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STUDY OF ACOUSTICAL PARAMETERS OF SUBSTITUTED 2-AMINOBENZOTHIAZOLES IN AQUEOUS DIOXANE AT DIFFERENT TEMPERATURES

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ABSTRACT: -
In a 1,4-dioxane-water mixture at 293, 295, and 297 K, throughout a wide range of concentration, the density, viscosity, and ultrasonic velocity of synthesised Schiff base 1,3-benzothiazol-2-amine and its substituted derivatives have been examined. The current work involved the analysis of acoustical parameters such as ultrasonic velocity (V), adiabatic compressibility (βs), apparent molar volume (ϕv), and intermolecular free length (L_f), which represent structural properties.

KEYWORDS: - Density, ultrasonic velocity, Heterocyclic, acoustic parameters, structural interactions.

I] Introduction

The study of certain acoustic properties, such as adiabatic compressibility(βs), apparent molar volume (ϕv), intermolecular free length(L_f) specific acoustic impedance(Z), relative association(Ra) etc. is related to the formation or breaking of a solvents structure. The ultrasonic velocity, together with density and viscosity, is a straight forward probe employed by physicists to ascertain these characteristics (1). According to review of the literature, ultrasonic analysis of liquid mixtures is very helpful in determining the type of molecular interactions and the physiochemical behaviour of molecules (2-4). Ultrasound is employed in a wide variety of Industries, including quality control and Medicine (5) in Industries for quality control, to expedite chemical reactions, in non-destructive testing of products and constructions etc. exploring the use of ultrasonography in ex-situ cleaning applications.

The nature of molecular interactions in pure liquids (6) fluid mixtures (7-9) and ionic interactions in electrolyte solutions (10) have all been adequately investigated using ultrasonic technology the ability of ultrasonic technology to detect very weak intermolecular interaction is a significant advantages by examining the acoustics at various concentrations and temperatures numerous researchers have made significant progress in comprehending the nature of molecular interaction and physicochemical behaviour of liquid mixtures.

The acoustical characteristics of the schiff base have been examined in the current analysis schiff bases are an important class of ligands in the study of coordination chemistry because of their great

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synthetic flexibility, coordinating ability and therapeutic value (11). Numerous schiff bases have been discovered to exhibit significant biological and catalytic properties and their analytical characteristics have been described (12-13). A study of wide variety of schiff bases utilized in metallic cation and anion sensing applications was recently published. Different biological and environmental mediums (14). There is a relationship between acoustic parameters and an accumulation of schiff bases.

Due to the amount of substitutions, heterocyclic molecules offer a synthetic and structural capabilities (15). T. the biological and pharmacological effects of antioxidants medicines depend heavily on benzothiazoles and their derivatives (16-17). They are widely distributed throughout nature and necessary for life in a number of ways (18) 2-aminobenzothiazoles and its substituted derivatives were synthesized in the laboratory by using microwave radiations over conventional route (19). The synthesized compounds were then characterized by their spectral analysis. In the present study, attempts have been made to study the molecular interactions of the following substituted schiff base ligands in the suitable percentage of 1,4 dioxane at different temperatures by acoustical investigations.

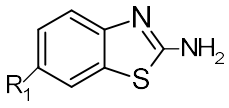
1) 1,3-benzothiazol-2-amine

2) 6-Nitro-1,3-benzothiazol-2-amine

3) 6-chloro-1,3-benzothiazol-2amine

4) 2-amino-1,3-benzothiazol-6-ol

Structure of ligand



Where R_1 is NO_2, Cl, NH_2

II) METHOD AND MATERIALS

I) METHOD

2-aminobenzothiazole and its substituted derivatives were synthesized in the laboratory using microwave radiations. The ligands solutions densities and ultrasonic velocities were measured according to procedure at 293, 295 and 297 K.

II) MATERIALS

LR grade compounds were employed in the synthesis before use the ligands (L_1 to L_4) underwent recrystallization. The 1,4-dioxane solvent was purified according to protocol. Deionized water was used to freshly prepare all the working solutions deionized water was used for all the purposes in this study to prevent any ionic contamination. For each ligand 0.01M solution was made in a different way (75%, 80%, 85 % & 90%)

III) INSTRUMENTATION

The densities of the solutions were measured using a conventional capillary with and internal capillary diameter of 1 mm and a bulb volume of approximately 10 cm using a Citizm CY 104 one pan digital balance. All of the weighing was done the ultrasonic velocity in liquid mixes and solutions was measured in the current study using a variable path. Ultrasonic interferometer from Mittal Enterprises New Delhi model MX-3, with an accuracy of 10.03 percent. The exact calculation of the wavelength (λ) serve as the foundation for the measurement of velocity(V).

