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Acoustic and volumetric properties of substituted heterocyclic compounds in dioxane-water mixture at 303K

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ABSTRACT

Acoustical and volumetric properties have been measured for substituted heterocyclic compounds drugs and compounds in dioxane-water mixture at 303K. The measurement have been perform to evaluate acoustical parameter such as adiabatic compressibility (βs), Partial molal volume (ϕ_v), intermolecular free length (L_f), apparent molal compressibility (ϕ_K), specific acoustic impedance (Z), relative association (R_A), salvation number (Sn).

Key word: Ultrasonic velocity, adiabatic compressibility, apparent molal volume.

INTRODUCTION

In the recent years, measurements of the Ultrasonic velocity are helpful to interpreted solute-solvent, ion-solvent interaction in aqueous and non aqueous medium [1-4]. Fumio Kawaizumi [5] have been studied the acoustical properties of complex in water. Jahagirdar et. al. has 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 different solute-solvent interaction due to their different size, shape and structure [6]. Meshram et. al. studies the different acoustical properties of some substituted Pyrazolines in binary mixture acetone-water and observed variation of ultrasonic velocity with concentration[7]. Palani have investigated the measurement of ultrasonic velocity and density of amino acid in aqueous magnesium acetate at constant temperature [8]. 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 has been studied the structural properties of

solution of lanthanide salt by measuring ultrasonic velocity [9].Syal et.al. has been studied the ultrasonic velocity of PEG-8000, PEG- study of acoustical properties of substituted heterocyclic compounds under suitable condition[10].Tadkalkar et.al. have studied the acoustical and thermodynamic properties of citric acid in water at different temperature[11]. Mishra et.al. have investigated ultrasonic velocity and density in non aqueous solution of metal complex and evaluate acoustic properties of metal complex[12].M. Arvinthraj et.al. have determined the acoustic properties for the mixture of amines with amide in benzene at 303K-313K .They also determined thermodynamic parameters[13].S.K. Thakur et.al. have studied the different acoustical parameters of binary mixture of 1-propanol and water [14].

After review of literature survey the detail study of substituted heterocyclic drugs under identical set of experimental condition is still lacking. It was thought of interest to study the acoustical properties of substituted heterocyclic drugs under suitable condition .

EXPERIMENTAL SECTION

The substituted heterocyclic drugs (Acarbose, Haloperidol, Silymarin, Digoxin, Rifampicin are used in the present study. Dioxane was purified by Vogel's standard method [15]. The double distilled dioxane is used for solution preparation of different drugs. The density was determined by using specific gravity bottle by relative measurement method with accuracy $\pm 1x10^{-5}$ gm/cm^3. The ultrasonic velocity was measure by using ultrasonic interferometer having frequency 2MHz (Mittal Enterprises, Model No F-81) .The constant temperature is mentioned by circulating water through the double wall measuring cell made up of steel.

In the present investigation different parameters such as adiabatic compressibility (βs), apparent molal volume (ϕ_v), intermolecular free length (L_f), apparent molal compressibility (ϕ_κ), specific acoustic impedance (Z), relative association (R_A), Solvation number (S_n) were studied.

$$\text{Adiabatic compressibility } (\beta s) = \frac{1}{U_s^2 d_s} \qquad (1)$$

$$\text{Adiabatic compressibility } (\beta 0) = \frac{1}{U_0^2 d_0} \qquad (2)$$

$$\text{Apparent molal volume } (\phi_v) = \left(\frac{M}{ds}\right) x \frac{(d_0\text{-}ds)\ x10^3}{mxdsxd_0} \qquad (3)$$

$$\text{Apparent molal compressibility } (\phi_\kappa) = 1000\ x\left(\frac{\beta s\ d_0 - \beta 0\ d_s}{Mxdsxd0}\right) + \frac{\beta s\ x\ M}{ds} \qquad (4)$$

$$\text{Specific acoustic impedance } (Z) = Us\ ds \qquad (5)$$

Intermolecular free length (L_f) = $K\sqrt{\beta s}$ (6)

Relative association (R_A) = $(ds / d_0) \times (U_0/U_s)^{1/3}$ (7)

Solvation number (S_n) = $\phi_\kappa / \beta 0 \times (M/ d_0)$ (8)

RESULTS AND DISCUSSION

In the present investigation , different thermodynamic parameters , such as adiabatic compressibility (βs), Partial molal volume (ϕ_v), intermolecular free length (L_f), apparent molal compressibility (ϕ_κ), specific acoustic impedance (Z), relative association (R_A), salvation number(Sn).

Table-1: Ultrasonic velocity, density, adiabatic compressibility (β_S), Specific acoustic impedance (Z) Intermolecular free length (L_f) in different percentage of dioxane-water mixture.

