

This is an example report of an investigation performed in General Chemistry lab. Pay attention to format and content, not on the results or the experiment itself. The report is best explored on screen or printed in color since editor comments are in red. The names have been withheld to protect the authors. This would be considered a very good report and a quality to aspire to in the General Chemistry I lab.

Determination of the Rate Law for Food Dye Bleaching with Hypochlorite

Author 1 Name, Author 2 Name, Author 3 Name
General Chemistry II Lab, Wednesday 6-9 p.m.

Note the title, authors, and affiliation. If this were a manuscript for publication the affiliation would be where the authors work or study.

Abstract

Normally, the abstract would go here but since the abstracts are handwritten, they can be stapled to the back.

Introduction (1) As a courtesy to the grader, identify the author number of this section for this week.

Common household liquid bleach is often a solution of sodium or calcium hypochlorite. Being a powerful oxidizing agent, the hypochlorite ion can decompose many organic substances. In this experiment, bleach will be used to decompose the FC&C blue dye #1, commonly found in blue-colored beverages and snacks.

Double-spacing (or 1.5 spacing) is better – it's easier for a reader.

We are exploring the relationship between the time it takes to completely – or nearly so – bleach the dye and the concentration of the bleach necessary to do so. There are several factors that affect the rate of a reaction, including concentration of reactants, surface area of a reactant in a heterogeneous reaction, temperature, pressure (if a reactant is a gas), and the presence of a catalyst. In this report, we present the chemical conditions necessary to achieve nearly complete decomposition of the dye in about 15 minutes.

We also present the rate law for the reaction



Notice that the equation is numbered so that it can be referenced in the text if necessary despite not having knowledge of the stoichiometry nor the products of the reaction. The general form of the rate law for the reaction can be written

$$\text{Rate} = k[\text{dye}]^x[\text{ClO}^-]^y \quad (2)$$

Since x and y are not directly related to the stoichiometry of the reaction the correct reaction stoichiometry doesn't need to be known. The values of x and y are the orders of the reaction in the respective reactant and k is the rate constant for the reaction.

Reaction progress is monitored spectroscopically using the Spectronic-20 spectrophotometer. The reaction orders can be obtained by the method of initial rates or by linearizing the concentration vs. time plot with the integrated rate law of the appropriate order (zeroth, first, or second order). The reaction will be forced into pseudo-order conditions by using a huge excess of hypochlorite and a limiting amount of dye. In this way, the $[\text{ClO}^-]$ will remain essentially unchanged over the course of the reaction and the experimentally-determined rate constant, k'

(also called the *apparent rate constant*), will be a composite of the actual rate constant, k , and the $[\text{ClO}^-]$:

$$k' = k[\text{ClO}^-]^y \quad (3)$$

In one experiment, the $[\text{dye}]$ vs time will be monitored at a fixed and known $[\text{ClO}^-]$. The curve will be linearized by plotting $\ln[\text{dye}]$ vs time and $[\text{dye}]^{-1}$ vs time and selecting the most linear plot to assign the reaction order in dye. The slope of the line is the apparent rate constant, k' . By changing the concentration of the hypochlorite and keeping the dye concentration constant, the experiment can be run again. A new k' will be measured and from the differences in the former and latter apparent rate constants and the $[\text{ClO}^-]$, the reaction order in hypochlorite, y , will be determined as well as the actual rate constant, k , for the reaction.

Experimental (3)

This experimental could be improved by having subheadings since there are 3 distinctly different parts to the experiment. Subheadings are shown in green italics

All spectroscopic measurements were performed with a Spectronic-20 spectrophotometer (Bausch & Lomb) set at 630 nm. Cylindrical cuvettes with a nominal pathlength of 1 cm were used for solutions to be analyzed. Deionized water was used for the 100%T reference on the spectrophotometer. The zero and 100%T were checked frequently during the experiment.

A stock solution of FD&C Blue #1 with a concentration of 4.72×10^{-6} M (*note that 1.89E-6 would be unacceptable*) was prepared in advance and available on the shelf in the laboratory. Undiluted commercial bleach (Chlorox) was provided in the laboratory. The concentration of hypochlorite reported for the bleach was 0.69 M.