IV) RESULT AND DISCUSSION

The major ultrasonic velocity is used to derive the acoustic parameters for the ligands L_1, L_2, L_3 & L_4 in varying percentage of dioxane examined at three different temperatures. The structural interactions of the solvent and solute is determined by the analysis of ultrasonic velocity (V), adiabatic compressibility (βs), apparent molar volume (ϕv), and intermolecular free length(L_f). It provides details about internal structure.

ADIABATIC COMPRESSIBILITY (βs)

one of the significant physical quantities in fluid mechanics is a liquids structure, which takes into account the geometric fit of the. Solute into the ordered from of the aqueous solvent surrounding the

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solutes including its shape, size, branching, presence of aromatic rings etc. (20). Adiabatic compressibility is crucial for understanding.

From the table 1-12 and figure 1-3 it is observed that the values of adiabatic compressibility of ligands decreases with percentage of solvents. With increasing concentration of solvent, molecules aggregate surrounding to the ions and the free ions number decreases, demonstrating that ionic association occurs as a result of strong ion-ion interactions (21). Additionally, a rise in temperature revels a very slight alteration in the values of all ligands. It is evident that the existence of electron withdrawing $–NO_2$ group and electron releasing $-CH_3$ group has an impact on the trend in values.

APPARENT MOLAR VOLUME (ϕv)

The density molarity, and molecular weight of the solute are all factors that affect apparent molar volume. From Table 1-12 and figure 3-6 the solute-solvent interaction is expressed by a thermodynamic characteristic of solution. At 293,295 and 297K, the values of apparent molar volume ϕv drop as the percentage of 1,4dioxane rises. Depending on salt concentration, solution and solvent densities, molecular weight, and variation in concentration (22).

INTERMOLECULAR FREE LENGTH (L_f)

The distance between the surfaces of the molecules is known as the intermolecular free length. From table 1-12 and figure 9-12 all the ligands in dioxane have positive values at various temperatures, showing the presence of dispersive forces between the mixtures molecules.

Table 1: Acoustic Parameters at different percentage of dioxane

Ligand L_1 Temp: 293K

% 1,4-Dioxane	ds x 10^3 (kg m^{-3})	V x 10^3 (m sec^{14}	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} m^3 mol^{-1} pa^{-1}	L_f x 10^{-1} m^{-1}
75%	1.227	1.573	0.2995	335.316	524.506
80%	0.998	1.649	0.3268	274.587	515.017
85%	0.821	1.501	0.3093	243.531	522.701
90%	0.533	1.453	0.2554	186.866	549.339

Table 2: Acoustic Parameters at different percentage of dioxane

Ligand L_2 Temp: 293K

% 1,4-Dioxane	ds x 10^3 (kg m^{-3})	V x 10^3 (m sec^{14}	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} m^3 mol^{-1} pa^{-1}	L_f x 10^{-1} m^{-1}
75%	0.9981	1.214	0.3186	333.766	523.29
80%	0.978	1.211	0.2778	131.898	588.083
85%	0.827	1.12	0.2803	314.348	548.282
90%	0.607	1.12	0.208	47.195	517.58

Table 3: Acoustic Parameters at different percentage of dioxane

Ligand L_3 Temp: 293K

% 1,4-Dioxane	ds x 10^3 (kg m^{-3})	V x 10^3 (m sec^{14}	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} m^3 mol^{-1} pa^{-1}	L_f x 10^{-1} m^{-1}
75%	0.992	1.451	0.2893	396.643	517.86
80%	0.983	1.123	0.2724	460.32	525.673
85%	0.954	1.226	0.2642	230.555	535.035
90%	0.913	1.026	0.2517	-96.27	531.603

Table 4: Acoustic Parameters at different percentage of dioxane

Ligand L_4 Temp: 293K

% 1,4-Dioxane	ds x 10^3 (kg m^{-3})	V x 10^3 (m sec^{14}	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} m^3 mol^{-1} pa^{-1}	L_f x 10^{-1} m^{-1}
75%	1.187	1.187	0.2716	346.785	527.532
80%	0.917	1.193	0.2443	370.086	520.267
85%	0.997	1.197	0.2553	283.325	535.27
90%	0.996	1.198	0.2362	130.502	531.603

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Table 5: Acoustic Parameters at different percentage of dioxane

