Extraction, Distribution Coefficient

Experiment 4A Calculation Worksheet

A. Prepare the Standard Benzoic Acid Solution

1. Calculate the molarity of your standard Benzoic Acid ($PhCO_2H$; Molecular Weight: 122.12) solution:

$$0.61\text{g } PhCO_2H \times \frac{1\text{ mole } PhCO_2H}{122\text{ g } PhCO_2H} = .005\text{ mole } PhCO_2H \text{ dissolved in 250 mL water}$$

Benzoic Acid
($PhCO_2H$ where Ph = C_6H_5)
M.W. = 122.12

$$\frac{.005\text{ mole } PhCO_2H}{250\text{ mL water}} = \frac{X\text{ mole } PhCO_2H}{1000\text{ mL water}}$$

Solve for X: X = 0.02 mole $PhCO_2H$ in 1000 mL water or 0.02 M $PhCO_2H$

B. Single 10 mL Extraction and Determination of Distribution Coefficient

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

$$50\text{ mL } 0.02M\ PhCO_2H \times \frac{0.02\text{ mole } PhCO_2H}{1000\text{ mL } 0.02M\ PhCO_2H} \times \frac{122.12\text{ g } PhCO_2H}{1\text{ mole } PhCO_2H} = 0.122\text{ g } PhCO_2H \text{ in starting aqueous solution.}$$

2. To calculate amount of $PhCO_2H$ remaining in aqueous solution after extraction with 10 mL of methylene chloride, titrate aqueous layer with 0.02M NaOH

$$\_\_\_\text{mL } 0.02M\ NaOH \times \frac{0.02\text{ mole NaOH}}{1000\text{mL } 0.02M\ NaOH} \times \frac{1\text{mole } PhCO_2H}{1\text{ mole NaOH}} \times \frac{122.12\text{ g } PhCO_2H}{1\text{ mole } PhCO_2H} = Y\text{ g } PhCO_2H \text{ remaining in aqueous layer}$$

3. Calculate the amount of $PhCO_2H$ extracted into the methylene chloride layer

0.122 g $PhCO_2H$ – Y g $PhCO_2H$ = Z g $PhCO_2H$ in 10 mL methylene chloride extract

4. Calculate K_d

$$K_d = \frac{C_{methylene\ chloride}}{C_{water}} = \frac{Z\text{ g } PhCO_2H / 10\text{ mL}}{(Y\text{ g } PhCO_2H) / 50\text{ mL}} = \frac{Z / 10}{Y / 50} = \text{Calculated } K_d$$

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Experiment 4A Calculation Worksheet (continued)

C. Two 5 mL Extractions

1. Calculate amount of Benzoic Acid ($PhCO_2H$) you are starting with:

$$50\text{mL } 0.02\text{M } PhCO_2H \times \frac{0.02 \text{ mole } PhCO_2H}{1000 \text{ mL } 0.02\text{M } PhCO_2H} \times \frac{122.12 \text{ g } PhCO_2H}{1 \text{ mole } PhCO_2H} = 0.122 \text{ g } PhCO_2H \text{ in starting aqueous solution.}$$

2. To calculate amount of $PhCO_2H$ remaining in aqueous solution after extraction with 2 x 5 mL of methylene chloride, titrate aqueous layer with ~0.02M NaOH

$$\_\_\_\text{mL } 0.02\text{M NaOH} \times \frac{0.02 \text{ mole NaOH}}{1000\text{mL } 0.02\text{M NaOH}} \times \frac{1\text{mole } PhCO_2H}{1 \text{ mole NaOH}} \times \frac{122.12 \text{ g } PhCO_2H}{1 \text{ mole } PhCO_2H} = Y \text{ g } PhCO_2H \text{ remaining in aqueous layer}$$

3. Calculate the total amount of $PhCO_2H$ extracted into the 2 x 5 mL methylene chloride layers

$0.122 \text{ g } PhCO_2H - Y \text{ g } PhCO_2H = Z \text{ g } PhCO_2H$ total amount in 2 x 5mL methylene chloride extracts

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4. Calculate theoretical amount of $PhCO_2H$ that should be removed by 2 x 5 mL methaylene 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:

$$K_d = \frac{C_{methylene\ chloride}}{C_{water}} = \frac{W \text{ g } PhCO_2H / 5 \text{ mL}}{(0.122 \text{ g } PhCO_2H - W \text{ g } PhCO_2H) / 50 \text{ mL}} = \frac{W / 5}{(0.122 - W) / 50} = \text{Calculated } K_d \text{ (value determined in B4)}$$

(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:

$$K_d = \frac{C_{methylene\ chloride}}{C_{water}} = \frac{A \text{ g } PhCO_2H / 5 \text{ mL}}{(0.122 \text{ g } PhCO_2H - W \text{ g } PhCO_2H - A \text{ g } PhCO_2H) / 50 \text{ mL}} = \frac{A / 5}{(0.122 - W - A) / 50} = \text{Calculated } K_d \text{ (value determined in B4)}$$

(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.