EXPERIMENT 2

Reaction Order

Introduction

How a reaction progresses over time is an indication of its reaction order. In the rate laws, $(Rate = k[A]^m[B]^n)$, found in the first experiment, you calculated the reaction order with respect to each of the reactants, (variables m and n), using the method of initial rates. This allowed you to predict how much the rate would increase when the initial concentrations of the reactants were changed. While these rate laws provided a means for predictably changing the rate of a reaction so that you could determine when a reaction would finish, no information could be gained about how the reaction was progressing. Questions such as "how much of my reactant is left after 5 minutes?" or "when will the reaction be finished?" could not be answered using the rate law alone. To find an answer to these questions, or any questions that relate time to the reactant concentration, a better understanding of the reaction orders is needed.

Reaction order

In experiment 1, we determined that reaction order with respect to all reactants can be determined experimentally by the method of initial rates. In this experiment we will find the reaction order graphically by plotting the decrease in reactant concentration over time and use it to write a new rate law, called the integrated rate law that can be used to better define our reaction in terms of time. The 3 most commonly studied reaction orders are referred to as zero order reactions, first order reactions and second order reactions.

For simplification when graphing to find the order of a reactant, we look only at one reactant at a time. Unlike the rate equation, where we had $A+B \rightarrow$ products, when finding the integrated rate law, the concentration of B is held constant so that you are only looking at a reaction that changes as a result of a single reactant, A. Therefore, the chemical equation effectively becomes $A \rightarrow$ products. To find the integrated rate law with respect to B, you would need to perform a separate set of experiments where B \rightarrow products and A is held constant.

Zero order reactions

Zero order reactions describe reactions where a reactant decreases at a steady rate regardless of the concentration. One example of a zero order reaction would be a reactant that breaks apart at a steady rate until there is no more reactant left at all in the reaction. It doesn't break up any faster due to higher concentrations. Combustion reactions are zero order reactions. It doesn't matter how much fuel you have, once you have reached a constant temperature, the fuel burns at a predictable rate. An increase in the amount of fuel initially will raise the intercept on the y-axis, but does not change the slope of the line which corresponds to the rate of the reaction. The rate of the burning would be constant regardless of how much fuel was present at any particular time. The first graph below is the result of the amount of fuel used versus time. The second graph demonstrates that when the initial amount of fuel is increased the rate of the reaction (slope) does not change. It is a constant that equals -0.02gallons/min for either graph.



The rate of the reaction is based on the linear equation y = mx + b which can be found by finding the slope of the line from the graph. "b" is the intercept on the y axis corresponding to your initial amount of reactant. The variables from the graphs are as follows:

y is the amount of your reactant at a particular time during the reaction x is a specific time during the reaction m is the slope of the line which is the rate of reaction (for combustion example = Δ fuel/ Δ time) b is the y intercept that correlates to the initial amount of a reactant

The correlation coefficient (R^2) shown below each graph gives an indication of how closely the line fits the data. In general, a correlation coefficient of .99 or greater is necessary to be confident that the equation for the line is correct.

First order reactions

First order reactions are extremely common. These are reactions where the reaction rate is fast at the beginning of the reaction and slows down as the reaction progresses. Unlike a zero order reaction that gives you a straight line when plotting reactant concentration vs. time, you will get a curve for a first order reaction. The rate is continually decreasing over time, thus the mathematical equation for this curved line is more complicated than plotting the concentration/time data directly. However, if the natural log (In) of the reactant concentration is plotted vs. time, you will now have a straight line which allows you to easily relate reaction time to reactant concentration. Radioactive decay is one example of a first order reaction.



Second order reactions

Like first order reactions, second order reactions start out quickly and then slow down as the reaction progresses. The relationship between time and concentration for a second order reaction becomes linear when the reciprocal of the concentration (1/conc.) is plotted vs. time. Also note that the linear plot in second order reactions results in a line with a positive slope which will be reflected in the integrated rate laws described in the next section.



Determining reaction order

Once you have recorded experimental data for the decrease of a reactant over time, make the following 3 plots. First, plot concentration vs. time directly (zero order) then In[A] vs. time (first order) and finally, 1/[A] vs time (second order). The graph with the line with the highest correlation coefficient, R^2 , is the one that best describes the reaction order with respect to the reactant that was plotted.

