Case File 9

Killer Cup of Coffee:
Using colorimetry to determine concentration of a poison

Determine the concentration of cyanide in the solution.

A Killer Cup of Coffee? GlobalTech Manager Dies

SOUTH PAINTER, Tuesday: It was a normal Monday morning at GlobalTech Industries until the mail boy discovered project manager Patrick Marchand dead in his cubicle, head on his desk. Mr. Marchand had died while writing an email, in a room full of people hard at work. An early examination of the crime scene yielded no clues.

Mr. Marchand was known to have a serious heart condition, and many signs pointed to cardiac arrest as the cause of his death. However, as police canvassed the office space, the distinct odor of bitter almonds was detected, and a vial containing a small amount of an unknown chemical was found discarded in a communal trash can.

Based on the bitter almond odor, police have tentatively identified the substance as cyanide. The existence of this possible poison has lead police to suspect foul play in Mr. Marchand's death. The police have no leads.

continued on p. D2

This vial, wrapped in a piece of tissue, was discovered in the bottom of a communal trash can near the GlobalTech office bathroom. It once contained an unspecified amount of cyanide.

LAB NOTES

Technician: Beverly Chin

-received vial containing 20 mL cyanide solution—concentration unknown
-reacted cyanide (CN^-) solution with potassium polysulfide (K_2S_x) to produce potassium thiocyanate (KSCN)
-reacted KSCN solution with iron(III)chloride ($FeCl_3$) to produce iron(III)thiocyanate ion ($FeSCN^{2+}$)
-determination of amount of $FeSCN^{2+}$ in reacted solution will allow estimation of concentration of CN^- in original solution
-included in package: $FeSCN^{2+}$ solution of unknown concentration

Science Objectives

- Use Beer's law to determine the concentration of simulated iron (III) thiocyanate ($FeSCN^{2+}$) in an unknown solution.
- Use colorimetry to determine the concentration of a colored species in a solution.
- Use a linear relationship to model the data (Beer's law).
- Learn the importance of carefully prepared standards.

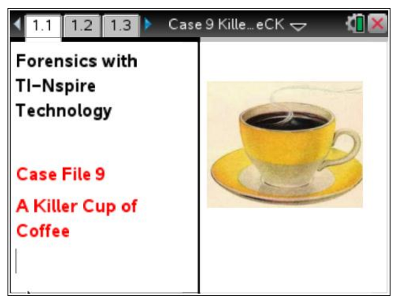
Activity Materials

- TI-Nspire™ technology
- *Case 9 Killer Coffee.tns* file
- Vernier EasyLink™ or TI-Nspire Lab Cradle
- Vernier Colorimeter
- 7 cuvettes
- colored wax pencil
- distilled water
- waste beaker
- two 5 mL beakers
- stirring rod
- goggles
- 5 mL of simulated $FeSCN^{2+}$ solution of unknown concentration in the suspicious vial
- two 10 mL pipettes or graduated cylinders
- 50 mL of 0.15 M stock simulated $FeSCN^{2+}$ solution
- 2 droppers
- 6 test tubes
- test tube rack
- lint-free tissues

Procedure

Open the TI-Nspire document *Case 9 Killer Coffee.tns.*

In this data-gathering activity, you will use Beer's law to determine the concentration of iron(III)thiocyanate (FeSCN2+) in an unknown solution.



Part 1 – Preparing the Solutions

Move to pages 1.2–1.7.

CAUTION: You should obtain and wear goggles during this experiment, and be careful not to ingest any solution or spill any on their skin. Inform your teacher immediately in the event of an accident.

1. Obtain and label the following with a wax pencil:

   a. Pour 50 mL of stock simulated 0.15 M $FeSCN^{2+}$ solution into a 50 mL beaker. Label the beaker "Simulated 0.15 M $FeSCN^{2+}$."

   b. Pour 30 mL of distilled water into a 50 mL beaker. Label the beaker "H_2O."

