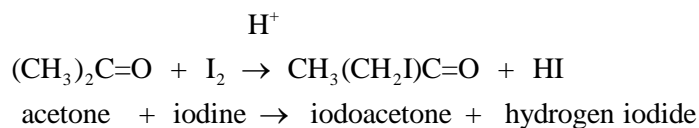


## KINETICS OF THE IODINATION OF ACETONE

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### Introduction

Solid iodine (I<sub>2</sub>) crystals have a dark red/black color. An aqueous iodine solution is yellow. When an aqueous iodine solution reacts with acetone in the presence of an acid, the yellow color slowly fades as the iodine is consumed. The products of the reaction are iodoacetone and hydrogen iodide. The hydrogen ion is a catalyst for this reaction.



The rate law for this reaction is of the form:

$$\text{rate} = k [\text{I}_2]^x [\text{H}^+]^y [(\text{CH}_3)_2\text{C}=\text{O}]^z$$

The rate of this reaction will be followed by watching the solution's yellow color fade over time.

$$\text{rate} = - \frac{\Delta[\text{I}_2]}{\Delta t}$$

The rate law can be written as:

$$\text{rate} = - \frac{\Delta[\text{I}_2]}{\Delta t} = k [\text{I}_2]^x [\text{H}^+]^y [(\text{CH}_3)_2\text{C}=\text{O}]^z$$

In this experiment you will use the method of initial rates to determine the value of the rate constant, *k*, and the orders of the reaction with respect to I<sub>2</sub> (the value of *x*), H<sup>+</sup> (the value of *y*), and (CH<sub>3</sub>)<sub>2</sub>C=O (the value of *z*).

You will perform four runs using different concentrations of reactants. For each run, you will produce an Absorbance vs. Time plot. The slope of each plot can be used to find the initial rate of the reaction for that particular run. This initial rate will be part of the data summarized in Table 2 of the Data and Analysis Sheet.

Since the iodine concentration is proportional to absorbance (*A*), we must also calculate the constant (*b*) relating Absorbance to iodine concentration for your spectrometer using the following equation.

$$A = b [\text{I}_2]$$

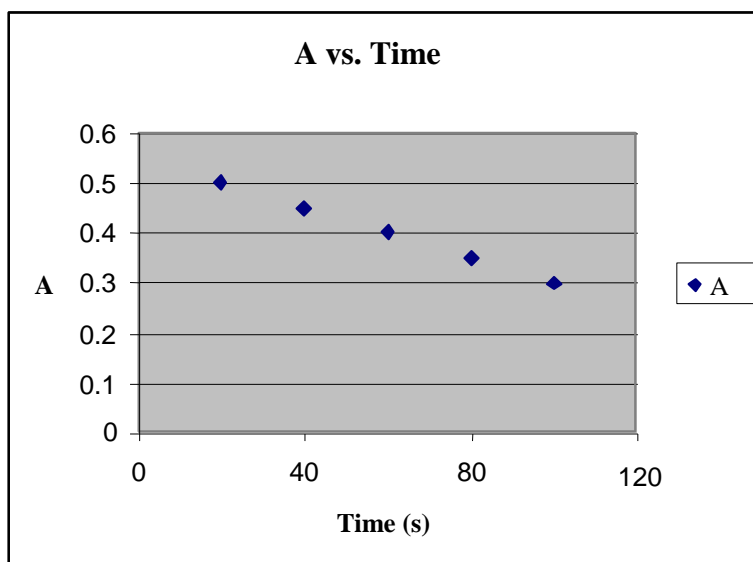
Because you are following the rate of the reaction by measuring the change in absorbance of the solution, you will need to divide the change in absorbance vs. time by the constant *b*.

$$\text{rate} = - \frac{\Delta[\text{I}_2]}{\Delta t} = - \frac{\Delta A}{b \Delta t}$$

In this manner, the Absorbance vs. time plot can be used to obtain the initial rate of the reaction in concentration per unit time.

