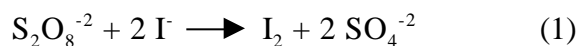


Experiment II¹ Chemical Kinetics

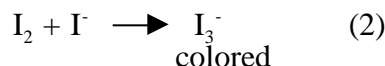
Introduction

A company that manufactures dyes has had problems with its newest shade of purple: crystal violet. With the recent '70's craze, they have been marketing crystal violet for use in the tie-dye process, which normally requires that the color be "set" in highly basic washing soda. However, many disgruntled customers have complained that crystal violet loses its color during the tie-dye process. The head of Quality Control attended the premiere of *Dracula* and noted the tremendous job that the Chemical Investigation Team did with the blood and has contacted you to investigate the dye decolorization dilemma. She suspects that base may be involved in the loss of color and would like CIT's interpretation of the role of hydroxide in the kinetics of crystal violet decolorization.

Because your company is relatively new, the company proposes to give you a system with which they are already familiar to investigate first. If your interpretation of this system agrees with what they already know, then they will have more confidence in your crystal violet studies. Therefore, it is prudent to put your best foot forward during the Week 1 analysis so that they will trust your Week 2 findings. The known reaction of Week 1 is the decomposition of peroxydisulfate, $S_2O_8^{2-}$, in the presence of iodide as follows:

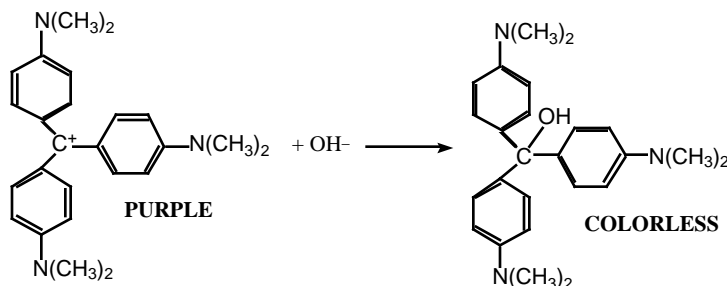


The rate of this reaction can be monitored with a spectrophotometer because the product I_2 reacts with excess I^- in the solution to form the colored species I_3^- , triiodide. The absorbance due to triiodide increases during the course of the reaction as it is being produced and can be used as a measure of the rate.



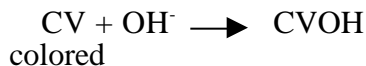
rate of disappearance of $S_2O_8^{2-}$ = rate of appearance of I_2 = rate of appearance of I_3^- = $k[S_2O_8^{2-}]^x[I^-]^y$

During Week 2, you will examine the reaction actually of interest to the dye company. In contrast to the peroxydisulfate reaction, it is proposed that crystal violet *loses* color over time in the presence of base:



This reaction can be represented as follows:

¹ Adapted from Chemistry The Central Science, Laboratory Experiments, 6th Edition, by J.H. Nelson and K.C. Kemp, the Colby College CH 142 Laboratory Manual edited by D. W. King, 2000, and Laboratory Inquiry in Chemistry, by R. C. Bauer, J. P. Birk, and D. J. Sawyer.



The kinetics of this reaction can also be monitored with a spectrophotometer by observing the *decrease* in absorbance of crystal violet, which can be used as a measure of the rate to determine the rate law:

$$\text{rate} = [\text{CV}]^x [\text{OH}^-]^y \quad (3)$$

Your task is to determine the form of the rate law and the rate constants for both of the reactions described above: the decomposition of peroxydisulfate and the decolorization of crystal violet. CIT's research guru Dr. Kim A. Kell-Wizz has prepared the following useful summary on chemical kinetics to prepare you for this task.

Chemical Kinetics

Chemical reactions occur at varying speeds with a vast spectrum of rates, ranging from very slow to extremely fast. For example, the rusting of iron is fairly slow, whereas the decomposition of TNT proceeds explosively fast. Experiments have shown that the rate of a homogeneous reaction in solution depends upon the nature of the reactants, their concentrations, the temperature of the system, and the use of catalysts.

