



# **Titrimetric Study of Solubility of Solute Benzoic Acid and Their Partition in Water and Benzene Solvents**

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## **Author's contribution**

*The sole author designed, analyzed, interpreted and prepared the manuscript.*

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## **ABSTRACT**

The solubility and distribution coefficient ( $K$ ) of solute in solvent is depends on temperature and solute-solvent interaction, where the solute is partitioned between two immiscible solvents phase and dissociated into ionic form. Here, we have reported the titrimetric study for solubility and partition or distribution coefficient of benzoic acid (solute) in aqueous water and in organic benzene which are using as solvents. The benzoic acid solubility (in g/100g of solvent) in water and in benzene solutions have determined by titrimetrically. There is partitioning and concentration of such acid in these solvent phase by shake-flask and acid-base titration method as well. The benzoic acid solubility and their distribution between water and benzene as in different pH buffer solutions have been analyzed at room temperature (25°C) in acidic, neutral and basic (pH 4.0, 7.0 and 9.0) medium, respectively.

*Keywords: Solubility; benzoic acid; distribution coefficient; pH effect; nernst's partition law.*

## **1. INTRODUCTION**

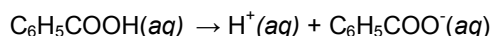
Indeed, the first study of solubility with partition ratio of solute in solvent have performed by Berthelot and Jungfleisch [1], but it clearly proved

by Nernst in 1891. A literature reveals about solubility and partition of solute with its application [2], the partitioning for where both solid-solid phase [3], and one molten and second as solid phase [4]. Liquid-liquid partition

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coefficients now have been determined by using methods of chromatographic separation with partition of solute between the stationary and mobile phase [5-6]. Solubility and dissociation of benzoic acid in water by titrimetrically [7], partition of octanol and water [8], and salivation thermodynamics in different solvents as water-chloroform system have also been well reported [9]. Concerning, the present study of benzoic acid solubility and its dissociation process between water and benzene solvents have been reported by adapting of various physico-analytical methods [10-11], at room temperature (25°C) with compatibility of Le Chatelier's principle [12]. In series of aromatic organic acids the benzoic acid (C<sub>6</sub>H<sub>5</sub>COOH) having less solubility in ordinary water through the carboxylic acid group polarization during on dissociation partially in water by forming hydrogen bonding attachment to produce benzoate anion (C<sub>6</sub>H<sub>5</sub>COO<sup>-</sup>) and hydronium cation (H<sub>3</sub>O<sup>+</sup>) [7].

In saturated aqueous solution (aq), a little molar solubility of benzoic acid which has following equilibrium-



The molar solubility of benzoic acid in aqueous (water) is determined by titrimetrically against NaOH solution as standard strong base, then equilibrium can be expressed as-

$$K = [\text{H}^+][\text{C}_6\text{H}_5\text{COO}^-] / [\text{C}_6\text{H}_5\text{COOH}(\text{aq})]$$

Where, the *K* is dissociation constant of benzoic acid.

Here, we have been reported the titrimetric study of benzoic acid's solubility and distribution coefficient between immiscible two solvents as hydrophilic aqueous water and hydrophobic organic benzene. In this work we are determined by using equation derived from Nernst distribution coefficient law, which have used and improved to finding an accurate results as compared to the reported its *K* value in the literature study [13]. Mathematically, the expression of Nernst distribution equation which is given as- '*K*' = C<sub>A</sub>/C<sub>B</sub>. Where, the C<sub>A</sub> and C<sub>B</sub> are concentration of reporting substances as for solvent A and B, and *K* is a constant of Nernst equation and it also known as partition or distribution coefficient where its value is independent of actual concentration of the solutions. In case when solute undergoing partition has molecular weight in one solvent say (organic solution) *n* times higher than water at

equilibrium, the distribution ratio *K* becomes-  $K = C(\text{aq})/C(\text{org})^{1/n}$  [14]. Here, C(aq) is equilibrium concentration of solute (benzoic acid) in aqueous solution (water), and C(org) is equilibrium concentration of solute in organic solvent (benzene). Since, benzoic acid exists as dimer in aprotic solvents like in benzene (i.e., *n*=2,3), hence the modified distribution law is valid i.e.,  $K = C(\text{aq})/n\sqrt{C(\text{org})}$ . Where, *n* is known as degree of association with *K* as partition ratio or coefficient.

