ACOUSTICAL PARAMETERS AND SOLVATION BEHAVIOR OF NIFURTIMOX DRUG IN DIFFERENT MIXED SOLVENTS AT 308 K

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Abstract

The density, viscosity and ultrasonic velocityforNifurtimox drug have been investigated by experimental procedures in order to understand the effect of solvents on molecular interactions in different medium at 308K inthe concentration range of 0.002 to 0.01 mol dm-3.Various acoustical parameters such as apparent molar compressibility (φk), apparent molar volume (φv), adiabatic compressibility (βs), specific acoustic impendence (Z), intermolecular, free length (Lf) etc. have been evaluated. Ultrasonic studies provide valuable information in understanding the molecular behavior and intermolecular interactions of Nifurtimox drug in different solvent mixtures. The variation of these acoustic parameters is explained in terms of solute-solvent molecular interaction occurring in drug solutions.

Introduction

Solvation describes the interaction of solvent with dissolved molecules. Both ionized and uncharged molecules interact with solvent, strength and nature of this interaction influence many properties of the solute as well as influencing the properties of the solvent such as viscosity and density. Ion-solvation is the back bone of solution chemistry [1-2].Ultrasonic waves and related thermodynamic parameterprovided valuable information about the structure of solid. The measurement of ultrasonic velocity has been adequately employed in understanding the nature of molecular interactions in pure liquids[3-6] and liquid mixtures[7-8]. Ultrasonic propagation parameters yield valuable information regarding the behavior of liquid systems, because intramolecular and intermolecular association, dipolar interactions, complex formation and related structural changes affect the compressibility of the system which in turn produces corresponding variations in the ultrasonic velocity. The acoustical and thermodynamical parameters obtained in ultrasonic study show that the ion solvation is accompanied by the destruction or enhancement of the solvent structure[9-12]. Excess thermodynamic properties of liquid mixtures are of great interest to conveniently design industrial processes and also to provide valuable information on the molecular interactions required for optimizing thermodynamic models. When two or more liquids are mixed there occur some changes in physical and thermodynamic properties because of free volume change, change in energy and change in molecular orientations. Derived thermodynamic and acoustical parameters like internal pressure, free volume and acoustic impedance are of considerable interest in understanding the intermolecular orientations in binary liquid mixtures[13-15]. Excess thermodynamic properties of mixtures are useful in the study of molecular orientations and arrangements[16-17]

For the present study Nifurtimox drug is selected.The Nifurtimox has an antiparasitic activity and used to treat Chages disease and also used in treating problem related to central nervous system. So, it was found important to study Ultrasonic and thermodynamic behavior of the dugs which may lead to some new findings. The acoustic properties of

Nifurtimox drug have been studied in 30% Methanol-water, 30%Dioxane-water and 30% DMF-water solutions at 308K

Experimental

For the present work methanol, dioxane and dimethyl formamide solvents used which are of AR grade and were purified and dried by the usual procedure. Densities, viscosities and ultrasonic velocities were measured at 308K over a wide range of composition. Densities were determined by using bicapillarypyknometer. The viscosities were measured by precalibrated Ostwald viscometer. Ultrasonic velocity measurements were made by using an ultrasonic interferometer (Mittal Enterprises, New Delhi) at a frequency of 2MHz with a tolerance of ± 0.005%. All the measurements were carried out at 308K

Theory

Acoustic parameters such as apparent molar compressibility (φ_k), apparent molar volume (φ_v), adiabatic compressibility (β_s), specific acoustic impendence (Z), intermolecular free length (L_f), Limiting apparent molar volume (φ^0_v), Limiting apparent molar compressibility (φ^0_k)were determined using following relations.

