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EFFECT OF Tert-BUTANOL ON SOLUBILITY OF BENZIMIDAZOLE AT (293.15 TO 313.15) K

Sachin S. Kale

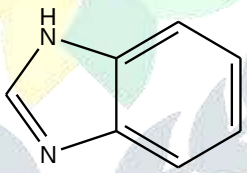
Department of Chemistry, A.C.S. College, Navapur, Dist - Nandurbar (Maharashtra) India

Abstract: Solubility of Benzimidazole in tert-Butanol have been experimentally measured using a gravimetric method at temperatures (293.15 to 313.15) K. Solubility values were correlated with temperature by the Apelblat equation, is used to fit experimental solubility data in tert-butanol solvents at constant temperature. Thermodynamic functions including ΔH_{soln}^0, ΔG_{soln}^0, and ΔS_{soln}^0 of Benzimidazole were obtained from the modified van't Hoff equation. The solubility of Benzimidazole in tert-butanol increases with temperature.

KEY WORDS: Benzimidazole, Solubility, tert-butanol, Apelblat equation, Thermodynamic functions.

I. INTRODUCTION

Benzimidazole is aromatic heterocyclic compound, having molecular formula $C_7H_6N_2$. It is bicyclic compound and consists of a fusion of imidazole and benzene. The structure of Benzimidazole is as



In medicinal chemistry, benzimidazole is privileged structure and one of the important pharmacophore. In many of therapeutic activity, it has an important role such as antibacterial, antifungal, antiulcer, analgesic, antihypertensive, antiviral, anti-inflammatory, antihelmintic and anticancer[1].

A basic step in characterization of a drug or any chemical substance is to determine its solubility behavior, which can give a demonstrative description of its physico chemical properties and thermodynamic functions[2].

Urszula Domanska determined the solubility of Benzimidazole in 1-propanol, 1-butanol, 2-butanol, 2-methyl-2-propanol, 1-hexanol. However there is no data for solubility of Benzimidazole in tertiary butanol and also for present study temperatures[3].

II. EXPERIMENTAL SECTION

Material

Benzimidazole was supplied by spectrochem with purity was 99 % and tert-Butanol was supplied by spectrochem with purity was (GC) 99.5 %.

Apparatus and procedure

An extra quantity of Benzimidazole was added to the solvents prepared by weight (Scale-Tec) with an uncertainty of ± 0.1 mg, in a specially designed 100 mL double jacketed flask. Water was moved at constant temperature between the inner and outer

walls of the flask. The temperature of the moving water was controlled by thermostat to within (± 0.1) K. The solution was constantly stirred using a magnetic stirrer for 1 hr. so that equilibrium is reached, no further solute dissolved, and the temperature of solution is same as that of moving water; the stirrer was switched off; and the solution was allowed to settle for 1 h. Then a fixed quantity of the supernatant liquid was removed from the flask in a weighing bottle by using pipette which is hotter than the solution. The weight of this sample was taken and the sample was kept in an oven at 343 K till the whole solvent was evaporated and the residue was fully dry. This was confirmed by weighing two or three times till a constant weight was obtained after putting the sample in an oven for another 30 min each time. From weight of solute and weight of solution the solubility was calculated. Every experimental value of solubility is an average of minimum three different measurements and the standard uncertainty of the experimental mole fraction solubility (x_B), value is ± 0.003 [4]. The saturated mole fraction solubility (x_B), were calculated using usual equations.

Table 1. Experimental $x_{B(exp.)}$ and calculated $x_{B(cal.)}$ values of solubility for Benzimidazole in tert-butanol at temperatures (293.15 to 313.15) K

Temperature	$x_{B(exp.)}$	$x_{B(cal.)}$	RD
293.15	0.0942	0.0945	-0.0032
295.15	0.0982	0.0981	0.0010
298.15	0.1040	0.1038	0.0019
300.15	0.1084	0.1077	0.0064
303.15	0.1134	0.1137	-0.0026
305.15	0.1175	0.1178	-0.0026
308.15	0.1237	0.1240	-0.0024
310.15	0.1280	0.1283	-0.0023
313.15	0.1354	0.1350	0.0030