Integrated Rate Laws

Once you have determined the order of your reaction, you can use the equation for that line to determine further information about your reaction. These equations are called <u>integrated rate laws</u> and are based on the chemical reaction: $A \rightarrow$ Products. By convention, the following variables are substituted for the variables found in the equation of a line, y = mx + b when generating the integrated rate laws.

Old Variable	Definition	New Variable
у	concentration of reactant	[A] or ln[A] or 1/[A]
m	slope =rate constant of reaction	k
Х	time	t
b	y-intercept=initial amount of A	$[A_0]$ or $In[A_0]$ or $1/[A_0]$

The resulting linear equations are as follows:

Order of reaction	Rate law equation	Integrated rate law	
Zero order:	Rate = k	$[A] = -kt + [A_0]$	
First order:	Rate = $k[A]$	$\ln[A] = -kt + \ln[A_0]$	Rearrange: $ln([A]/[A_0]) = -kt$
Second order:	Rate = $k[A]^2$	$1/[A] = kt + 1/[A_0]$	

The integrated rate law is based on a single reactant going to products. The concentration of all other reactants must be held constant. For example, if you have a reaction $A + B \rightarrow$ products, and both were found to be first order and the rate constant = 0.5, your rate equation would look like the following:

Rate = 0.5[A][B]

If [B] was always 1M, then your rate would be based on the concentration of A only.

Rate = $0.5[A] \times [1] = 0.5[A]$ k = .5

However, [B] was increased to 4M for a second reaction, but still held constant throughout the experiment, the effect of [B] can be incorporated as part of the rate constant.

Rate = $0.5[A] \times [4] = 2[A]$ k = 2

Therefore, if the concentration of [B] is changed, the change will be reflected in the rate constant, k.

One point to note, [B] naturally decreases by reacting with A so you must make sure that [B] is much greater than that of [A] when setting up the reaction. To minimize this effect and keep [B] relatively unchanged, we must always use an excess of [B] so that the amount of B used up in the reaction with A is minimal relative to the total amount of B.

Reaction of Crystal Violet with Sodium Hydroxide

The Reaction

In your experiment, you will be reacting a purple solution of crystal violet with sodium hydroxide. The sodium hydroxide acts as a bleaching agent by gradually lightening the purple color of the solution. The chemical equation associated with this reaction is given below.



Crystal Violet (purple) \rightarrow Product (colorless)

Colorimetric Analysis

While the bleaching effect of the hydroxide on the crystal violet is visible to the naked eye, it is impossible to get a precise measurement of just how much crystal violet has been converted to product at any particular time during the experiment. A method is needed that will allow you to monitor this color change in such a way that the gradual bleaching of color can be recorded with numerical values. One way to do this is by using an instrument called a colorimeter that measures the absorbance of light by a sample and gives a numerical reading that correlates to the sample's concentration. A colorimeter works by shining a known amount of light through a sample and measuring how much light comes out through the other side. The "absorbance" is a measurement of the amount of light that does not come out, but rather is absorbed by the sample. This is analogous to shining a light through a glass of water versus a glass of grape juice. The grape juice, being darker, will absorb more light, thus the amount of light coming out the other side of the glass is less than that seen through a glass of water.

A colorimeter assigns numerical values that correspond to the amount of light that is absorbed by a solution. These <u>absorbance</u> values can be correlated to the concentration of the solution. A colorless solution will allow light to go through uninhibited and therefore the value of the absorbance will be very small. As the concentration of a colored solution increases, it gets darker and absorbs more light. The absorbance values will increase at a linear rate as the concentration of the solution increases. In the crystal violet experiment, you will use the colorimeter to monitor the decrease in absorbance over time which correlates to the decrease in the concentration of the purple crystal violet in your solution as it is converted to colorless product.

Graphically determining the Order of a Reactant

Once you have started your reaction, you will record the absorbance of the solution every minute. At the end of the experiment, your raw data will consist of a series of times and absorbance readings. After converting the absorbance to concentration, you will then determine the order of the reaction with respect to the crystal violet by making 3 plots. The first will be a graph of time versus concentration. The second is time versus the natural logarithm of the concentration and the third is a plot of time versus the inverse of the concentration (1/concentration). The plot that has the correlation coefficient (R^2) closest to 1 will be the one that tells you the reaction order with respect to crystal violet.

