Average each pair of times for each experiment then calculate the **rate** of the reaction.

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

Solution: The rate of reaction is equal to the concentration of iodine divided by the time elapsed (see the introduction section for more details; do *not* use [HCl]/time or [acetone]/time in this lab). Using the concentrations from the above examples, we can calculate rate thusly:

rate (experiment #1) = $[I_2]$/(average time in seconds) = 0.0010 M / 240 s = $\mathbf{4.2 * 10^{-6}\ M\ s^{-1}}$.

rate (experiment #2) = $[I_2]$/(average time in seconds) = 0.0020 M / 496 s = $\mathbf{4.0 * 10^{-6}\ M\ s^{-1}}$.

3. Next determine the **order** of the reaction with respect to each reactant (**m**, **n**, and **p**). Show your work clearly in your lab report as to how you solved for m, n ***and*** p.

Example: Find the order of reaction with respect to iodine (p) using the information calculated above.

Solution: Notice how in experiment #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 ($4.0 * 10^{-6}$ M s^{-1} versus $4.2 * 10^{-6}$ 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:

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

The values of k, [acetone] and [HCl] remain constant between experiment 1 and experiment 2 (only $[I_2]$ changes), so the expression reduces to

$$\frac{\text{rate 2}}{\text{rate 1}} = \frac{4.0 * 10^{-6}}{4.2 * 10^{-6}} = \frac{[0.0020]^p}{[0.0010]^p} = 2^p$$

$$0.95 = (2)^p$$

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**.

4. Calculate k for each experiment .

Example: Find the value of k for experiment #1 using the values supplied above and assuming that the order with respect to acetone (m) is one and the order with respect to HCl (n) is one.

Solution: Using the information in experiment #1, the diluted concentration of acetone is 0.80 M and the HCl is 0.20 M (confirm this on your own). Using the values for rate 1 and the order of iodine from above, we can calculate k from the following equation:

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

$$4.2 * 10^{-6} = k[0.80]^1[0.20]^1[0.0010]^0$$

and solving for k we get a value of $\mathbf{k = 2.6 * 10^{-5}\ M^{-1}\ s^{-1}}$

5. Find the average value of k and conduct a parts per thousand analysis on your k values.

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.)

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_2O.
   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?