2. Prepare the unknown and standard solutions.

    a. Label five clean, dry test tubes with numbers 1 through 5.

    b. The following table (and on page 1.5) shows how much water and stock simulated $FeSCN^{2+}$ solution to add to each test tube. Use a pipette or a dropper and graduated cylinder to measure the correct amount of simulated $FeSCN^{2+}$ solution into each test tube. **Note:** Use a separate pipette or graduated cylinder and dropper for the water and the simulated $FeSCN^{2+}$.

    c. Carefully stir the contents of each test tube with a clean stirring rod. (Clean the stirring rod with distilled water and dry it thoroughly in between each test tube.)

    d. Label a sixth test tube with a "U" for unknown. Use a pipette or a dropper and graduated cylinder to measure 5 mL of simulated $FeSCN^{2+}$ solution of unknown concentration into the test tube.

Test Tube	$FeSCN^{2+}$ Solution (mL)	Distilled Water (mL)	Final Concentration of $FeSCN^{2+}$ (mol/L)
1	10	0	0.15
2	8	2	0.12
3	6	4	0.09
4	4	6	0.06
5	2	8	0.03

3. Prepare the blank, the five standard solutions, and the unknown for colorimetry.

    a. For each standard solution, rinse an empty cuvette twice with about 1 mL of the sample.

    b. Fill each cuvette 3/4 full with the sample, and seal it with a lid.

    c. Label the lid with the sample number.

    d. Wipe the outside of each cuvette with a tissue.

    e. Repeat Steps 3a–3d for the unknown sample. Label the lid with a "U".

    f. Repeat Steps 3a–3d using distilled water for the blank. Label the lid with a "B".

Remember the following:

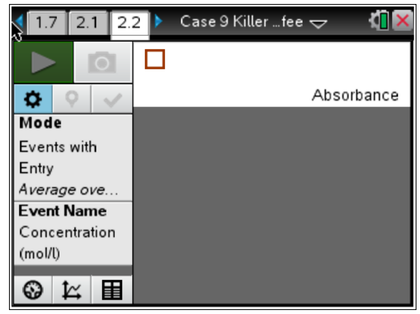
- All cuvettes should be clean and dry on the outside.
- Handle cuvettes only by the top edge or the ribbed sides.
- All solutions should be free of bubbles.

Part 2 – Collecting Data

Move to pages 2.1-2.4.

4. In your Evidence Record below, enter the volume of the suspicious vial.

5. On page 2.2, connect the Colorimeter to TI-Nspire.

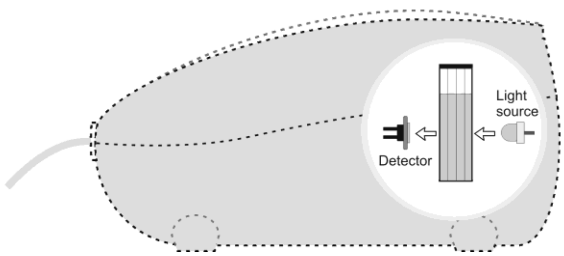


6. Calibrate the Colorimeter.

   a. Open the Colorimeter lid. Place the blank cuvette containing distilled water, in the cuvette slot of the Colorimeter. Make sure that one of the transparent faces of the cuvette is pointing toward the white reference mark. Close the lid of the Colorimeter.

   b. Press the < or > button on the Colorimeter to select a wavelength of 470 nm (Blue).

   c. Press the CAL button until the red LED begins to flash. Then release the CAL button. When the LED stops flashing, the calibration is complete.



7. You are now ready to collect absorbance-concentration data at 470 nm for the solutions.

   a. Start data collection ▶.

   b. Place cuvette 1 in the Colorimeter. Be sure the cuvette is clean, dry, and has a transparent face pointing toward the reference mark.

   c. After closing the lid, wait for the absorbance value displayed on the monitor to stabilize, and then select Keep button.

   d. Enter the concentration of the solution (from the table in Step 2) and select OK. The data pair you just collected should now be plotted on the graph.

   e. Remove the cuvette from the Colorimeter.

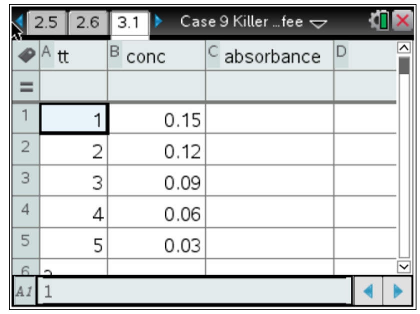
   f. Repeat this process for the remaining standards in cuvettes 2 through 5.