Determining the Rate Equation (Review Experiment 1)

You will monitor the bleaching of the crystal violet with 2 different concentrations of sodium hydroxide. This will allow you to use the method of initial rates covered in experiment 1 to determine the order of reaction for the sodium hydroxide, calculate the rate constant of the overall reaction and finally write the rate equation associated with the reaction.

Determining the Integrated Rate Law for a Reaction

One restriction to the integrated rate law for the crystal violet/sodium hydroxide reaction is that the integrated rate law written applies only when a designated concentration of sodium hydroxide is use. Thus, the new rate constant will incorporate the effect of a constant concentration of an additional reactant. This accounts for the difference in the values of the rate constants observed when plotting the graphs from the time/concentration studies for different concentrations of sodium hydroxide.

In your lab, you will be doing the experiment using 2 different concentrations of sodium hydroxide to determine how the change in concentration affects the rate constant of the crystal violet/sodium hydroxide reaction. After determining the order of reaction for the crystal violet from one of the graphs, you will use the equation for a line defined by your data to find the intercept and the slope in the equation for your integrated rate law. You will find the integrated rate laws for both concentrations of sodium hydroxide and observe how the rate constant varies as a result of the change in hydroxide concentration. Your discussion questions will require you to use the rate laws you calculated to predict the results of hypothetical experiments.

Laboratory Equipment Procedures

Chemical Hazards

Crystal Violet Solution

NFPA RATING: HEALTH: 2 FLAMMABILITY: 0 REACTIVITY: 0

DERMAL EXPOSURE: Wash off with soap and plenty of water. Stains clothing and skin. **EYE EXPOSURE:** Flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Contact your TA immediately.

Sodium Hydroxide Solutions

NFPA RATING: HEALTH: 0 FLAMMABILITY: 0 REACTIVITY: 1

ORAL EXPOSURE

Caustic. If swallowed, wash out mouth with water provided person is conscious. Do not induce vomiting. Contact your TA immediately.

DERMAL ÉXPOSURE

Caustic. In case of extensive skin contact, flush with copious amounts of water for at least 15 minutes. Remove contaminated clothing and shoes. Contact your TA immediately.

EYE EXPOSURE

Caustic. In case of contact with eyes, flush with copious amounts of water for at least 15 minutes. Assure adequate flushing by separating the eyelids with fingers. Contact your TA immediately.

Equipment Procedures

Using the MeasureNet System for Colorimetry

The colorimeter should already be connected to the MeasureNet system at the start of lab. Follow the instructions below to set up for absorbance measurements.

Colorimeter Calibration

- 1. Fill a wash bottle with distilled water.
- 2. Use the wash bottle to fill 2 cuvettes with distilled water.
- a. Remember to avoid touching the sides of the cuvette near the midpoint.
- 3. Dry the sides of the cuvettes with a kimwipe.
- 4. Gently place the 2 cuvettes containing the water in the reference and sample cell holders in the colorimeter. See your TA if they will not go in easily, DO NOT FORCE THEM INTO THE HOLDER.
- 5. Close the lid of the colorimeter
- 6. Press the following keys on the workstation to start the kinetics program.
 - a. Press **ON/OFF** on the workstation.
 - b. Press MAIN MENU.
 - c. Press F6- Colorimetry/Fluor./Trb./Lum.
 - d. Press F1-Colorimetry.
 - e. Press **F2**-Green LED (wavelength = 515 nm)
 - f. Press F1- Kinetics
 - g. Press **ENTER** to calibrate your zero point on the Y axis (absorbance)
- 7. Wait until green light shows on colorimeter and you hear a beep acknowledging that the calibration is complete.
 - Set your X and Y graphing limits by using the following sequence:
 - a. Press **SETUP** to enter your X and Y graphing limits.
 - b. Press F1-Set limits for new acquisition.
 - c. Enter \rightarrow twice to move down to the X max limits.
 - d. Enter "1800" for the X max limits to 30 minutes.
 - e. Press ENTER to accept the new value.
 - f. Press **DISPLAY** to accept the new value for the new settings.
- 9. Press START/STOP to enter the Kinetics program.
- 10. Remove the sample cuvette (S) and dump the water into the sink. Do not remove the reference cuvette.
- 11. Dry the inside of the sample cuvette with a kimwipe before proceeding to the next section.