Although, in early 20<sup>th</sup> century, the salt of benzoic acid have been used for domestic, industrial and medicinal purposes [15-16]. The benzoic acid (M.F. C<sub>6</sub>H<sub>5</sub>COOH and M.P. 121°C) is a colorless crystalline solid substance with pleasant smelling [17]. In present study we have been selected a benzoic acid because its suite solubility in variety of polar and non-polar solvents such as benzene (C<sub>6</sub>H<sub>6</sub>), carbon tetrachloride (CCl<sub>4</sub>), chloroform (CHCl<sub>3</sub>), alcohol (C<sub>2</sub>H<sub>5</sub>OH), acetone (CH<sub>3</sub>COCH<sub>3</sub>) and in liquor ammonia (liq.NH<sub>3</sub>) [18], etc. The benzoic acid solubility in water and benzene solutions with pH value as in acidic (4.0), neutral (7.0) and basic (9.0) medium are determined by using titration method and partitioning study of that acid in both liquid solvents by shake-flask method. The solute benzoic acid concentration in water and benzene solution is analyzed by applying acid-base titration method as well.

## 2. METHODOLOGY

In experimental procedure, the all required chemicals and solvents which are used in this study as an analytical reagent grade on laboratory based as well as the solvent distilled water is also freshly prepared which is used during throughout the work. The carbonate free sodium hydroxide (NaOH) solutions are prepared as work suggested by Vogel [19]. A Research Lab Fine Chemicals Industries, Mumbai, have provided solid benzoic acid, (C<sub>6</sub>H<sub>5</sub>COOH) and the Merck Specialties (Pvt.) Limited, Mumbai, to buffer solutions as of pH 4.0, 7.0 and 9.0 value.

At 25°C temperature we are applying the acid-base titration method, for estimation of benzoic acid solubility at varies pH buffer solution. Now, in different beakers take 100ml buffer solution of pH 4.0, pH 7.0 and pH 9.0, and then in every beaker we added solid benzoic acid about 200mg, and for producing saturated solution it stirred with glass rod. Notably, some solid un-dissolved and must be left. If required these solution is heated.

At 25°C, cooling these solution which are prepared and into dry conical flask (say  $W_1$ ) it withdrawn a 5.0ml of these solution. Again weight (say  $W_2$ ) of 5.0ml solution contained conical flask and indicator phenolphthalein is used and it titrate against to these solution with prepared of 0.05N NaOH solution. Records the burette reading (V) as appearing pink colour show it end point. As given below described formula we determine the benzoic acid solubility (S) in gram/100gram of solvents and to compare with water (distilled) as blank against solubility [18].

Concerning, if

the conical flask weight (empty) =  $W_1$   
 the conical flask weight with solution (5.0ml) =  $W_2$   
 the solution weight, ( $W_2 - W_1$ ) gram =  $W_3$   
 the solute weight ( $C_6H_5COOH$ ) =  $W_4$   
 here,  $W_4$  is (gram of substance x N of solution x ml of solution used) as  $0.12g \times 0.05N \times V$   
 the solvent weight, ( $W_3 - W_4$ ) =  $W_5$   
 thus,  $S = \text{solute weight } (W_4) \times 100 / \text{solvent weight } (W_5)$ .

By the using acid-base and shake-flask method we estimated partition coefficient (K) of benzoic acid at different pH. Where, in a beaker we prepared 10 % benzoic acid solution in benzene (say 2B solution). Here, the four different type of solutions are prepared in separating funnel, where buffer solution having the same pH 4.0 for each, is given below-

- (1). Buffer solution, (40 ml) + 2B solution, (20 ml) + benzene, (20 ml).
- (2). Buffer solution, (40 ml) + 2B solution, (25 ml) + benzene, (15 ml).
- (3). Buffer solution, (40 ml) + 2B solution, (30 ml) + benzene, (10 ml).
- (4). Buffer solution, (40 ml) + 2B solution, (40 ml).

At 25°C, we used a water-bath incubator shaker for where all prepared solutions with in flasks have been shaken for one day (24hours) and allowing to stand it about half hour to get equilibrium. After then we obtained that the used separating funnel or flask is containing lower aqueous with upper as benzene layer. In dry beaker, firstly we removed the lower layer (aqueous) from each flask by retaining of upper layer (benzene) within separating flask. Now, in a dry conical flask we pipette out aqueous layer of 10 ml, and against with 0.01N NaOH solution we

titrated it, by using indicator as phenolphthalein. The pink colour as it end point. We record this reading well. Benzene layer (5.0 ml) is pipette out in a another using dry conical flask with adding a 10 ml of distilled water. Using of indicator as phenolphthalein also, these prepared solution with 0.1N NaOH solution against titrated. A pink colour is appearance as it end point of reaction and record this observe burette reading. Notably, we have followed for buffer solution of pH 7.0 and pH 9.0, the same above described procedure with to blank sample as distilled water. By applying normality and modify Nernst partition formula for aqueous water and organic benzene phase or layer, we are estimate as well as to calculate the partitioning (K) behavior of solute in solvent. The following formula have been given below-

