

## Extraction, Distribution Coefficient

### Experiment 4A. Calculation Worksheet

#### A. Prepare the Standard Benzoic Acid Solution

1. Calculate the molarity of your standard Benzoic Acid ( $\text{PhCO}_2\text{H}$ ; Molecular Weight: 122.12) solution:

$$0.61\text{g PhCO}_2\text{H} \times \frac{1\text{ mole PhCO}_2\text{H}}{122\text{ g PhCO}_2\text{H}} = .005\text{ mole PhCO}_2\text{H dissolved in 250 mL water}$$

Benzoic Acid  
( $\text{PhCO}_2\text{H}$ )  
M.W. = 122.12

$$\frac{.005\text{ mole PhCO}_2\text{H}}{250\text{ mL water}} = \frac{X\text{ mole PhCO}_2\text{H}}{1000\text{ mL water}} \quad \text{Solve for X: } X = 0.02\text{ mole PhCO}_2\text{H in 1000 mL water or } 0.02\text{ M PhCO}_2\text{H}$$

#### B. Single 10 mL Extraction and Determination of Distribution Coefficient

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

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

2. To calculate amount of  $\text{PhCO}_2\text{H}$  remaining in aqueous solution after extraction with 10 mL of methylene chloride, titrate aqueous layer with 0.02M NaOH

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

3. Calculate the amount of  $\text{PhCO}_2\text{H}$  extracted into the methylene chloride layer

$$0.122\text{ g PhCO}_2\text{H} - Y\text{ g PhCO}_2\text{H} = Z\text{ g PhCO}_2\text{H in 10 mL methylene chloride extract}$$

4. Calculate  $K_d$

$$K_d = \frac{C_{\text{methylene chloride}}}{C_{\text{water}}} = \frac{Z\text{ g PhCO}_2\text{H} / 10\text{ mL}}{(Y\text{ g PhCO}_2\text{H}) / 50\text{ mL}} = \frac{Z / 10}{Y / 50} = \text{Calculated } K_d$$

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Experiment 4A Calculation Worksheet (continued)

C. Two 5 mL Extractions

1. Calculate amount of Benzoic Acid ( $\text{PhCO}_2\text{H}$ ) you are starting with:

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

2. To calculate amount of  $\text{PhCO}_2\text{H}$  remaining in aqueous solution after extraction with 2 x 5 mL of methylene chloride, titrate aqueous layer with ~0.02M NaOH

$$\underline{\hspace{2cm}} \text{ mL } 0.02\text{M NaOH} \times \frac{0.02 \text{ mole NaOH}}{1000\text{mL } 0.02\text{M NaOH}} \times \frac{1 \text{ mole PhCO}_2\text{H}}{1 \text{ mole NaOH}} \times \frac{122.12 \text{ g PhCO}_2\text{H}}{1 \text{ mole PhCO}_2\text{H}} = \underline{Y} \text{ g PhCO}_2\text{H} \text{ remaining in aqueous layer}$$

3. Calculate the total amount of  $\text{PhCO}_2\text{H}$  extracted into the 2 x 5 mL methylene chloride layers

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

4. Calculate theoretical amount of  $\text{PhCO}_2\text{H}$  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.