Extraction, Distribution Coefficient

Experiment 4A Calculation Worksheet

A. Prepare the Standard Benzoic Acid Solution

1. Calculate the molarity of your standard Benzoic Acid (PhCO₂H; Molecular Weight: 122.12) solution:

   \[
   \frac{0.61 \text{ g PhCO}_2\text{H}}{122 \text{ g PhCO}_2\text{H}} \times \frac{1 \text{ mole PhCO}_2\text{H}}{0.005 \text{ mole PhCO}_2\text{H}} \times \frac{1000 \text{ mL water}}{250 \text{ mL water}} = 0.02 \text{ M PhCO}_2\text{H}
   \]

   Solve for \( X \): \( X = 0.02 \text{ mole PhCO}_2\text{H} \) in 1000 mL water or \( 0.02 \text{ M PhCO}_2\text{H} \)

B. Single 10 mL Extraction and Determination of Distribution Coefficient

1. Calculate amount of Benzoic Acid you are starting with:

   \[
   \frac{50 \text{ mL 0.02M PhCO}_2\text{H}}{1000 \text{ mL 0.02M PhCO}_2\text{H}} \times \frac{0.02 \text{ mole PhCO}_2\text{H}}{1 \text{ mole PhCO}_2\text{H}} = 0.01 \text{ mole PhCO}_2\text{H}
   \]

2. To calculate amount of PhCO₂H remaining in aqueous solution after extraction with 10 mL of methylene chloride, titrate aqueous layer with 0.02M NaOH

   \[
   \frac{\text{mL 0.02M NaOH}}{1000 \text{ mL 0.02M NaOH}} \times \frac{0.02 \text{ mole NaOH}}{1 \text{ mole NaOH}} \times \frac{1 \text{ mole PhCO}_2\text{H}}{122.12 \text{ g PhCO}_2\text{H}} = \frac{Y \text{ g PhCO}_2\text{H}}{1000 \text{ mL 0.02M NaOH}} \times \frac{1 \text{ mole PhCO}_2\text{H}}{1 \text{ mole PhCO}_2\text{H}}
   \]

3. Calculate the amount of PhCO₂H extracted into the methylene chloride layer

   \[
   \frac{0.122 \text{ g PhCO}_2\text{H}}{1 \text{ mole PhCO}_2\text{H}} = \frac{Z \text{ g PhCO}_2\text{H}}{10 \text{ mL}}
   \]

4. Calculate \( K_d \)

   \[
   K_d = \frac{C_{\text{methylene chloride}}}{C_{\text{water}}} = \frac{Z \text{ g PhCO}_2\text{H}}{10 \text{ mL}} \times \frac{1000 \text{ mL}}{50 \text{ mL}} = \frac{Z}{10} = \text{Calculated } K_d
   \]

(Continued on other side)
C. Two 5 mL Extractions

1. Calculate amount of Benzoic Acid (PhCO₂H) you are starting with:

\[
\frac{50\text{mL} \times 0.02\text{M PhCO}_2\text{H} \times 122.12\text{ g PhCO}_2\text{H}}{1000\text{mL} \times 0.02\text{M PhCO}_2\text{H} \times 1\text{ mole PhCO}_2\text{H}} = 0.122\text{ g PhCO}_2\text{H} \text{ in starting aqueous solution.}
\]

2. To calculate amount of PhCO₂H remaining in aqueous solution after extraction with 2 x 5 mL of methylene chloride, titrate aqueous layer with ~0.02M NaOH

\[
\frac{\text{mL} \times 0.02\text{M NaOH} \times 1\text{ mole PhCO}_2\text{H}}{1000\text{mL} \times 0.02\text{M NaOH} \times 1\text{ mole PhCO}_2\text{H}} = \frac{122.12\text{ g PhCO}_2\text{H}}{1\text{ mole PhCO}_2\text{H}} = Y\text{ g PhCO}_2\text{H} \text{ remaining in aqueous layer}
\]

3. Calculate the total amount of PhCO₂H extracted into the 2 x 5 mL methylene chloride layers

\[
0.122\text{ g PhCO}_2\text{H} - Y\text{ g PhCO}_2\text{H} = Z\text{ g PhCO}_2\text{H} \text{ total amount in 2 x 5 mL methylene chloride extracts}
\]

4. Calculate theoretical amount of PhCO₂H that should be removed by 2 x 5 mL methylene chloride extractions using K_d calculated in Step B4. For the first 5 mL extraction with methylene chloride where W is the amount of benzoic acid extracted into methylene chloride:

\[
K_d = \frac{C_{\text{methylene chloride}}}{C_{\text{water}}} = \frac{W\text{ g PhCO}_2\text{H} / 5\text{ mL}}{(0.122\text{ g PhCO}_2\text{H} - W\text{ g PhCO}_2\text{H}) / 50\text{ mL}} = \frac{W / 5}{(0.122 - W) / 50} = \text{ Calculated } K_d \text{ (value determined in B4)}
\]

(K_d = known quantity; solve equation for W).

Repeat this calculation for the second 5 mL extraction using the W value determined above and where A is the amount of benzoic acid extracted into the second 5 mL portion of methylene chloride:

\[
K_d = \frac{C_{\text{methylene chloride}}}{C_{\text{water}}} = \frac{A\text{ g PhCO}_2\text{H} / 5\text{ mL}}{(0.122\text{ g PhCO}_2\text{H} - W\text{ g PhCO}_2\text{H} - A\text{ g PhCO}_2\text{H}) / 50\text{ mL}} = \frac{A / 5}{(0.122 - W - A) / 50} = \text{ Calculated } K_d \text{ (value determined in B4)}
\]

(W, K_d = known quantities; solve equation for A).

Combine calculated W and A values to get theoretical amount of acid removed by two 5 mL extractions and compare with the amount experimentally found.