[1]- *In moles/litre, the solute (benzoic acid) concentration for aqueous (water) phase;*

As determination of normality it is calculated by applying following normality equation-

$$N_1V_1 = N_2V_2 \dots\dots\dots (i)$$

Here,  
 the  $N_1$  is aqueous layer normality written as,  $N(aq)$  and the  $N(aq) = 0.01 V_2 / 10 \dots\dots(ii)$   
 and, the  $N_2$  is normality of base NaOH which involve for titration as  $N(org) = 0.01 N$ , thus, the

$$N(aq) = C(aq) \dots\dots\dots (iii)$$

The  $V_1$  is taken volume of aqueous layer (10 ml), and  $V_2$  the consumed as burette reading of volume of base NaOH.

[2]- *In moles/litre, the solute (benzoic acid) concentration for organic (benzene) phase;*

As determination of normality it is calculated by applying following normality equation-

$$N_3V_3 = N_4V_4 \dots\dots\dots (iv)$$

Here,  
 the  $N_3$  is organic layer normality as  $N(org)$ , = 0.1

$$V_4 / 5 \dots\dots\dots (v)$$

and the  $N_4$  is normality of base NaOH which used for titration as  $N(org) = 0.1 N$ , thus the,

$$N(org) = C(org) \dots\dots\dots (vi)$$

The  $V_3$  is taken volume of organic layer (5.0 ml), and  $V_4$  as the burette reading (consumed) of volume of base NaOH.

[3]- The partition coefficient ( $K$ ) of solute for water and benzene solvents;

The partition coefficient of aqueous-organic solvents system which is determined from applying equation-

$$\text{Hence, } K = \frac{C(\text{org})}{C(\text{aq})}, \text{ or } = \frac{C(\text{aq})}{C(\text{org})^{1/2}} \dots \dots \quad (\text{vii})$$

At equilibrium,

$$K = \frac{[\text{Aqueous layer Concentration } (C_w)]}{[\text{Organic layer Concentration } (C_o)^{1/2}]}$$

Where,  $C$  is stand for concentration of solute (benzoic acid) in aqueous water and organic benzene layers.

### 3. RESULTS AND DISCUSSION

The solubility of solute is depends on various factors such as temperature, pressure, interaction of solute-solvent with solute dissociation in solvent to ionic form and H-bonding formation etc. The addition of salts in water gives rise a slight changing because solute-solute and solute-solvent interaction [20]. The solute benzoic acid in aqueous solution has less solubility and having weaker electrolyte behaviour [21]. From Table 1 we have reported that the solute benzoic acid's solubility in gram/100gram of solvent, at room temperature about 25°C, as in water (as distilled) is being to  $0.142 \pm 0.033$  and at three pH 4.0, pH 7.0 and pH 9.0 it is varies to  $0.153 \pm 0.012$ ,  $0.186 \pm 0.145$  and  $0.148 \pm 0.708$  g/100g with solvent for benzene-buffer solution, respectively. This observation reveals that the value is being maximum at neutral pH (7.0) for benzene and buffer solution. Here the result analysis of benzoic acid solubility (in g/100g of solvent) is at

room temperature (25°C) where it expressed as;  $n=3$ , and, Mean  $\pm$  SD.

The Fig. 1 have shown benzoic acid solubility with pH effect, where graph is plotting between solubility of solute in g/100g of solvent versus varied pH of buffer solutions and water. These suggested that the acid solubility as in acidic range is becoming higher slightly in comparison of basic medium due to their strength of ionic dissociation [21].

In analytical way from the Table 2, we have reported the pH behaviour on partitioning of benzoic acid in phase system of water and benzene with acidic, neutral and basic buffer solutions. Where, the value for benzene-water phase it is being 0.636 as well as the combine value as 0.841, 0.624 and 0.589 is being for benzene-buffer solutions at different range pH 4.0, 7.0 and 9.0, respectively.

The Fig. 2 has been shown, where, the graph is plotted between partitioning ( $K$ ) and the buffer solutions of different pH value. Graph observation indicate that, the benzoic acid's distribution coefficient in acidic pH medium is higher than in comparison that of neutral as well as in basic medium.

