Experiment 13G

FV 23Dec06

REACTION KINETICS

MATERIALS: Solid $Na_2S_2O_8$; 0.875M KI and 0.35 M NaF aqueous solutions; standard aqueous I_2/I^- solution (1.00×10^{-3} M I_2/0.20 M I^-); Spectronic-20; round cuvettes with rubber stoppers; 50 mL beakers (2); 25 mL volumetric flasks (2); volumetric pipets: 1-mL, 2-mL, 5-mL and 10-mL; 5-mL graduated pipet; 10 mL graduated cylinder; acetone; Styrofoam cups; digital thermometer; ice; capped vials

PURPOSE: The purpose of this experiment is to determine the rate law for a reaction, including the value for the rate constant, and to determine the activation energy for the reaction.

LEARNING OBJECTIVES: By the end of this experiment, the student should be able to demonstrate the following proficiencies:

1. Properly make aqueous solutions, given target volumes and molarities.
2. Relate absorbance measurements to concentrations, using the Beer-Lambert Law.
3. Apply the method of comparing initial reaction rates to determine the order of reaction with respect to reactants.
4. Apply the graphical (integrated rate law) method to determine the order of reaction with respect to one reactant.
5. Determine the activation energy of a reaction by comparing rate information for at least two different temperatures.
6. Perform dilution calculations in order to determine initial concentrations of reactants.
7. Control experimental conditions as needed to assure proper comparison of rate information.

PRE-LAB: Complete the Pre-Lab Assignment at the end of this document **before** going to lab. You will need some of the answers to these questions in order to get started with the experiment.

DISCUSSION:

Basic Rate Laws. Many reactions have rate laws which depend only on the concentrations of the reactants, i.e.,

$$\text{rate} = k[A]^x[B]^y \tag{1}$$

where A and B are reactant species, x and y are the orders of the reaction with respect to these species, and k is the rate constant. This experiment involves such a reaction. When colorless aqueous solutions of potassium iodide, KI, and sodium persulfate, $Na_2S_2O_8$, are mixed, an increasingly yellow solution results, indicative that the product iodine (I_2) is being produced. The persulfate ion splits apart into sulfate ions, which are also colorless. (You should be able to write the reaction based on this information.) The experimental work will provide information that will allow the complete rate law for this reaction to be determined, including the orders of reaction and the specific value for the rate constant.

Method of Initial Rates. All general chemistry textbooks outline a simple method, known as the Method of Initial Rates, for determining orders of reaction. This method simply involves a comparison of two different trials, the only difference between the trials being the initial concentration of one of the reactant species. Details of this method are outlined in any textbook. Part of this experiment includes performing this kind of analysis for determining the order of reaction for one of the reactant species.

Pseudo Rate Law Method (graphical). Another method outlined in general chemistry textbooks involves determining whether a reaction follows certain graphical profiles. However, this method can only be applied if the rate law for the reaction involves only one reactant. This may appear rather limiting, since most chemical reactions involve at least two reactants. As shown below, however, there is a way, in principle, to cause a reaction involving multiple reactants to appear to include the change in only one reactant. This method is known as the pseudo rate law method.

Consider a reaction involving two reactants, A and B, whose rate law is given by Eq. (1) above. If an experiment is performed where one of the reactants, A, has an initial concentration over *100* times as great as the other reactant, B, then the rate law effectively (to a very good approximation) becomes

$$\text{rate} = k'[B]^y \tag{2}$$

where k' is equal to k[A]', and is essentially a constant. This is true because the percent change of the concentration of substance A is very small due to its overwhelmingly large initial concentration. Once this pseudo rate law condition is achieved, the graphical methods involving simple integrated rate laws outlined in general chemistry texts can be used to determine the order of reaction with respect to the less concentrated species.

