Activation Energy in Chemical Kinetics

Objective

The objective of this at-home experiment is to demonstrate how the rate of a chemical reaction is temperature dependent. The reaction of blue food dye with sodium hypochlorite as represented by the following reaction equation:

Blue dye (aq) + NaOCI $(aq) \rightarrow$ Colourless Products (aq)

will be carried out at various temperatures in order to evaluate its activation energy.

Introduction

Based on the *collision model*, a reaction occurs when there is enough energy in the collision between the reactant molecules to disrupt the bonds. At any particular temperature, reactant molecules will move through space with a certain amount of kinetic energy. When reactant molecules collide, the energy is then changed to potential energy. If the potential energy exceeds the energy of the bonds in the reactant molecules, the bonds can break and allow for the atoms to rearrange into new product molecules.

The point at which rearrangement occurs is known as the *activated complex*, or *transition state*. It can be described as the potential energy 'hill' or barrier. For a reaction to occur, the energy associated with the collision must equal or exceed the potential energy of the system at the top of the 'hill'. This energy is referred to as the activation energy, E_a, which represents the minimal or threshold energy of the reaction.

A reaction also requires the reactant molecules to be in the correct orientation such that the new bonds for the products can form. By taking the two requirements of the collision model into account, the rate constant can be represented by the following equation, which is also known as the *Arrhenius equation*:

$$k = Ae^{-Ea/RT}$$
(1)

where

The frequency factor (A) is related to the frequency of collisions with effective orientations between the reactant molecules. Whereas the exponential factor ($e^{-Ea/RT}$) represents the fraction of collisions with energy Ea or greater at temperature T. The equation can also be expressed as

$$\ln k = -\frac{E_a}{R} \left(\frac{1}{T}\right) + \ln A$$
⁽²⁾

which is a linear equation. By examining the temperature dependence of the rate constant for a chemical reaction, the activation energy can be determined.

In this experiment, the rate of the reaction of NaOCI (sodium hypochlorite), from bleach, with the pigment in blue food colouring is studied at various temperatures. The reaction can be represented as follows:

Blue dye
$$(aq)$$
 + NaOCI $(aq) \rightarrow$ Colourless Products (aq) (3)

where the reaction obeys a second-order bimolecular rate law

$$R = k[Blue dye][NaOCI]$$
(4)

As seen in the at-home chemistry experiment called 'The Rate Law in Chemical Kinetics Using Blue Food Dye', the rate constant, *k*, can be calculated using the following equation:

$$k_{obs} = k[\text{NaOCI}] \tag{5}$$

where k_{obs} is obtained from the slope of the integrated rate law plot.

Once again, the smartphone will be used as a spectrophotometer to monitor the reaction progress over time by measuring the absorbance of the red light. Additionally, due to the limitations of the at-home experiment, the absorbance values will be assumed to be the concentration values of the absorbing species in mol/L (M), and as such, this experiment can give only an approximated rate constant.

Based on equation (2), a plot of ln k vs T^{-1} will yield a straight line. The activation energy can then be extracted from the slope.

Materials

- Water
- Bleach (must have concentration of sodium hypochlorite indicated)**
- Blue food dye*
- ¹/₂ cup Measuring cup (125 mL)
- Teaspoon (5 mL)
- Thermometer
- Metal spoon

- Red construction paper
- Standard size (~10 oz) colourless drinking glass used *only for chemistry experiments*.
- Smartphone
- Glass or ceramic plate
- Timer
- Stand for smartphone (can be a taller drinking glass, preferably colourless)

* Can be from a 'Club House' pack of regular colours, do not use the neon colour set. ** Not all household bleach shows the concentration NaOCI on the label. However, some do specify the concentration and it may be in the fine print. See figure 1 below for an example. The bottle should also not be older than **6 months** from the time it was first opened. Older bottles will no longer have the same concentration of NaOCI due to decomposition.

WARNING				
Bleach Bleach must be handled carefully. It may irritate eyes and skin. Dangerous fumes form when mixed with other products.	CORROSIVE			
Do not mix with acid products or household ammonia, rust remover or toilet bowl cleaner. Do not get in eyes. Do not get on skin or clothing. Do not breathe fumes. Keep out of reach of children. In case of spillage, wash your working area and hands immediately. Do not leave bleach unattended.				
Wear your <i>lab coat</i> and <i>lab glasses</i> for this experiment.				

Procedure

The procedure will be similar to what was done in the 'The Rate Law in Chemical Kinetics Using Blue Food Dye' experiment with the exception of using only one concentration of the NaOCI throughout the experiment, and varying the temperature of the water used in the reaction.

Part A – Reaction at Room Temperature (Run 1)

1. Record the brand name of your bleach and the concentration of the NaOCI onto the data sheet. See figure 1 as an example.