Consider the hypothetical reaction:



The rate of this reaction may be measured by observing the rate of disappearance of the reactants A or B, or the rate of appearance of the products C or D. Which species is observed is a matter of convenience. For example if A, B, and C are colorless and D is colored, the rate of appearance of D can be conveniently measured by observing an increase in the intensity of the color of the solution as a function of time. Mathematically, the rate of reaction may be expressed as follows:

$$\text{Rate of disappearance of A} = \frac{\text{Change in the concentration of A}}{\text{Change in time}} = - \frac{[\text{A}]}{t}$$

$$\text{Rate of appearance of D} = \frac{\text{Change in the concentration of D}}{\text{Change in time}} = \frac{[\text{D}]}{t}$$

In general, the rate of the reaction depends upon the concentration of one or more of the reactants. Thus, the rate of the hypothetical reaction above may be expressed as:

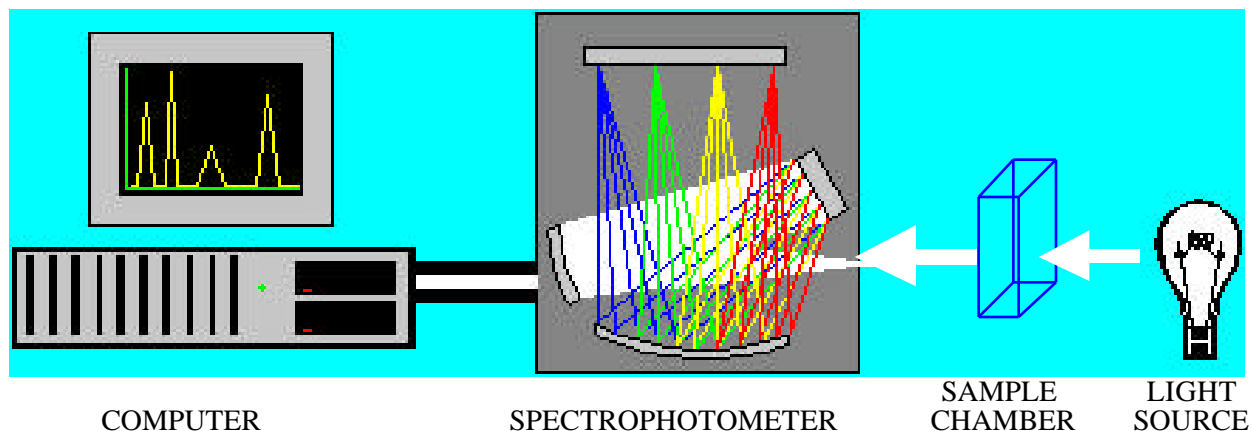
$$\text{Rate} = k[\text{A}]^x [\text{B}]^y$$

where [A] and [B] are the molar concentrations of A and B, x and y are the powers to which the respective concentrations must be raised to describe the rate, and k is the specific rate constant. The values of x and y must be determined experimentally. For example, if x = 2 and y = 1, then the rate law is:

$$\text{Rate} = k[\text{A}]^2[\text{B}]$$

This reaction is first order in B, meaning that doubling the concentration of B while keeping A constant causes the reaction rate to double. Simultaneously, this reaction is second order in A, meaning that doubling the concentration of A while keeping B constant causes the rate to increase by a factor of four since the rate of the reaction is proportional to the square of the concentration of A. The overall order of the reaction is the sum of the exponents: or third order in this case. It is possible to determine these orders experimentally by noting the effects of changing reagent concentrations on the rate of the reaction. The specific rate constant, k , has a definite value that is independent of the concentration. The rate constant is characteristic for a given reaction and varies only with temperature. Once the rate is known for a given set of concentrations, the value of k can be calculated.

For both of our reactions of interest, the rate law will be determined by spectrophotometrically measuring either the amount of reactant disappearing or the amount of product appearing as a function of time. The values of x and y as well as the rate constant k will be determined for the rate law: $\text{rate} = k[A]^x [B]^y$. CIT is fortunate that Colby was recently awarded a sizeable grant from the Howard Hughes Medical Institute that allowed the Chemistry Department to purchase the mini-spectrophotometers from Ocean Optics that we will use. A cartoon of the instrument is provided below.