Preparation of the Beer's Law Calibration Plot

Three 25 mL calibration solutions of FD&C Blue #1 were prepared from dilutions of the stock dye solution. A 10 mL aliquot of the stock dye solution was dispensed from a burette into a 25 mL volumetric flask and diluted to the mark with water to give a 1.89×10^{-6} M solution of dye. A 15 mL aliquot of the stock dye solution was transferred into the second and 20 mL into the third 25 mL volumetric flask and diluted to the mark to give 2.83×10^{-6} M and 3.78×10^{-6} M dye solutions, respectively. The stock dye solution was used undiluted as the fourth calibration solution. The percentage transmittance of each calibration solution was measured once. The percentage transmittances were converted to absorbance with the equation

$$A = -\log(\%T) \quad (4)$$

The calibration data are summarized in Table 1. A Beer's law calibration plot was prepared by plotting absorbance vs. concentration (Figure 1) yielding a best-fit equation of the line of $A = 1.220 \times 10^5 \text{M}^{-1}c + 0.00161$.

Notice that Table 1 has a descriptive caption, the exponential data are presented in the customary format and the displayed precision is correct. It is possible that the precision used to prepare the Beer's law plot was higher but the displayed precision is correct for the context of the table.

It is unusual to present both a table of data and the plot of the same data but it's ok here. Also notice that the authors were very selective about what data to show and did not include every single scrap of data; only the data necessary for the reader to reproduce the calibration are shown.

Table 1. Calibration data for the concentrations of FD&C Blue #1 ([dye]) and the respective absorbances at 630 nm.

[dye] (M)	Absorbance (630 nm)
1.89×10^{-6}	0.2343
2.83×10^{-6}	0.3468
3.78×10^{-6}	0.4559
4.72×10^{-6}	0.5817

The units are included in the table headers. This is important.

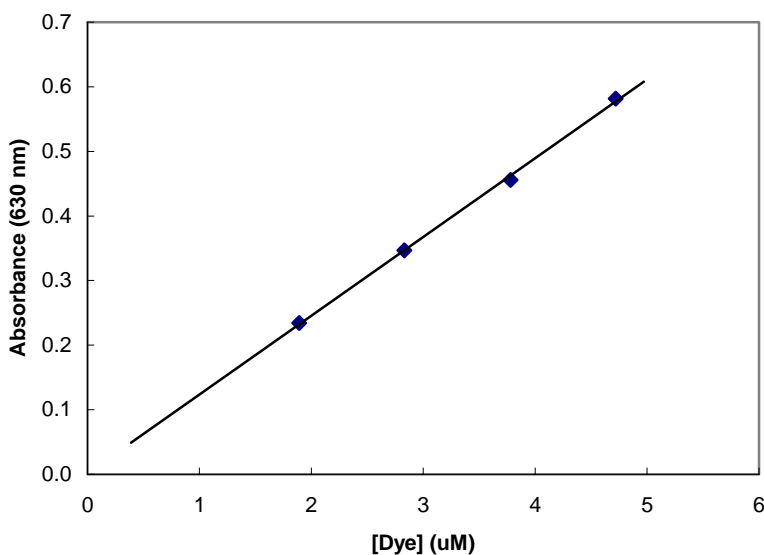


Figure 1. Beer's law plot of absorbance vs. [dye] (μM) for the calibration data shown in Table 1. The line is the least-squares fit of the data.

The authors performed a transformation of the concentrations to micromolar so that the plot looked prettier. This is acceptable. This is a nice looking graph since the axes are labeled, the line is about 45° and fills the panel, the data points are adequately sized, and there is no "connect-the-dots" of the data points. In this case the authors could have included the 0,0 point in their least-squares fit but elected not to do so.

Empirical Determination of Optimum Experimental Conditions

In order to determine the concentrations of dye and hypochlorite necessary to give a bleaching time of about 15 minutes, different volumes of undiluted bleach were mixed with 25 mL of stock dye solution and timed for the complete disappearance (at least by visual determination). The results are summarized in Table 2. By including this information, the person reading this can see the logic of using the concentrations which will be used later in the experiment.

