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Forensic Chemistry: Colorful Chemical Kinetics

Experiment

Color Countdown Timer

- Go Direct Colorimeter

Workshop Presenter

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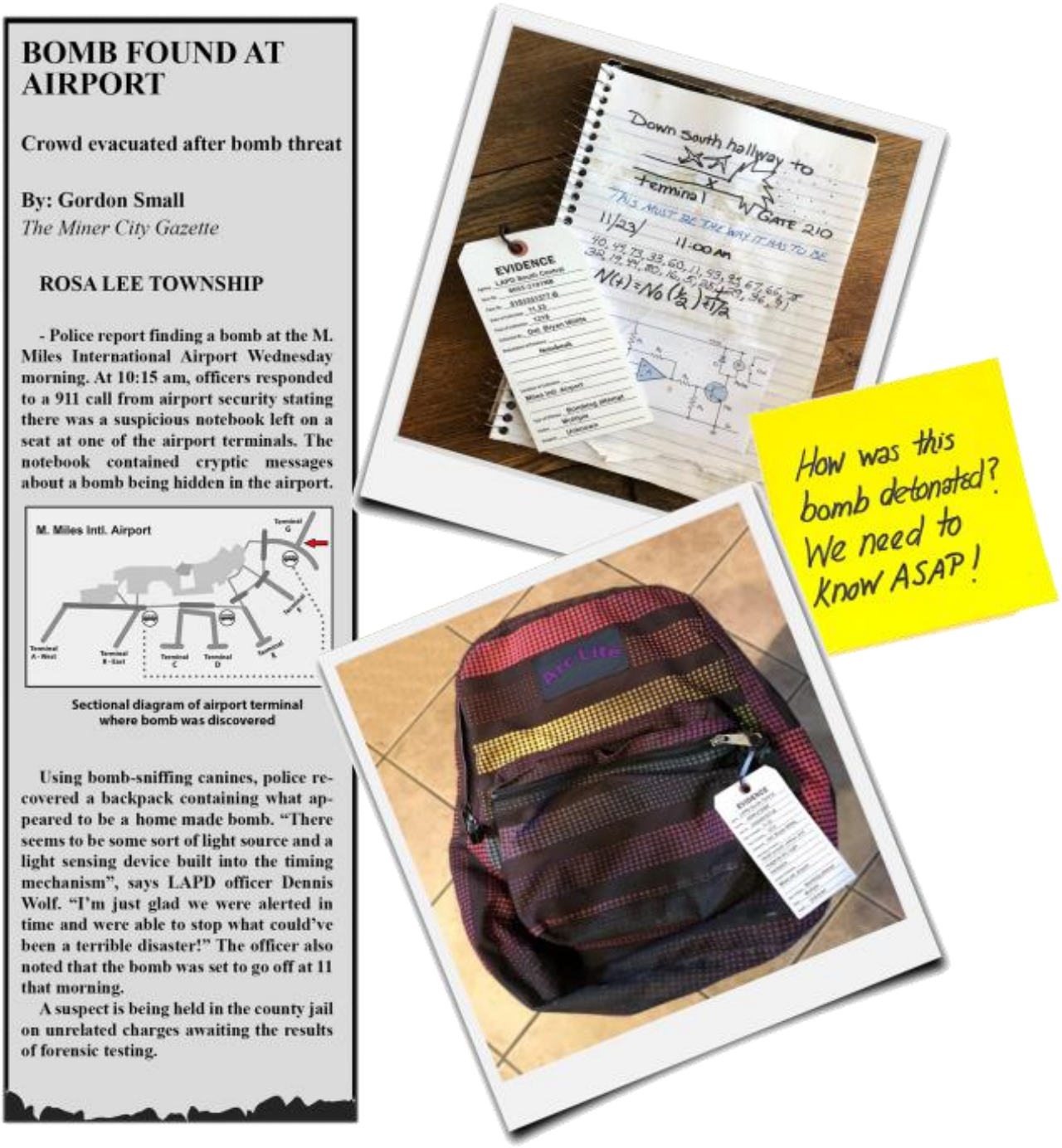
Color Countdown Timer (Colorimeter)



BOMB FOUND AT AIRPORT

Crowd evacuated after bomb threat

By: Gordon Small
The Miner City Gazette

ROSA LEE TOWNSHIP

- Police report finding a bomb at the M. Miles International Airport Wednesday morning. At 10:15 am, officers responded to a 911 call from airport security stating there was a suspicious notebook left on a seat at one of the airport terminals. The notebook contained cryptic messages about a bomb being hidden in the airport.