% of dioxane	Density(ds) Kg m^{-3}	Ultrasonic velocity (Us) m s^{-1}	Adiabatic compressibiliy (β_S) $x10^{-10}m^2N^{-1}$	Intermolecular free length (L_f) $x10^{-11}$m	Specific acoustic impedance ($Zx10^6$)kg m^{-2} s^{-1}
Acarbose + Dioxane					
45	1019.95	1596.32	3.8475	3.9450	1.6282
55	1021.76	1518.88	4.2423	4.1425	1.5519
65	1023.77	1444.80	4.6793	4.3506	1.4791
75	1025.78	1367.68	5.2117	4.5914	1.4029
Haloperidol + Dioxane					
45	1023.08	1446.56	4.6711	4.3468	1.4628
55	1024.89	1441.12	4.6981	4.3593	1.4703
65	1026.90	1434.56	4.7319	4.3750	1.4799
75	1028.91	1429.76	4.7544	4.3854	1.4884
Silymarin + Dioxane					
45	1024.18	1524.32	4.2022	4.1228	1.5387
55	1025.99	1519.68	4.2204	4.1317	1.5538
65	1027.99	1514.40	4.2416	4.1421	1.5568
75	1029.98	1502.40	4.3013	4.1711	1.5653
Digoxin + Dioxane					
45	1027.15	1599.80	3.8040	3.9226	1.3938
55	1028.96	1529.20	4.1560	4.1001	1.4842
65	1030.98	1442.40	4.6621	4.3426	1.5766
75	1032.98	1356.96	5.2574	4.6115	1.6526
Rifampicin + Dioxane					
45	1027.61	1523.04	4.1952	4.1194	1.5384
55	1029.38	1519.36	4.2083	4.1258	1.5579
65	1031.40	1513.44	4.2329	4.1379	1.5671
75	1033.41	1497.04	4.3178	4.1792	1.5739

Table-2: Concentration (m), Relative association (R_A), apparent molal compressibility (ϕ_κ), Apparent molal volume (ϕ_v), Solvation number (S_n)-

% of dioxane	Apparent molal volume (ϕ_v) m^3mole^{-1}	Apparent molal compressibility (ϕ_κ)x0^{-9} $m^2 N^{-1}$	Relative association (R_A)	Solvation number (S_n)
Acarbose + Dioxane				
45	0.6955	0.9742	1.0169	1.1005
55	0.6942	1.0722	0.9988	0.9882
65	0.6927	1.1804	0.9788	0.8756
75	0.6912	1.3121	0.9120	0.5725
Haloperidol + Dioxane				
45	0.7299	0.6865	1.0541	1.3320
55	0.7280	0.6893	1.0196	1.0911
65	0.7258	0.6929	0.9097	0.8827
75	0.7237	0.6948	0.9014	0.5207
Silymarin + Dioxane				
45	0.9385	0.7918	1.0370	1.1894
55	0.9360	0.7938	1.0028	0.9729
65	0.9323	0.7962	0.9685	0.7854
75	0.9287	0.8059	0.8873	0.4676
Digoxin + Dioxane				
45	1.5101	1.1569	1.0234	1.0803
55	1.5061	1.2617	1.004	0.9613
65	1.5026	1.4126	0.9864	0.8662
75	1.4973	1.5699	0.9209	0.5663
Rifampicin + Dioxane				
45	1.5942	1.3439	1.0408	1.1909
55	1.5862	1.3457	1.0062	0.9730
65	1.5825	1.3510	0.9711	0.7862
75	1.5779	1.5136	0.9059	0.5181

From table-1, these found that ultrasonic velocity decreases with increase in percentage of dioxane for all systems. 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 propagation proposed by Eyring and Kincaid [16]. It was found that, intermolecular free length increases linearly on increasing the percentage of dioxane in solution. The intermolecular free length increase 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 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 (Z) decreases with increase in percentage of dioxane in all substituted heterocyclic compounds in dioxane. The increase of adiabatic compressibility with increase of percentage of dioxane in solution may be due to 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.

From table-2, it is observed that apparent molal volume decreases with increase in percentage of dioxane in all system indicates the existence of weak ion-solvent interaction. The value of apparent molal compressibility is increase with increase in percentage of dioxane of all systems. It shows strong electrostatic attractive force in the vicinity of ions. It can be concluded that strong molecular association is found in all systems. The value of relative association decreases with increase in percentage of dioxane in all systems. It is found that there is weak interaction between solute and solvent.

The Solvation number decrease with increase in percentage of dioxane due to weak solute-solvent interaction. There is regular decrease in Solvation number with increase in percentage of dioxane indicates the decrease in size of secondary layer of Solvation. The Solvation number in all system decreases with increase in percentage of dioxane indicates the solvent molecule forms weak coordination bond in primary layer.

CONCLUSION

In the present study mentions the experimental data for ultrasonic velocity, density and at 303 k for all substituted heterocyclic drugs in 1, 4 dioxane-water mixture. From experimental data calculated acoustical parameters 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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