Figure 1: Choose a bleach that indicates the concentration of sodium hypochlorite (NaOCl)I on the label

2. Place the standard size drinking glass that is colourless in the middle of the red construction paper (make sure you somehow mark this glass so you know it is used *only for chemistry experiments and not for drinking!*). Draw a circle around the reaction glass, as well as a mark on the glass in line with a mark on the construction paper (figures 2 and 3). This will allow you to always put the reaction glass in the same position in order to keep the pathlength of the red light readings consistent.



Markings on reaction glass AND construction paper

Figure 2: Mark the construction paper and glass, and trace out a circle on the red construction paper, to align the glass in the same position for each absorbance reading.



Figure 3: Materials needed for the experiment. Identify the glass that is intended just for the experiment. A taller drinking glass can be used to elevate the smartphone.

3. Set up your timer, smartphone and a stand to hold your smartphone as seen in Figure 4. Make sure the bottom of the reaction glass is centered in the camera view.



Bottom of glass should be centered in the camera view

Figure 4: Positioning of the smartphone camera centered over the glass

4. Take the reaction glass off the red construction paper. Add ½ cup (125 mL) of room temperature water and *1 teaspoon* of bleach (5 mL) into the reaction glass. Stir with a metal spoon to mix the solution. Place the spoon on a glass or ceramic plate. Be careful not to spill the reaction mixture as the bleach can damage clothing, irritate your skin, and damage surfaces.

If the concentration of NaOCI in your bleach is greater than 5%, you will need to use a more dilute mixture for your reaction solution. In a separate container (something that pours well and is *marked for chemistry use only*), add 1 cup (250 mL) of room temperature water and **1 teaspoon** of bleach. Stir with a metal spoon to mix the solution. Place the spoon on a glass or ceramic plate. Be careful not to spill the reaction mixture as the bleach can damage clothing, irritate your skin, and damage surfaces. Transfer ½ cup (125 mL) of the diluted bleach solution into the reaction glass. Then proceed with the steps below.

- 5. Measure the temperature of the solution with the thermometer and record it on your data sheet. Rinse the thermometer and place it aside.
- 6. Make sure the reaction glass is dry, then place it back on the construction paper on the circle, with the marking on the glass in line with the marking on the construction paper. The reaction glass should be centered in the camera view. If not, make adjustments by moving the smartphone and/or stand.
- 7. Ensure there are **no shadows** casted onto the glass during the entire time of the experiment, and the reaction is not directly in any sunlight.
- 8. Open the 'Color Name' app on your smartphone. Alternatively, you can use any other app that detects color and is able to give an RGB reading. Select 'Live view' and after a few seconds, tap the color identifier box (the white box), and record the first number of the RGB value onto your data sheet. This corresponds to the initial Red value (R_o). It is the amount of red light that is passing through the solution before the blue dye is added. It is being detected by the smartphone camera. See figures 5 and 6.



Figure 5: Select the 'Live View' within the 'Color Name AR' app



Figure 6: The R values are obtained by (a) tapping on the color identifier box and (b) recording the first value from the RGB reading

- 9. From this point on, *do not* move the smartphone, and do not cast any shadows onto the glass as you observe and record the data. (*Test your hand movements to be sure the smartphone does not move.*)
- 10. Go back to the live view on the app by tapping on 'back'.
- 11. Slide the reaction glass out far enough so that you can add one drop of the blue dye into the glass. **Start the timer** the moment the blue dye is added to the reaction.
- 12. Quickly mix the solution with the same metal spoon so that it's homogeneous. Be careful not to spill.
- 13. Slide the reaction glass back into the circle, lining up the marking on the glass with the marking on the construction paper.
- 14. At 30 seconds, tap the color identifier box, record the red value on your data sheet, then return back to the live view.
- 15. Continue recording the red value every 30 seconds until the red color value no longer changes. The solution will be, or close to being, colourless at this point.
- 16. Leave the smartphone and stand in place, do not move them. Dispose the bleach solution immediately down the drain and rinse the reaction glass with lots of water. Also rinse the teaspoon, metal spoon and the plate holding the spoon.
- 17. Dry all the equipment, including the thermometer.

Part B - Reaction at Cooler Temperature (Run 2)

- 18. Repeat steps 5 17, except measure out ½ cup (125 mL) of *cold water* that is between 5 to 8 °C lower than the room temperature from Run 1. Measure the temperature of the water before adding the bleach, to be sure the temperature is in the desired range. Once the bleach is added and the solution is stirred, measure the temperature again and this time record it on your data sheet (continue on from step 5).
- 19. At the end of the run, rinse and dry all equipment and remember not to move the smartphone and stand.