Table 2. Determination of the amounts of FD&C Blue #1 and bleach to give a particular time of bleaching

Trial	Volume dye (mL)	Volume Bleach (mL)	[dye] ^a (M)	[ClO ⁻] ^a (M)	Time ^b (min)
1	25	2	4.37×10^{-6}	0.051	4
2	25	1	4.54×10^{-6}	0.027	6
3	25	0.7	4.59×10^{-6}	0.019	10
4	25	0.5	4.62×10^{-6}	0.014	13

^a Concentration after dilution from the mixing of the dye and bleach solutions

^b Time to complete disappearance of color

Trial 4 was sufficiently close to the desired 15 minutes for an individual experiment that we elected to use those conditions. We found that accurately measuring 0.5 mL from the burette difficult so we carefully prepared a 50:50 mixture of bleach with water resulting in a [ClO⁻] of 0.35 M and used that solution for all subsequent experiments.

Acquisition of Kinetic Plots

The spectrophotometer was prepared for acquiring the kinetic data by checking the zero and 100%T then placing an empty cuvette in the sample holder. A 25 mL volume of dye was dispensed from a volumetric pipette into a small beaker. In one step, 1.00 mL of the diluted bleach was added to the beaker from a burette, the beaker swirled, the timer started, and two squirts of the solution from a pasteur pipette placed in the cuvette. The diluted concentrations of the dye and the hypochlorite were 4.54×10^{-6} M and 0.0133 M, respectively. (←This sentence construction is considered awkward and should be avoided when possible.) The percentage transmittance was recorded as soon as possible after the transfer and the time recorded. This procedure necessarily meant that the absorbance at time zero was not obtained. The percentage transmittances were recorded every 30 seconds until the percentage transmittance changed by no more than 0.1 %T over 1 minute. Each percentage transmittance was converted to absorbance with equation 4. The kinetic run was performed only once. The data are summarized in Table 3. A single run may not have been a good idea but time may have been short. Credit may or may not be lost for not performing replicates.

A second kinetic run was performed with the [ClO⁻] one-half of the first run. A new 25 mL aliquot of the dye was placed in a small beaker. From a burette containing only water, 0.5 mL of water was dispensed into the beaker. The [ClO⁻] in this kinetic run was 0.00665 M. Using the identical procedure as before, the kinetic data were obtained and are summarized in Table 4. This method to get one-half [ClO⁻] is pretty clever but other ways could have been used. The authors already said that accurately dispensing 0.5 mL then used that volume.

Data and Results (3)

Here's where the important data and results can be found

Table 3 shows the results of the kinetic run with the highest concentration of hypochlorite. The absorbances were converted to concentration using the best-fit equation from the Beer's law plot.

Table 3. Kinetic data for the decomposition of 4.54×10^{-6} M FD&C Blue #1 with 0.0133 M ClO^- .

Time (min)	Absorbance (630 nm)	[dye] (M)
0.5	0.4792	3.92×10^{-6}
1.0	0.4171	3.41×10^{-6}
1.5	0.3632	2.96×10^{-6}
2.0	0.3162	2.58×10^{-6}
2.5	0.2752	2.24×10^{-6}
3.0	0.2396	1.95×10^{-6}
3.5	0.286	1.70×10^{-6}
4.0	0.1816	1.48×10^{-6}
4.5	0.1581	1.28×10^{-6}
5.0	0.1376	1.12×10^{-6}
5.5	0.1198	9.69×10^{-7}
6.0	0.1043	8.42×10^{-7}
6.5	0.098	7.31×10^{-7}
7.0	0.0791	6.35×10^{-7}
7.5	0.688	5.51×10^{-7}
8.0	0.0599	4.78×10^{-7}
8.5	0.0522	4.15×10^{-7}
9.0	0.0454	3.59×10^{-7}
9.5	0.0395	3.11×10^{-7}
10.0	0.0344	2.69×10^{-7}
10.5	0.03	2.33×10^{-7}
11.0	0.0261	2.01×10^{-7}
11.5	0.0227	1.73×10^{-7}
12.0	0.0198	1.49×10^{-7}
12.5	0.0172	1.28×10^{-7}
13.0	0.015	1.10×10^{-7}
13.5	0.013	9.38×10^{-8}
14.0	0.0114	7.99×10^{-8}
14.5	0.0099	6.79×10^{-8}
15.0	0.086	5.74×10^{-8}

The absorbances in the table are reported with inconsistent precision. This should have been noticed and corrected before submitting the report. There is a font face change in the table. This should be avoided.

