Experiment 28

FV 12/19/08

DETERMINATION OF AN EQUILIBRIUM CONSTANT AND HYDROGEN BONDING[1]

MATERIALS:

50 mL buret, 5-250 mL Erlenmeyer flasks, 4 rubber stoppers, 50 mL graduated cylinder, 0.50 M NaOH solution, 25 mL pipet, toluene, pentanol, 4 M stock solution of butyric acid (in hoods!), phenolphthalein.

DISCUSSION:

Chemical substances dissolve in solvents according to the nature and strength of the intermolecular forces which can be formed between solute and solvent. It is possible to measure absolute solubilities and thus gain insight into the solute-solvent interactions. An alternate method is to examine the relative amounts of a solute which is found in two nonmiscible solvents, both of which may be solvents for the solute. This is not unlike placing a group of students in a two room apartment in which there is a television set in one room and a radio in the second room. After a time, some number of students will be in the television room and the rest will be in the radio room. The simple ratio of the students in these two rooms would be equivalent to the equilibrium constant, K. For this example:

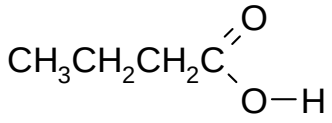
$$K = [\text{no. in TV room}]/[\text{no. in radio room}]$$

For a solute, a similar process can be explored by first dissolving the solute in one solvent and then adding the second solvent and shaking the mixture until the solute has reached its equilibrium concentrations in the two solvents. The resulting equilibrium constant (called a "Distribution Coefficient" or K_d) is formulated as:

$$K_d = [\text{solute}]_{\text{layer 1}}/[\text{solute}]_{\text{layer 2}}$$

and is a direct measure of the relative intermolecular forces between the solute and the two solvents.

In the current experiment, the solute to be examined is butyric acid (a foul smelling component of rancid butter), an organic acid which has the chemical structure:



The carboxylic acid end of this molecule ($-CO_2H$) is polar and capable of strong hydrogen bonding, while the hydrocarbon end ($CH_3CH_2CH_2-$) is nonpolar and has no hydrogen bonding capability. The compound is soluble to some extent in both water and organic solvents.

In this experiment the relative solubility of butyric acid will be studied using water, pentanol and toluene as solvents. Water is not very soluble in either pentanol or toluene while pentanol is fairly soluble in toluene. Therefore, the comparisons will be made between pentanol and water and separately between toluene and water. By comparing the two equilibrium constants it will be possible to develop a relative order for butyric acid solubility in the three solvents. The amount of butyric acid present in the water at equilibrium is determined by titration of the water phase of the mixtures. (Titrations of nonaqueous solutions are possible but difficult and are unnecessary in this case.)

[1] See: Koubek, E., Johnstone, P., Journal of College Science Teaching. 3, 241 (1978).

PROCEDURE:

Note: Butyric acid has a strong, unpleasant odor. To minimize exposure, each hood contains 4 M butyric acid solution and a waste beaker. Do not remove any solutions containing butyric acid from your hood.

Work in groups of four for this lab. Each midshipman should run the experiment with one solution.

Make up four solutions in 250 mL flasks (in the hood) as outlined in the following table. One half of the class will use toluene. The other half will use pentanol. Your instructor will indicate which solvent you are to use. At the conclusion of the experiment, obtain data for the other solvent, again following the directions of your instructor as to how this is to be done.

Solution #	4 M butyric acid	H_2O	organic solvent
1	5 mL	45 mL	50 mL
2	10 mL	40 mL	50 mL
3	20 mL	30 mL	50 mL
4	30 mL	20 mL	50 mL

Stopper each flask with a rubber stopper covered with polyethylene and shake vigorously for 15 minutes. Take care not to lose any of the solution. After this time remove 25 mL of the aqueous phase of each mixture with a 25 mL pipet and titrate with the 0.5 M NaOH provided using phenolphthalein as your indicator. Also titrate 5 mL of the original 4M butyric acid solution with the same base in order to get the mols of butyric acid used in each experiment to 3 significant figures.

DATA:

Solvent _____

1. _____ final buret reading

   _____ initial buret reading

   _____ vol. of 0.50 M NaOH

2. _____ final buret reading

   _____ initial buret reading

   _____ vol. of 0.50 M NaOH

3. _____ final buret reading

   _____ initial buret reading

   _____ vol. of 0.50 M NaOH

4. _____ final buret reading

   _____ initial buret reading

   _____ vol. of 0.50 M NaOH

5 mL of butyric acid

_____ final buret reading

_____ initial buret reading

_____ vol. of 0.50 M NaOH

DATA ANALYSIS:

Organic solvent used_____

Fill in the following table (Note that each experiment contains 50 mL of water and 50 mL or organic solvent). Attach the calculations used in your experiment on a separate page.

Exp.	Total mols of butyric acid	Mols of butyric acid in water layer	Mols of butyric acid in organic layer	$[\text{butyric acid}]_{water}$	$[\text{butyric acid}]_{organic}$	K_d
1						
2						
3						
4						

Calculate the average K_d for your solvent: _____

Get the average K_d from a group that used the other solvent.

K_d _____ Solvent _____ Data from Midns _____

Use these distribution constants to rank the solubility of butyric acid in water, pentanol, and toluene.

Find the chemical structures of pentanol and toluene and draw them below:

Using your knowledge of molecular dipoles and intermolecular bonding, explain the order of relative solubilities that you obtained in this experiment.