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Physico-Chemical Behaviour of Benzophenone with Benzene At 303.15 K Using Ultrasonic Measurements

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Abstract — ***Ultrasonic investigations throw a light on the molecular interactions between solute and solvent molecules. The ultrasonic velocities, densities and viscosities have been measured for the binary liquid mixtures benzophenone and benzene of different mole fractions at 303.15 K. The obtained experimental data are used to calculate the acoustical parameters like adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π_i), interaction parameter (χ) and acoustic impedance (Z). The deviations in the parameters suggest the structure breaking tendency of the solvent molecules.***

Keywords — ***Ultrasonic velocities, Benzophenone, Benzene, Acoustical parameters, Molecular interactions.***

I. Introduction

Ultrasonic velocity investigation acts as a key to study the physico-chemical behaviour of binary liquid mixtures and nature of intermolecular interactions as well as energy transfer reactions. The study of physical, chemical and transport properties of liquid mixtures helps in many industrial processes. Benzophenone ($C_{13}H_{10}O$), an organic diphenyl ketone compound is used extensively in the manufacture of many organic compounds like dyes, pesticides and drugs. UV radiation possesses higher energy than visible light; in such cases Benzophenone is used as UV ray blocker to protect degradation of organic substances, especially in plastics, scents, soaps sun-screen lotions, and as a photo initiators in adhesives, paints, ink and printed circuit boards [1]. Benzene is a commercial solvent used in many industries like dye stuffs, pesticides and petrochemicals.

The present study involves the interaction between the polar Benzophenone molecule and the non-polar Benzene molecule by using ultrasonic velocity, density and viscosity data of the binary liquid mixtures in the room temperature - 303.15 K. An exhaustive literature survey reveals that the work has not been done earlier using ultrasonic techniques, but supported by Viji and Srivastava, dielectric studies on Benzophenone and Benzene [2].

II. Material and Methodology

2.1. Experimental Details

Chemicals used were of analytical grade. Benzophenone (SD Fine chemicals) and Benzene (Merck), purity >99% were redistilled and used [3]. Ultrasonic velocities of liquids have been measured using quartz crystal ultrasonic interferometer (Mittal Enterprises, New Delhi- 0.1% accuracy) having 2 MHz frequency. Velocity measurements were carried out at 303.15K using thermostatically controlled water bath with temperature accuracy (0.1%). The viscosities of the liquids were measured using Ostwald Viscometer by observing flow time of liquid and liquid mixtures using digital stop watch. Densities of liquids were measured using 20 ml specific gravity bottle. Velocity, density and viscosity values were being calibrated using double distilled water and closely related with literature survey values [4]. The study of various acoustical parameters helps us to understand the structure of liquid systems. Ultrasonic studies on the acoustical parameters for binary liquid mixtures have been calculated to predict the type of interaction between Benzophenone and benzene over various mole fractions at 303.15 K.

2.2. Theoretical Concepts

Using the ultrasonic velocity, density and viscosity data for the binary liquid mixtures, various thermo - acoustical parameters like adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π_i), interaction parameter (χ) and acoustic impedance (Z) were calculated using standard formulae [5].

2.2.1. Adiabatic compressibility (β): The structural arrangement or orientation may affect the adiabatic compressibility.

$$\beta = 1/u^2\rho$$

Where u is the ultrasonic velocity, ρ is the density of the system.

2.2.2. Free length (L_f): The intermolecular free length is one of the important acoustical parameters, which is used to study the nature and strength of molecular interaction [6].

$$L_f = K/ \beta^{1/2}$$

Where K is a temperature independent constant.

2.2.3. Free volume (V_f): The change in size and shape of the molecules results in structural re-arrangement of molecules in the mixture [7].

$$V_f = [M_{eff}\, u / \eta\, K]^{3/2}$$

Where **K** is a constant of value 4.28×10^9 and independent of temperature for all types of liquids and $\mathbf{M_{eff}}$ is the effective molecular weight of the system.

2.2.4. Internal pressure (π_i): The internal pressure is the only tool, which depends on all types of interactions such as solvent–solvent, solute–solvent and solute–solute.