Sample Analysis

- 1. You will always be using the sample cuvette (S) when measuring any absorbance.
- 2. Make sure the cover is completely closed before recording absorbance values.
- 3. Remember to avoid touching the sides of the cuvette near the midpoint.
- 4. If making a series of absorbance values, you do not need to press any further buttons on the workstation, just insert the cuvette and record the values.

Laboratory Procedures

Part 1: Absorbance of Initial Solution

- 1. Calibrate the colorimeter according to the Equipment Procedure.
- 2. Record the concentration of the crystal violet in your laboratory notebook.
- 3. Dispense 2 mL of distilled water into a 10 mL graduated cylinder.
- 4. Pour the water into the sample cuvette.
- 5. Dispense 2 mL of 1 x 10^{-5} M of crystal violet into a second 10 mL graduated cylinder.
- 6. Carefully pour the crystal violet solution into the same sample cuvette
- 7. Cap the cuvette, invert to mix the contents and wipe the sides with a kimwipe.
- 8. Place the cuvette in the sample holder (S) and close the cover on the colorimeter.
- 9. Record the absorbance in your laboratory notebook.
- 10. Remove the sample cuvette and dump the contents into a 100 mL waste beaker.
- 11. Rinse the cuvette with distilled water and dry the inside of the cuvette with a kimwipe before proceeding.
- 12. Dispose of solution in a 50 mL waste beaker.

Part 2: Monitoring the Reaction of Crystal Violet and Sodium Hydroxide

- 1. Record the concentration of the 2 NaOH solutions in your laboratory notebook.
- 2. Dispense 2.00 mL of 1.0×10^{-5} M of crystal violet to a 10 mL graduated cylinder.
- 3. Transfer the solution to your sample cuvette.
- 4. Dispense 2.00 mL of 0.010M NaOH into a second graduated cylinder.
- 5. Pour the sodium hydroxide into the sample cuvette.
- 6. Immediately press **START/STOP** on the MeasureNet station.
- 7. Cap the cuvette, mix quickly by inverting the cuvette and wipe the sides with a kimwipe.
- 8. Place the cuvette in the sample holder (S) and close the cover on the colorimeter.
- 9. Press **START/STOP** to start the data acquisition.
- 10. Record the absorbance after 30 seconds and at 60 seconds in your laboratory notebook.
- 11. Note: If you miss the 30 second mark, immediately record the time and absorbance as soon as possible.
- 12. Continue recording the absorbance at one minute intervals until you reach 1800 seconds.
- 13. Remove the sample cuvette and dump the contents into the waste beaker.
- 14. Dry the inside of the cuvette with a kimwipe before proceeding.
- 15. Repeat previous steps of Part 2 using the 0.020M NaOH.
- 16. Be careful to fully rinse out both cuvettes with water before returning them to your drawer.
- 17. Dispose of waste solution in waste container in the hood when finished.

Laboratory Data

Create tables for the following data in your lab notebook before coming to class. Record the data shown in your laboratory notebook during the lab in pen. Include the **signed** white copy of this table when you turn in your lab report. Include the correct number of significant figures for each measurement.

Concentration of stock solution of crystal violet	M
Concentration of stock solution of sodium hydroxide	M
Abs of diluted crystal violet (abs of time 0)	

You will need separate tables that each go up to 1800sec for each NaOH solution.

	0.010M NaOH			0.020M NaOH	
Time		Absorbance	Time		Absorbance
	_sec			sec	

Laboratory Results

Graphs

Include a table of these results for each time/abs pair in your lab report for each experiment. The tables must be typed but can be taken directly from the Excel spreadsheet.

()					
Time(s)	Time (min)	absorbance	concentration	In concentration	1/concentration

Include the 6 graphs created from these data. There should be 3 graphs from each concentration of NaOH used.

