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ULRASONIC BEHAVIOUR AND STUDY OF MOLECULAR INTERACTION OF SUBSTITUTED 3,5-DIARYL ISOXAZOLINE IN 70% DMF-WATER MIXTURE AT 32°C

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ABSTRACT

The acoustical properties have been investigated from the ultrasonic velocity and density measurement of 3-(2-hydroxy-3-bromo-4-nitro-5-methyl)-5-(3-nitrophenyl)isoxazoline(L_1) in 70% DMF-water mixture have been carried out in the concentration range $1 \times 10^{-2} - 5 \times 10^{-2}$ mol dm^{-3} and in different percentages of DMF-water mixture. The measurement have been perform to evaluate acoustical parameters such as –Ultrasonic Velocity (Us), Density (ds), Adiabatic compressibility (βs), Intermolecular length (L_f), Apparent molal volume (ϕ_v), Apparent adiabatic compressibility ($\phi_{k(s)}$), relative association (R_A), specific acoustic impedence (Z_s). The result have been interpreted in terms of solute-solvent interaction.

Key words: Acoustical study, Mixed solvent.

INTRODUCTION

Ultrasonic is an interesting field of study, which makes an effective contribution to many areas of human endeavor. In recent years, many attempts have been made in the field of physical acoustics and ultrasound on solids, liquids and gases. The ultrasonic velocity and adsorption coefficient measurement have furnished method for studying molecular and structural properties of liquid. There exist a close relationship between ultrasonic velocity and chemical or structural characteristics of molecules of fluid. In the recent years, measurement of the ultrasonic velocity are helpful to interpreted solute-solvent, ion-solvent interaction in aqueous medium and non-aqueous medium[1-4]. Kawaizumi et al.[5] have studied the acoustic properties of complex in water. Jahagirdar et al.[6] have studied the acoustical properties of four different drugs in methanol and he drawn conclusion from adiabatic compressibility. The four different drugs compress the solvent methanol to the same extent but it shows the different solute-solvent interaction due to their different size, shape and structure. Meshram and Narwade[7] studies the different acoustical properties of some substituted pyrazolines in binary mixture acetone-water and observed variation of ultrasonic velocity with concentration[7]. Palani and Saravanan[8] have investigated the measurement of ultrasonic velocity and density of amino acid in aqueous magnesium acetate at constant temperature. Syal et al.[9] have studied the ultrasonic velocity of PEG-8000, PEG-study of acoustical properties of substituted hetrocyclic compounds under suitable condition. M. Arvinthraj et al.[10] have determined the acoustic properties for the mixture of

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amines with amide in benzene at 303 K-313 K. They also determined thermodynamic parameters. Thakur and Chauhan[11] have studied the different acoustical parameters of binary mixture of 1-propanol and water. Tadkalkar et al.[12] have studied the acoustical and thermodynamic properties of citric acid in water at different temperature. Mishra and Mishra[13] have investigated ultrasonic velocity and density in non aqueous solution of metal complex and evaluate acoustical properties of metal complex. The ion-dipole interaction mainly depends on ion size and polarity of solvent. The strength of ion-dipole attraction is directly proportional to the size of the ions, magnitude of dipole. But inversely proportional to the distance between ion and molecules. Voleisines and Veloisis[14] have studied the structural properties of solution of lanthanide salt by measuring ultrasonic velocity. After review of literature survey, the detail study of substituted heterocyclic drug under identical set of experimental condition is still lacking. It was thought of interest to study the acoustical properties of substituted isoxazoline under suitable condition.

EXPERIMENTAL

The substituted 3-(2-hydroxy-3-bromo-4-nitro-5-methyl)-5-(3-nitrophenyl) isoxazoline (L_1) is used in the present study. DMF was purified by Vogel's standard method[15]. In the present study, the DMF was used for solution preparation of different compound. The density was determined by using specific gravity bottle by relative measurement method. The ultrasonic velocity was measure by using ultrasonic interferometer having frequency 1 MHz (Mittal Enterprise, Model MX-3) of accuracy of ± 0.03%. The constant temperature was maintained by circulating water through the double wall measuring cell made up of steel. In the present investigation different parameters such as adiabatic compressibility (β_s), appearent molal volume (φ_v), intermolecular free length (L_f), apparent molal compressibility ($\varphi_{k(s)}$), specific acoustic impedance (Z_s), relative association (R_A), were studied.

Adiabatic compressibility $(\beta_s) = 1 / U_s^2 d_s$ …(1)

Adiabatic compressibility $(\beta_o) = 1 / U_0^2 d_0$ …(2)

Apparent molal volume $(\phi_v) = [M/d_s] \times (d_0 - d_s) \times 10^3 / m \times d_s \times d_0$ …(3)

Apparent molal compressibility $(\phi_{k(s)}) = 1000 \times [\beta_s d_0 - \beta_o d_s/M \times d_s \times d_0] + \beta_s \times M / d_s$ …(4)

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

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

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

RESULTS AND DISCUSSION

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 DMF-water mixtures and at different concentrations of solute are determine at 305 K and presented in Table 1. From Table 1, it is found that apparent molal volume increases with increases in the percentage of the DMF. The value of the apparent adiabatic compressibility is increased with increase in the percentage of the DMF. It shows strong electrostatic attractive force in the vicinity of ions. 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 DMF in systems. It is found that there is weak interaction between solute and solvent.