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$$\pi_i = bRT\,[K\,\eta/\,u]^{1/2}\,[\rho^{2/3} / M_{eff}^{7/6}]$$

Where ***b*** stands for cubic packing factor which is assumed to be 2 for all liquids and solutions, and **K** is the temperature independent constant.

2.2.5. Interaction parameter (χ): Molecular interaction parameter helps to predict the stronger and weaker interactions between the component molecules.

$$\chi = (u_{exp}^2/u_{ideal}l^2)-1$$

Where u_{exp} is the experimental velocity and $u_{ideal}l=x_1u_1+x_2u_2$ stands for ideal mixing velocity.

2.2.6. Acoustic impedance (Z): The specific acoustic impedance **z** is related to velocity and density by the relation,

$$Z= u\rho$$

The **Z** depends upon the structure of liquids and the molecular packing.

III. Results and Discussions

The experimentally determined values of ultrasonic velocity (u), density (ρ) and viscosity (η) are shown in Table 1 and computed thermo - acoustical parameters like adiabatic compressibility (β), free length (L_f), free volume (V_f), acoustic impedance (Z), interaction parameter (χ) and internal pressure (π_i) for the binary liquid mixtures Benzophenone with Benzene at 303.15K are summarized in Table 2 & Table 3.

Table 1: Values of Ultrasonic Velocity (u), Density (ρ), Viscosity (η) for the binary liquid systems-Benzophenone + Benzene at 303.15K.

mole fraction $X_{C13H10O}$	**u** m s^{-1}	**ρ** kg m^{-3}	**η** Pa s
0.0016	1274.47	847.70	287.54
0.0032	1257.50	849.00	287.25
0.0048	1265.20	849.90	284.54
0.0065	1287.20	851.90	285.91
0.0081	1289.05	852.00	286.89
0.0096	1273.20	853.30	287.69
0.0112	1278.11	853.80	287.86
0.0128	1277.30	854.40	290.85
0.0144	1297.82	855.60	292.14

Benzophenone is a polar molecule having carbonyl functional group interacts with non-polar Benzene molecule. Π electrons of the Benzene ring clouds attracted by C=O group Carbon atom of Benzophenone molecule as shown in Fig.1. Due to the steric hinderance of the bulky phenyl groups in both the solute and solvent molecules Table 1 & Fig. 2 show an increase in ultrasonic velocity, this signifies strong intermolecular interaction between Benzophenone and Benzene as the mole fraction of Benzophenone is increased. Yadava and Yadav show similar kind of variation of ultrasonic velocity in liquids [8].

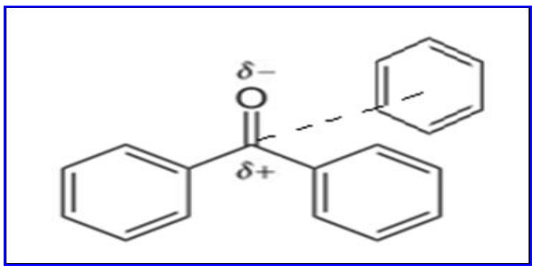

Fig. 1- Dipole-induced dipole interaction in Benzophenone + Benzene liquid systems

Table 2 & Fig. 3 show the non-linear increasing trend of viscosity and density with the concentration of solute particles is due to the frictional resistance forces created between the unlike molecules. The solvent behaves as the structure breaker with increasing velocity of the components [9].

