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Molecular Interaction studies in Phenol-Water system at its Critical Solution Temperature

M. S. Wagh¹, P. S. Agrawal², L. J. Paliwal³

1. Department of Chemistry, Kamla Nehru Mahavidyalaya, Nagpur-440009, (M.S.), India.

2. Department of Chemistry, Laxminarayan Institute of Technology, Nagpur-440010, (M.S.), India.

3. Department of Chemistry R.T.M. Nagpur University, Mahatma Jyotiba Phule Educational Campus, Nagpur-440033 (M.S.), India.

Abstract: The ultrasonic velocity, density and viscosity have been measured for a versatile precursor to a large collection of drugs that is Phenol in water. The experimental data is obtained for Phenol-Water system at its miscibility temperature in the concentration range of (0.02 to 0.16). The derived parameters such as Adiabatic Compressibility (β), Free Length (L_f), Acoustic Impedance (Z). The molecular interactions through Hydrogen bonding has been studied in the light of various acoustical parameters. The trends in the variation of the solution property indicate the existence of positive molecular interactions of Phenol in water.

Key words: Ultrasonic Velocity (U), Adiabatic Compressibility (β_s), Free Length (L_f), Acoustic Impedance (Z)

I. Introduction

Phenol is also a versatile precursor to a large collection of drugs, most notably aspirin but also many herbicides and pharmaceutical drugs. Phenol is also used as an oral anesthetic/analgesic in products such as Chloraseptic or other brand name and generic equivalents, commonly used to temporarily treat pharyngitis. Phenol, also known as carbolic acid, hydroxybenzene and phenyl alcohol, is produced at the rate of millions of tons per year, mostly from isopropyl benzene ("cumene"). Phenol is a starting material in the manufacture of plastics and drugs. It was used as an antiseptic beginning in the 1860's. However, phenol is poisonous.

Aqueous phenol solutions have been used pharmaceutically [1]. At low and high percentages of phenol, water and phenol mix completely, forming a single liquid phase. However, at intermediate compositions (and below the critical temperature) mixtures of phenol and water separate into two liquid phases. Above the critical temperature, phenol and water are completely miscible. The miscibility of phenol and water is reduced by addition of many common salts such as alkali and alkaline-earth halides [2-3].

The study of behaviour of propagation of ultrasonic waves in liquid systems and solids is now rather well-established as an effective means for examining certain physical properties of the materials. It is particularly well-adopted to examine changes in such physical properties while they occur. The data obtained from ultrasonic propagation parameters such as ultrasonic velocity, adiabatic compressibility, molar volume, free length, etc. and their variations with concentration of the medium are useful in understanding the nature of molecular interaction in terms of physical parameters owing to the sensitivity to very populated densities at high energy states, ultrasonic methods have been preferred and are reported to be complementary to other techniques like dielectric relaxation, IR spectroscopy, NMR, etc. Hence, the author preferred to study the ultrasonic velocity, density and viscosity measurement of phenol water system. Structure, stability and hydrogen-bonding interaction in phenol, water and phenol-water clusters have been investigated using *ab initio* and density functional theoretical (DFT) methods and using various topological features of electron density [4]. Several theoretical studies have been made on the interaction of phenol with water [5-10]. Various theoretical and experimental studies revealed that the hydrogen bonding of phenol in water is similar to that of water [11] Clusters (H₂O)_n, n = 8-20:

II. Materials and Methods

The chemical Phenol used in the study was the product from S.D. Fine Chem. Ltd. and E-Merck. All compounds were of AR grade with minimum assay of 99.9%. Therefore, it was used without further purification. The temperature was maintained by a thermostatically controlled water bath LTB-10. The density of the solution was measured at 339.95 K by the hydrostatic plunger method. A mono-pan digital balance of least count 0.0001g was used to record change in plunger weight dipped in solutions. A thoroughly cleaned and dried Ostwald viscometer filled with the experimental liquid was placed vertically in a glass-fronted, well-stirred water bath. Once the thermal equilibrium was attained, the flow times of the liquid were recorded with an accurate stopwatch (± 0.01 s). The viscosities were calibrated with double distilled water. Ultrasonic velocity measurements were made by variable path single crystal interferometer (Mittal Enterprises, Model F-81) at 2MHz with the accuracy of ± 0.03 %. The densities of pure water at required temperatures were taken from the literature [5].

III. Experimental and Computed data:-

Table-1:

DENSITY, ULTRASONIC VELOCITY ADIABATIC COMPRESSIBILITY (β_s), INTERMOLECULAR FREE LENGTH (Lf) AND SPECIFIC ACOUSTIC IMPEDANCE (Z) IN DIFFERENT MOLE FRACTION OF PHENOL-WATER MIXTURE AT 339.95 K