Part C – Reaction at Elevated Temperatures (Runs 3-5)

- 20. Repeat steps 5 17 three more times. For each run:
 - Measure out ½ cup (125 mL) of water that is *warmer* than the room temperature run. The temperatures should be between room temperature and 45 °C, with 5-8 °C difference between each run (for ex. 30 °C, 37 °C and 45 °C). The water can be used from the hot water tap and mixed with colder water to achieve the desired temperatures.
 - b. Record the red values every **15 seconds**
- 21. At the end of each run, rinse and dry all equipment and remember not to move the smartphone and stand.
- 22. Take a picture of your experimental set up and include it in your lab report.

Calculations and Data Analysis

For the analysis of the data, use Microsoft Excel to carry out the calculations and to plot the graphs.

- 1. For each temperature run:
 - a. Prepare the following table of data (each trial should be on separate worksheets):
 - i. *Time* (s) Convert the time readings into total time based on seconds.
 - ii. *Absorbance, A* Calculate the absorbance of red light at each time point using the following equation:

$$A = -\log\left(\frac{R}{R_o}\right)$$

- iii. In A Calculate the natural logarithm (In) of each absorbance value
- b. Plot a graph of In A vs Time. Provide an appropriate title and include labels for the axes. As in the previous experiment, 'The Rate Law in Chemical Kinetics Using Blue Food Dye', we will treat the absorbances as concentration values when plotting the graphs.
- c. Determine k_{obs} from the slope of the line. When adding the linear trendline, exclude data points near the end of the reaction that have the same values of A and/or do not fall on the trendline.
- 2. Calculate the concentration of NaOCI, [NaOCI], (M) using the concentration of NaOCI provided on the bottle of bleach. Ignore the volume of the blue dye as it's relatively small. The total volume of the solution is based on the volume of bleach and water used. The concentration of bleach on the bottle is expressed as a % NaOCI w/w. Assume this represents the percentage of NaOCI in grams, per 100 g of solution (e.g. 1.5% NaOCI w/w is equivalent to 1.5 g of NaOCI in 100 g of solution). Assume the density of the bleach solution is 1.00 g/mL.
- 3. Calculate the value of *k* using equation (5)

$$k_{obs} = k[\text{NaOCI}] \tag{5}$$

- 4. Fill in the Part D data table.
- 5. Plot ln *k* vs T⁻¹. Provide an appropriate title and include labels for the axes. From the slope of the line, determine E_a.

Name

Section

Date

Activation Energy in Chemical Kinetics

Data

Brand name of bleach:

Concentration of NaOCI in bleach (as indicated on the bottle):

Red Value

Part A – Room Temperature

Part B – Colder Temperature

Run 2				
Temp (°C)				
Initial Red value (bleach + water)				
Ro				
Reaction Time	Red Value			
0:30				
1:00				
1:30				

Part C – Warmer Temperatures

Run 3			
Temp (°C)			
Initial Red value (bleach + water) R₀			
Reaction Time	Red Value		
0:30			
0:45			
1:00			

Run 4				
Temp (°C)				
Initial Red value (bleach + water)				
Ro				
Reaction Time 0:30	Red Value			
0:45				
1:00				

Run 5				
Temp (°C)				
Initial Red value (bleach + water)				
R₀ Reaction Time	Red Value			
0:30				
1:00				

Part D – Summary of the data

Run	T (°C)	Т (К)	T ⁻¹ (K ⁻¹)	<i>k</i> _{obs} (s ⁻¹)	<i>k</i> (M ⁻¹ s ⁻¹)	ln <i>k</i>
1						
2						
3						
4						
5						

Activation Energy, E_a (kJ, mol) _____

References

Department of Chemistry. (2019, Fall). 'Kinetics of the Bleaching of a Food Dye', *Chemistry NYB Lab Manual*. Sainte-Anne-de-Bellevue, QC: John Abbott College

Kuntzleman, Tom. "Chemical Kinetics with a Smartphone." *Chemical Education Xchange*, 27 Nov. 2019, <u>www.chemedx.org/blog/chemical-kinetics-smartphone</u>.

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Using Bleach to Help Flower Bouquets (Optional)

Fill a vase with 3 drops of bleach and 1 teaspoon of sugar in one quart (1 liter) of water before adding the flowers. The bleach and sugar not only helps the freshly cut flowers last longer, but it also prevents harmful bacteria from growing in the water, and keeps the water clearer.



Reference: Editors, Reader's Digest. "How to Make Flowers Last Longer: 8 Pro Tricks." *Reader's Digest*, Reader's Digest, 13 Feb. 2019, www.rd.com/home/decorating/how-tomake-flowers-last-longer/#:~:text=Bleach,inhibit the growth of bacteria.