Activation Energy Determination. Finally, reactions carried out at different temperatures provide information that allows the determination of the activation energy, E_a, of the reaction. If the rate constants (k values) are determined at several different temperatures then the activation energy is found by making a plot of ln k vs. 1/T, since:

$$\ln(k) = -\frac{E_a}{R}\left(\frac{1}{T}\right) + \ln(A) \tag{3}$$

Thus the slope of the line equals $-E_a/R$, and the intercept provides the frequency factor A. (If only two such pairs of data points (k_j, T_j) are available, the equation reduces to $\ln(k_1/k_2) = (E_a/R)(1/T_2-1/T_1)$, as derived in your textbook.)

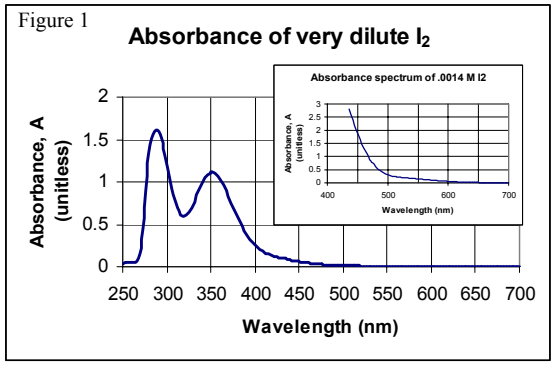
Maintaining Constant Conditions. Temperature is one condition which must be maintained as constant as possible during any given kinetics trial. Since reaction rates depend strongly on temperature, changing temperature during the course of a single kinetics trial would result in data that would be essentially impossible to analyze correctly.

How can the temperature of a reaction system be maintained constant? Though there are sophisticated methods available for accomplishing this, a simple way that will be used in this experiment is simply to keep the reaction system immersed in a "constant temperature bath" as much as possible during the course of a given trial. This can most simply be accomplished by having a large beaker of water in which the reaction vessel (a spectrophotometer cuvette in this case) can be kept between measurements. If the water bath is large enough, it will be able to absorb any energy produced by the reaction that would otherwise raise its temperature, thus keeping the temperature more or less constant. Periodic measurements of the temperature of the reaction system will provide evidence that the temperature was maintained essentially constant during a given trial.

Another reaction system condition that must be maintained constant for reactions involving ions, as in this experiment, is known as the *ionic strength* of the solution. This is a concept whose theoretical details are beyond the scope of general chemistry courses, but it can easily be achieved experimentally. It simply means that the abundance or concentration of ions must be more or less the same for the various kinetics trials that are performed in the experiment. For example, if one of the reactant ion concentrations is different in two different trials, as would be the case when applying the Method of Initial Rates, non-reactive ion solutions must be used to assure that the total ionic concentrations are about the same in the two trials.

Spectrophotometric Issues. Because one substance in the reaction (aqueous I_2) is colored, and all others are colorless, spectrophotometry can be used to follow the kinetics of the reaction. Unfortunately, the use of I_2 as the marker creates some problems. This molecule does absorb in the visible region (hence the color), but has no absorption peak where the Spectronic 20 instrument is sensitive. You should recall (Appendix I) that the absorption peak would be the best wavelength for the measurement. It does have absorption peaks in the ultraviolet, at wavelengths the instrument cannot detect (see Figure 1). Furthermore, those peaks are so strong that reliable spectroscopic data would require very dilute solutions (Appendix I), but that would make the kinetic runs very slow. Consequently, a compromise is required. We will record our results at 460 nm. While this is not optimum, due to its location on the side of a peak, it is about the lowest wavelength (and hence strongest signal and most sensitive detection) that does not result in unreliable absorbance or transmittance measurements for the concentrations used in the experiment (see Figure 1 inset).

Figure 1



PROCEDURE: Work in pairs. Some of the steps below may require information from the pre-lab exercises.

Part A. Solution and Equipment Preparation

1. Using the stock solution of KI and the appropriate glassware, use dilution to accurately prepare 25.00 mL of an aqueous KI solution having a concentration of approximately 0.350 M. Be sure to record the exact concentration of your solution. At the end of the day, store your solution in a clean, dry labeled container.

