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Assessment of Molecular Interactions of 4-Ethyl Thiocarbamidophenol on Acoustic Parameters Base

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ABSTRACT

Acoustic parameters assessment significantly able to disclose molecular and intermolecular interaction briefly. These parameters measured more significant by ultrasonic interferometer. Present research scheme concern to measurements of ultrasonic velocity and density for solutions of 4-ethylthiocarbamidophenol (ETP) at different molar concentrations (i.e. 0.1M, 0.075M, 0.050M and 0.025M) and 300 K, in 70% compositions of ethanol-water mixtures. These determinations sustain estimation of adiabatic compressibility (β), apparent molal compressibility (k), apparent molal volume (v), intermolecular free length (Lf), relative association (RA) and specific acoustic impedance (Z). These properties were help to know about solute-solute and solute-solvent interactions in solvent. Internal structure and molecular association can be possible to understand through current investigation.

Keywords: 4-ethylthiocarbamidophenol (ETP), Interferometric measurements, Intermolecular interactions and acoustic parameters.

INTRODUCTION

Molecular structure and their interactions in solution is always received importance in various field of sciences. Ultra sound and ultrasonic interferometer significantly used in

estimation of molecule interactions such as inter and intra ionic or molecular interactions. Since from last few decades ultra sound and ultrasonic interferometric investigation extensively used to understand molecular interactions in liquid. This investigation has important to know the properties and significances of molecules. Ultra sound and ultrasonic wave's measurements widely applicable in many evolutions and new concepts in engineering, applied, industrial, mechanics, agricultural, medicinal, forensic sciences and space research development and updating. Ultrasonic is a branch of science, which deals with waves of high frequencies. A Thiocarbamido phenol nucleus has various significances in different industrial and life sciences. Valuable information regarding internal structure, molecular association, complex formation, internal pressure and stability[1] obtained from the study of ultrasonic parameters investigation in liquid phase[2-4], liquid mixture[5-6] and electrolyte solution[7-9]. Ultrasonic interferometric study of 4-(p-chloro)phenylthiocarbamido phenol in mixed solvent media carried out by Isankar *et al*[10]. Comparative study of intermolecular interaction by inteferometric measurements of α-bromoacetophenones and cumaran-3-ones in ethanol and dioxan solvents was studied by Aswale *et al*[11] and acoustical studies on ternary mixture of toluene in cyclohexane and nitrobenzene at 308 K was studied[12]. Ultrasonic velocity and density of binary liquid mixture of diethyl ether with three non-polar solvents such as CCl_4, CS_2 and C_6H_6 at 303.15K were investigated[13] and interferometric investigated 4-ethylthiocarbamdiophenol in 60% mixed solvent media[14].

Ultrasonic investigation received more important to understand the ion solvent and solvent-solvent and structure breaking and making properties of solutes. Organic ligands solutions used through the current investigation and this study provide an excellent information concern to intra as well as intermolecular interactions. In present investigation, mainly concentrate on the assessment of ultrasonic velocity and density for solutions of 4-ethylthiocarbamidophenol (ETP) at different molar concentrations and 300K, in 70% compositions ethanol-water mixtures and estimation of adiabatic compressibility (β), apparent molal compressibility (k), apparent molal volume (v), intermolecular free length (Lf), relative association (RA) and specific acoustic impedance (Z). In the view of above current research scheme designed as "Assessment of molecular interactions of 4-ethylthiocarbamidophenol on acoustic parameters base". This investigation regarding to know effect of concentrations on various acoustical properties and effect of acoustic parameters on molecular interactions.

MATERIAL AND METHODS

All AR grade chemicals used through current work. Freshly prepared solution used during study. The solvents were purified by standard method. 0.1M, 0.075M, 0.050M and 0.025M solutions of ETP in 70% ethanol-water mixture were prepared. Ethanol was purified by standard procedure[15]. Densities were measured with the help of bicapillary pyknometer (10.1 % kg m^{-3}). Pyknometer used is of Borosil make. Weighing was made on Citizen CY 104 one pan digital balance (± 0.0001 gm). A special thermostatic arrangement was done for density and ultrasonic velocity measurements. Elite thermostatic bath was used in which continuous stirring of water was carried out with the help of electric stirrer and temperature

variation was maintained within ± 0.1 ^{0}C. The speed of sound waves was obtained by using variable path, Single crystal interferometer (Mittal Enterprises, Model MX-3) with accuracy ± 0.03% and frequency 1 MHz was used in the present work. The densities and ultrasonic velocity of liquids in ethanol solvent were measured at 300 K for the calculation of intermolecular free length and the value of Jacobson's constant[16] (K = 631) was taken.

