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Effect of Concentration of Substituted Pyrazoline on Acoustic Parameters

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Abstract: ***Substituted pyrazoline have been reported to show broad spectrum of biological activities mainly as anti-microbial, anti-inflammatory, anti-depressant, antipyretic, anti-fungal, anti-filarial etc. It is also widely used as a photoluminescence and electroluminescence. Therefore, present work is carried out to study the substituted pyrazoline with different concentrations at 303.15K. . Ultrasonic velocities and densities of substituted pyrazoline have been measured in the different concentration in binary mixtures of dioxane-water (Dx-water) at 303.15 K. The acoustical parameters; adiabatic compressibility, linear free length, acoustic impedance, relative association, apparent molal compressibility and volume of system have been calculated with experimental data of density and ultrasonic velocity. It is observed that values of apparent adiabatic compressibility and volume are found to be decreases with rise in concentration of ligand. The linear free length, relative association and acoustic impedance increases linearly with increasing the concentration of ligand.***

Keywords: acoustical parameter, density, Dx-water mixture, substituted pyrazoline, ultrasonic velocity.

1. Introduction

Spectacular developments in organic chemistry during recent years have greatly accelerated the advanced in pharmacology. Pyrazoline derivatives are found to be bactericidal[1], fungicidal[2] and biodegradable agrochemical[3] also, used as intermediate in the dye industry[4]. The substituted pyrazoline effectively utilized as antitumer[5], antidiabatic[6], anaesthetic[7] and analgesic[8]. While the pyrazoline structure has shown a special ability to interact with UV and VIS radiation in linear and nonlinear optical sense; and some of them used as drugs for prevention and diagnosis of many diseases[9]. Also, pyrazoline derivatives with different substitution show the electroluminescence and photoluminescence in OLED[10].

The nature and relative strength of the molecular interaction between the components of the liquid mixtures have been successfully investigated by the ultrasonic method[11-12]. This interaction helps in better understanding the nature of solute and solvent i.e. whether the solute modifies or distorts the structure of the solvent. The measurement of ultrasonic speed enables the accurate determination of some useful acoustical and thermodynamic parameters, which is highly sensitive to molecular interactions in liquid mixtures.

Ultrasonic waves used to detect a wide variety of anomalous conditions such as tumors, pregnancy and heart valve action. Ultrasound is more sensitive than X-rays in distinguishing various kinds of tissues, selective pathological tissue and find usefulness in the treatment of certain cancers as well as arthritis and related diseases[13]. Thermodynamic and transport properties of binary and ternary mixtures with different organic liquids have been studied by many workers[14-16]. Data on some of the properties associated with the liquids and liquid mixtures like densities, viscosities, ultrasonic velocities and refractive indices find extensive application in chemical engineering process stimulation, solution theory and molecular dynamics[17]. The studies in regard to the determination of densities, viscosities, refractive indices of organic liquid mixture are reported by many workers[18-21].

1, 4-Dioxane (Dx) has been widely used as a solvent, stabilizer for chlorinated solvent such as methyl *tert*-butyl ether and dichloromethane, greasing agents, components of paint, varnish removers, biosensors, pharmaceuticals, chemical technologies and dispersion agents in the textile industry. The Dx is a hetero cyclic diethyl ether with each of its two oxygen atoms forming an ether functional group. The molecular structure of Dx may be related to ethanediol and methoxy ethanol, but is an almost apolar, aprotic and protophilic solvent[22]. It has very low dipole moment and there is no H-bond pair formation between two Dx molecules in pure liquid state, which is mainly due to the fact that in Dx molecule ether oxygen's offer H-bond acceptor sites, but it cannot self-associate due to lack of H-bond donor positions[23].

The work follows systematic studies on densities and ultrasonic velocities of substituted pyrazolines have been measured in the different concentration in binary mixtures of Dx-water at 303.15 K. The acoustical parameters; adiabatic compressibility, linear free length, acoustic impedance, relative association, apparent molal compressibility and volume of system also have been calculated with experimental data. All calculations made by computer based Excel programmed.

Theory: The adiabatic compressibility (β_s) was calculated from Newton-Laplace equation:

$$\beta_s = \frac{1}{\rho_s u_s^{\,2}} \text{-------(1)}$$

Where $\rho_s =$ density of solution, $u_s =$ Speed of sound

The intermolecular free length (L_f) is calculated by using the standard expression;

$$L_f = K\sqrt{\beta_s} \text{------(2)}$$

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Where 'K' is a temperature dependent constant known as Jacobson constant[24].