With a concentration of dye nearly 4 orders of magnitude smaller than the $[\text{ClO}^-]$ (it's not immediately obvious but the author of this section is using a different convention for the ClO^- ion – this author is using ClO^-), the concentration of hypochlorite remains essentially unchanged during the run. Thus, the rate law (eq 2) can be simplified to

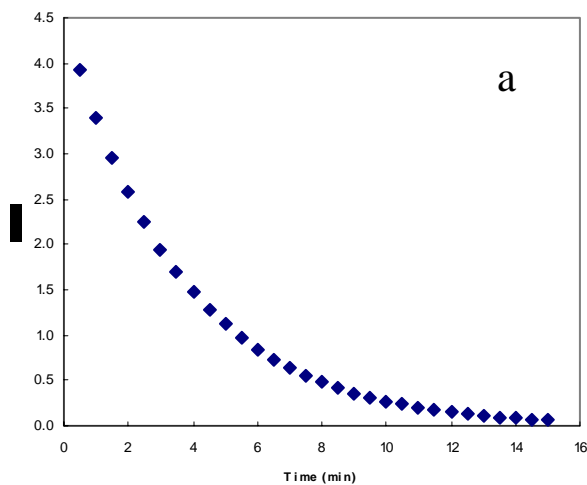
$$\text{Rate} = k'[\text{dye}] \quad (5)$$

The result of this simplification is that the rate law can be determined graphically using the well-characterized integrated rate laws. If a plot of concentration vs. time is linear then the reaction is zeroth order in dye. A linear plot of $\ln[\text{dye}]$ vs. time indicates first-order kinetics and a straight line plot of $[\text{dye}]^{-1}$ vs. time indicates second-order kinetics in dye.

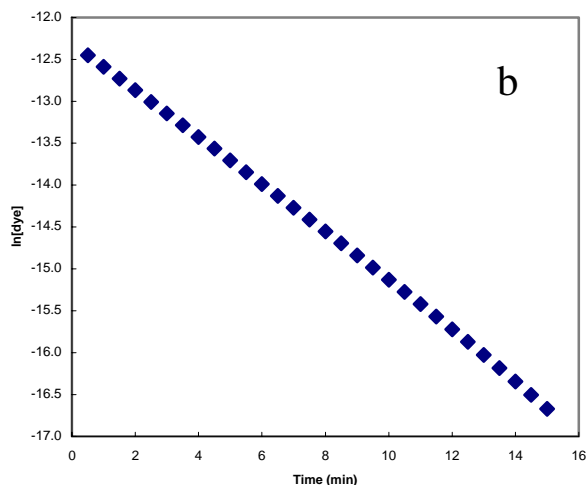
The concentration vs. time data were plotted as shown in Figure 2a. Since the plot is nonlinear, it is clear that the kinetics are not zeroth-order in dye. Figure 2b is a plot of the data transformed to $\ln[\text{dye}]$ and Figure 2c is a plot of the data as $[\text{dye}]^{-1}$ vs time.

Look carefully.
Something is missing from the axis label.

(it's the unit of measure)



There was a data transformation in 2a that is not explained (each concentration has been multiplied by 10^6). This is an acceptable transformation but unacceptable omission.



The plots were simply pasted in from Excel and the labels were added with text boxes overlaid on the graphs.

While the graphs are well-done, the axis fonts are a bit too small and should be resized before importing

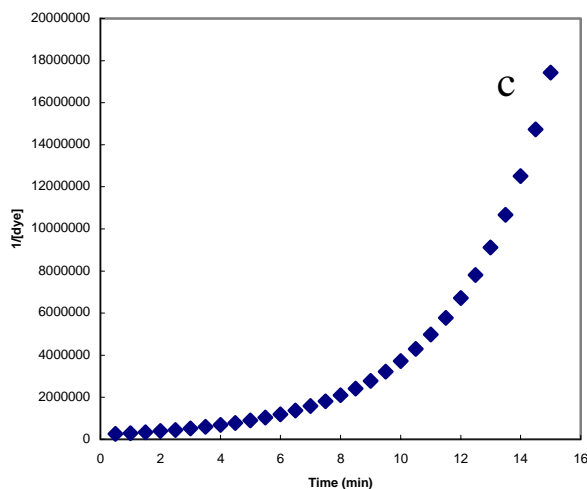


Figure 2. Plots of the kinetic data from Table 3 treated as (a) 0th, (b) 1st, and (c) 2nd order.

