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STUDIES IN ACOUSTICAL PROPERTIES OF NITRO AND BROMO-NITRO SUBSTITUTED ISOXAZOLINES IN DIFFERENT CONCENTRATION AND DIFFERENT PERCENTAGES IN DMSO-WATER MIXTURE

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ABSTRACT

The acoustical properties of 3-(2-hydroxy-3-nitro-5-methylphenyl)-5-(3-nitrophenyl) isoxazoline(L_1) and 3-(2-hydroxy-3-bromo-4-nitro-5-methyl)-5-(3-nitrophenyl) isoxazoline (L_2) have been investigated from the ultrasonic velocity and density measurements at different concentration and different percentages in DMSO-water mixture at 307 K. The adiabatic compressibility (βs), acoustic impedence (Z_s), intermolecular free length (L_f), apparent molal volume (ϕ_v) and relative association (R_A) values have been calculated from the experimental data of velocity and density measurement at concentration range 0.01-0.05 mol/lit and 60%,70%, 80%,90%,100% DMSO-water mixture. These above parameters are used to discuss the structural and molecular interactions.

INTRODUCTION

The study of intermolecular interaction plays an important role in the development of molecular Sciences. The effect of dioxane on substituted thiocarbamide,pyrazolines have been studied by ultrasonic method [1, 2].The acoustical properties were studied by many workers.[3-9] For interpreting solute-solvent, ion-solvent interaction in aqueous and non – aqueous medium was helpful from Ultrasonic velocity measurements in recent year[10-13]. Ultrasonic waves used to detect a wide variety of anomalous condition such as pregnancy, tumors and a study various phenomena such as heart valve action. This Ultrasonic wave is more sensitive than X-rays. Due to this ultrasonic technique used in the treatment of certain cancer as well as arthritis and related diseases [14]. Recently, the acoustical properties of amino acids in aqueous magnesium acetate at constant temperature were studied from the measurement of ultrasonic velocity and density [15]. The studied of the determination of densities, viscosities, refractive indices of organic liquid mixture are reported by many workers[16-19]. The studied the acoustical properties and viscosity coefficient of substituted heterocyclic drugs under suitable condition [20]. The work follow systematic studies of nitro and bromo nitro substituted isoxazolines in different concentration and different percentage in DMSO-water mixture and measure the ultrasonic velocities and densities, from that values, evaluated the acoustic properties.

MATERIALS AND METHODS

All chemicals used were of analytical grade was purified by Vogel's standard method[21].The distilled DMSO was used for preparation of different concentration and different percentages of nitro and bromo nitro substituted isoxazolines solution. Acetone was used for washing purpose. The acoustical properties require the measurement of ultrasonic velocity and densities. The densities of pure solvent and their solution were measured by using a bicapillary Pyknometer (Borosil) (±0.2%) having a bulb volume of about 10 cm3 and capillary having an internal diameter of 1 mm. The ultrasonic velocities were measured by using single crystal interferometer (Mittal Enterprises, Model MX-3) with accuracy of ± 0.03 % and frequency 1MHz. In the present work, different properties such as adiabatic compressibility (β_s), apparent molal volume (ϕ_v), intermolecular free length (L_f), apparent molal compressibility ($\phi_{k(s)}$), acoustic impedance (Z_s), relative association (R_A) have been evaluated from following equations. The adiabatic compressibility (β_s) was calculated from Newton-Laplace.

Equation:

$b_s = 1/U_s2 \times d_s$ ……… [for solution] ……………(i)

$b_o = 1/U_o2 \times d_o$ ……… [for solvent] ……………..(ii)

Where, d_o, d_s and U_o, Us are the densities of pure solvent, solution and ultrasonic velocities of pure solvent and solutions, respectively

The apparent molal compressibility ($\phi_{k(s)}$) has been calculated by using the relation.

Adiabatic compressibility (β_s) = $1 / U_s^2 d_s$ ------(1)

Adiabatic compressibility (β_o)= $1 / U_0^2 d_0$ ------(2)

Apparent molal volume (ϕ_v) =[M/d_s] x (d_0-d_s) x10^3 / m x d_s x d_0 -----------(3)

Apparent molal compressibility

($\phi_{k(s)}$) =1000 x [$\beta_s d_0$- $\beta_o d_s$ / M x d_s x d_0] + β_s x M / d_s -------(4)

Specific acoustic impedence (Z_s) = $U_s d_s$ ----------(5)

Intermolecular free length (L_f) =$K\sqrt{\beta_s}$ ------------(6)

Relative association (R_A) =(d_s/d_o) x $(U_o/U_s)^{1/3}$ -----------(7)

Where 'K' is a temperature dependent constant known as Jacobson constant [25].