Graphically study for benzene-water system, where both graphs are plotted in respect of solubility ( $S$ ) and partitioning or distribution coefficient ( $K$ ) of solute in solvents with different pH containing buffer solutions and effect of pH on solubility and partitioning of benzoic acid. For distribution of solute in aqueous-organic solvents, the study reveals that as  $C_w$  and  $C_o^{1/n}$  (concentration of water and organic layer) ratio is remain constant, whereas, the  $C_w$  and  $C_o$  ratio may not remain constant. It indicates the formation of H-bonding by association of molecules in dimerization or dimer form between molecules of benzoic acid in organic layer and in aqueous layer the remaining monomer molecules [22].

**Table 1. At 25°C, Solubility analysis of Benzoic Acid [18]**

S.N.	Using solvents	pH	Mean solubility (S) (in g/100g of solvent)
1-	Water (distilled)	-	$0.142 \pm 0.033$
2-	Benzene-buffer solution	4.0	$0.153 \pm 0.012$
3-	Benzene-buffer solution	7.0	$0.186 \pm 0.145$
4-	Benzene-buffer solution	9.0	$0.148 \pm 0.708$

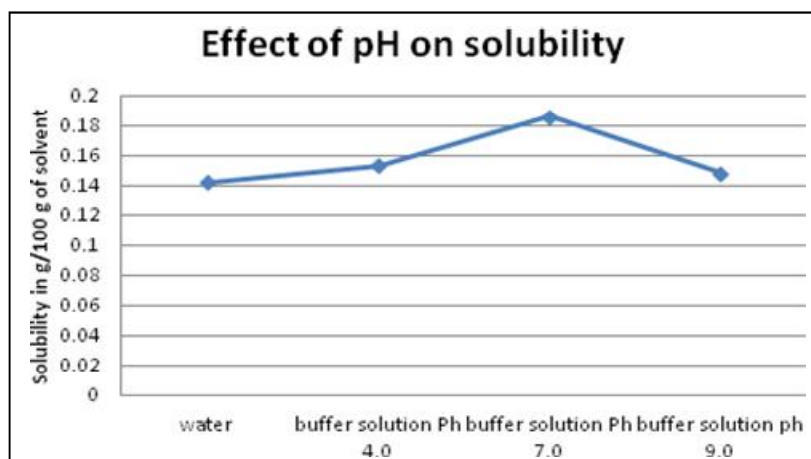


Fig. 1. The pH effect on benzoic acid solubility [18]

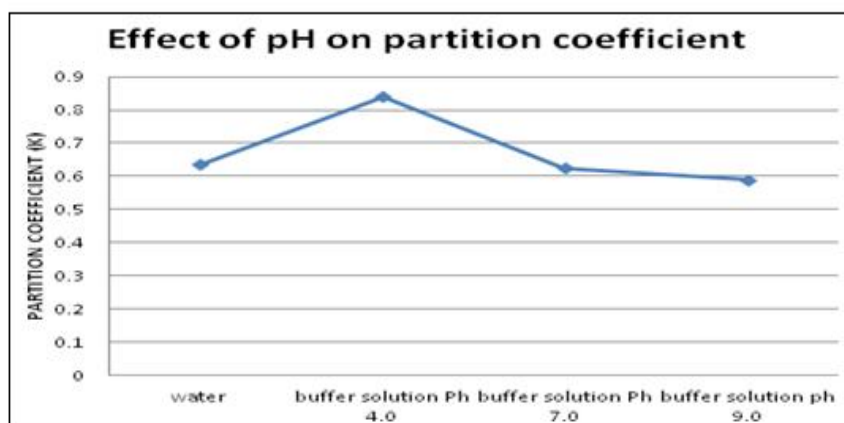


Fig. 2. The pH effect on partition coefficient of benzoic acid [18]

Table 2. pH analysis on partition coefficient of Benzoic Acid [18]

S.N.	Using Solvents	pH	Partition coefficient (K)
1-	Benzene-water solvent	-	0.636
2-	Benzene-buffer solution	pH 4.0	0.841
3-	Benzene-buffer solution	pH 7.0	0.624
4-	Benzene-buffer solution	pH 9.0	0.589

#### 4. CONCLUSION

In conclusion, we have been reported the titrimetric study of solubility and partition or distribution coefficient ( $K$ ) of solute benzoic acid at room temperature (25°C) in water and benzene as two immiscible liquid-liquid solvents. The benzoic acid solubility between water and benzene solution are analyzed by applying titration method. The distribution of benzoic acid in water and benzene solvents have determined by shake-flask method, and the concentration of

acid in these solvents by acid-base titration method. The solubility (in gram/100g of solvent) and partitioning of benzoic acid in water and benzene in different buffer solutions have studied at pH 4.0, 7.0 and 9.0 as in acidic, neutral and basic medium, respectively.

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## COMPETING INTERESTS

Author has declared that no competing interests exist.

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