Techni Science.

Case

Killer Cup of Coffee

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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.

MATERIALS

LabQuest
LabQuest App
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

CAUTION: Obtain and wear goggles during this experiment. Be careful not to ingest any solution or spill any on your skin. Inform your teacher immediately in the event of an accident.

Part I Preparing the Solutions

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 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. (Carefully clean the stirring rod with distilled water and dry it with a tissue before using it in the next 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 II Collecting Data

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

5. Connect the Colorimeter to LabQuest and choose New from the File menu. If you have an older sensor that does not auto-ID, manually set up the sensor.

6. Set up the data-collection mode.
   a. On the Meter screen, tap Mode. Change the mode to Events with Entry.
   b. Enter the Name (Concentration) and Units (mol/L). Select OK.

7. 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.

8. 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, with the cuvette clean, dry, and with a transparent face pointing toward the reference mark.
   c. After closing the lid, wait for the absorbance value displayed on the monitor to stabilize, then tap Keep.

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.

10. In your Evidence Record, write down the absorbance values displayed in the Data Table.

Part III: Analyzing the Data

11. Tap 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 and write it in your Evidence Record.

12. To determine the concentration of $FeSCN^{2+}$ in the unknown solution, fit a straight line to the graph of absorbance vs. concentration.
    a. Tap the Graph tab.
    b. Choose Curve Fit from the Analyze menu.
    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. The linear relationship between absorbance and concentration is known as Beer's law. Select OK.
    e. Choose Interpolate from the Analyze menu. 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.

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

1. 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 $y = 3x + 6$.

2. 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?

3. 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 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.

4. 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 your work.

5. 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.

6. 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 the graph. What factors could have caused that to happen?