It is clear from the plots in Figure 2 that the reaction is first-order in dye. The reaction, therefore, obeys the integrated rate law

$$\ln[\text{dye}]_t = \ln[\text{dye}]_o - k't \quad (6)$$

where $[\text{dye}]_o$ is the initial concentration of the dye, $[\text{dye}]_t$ is the concentration of dye at each time interval, and k' is the apparent rate constant and can be calculated from the slope of the line. The apparent rate constant obtained from Figure 2b is 0.277 min^{-1} .

Knowing that the reaction is first order in dye makes it possible and, in fact, easy to determine the order of the reaction in hypochlorite. The data of the second kinetic run with a $[\text{ClO}^-]$ 0.00655 M (notice that this has been erroneously copied from the experimental or lab notebook. The correct value is 0.00665 M) are shown in Table 4. Since we know from the first experiment that the reaction is first order in dye it is not necessary to prepare any graph except the $\ln[\text{dye}]$ vs time plot (Figure 3).

Table 3. Kinetic data for the decomposition of 4.54×10^{-6} M FD&C Blue #1 with 0.00665 M ClO^- .

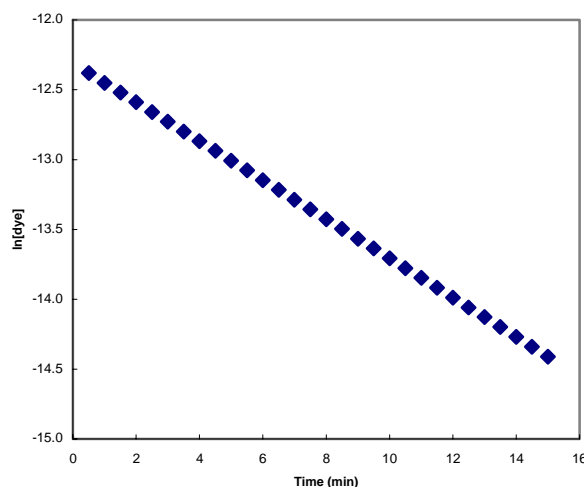
Time (min)	Absorbance (630 nm)	[dye] (M)
0.5	0.5135	4.20×10^{-6}
1.0	0.4792	3.92×10^{-6}
1.5	0.4471	3.65×10^{-6}
2.0	0.4171	3.41×10^{-6}
2.5	0.3892	3.18×10^{-6}
3.0	0.3632	2.96×10^{-6}
3.5	0.3388	2.77×10^{-6}
4.0	0.3162	2.58×10^{-6}
4.5	0.2950	2.41×10^{-6}
5.0	0.2752	2.24×10^{-6}
5.5	0.2568	2.09×10^{-6}
6.0	0.2396	1.95×10^{-6}
6.5	0.2236	1.82×10^{-6}
7.0	0.2086	1.70×10^{-6}
7.5	0.1946	1.58×10^{-6}
8.0	0.1816	1.48×10^{-6}
8.5	0.1694	1.38×10^{-6}
9.0	0.1581	1.28×10^{-6}
9.5	0.1475	1.20×10^{-6}
10.0	0.1376	1.12×10^{-6}
10.5	0.1284	1.04×10^{-6}
11.0	0.1198	9.69×10^{-7}
11.5	0.1118	9.04×10^{-7}
12.0	0.1043	8.42×10^{-7}
12.5	0.0973	7.85×10^{-7}
13.0	0.0908	7.31×10^{-7}
13.5	0.0847	6.82×10^{-7}
14.0	0.0791	6.35×10^{-7}
14.5	0.0738	5.92×10^{-7}
15.0	0.0688	5.51×10^{-7}

got the concentration correct in the caption.