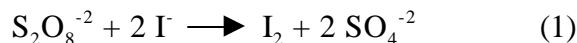
White light illuminates the sample and can be absorbed. The remaining light enters an optical fiber and is efficiently transmitted to the spectrophotometer and then analyzed by a computer. The amount of light absorbed by the sample can be determined by measuring the light signal with the sample in the optical path relative to a reagent blank. Recall from Experiment I that Beer's Law relates the measured absorbance, A , to concentration, C , of the chromophore as follows:

$$A = \epsilon b C$$

where b is the path length, which is 1 cm in our case, and ϵ is the molar extinction coefficient

Peroxydisulfate Decomposition

The reaction of interest is as follows:



Recall that the rate of the chemical reaction is equal to the change in concentration of either products or reactants with time and can be expressed in several different ways:

$$\text{rate} = \frac{-[\text{S}_2\text{O}_8^{2-}]}{\text{time}} = \frac{[\text{I}_2]}{\text{time}} = k [\text{S}_2\text{O}_8^{2-}]^x [\text{I}^-]^y \quad (4)$$

We are assuming that the change in I_2 concentration ($[I_2]$) can be measured by the change in color of the solution, which is really the change in $[I_3^-]$. The change in time (t) is the time between absorbance measurements. This is an approximation because the rate changes over the course of the reaction and is not constant. For example, the rate of appearance of I_2 versus time is not linear because the overall order of the reaction could follow a complicated polynomial and/or exponential dependence. However, since we are only studying the *initial rate* of this reaction, it is reasonable to assume a linear relationship between concentration and time. Initial rate experiments are performed so that the concentration of reactants remains within 1% of their starting values.

Beer's Law allows calculation of the concentration of triiodide using the literature value of ($15,000 \text{ M}^{-1}\text{-cm}^{-1}$ at 360 nm). Thus,

$$[I_3^-] = \text{Absorbance} / (15,000 \text{ M}^{-1}\text{-cm}^{-1}) (1 \text{ cm}) \quad (5)$$

The key to our kinetic analysis is the assumption that $[I_3^-] = [I_2]_{\text{formed}}$, which is true because this subsequent reaction is very fast in the presence of excess I^- compared to the reaction that we are studying.

A practical approach to find the order of the chemical reaction by the initial rate method is to vary the concentration of one reactant while leaving the concentration of the other reactants constant. We will determine the order of the reaction for each reactant by collectively running two sets of experiments: Group 1 will vary $[S_2O_8^{2-}]$ while keeping $[I^-]$ constant; Group 2 will vary $[I^-]$ while keeping $[S_2O_8^{2-}]$ constant. You will run either Group 1 or Group 2 experiments in lab. You will then obtain data for the other group from fellow CIT members to perform your final determination of the rate law.

Because this reaction has two reactants and is likely to follow a complicated mechanistic pathway to products, it may not have simple whole number values for reaction orders. Therefore, we cannot determine the reaction order through the simple linear plots we have used to solve problems in the textbook to determine whether a reaction is zero, first, or second order. Instead, we will use a mathematical trick in our analysis. Taking the (log) of both sides of the rate equation,

$$\text{rate} = k [S_2O_8^{2-}]^x [I^-]^y, \text{ gives:}$$

$$\log(\text{rate}) = \log(k) + x \log [S_2O_8^{2-}] + y \log [I^-]$$

For Group 1, the term $y \log [I^-]$ is constant because the $[I^-]$ is constant. The term $\log(k)$ is also constant since the rate constant, k , is characteristic of each reaction. Therefore, a plot of $\log(\text{rate})$ vs. $\log [S_2O_8^{2-}]$ should give a straight line with a slope of x , the rate order with respect to $S_2O_8^{2-}$. Similarly, for Group 2 both the terms $x \log [S_2O_8^{2-}]$ and $\log(k)$ are constant. Thus, the rate order with respect to I^- can be determined through a plot of $\log(\text{rate})$ vs. $\log [I^-]$. Note that it is unlikely that you will calculate whole number values for these reaction orders: do **not** round the values that you calculate to the nearest whole number when calculating your rate constants.