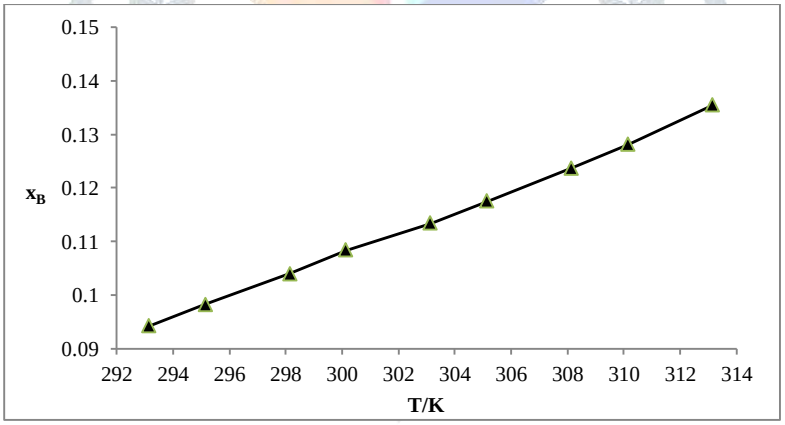


Figure 1. Mole fraction solubility (x_B) of Benzimidazole in tert-butanol with temperature (T/K)

IV. RESULTS AND DISCUSSION

Solubility of Benzimidazole

Table 1 shows the experimental and calculated values of solubility (x_B) of Benzimidazole at 293.15 to 313.15 K in tert-butanol. Variation of solubility with temperature is shown in Figures 1. The solubility of Benzimidazole in tert-butanol increases with temperature.

Table 2. Slope and intercept of plot of x_B versus T

Solvents	m	c	R^2
Tert-butanol	0.002	-0.498	0.998

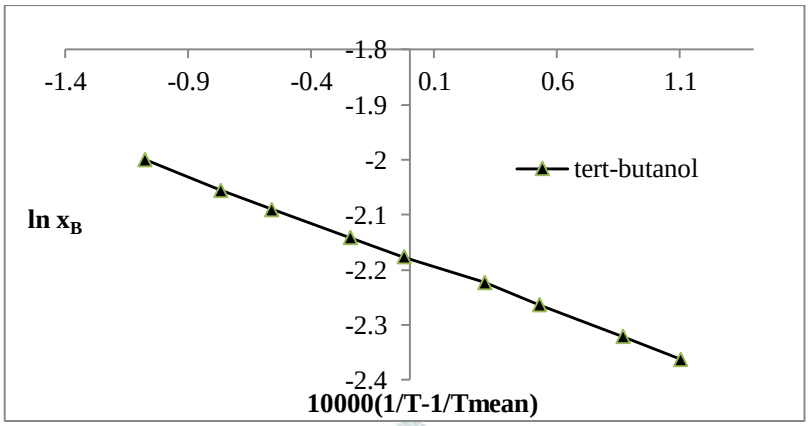


Figure 2. Plot of lnx_B vs. 10000(1/T − 1/T_{mean}) for Benzimidazole in tert-butanol.

Table 3. Slope (m) and intercept (c) of the lnx_B vs. 10000(1/T − 1/T_{mean}) plot along with R^2

Solvents	m	c	R^2
Tert-butanol	0.163	-2.178	0.999

Apelblat Model

It has been generally deemed that the Apelblat equation was successfully used in correlating the solubility in pure solvent[5], the equation, shown as equation (1), was deduced from ideal solid liquid equilibrium equation[6].

$$\ln x_{B=} A + \frac{B}{T} + C\ln T \quad \ldots\ldots\ldots\ldots (1)$$

Where, A, B and C were set to be parameters of the equation. The parameter values for Benzimidazole solubility correlation were regressed from the experimental values and given in table 4. Using the parameters obtained, the calculated solubilities of Benzimidazole at temperature were obtained according to equation (1). The relative deviations (RD) were defined as equation (2) to evaluate the fitting effect.

$$RD = \frac{x_B^{exp.} - x_B^{cal.}}{x_B^{exp.}} \quad \ldots\ldots\ldots\ldots\ldots (2)$$

Where, $x_B^{exp.}$ and $x_B^{cal.}$ were the experimental and calculated mole fraction solubility respectively. Calculated and experimental values along with relative deviations are listed in table 1.

