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ULTRASONIC STUDIES ON MOLECULAR INTERACTION OF SUBSTITUTED HETEROCYCLIC COMPOUNDS IN ACETONE-WATER MIXTURE AT 303K

A. N. Sonar*, N. S. Pawar[1] , M.D. Khairnar[2]

*Shri V.S. Naik College, Raver. Dist.Jalgaon (M.S.) India
[1]Pratap College, Amalner
[2]Arts.Com. and Science. College, Yawal

ABSTRACT: Acoustical and volumetric properties have been measured for substituted heterocyclic compounds drugs and compounds in acetone-water mixture at 303K. The measurement have been perform to evaluate acoustical 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).

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[5] have been studied the acoustical properties of complex in water. Jahagirdar[6] 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. 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

The substituted heterocyclic drugs (Acarbose, Haloperidol, Silymarin, Digoxin, Rifampicin are used in the present study. Acetone is used for solution preparation of different drugs. The density was determined by using specific gravity bottle by relative measurement method with accuracy $\pm$ $1x10^{-3}$ 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), and Solvation number (S_n) were studied.

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

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

$$\text{Apparent molal volume } (\phi_v) = \left(\frac{M}{ds}\right) x \frac{(d_0 - ds)\, x 10^3}{mxdsxd_0} \quad (3)$$

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

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

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

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

$$\text{Solvation number } (S_n) = \phi_\kappa\ /\ \beta 0 \text{ x } (M / d_0) \quad (8)$$

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), solvation number (Sn) were studied in acetone-water mixture.

From table-1, these found that ultrasonic velocity decreases with increase in percentage of acetone 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[15]. It was found that, intermolecular free length increases linearly on increasing the percentage of acetone 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 acetone in all substituted heterocyclic compounds in acetone. The increase of adiabatic compressibility with increase of percentage of acetone in solution may be due to collection of solvent molecule around ions, this supporting weak ion-solvent interaction[16]. 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 acetone in all system indicates the existence of weak ion-solvent interaction. The negative values of apparent molal volume in mixture indicate the presence of ion-solvent interaction. The value of apparent molal compressibility is increase with increase in percentage of acetone 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 acetone in all systems. It is found that there is weak interaction between solute and solvent.

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

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

% of Acetone	Density(ds) Kg m^{-3}	Ultrasonic velocity (Us) m s^{-1}	Adiabatic compressibiliy (βs) $x10^{-9} m^2 N^{-1}$	Intermolecular free length (L_f) $x10^{-11} m$	Specific acoustic impedance ($Zx10^6$)kg m^{-2} s^{-1}
Acarbose + acetone					
45	897.15	1513.92	1.9531	4.4353	1.3582
55	876.17	1442.40	2.1943	4.7106	1.2638
65	855.20	1352.54	2.5564	5.0844	1.1567
75	835.21	1291.04	2.8733	5.3904	1.0783
Haloperidol + acetone					
45	900.28	1447.68	2.1200	4.6302	1.3033
55	879.30	1424.16	2.2429	4.7624	1.2523
65	858.10	1354.08	2.5423	5.0704	1.1619
75	838.00	1290.24	2.8631	5.3175	1.0949
Silymarin + acetone					
45	901.38	1451.84	2.1053	4.6141	1.3087
55	880.40	1444.46	2.1785	4.6926	1.2717
65	859.18	1438.88	2.2487	4.7686	1.2363
75	839.08	1431.84	2.3252	4.8491	1.2014
Digoxin + acetone					
45	904.40	1517.28	1.9212	4.4077	1.3722
55	883.37	1440.16	2.1832	4.6987	1.2733
65	862.20	1375.04	2.4537	4.9812	1.1856
75	842.10	1282.08	2.8862	5.4058	1.0796
Rifampicin + acetone					
45	904.77	1499.21	1.9670	4.4599	1.3564
55	883.79	1439.84	2.1831	4.6986	1.2725
65	862.57	1367.84	2.4791	5.006	1.1709
75	842.48	1348.11	2.6129	5.1399	1.1358

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

% of Acetone	App. molal vol. (ϕ_v)m^3mole^{-1}	App. molal comp. (ϕ_κ)x$0^{-9}m^2N^{-1}$	Relative association(R_A)	Solvation number (S_n)
Acarbose + acetone				
45	-0.2605	0.8863	1.0349	0.7746
55	-0.2998	0.9131	1.0165	0.6185
65	-0.3297	0.9422	1.0011	0.4873
75	-0.3579	0.9676	0.9302	0.2796
Haloperidol + acetone				
45	-0.0508	0.8867	1.0544	1.3309
55	-0.0792	0.9595	1.0242	1.1164
65	-0.0803	1.1136	1.0041	0.9892
75	-0.0950	1.2791	0.9335	0.6348
Silymarin + acetone				
45	-0.0687	1.1280	1.0547	1.3108
55	-0.1008	1.1941	1.0210	1.0757
65	-0.1034	1.2619	0.9852	0.8679
75	-0.1222	1.3315	0.9029	0.5116
Digoxin + acetone				
45	-0.1109	1.6594	1.0428	1.1987
55	-0.1466	1.9303	1.0254	1.0809
65	-0.1668	2.2223	1.0033	0.9501
75	-0.1972	2.6741	0.9396	0.6387
Rifampicin + acetone				
45	-0.1000	1.7896	1.0474	1.2268
55	-0.1533	2.0331	1.0259	1.0803
65	-0.1682	2.3651	1.0060	0.9596
75	-0.2034	2.5495	0.9206	0.5779

CONCLUSION

In the present study mentions the experimental data for ultrasonic velocity, density and at 303 k for all substituted heterocyclic drugs in acetone-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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