Potassium nitrate solution will be added to each reaction mixture to maintain the same concentration of ions and solution volume; it does not enter into the reaction in any way. Ethylene diamine tetraacetic acid (EDTA) is added to each mixture to complex metals that can interfere with the reaction. These metals are present in trace amounts, but even these trace amounts are enough to catalyze the reaction and thus affect the rate measurement.

Crystal Violet Decolorization

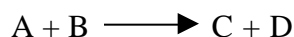
Many of the above principles hold true for the reaction of interest for Week 2. The rate of this chemical reaction is equal to the change in concentration of crystal violet with time.

$$\text{rate} = \frac{-[\text{CV}]}{\text{time}} = k [\text{CV}]^x [\text{OH}^-]^y \quad (6)$$

The first step in this analysis will be to determine the wavelength that can be used to monitor the disappearance of crystal violet and the extinction coefficient at that wavelength. Next, two different sets of experiments will be performed: Group 1 that varies the concentration of hydroxide and allows determination of y in equation (6), and Group 2 that varies the concentration of crystal violet and allows determination of x in equation (6). The plots of $\log(\text{rate})$ vs. concentration for Group 1 and Group 2 can then be used to determine the values of y and x , respectively.

Example Analysis

Use the kinetic data provided below for the hypothetical reaction:



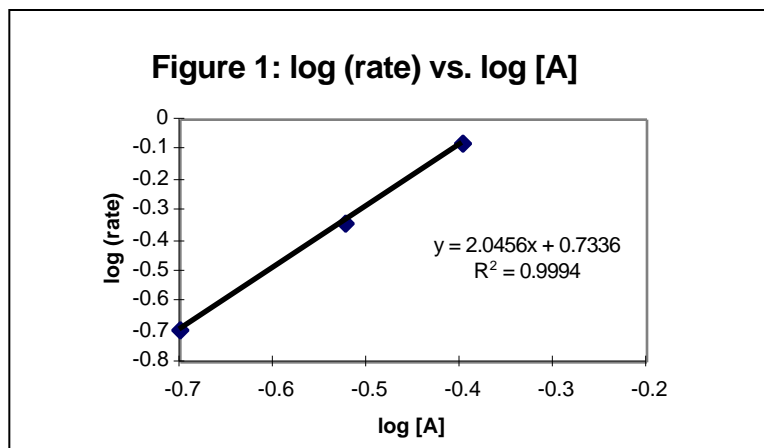
1. To determine the order of the reaction with respect to A.
2. To determine the order of the reaction with respect to B.
3. To write the rate expression for the reaction.
4. To calculate the rate constant of the reaction.

EXPERIMENT	[A] (M)	[B] (M)	RATE (M/SEC)
1	0.1	0.1	0.0101
2	0.1	0.2	0.0206
3	0.1	0.4	0.0403
4	0.2	0.5	0.203
5	0.3	0.5	0.452
6	0.4	0.5	0.841

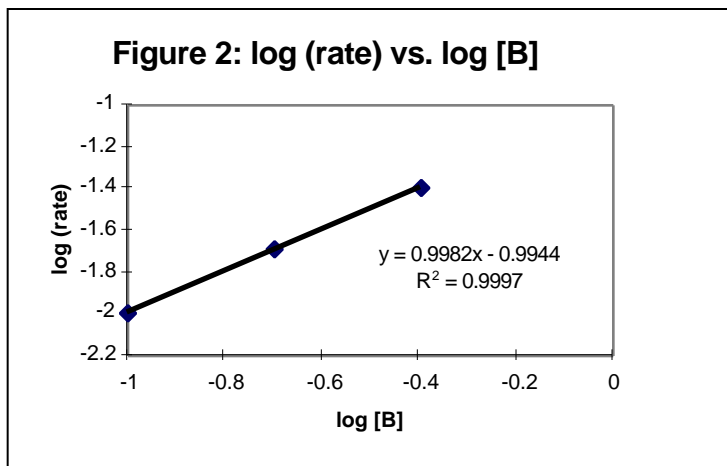
Solution

$$\text{Rate} = k [\text{A}]^x [\text{B}]^y$$

1. To determine “ x ”, the data from experiments 4-6 are used because [A] varies while [B] remains constant in these experiments. A plot of $\log(\text{rate})$ vs. $\log[\text{A}]$ for experiments 4-6 gives a slope of about 2 (Figure 1). Therefore $x \sim 2$.