Precision is consistent. Much better table.

Still has a font face change.

The slope of the linearized kinetic plot (Figure 3) is 0.139 min^{-1} which is the apparent rate constant for the reaction when the reactant in large excess is one-half the original concentration.



There is no least-squares fit line on these data. Since the slope of the graph is used to calculate k' , the fit line should be shown. The equation of the line and correlation coefficient are optional.

Figure 3. Plot of the kinetic data from Table 4 treated as 1st order kinetics.

The apparent and actual rate constants are related by eq 3. If we ratio the apparent rate constants and $[\text{ClO}^-]$ (missing right bracket) values for the two experiments, *i.e.*,

$$\frac{k_1'}{k_2'} = \frac{k [\text{ClO}^-]_1^y}{k [\text{ClO}^-]_2^y} \quad (7)$$

it is possible to determine the value of y , the order of the reaction in ClO^- . The ratio of apparent rate constants for the two experiments is 1.99 while the ratio of the ClO^- is 2.0. Thus, the value of y is 1 and the order of the reaction in ClO^- is first order. The reaction is second-order overall.

Finally, the actual second-order rate constant is calculated from eq 3 as $k = 20.9 \text{ M}^{-1}\text{min}^{-1}$. The complete rate law is

$$\text{Rate} = 20.9 \text{ M}^{-1}\text{min}^{-1}[\text{dye}][\text{ClO}^-] \quad (8)$$

Discussion (2)

Even without knowing the correct stoichiometry of the reaction, it is possible to determine the rate law for this reaction. However, we are unconvinced that our results, or in fact anyone's, are accurate. A comparison of our rate constant to other investigators' in the same laboratory showed results ranging from a lowest of $20.9 \text{ M}^{-1}\text{min}^{-1}$ to $658 \text{ M}^{-1}\text{min}^{-1}$. The highest value we attribute to a concentration calculation error but, even ignoring this highest value, the average of three investigation groups gives a rate constant of $51 \text{ M}^{-1}\text{min}^{-1}$. Had replicate trials been performed by the authors, we could comment more directly on the reliability of our data.

We suggest that the differences in reaction rates (thus, the rate constants) observed by different investigators may be, in part, due to differences in the origins of the bleach and the age of the bleach. The hypochlorite concentration was estimated¹ from the percentage concentration on the bottle label. Based on our experience with consumer labeling, the accuracy of the label is suspect². Although difficult to measure quickly, knowing the actual concentration of the hypochlorite in the bleach used would certainly improve the accuracy of the determination.

Despite our concerns of reproducibility between investigators, what is notable is the quality of the data obtained. The linearity of the $\ln[\text{dye}]$ vs. time plots both have correlation coefficients of 0.9997. This level of linearity is unusual³ but not unheard of.

The reaction conditions used in this experiment are known as *pseudo-first-order* conditions.⁴ In pseudo-first-order conditions, also known as flooding, one reactant's concentration is held constant by making it very large in concentration. Forcing a reaction into pseudo-first-order conditions greatly simplifies the analysis of the data. An attempt to integrate eq 2 (where x and y both equaled 1) to give an integrated rate law similar to that with which we are familiar was difficult. According to reference 4, it is not recommended to analyze "mixed-second-order" reactions without first resorting to pseudo-first-order conditions.

Conclusion (1)

The reaction of FD&C Blue #1 with hypochlorite is a second order reaction with a measured rate constant of $20.9 \text{ M}^{-1}\text{min}^{-1}$. The scenario presented was that undiluted bleach in the wash water must decolorize the dye from a consumer ice-pop in 15 minutes or less. We are unable to accurately comment on whether the requirements of the scenario have been met since the ratio of the volumes of bleach added to the wash water and the amount of water in the washing machine ultimately determine the rate of reaction. However, the rate of the reaction was so fast that the concentrations of both the dye and bleach had to be kept low to get a reaction to last a full 15 minutes.

References

¹ Malia Rose, personal communication.

² Author A, Author B. *Titrations of Acids and Bases* General Chemistry I, 2006.

³ David Green, personal communication.

⁴ Espenson, J.H. *Chemical Kinetics and Reaction Mechanisms* McGraw Hill, 1981.