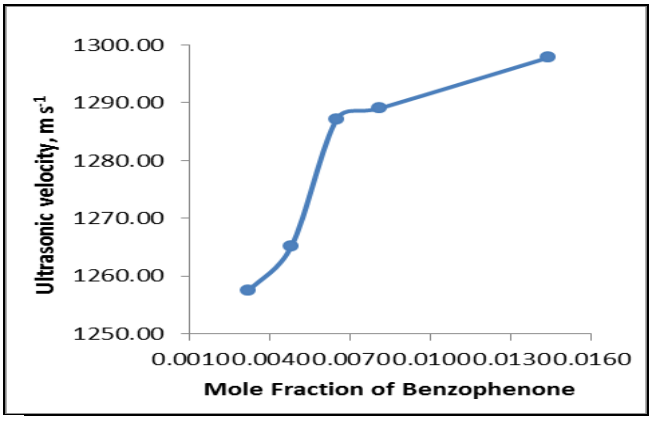

Fig. 2 - u versus mole fraction of Benzophenone

In Table 2 & Fig. 4, Adiabatic compressibility exhibits a non-linear variation similar to that of velocity, but maintains an inverse relationship. This observation is similar to that of a liquid mixture where the non-ideal behaviour is attributed to strong intermolecular interactions between the molecules of the solutions [10]. The compressibility factor, a measure of intermolecular attraction, leads to structural arrangements of the constituent particles and decreases the compressibility value. Adiabatic compressibility gives the electrostriction between the solute and solvent molecules. Decrease in compressibility between the two interacting molecules signifies interaction between the component molecules.

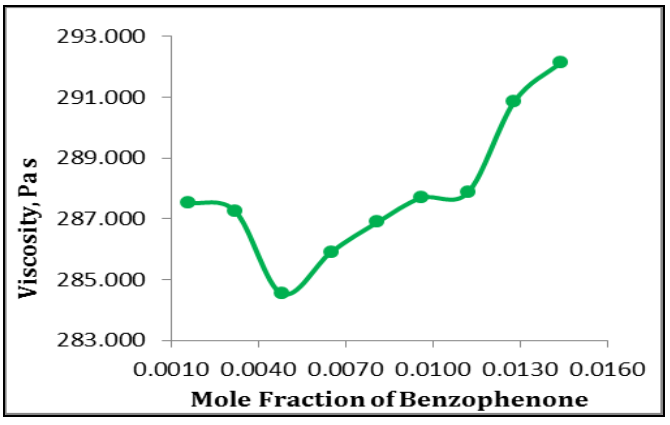

Fig. 3- η versus mole fraction of Benzophenone

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In Table 2, fig. 4 and 5, the parameters such as adiabatic compressibility and intermolecular free length decreases with increase in the concentration of Benzophenone, and show that there is specific interaction between the solute and solvent molecules [11] through dipole – induced dipole interaction.
Free Length is the distance between the Benzophenone and Benzene molecules. Free length decreases with increase in concentration signify the molecular interaction between Benzophenone and Benzene. According to Eyring and Kincaid, the non-linear trends in free length indicate the presence of structural arrangements between the components of the molecules [7].

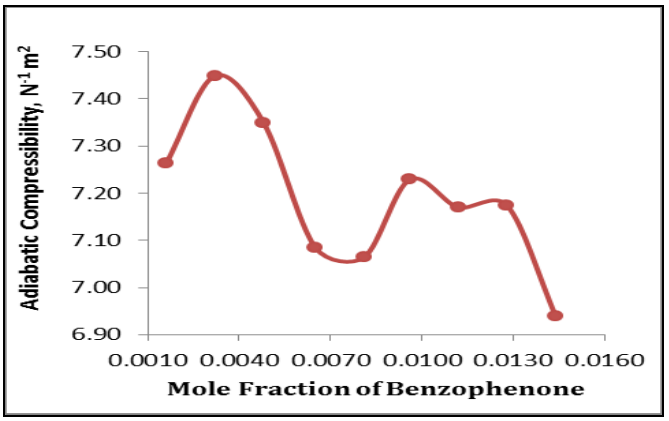

Fig. 4 - β versus mole fraction of Benzophenone

Table 2: Values of Adiabatic Compressibility (β), Free Length (L_f), Free Volume (V_f) of Benzophenone + Benzene at 303.15K.

mole fraction $X_{C13H10O}$	β 10^{-10} $N^{-1} m^2$	L_f Å	V_f 10^{-10} $m^3 mol^{-1}$
0.0016	7.263	0.5390	0.2308
0.0032	7.449	0.5458	0.2273
0.0048	7.350	0.5422	0.2334
0.0065	7.085	0.5323	0.2386
0.0081	7.064	0.5315	0.2386
0.0096	7.229	0.5378	0.2340
0.0112	7.170	0.5355	0.2359
0.0128	7.174	0.5357	0.2327
0.0144	6.939	0.5268	0.2375

From Table 2& 3, Fig. 6, 7 & 8, it is observed that free volume (V_f), acoustic impedance (Z) and interaction parameter (χ) decreases with increase in the concentration of Benzophenone shows interaction between the unlike molecules.