Calculated Results

Remember to show one example of each calculation either handwritten or typed on a separate sheet. Data determined from Excel, such as the correlation coefficient or the slope, is considered part of the graph and does not need to be hand calculated.

Include a typed copy of this table with your lab report.	0.010M NaOH	0.020M NaOH
Plot that gives the best straight line Order of reaction with respect to crystal violet:		
Diluted concentration of sodium hydroxide Diluted concentration of crystal violet	M	M
Absorbance per molar concentration		abs/M
Rate of disappearance of crystal violet: Order of reaction with respect to sodium hydroxide:		
Average rate constant, k: Overall rate law equation:		
Equation for each line:		

Calculations: Excel

Using Excel for Data Analysis

Microsoft Excel is a program that allows you to perform mathematical manipulations and graphs easily and professionally. It is widely used in academia as well in most industries, thus it is a valuable skill to learn. You will be expected to use Excel to generate data tables and graphs and include them as part of your lab reports. Contact your TA or a TA in the help office if you have questions on using Excel.

For this experiment, you will need to enter all of your data into Excel and then create 6 different plots for your lab report. If you do not have a personal copy of Excel, the computers in the library computer lab do have Excel and are available for your use. These instructions are written for Excel 2003, but are applicable to other versions. Some of the most basic features will be described here, but the more you use the program, the more features you will discover and the easier the program is to use. If you currently use Open Office, you are welcome to use the spreadsheet associated with that free software, but be aware that the TAs may not be familiar with this program.

Entering time and absorbance data

- 1. Open the Excel program and click on cell 1A.
- 2. Label cell 1A "Time (sec)". Use "enter" to move to the next cell. (2A)
- 3. Enter 0 in cell 2A . Hit enter to move to cell 3A.
- 4. Enter all the times that you recorded for your time data starting in cell 3A.
- 5. Click on cell 1B and label the cell "Absorbance". Hit "enter" to move to next cell.
- 6. Enter the absorbance recorded for the diluted concentration of crystal violet. Hit enter to move to cell 3B.
- 7. Enter the all the absorbance values that you recorded for your absorbance data starting in cell 3B.

Converting time in seconds to time in minutes

- 1. Click on cell 1C and label cell "Time (min)".
- 2. Hit "Enter" to move to the next cell (2C).
- 3. Enter "=A2/60" to convert the time in seconds to time in minutes. Do not hit Enter!
- 4. To copy this formula into the remaining cells, click on cell C2 and move cursor to lower right hand corner until a + sign appears. **Do not hit Enter!**
- 5. Click and hold the + sign and drag down the column until the last cell containing the data from the last time value is reached.
- 6. Release the cursor and the remaining cells will have the copied formula that calculates the remaining data.

Note: Do a reality check to make sure that you end up with 30 minutes if your last value is 1800 seconds.

Converting absorbance to concentration

- 1. Click on cell 1D and label cell "Concentration (M)
- 2. Hit "Enter" to move to the next cell (D2).
- 3. Calculate the diluted concentration of crystal violet and the absorbance per molar concentration in the calculations section. (abs/M). Use the abs/M value as the conversion factor for converting all the absorbance values to concentration in the following manner.
- 4. Enter "= b2/(abs/M value)" into cell D2. Do not hit Enter!
- 5. To copy this formula into the remaining cells, click on cell D2 and move cursor to lower right hand corner until a + sign is appears. **Do not hit Enter!**
- 6. Click and hold the + sign and drag down the column until the last cell containing the data from the last time value is reached.
- 7. Release the cursor and the remaining cells contain the copied formula that converts absorbance to concentration.

Note: your values should be in the e⁻⁶ range if you used absorbance values greater than 1.

Generating logarithmic and invers functions

- 1. Click on cell E1 and label cell E1 "In([CV])".
- 2. Hit Enter to move to the next cell (E2).
- 3. Enter "=LN(D2)" to generate the natural logarithm of the concentration recorded in cell D2.
- 4. Copy this formula into the remaining cells as you did with the time data.
- 5. Click on cell F1. Enter "1/[CV]" as a label.
- 6. Hit Enter to move to the next cell (F2).
- 7. Type "=1/(D2)" to generate the inverse of the concentration recorded in cell D2.
- 8. Copy this formula into the remaining cells as you did with the time data.