Mole fraction of Phenol (X1)	Mole Fraction of Water (X2)	Density(ρ_s) Kg m ⁻³	Ultrasonic velocity (Us) ms ⁻¹	Adiabatic compressibility $\beta_s \times 10^{-10}$ Nm ⁻²	Intermolecular free length (Lf) m	Specific acoustic impedance $Z \times 10^6$
0.020	0.970	1050.01	1274.2	5.86586	1.457	1.337
0.040	0.950	1051.02	1290.5	5.71312	1.438	1.356
0.060	0.940	1059.03	1316.5	5.44816	1.404	1.394
0.080	0.920	1060.00	1421.3	4.67006	1.300	1.506
0.100	0.900	1062.50	1523.0	4.05762	1.212	1.618
0.120	0.880	1063.80	1595.1	3.69457	1.156	1.696
0.130	0.870	1068.90	1610.2	3.60831	1.143	1.721
0.140	0.850	1069.40	1639.8	3.47759	1.122	1.753
0.160	0.830	1070.1	1705.6	3.21234	1.078	1.825

IV. Results and Discussion:

In the present investigation different thermodynamic parameters such as adiabatic compressibility (β_s), intermolecular free length (Lf), specific acoustic impedance (Z), were studied in phenol-water mixture. From table-1, it is reflected that ultrasonic velocity increases with increase in mole fraction of phenol. Variation of ultrasonic velocity in solution depends upon the increase or decrease of molecular free length after mixing the component based on a model for sound propagation proposed by Eyring and Kincaid [12]. Study reveals that, intermolecular free length decreases linearly as a result of mixing. The intermolecular free length decreases due to greater force of interaction between phenol and water bath formation of hydrogen bonding. This is in accordance with previous studies [13]. Further this trend is an indication of clustering of the molecules into some cage like agglomerates due to associative effect of the polar group which predominates over the other type of interactions [14]. Values of acoustic impedance (Z) are found to be increased. When an acoustic wave travels in a medium, there is a variation of pressure from particle to particle. The ratio of the instantaneous pressure excess at any particle of the medium to the instantaneous velocity of that particle is known as 'specific acoustic impedance' of the medium. This factor is governed by the inertial and elastic properties of the medium. It is important to examine specific acoustic impedance in relation to concentration and temperature. When a plane ultrasonic wave is set up in a liquid, the pressure and hence density and refractive index show specific variations with distance from the source along the direction of propagation. In the present investigation, it is observed that these acoustic impedance (Z) values increase with increasing concentration of phenol. Such an increasing values of acoustic impedance (Z) further supports the possibility of molecular interactions due to H-bonding between the water-phenol molecules.

Adiabatic compressibility β_s is found to be decreased with increasing concentration of phenol. It is primarily the compressibility that changes with structure which leads to change in ultrasonic velocity. The change in adiabatic compressibility (β_s) in liquid mixtures indicates that there is a definite contraction on mixing and the variation may be due to complex formation. This clearly shows that there is significant interaction between the phenol-water molecules [15]. The decrease in the values of adiabatic compressibility and the free length with increase in ultrasonic velocity (U) further strengthens the strong molecular association between the unlike molecules through hydrogen bonding.

The decrease of adiabatic compressibility with increase of percentage of phenol in solution may be due to collection of water molecules around phenol, supporting weak water-water interaction and more phenol-water interactions. Intermolecular interaction in phenol clusters is slightly stronger than in water clusters. However, fusion of phenol and water clusters leads to stability that is akin to that of H₂O clusters.

Dielectric constant of phenol is low as revealed from the literature. It is the indication of weaker tendency to keep the water molecules away from each other. So interaction between phenol-water is strong at elevated temperature.

References

- [1]. Sinko, J. Patrick, Martin's Physical Pharmacy and Pharmaceutical Sciences, 5th ed., Lippincott Williams & Wilkins, 2005. pp 51.
- [2]. Singh, Man Journal of Chemical Thermodynamics, vol 39, 2007, pp 240.
- [3]. S Ghizellaoui, A.H Meniai, Desalination, 185, 2005, pp 457.
- [4]. R. Parthasarathi, V. Subramanian and N. Sathyamurthy J. Phys. Chem. A, vol 5, 109, 2005, pp 843.
- [5]. S. L. Abd-EL-Messieh, Indian J. Phys. 70B vol 2, 1996, pp 119.
- [6]. T. Ebata, M. Kayano, S. Sato and N. Mikami, J. Phys. Chem. A, vol 105, 2001, pp 8623.
- [7]. D. M. Benoit, A. X. Chavagnac and David C. Clary. Chem. Phys. Lett. 283, 1998, pp 269.
- [8]. D. M. Benoit and D. C. Clary. J. Phys. Chem. A. 104, 2000, pp 5590.

- [9]. A. K. Chandra and T. Uchimar. Int. J. Mol. Sci. vol 3, 2002, pp 407.
- [10]. K. Sagarik and P. Asawakun Chem. Phys. 219, 1997, pp 173.
- [11]. S. Maheshwary, N. Patel, N. Sathyamurthy, A. D. Kulkarni and S. R. Gadre. J. Phys. Chem. A. 105, 2001, pp 10525.
- [12]. J. F. Kincaid and H. Eyring, J. Chem. Phys., vol 5, 1937, pp 587 .
- [13]. R. Parthasarathi, V. Subramanian, and N. Sathyamurthy J. Phys. Chem. A, vol 109 (5), 2005, pp 843.
- [14]. B Hemalatha, Ph. D. Thesis, Department of Chemistry, Annamalai University, 2004.
- [15]. K. Mohankrishnan, K. Rambabu, D. Ramachandran and G. K. Raman. Phys. Chem. Liq. (UK). vol. 29, 1995, pp 257.