A plot of Absorbance vs. Time will look like Figure 1 below.

**Figure 1.**



The key feature of this plot is that the slope of the line is constant and therefore the rate of the reaction (initial and after some time has elapsed) is constant. In other words, for each set of reaction conditions, the slope of the line plotted above divided by your constant, b, will give you the initial rate of the reaction in  $[\text{I}_2]/\text{s}$  units.

### Overview and Important Details

You will be measuring the rate of decolorization of iodine in reaction mixtures containing varying amounts of each reactant. By using this procedure, it is possible to calculate the order of reaction with respect to each reactant and the rate constant for the reaction. **It would be very beneficial to complete the initial concentration columns (columns 2 through 4) in Table 2 prior to coming to lab lab.**

In this experiment you will be using the spectrometer. However, you will not create a calibration curve showing Absorbance vs. Concentration as you have done in previous colorimetry experiments. Instead you will create a graph of Absorbance vs. Time for each experimental run. The equation of the line for each graph will be determined. This data will then be used to determine the rate constant and order of reaction with respect to each of the reactants.

## PROCEDURE

1. Double click the “Logger Pro” icon and allow the screen to open.
2. The Spectrometer needs to be powered for about 5 minutes before using so do this step before preparing your solutions. Do not use the Go!Link with the spectrometer. Plug the Spectrometer via provided USB cable to the computer USB port.
3. Label a set of clean dry test tubes so that there is a test tube for each experiment shown in Table 1. Add the components, **except iodine**, for each experiment into the corresponding test tube. (Example: Exp 1 would have 1 mL of acetone, 1 mL of HCl and 2 mL of deionized water.)
4. Label another set of clean dry test tubes so that there is a second test tube for each experiment. Deliver 1.0 mL of stock iodine solution into the test tubes labeled Exp 1, Exp 2 and Exp 3. Deliver 2.0 mL of stock iodine solution into the test tube labeled Exp 4.

**Table 1. Volume (mL) of Reactants for each Iodination Experiment**

<b>Reactant→</b>	<b>Acetone</b>	<b>HCl</b>	<b>H<sub>2</sub>O</b>	<b>Iodine</b>
<b>[Reactant]→</b>	<b>4.0 M</b>	<b>1.0 M</b>		<b>0.0025 M</b>
<b>Exp 1</b>	1.0 mL	1.0 mL	2.0 mL	1.0 mL
<b>Exp 2</b>	2.0	1.0	1.0	1.0
<b>Exp 3</b>	1.0	2.0	1.0	1.0
<b>Exp 4</b>	1.0	1.0	1.0	2.0

5. Calibrate the Spectrometer ; Do not unplug the spectrometer during this experiment or you will have to start over.
  - a. Return to the Logger Pro screen on the computer. Click: Experiment ; Calibrate ; Spectrometer:1.
  - b. Allow the lamp to warm up for 90 seconds as displayed on the computer screen.
  - c. Only touch the ridged faces of the cuvette, never touch the clear faces. Rinse and fill one cuvette (about  $\frac{3}{4}$  full) with the blank (deionized water). **Gently blot** (don't scratch the sides of the cuvette) any drips on the outside of the cuvette with a Kimwipe.
  - d. Place the cuvette containing the blank in the spectrometer so that one of the clear sides is aligned with the white arrow at the top of the cuvette slot. Click: “Finish Calibration” ; OK. Remove the cuvette from the spectrometer.