2. The value of “y” can be determined by plotting $\log(\text{rate})$ vs. $\log[B]$ for experiments 1-3. This yields a slope of about 1 (Figure 2). Therefore $y \sim 1$.



3. $\text{Rate} = k [A]^2 [B]$.
4. The rate constant “k” can be determined from the data in any experiment. For example, using the data in experiment 3: $0.0403 \text{ M/sec} = k (0.1 \text{ M})^2 (0.4 \text{ M})$, or $k = 10.1 \text{ M}^{-2}\text{sec}^{-1}$.

Pre-Laboratory Assignment

In addition to the usual summary of the experimental procedure in your notebook, please also prepare answers to the following questions:

Week 1 Calculate the concentrations of I^- (from the 0.2 M stock solution of KI) and $\text{S}_2\text{O}_8^{2-}$ (from the 0.2 M stock solution of $(\text{NH}_4)_2\text{S}_2\text{O}_8$) in each of the 10 reactions described in Tables 1 and 2 below. Assume that the total final volume of each reaction is 2.37 mL. Note that a microliter (μL) = $1 \times 10^{-6} \text{ L}$ or $1 \times 10^{-3} \text{ mL}$.

Week 2 Calculate the concentrations of crystal violet and hydroxide in a solution that has a total final volume of 3.0 mL and contains 200 μL of crystal violet (stock concentration of $1.0 \times 10^{-4} \text{ M}$) and 200 μL of sodium hydroxide (stock concentration of 1 M).

Experimental Procedure- Week 1

Note that you will use automatic micropipettors in this experiment. Although many of you may have used these before in Biology laboratories, a few notes on their proper use follows. There are three sizes of pipettors in the lab: 20 μL , 200 μL , and 1000 μL . These can be identified either by the button color if the pipettors are “Fisherbrand” Finnpiettes (orange is the 20; yellow, the 200; blue, the 1000) or by the number on the top if they are “Rainin” brand (**P20** is the 20; **P200**, the 200; and **P1000**, the 1000). These numbers refer to the maximum volume **in microliters** (μL) that can be achieved; e.g., the P200 can dispense a maximum of 200 microliters. Never dial a pipettor past the maximum volume. To adjust the volume that will be dispensed by the pipettor, turn the dial at the top until the number in the window reads the desired volume. For example, to dispense 100 μL with the P200, the dial should read **100**. To dispense 50 μL , the dial should read **050**. The P1000 is a little tricky: for volumes less than 1000 μL , the first digit should be a red zero and the last digit of the volume does not appear on the dial. That is, to dial the P1000 to 250 μL , the display

should say **025**. The 1000 μL pipettors take the blue tips; the 20 μL and 200 μL take the yellow tips. To draw up the sample into the pipette tip, push the button down to the first notch, immerse the tip in the sample, and slowly release the button. Check the tip to make sure you didn't capture any air bubbles. To dispense the sample, push the button all the way down. **If you have any questions about the micropipettors, please ask your instructor or TA before use.** Micropipettors can be severely damaged if they are incorrectly dialed.

A. Preliminary Experiment to Determine λ_{max} of the Chromophore

1. Add 100 μL of 0.2 M KI, 200 μL of 0.1 M KNO_3 , and 2 mL of water to a cuvette and mix thoroughly.
2. Use this mixture as your reference sample and perform a light and dark signal blank on an Ocean Optics spectrophotometer as described in the "oceanoptics.pdf" document available on the web.
2. Add 100 μL of 0.2 M $(\text{NH}_4)_2\text{S}_2\text{O}_8$ solution to the cuvette and invert to mix.
3. Wait 2 minutes (the solution should be visibly colored) and then measure the wavelength of maximal absorbance (λ_{max}), which should be around 360 nm. See your instructor about whether to use this wavelength in subsequent determinations or a slightly higher wavelength, depending on the stability of the signal of your particular spectrophotometer at this wavelength.

