Acoustical Behavior of (S)-2-(2-oxopyrrolidin-1-yl) Butanamide Drugs in Different Mixture of Solvents at 308K

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ABSTRACT

The Measurements of density, speed of sound and viscosity at different concentration of (S)-2-(2-oxopyrrolidin-1-yl) Butanamide drug in70% Ethanol-water, 70% Acetone-water and 70% DMF-water solutions at 308K. Acoustic parameter studies provide information in understanding molecular behavior and intermolecular interactions of (S)-2-(2-oxopyrrolidin-1-yl) Butanamide drug in solvent mixtures. From the experimental data various acoustical 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) and relative association has been evaluated. The variation of these acoustic parameters is explained in terms of solute -solvent molecular interaction occurring in Drug solutions. Compressibility has been found to decrease with the increase in concentration for all compositions indicating the increase in ion-solvent interaction. The concentration range is 0.002 to 0.01 mol dm^{-3}.

Key word- Acoustical Behavior, Sound velocity, Drugs, ion-solvent interaction.

Introduction

Ultrasonic velocity studies in aqueous and several non-aqueous electrolyte solutions have led to new insight in the solvation process[1-3]. Ultrasonic waves provided valuable information about the structure of solid[4]. The measurement of ultrasonic velocity has been adequately employed in understanding the nature of molecular interactions in pure liquids[5-6] and liquid mixtures[7-11].

Ultrasonic propagation parameters yield valuable information regarding the physio-chemical 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 thermo dynamical parameters obtained in ultrasonic solvent structure[8-11]Excess thermodynamic properties of liquid mixtures are of great interest to conveniently design industrial processes and also to provide useful 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[12-14]. Excess thermionic properties of mixtures are useful in the study of molecular orientations and arrangements[15-17]

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For the present study (S)-2-(2-oxopyrrolidin-1-yl) Butanamide drug is selected. This drug is an antihistamine that reduces the effects of natural chemical histamine in the body. It is used for the treatments of sneezing, runny nose, watery eyes, hives, skin rash, itching and other cold or allergy symptoms. The acoustic properties of (S)-2-(2-oxopyrrolidin-1-yl) butanamide Drug has been studied in70% Ethanol-water, 70% Acetone-water and 70% DMF-water solutions at 308K.

Experimental

Solvents Ethanol, Acetone and Dimethyl formamide used in the present work were 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 bicapillary pyknometer. The viscosities were measured by precalibrated Ostwald type 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 volume (φ_v), apparent molar compressibility (φ_k), specific acoustic impendence (Z), adiabatic compressibility (β_s), intermolecular free length (L_f), Limiting apparent molar compressibility(φ^0_k),Limiting apparent molar volume (φ^0_v), relative association(R_A) were determined using following relations.

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

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

Apparent molar volume $\varphi_v = 10^3(d_0-d_s)/m-d_0 d_s + M/d_0$---------- (iii)

Apparent molar compressibility $\varphi_k = 10^3(d_0\beta_s-d_s\beta_0)/m-d_s d_0 + \beta_s M/d_s$---- (iv)

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

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

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

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

Relative Association $R_A = d/d_0 [u_0/u]^{1/3}$ ---------- (ix)

Table no.1

Experimental Data of Density, Ultrasonic Velocity and Viscosity (S)-2-(2-oxopyrrolidin-1-yl) Butanamide Drug in different solvent at 308K

Solvents	Conc.mol.dm^{-3}	Density dS Kgm^{-3}	Ultrasonic Velocity(u)m/s	Viscosityx10^{-3} Nsm^{-2}
70% EtOH-Water Medium	0.002	822.95	1512.1	1.98956
	0.004	823.11	1518.8	1. 98977
	0.06	823.26	1524.3	1. 98989
	0.008	823.47	1529.4	1. 99008
	0.01	823.89	1532.8	1.99021
70% Ac-Water	0.002	791.88	1575.4	0.94233
	0.004	791.96	1578.6	0.94952

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Medium	0.006	792.03	1581.1	0.95281
	0.008	792.14	1584.6	0.95343
	0.01	792.21	1589.8	0.95955
70% DMF-Water Medium	0.002	1007.61	1591.00	1.79009
	0.004	1007.82	1594.30	1.79962
	0.06	1007.98	1597.80	1.80725
	0.008	1008.14	1600.01	1.80479
	0.01	1008.26	1602.10	1.82392

Table no.2-Variation of some acoustical parameters with concentration of (S)-2-(2-oxopyrrolidin-1-yl) Butanamide Drug in different solvents at 308K