Ligand L_1 Temp:295K

% 1,4-Dioxane	ds x 10^3 ($kg\ m^{-3}$)	V x 10^3 ($m\ sec^{14}$)	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} $m^3\ mol^{-1}\ pa^{-1}$	L_f x 10^{-1} m^{-1}
75%	1.062	1.5096	0.24182	132.852	381.109
80%	1.041	1.4873	0.2544	562.644	377.392
85%	0.998	1.4616	0.24376	603.086	385.562
90%	0.912	1.465	0.2335	339.966	393.937

Table 6: Acoustic Parameters at different percentage of dioxane

Ligand L_2 Temp:295K

% 1,4-Dioxane	ds x 10^3 ($kg\ m^{-3}$)	V x 10^3 ($m\ sec^{14}$)	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} $m^3\ mol^{-1}\ pa^{-1}$	L_f x 10^{-1} m^{-1}
75%	0.9985	1.588	0.23442	162.004	393.147
80%	0.9527	1.7543	0.2594	112.903	373.773
85%	0.9419	1.4683	0.21679	106.098	408.917
90%	0.9142	1.4116	0.20932	365.151	416.077

Table 7: Acoustic Parameters at different percentage of dioxane

Ligand L_3 Temp:295K

% 1,4-Dioxane	ds x 10^3 ($kg\ m^{-3}$)	V x 10^3 ($m\ sec^{14}$)	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} $m^3\ mol^{-1}\ pa^{-1}$	L_f x 10^{-1} m^{-1}
75%	1.0447	1.567	0.20932	160.226	396.132
80%	0.9882	1.6266	0.23094	494.857	431.512
85%	0.9817	1.3113	0.19461	836.4	432.016
90%	0.9211	1.4226	0.19417	208.456	416.865

Table 8: Acoustic Parameters at different percentage of dioxane

Ligand L_4 Temp:295K

% 1,4-Dioxane	ds x 10^3 ($kg\ m^{-3}$)	V x 10^3 ($m\ sec^{14}$)	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} $m^3\ mol^{-1}\ pa^{-1}$	L_f x 10^{-1} m^{-1}
75%	1.2079	1.6063	0.20853	266.208	338.782
80%	0.9912	1.578	0.31569	116.655	346.503
85%	0.9714	1.5073	0.30179	684.88	362.101
90%	0.9402	1.5496	0.27638	561.851	353.133

Table 9: Acoustic Parameters at different percentage of dioxane

Ligand L_1 Temp:297K

% 1,4-Dioxane	ds x 10^3 ($kg\ m^{-3}$)	V x 10^3 ($m\ sec^{14}$)	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} $m^3\ mol^{-1}\ pa^{-1}$	L_f x 10^{-1} m^{-1}
75%	1.5335	1.7756	0.39106	552.318	305.18
80%	0.9095	1.4814	0.54479	120.764	367.36
85%	0.9224	1.2472	0.67271	184.497	403.92
90%	0.9213	1.0616	0.53948	89.8341	450.36

Table 10: Acoustic Parameters at different percentage of dioxane

Ligand L_2 Temp:297K

% 1,4-Dioxane	ds x 10^3 ($kg\ m^{-3}$)	V x 10^3 ($m\ sec^{14}$)	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} $m^3\ mol^{-1}\ pa^{-1}$	L_f x 10^{-1} m^{-1}
75%	1.5442	1.2185	0.47695	120.7709	344.89
80%	0.9312	1.4814	0.47578	199.1365	339.98
85%	0.9014	1.5185	0.81968	855.4561	447.46
90%	0.9001	1.112	0.53146	178.4113	361.21

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Table 11: Acoustic Parameters at different percentage of dioxane

Ligand L_3 Temp:297K

% 1,4-Dioxane	ds x 10^3 (kg m^{-3})	V x 10^3 (m sec^{14}	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} m^3 mol^{-1} pa^{-1}	L_f x 10^{-1} m^{-1}
75%	1.4982	1.6173	0.46563	105.304	336.15
80%	0.9719	1.4121	0.61442	215.901	385.18
85%	0.9821	1.5874	0.48482	743.932	344.14
90%	0.9715	1.5002	0.47878	487.167	339.74

Table 12: Acoustic Parameters at different percentage of dioxane

Ligand L_4 Temp:297K

% 1,4-Dioxane	ds x 10^3 (kg m^{-3})	V x 10^3 (m sec^{14}	βs x 10^{-10} (pa^{-1})	ϕv x 10^{-3} m^3 mol^{-1} pa^{-1}	L_f x 10^{-1} m^{-1}
75%	1.3725	1.6122	0.46591	165.782	339.31
80%	0.9516	1.4585	0.57218	753.352	362.8
85%	0.9319	1.6176	0.47248	172.733	344.24
90%	0.981	1.066	0.45761	967.148	339.9