B. Kinetics Experiments

You will work in groups of 3 for this experiment. Ten different reactions will be run in the lab: each group will run either the 5 different reactions in **Table 1** or the 5 different reactions in **Table 2**. These two experiments vary either the $[\text{S}_2\text{O}_8^{2-}]$ (Table 1) or the $[\text{I}^-]$ (Table 2) while keeping the concentration of the other reagent constant. Data will be pooled so that everyone has data for all 10 different reactions to allow determination of the order of the reaction with respect to each reactant. After you are assigned to either group 1 or group 2, follow the recipes given in the appropriate table to do your 5 reactions. Prepare the solutions for your experiment one at a time just before the measurements are made and proceed as follows with each reaction.

1. Prepare solution A, adding both reagents (KI and KNO_3), in a spectrophotometer cuvette.
2. Add 2.0 mL deionized water and 20 μL of 0.1 M EDTA solution to the cuvette. Carefully place a stir bar in the cuvette and wipe the sides of the cuvette with a Kimwipe.
3. Place the cuvette in the sample chamber of the spectrophotometer, making sure that the stir bar is spinning gently (the stir plate will probably be on a low setting to achieve this).
4. Configure and blank the spectrophotometer (each reaction has a different blank so you must do this **each** time!) according to the instructions found in part **I** of the "Using the Ocean Optics Spectrophotometers" hand-out (available on the Web). Proceed to **III. Measuring and Storing Kinetics Data** and follow the instructions. Note that the **time between scans** should be entered for each experiment as shown in the tables below.
5. Fill a micropipette with the appropriate volume of solution B, inject solution B into the cuvette all at once, and **start** acquiring data as described in the hand-out. Make sure that once you are ready to add solution B, you work quickly. **THOROUGH MIXING IS CRUCIAL TO THE**

SUCCESS OF THIS EXPERIMENT. Please make sure that you invert your tubes two times to mix as described in the Ocean Optics hand-out.

- Allow the spectrophotometer to acquire data for between 2 and 3 minutes (less time for reactions with shorter times between scans like Experiment 5 and more time for reactions with longer times between scans like experiment 1). When the reaction has proceeded for long enough, **stop** collecting data as described in the hand-out. During the data collection phase, you will see the absorbance spectrum on the screen and should be able to witness the absorbance increase over time due to the production of triiodide.
- Follow the instructions on the hand-out for saving your data.

Table 1. Volumes of reagents for Solutions A and B to add for Group 1. Remember that you should also add 2.00 mL of deionized water and 20 μL EDTA to Solution A.

Experiment	Solution A		Solution B	t between scans
	μL KI (0.2 M)	μL KNO_3 (0.1 M)	μL $(\text{NH}_4)_2\text{S}_2\text{O}_8$ (0.2 M)	(sec)
1	100	200	50	10
2	100	150	100	8
3	100	100	150	6
4	100	50	200	4
5	100	0	250	2

Table 2. Volumes of reagents for Solutions A and B to add for Group 2. Remember that you should also add 2.00 mL of deionized water and 20 μL EDTA to Solution A.

Experiment	Solution A		Solution B	t between scans
	μL KI (0.2 M)	μL KNO_3 (0.1 M)	μL $(\text{NH}_4)_2\text{S}_2\text{O}_8$ (0.2 M)	(sec)
1	50	200	100	10
2	100	150	100	8
3	150	100	100	6
4	200	50	100	4
5	250	0	100	2

C. Data Analysis

The spectrophotometer will record absorbance measurements every X seconds (where X is the time between scans), but you must save this data immediately after acquisition or it will be lost during the next trial. Save the data for each reaction in a folder on the hard-drive or on the Chemistry Server. After you have completed your 5 reactions, open your data in Excel. You will see a column of absorbance data that reflects the solution absorbance at your wavelength of maximal absorbance. Insert a new column A and put in the corresponding times in seconds (this will differ for each experiment depending on the **time between scans**).

