

# Lab Project #1

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## Part 1. Solubility as a function of pH.

*Table 1 - Effect of pH on Solubility*

Compound	Soluble/Not Soluble and Observations		
	Water	1M NaOH	1M HCl
Benzoic Acid	no	yes	yes
Caffeine	no	no	yes
Naphthalene	no	no	no

Why certain compounds became soluble in aqueous solutions?

- Breaking bonds require energy and it highly depends on the polarity of the solute and the compound. We know that polar molecules are BEST solvated by polar solvent; the same can be said for nonpolars. So, regarding the cases in the table above, benzoic acid is nonpolar so, it can be visibly solvated in NaOH and HCl solutions which are nonpolar too. As for caffeine, it is a polar molecule so it can be dissolved in H<sub>2</sub>O and since it is slightly basic, the equilibrium will shift when added HCl to lower pH. For Naphthalene, we can argue that it cannot dissolve in water because it is nonpolar.
- Compounds can be separated into a conjugate acid form and a conjugate base form. When we do this separation, energy is needed and bonds between the cation and anion in the compounds need to be broken usually by the anions in the aqueous solutions. If the bonds in the compounds are strong enough to withstand the dissociation by the aqueous anions, then the compounds are not soluble in said solutions and vice versa.

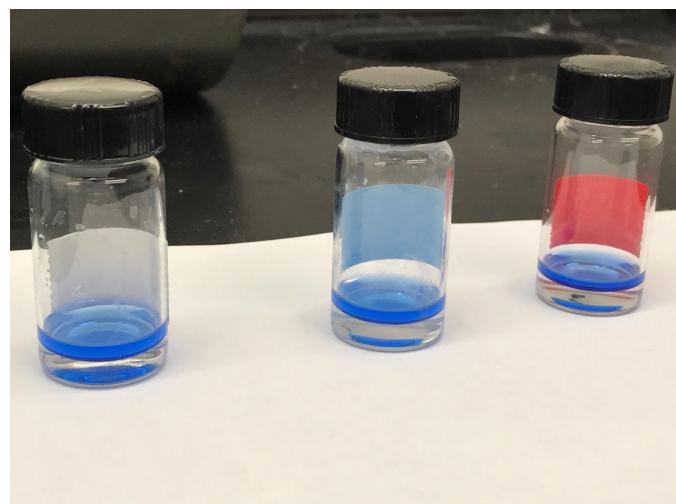
## Part 2. Solubility tests of dyes.

*Table 2 - Testing Compound Solubility*

Dye	In which phase it dissolved: organic (hexane) or aqueous (water)		
	Acidic	Neutral	Basic
Sudan Blue	hexane	hexane	hexane
Sudan Orange	water	hexane	water
Congo Red	water	water	water

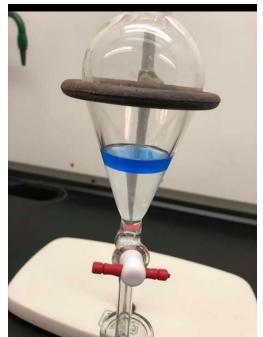
- For the sudan Blue dye, we can notice that the only force that is applied is the dispersion force. In fact, dispersion force is the only force that is used in hexane too so after testing the acidic, neutral and basic sudan Blue, we noticed that the Sudan Blue is miscible with the hexane since they share the same intermolecular force which is the dispersion force in this case.
- For the Sudan Orange dye, it is not exactly the same case since the acidic and the basic parts will form H-Bond which will allow them to be miscible in water. in contrast, the neutral can not form a H-Bond so the only force that is applied on it is the dispersion force which will lead the neutral to be soluble in hexane since they both share the same intermolecular force which is the dispersion force.
- For the Congo Red, the neutral, basic and acidic will be soluble in water since in all these three conditions, the intermolecular forces between them and the water is similar. In fact, the congo red in acidic, basic and even neutral can be miscible with water.

*Photos taken:*



## Part 3. Using liquid-liquid extractions to separate compounds based on solubility differences.

### First Dye

Before Mixing	After Mixing	After adding NaOH		
Phase 1: Hexane Dye A	Phase 1: Hexane Dye A	Phase 1: Hexane Dye A		
Phase 2: Aqueous Trace Amounts of Dye A	Phase 2: Aqueous No Dye	Phase 2: NaOH No Dye		

### Second Dye

Before mixing	After mixing	Added NaOH		
Phase 1: Hexane Dye B	Phase 1: Hexane Dye B	Phase 1: Hexane Dye B (non polar parts)		
Phase 2: Aqueous Traces of Dye B	Phase 2: Aqueous No Dye	Phase 2: NaOH Dye B (polar parts)		

#### Reasoning behind graph:

Water and NaOH have greater densities than Hexane, so naturally Hexane will float on top of them. In our first experiment with dye a, you can see that the dye has a high partitioning coefficient as it is only found with the organic phase. This is reinforced when we added the NaOH to the Hexane. As for dye B, we can determine that its partitioning coefficient is low enough for there to be a great amount of separation between it and the water, but high enough that it can be observed when NaOH is added. By the Colour of the NaOH, we can assume that most of the dye is still with the Hexane, and thus the dye isn't very polar.