Solvents	Conc.mol. dm^{-3}	$\beta s \times 10^{-10}$ Pa^{-1}	$\Phi v \times 10^{4}$ m^3mol^{-1}	$\Phi k \times 10^{-14}$ $m^3mol^{-1}Pa^{-1}$	$Lf \times 10^{-11}$ (m)	$Z \times 10^{5}$ Kg m^{-2} sec^{-1}	$RA \times 10^{-2}$
70% EtOH-Water Medium	0.002	5.315	38.3796	391.6978	1.370626	12.44383	82.2554
	0.004	5.267	38.3402	368.9479	1.374023	12.50139	82.1502
	0.006	5.228	38.3032	350.4436	1.378796	12.54895	82.0663
	0.008	5.192	38.2514	333.2745	1.383915	12.59415	81.9959
	0.01	5.166	38.1479	321.1907	1.390182	12.62859	81.9774
70% Acetone-W	0.002	5.08814	46.2214	272.9187	1.360249	12.47528	78.0753
	0.004	5.06702	46.2007	263.2446	1.357423	12.50188	78.0304
	0.006	5.05056	46.1826	255.7071	1.355217	12.52279	77.9961
	0.008	5.02758	46.1542	245.1818	1.35213	12.55225	77.9495
	0.01	4.99008	45.9632	228.1659	1.347078	12.60521	77.9371
70% DMF-Water Medium	0.002	3.92073	-22.018	-335.03	1.19405	1603108	99.0194
	0.004	3.90347	-22.433	-345.054	1.191454	1606767	98.9717
	0.006	3.88656	-22.750	-355.458	1.188725	1610550	98.9152
	0.008	3.87423	-23.066	-362.402	1.186947	1613125	98.8833
	0.01	3.86421	-23.303	-368.367	1.185395	1615333	98.8539

Table- 3

Limiting values of $\phi^0 v$ and $\phi^0 k$ along with slope (Sv & Sk) for (S)-2-(2-oxopyrrolidin-1 Butanamide Drug different medium at 308K temperature

Temp. T (K)	Medium	Parameters			
		$\phi^0 v \times 10^4$ m^3mol^{-1}	$Sv \times 10^4$ $m^3mol^{-3/2}dm^{3/2}$	$\phi^0 k \times 10^{-14}$ $m^3mol^{-1}pa^{-1}$	$Sk \times 10^{-14}$ $m^3mol^{-3/2}dm^{3/2}pa^{-1}$

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308K	70% EtOH-W	37.97	4.092	258.6	1259
	70% Acetone-W	45.82	4.329	193.8	789.8
	70% DMF-W	-24.432	-398.1	611.21	598.3

Table-4. A and β coefficient values at 308K in different medium for (S)-2-(2-oxopyrrolidin-1-yl) Butanamide Drug

Medium	Coefficient	Temp 308K
70%Ethanol-Water medium	A	**0.830**
	β	**-0.163**
70 %Acetone-Water medium	A	**1.635**
	β	**-0.186**
70% DMF-Water medium	A	**0.601**
	β	**-0.091**

Results and discussion:

The density (d), ultrasonic velocity (u) and viscosity (η) increases with increase in concentration for all three systems are presented in Table 1. The increase in ultrasonic velocity is due to decrease in intermolecular free length (Lf). Intermolecular free length (Lf) denotes the magnitude of either the ion-ion interaction or the ion-solvent interaction. Intermolecular free length is a predominant factor in solvation chemistry [18] and inversely related to ultrasonic velocity. Calculated values of Lf for all the concentration and compositions are in shown in table 2. This suggests that there is a strong interaction between (S)-2-(2-oxopyrrolidin -1-yl) Butanamide Drug and solvent molecule. Adiabatic compressibility (βs) is a measure of intermolecular association or repulsion calculated from the measured ultrasonic velocity (u) and density (d). 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[6] 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 (φk) explains the solute-solvent and solute- solute interactions in solution and was calculated by using the equation no.(iv). The apparent molar

volume (φv) 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 $\varphi^0 k$ values are positive for 70% EtOH-water, 70% Acetone-water

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and 70%DMF-water. This positive values of $\varphi^0 k$ are due to solute- solute interaction, is further confirmed by $\varphi^0 v$ values which are positive for 70% EtOH-water and 70% Acetone-water and negative for 70%DMF-water of the drug. Sv is a measure of solute – solvent interaction. It is observed from the table 3 that Sv values are higher in 70% EtOH-water and 70% Acetone-water and low in 70% DMF-water solution. This confirms that in 70% DMF-water solution solute- solute interactions and in70% EtOH-water and 70% Acetone-water solute – solvent interaction predominate.

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

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

Where $\frac{\eta}{\eta^0} = \eta r$ is the relative viscosity, η and η^0 are the viscosities of solution and of the pure solvent, C is the concentration and A and β are the viscosity coefficient characteristics of the solute and solvent respectively. 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 $\eta r - 1 / C^{1/2}$ 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.[10-12]

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 70% Ethanol -water, 70% Acetone-water and 70% 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 to arise 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 Singh et al.[19-25]

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