RESULT AND DISCUSSION

The experimental values of density and ultrasonic velocity at different concentration of ligand (L_1 & L_2) and different percentage in DMSO -water mixtures at 307 K are given in the tables 1-2. From these experimental data,

Table 1:-

(a) Acoustic parameters of HNMP3NI L_1 at different percentage of solute in 70% DMSO-water mixture

% DMSO	Ultrasonic Velocity (U_s) (m/sec) × 10^3	Density ds (g/m^3) ×10^6	Adiabatic Compressibility β_s (bar^{-1}) ×10^{-10}	Intermolecular Free Length L_f (A^o) × 10^2	Apparent molal volume (ϕ_v) (m^3/mol)x10^{-6}	Apparent molal compressibility ($\phi_{K(S)}$) (m^{3}mol^{-1}bar^{-1})x10^{-10}	Relative Association (R_A)	Specific acoustic impedance Zs(kgm^{-2}s^{-1})x10^6
100	1.3916	1.0831	47.68	4.387	1274	59.68	1.01014	1.5072
90	1.5608	1.0813	37.96	3.915	1382	-34.72	0.98589	1.6876
80	1.5915	1.0809	36.53	3.84	1302	6.906	0.99122	1.7203
75	1.6723	1.0803	33.31	3.667	1254	4.039	0.99033	1.8066
70	1.6761	1.0802	32.95	3.648	1062	4.008	0.99385	1.8110
60	1.6787	1.0799	32.86	3.642	1279	6.507	0.99367	1.8128

(b) Acoustic parameters of HNMP3NI L_1 at different concentration of solute in 70% DMSO-water mixture

% DMSO	Ultrasonic Velocity (U_s) (m/sec) × 10^3	Density ds (g/m^3) ×10^6	Adiabatic Compressibility β_s (bar^{-1}) ×10^{-10}	Intermolecular Free Length L_f (A^o) × 10^2	Apparent molal volume (ϕ_v) (m^3/mol)x10^{-6}	Apparent molal compressibility ($\phi_{K(S)}$) (m^{3}mol^{-1}bar^{-1})x10^{-10}	Relative association (R_A)	Specific acoustic impedance Zs(kgm^{-2}s^{-1})x10^6
1×10^{-2}	1.5105	1.082	40.5034	4.029	1418	-49.08	0.964	1.635
2×10^{-2}	1.5810	1.083	36.9478	3.849	852.5	0.946	0.95	1.712
3×10^{-2}	1.6109	1.083	35.5790	3.777	675.1	-30.88	0.944	1.745
4×10^{-2}	1.6907	1.084	32.2758	3.597	575.6	-28.59	0.93	1.826
5×10^{-2}	1.7006	1.085	31.8835	3.575	519.3	-25.06	0.929	1.844

Table 2

(a)Acoustic parameters of HBNMP3NI L_2 at different percentage of solute in 70% DMSO-water mixture

% DMSO	Ultrasonic Velocity (U_s) (m/sec)x 10^3	Density ds (g/m^3) ×10^6	Adiabatic Compressibility β_s (bar^{-1}) ×10^{-10}	Intermolecular Free Length L_f (A^o) × 10^2	Apparent molal volume (ϕ_v) (m^3/mol)x 10^{-6}	Apparent molal compressibility ($\phi_{K(S)}$) (m^{3}mol^{-1}bar^{-1})x10^{-10}	Relative association (R_A)	Specific acoustic impedance Zs(kgm^{-2}s^{-1})x10^6
100	1.4856	1.089	41.62	4.099	840.1	1.729	0.993	1.617
90	1.5820	1.088	36.71	3.85	760.7	-15.5	0.988	1.722
80	1.6169	1.088	35.16	3.768	597.8	-11.42	0.992	1.759
75	1.7021	1.088	31.73	3.579	454.6	-18.01	0.992	1.851
70	1.7039	1.086	31.72	3.578	3.998	-14.5	0.994	1.85
60	1.7118	1.086	31.43	3.562	401.8	-18.44	0.993	1.859

