



ULTRASONIC VELOCITY, DENSITY AND VISCOSITY MEASUREMENT OF SUBSTITUTED HETEROCYCLIC DRUGS IN 1, 4-DIOXANE AT 303 K

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ABSTRACT

The acoustical properties have been investigated from the ultrasonic velocity and density measurements of substituted heterocyclic drugs (Acarbose, haloperidol) in 1, 4-dioxane at 303K. The viscosity coefficient (A, B) have been investigated from the viscosity and density measurements of drugs. The results were fitted by John–Dole equation. These properties throw the light on the solute-solvent interaction and solute-solute interaction.

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

INTRODUCTION

For interpreting solute-solvent, ion-solvent interaction in aqueous and non aqueous medium was helpful from Ultrasonic velocity measurements in recent year¹⁻⁴. The acoustical properties of four different drugs in methanol have been studied and drawn conclusion from adiabatic compressibility⁵. Variations of ultrasonic velocity with concentration of some substituted Pyrazolines in binary mixture acetone–water were observed⁶. The acoustical properties of amino acids in aqueous magnesium acetate at constant temperature were studied from the measurements of ultrasonic velocity and density⁷. The ion-dipole interaction mainly depends on ion size and polarity of solvent. The structural properties of solution of lanthanide salt were studied from measurements of ultrasonic velocity⁸. The ultrasonic velocity and viscosity of PEG-8000, PEG-20000 in acetonitrile and water mixture was studied⁹. The hydrogen bond complex of Benzamide in 1,4 dioxane with alcohols at different temperature were studied from measurements of the ultrasonic velocity, density and viscosity¹⁰.

The acoustical properties and viscosity coefficients of glycine in aqueous solution were investigated¹¹.

In this work, we are interested in studying the acoustical properties, viscosity coefficient of substituted heterocyclic drugs under suitable condition.

EXPERIMENTAL

In the present study, the drugs Acarbose, Haloperidol were used. Dioxane was purified by Vogel's standard method¹². The double distilled dioxane was used for preparation of different concentration of drugs solution. The densities were determined by using specific gravity bottle by relative measurement method with accuracy $\pm 1 \times 10^{-5}$ gm/cm³. The ultrasonic velocities were measured by using ultrasonic interferometer having frequency 2MHz (Mittal Enterprises, Model No F-81). The constant temperature was maintained by circulating water through the double wall measuring cell, made up of steel. For viscosity measurement Ostwald viscometer (10 ml) was used. The flow time was also measured by using digital clock (0.01 Sec).

In the present investigation, different properties such as adiabatic compressibility (β_s), 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), limiting apparent molal compressibility

(ϕ_{κ}^0) , limiting apparent molal volume(ϕ_v^0) and their constant (S_k, S_v). Viscosity coefficient (A, B) were investigated from equations 1-11.

Theory

Adiabatic compressibility (β_s) is given by:

$$\beta_s = \frac{1}{U_s^2 d_s} \quad (1)$$

Apparent molal compressibility (ϕ_{κ}) has been calculated by using the relation,

$$(\phi_{\kappa}) = 1000 \times \left[\frac{\beta_s d_0 - \beta_0 d_s}{m x d_s x d_0} \right] + \frac{\beta_s \times M}{d_s} \quad (2)$$

Where β_s, d_0 and $\beta_0 d_s$ are the adiabatic compressibility and density of solution and solvent respectively. m is molal concentration of solute, M is molecular weight of solute.

$$\text{Apparent molal volume } (\phi_v) = \left[\frac{M}{d_s} \right] \times \frac{(d_0 - d_s) \times 10^3}{m x d_s x d_0} \quad (3)$$

$$\text{Specific acoustic impedance } (Z) = U_s d_s \quad (5)$$

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

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

The entire viscosity data have been analyzed by using Jones-dole equation.

$$\eta_{sp} / \sqrt{c} = A + B \sqrt{c} \quad (8)$$

RESULTS AND DISCUSSION

In the present investigation, different acoustical properties such as ultrasonic velocity (U_s), adiabatic compressibility (β_s), intermolecular free length (L_f), specific acoustic impedance (Z), are listed in table-1. Partial molal volume (ϕ_v), apparent molal compressibility (ϕ_{κ}), relative association (R_A), solvation number (S_n) are listed in table-2. Limiting apparent molal compressibility (ϕ_{κ}^0), limiting apparent molal volume(ϕ_v^0) and their constant (S_k, S_v) are listed in table-3. The viscosity coefficient (A, B) have been calculated at 303^oK in 1, 4 dioxane are listed in table-4. It was found that the ultrasonic velocity decreased with the increase in concentration for both systems (Table-1). Variation of ultrasonic velocity in solution depends upon the increase or decrease of molecular free length after mixing the component. This is based on a model for sound propagation proposed by Eyring and Kincaud¹³. Intermolecular free length increased linearly on increase in concentration of substituted heterocyclic drugs (Acarbose, Haloperidol) in 1,4 dioxane. Hence, decreased in ultrasonic velocity with increase in concentration of drugs. It happened because there was significant interaction between ions and solvent molecules suggesting a structure promoting behavior of the added electrolyte. The specific acoustic impedance (Z) increased with the decrease in concentration in both drugs in dioxane. When concentration of electrolyte was increased, the thickness of oppositely charged ionic atmosphere increases due to decrease in ionic strength. This is