The variation in the free volume shows the structure breaking [12] tendency of the solvent molecules as reported by Ali et al.

The non-linear variation in Z indicates the presence of specific interactions between two components in the binary liquid mixture which further indicates that the formation of cluster between the components due to specific interactions.

Molecular interaction parameter (in fig. 8) is positive and small in magnitude signifying the interaction between polar Benzophenone and non-polar Benzene molecules. MIP depends upon the shape, size and polarity of the molecule. Zareena Begum and co-workers reported that the positive magnitude of molecular interaction parameter along with the increasing concentration represents the strong dipole-induced dipole interaction [13] between the binary liquid mixtures.

Table 3: Values of Acoustic Impedance (Z), Internal Pressure (π_i), Interaction Parameter (χ) of Benzophenone + Benzene at 303.15K.

mole fraction $X_{C13H10O}$	Z 10^6 kg m^{-2} s^{-1}	χ no unit	π_i 10^5 Pascal
0.0016	1.080	0.0374	554.40
0.0032	1.068	0.0100	588.45
0.0048	1.075	0.0224	615.26
0.0065	1.097	0.0579	644.39
0.0081	1.098	0.0609	678.37
0.0096	1.086	0.0351	719.11
0.0112	1.091	0.0429	754.45
0.0128	1.091	0.0416	796.86
0.0144	1.110	0.0747	832.29

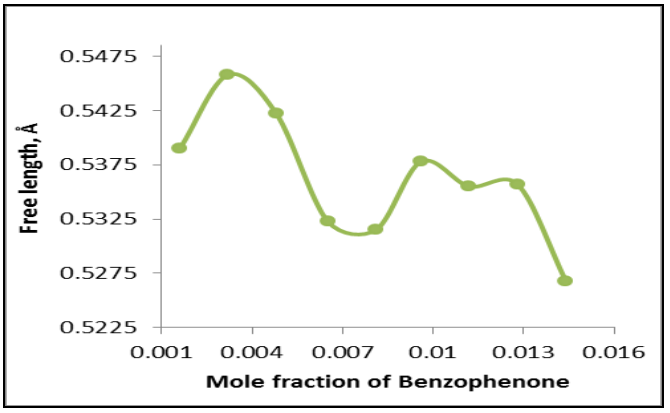

Fig. 5- L_f versus mole fraction of Benzophenone

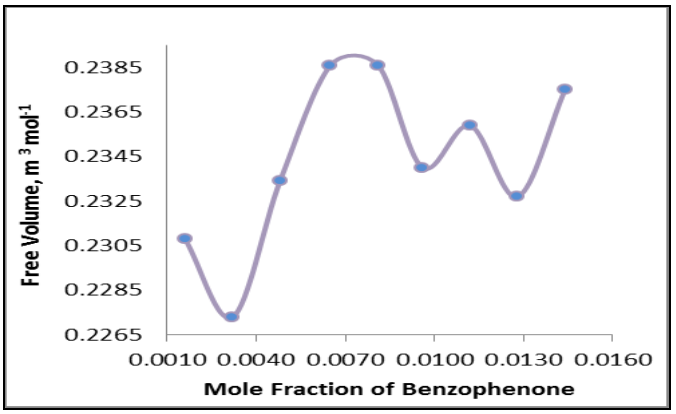

Fig. 6 - V_f versus mole fraction of Benzophenone

Table 3 & Fig. 9 show the increasing tendency of internal pressure along with the increase in concentration of solute molecules those reveal the orientation of the solvent molecules around the ions present in this solution. This may be due to the

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electrostatic field of the ions. This indicates the heteromolecular associative tendency of the molecules [14].