2. Starting from solid sodium persulfate, $Na_2S_2O_8$, prepare 25.00 mL of an aqueous solution that is about 0.00800 M $Na_2S_2O_8$. Be sure to record the exact concentration of your solution. At the end of the day, store your solution in a clean, dry labeled container.

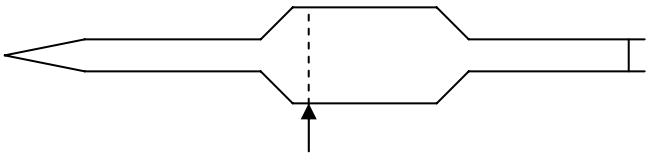
3. As described in the discussion section, a wavelength of 460 nm will be used to observe the formation of I_2(aq) over time. Prepare the Spectronic-20 instrument by setting the wavelength and filter appropriately. Using some of your KI solution as a "blank," calibrate the spectrophotometer at the 0% and 100% transmittance values. Save the "blank" so that you can periodically verify that the calibration is still valid.

4. Obtain about 10 mL of the calibration solution of iodine/iodide water (I_2(aq)/I^-(aq)). Record the exact I_2 concentration marked on the bottle. Rinse the cuvette with some of the solution, refill the cuvette and measure the percent transmittance or absorbance at 460 nm.

Part B. Determining the Average and Instantaneous Rates of a Reaction

1. Rinse a 5 mL pipet with your KI solution. Prepare a clean dry cuvette; acetone may be used to help dry the cuvette if necessary. Pipet 5.00 mL of the KI solution into the dry cuvette. Place this cuvette in a Styrofoam cup about 2/3 full of water (at room temperature) and measure the temperature of the solution in the cuvette until it stabilizes. Record the final stable value. *Carefully drain and dry off the thermometer whenever you remove it from the cuvette in order to maintain the concentrations and avoid contamination.*

2. Rinse the 1 mL pipet with your $Na_2S_2O_8$ solution. Use a marker to make a mark on your rinsed 1 mL pipet about ¼ of the way up the bulb of the implement, as suggested by the arrow in the figure below. (This is about where the glass of the bulb becomes straight.) When delivering solution from the pipet, about ½ will be added before the liquid reaches this line, and about ½ after. Although not a perfect method, this provides a convenient zero point to start the timing of your reactions.



For kinetics, timing matters! Read the next three steps in their entirety before performing step 3, so you will have a plan to follow!

3. Using your marked pipet, add 1.00 mL of the $Na_2S_2O_8$ solution to the reaction cuvette containing the KI solution, starting the time measurement as the liquid reaches the line you inscribed on it in Step 2. Quickly stopper the cuvette and shake/invert the tube two or three times. Remove the stopper and return the cuvette to the water bath. Keep the cuvette in the water bath except when making a measurement.

4. Every 30 or 45 seconds or so, dry off the outside of the cuvette and record a percent transmittance or absorbance reading and the time of the reading. <u>Knowing</u> the reaction time is much more important than maintaining specific intervals. Be sure to close the cover of the sample compartment during the measurement. Quickly return the cuvette to the bath after taking a reading.

5. Continue recording data for 12-15 minutes. About half way through the run, and at the end of the run, record the temperature of the solution while it is in the bath. If the temperature changes slightly during the course of the reaction, the "temperature" for the reaction is just the average of these periodic temperature measurements. While the reaction will not have gone to completion during the 15 minute run, this is long enough to determine kinetic parameters for the process.

Part C. Method of Initial Rates for Determining the Order of Reaction with respect to I^-

1. Note the volumes and concentrations of the KI and $Na_2S_2O_8$ reactants used in Part B. Determine a way to perform a second trial such that the initial $Na_2S_2O_8$ concentration <u>in the reaction cuvette</u> is the same as before, but the initial KI concentration <u>in the cuvette</u> is different. *Don't mix anything until step 3, after you develop a plan and discuss it with your instructor!* You may use either the 1-mL and 2-mL volumetric pipets or the graduated pipet as needed to alter the reaction mix from that used in Part B. Make up the "missing" volume with the 0.35 M NaF solution provided so that the total ionic concentrations are the same as the first trial. (This works because your KI and the stock NaF solutions have the same charges and concentrations.)