1. Calculate the I_3^- concentration in a third column, using Beer's Law as described above [see equation (5)].
2. Plot $[I_3^-]$ vs. time in Excel via a scatter plot to achieve a straight line that provides a measure of the rate of reaction for that experiment. The slope of the best-fit line gives you the rate of the reaction. Note that it is likely that you will not plot all 50 data points- early time points when you were mixing should not be plotted. Late time points when you were not collecting data should also not be plotted. Check your significant figures for the slopes of the line- you should have at least 3 significant figures for these values. You must include at least one of the plots that you personally acquired in your notebook (i.e., each person in the group of 3 must acquire at least 1 of the 5 sets of kinetic data) and **provide a sample of all calculations in your lab notebook**.
3. Before leaving lab, enter your rate data for each concentration in the spreadsheet at the front of the lab for your group's 5 reactions. You may access the class data on the web (in the laboratory folder) after everyone has completed the lab in order to perform your analysis. Please note that some data may be better than other data. You are welcome to be selective in the use of this data and choose the set of data for Group 1 and Group 2 from your laboratory section that appears to be the most well-behaved, even if it is not your own data. You should include the spreadsheet of the entire lab's data in your notebook and **clearly reference** the source of the data actually used in your write-up.
4. Determine the reaction order for each of the reactants as follows:
 - a) Group 1: plot $\log(\text{rate})$ vs. $\log[S_2O_8^{2-}]$. The slope of the best-fit line is the reaction order for $S_2O_8^{2-}$ ("x" in the rate law equation (4) above).
 - b) Group 2: plot $\log(\text{rate})$ vs. $\log[I^-]$. The slope of the best-fit line is the reaction order for I ("y" in the rate law equation (4) above).
5. After you have determined the values of "x" and "y", determine the value of the rate constant, k, for each of the 5 experiments in group 1 and then the 5 experiments of group 2 separately using the expression: $\text{rate} = k[S_2O_8^{2-}]^x[I^-]^y$. Show a sample calculation in your lab notebook. Calculate the mean and the standard deviation for both group 1 and group 2. (Question: why are you analyzing the data separately, when k should be a constant that is independent of reaction conditions?)

Experimental Procedure- Week 2

Again, the first step in your analysis will be to determine the wavelength of maximal absorbance of the chromophore (crystal violet in this case). You will use the absorbance of a solution of known concentration of crystal violet to calculate the value of the extinction coefficient at this wavelength. Two sets of experiments will be performed collectively by the CIT members: one which holds the concentration of crystal violet constant while varying the hydroxide concentration (Group 1) and the other which holds the concentration of hydroxide constant while varying the crystal violet concentration (Group 2). These two sets of experiments will allow you to determine the reaction order for hydroxide and crystal violet, respectively, and thus the rate law. Note that your reference cuvette should contain water for all blanking procedures below.

A. Preliminary Experiment to Determine λ_{max} and ϵ

1. Keeping your total solution volume 3.00 mL in all cases, take the absorbance of a solution of crystal violet in water. A stock solution of 1.00×10^{-4} M will be available for you to use, and

you should try to keep the maximum absorbance value at around 1.5 or lower. It may take you a few dilutions to obtain a good spectrum, but you can collaborate with another research team to zone in on an appropriate amount of crystal violet that will be on-scale. Be as accurate as possible when making up your solution as you will use the concentration to calculate the extinction coefficient.

2. Once you find an appropriate dilution, make sure that you record both the λ_{max} and the absorbance at that wavelength on your own spectrophotometer. Wavelengths may differ from spectrophotometer to spectrophotometer.
3. Use Beer's Law to calculate the value of ϵ for crystal violet based on your measured absorbance value and your concentration (the path length is 1 cm).

B. Kinetics Experiments to Determine Reaction Order for Hydroxide (Group 1)

1. Again, the total volume of each trial should be 3.00 mL. Your first kinetics trial should contain a volume of crystal violet that will give an absorbance of about 1.2-1.5 (based on your findings from **Part A**). Plan to add the same volume of 1.00 M NaOH as you have of crystal violet, but don't add it yet! Add the crystal violet to your cuvette, then the appropriate volume of water that will make your final volume 3.00 mL (be sure to account for the NaOH that you're about to add). Finally, add the NaOH, mix with the pipette tip, and immediately start collecting kinetic data with the Ocean Optics spectrophotometer. You should see the signal drop as the crystal violet decolorizes in the presence of base. Collect data every few seconds for a couple of minutes then stop collecting, extract the data at the λ_{max} , and save the data as described in the Ocean Optics hand-out.
2. Set up another 3.00 mL reaction that contains less hydroxide than the first trial (but make sure that you know this concentration). Again, add crystal violet, water (make sure that you increase the volume of water to make up for the decrease in the amount of sodium hydroxide), and the new, reduced volume of 1.00 NaOH. Collect kinetics data again and save this data to disk.
3. Repeat until you have four or five kinetics trials, each with a total volume of 3.00 mL, a constant volume of crystal violet, and a known, varying amount of sodium hydroxide.