The specific acoustic impedance (Z) is obtained by;

$$Z = u_s \rho_s \text{ -------(3)}$$

The relative association (R_A) was calculated by the following equation;

$$R_A = \left(\frac{\rho_s}{\rho_o}\right)\left(\frac{u_o}{u_s}\right)^{1/3} \text{ ------(4)}$$ Where ρ_o = density of solvent, u_o = velocity of solvent

2. Materials and Methods

Substituted pyrazolines; 3-(2-hydroxy-5-methyl phenyl)-5-phenyl-Δ^2pyrazoline [L1] and 3-(2-hydroxy-5-methylphenyl)-1, 5-di-phenyl-Δ^2pyrazoline [L2] were synthesized by known method[25]. The different concentration of solute prepared in 70% Dx-water mixture. The densities and sound velocities were measured with a densitometer (Anton Paar, DMA-35) and ultrasonic interferometer (Mittal enterprises, F-81s) at 2 MHz with frequency tolerance was ± 0.03%. The accuracy of instrument was examined with distilled water at 303.15 K and compare with literature value (table 1) All measurements done on analytical balance (ADG-200, Accuracy = 0.001gms).

3. Results and Discussion

The experimentally measured ultrasonic velocity in pure liquids of Dx and water with their density value are given in the table-1. The calculated values of ultrasonic velocity and density are in good concordance with literature values.

Table 1: Comparison with literature values for ultrasonic velocity and density of pure liquids at 303.15 K reported in this work

Liquid	Ultrasonic velocity m/s		Density kg.m^{-3}	
	This work	Literature value	This work	Literature value
Dx	1328	1343[26]	1027	1028.4[26]
Distilled water	1507	1499[26]	997.7	996.0[26]

Table 2: Values of ultrasonic velocity (u), density (ρ) adiabatic compressibility (β_s), acoustic impedance (Z), intermolecular free length (L_f) and relative association (R_A) of different concentration of solute in Dx-water at 303.15K

Conc.	ρ kg.m^{-3}	u m.s^{-1}	β_s x10^{-10} m^2.N^{-1}	L_f x10^{-10} m	Z x10^{-6} N. m^{-2}	R_A x10^{-7} m^3.mol^{-1}	Φ_β x 10^{-10} m^5.m^{-1}.N^{-1}	Φ_V
L1								
0.002	984.2	1363	5.4692	4.9769	1.3414	5.4692	0.2732	-2.6137
0.004	984.5	1367	5.4355	4.9860	1.3426	5.3569	0.2737	6.42130
0.006	986.4	1354	5.5298	5.0124	1.3227	5.6375	0.2755	14.0127
0.008	994.0	1327	5.7130	5.0553	1.3120	5.8659	0.2783	25.3972
0.010	998.6	1302	5.9072	5.1466	1.3001	5.9072	0.2946	80.5928
L2								
0.002	1005.5	1276	6.0780	4.9193	1.2893	4.9617	0.2821	-1.4660
0.004	1004.1	1262	6.2099	4.9724	1.2760	4.9975	0.2829	8.5928
0.006	1005.6	1250	6.3079	5.0115	1.2682	5.1429	0.2855	16.5760
0.008	1016.7	1235	6.4550	5.0696	1.2543	5.4253	0.2872	27.0134
0.010	1016.8	1227	6.5324	5.0999	1.2476	5.4728	0.2962	83.5153

The values of densities and ultrasonic velocities at 303.15 K are presented in table 2. The values are correlated with concentration of solute. It is observed trends of ρ and u are in L2 > L1 listed in table 2 showed that increases and decreases respectively with increase in concentration all systems.

Density is a measure of solvent-solvent and ion-solvent interaction increases in density with concentration indicates an increases in solvent-solvent and solute-solvent interaction and this may be due to shrinkage in volume owing to the presence of solute molecules. This can be attributed to the structure making ability of the solute in the presence of solvent. The linear increase of ρ and u with concentration of solute confirmed an increase of cohesive forces because of strong molecular interactions.

The adiabatic compressibility, free length and acoustic impedance show an opposite trend to that of velocity. According to a model proposed by Erying and Kinkaid[27], ultrasonic velocity decreases with increase in free length and vice versa. This is also in accordance with the expected molecular interaction between the solute-solvent, increases in compressibility. The calculated values of ultrasonic velocity and adiabatic compressibility are in good concordance with reported work[28-29].

The acoustic impedance is the parameter related to the elastic properties of medium, therefore it is essential to examine. It shows from table 2, the variation of acoustic impedance values decreases with increase concentration of solute. The nonlinear behavior further suggests the possibility of molecular interaction between solute and solvent through hydrogen bonding.

The values of relative association are presented in table 2. It shows an increasing trend with increasing concentration. A close examination of relative association values are close to each other indicates the system under investigation is essentially ideal in nature [30]. It can be seen from table 2, that the apparent molar compressibility increases with increase concentration. The larger the values of Φ_β in solutions are

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attributed the strong attractive interactions due to the hydrogen bond formation; solute and water molecules induce the dehydration of ions and therefore increase Φ_β.

The apparent molar volume increases with increase concentration (table 2). The larger the values of Φ_V in solutions are attributed the strong attractive interactions due to the hydrogen bond formation; solute and water molecules induce the dehydration of ions and therefore increase Φ_V [31].

4. Conclusion

Densities and ultrasonic velocities of substituted pyrazoline in Dx-water have been experimentally determined over entire mole fraction range at 303.15 K. It suggests a linearly increases and decreases respectively. Its indicate that a strong solute-solvent interaction.

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