2. Make sure that your water bath is at the same temperature as that used in Part B. If the temperature of the water bath needs to be adjusted up or down, use either warm tap water or small amounts of ice, as necessary. Prepare a clean dry cuvette for the reaction; acetone may be used to help dry the cuvette if necessary. Prepare the Spectronic 20 spectrometer for use as before.

3. Using pre-rinsed pipets, add the volumes of KI and NaF solutions you just determined to the reaction cuvette. Place this in the water bath, and measure the temperature of the solution until it stabilizes; record that value. *Carefully drain and dry off the thermometer whenever you remove it from the cuvette in order to maintain the concentrations and avoid contamination.*

For kinetics, timing matters! Plan what you are going to do before performing step 4!

4. Add the appropriate amount of $Na_2S_2O_8$ solution (with proper timing) and mix properly to perform the kinetic trial, following the same general procedure as used in Part B. Follow the reaction for 12-15 minutes as before.

5. If directed by your instructor, repeat Part C, again changing the initial concentration of KI, while keeping the same initial concentration of $Na_2S_2O_8$, and making up the "missing" volume with 0.35 M NaF solution.

6. As directed by your instructor, perform the analysis described in the In-Lab Worksheet on p. 6.

Clean-Up.

1. All chemicals may be disposed of via the regular drains. Rinse with plenty of water.

2. Rinse your pipets and flasks with distilled water, especially those used for KI solutions.

Part D. Pseudo Rate Law Method for Determining the Order of Reaction with respect to $S_2O_8^{2-}$

You have already collected all of the data necessary to determine the order of the reaction with respect to $S_2O_8^{2-}$ by graphical means. If your instructor indicates that your data looks good, there is no need to repeat the run. If not, repeat the run of Part B.

Part E. Determining the Activation Energy for the Reaction

1. IF NECESSARY, prepare new solutions of 0.350 M KI and 0.00800 M $Na_2S_2O_8$, as done previously in Part A. (If you have ample stored solution, use that.) Recalibrate your spectrometer with KI solution as done in Part A. It is NOT necessary to repeat step 4 of Part A, as you already know ε for I_2.

2. Prepare a warm water temperature bath by obtaining warm tap water. Place the water in a well-insulated container consisting of two Styrofoam cups. This will help keep the temperature of the water bath fairly constant as time elapses. Make sure that the temperature is higher than that of the first trial (Part B) by at least 7°C or 8°C.

3. Perform a kinetics run exactly as done in Part B, except now using the higher temperature water bath. To ensure that the reaction starts at the higher temperature of the new bath, let the 5 mL of KI solution come to a stable temperature in the reaction cuvette before adding the $Na_2S_2O_8$ solution. Remember to start timing the reaction exactly as done in Part B, and record data with the same frequency and duration as in that Part. Also, be sure to make a few temperature measurements as done in Part B.

4. Rinse and dry your cuvette and prepare for another run. Use hot tap water to create an even higher temperature bath (7-8°C above the last), and repeat the kinetic run. It may be necessary to measure more often at these higher temperatures, as the reaction may speed up considerably.

Clean-Up.

1. All chemicals may be disposed of via the regular drains. Rinse with plenty of water.

2. Rinse your pipets and flasks with distilled water, especially those used for KI solutions.

Name _____ Section _____

IN-LAB WORKSHEET - DAY 1
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Complete these questions during or after lab on Day 1, as directed by your instructor.

Part A

1. Use your measured percent transmittance or absorbance of the $I_2(aq)/I^-(aq)$ calibration solution, and the known concentration of $I_2(aq)$ in the solution, to determine the molar absorptivity (ε) value for $I_2(aq)$ at 460 nm.

Part B

1. As directed by your instructor, use Beer's Law and your calculator or Excel to determine the concentration of $I_2(aq)$ at each point in the reaction of Part B. The table below is provided for your convenience. SHOW the calculations for the first point in the space below the table.