Ultrasonic velocity $u = \lambda\upsilon$ ---------- (i)

Adiabatic compressibility $\beta_s = 1/u^2{}_s\rho_s$ ---------- (ii)

Apparent molar volume $\varphi_v = 10^3(\rho_0-\rho_s)/m-\rho_0\rho_s + M/\rho_0$ ---------(iii)

Apparent molar compressibility $\varphi_k = 10^3(\rho_0\beta_s-\rho_s\beta_0)/m-\rho_s\rho_0 + \beta_s M/\rho_s$---(iv)

Intermolecular free length $L_f = K(\beta_s)^{1/2}$ ---------- -------(v)

Specific acoustic impendence $Z = \rho.u$ --------- ----- ----------(vi)

Limiting apparent molar volume $\varphi_v = \varphi^0_v + S_vC^{1/2}$ ---------- (vii)

Limiting apparent molar compressibility $\varphi_k = \varphi^0_k + S_k^{1/2}$----------(viii)

Table no.1

Experimental Data of Density, Ultrasonic Velocity and Viscosity of Nifurtimox Drug in Different Solvents at 308 K

Solvents	Conc.mol.dm^{-3}	Density ρ,Kgm^{-3}	Ultrasonic Velocity(u)m/s	Viscosityx10^{-3} Nsm^{-2}
30% MeOH-Water Medium	0.002	928. 07	1543.7	1.1251
	0.004	928.28	1554.0	1.1312
	0.006	928.65	1576.7	1.1314
	0.008	928.79	1588.3	1.1355
	0.01	928.86	1595.9	1.1387
30% Dioxane-Water Medium	0.002	1054.44	1649.3	1.24351
	0.004	1054.56	1661.2	1.24692
	0.006	1054.61	1675.6	1.24854
	0.008	1054.72	1681.9	1.24958
	0.01	1054.95	1689.7	1.24850
30% DMF-Water Medium	0.002	1012.41	1543.3	0.95234
	0.004	1012.52	1567.5	0.95457
	0.006	1012.73	1571.6	0.95582
	0.008	1012.84	1582.5	0.95649
	0.01	1012.96	1599.8	0.95963

Table no.2

Variation of some acoustical parameters with concentration of NifurtimoxDrug in different Solvents at 308K

Solvents	Conc.mol.dm^{-3}	β_s x10^{-10} Pa^{-1}	Φ_vx10^{-5} m^{3}mol^{-1}	Φ_k x10^{-14} m^{3}mol^{-1} Pa^{-1}	L_fx10^{-11} (m)	Z x 10^5 Kg m^{-2} sec^{-1}
30%MeOH-Water Medium	0.002	4.3873	-82.55	-53.658	3.2246	14.4144
	0.004	3.3634	-61.49	-38.577	3.2116	14.4512
	0.006	3.3459	-12.56	-25.343	3.1697	14.4523
	0.008	3.3223	8.66	-2.117	2.1156	14.4549
	0.01	3.2898	14.97	-5.1773	2.0194	14.4852
30%Dioxane-	0.002	6.8677	-49.4	-81.7969	4.9345	14.3493
	0.004	6.7953	-8.81	-44.6467	4.1272	15.3532

Water Medium	0.006	6.7851	7.98	-22.6674	4.0657	15.3571
	0.008	6.7128	9.82	-18.5594	4.0117	15.3598
	0.01	6.6232	15.94	-16.5892	4.0012	15.3612
30% DMF-Water Medium	0.002	4.7223	12.56	298.7213	4.4677	14.4249
	0.004	4.6239	17.34	134.5842	4.4566	14.6552
	0.006	4.5612	22.26	114.4264	4.4432	14.6767
	0.008	4.5457	24.35	78.1877	4.4356	14.6953
	0.01	4.5258	25.49	65.4595	4.4253	14.7661

Table-3

Limiting values of ϕ^0_v and ϕ^0_k along with slope (S_v&S_k) for Nifurtimox Drug different medium at 308K temperature

Temp. T (K)	Medium	Parameters			
		$\phi^0_v \times 10^{-5}$ m^3mol^{-1}	$\phi^0_k \times 10^{-14}$ $m^3mol^{-1}pa^{-1}$	$S_v \times 10^{-5}$ $m^3mol^{-3/2}dm^{3/2}$	$S_k \times 10^{-14}$ $m^3mol^{-3/2}dm^{3/2}pa^{-1}$
308K	30% M-H_2O	- 148.634	-77.65	473.88	326.95
	30% D- H_2O	-76.643	-256.17	448.771	409.523
	30% DMF- H_2O	4.854	545.26	61.342	-1483.37