Fig-1

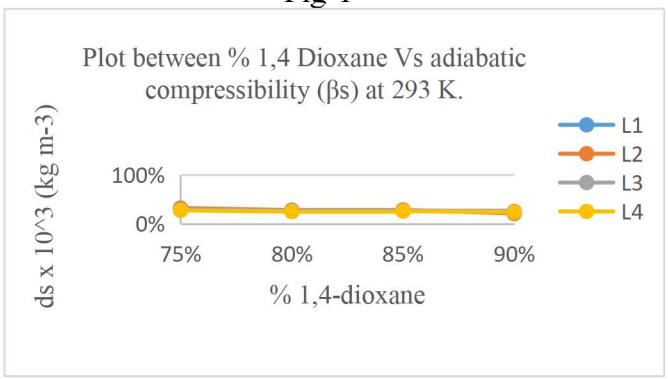

Fig -2

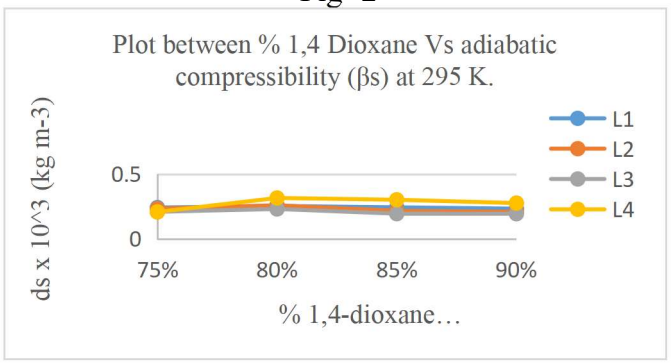

Fig- 3

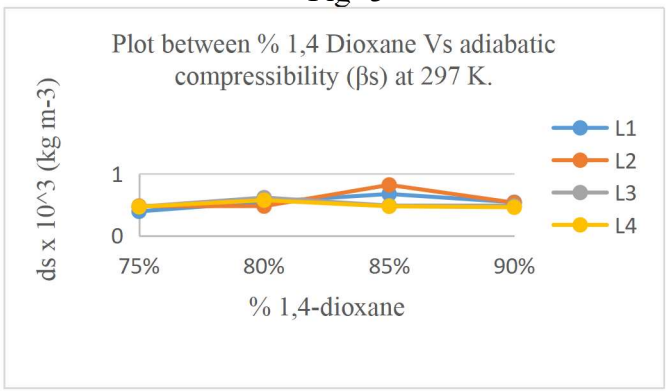

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Fig. 4

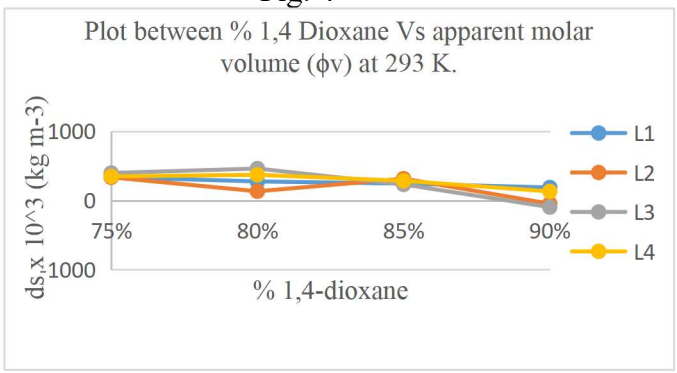

Fig.5

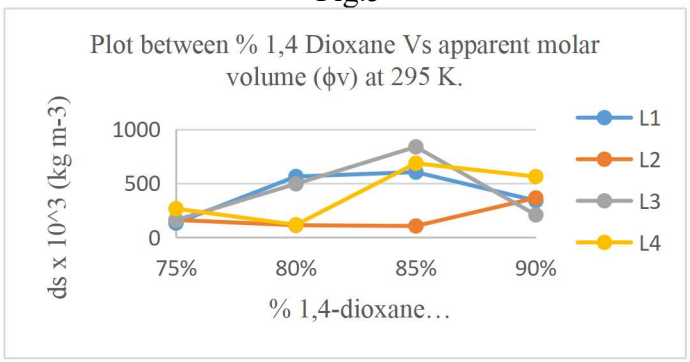

Fig.6

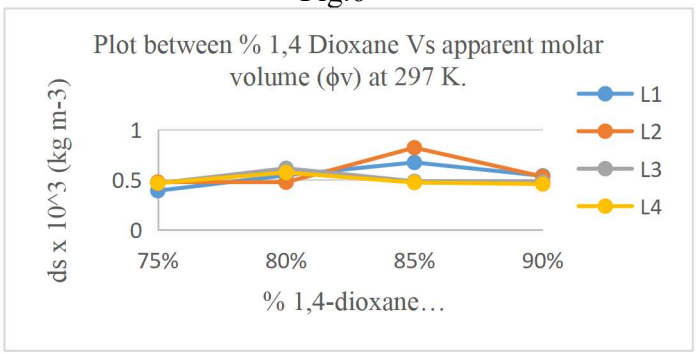

Fig.7

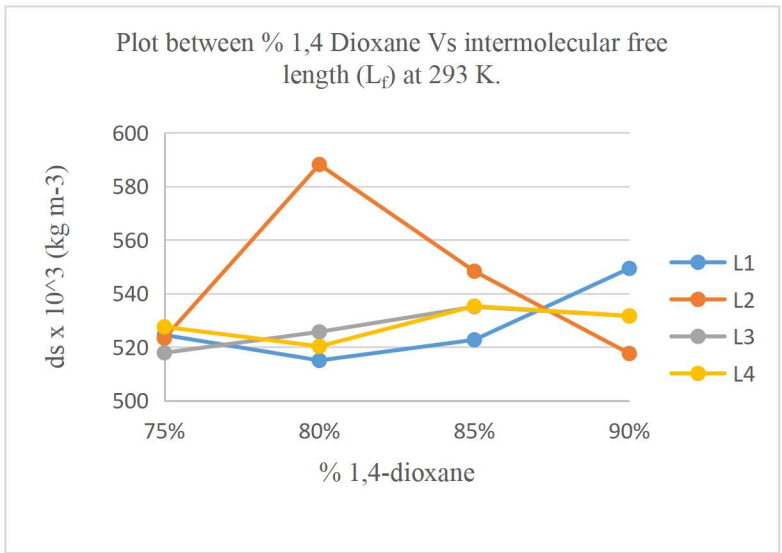

Fig .8

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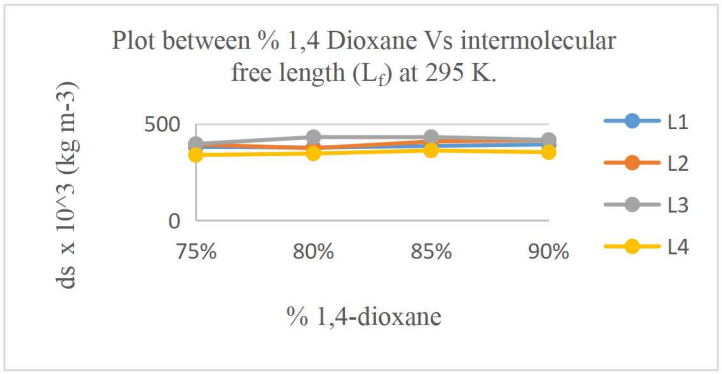
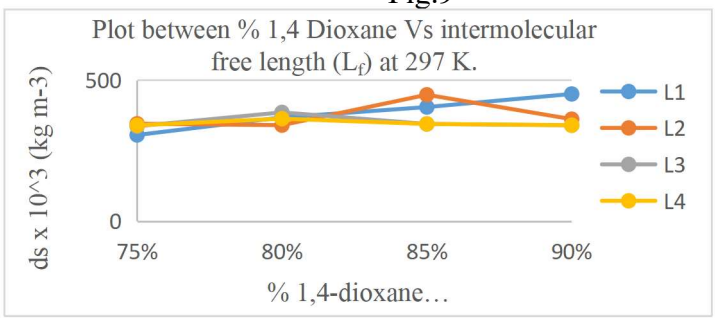


Fig.9



V) CONCLUSION: -

From available research one can easily clarify that, when the value of βs is low there is higher association of molecules showing the solute-solvent interactions. Similarly, when the value of ϕv and is positive, in dioxane it shows strong interaction between ion and solute Hence, ultrasonic velocity measurement technique can be used to analyse and study solute-solvent, solute- solute, and ion-solute interactions. In addition to this, acoustic properties help in studying and analysing the varied interactions occurring in the Process of making and breaking the structures. With these technical know-how one can easily study the detailed insight of stability of ligands in the solution."

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