Sectional diagram of airport terminal where bomb was discovered

Using bomb-sniffing canines, police recovered a backpack containing what appeared to be a home made bomb. "There seems to be some sort of light source and a light sensing device built into the timing mechanism", says LAPD officer Dennis Wolf. "I'm just glad we were alerted in time and were able to stop what could've been a terrible disaster!" The officer also noted that the bomb was set to go off at 11 that morning.

A suspect is being held in the county jail on unrelated charges awaiting the results of forensic testing.

Detectives need your help with understanding how this chemical reaction works as a timer. There was a food dye and bleach solution recovered from the backpack in the airport terminal. How can these be used as a timer?

In Part I you will measure the absorbance of a food dye solution at different wavelengths and identify the wavelength of maximum absorbance, λ_{max}.

In Part II you will collect data observing the reaction between the food dye and bleach, using the wavelength you determined in Part I. Common bleaches contain sodium hypochlorite, NaClO. In solution, this ionic compound dissociates to form sodium ion, Na^+, and hypochlorite ion, ClO^-.

As the reaction between the food dye and bleach proceeds, the food dye color will fade and the absorbance of light will decrease.

Here is an equation for this reaction:

$$\text{FoodDye} + OCl^- \rightarrow \text{colorless molecule}$$

The kinetics or speed of this reaction is related to the concentration of the reactants. As the concentration of either reactant is changed, you can determine how this affects the rate of the reaction. As this reaction proceeds, the concentration of food dye will drop over time. You will determine the order of the reaction with respect to the food dye and write the rate law based on your analysis of the graph of absorbance *vs*. time.

A typical rate expression might look something like this:

$$\text{rate} = k[\text{FoodDye}]^x[\text{bleach}]^y$$

Where *k* is called the rate constant, [FoodDye] and [bleach] represent the concentration of each reactant. The exponents *x* and *y* are related to the effect of changing the concentration of each reactant has on the rate of the reaction.

Food dye concentrations are typically around 10^{-6} mol/L in the foods that we consume. On the other hand, the concentration of the bleach is on the order of 1 mol/L or 10^6 times as concentrated. Since the concentration of the bleach is so much larger than that of the food dye, the concentration of the bleach will not change much during the reaction. We can concentrate on how the change in concentration of the food dye affects the kinetics and only examine that reactant in the expression,

$$\text{rate} = k[\text{FoodDye}]^x$$

Using your data and some analysis, you will determine the value of the exponent, *x*, on [FoodDye] in the expression. If the value of *x* is 0, changing the concentration of the reactant has no effect on rate of reaction.

If the value of *x* is 1, that means increasing or decreasing the concentration of FoodDye causes a direct change in the rate of the reaction. If the concentration is doubled, the rate doubles and so on. If the concentration is halved, the rate will drop in the same proportion.

If the value of *x* is 2, the rate of the reaction would quadruple if the concentration of FoodDye is doubled or drop by 1/4 if the concentration is halved.

Finally, you will write a summary that the district attorney can use in court to explain how this reaction was used as a timer by the suspect.

OBJECTIVES

- Apply scientific principles and evidence to provide an explanation about the effect of blue food dye concentration on the rate of reaction between bleach and food dye.
- Analyze and interpret absorbance spectra to identify the wavelengths of maximum absorbance for blue food dye.
- Use mathematical representations to determine the rate constant for the reaction between blue food dye and bleach and the half-life of the reaction.
- Communicate technical information about the process used to identify the rate of change of blue food dye concentration using absorbance data.
- Write a Case Report to help detectives present the case in court.

MATERIALS

Chromebook, computer, **or** mobile device
Graphical Analysis Pro app
Go Direct Colorimeter
two cuvettes and caps
cuvette rack
100 mL beaker
two 10 mL graduated cylinder
two Beral pipettes
blue food dye solution
diluted commercial bleach, OCl^-
distilled water
tissues, lint free

PRE-LAB ACTIVITY

The part of the electromagnetic spectrum that we call visible light extends from about 400 to 700 nm in wavelength. Commonly, we can remember the order of the colors in the spectrum of visible light using "ROY G. BIV". Name the colors that correspond to each wavelength in Table 1.