Table-4 A and β, coefficient values at 308 K in different medium for NifurtimoxDrug

Medium	Coefficient	308K
30%Methanol-Water medium	A	1.564
	β	-0.253
30%Dioxane-Water medium	A	1.852
	β	-0.384
30% DMF-Water medium	A	0.453
	β	-0.118

Results and discussion:

Table 1 shows that density (ρ), ultrasonic velocity (u) and viscosity (η) increases with increase in concentration for all three systems. The increase in ultrasonic velocity is due to decrease in intermolecular free length (L_f) as shown in table 2. This suggests that there is a strong interaction between Nifurtimox drug and solvent molecule. Adiabatic compressibility (β_s) is a measure of intermolecular association or repulsion calculated from the measured ultrasonic velocity (u) and density (ρ). Adiabatic compressibility is found to decrease with increase in concentration. Since adiabatic compressibility is inversely related to the product of density and ultrasonic velocity based on this the compressibility is expected to decrease which has observed in the present case. When the sound waves travels through the solution, certain part of it travels through the medium and rest gets reflected by the ion i.e. restriction for flow of sound velocity by the ions. The character that determines the restriction movement of sound waves is known as acoustic impendence (Z). It has been found that acoustic impendence increases with increase in concentration. The apparent molar compressibility (φ_k) explains the solute-solvent and solute- solute interactions in solution and was calculated by using the equation no. (iv). The apparent molar volume (φ_v) is defined as the change in volume of solution for the added one mole of a particular component at constant temperature and pressure. It is thermodynamic property which helps in elucidating solvation behavior of electrolyte in solution. Apparent molar volume was evaluated from the density of solution and solvent.

It is evident from the table 3 that φ^0_k values are negative for 30%MeOH-water and 30%Dioxane-water but for 30%DMF-water φ^0_k values are positive. The negative φ^0_k values are suggest solute- solvent interaction whereas positive values are due to solute- solute interaction, is further confirmed by φ^0_v values which are positive for 30% DMF-water and negative for 30%MeOH-water and 30%Dioxane-water of the drug. Sis a measure of solute – solvent interaction. It is observed from the table 3 that S values are higher in 30%MeOH-

water and 30%Dioxane-water and low in 30% DMF-water solution. This confirms that in 30% DMF-water solution solute- solute interactions and in30%MeOH-water and 30%Dioxane-water solute – solvent interaction predominate.

The viscosity B-Co-efficient has been derived from Jones-Dole equation

$$(c> 0.1m)\eta_r\text{-}1 / C^{1/2} = A+B\ C^{1/2}$$

Where $\frac{\eta}{\eta_0} = \eta_r$ is the relative viscosity A and β are the characteristics of the solute and solvent. A is Falkenhagen coefficient represent the contributor from solute-solute interaction and β is Jones Dole coefficient known to depend on the size of the solute particle and on the interaction between solute and solvent.

They were obtained by a least – squares treatment as intercept and slope of the linear plot of $\eta r\text{-}1 / C^{1/2}$ Vs $C^{1/2}$.The graph for each system given linear straight line showing validity of Jones-Dole equation. The slope of straight line gives value of β co-efficient.

The viscosity A coefficient represent the ion-ion interactions and negative values have shown some physical significance. However negative 'A' values have also been reported to be in other solvents in some studies. The large and small value of 'A' shows the stronger and weaker solute – solute interactions respectively. When solute is introduced into solvent of organic-water mixture it will interfere with the ordered structure of water in the solutes co-sphere. As only one solute is present so such variation in the values of A can be explained.

In the present study viscosity of liquid solutions increases with increase in concentration of drugs solution in 30% methanol-water, 30%dioxane-water and 30% DMF-water mixture. The increase in viscosity with increase in concentration may be attributed to the increase in solute solvent interactions.

Viscosity β coefficients have been established from ion- solvent interactions and are responsible for introducing order or disorder in the structure of the solvent. Solute with negative β Coefficient is characterized as structure breakers indicating weak solute-solvent interactions. Such type of results is also shown by Reddyet al.[18-21]

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