6. Determine the Wavelength of Maximum Absorbance
  - a. Record the concentration of the standard iodine solution on the report sheet. Rinse and fill a cuvette with the standard iodine solution. **Gently blot** (don't scratch the sides of the cuvette) any drips on the outside of the cuvette with a Kimwipe.
  - b. Place the cuvette containing the standard iodine solution in the spectrometer. Click: Experiment ; Data Collection ; Full Spectrum ; Done. Click the rainbow icon labeled "Absorbance=..." in the upper left hand corner of the window. Change the "Wavelength Range" to 380-750nm. Close this box by clicking the "x" in the upper right hand corner of the window.
  - c. Click the small green triangle in the toolbar labeled "Collect". After the line graph appears on the screen, click the small red square in the toolbar labeled "Stop".
  - d. To automatically store the maximum wavelength go to the toolbar and select: Experiment ; Store Latest Run.
  - e. Record the absorbance of the standard iodine solution at the wavelength of maximum absorbance on the report sheet. Remove the cuvette from the spectrometer.
7. Choose: Experiment ; Data Collection. In the collection tab choose: Time Based. The Sample at Time Zero box needs to be checked and the Repeat box should not be checked. Set Duration to 200 s and Sampling Rate to 2 s/sample. Done.
8. Each of the four experiments will generate a graph of absorbance (y-axis) vs. time (x-axis). Title the graph and check that the axes are labeled appropriately. You will need to be careful to keep track of which experiment is being run. Double click on the data table title on the left of the screen. Replace "Data Set" or "Latest" with Exp 1.

Do the next steps quickly: the solution will start losing color as soon as reactants are mixed together and you want to follow as much of the initial reaction as possible.

  - a. Do not rinse the cuvette with the solution to be analyzed.
  - b. Add the reactants contained in the first test tube for Exp 1 to the second test tube containing the iodine solution for Exp 1.
  - c. **Mix well, then quickly** fill the cuvette about  $\frac{3}{4}$  full, blot it dry, and place it in the spectrometer.
  - d. Immediately touch the data collection button (white triangle in green rectangle) on the upper portion of the computer screen.
  - e. After 200 seconds data collection will automatically stop.
  - f. Choose: Experiment ; Store Latest Run.
9. Repeat Step 7 (just to be sure everything is still as it should be) and Step 8 for each experiment. Be sure to replace "Data Set" or "Latest" with the correct experiment number and don't forget to store your latest run.
10. The curves for all four experiments should be visible on the same graph.

- a. Choose: Analyze ; Autoscale ; Autoscale.
  - b. Highlight the initial, linear portion of the graph for Exp 1. Choose: Analyze ; Linear Fit. Check the Exp 1 box.
  - c. Repeat Part b for the remaining experimental runs.
  - d. If necessary, click on the graph to remove the linear analysis shaded areas and move the analysis boxes around to visually clean up the graph.
11. Each lab partner's report must have a Logger Pro generated printout of a single graph containing the plots and linear analysis for all four runs of the experiment.

Once you are ready to print out the graph, Click: File ; Print. Change the "orientation" to landscape under properties. Be sure that the names of all lab partners are entered in the "Name" section and that the date box is checked.

12. When you are done, return your bin to Lab Services

### DATA AND ANALYSIS SHEET EXAMPLE

1. Concentration of the standard iodine solution: \_\_\_\_\_

Absorbance of the standard iodine solution: \_\_\_\_\_

Use the equation:  $A = b [I_2]$  to calculate  $b$ .  $b =$  \_\_\_\_\_

2. The information for the last three columns, initial rate information for each experiment and the rate constant, is determined in the laboratory.

**Table 2.** Initial Molar Reactant Concentration/Iodination Experiment Data Table

Experiment	[acetone]	[HCl]	[I <sub>2</sub> ]	Initial Rate (A/s)	Initial Rate (M/s)	Rate Constant
Exp 1						
Exp 2						
Exp 3						
Exp 4						
Average value of the rate constant						

3. Determine the order with respect to each reactant and the overall order for the reaction.

4. Calculate the value of the rate constant for each of the four runs of the experiment and an average value of the rate constant. Show your work and include the correct units.

5. Rewrite the rate law (in the form:  $\text{rate} = k [I_2]^x [H^+]^y [(CH_3)_2C=O]^z$ ) for the reaction substituting in the numerical values you calculated for  $k$  (average),  $x$ ,  $y$ , and  $z$ .

6. Be sure a copy of the graph is attached to your lab report.