You have now generated a table that starts out similar to the one below. Your table should have at least 1800 seconds as the last time value. If in the future you want to use other formulas, look for the Σ sign on the toolbar at the top of the page. Click on the down arrow to bring up commonly used functions. Click on the one you want to use. If the function you need is not listed, click on the "More Functions" tab at the bottom of the box to bring up a list of additional functions.

: 2	<u>File E</u> dit	⊻iew <u>I</u> nsert	F <u>o</u> rmat <u>T</u> o	ols <u>D</u> ata <u>W</u> indow	Help	\cap			
1	💕 📙 🔮) 🛃 🛕 🎁	🍄 🛍 X	(🗈 🛍 - 🛷 K) = (21 =	😫 (Σ)- 👌	🖡 🕺 🛍	46 100%	- 🕜 📮
Ari	Arial • 10 • B I U = = = = 🔤 \$ % , 🐝 🚧 🗄 • 🖄 • 🗛 •								
	19	▼ <i>f</i> _x							
	A	В	C	D	E	F	G	Н	
1	Time (sec)	Absorbance	Time (min)	Concentration (M)	Ln([CV]	1[CV]			
2	0	469	0	0.000075	-11.8006	133333.3			
3	30	454	0.5	7.26013E-06	-11.8331	137738.6			
4	60	439	1	7.02026E-06	-11.8667	142445			
5	120	399	2	6.3806E-06	-11.9622	156725.1			

Graphing Data in Excel

- 1. Highlight the data for your first graph by clicking on cell C1 and dragging across to cell D1 and down to the end of your data table. When you release the cursor, your data should show up with a darker background.
- Click on the chart wizard icon shown below. This will bring up a box with instructions to generate different types of graphs. Alternatively, you can click on Insert at the top of the toolbar to bring up a pull-down menu containing a "chart" option. Click on chart to bring up the same box shown below.

:	Eile Edit	<u>V</u> iew <u>I</u> nsert	Format <u>T</u> o	ols <u>D</u> ata <u>W</u> indow	Help		Type a question for help 🗸 🗕 🗗		
10) 💕 🖬 🔒	🛃 🛕 🎁	ABÇ 🔣 👌	6 🗈 🖺 • 🛷 🗉	7 - (24 - 1	😫 Σ 🗕 🤶	t X↓ III 45 100% - @ -		
A	rial	• 10 •	BIU		\$ % ,	+.0 .00	崔 律 I II · ③ · A ·]		
1	 ✓ fx Time (min) 								
	A	В	C	D	E	F	Chart Wizard - Step 1 of 4 - Chart Type		
1	Time (sec)	Absorbance	Time (min)	Concentration (M)	Ln([CV]	1[CV]			
2	0	469	0	0.0000075	-11.8006	133333.3	Standard Types Custom Types		
3	30	454	0.5	7.26013E-06	-11.8331	137738.6	Chartering Charterin Lings		
4	60	439	1	7.02026E-06	-11.8667	142445			
5	120	399	2	6.3806E-06	-11.9622	156725.1			
6	180	367	3	5.86887E-06	-12.0458	170390.6			
7	240	339	4	5.42111E-06	-12.1252	184464.1			
8	300	314	5	5.02132E-06	-12.2018	199150.7			
9	360	291	6	4.65352E-06	-12.2779	214891.2			
10	420	269	7	4.30171E-06	-12.3565	232465.9			
11	480	250	8	3.99787E-06	-12.4297	250133.3			
12	540	231	9	3.694U3E-U6	-12.5088	2/0/07.1	Radar IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII		
13	600	215	10	3.4381/E-U6	-12.5806	290852.7	Surface		
14	660	198	11	3.16631E-06	-12.6629	315824.9			
15	720	184	12	2.94243E-06	-12.7363	339855.1			
15	780	170	13	2.71855E-06	-12.8154	36/843.1	Scatter. Compares pairs of values.		
10	040	100	14	2.52005E-00	10.0000	395700.0 400040.5			
10	900	140	10	2.334/5E-06	12.9070	420310.5			
19	960	130	10	2.17404E-00	12 1200	400003.9	Divoce and Hold to View Sample		
20	1020	124	12	1.90294E-00	13,1309	504301.1 534472.9	Press and Hold to vew Sample		
21	1140	108	10	1 72708E 06	13,7691	570012.3			
22	1740	100	20	1.63113E.06	13 3363	613071.0	Cancel < Back Next > Einish		
23	1200	102	20	1.03113E-00	-13.3202	013071.5			