9. Stop data collection when you have collected data for all the samples. You will NOT have done the unknown!

10. In your Evidence Record and/or on page 3.1 (as directed by your teacher), write down the absorbance values displayed in the Data Table from page 2.2.

Part 3 – Analyzing the Data

Move to page 2.5-3.1



11. Select the Meter tab. Place the cuvette with the unknown solution in the Colorimeter. Monitor the absorbance value displayed on the screen. When this value has stabilized, round it to the nearest 0.001.

12. To determine the concentration of $FeSCN^{2+}$ in the unknown solution, fit a straight line to the graph of absorbance vs. concentration.

    a. Select the Graph tab on page 2.2 to see the graph.

    b. Press the **menu** key and choose **Analyze > Curve Fit > Linear**.

    c. Select Linear for the Fit Equation. A best-fit linear regression line will be shown for your five data points. This line should pass near or through the data points *and* the origin of the graph. The equation for a straight line is $y = mx + b$, where y is absorbance, x is concentration, m is the slope, and b is the y-intercept.

    d. The displayed values of m and b give the best fitting line to your data points. The correlation coefficient indicates how well the data points match the linear fit. A value of 1.00 indicates a perfect fit. Record the values of m, b, and the correlation in the Evidence Record and/or on page 3.2 in the .tns file (as directed by your teacher). The linear relationship between absorbance and concentration is known as Beer's law. Select OK.

    e. Press the **menu** key. Choose **Analyze > Interpolate**. Interpolate along the regression curve to determine the concentration of the unknown solution. Tap any point on the regression curve (or use the ► or ◄ keys) to advance to the absorbance value that is closest to the absorbance reading you obtained. The corresponding concentration value is the concentration of the unknown $FeSCN^{2+}$ solution, in mol/L. Write this value in the Evidence Record and/or on page 3.3 in the .tns file (as directed by your teacher)

Name _______________
Class _______________

Evidence Record

Volume of the suspicious vial ___________________________

Solution Number	Concentration of Simulated FeSCN2+ in Solution (mol/L)	Absorbance
1	0.15	
2	0.12	
3	0.09	
4	0.06	
5	0.03	
U	Unknown	

Concentration of $FeSCN^{2+}$ in the unknown solution ___________________________

y	*mx* + *b*
m	
b	
correlation	

Case Analysis

Answer the following questions here, in the .tns file, or both.

Q1. Write the equation for the line in the form $y = mx + b$, using the values for m and b that you recorded in the Evidence Record. For example, if $m = 3$ and $b = 6$, then the equation for the line is $y = 3x + 6$.

Q2. Use the equation to calculate the concentration of $FeSCN^{2+}$ in the unknown solution. How does the value you calculate compare with the value you read from the graph?

Q3. The volume of the cyanide solution that was found at the scene was 20 mL. Based on the calculated concentration of $FeSCN^{2+}$ in the unknown solution, determine the concentration of potassium cyanide, KCN, in the original poison. Show all of your work. Give your answer in milligrams of KCN per milliliter of solution. **Hint:** One mole of KCN will produce one mole of $FeSCN^{2+}$. Assume that all of the KCN in the poisoned solution reacted to form $FeSCN^{2+}$. Assume that the 20 mL of original solution was not diluted during the reaction to form $FeSCN^{2+}$ and that the sample you received was also undiluted. The molecular weight of $FeSCN^{2+}$ is 114 g/mol. The molecular weight of KCN is 65 g/mol.

Note: Page 4.5 is a calculator page to help with this.

Q4. For most people, swallowing 300 mg of KCN is fatal. Based on the concentration of KCN in the poison that you calculated in Question 3, determine the approximate volume of poison that the victim would have to have swallowed for it to have killed him. Show all of your work.

Note: Page 4.7 is a calculator page to help with this.

Q5. Is it likely that the poison was the direct cause of death? Explain your answer. **Hint:** Remember that the vial was mostly empty and may, at one time, have held more than 20 mL.

Q6. Suppose you found out that the concentration of $FeSCN^{2+}$ in the unknown was actually very different from the value you calculated in Question 2 and the value you read off of the graph. What factors could have caused this difference?