(b)Acoustic parameters of HBNMP3NI L_2 at different concentration of solute in 70% DMSO-water mixture

% DMSO	Ultrasonic Velocity (U_s) (m/sec) × 10^3	Density ds (g/m^3) ×10^6	Adiabatic Compressibility β_s (bar^{-1}) ×10^{-10}	Intermolecular Free Length L_f (A^o) × 10^2	Apparent molal volume (ϕ_v) (m^3/mol)x10^{-6}	Apparent molal compressibility ($\phi_{K(S)}$) (m^{3}mol^{-1}bar^{-1})x10^{-10}	Relative association (R_A)	Specific acoustic impedance Zs(kgm^{-2}s^{-1})x10^6
1×10^{-2}	1.5221	1.088	39.68	4.009	966.3	-58.59	0.967	1.656
2×10^{-2}	1.5926	1.088	36.24	3.832	672.4	-44.48	0.952	1.733
3×10^{-2}	1.6230	1.088	34.89	3.76	571.5	-33.4	0.941	1.766
4×10^{-2}	1.7123	1.089	31.33	3.563	514.6	-33.06	0.93	1.864
5×10^{-2}	1.7159	1.089	31.19	3.555	483.9	-26.48	0.93	1.869

In the present investigation, different acoustical properties such as ultrasonic velocity (Us), adiabatic compressibility (β_s), intermolecular free length (L_f), specific acoustic impedance (Z_s),apperent molal volume (φ_v), apparent molal compressibility ($\varphi_{\kappa(s)}$), relative association (R_A) of the solution in different percentage of DMSO-water mixtures and at different concentrations of solute are determine at 300K and presented in table 1-2. From above tables, it is found that apparent molal volume increases with increases in the percentage of the DMSO.The value of the apparent adiabatic compressibility is increases with increase in the percentage of the DMSO.It shows strong electrostatic attractive force in the vicinity of ions.In L_2 at different percentage of DMSO ($\varphi_{\kappa(s)}$)increases first then again decreases &increases with increase in concentration of L_1 ,this may b due to weakening intermolecular interaction . It can be concluded that strong molecular association is found in systems. The value of the relative association is increases with increase in the percentage of DMSO in systems. It is found that there is weak interaction between solute and solvent.From Table 1&2, it is found that the ultrasonic velocity increases with increase in the concentration of the ligand L_1 & L_2 in 70% DMSO-water mixture at 34^0C temperature.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 propogation proposed by Erying and Kincaid[22]. It was found that, intermolecular free length decreases linearly on increasing the concentration ligand L_2 in 70% DMSO-water mixture at 34^0C temperature.The intermolecular free length (Lf) is found to be similar behavior,increase in free length results decrease ultrasonic velocity on the basis of sound propagation in the liquid [23, 24]. This is in good concordance with Naik and Co-workers [25]. These results showed that there is weak solute-solvent interaction. This was happened because there is significant interaction between ions and solvent molecules suggesting a structure promoting behavior of the added electrolyte. This may also indicates that decrease in number of free ions showing the occurrence of ionic association due to weak ion-ion interaction. The value of specific acoustic impedance (Zs) increases with increase in the concentration of ligand L_1 &L_2 in 70% DMSO-water mixture. The value of adiabatic compressibility is increase with the increase in the concentration of the ligand L_2 in 70% DMSO water mixture at 34^0C temperature and at ultrasonic frequency is 1 MHz is given in table. The first decrease of adiabatic compressibility then again increase with increase in the percentage of DMSO in solution may be due to the collection of solvent molecule around ions, this supporting weak ion-solvent interaction[26].This indicate that there is significant solute-solvent interaction.The increase in adiabatic compressibility following a decrease in ultrasonic velocity showing there by weakening intermolecular interaction.

CONCLUSION

The present study mentions the experimental data for ultrasonic velocity, density and at 34^0C for substituted 3,5-diaryl isoxazolines in DMSO -water mixture. From experimental data acoustical parameters calculated and studied to explan solute-solvent interaction and ion-ion & solute-solute interaction are existing between drugs and organic solvent mixture. From experimental data it can be conclude that weak solute solvent interaction in all systems.

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