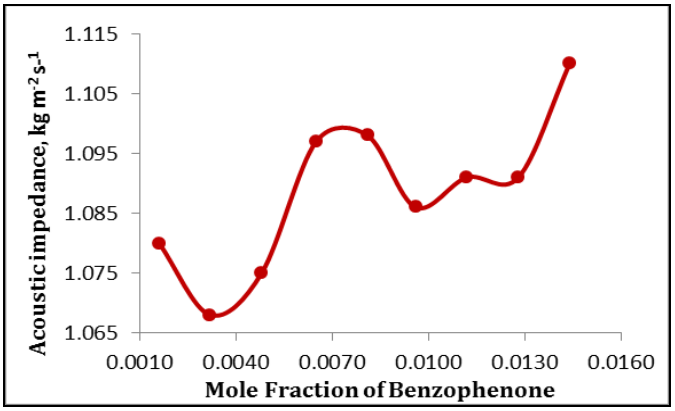

Fig. 7 -Z versus mole fraction of Benzophenone

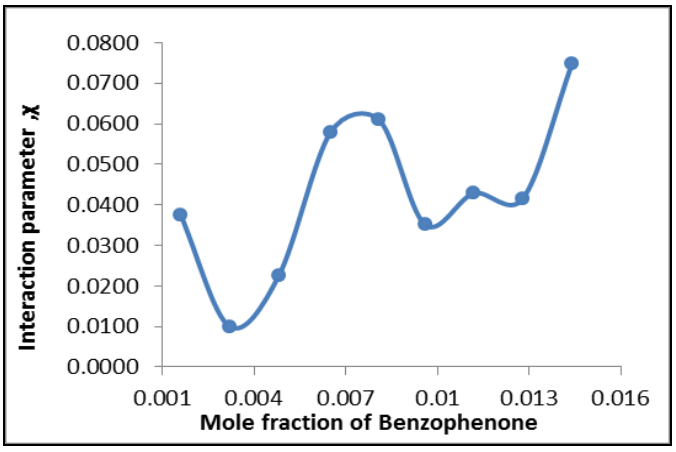

Fig. 8 - χ versus mole fraction of Benzophenone

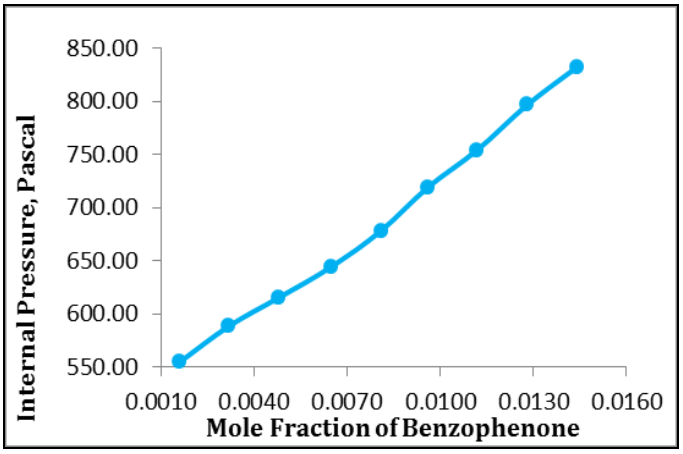

Fig. 9 - π_i versus mole fraction of Benzophenone

IV. Conclusion

From the Ultrasonic viscosities, densities and viscosities data, the thermo - acoustical parameters like adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π_i), interaction parameter (χ) and acoustic impedance (Z) for binary liquid mixtures have been calculated to predict the intermolecular interaction between Benzophenone and Benzene over various mole fractions at 303.15K. The increasing and decreasing trend of the above parameters attribute the dispersive nature of the solute molecules. Adiabatic compressibility and free length data shows the specific interaction between the unlike molecules. The non-linear variation in the parameters is due to the frictional resistance forces created by the bulky side groups of the solute particles.

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