Time (___)	Abs or %T	$[I_{2(aq)}]$ (M)
0	--------	0

Time (___)	Abs or %T	$[I_{2(aq)}]$ (M)

Time (___)	Abs or %T	$[I_{2(aq)}]$ (M)

2. Calculate $\Delta[I_2]/\Delta t$, the <u>average rate</u> of formation of $I_2(aq)$ over the course of the reaction. SHOW your work.

3. Calculate $\Delta[I_2]/\Delta t$, the average rate of formation of $I_2(aq)$ over only the <u>first</u> 5 minutes of the reaction. Calculate $\Delta[I_2]/\Delta t$ over only the <u>last</u> 5 minutes of the reaction. How does the average rate change as the reaction proceeds?

4. As directed by your instructor, use your calculator, a hand graph or Excel to find the tangent to the data curve at time zero. (Methods for finding the tangent line can be found on p. 11.) The slope of this tangent line is the instantaneous rate of the Part B reaction at time zero (also called the initial rate). Write out the value for the initial rate, including units.

5. An approximate way of obtaining the initial rate is simply to calculate the change in concentration with time very early in the reaction. If the points are close together (in time) and very close to the start, this value approximates the slope of a tangent line at the center point. Use your data and calculate $\Delta[I_2]/\Delta t$ for the time period from zero up to three minutes. (If you had no readings at three minutes, use the next lower values.) How does this compare with the computed or graphed value from question 4?

Part C

1. As directed by your instructor, use Beer's Law and your calculator or Excel to determine the concentration of I_2(aq) at each point in the reaction of Part C. The table below is provided for your convenience.

Time (___)	Abs or %T	$[I_{2(aq)}]$ (M)

Time (___)	Abs or %T	$[I_{2(aq)}]$ (M)

Time (___)	Abs or %T	$[I_{2(aq)}]$ (M)

2. As directed by your instructor, use the approximation method or any of the graphical methods (calculator, Excel or hand graph) to find the initial rate of the Part C reaction. Write out the value for the initial rate, including units.

3. Fill in the table below, based on your data and analysis from Part B and Part C. If you did a second run of Part C, analyze that in a similar way.

Reaction	Initial $[S_2O_8^{2-}]$ (M)	Initial $[I^-]$ (M)	Initial Rate $\Delta[I_2]/\Delta t$ (M/___)
Part B			
Part C			

4. Based on your data, what is the order of the reaction with respect to iodide ion, I^-? Show and/or explain your reasoning.

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POST-DAY 1 EXERCISES
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Part D

1. Write out the molecular and net ionic equation for the reaction of KI(aq) with $Na_2S_2O_8$ (aq) which you observed.

2. According to the net ionic equation, how many moles of $S_2O_8^{2-}$ (aq) are consumed every time one mole of I_2 (aq) is formed? Since both species are in the same solution, with the same total solution volume (that remains constant), how will the concentrations (molarities) change as the reaction proceeds?

3. Use the information above and your data/analysis from Part B to complete the table for the initial (time = 0) values and your first 4 data points. This will help you establish the pattern of changes in concentrations.

Time (___)	**$[I_2]$ (M)**	**$[S_2O_8^{2-}]$ (M)**
0	0	

4. Using the patterns identified in questions 2 and 3 above, create an Excel spreadsheet to analyze your data from Part B. Use formulas in Excel (NOT a calculator!) to determine the $[S_2O_8^{2-}]$ at every time point measured. Use formulas in Excel (NOT a calculator!) to determine the quantities $\ln[S_2O_8^{2-}]$ and $1/[S_2O_8^{2-}]$ at every time point measured.

5. Use Excel to make plots of $[S_2O_8^{2-}]$ vs. time, $\ln[S_2O_8^{2-}]$ vs. time, and $1/[S_2O_8^{2-}]$ vs. time. Use the plots to determine the order of the reaction with respect to the $S_2O_8^{2-}$ reactant ion, and the pseudo rate law rate constant k' (see discussion associated with Eq. 2). Explain your reasoning.