Table 1							
Wavelength	400 nm	450 nm	500 nm	550 nm	600 nm	650 nm	700 nm
Color							

When white light falls on a colored surface your eyes can only see the color(s) of light NOT absorbed by the surface. A blue surface looks blue since all the other colors of the visible spectrum are absorbed by the surface and not reflected back to your eyes. Artists sometimes use a color wheel to match up complimentary colors, colors of light that absorb one another.

You will be using a blue food dye solution in this experiment. When the solution is mixed with sodium hypochlorite (bleach) the intensity of the blue color will drop over time. A graph of this change will be produced from which you will determine a mathematical relationship between concentration of the food dye and time called a reaction rate expression.

In this type of study, the color of light or wavelength of maximum absorbance, λ_{max}, is used to get the best results.

Which color of light will the blue food dye absorb the most?

PROCEDURE

Part I Find λ_{max}

In this section you will determine λ_{max} for the blue dye.

1. Obtain and wear goggles.

2. Prepare a blank by filling a cuvette 2/3 full with distilled water. To correctly use cuvettes, remember

    - Wipe the outside of each cuvette with a lint-free tissue.
    - Handle cuvettes only by the top edge of the ribbed sides.
    - Dislodge any bubbles by gently tapping the cuvette on a hard surface.
    - Always position the cuvette so the light passes through the clear sides.

3. Prepare a second cuvette of blue food dye solution. Fill the cuvette less than 1/2 with blue food dye solution and then about 1/2 with water. Place a cap on the cuvette and invert it a couple of times to mix the water and food dye.

4. Launch Graphical Analysis. Connect the Go Direct Colorimeter to your Chromebook, computer, or mobile device.

5. Set up the data-collection mode.

   a. Click or tap Mode to open Data Collection Settings. Change Mode to Event Based.

   b. Enter **Wavelength** as the Event Name and **nm** as the Units. Click or tap Done.

   c. Click or tap View Options, ⊞, and turn on Meters. Then, dismiss the View Options menu.

   d. Tap or click Graph Options, 📈, and choose Edit Graph Options. Then, adjust the following settings:

      Appearance: ☑ Bars

x-axis range	y-axis range
Left: 400 Right: 700 Scaling: Manual Scaling	Bottom: 0 Scaling: Always Show 0

   e. Click or tap outside the Graph Options window to exit.

6. You are now ready to collect absorbance-wavelength data.

   a. Click or tap Collect to start data collection.

   b. Place the blank cuvette into the colorimeter. Make sure to align the light path correctly.

   c. Press the < or > buttons on the Colorimeter to set the LED to the lowest wavelength, 430 nm. Then calibrate by pressing the CAL button on the Colorimeter. When the LED stops flashing, the calibration is complete.

   d. Replace the blank cuvette with the blue food dye cuvette.

   e. When the value has stabilized, click or tap Keep and enter the wavelength of the LED, 430 nm, being used on the colorimeter. Click or tap Keep Point. The absorbance and wavelength values have now been saved for the first LED.

   f. Replace the blue food dye cuvette with the blank cuvette into the colorimeter. Make sure to align the light path correctly.

   g. Press the < or > buttons on the Colorimeter to set the LED to the next wavelength, 470 nm. Then calibrate by pressing the CAL button on the Colorimeter. When the LED stops flashing, the calibration is complete.

   h. Replace the blank cuvette with the blue food dye cuvette.

   i. When the value has stabilized, click or tap Keep and enter the wavelength of the LED, 470 nm, being used on the colorimeter. Click or tap Keep Point. The absorbance and wavelength values have now been saved for the first LED.

   j. Repeat h and i of this step for the rest of the LEDs on the colorimeter.

   k. Click or tap Stop to stop data collection.

7. To examine the data pairs on the displayed graph, click or tap the graph. Take note of the wavelength that results in the highest absorbance value. This is λ_{max}. Record this value in the Evidence Record.