- 3. Click on XY (Scatter) to generate a plot using the data in column C as your x-axis and the data in column D as your y-axis. Click Next>
- 4. Select subtype "Scatter". This only shows the data points, not a line. Click Next>.
- 5. Your data range will show up in the next box, Click Next> again.
- 6. The next data box allows you to enter titles for the graph and x and y axes. Enter appropriate titles and click Next>.
- 7. Click Next> to move the next box.
- 8. Click Finish to accept your graph.



Note: To make additional graphs with data that is not in adjacent columns, click on cell C1 and select the time data as done before. Now, instead of dragging to the next column, hold down the Ctrl key and then click on cell E1 and drag down to select the logarithmic data. You should then have 2 columns highlighted. This is the data that will be plotted. The first column will be your time data that will be plotted on the x-axis and the second column selected is the y-axis data. Follow the instructions above to generate the graph associated with a first order reaction. Repeat these instructions for the final graph which will be 1/A vs. time.

Data Analysis in Excel

To determine the linearity of a graph, you need to find the correlation coefficient, R², and the equation for the line. Use the following instructions to add a trendline and these statistics to your graph.

- 1. Click on a data point , right click to open up a selection box and select "Add Trendline".
- 2. A selection of options for adding trendlines will arise. Make sure the box labeled "linear" is selected and then click on the Options tab.
- 3. Select "Display Options" on Chart
- 4. Click on box in front of "Display R² Value on Chart and "Display Equation on Chart" to put arrows in the selection boxes.
- 5. Click OK.
- 6. Your graph will now have these statistics on the graph.



Formatting Graphs in Excel

You will need to format your graph to make it easier to read. Use the following instructions to change the graph as needed.

Text boxes

All 3 titles and the legend box act as text boxes and can also be directly edited as a text box. The box within the graph containing the statistics also can be manipulated as a text box. Right clicking on "clear" will remove the box.

Axes

You can format the axes by clicking on the axis and right clicking to bring up the format axis box. There are several tabs that allow you to change the scale on the axis and edit the font, alignment and several other attributes associated with the axes.

Other graph features

The legend box to the right of the graph, the gridlines and the plot area can all be edited by clicking on them and then right clicking to bring up a text box with different options. Clicking Clear will remove the legend box, gridlines and the color of the plot area.

Size and shape of graph

Clicking in an open area of the graph treats the graph as an object and allows you to stretch it or shrink it horizontally or vertically to achieve the look you desire.

Importing graph into other programs

Click on the graph so that small black boxes show up on the outer borders of the graph. Right click to bring up a dropdown menu of options. Click "copy" to copy the graph and then "paste" into other document. If you prefer to print each graph separately, when the black boxes are showing on the graph, it is all set to print out as a full-size page.

Calculations: May be hand written unless designated otherwise

Diluted concentration of reactants

Since you used equal amounts of both sodium hydroxide and crystal violet, you must divide the original concentrations of each reactant by 2 to account for dilution when mixing the two solutions together.

Absorbance per molar concentration of crystal violet.

The absorbance is linearly related to the concentration of crystal violet. Divide the absorbance of the diluted crystal violet by the concentration of the crystal violet to get the absorbance units/Molar unit. Make the assumption that a solution with no crystal violet has no absorbance. This value will be the same for both concentrations of NaOH, as the absorbance of NaOH is essentially zero.

Abs/M = (abs of diluted CV solution -0abs)/([diluted CV]- 0)

Converting Absorbance to Concentration

Enter each of your absorbance values into Excel and then create a new column for the concentration values by dividing each value by the Abs/M value you calculated in the previous step.

Creating data table for graphed data

Determine the natural logarithm of concentration (In concentration) and the reciprocal of the concentration (1/concentration) for each recorded concentration. This should be done in Excel and not handwritten.

Plotting a zero order reaction

Plot time in seconds on the X-axis and concentration on the Y axis in Excel. Your times should go from 0 to 30 minutes.