6. You now know the order of the reaction with respect to I^- and the order with respect to $S_2O_8^{2-}$. Write out the complete rate law for the reaction.

7. Use the complete rate law, and your initial concentrations and initial rates for Parts B and C (tabulated in the Day 1 worksheet above) to calculate the value of the true rate constant k in each case. How 'constant' is the rate constant?

DATA ANALYSIS:

PART A. (If you completed the In-Lab Worksheet for Day 1 then you have already performed this analysis.)

1. Use the known concentration of the I_2 (aq) calibration solution and your measured absorbance or percent transmittance to determine the value of the molar absorptivity (ε) for I_2(aq) at 460 nm.

PART B. (If you completed the In-Lab Worksheet for Day 1 then you have already performed this analysis.)

1. Use Beer's Law and your measured absorbance or percent transmittance values to determine the concentration of the I_2 (aq) product formed at each time point in the reaction.

2. Calculate the average rate of formation of I_2, $\Delta[I_2]/\Delta t$ over the entire time of the reaction. Calculate the same quantity over the first 5 minutes of the reaction, and over the last 5 minutes of reaction. Compare these average rate values.

3. Use approximation methods, hand graphs, Excel, or your calculator to determine the instantaneous rate at time zero (the "initial rate") for the reaction measured in Part B.

PART C. (If you completed the In-Lab Worksheet for Day 1 then you have already performed this analysis.)

1. Use Beer's Law and your measured absorbance or percent transmittance values to determine the concentration of the I_2 (aq) product formed at each time point in the reaction.

2. Use approximation methods, hand graphs, Excel, or your calculator to determine the "initial rate" for the reaction measured in Part C.

3. Create a "Method of Initial Rates" table summarizing the initial concentrations of the I^- and $S_2O_8^{2-}$ reactants and the initial rates of reaction for the kinetic runs of Parts B and C. Use these to determine the order of the reaction with respect to I^- ion.

PART D. (If you completed the Post-Day 1 Exercises then you have already performed this analysis.)

1. Using the data from Part B, and the stoichiometry of the reaction, create an Excel spreadsheet which uses formulas to determine the $[S_2O_8^{2-}]$ at every time point measured. Use formulas in Excel (NOT a calculator!) to determine the quantities $\ln[S_2O_8^{2-}]$ and $1/[S_2O_8^{2-}]$ at every time point measured.

2. Use Excel to make plots of $[S_2O_8^{2-}]$ vs. time, $\ln[S_2O_8^{2-}]$ vs. time, and $1/[S_2O_8^{2-}]$ vs. time. Use the plots to determine the order of the reaction with respect to the $S_2O_8^{2-}$ reactant ion, and the pseudo rate law rate constant k' (see discussion associated with Eq. 2).

3. Write out the complete rate raw. Use the complete rate law, and your initial concentrations and initial rates for Parts B and C (tabulated in the Day 1 worksheet above) to calculate the value of the rate constant k in each case. How 'constant' is the rate constant?

PART E.

1. Make plots of $\ln[S_2O_8^{2-}]$ vs. time for the two (or more) high-temperature runs of Part E. Use the plots to determine the pseudo rate law rate constant k' at those temperatures. (Since the reactions were performed at different temperatures, these values should be different.)

2. Using the rate constants (k') from the room temperature reaction (Part B) and the two high temperature reactions (Part E), graphically determine the activation energy of the reaction.

QUESTIONS FOR CONSIDERATION:

1. Draw reasonable Lewis structures for the sulfate and persulfate ions, applying the formal charge concept as a guide to the best structure. For hints on persulfate, note that this ion splits apart into two SO_4^{2-} ions over the course of the reaction, and also that the prefix "per" frequently describes cases where O atoms are bonded to other O atoms, as in hydrogen peroxide.

2. For the trial of Part B, determine the initial and final concentrations of the iodide ion. Does this justify the assumption that the rate law depends only on the persulfate ion for this trial?