8. Click or tap File, 🗋, and choose Save to save your data file.

9. Empty and rinse the food dye cuvette.

Part II Reaction of Food Dye with Bleach

In this section you will measure the absorbance over time, which is a measure of the food dye concentration.

1. Click or tap File, 🗋, and start a New Experiment in Graphical Analysis.
2. Place 10 mL of blue food dye solution into one 10 mL graduated cylinder and 10 mL of diluted bleach solution in a second 10 mL graduated cylinder. Beral pipettes can help you to be more accurate.
3. Calibrate the Colorimeter.
   a. Place the blank in the cuvette slot of the Colorimeter, making sure to align the light path correctly, and close the lid.
   b. Press the < or > buttons on the Colorimeter to set the wavelength to the value that resulted in the highest absorbance in Part I, λ_{max}. Then calibrate by pressing the CAL button on the Colorimeter. When the LED stops flashing, the calibration is complete.
4. Click or tap Mode to open Data Collection Settings. Change Rate to 2 samples/s and End Collection to 200 s. Click or tap Done.
5. **READ THIS STEP COMPLETELY FIRST**, then QUICKLY complete the entire step:
   a. Have a clean, empty cuvette ready.
   b. Pour the contents of the 10 mL graduated cylinder of food dye into a 100 mL beaker.
   c. Pour the contents of the 10 mL graduated cylinder of dilute bleach into the 100 mL beaker with the food dye.
   d. Swirl the beaker and fill the cuvette about 3/4 full.
   e. Place the cuvette into the colorimeter, aligning it correctly. Close the Colorimeter lid.
   f. Watch the absorbance meter. When the reading reaches the highest value, click or tap Collect to start data collection.
6. While data is being collected, observe the remainder of the solution in the beaker. Note your observations in the Case Evidence section.
7. Absorbance data will be collected for 200 seconds and will stop automatically. Discard the contents of the beaker, graduated cylinders, and cuvette as directed by your instructor.

EVIDENCE RECORD

λ_{max} = _____

Observations of test tube containing reaction mixture:

_____

_____

_____

Table 2			
	Slope, *m*	y-intercept	Correlation coefficient, *r*
First order plot			
Second order plot			

PROCESSING THE DATA

1. Analyze the data graphically to decide if the reaction is zero, first, or second order with respect to food dye.

   - Zero Order: If the current graph of absorbance *vs*. time is linear, the reaction is *zero order*. In the rate expression, the exponent on the concentration of this reactant would be 0.
   - First Order: To see if the reaction is first order, plot a graph of the natural logarithm (ln) of absorbance *vs*. time. If this plot is linear, the reaction is *first order*. In the rate expression, the exponent on the concentration of this reactant would be 1.
   - Second Order: To see if the reaction is second order, plot a graph of the reciprocal of absorbance *vs*. time. If this plot is linear, the reaction is *second order*. In the rate expression, the exponent on the concentration of this reactant would be 2.

2. To test for first-order kinetics with respect to the food dye, create a calculated column, ln (Absorbance), and add a linear curve fit to the graph ln (Absorbance*) vs*. time:

   a. Click or tap View Options, ⊞, and turn on Data Table. Then, dismiss the View Options menu.

   b. In the Absorbance column header in the table, click or tap Column Options, ⋯, and choose Add Calculated Column.

   c. Enter **ln (Absorbance)** as the Name and leave the Units field blank.

   d. Click or tap Insert Expression and choose A ln(X) as the expression.

   e. Enter **1** as Parameter A and select Absorbance as Column X.

   f. Click or tap Apply. A graph of ln (Absorbance) *vs*. time is displayed. Double-click the graph to autoscale the graph. If the y-axis does not change automatically to ln (Absorbance), click or tap on the y-axis label, select ln (Absorbance) and deselect Absorbance. Click or tap the y-axis label again to close the menu.

   g. To determine if the relationship is linear, click or tap Graph Options, ⌞⋰, and choose Apply Curve Fit.

   h. Select Linear as the curve fit and dismiss the Curve Fit box.

   i. Record the slope, *m*, and the correlation coefficient, *r*, in the Evidence Record. Dismiss the Linear curve fit box.