RESULTS AND DISCUSSION

Ultrasonic velocities and densities of ETP in 70% ethanol-water mixture investigated through present work and it is tabulated in following Table No.1.

Table-1.1: Average Ultrasonic Velocity of Water at 300K.

Sr. No.	No. of Rotation of Screw	Micrometer Reading (mm)	Difference Between Reading (mm)	Distance Travelled By Screw in One Rotation	Average Ultrasonic Velocity (m/sec)
1	5	26.4705	1.6105	0.61465	1398.708956
2	10	24.8642	5.5300	2.18285	
3	15	19.3372	3.0708	1.20041	
4	20	16.2664	4.4071	1.73277	
5	25	11.8593	4.5219	1.78301	
6	30	7.3374	4.0715	1.6004	
7	35	3.2659	2.0059	1.17213	
8	40	1.2663		10.45377	

Table-1.2: Average Ultrasonic Velocity of Pure Ethanol 300K (β_0)

Sr. No.	No. of Rotation of Screw	Micrometer Reading (mm)	Difference Between Reading (mm)	Distance Travelled By Screw in One Rotation	Average Ultrasonic Velocity (v_0) (m/sec)	Density (d_0) (Kg. m^{-3})	$\beta_0 \times 10^{-10}$ (Pa^{-1})
1	5	15.2623	4.9016	1.9321	1243.64	1030.00	5.843517555
2	10	10.3686	2.0211	0.7845			
3	15	8.3374	3.1108	1.2161			
4	20	5.2265	3.3795	1.3199			
5	25	1.8569		5.4374			

Table-1.3: Average Ultrasonic Velocity of 70% Ethanol 300K (β_0)

Sr. No.	No. of Rotation of Screw	Micrometer Reading (mm)	Difference Between Reading (mm)	Distance Travelled By Screw in One Rotation	Average Ultrasonic Velocity (v_0) (m/sec)	Density (d_0) (Kg. m^{-3})	$\beta_0 \times 10^{-10}$ (Pa^{-1})
1	5	16.8193	3.5422	1.39301	1336.98	1030.52	5.172074651
2	10	13.2705	3.9280	1.52925			
3	15	9.3775	3.1075	1.21513			
4	20	6.2752	3.8942	1.48981			
5	25	2.4757		6.65083			

Table-1.4: Acoustic Parameters at Different Concentration of [ETP] at 300 K in 70% E-W

Conc. C (Mole/lit)	Average Ultrasonic Velocity Us (m/sec)	Density d_s ($Kg.m^{-3}$)	$\beta s x10^{-10}$ (pa^{-1})	ϕ_V (m^3mol^{-1})	ϕ_k $x10^{-10}$	L_f (A_0)	R_A	$Z * 10^4$ ($Kgm^{-2} sec^{-1}$)
0.1	1593.587	1034.32	3.7714	0.1885	-8.9981	0.0155	0.982	161.741
0.075	1445.427	1027.52	4.6011	0.256	-1.0204	0.0168	1.007	145.301
0.050	1270.737	1025.12	5.941	0.2771	21.855	0.0186	1.048	126.999
0.025	1172.687	1021.12	6.9857	0.3158	53.761	0.0199	1.072	116.430

CONCLUSION

Table-1.4 reveals acoustic parameters of ETP at different concentration such as 0.1M, 0.075M, 0.050Mand 0.025M and 300K in 70% ethanol-water mixture. Table-1.4 reveals that Ultrasonic Velocity (Us), Density (ds) and decreases along with decreasing concentration from 0.1M to 0.025M. Acoustic parameters such as adiabatic compressibility (βs), Apparent molar volume (φv), Apparent molar compressibility (φk), Intermolecular free length (Lf), Relative association (RA) increases and Specific acoustic impedance (Z) decreases along with decreasing concentration from 0.1M to 0.025M. This acoustic parameters investigation help to understand molecular interactions occur and responsible for breaking and making of their structure in solution.

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