Table 4. Parameters and correlation errors of experimental values with the Apelblat equation

Solvents	Parameters			R^2
	A	B	C	
tert-butanol	11.4849	-2009.18	-1.23057	0.9992

Thermodynamics functions

In this work the thermodynamic functions in the process of solution of Benzimidazole are calculated on the basis of the solubility of Benzimidazole in tert-butanol.

According to the van't Hoff equation, the standard molar enthalpy change of solution ΔH^0_{soln} is generally obtained from the slope of the lnx_B vs 1/T plot. Average temperature T_{mean} is used to get a single value of ΔG^0_{soln} and ΔS^0_{soln} in the temperature range considered

$$T_{mean} \frac{n}{\sum_{i-1}^{n}\left(\frac{1}{T}\right)} \quad \ldots\ldots\ldots\ldots (3)$$

Where, n is the number of experimental points. In the present work, T_{mean} = 302.92 K and the temperature range is (293.15 to 313.15) K in pure solvent. Heat capacity of the solution can be assumed as constant. So values of ΔH^0_{soln} are derived using eq 4.

$$\Delta H^0_{sol} = -R\left(\frac{\partial \ln x_B}{\partial 1/T}\right) - R\left[\frac{\partial \ln x_B}{\partial\left(\frac{1}{T}-\frac{1}{T_{mean}}\right)}\right] \quad \text{..... (4)}$$

The $\ln x_B$ versus 10000 (1/T − 1/Tmean) plot of different solutions including pure solvent are displayed in Figure 2. From figures, it is observed that a trend of increasing solubility with temperature is observed. The slope and the intercept for solvent are listed in Table 3. The modified van't Hoff equation can be supposed to be fit to calculate the enthalpy change of solution. The standard molar Gibbs energy change for the solution process ΔG^0_{soln}, can be calculated in the way similar to Krug et al [7] as

$$\Delta G^0_{sol} = -RT \times \text{intercept} \quad \text{..... (5)}$$

The intercept used is that obtained in plots of $\ln x_B$ as a function of (1/T − 1/Tmean). The standard molar entropy change ΔS^0_{soln} is calculated from

$$\Delta S^0_{Sol} = \frac{\Delta H^0_{Sol} - \Delta H^0_{Sol}}{T_{mean}} \quad \text{..... (6)}$$

Both ΔG^0_{soln} and ΔS^0_{soln} pertain to the mean temperature T_{mean} = 302.92 K.

The results are shown in Table 5, together with ζH and ζTS. It is worthy to note that relative contribution of enthalpy ζH and ζTS which are defined as

$$\zeta_H = \frac{\Delta H^0_{Sol}}{|\Delta H^0_{Sol}| + |T\Delta S^0_{Sol}|} \quad \text{..... (7)}$$

$$\zeta_{TS} = \frac{|T\Delta S^0_{Sol}|}{|\Delta H^0_{Sol}| + |T\Delta S^0_{Sol}|} \quad \text{..... (8)}$$

can be simply used to calculate the main contributors of enthalpy or entropy on ΔG^0_{soln} [8].

The values of ΔH^0 and ΔS^0 for all solutions are positive indicating the solution process as endothermic. The contribution of enthalpy to positive molar Gibbs energy is high as compared to entropy for all solutions.

Table 5. Thermodynamic functions relative to solution process of Benzimidazole at T_{mean} = 302.92 K

Solvents	ΔH^0sol/kJ·K^{-1}·mol^{-1}	ΔG^0soln/kJ·K^{-1}·mol^{-1}	ΔS^0soln/KJ·K^{-1}·mol^{-1}	$T\Delta S^0$soln/KJ·K^{-1}·mol^{-1}	ζH	ζTS
tert-butanol	13.5518	5.4854	0.0266	8.0664	0.6269	0.3731

CONCLUSION

The purpose of this study is to report the examination of solid-liquid equilibria in binary mixtures of Benzimidazole in tert-butanol using gravimetric method. The solubility of Benzimidazole in tert-butanol increases with temperature. The experimental data will be useful for the testing of new theories of liquid mixtures for determining the thermodynamic properties of mixture containing Benzimidazole and ionic liquids.

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