3. To test for second-order kinetics with respect to the blue food dye, create a calculated column, 1/Absorbance, and then plot a graph of 1/Absorbance *vs*. time:

   a. In the data table, click or tap Column Options, ⋯, in the Absorbance column header, and then choose Add Calculated Column.

   b. Enter **1/Absorbance** as the Name and leave the Units field blank.

   c. Click or tap Insert Expression and choose A/X as the expression.

   d. Enter **1** as Parameter A and select Absorbance as Column X.

   e. Click or tap Apply.

   f. Click or tap the y-axis label and select only 1/Absorbance to display a graph of 1/Absorbance *vs*. time.

   g. To determine if the relationship is linear, click or tap Graph Options, ⋰, and choose Apply Curve Fit.

   h. Select Linear as the curve fit and dismiss the Curve Fit box.

   i. Record the slope, *m*, and correlation coefficient, *r*. Dismiss the Linear curve fit box.

4. (Optional) To see any of the three graphs again, click or tap the y-axis label and choose the column you want to display.

5. Export, download, or print the most linear graph.

CASE ANALYSIS

1. Was the reaction zero, first-, or second-order with respect to the concentration of food dye? Explain.
2. Write a *rate expression* for this reaction with respect to food dye concentration based on your data and graphs.
3. Determine the rate constant, *k*, using the slope of the linear regression line for your linear curve (*k* = –slope for zero and first order, *k* = slope for second order). Be sure to include correct units for the rate constant. **Note**: This constant is sometimes referred to as the *pseudo rate constant*, because it does not take into account the effect of the other reactant, OCl^-.
4. For first order kinetics, a common mathematical equation looks like this:

$$\ln [A]_t = -kt + \ln [A]_0$$

   where $[A]_0$ is the initial concentration of reactant A, $[A]_t$ is the concentration of A at some later time, *t*, and *k* is the slope of the graph of ln [A] *vs*. time. For this reaction, the absorbance of the food dye is directly proportional to the concentration of the food dye, [FoodDye]. It is reasonable to use (Abs) in place of [FoodDye].

   Write a mathematical equation for a first order reaction from the linear regression equation on your graph, $y = mx + b$, substituting from your graph and linear regression data.

5. The timer actuates the device when the reaction is halfway completed. This time is commonly called the half-life or $t_{1/2}$. Your teacher will tell you which method below to use to calculate the half-life of the reaction.

METHOD 1 DETERMINE REACTION ORDER FROM THE GRAPH OF ABSORBANCE *VS*. *T*

6. You will use your graph to estimate the half-life of the reaction. The half-life is the amount of time for the Absorbance to decrease to half of its original value. The absorbance of the food dye is directly proportional to the concentration of the food dye, [FoodDye]. You can use Absorbance in place of [FoodDye].
   a. Click or tap the graph and determine the Absorbance at $t = 0$. Record the value in the table.
   b. Click or tap the graph to determine the time when the Absorbance is half of its value at $t = 0$. Record the time and absorbance values in Table 3.
   c. Repeat the previous step, using to determine the time when the Absorbance is decreased to half of the previous value. Record the time and absorbance values in Table 3. Repeat this process as many times as possible, until you reach the end of the data.
   d. Calculate each half-life and record in the table. Compare the half-life values. Is the half-life constant? Remember, this method is an estimate for half-life. For first order kinetics reactions, the half-life values will be constant.

Table 3

Time (s)	Absorbance	Half-life (s)
0		
53		
102		
152		

METHOD 2 DETERMINE REACTION ORDER FROM THE EQUATION

6. For a more accurate determination of half-life, use the equation in Case Analysis Question 4. When the concentration of the reactant drops to 1/2 the original value, the expression can be simplified to look like this:

$$t_{1/2} = \frac{\ln 2}{k}$$

   where k = slope from your graph of ln Abs *vs*. time.

   Calculate the half-life using the rate constant, k, from your graph of ln Abs *vs*. time.

7. There was a light sensing mechanism found in the backpack. The timer was meant to actuate the device when the absorbance value reached $t_{1/2}$. Calculate the absorbance of the solution when it has reached its half-life.

CASE REPORT

When you write your case report, make sure to include graphs, supporting data, and

- Explain why it was important to determine the λ_{max}.
- Describe what happened to the absorbance of the solution as the reaction progressed.
- Write the rate expression for this reaction with respect to food dye.
- Explain how you determined when the timer would actuate the device.