C. Kinetics Experiments to Determine Reaction Order for Crystal Violet (Group 2)

1. Again, the total volume of each trial should be 3.00 mL. Your first kinetics trial should contain a volume of crystal violet that will give an absorbance of about 1.2-1.5 (based on your findings from **Part A**). Plan to add the same volume of 1.00 M NaOH as you have of crystal violet, but don't add it yet! Add the crystal violet to your cuvette, then the appropriate volume of water that will make your final volume 3.00 mL (be sure to account for the NaOH that you're about to add). Finally, add the NaOH, mix with the pipette tip, and immediately start collecting kinetic data with the Ocean Optics spectrophotometer. You should see the signal drop as the crystal violet decolorizes in the presence of base. Collect data every few seconds for a couple of minutes then stop collecting and save the data as described in the Ocean Optics hand-out.
2. Set up another 3.00 mL reaction, this time with less crystal violet than in the first trial (but make sure that you know this concentration). Again, add crystal violet, water (make sure that you increase the volume of water to make up for the decrease in the amount of crystal violet), and the same volume of 1.00 NaOH as before. Collect kinetics data again and save this data to disk.

3. Repeat until you have four or five kinetics trials, each with a total volume of 3.00 mL, a constant volume of 1.00 M NaOH, and a known, varying amount of crystal violet.

D. Data Analysis

1. Open your absorbance data in Excel and insert a new column A of time in seconds.
2. Insert a new column B of crystal violet concentration, using the absorbance data and your extinction coefficient calculated in **Part A** above to determine these values ($c = A/\epsilon l$; path length is 1).
3. Plot [crystal violet] versus time in Excel. The slope of the best-fit line is the rate of the reaction for that experiment.
4. Before leaving lab, enter your rate data in the spreadsheet at the front of the lab for your group's reactions. You may access the class data, which will be posted on the web after everyone has completed the lab, in order to perform your analysis. Please note that some data may be better than other data. You are welcome to be selective in the use of this data and choose the set of data for Group 1 and Group 2 from your laboratory section that appears to be the most well-behaved, even if it is not your own data. You should include the spreadsheet of the entire lab's data in your notebook and **clearly reference** the source of the data actually used in your write-up.
5. Determine the reaction order for each of the reactants as follows:
 - a) **Group 1**: plot $\log(\text{rate})$ vs. $\log[\text{hydroxide}]$. The slope of the best-fit line is the reaction order for hydroxide ("y" in the rate law equation (6) above).
 - b) **Group 2**: plot $\log(\text{rate})$ vs. $\log[\text{crystal violet}]$. The slope of the best-fit line is the reaction order for crystal violet ("x" in the rate law equation (6) above).
6. After you have determined the values of "x" and "y", determine the value of the rate constant, k, for each of the 5 experiments in group 1 and then the 5 experiments of group 2 separately using the expression: $\text{rate} = k[\text{CV}]^x[\text{OH}^-]^y$. Show a sample calculation. Calculate the mean and the standard deviation for both group 1 and group 2. (Question: why are you analyzing the data separately, when k should be a constant that is independent of reaction conditions?)

Report

Prepare a **ONE-PAGE typed report** summarizing your findings for the dye company that hired you. You should attach to this report all spreadsheets and graphs that you used to make your findings. Make sure that your report is at an appropriate level for your audience: in this case, the quality control manager at the dye company who not only has had college-level chemistry but also postulated that base was involved in the decolorization dilemma. Present your findings for both Week 1 and Week 2, but keep in mind that it is the crystal violet reaction that really interests them. Can you make any suggestions as to how the tie-dye process could be modified to accommodate this base-sensitive dye? Make sure that you include an error analysis in your report, referring to the CH142 Error Analysis document (error.pdf) available on the web.