Plotting a first order reaction

Plot time on the X-axis and In(concentration) on the Y axis in Excel.

Plotting a second order reaction

Plot time on the X-axis and 1/concentration on the Y axis in Excel.

Determining the order of the reaction with respect to crystal violet

The graph that gives the highest correlation coefficient, R² is the one that is considered to be the best representation of the order of the reaction.

This is the graph that corresponds to the order of the reaction with respect to crystal violet.

The order of reaction with respect to the crystal violet should be the same for both experiments.

Rate of disappearance of crystal violet (\(\Delta\)conc/\(\Delta\)time)

The equation for the line is in the form of y=mx+b. The slope is m. This corresponds to the change in concentration over time. You will have a different rate (slope) for each concentration of sodium hydroxide used. Record the slope from the graph that you used to find the order of reaction of crystal violet for each concentration of NaOH.

Determining the order of the reaction with respect to sodium hydroxide

Use the initial rates method covered in experiment 1 and the rate law equation: Rate = $k[CV]^{m}[OH]^{n}$ to find the order of the reaction with respect to sodium hydroxide. Remember, you already have the order of reaction with respect to the crystal violet from your graphs. The rates used in the equation are the two calculated rates of disappearance of crystal violet.

Determining the rate constant for the rate law equation

You now have all of the variables except k in the rate law equation above. Rearrange the rate law equation to solve for k using both concentrations of sodium hydroxide. The rate constants should be relatively close. Average the two numbers to get a final value.

Determining the overall rate law equation

The general rate equation is $Rate = k[CV]^{m}[OH]^{n}$. Fill in the orders of each reactant average rate constant found above into this equation. You now have an equation that allows you to monitor the rate of reaction for any combination of crystal violet and sodium hydroxide concentrations.

Determining the integrated rate Laws for experiments 1 and 2

Use the table below to find the integrated rate law that corresponds to the order of reaction with respect to the crystal violet.

Order of reaction	Rate equation	Integrated rate law	
Zero order:	Rate = k	$[CV] = -kt + [CV_0]$	
First order:	Rate = $k[CV]$	$\ln[CV] = -kt + \ln[CV_0]$	Rearrange: $ln([CV]/[CV_0]) = -kt$
Second order:	Rate = $k[CV]^2$	$1/[A] = kt + 1/[A_0]$	

Record the equations for a line from each of the graphs that you used to determine the order of reaction with respect to crystal violet.

Writing the integrated rate laws for experiments 1 and 2

Use the table below to make the correct substitutions to convert the equation for a line that you used to find the order of reaction for crystal violet into the integrated rate law for each experiment. Note that the two integrated rate laws be different because the rate of disappearance of crystal violet varies due to the concentration of the sodium hydroxide.

Old Variable	Definition	New Variable
У	concentration of reactant (M)	[CV] or In[CV] or 1/[CV]
m	slope =rate constant of reaction	k (not same k as found in initial rates)
Х	time in minutes	t
b	y-intercept=initial amount of CV (M)) $[CV_0]$ or $ln[CV_0]$ or $1/[CV_0]$

Discussion Questions

You must use your data to answer these questions. If the answer you give does not reflect YOUR data and results, you will receive no credit for the question.

- 1) Write the rate law equation that you developed for the crystal violet/sodium hydroxide reaction. Based on this experimentally determined rate law equation, calculate the reaction rate if you doubled the initial concentration of crystal violet. Show all work. (This problem may be hand written)
- 2) Give two specific sources of error in your experiment. Explain the impact of these errors on generating the order of the reaction with respect to the crystal violet. Explain how they could be minimized in the future. (If you use the phrase "human error" in your experiment, you lose all credit!)
- 3) Write the two integrated rate law equations for your two experiments. Explain why there are differences between these two equations. What restrictions were required for you to generate the integrated rate law equations?
- Calculate the concentration of crystal violet in the solution after 5.0 minutes using your integrated rate law equation when the concentration of sodium hydroxide is 0.01M and again at 0.02M. Show all work. (This problem may be handwritten)
- 5) Give 1 example each explaining how knowing the rate law equation and the integrated rate law can help you to modify a reaction.