Table 1: Acoustic parameters of HBNM3NI L_1 at different percentage of solute in 70% DMF-water mixture

System – HBNM3NI (L_1)   Temp : 32± 0.1 °C   Ultrasonic frequency – 1 MH_Z

% DMF	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^0) × 10^2	Apparent molal volume (ϕ_v) (m^3/mol) x 10^{-6}	Apparent molal compressibility ($\phi_{K(S)}$) ($m^3mol^{-1}bar^{-1}$) x 10^{-10}	Relative association (R_A)	Specific acoustic impedance Zs ($Kgm^{-2}s^{-1}$) x 10^6
100	1.2571	0.938	67.49	5.202	1474	84.9	1.027	1.179
90	1.2965	0.939	63.37	5.041	1461	68.14	1.021	1.217
80	1.3121	0.941	61.75	4.976	1443	84.25	1.023	1.234
75	1.3473	0.942	58.49	4.843	1343	76.51	1.02	1.269
70	1.3949	0.944	54.46	4.673	1117	55.23	1.014	1.316
60	1.4333	0.952	51.15	4.529	864.6	64.11	1.015	1.364

Table 2: Acoustic parameters of HBNM3NI L_1 at different concentration of solute in 70% DMF-water mixture

% DMF	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^0) × 10^2	Apparent molal volume (ϕ_v) (m^3/mol) x 10^{-6}	Apparent molal compressibility ($\phi_{K(S)}$) ($m^3mol^{-1}bar^{-1}$) x 10^{-10}	Relative association (R_A)	Specific acoustic impedance Zs ($Kgm^{-2}s^{-1}$) x 10^6
1×10^{-2}	1.4173	0.939	53.04	4.612	2037	-58.39	0.964	1.33
2×10^{-2}	1.4375	0.941	51.42	4.541	1094	-37.49	0.963	1.353
3×10^{-2}	1.4533	0.943	50.22	4.487	817.7	-28.82	0.961	1.37
4×10^{-2}	1.4822	0.951	47.86	4.381	486.8	-28.58	0.963	1.41
5×10^{-2}	1.4848	0.952	47.65	4.371	459.9	-22.97	0.962	1.418

From Table 2, it is found that the ultrasonic velocity increases with increase in the concentration of the ligand L_8 in 70% DMF-water mixture at 32°C 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[16]. It was found that, intermolecular free length decreases linearly on increasing the concentration ligand L_1 in 70% DMF-water mixture at 32°C temperature. The intermolecular free length increases due to greater force of interaction between solute and solvent by forming hydrogen bonding. This was happened because there is significant interaction between ions and solvent molecules suggesting a structure promoting behavior of the added electrolyte. This 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 in 70% DMF-water mixture. The value of adiabatic compressibility is increased with increase in the concentration of the ligand L_1 in 70% DMF water mixture at 32°C temperature and at ultrasonic frequency is 1 MHz as given in Table. The first decrease of adiabatic compressibility then again increase with increase in the percentage of DMF in solution may be due to the collection of solvent molecule around ions, this supporting weak ion-solvent interaction[17]. This indicates 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 shows the experimental data for ultrasonic velocity, density at 32°C for substituted 3,5-diaryl isoxazoline in DMF and DMF-water mixture. From experimental data, acoustical parameters were calculated and studied to explanation 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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REFERENCES

1. S. Baluja and S. Oza, Fluid Phase Equibria, **200(1)**, 49-54 (2005).
2. M. K. Rawat and Sangeeta, Ind. J. Pure Appl. Phy., **46**, 187-192 (2008).
3. A. Ali and A. K. Nain, Acoustics Lett., **19**, 53 (1996).
4. H. Ogawa and S. J. Murakami, J. Solution. Chem., **16**, 315 (1987).
5. F. Kawaizumi, K. Matsumoto and H. Nomura, J. Phys. Chem., **87(16)**, 3161-3166 (1983).
6. D. V. Jahagirdar, B. R. Arbad, S. R. Mirgane, M. K. Lande and A. G. Shankarwar, J. Molecular Liq., **75**, 33-43 (1998).
7. Y. K. Meshram and M. L. Narwade, Acta Clencia Indica, **XXVII.C No. 2**, 67-70 (2001).
8. R. Palani and S. Saravanan, Res. J. Phys., **2(1)**, 13-21 (2008).
9. V. K. Syal, A. Chauhan and S. Chauhan, J. Pure Ultrasound, **27**, 61-69 (2005).
10. M. Arvinthraj, S. Venktesan and D. Meera, J. Chem. Pharm. Res., **3(20)**, 623-627 (2011).
11. S. K. Thakur and S. Chauhan, J. Chem. Pharm. Res., **3(2)**, 657-664 (2011).

12. A. Tadkalkar, P. Pawar and G. K. Bichile, J. Chem. Pharm. Res., **3(3)**, 165-168 (2011).
13. A. P. Mishra and D. K. Mishra, J. Chem. Pharm. Res., **3(3)**, 489-498 (2011).
14. B. Voleisiene and A. Voleisis, J. Ultrasound, **63(4)**, 7-18 (2008).
15. Vogel's, G. H. Jaeffery, S. Bassetl and R. C. Denney, Text Book of Quantitative Chemical Analysis, V^{th} Ed., ELBS Longman (1997) p. 53.
16. H. Eyring and J. F. Kineaud, J. Chem. Phys., **6**, 620-629 (1938).
17. J. D. Pandey, A. Shukla, R. D. Rai and K. J. Mishra, J. Chem. Eng. Data., **34**, 29 (1989).