## Part 4. “Tuning” pH to affect solubility.

*Table 3 - Tuning the pH*

Compound	pKa	Soluble/Not Soluble and Observations		
		Water	1M NaOH	Weak Base
Benzoic Acid	4.20	no	yes	Partial
$\beta$ -Naphthol	9.51	no	yes	no

- The solution that showed different solubility between benzoic acid and beta-naphthol is 1M HCl.

- Calculating the pH of 1M NaOH (100% dissociation, strong base):

$$pOH = -\log[OH^-] = -\log(1) = 0 \rightarrow pH = 14 - 0 = 14$$

- Calculating the pH of 1M HCl (100% dissociation, strong acid):

$$pH = -\log[H^+] = -\log(1) = 0 \rightarrow pH = 0$$

The results can be explained by taking into account how benzoic acid reacts with the NaOH solution to form a salt which is then soluble in water (which is readily available in the aqueous solution).

- For Beta-Naphthol, it is a polar molecule which is expected to be soluble in water (like dissolves like) but our experimental result shows the opposite. This inconsistency compared to the theory could be due to the fact that we did not have the necessary equipment to measure exactly how much it was dissolved and used only eye observation to determine its solubility in water. For why it dissolves in 1M NaOH solution, Beta-Naphthol is an acid so it has to react to NaOH to some degree to create 2 new acid and base species that are soluble in NaOH.
- Beta-Naphthol is insoluble in a weak base solution because the ions in the weak base have weak IMF therefore cannot separate the Beta-Naphthol molecules in order to solvate them.

## Part 5.

### 1. Derivation of equation (4)

At first, we have to understand that  $\alpha$  is the ratio of unprotonated acid in the solution, therefore we have to understand that  $\alpha = [\text{HA}]$ , therefore  $= (1 - \alpha)$ . Now let's use the acid equilibrium and plug in those two values

$$Ka = [H^+][A^-] \div [HA]$$

$$Ka = [H^+](1 - \alpha)/\alpha$$

$$Ka = ([H^+] - \alpha[H^+])/\alpha$$

$$Ka = ([H^+]/\alpha) - [H^+]$$

$$Ka + [H^+] = [H^+]/\alpha$$

therefore:

$$\alpha = [H^+]/([H^+] + Ka)$$

### 2.

The meaning of equation 3 is simple, it is a way to find the partition coefficient of any compound, preferably acids or base, when the pH of said acid or base is near its pKa. Which means that the compound is at equilibrium. It makes sense to add the  $\alpha$  times the partition coefficient of the un-ionized part of the compound to the  $(1 - \alpha)$  time the ionized partition coefficient; since the  $\alpha$  is already the ratio of un-ionized molecules in the solution and  $(1 - \alpha)$  is just the ration of the ionized molecule, by multiplying each ratio of ionized and unionized to their respective partition coefficients we can have the respective proportion of each partition coefficient in the solution and by adding them together we should find the overall partition coefficient of the whole reaction.

### 3.

The graph represents the relation the between the partition coefficient of benzoic acid and aniline and the pH of the solutions. Benzoic acid is, as the name says, an acid with pKa of 4.20 and here is the chemical reaction of dissolution in water:

$C_7H_6O_2 + H_2O \rightleftharpoons C_7H_5O^-_2 + H_3O^+$ , and here is the equation for aniline which is a weak base with pKb of 4.63:  $C_6H_5NH_2 + H_2O \rightleftharpoons C_6H_5NH_3^+ + OH^-$ . In the plot we can see that the relation between the partition coefficient of Benzoic acid is inversionally proportional to the value of the pH, as the value of the pH gets stronger the value of the partition coefficient of Benzoic acid gets weaker. On the contrary, its seems that the value of the partition coefficient of aniline is proportional to the value of the pH, meaning that it increase as the value of the pH increase.. We can see a slight increase in the partition coefficient of I-butanol, but since it isn't soluble in water it is negligible. Something important to see is that when the pH is equal to the value of the pKa of Benzoic acid and to the value of the pKb of aniline, the partition coefficient of the compound is relatively the same with a value of 4,5.

## Part 6. Conclusions

In conclusion, we are able to know if two compounds are miscible or not by comparing their intermolecular forces. In fact, if they have similar forces then they can be mixed together.