3. Based on the rate law determined from this experiment, what can be said about the overall mechanism for this reaction? What is the correct stoichiometry for the reactants in the rate-determining step?

4. Both reactants studied in this experiment are anions, and the reaction is relatively slow compared to most (many minutes required for complete reaction). The reaction between persulfate ion and Fe^{2+}, yielding sulfate and Fe^{3+} ions, is much faster, even though the reaction follows basically the same overall mechanism. How might the different types of ionic charges (anions and cations) result in a lower activation energy for this case?

5. For the second trial (Part C) performed in this experiment, what are the initial rates of <u>disappearance</u> of I^- and $S_2O_8^{2-}$, respectively?

6. Using the rate law and rate constant determined from your data, predict the % T of a solution made by mixing 4.0 mL of 0.25 M $Na_2S_2O_8$ and 1.0 mL of 0.0030 M KI, after 500 seconds have elapsed. Ignore any effects that might arise due to a different ionic strength (we wouldn't know how to deal with them anyway!).

7. The ΔH_f^o for persulfate ion and aqueous I_2 are not readily available in most thermodynamic tables, and so are given here: -1344.7 kJ/mol and +20.9 kJ/mol, respectively. What would have been the temperature rise for the mixture prepared in the first trial of this experiment? Assume no heat was lost from the solution, and assume that the heat capacity of the solution is the same as that for the same volume of pure water. What does this result indicate about the need for a water bath for maintaining a constant temperature during the course of the trial?

METHODS FOR FINDING A TANGENT TO A CURVE TO DETERMINE THE INSTANTANEOUS RATE

1. Manual

a) Make a plot of Concentration vs. Time. Draw a smooth line through the points.

b) Place a mark where you want to draw the tangent line.

c) Hold a small mirror at the marked point, with the reflective surface perpendicular to the paper. Pivot the mirror around the point, watching how the curve on the paper, and the mirror image of the curve, line up. When the curve and its mirror image appear continuous, the edge of the mirror is perpendicular to the curve at that point. Draw a line along the edge of the mirror.

d) Remove the mirror. Use a ruler or square to draw a line perpendicular to the mirror edge line just inscibed. This line will be tangent to the curve at the original spot.

e) Find the slope of the tangent line to determine the instantaneous rate.

2. Using the TI *Voyage 200* Calculator

a) Given the magnitudes of the values involved, it is a good idea to use the **MODE** button to set the **Display Digits** to **Float 9**, or to set the **Exponential Format** to **Scientific**.

b) Open the **Data/Matrix Editor**. Enter the time data in column **c1** and the concentration data in column **c2**.

c) Press **F5 Calc**. Change the **Calculation Type** to **A:Quart Req** (i.e., fit the data to a 4th-order polynomial). Set the **x** data cells to **c1** and **y** data cells to **c2**. Select **Store RegEQ** to **y1(x)** (or other empty variable.) Hit **Enter.** The fitting equation will be displayed. It is NOT necessary to record this equation if you stored the RegEQ as instructed. Hit **Enter** again.

d) Press **F2 Plot Setup**. Press **F1 Define**. Set **x** as **c1** and **y** as **c2**, as before. Hit **Enter**.

e) Press **◊-GRAPH**. The display will show your data, with the fitted polynomial overlaid. If you cannot see the plot, press **F2 Zoom** and **9:ZoomData** to adjust scales to fit the data.

f) With the graph showing, press **F5 Math**. Select **A:Tangent**. A crosshair will appear on the plot, and the display will read **Tangent at?**. Use the cursor keys to move the crosshair to the point where you want to draw a tangent. Press **Enter**.

g) The calculator will compute and draw the tangent line, and show the equation for that line. Record the equation of the tangent line and use it to determine the instantaneous rate.

3. Using Excel

a) Open a new Excel spreadsheet. Enter time and concentration data.

b) Create a **Chart** with time values on the x axis and concentration values on the y-axis.

c) Open the **Chart** and **Select** the **First Series** (your data). Righ-click and select **Add Trendline**. Select the **Polynomial** function and change the **order** to 4. On the **Options** tab, select **Display Equation** and **Display R^2** value on the chart. Click **OK**. When the equation is displayed, carefully write down the equation. Make sure that the numeric format for the trendline equation is Scientific, with at least two decimal points showing.

d) Create two new columns in the spreadsheet; label one x and the other y. In the first cell of the x column, enter the x (time) value where you want to determine the tangent. In the second cell of the x column, enter another time value only slightly larger than the first. (E.g., for intial rates, your first x value would be zero, and the second might be 0.1 minutes.)

e) In the first cell of the y column, enter the 4th order polynomial equation fit to your data. For the x values, refer to the cell with the first x value just created. (E.g., if the trendline equation were y = 3.67E-15x4 - 3.48E-12x3 - 1.15E-09x2 + 2.87E-06x - 5.29E-06, and your first x value was in cell C100, then you should go to the cell D100 and enter the equation: = 3.67E-15*C100^4 - 3.48E-12*C100^3 - 1.15E-09*C100^2 + 2.87E-06*C100 - 5.29E-06.)

f) Copy the equation from the cell just defined to the second cell in the y column.

g) **Select** the **Chart**. Right-Click to select **Source Data**, choose the **Series** tab and **Add** a second series. Select the x and y values of series2 as the two columns just defined with the polynomial equation. Press **OK**.

h) Select **Chart** from the menu, and **Add Trendline**. Select the **Linear** trendline and, in the **Based on Series...** box, choose **Series2**. Choose the **Options** tab and choose to **display the equation** and **R^2** values on the chart. In the **Forecast** box, choose **Forward ____ units**. Set the number of units to be the same as the maximum x value in your data. (This will mostly prevent the chart from changing scales.) Hit **OK**.

i) Excel will draw the tangent line and show the equation. Be sure to set the numeric format for the equation as above, to give at least two significant figures. Use the slope of the line to determine the instantaneous rate.

Name _____ Section _____
Date _____

PRE-LAB QUESTIONS
Experiment 13G

Complete these questions prior to attending lab. Some of the results will be useful in conducting the experiment, so you should record those results in the appropriate section of the lab as well.

1. In Part A, step 1, you are directed to use dilution to prepare 25.00 mL of an aqueous KI solution having a concentration of approximately 0.350 M, starting from a stock solution of approximately 0.875 M KI. What two SPECIFIC pieces of volumetric glassware (list amounts or sizes) will you need to perform this step? Note that your solution concentrations will need to be accurate to <u>at least</u> three significant figures.

2. In Part A, step 2, you are directed to prepare 25.00 mL of an aqueous solution that is about 0.00800 M $Na_2S_2O_8$, starting from the solid sodium persulfate. What mass of the solid will you need? What type of balance and vessel will you use to ensure an accurate mass and volume, and thus accurate concentration?

3. As presented in the discussion, this experiment involves the reaction between aqueous solutions of potassium iodide (KI) and sodium persulfate ($Na_2S_2O_8$). The products of the reaction are aqueous molecular iodine (I_2), aqueous sodium sulfate, and aqueous potassium sulfate. Write out the reaction in both molecular form and net ionic form. (Be sure to include states of matter, to help you identify what is going on!) You will need the correct net ionic reaction to perform several steps in the Data Analysis of Part D.

molecular

net ionic

5. Analysis of Parts B and C data involves determining the rate of the reaction. If the concentration of the I_2 <u>product</u> (initially zero) is 0.000514 M after 205 seconds of reaction, what is the average rate of appearance of iodine, $\Delta[I_2]/\Delta t$?

4. You will use graphical methods to analyze your Part B data to determine the order of the reaction with respect to the persulfate ion, $S_2O_8^{2-}$. Use your textbook (Sec. 13.3) and sketch the plots that would be expected if the reaction shows the following behaviors. Be sure to label the axes!

zero order in $S_2O_8^{2-}$

first order in $S_2O_8^{2-}$

second order in $S_2O_8^{2-}$