suggested by decrease in acoustic impedance with concentration in both systems. It was seen that the intermolecular free length increased with the increase in concentration in both system. The intermolecular free length increased due to greater force of attraction between solute and solvent by forming hydrogen bonding. The adiabatic compressibility increased with the increase in concentration of solution. It happened due to collection of solvent molecule around ions, this supporting weak ion-solvent interaction. This indicates that there is significant solute-solvent interaction.

It was observed that apparent molal volume increased with concentration in both systems. It indicates the existence of strong ion-solvent interaction. It was found that the value of apparent adiabatic compressibility was increased with the increase in concentration of acarbose in dioxane. It shows strong electrostatic attractive force in the vicinity of ions. From the data, we were concluded that strong molecular association was found in acarbose than haloperidol. The value of apparent adiabatic compressibility in haloperidol decreased with concentration, which indicates weak ion-solvent interactions in the system. The value of relative association increased with the increase in concentration in both systems. It has been found that there was strong interaction between solute and solvent. In Haloperidol system the solvation number decreased with the increase in concentration due to weak solute-solvent interaction. There were regular decreases in solvation number with the increase in concentration. It indicates the decrease in size of secondary layer of Solvation. The solvation number in Acarbose-dioxane system increased with concentration, it indicates the solvent molecule forms strong coordination bond in primary layer. The limiting molal compressibility was positive in both cases. The value of S_k exhibits positive. It indicates the existence of ion-ion or solute-solute interactions in Acarbose system. The value of S_k exhibits negative, it indicates the weak existence of ion-ion or solute-solute interactions in Haloperidol system. From table-3, it was found that the value of limiting apparent molal volume was positive in both systems. It indicates that the ion-dipolar interaction in Acarbose, Haloperidol and 1, 4 dioxane. The positive value of S_v indicates the strong solute-solvent interaction. These value indicates an induced effect of 1, 4 dioxane on solute-solvent interaction. The value of S_k and S_v has been determine from Fig. 1 and 2.

From Table-4 it was observed that the value of 'A' (Falkenhagen coefficient) was positive in both studied system. 'A' measures of ionic interaction. It indicates that there is a strong solute-solute interaction in solute molecules. The Jones-Dole coefficient measures solute-solvent interaction. The value of "B" coefficient was negative in both the drugs, which measured the solute-solvent interactions. The value of A and B was determined from Fig. 3.

CONCLUSION

The present study shows the experimental data for ultrasonic velocity, density and viscosity at 303K for substituted heterocyclic drugs in 1,4 dioxane. From experimental data, the acoustical properties were calculated. The solute-solvent interaction and ion-ion / solute-solute interaction existing between drugs and 1,4dioxane were also studied with the help of experimental data. Lastly it has been concluded from the experimental data, that the solute-solvent interaction in drugs-1, 4dioxane systems are weak.

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Table-1: Ultrasonic velocity, density, adiabatic compressibility (β_s), Specific acoustic impedance (Z) Intermolecular free length (L_f).

Concentration moles lit ⁻¹ (m)	Density (ds) kg m ⁻³	Ultrasonic velocity (Us) m s ⁻¹	Adiabatic compressibility (β_s) x10 ⁻¹⁰ m ² N ⁻¹	Intermolecular free length (L_f) x10 ⁻¹¹ m	Specific acoustic impedance (Zx10 ⁶) kg m ⁻² s ⁻¹
Acarbose + 1,4 Dioxane					
0.00	1022.13	1321.25	5.60433	4.76123	1.3505
1x10 ⁻³	1022.26	1317.21	5.63805	4.77563	1.3465
2x10 ⁻³	1022.37	1312.61	5.67702	4.79201	1.3420
3x10 ⁻³	1022.46	1306.85	5.72667	4.81292	1.3362
4x10 ⁻³	1022.53	1302.95	5.76061	4.82716	1.3323
5x10 ⁻³	1022.61	1298.11	5.80319	4.84497	1.3275
6x10 ⁻³	1022.67	1293.54	5.84393	4.86194	1.3229
7x10 ⁻³	1022.72	1287.68	5.89695	4.88935	1.3169
8x10 ⁻³	1022.77	1283.45	5.93559	4.89992	1.3127
9x10 ⁻³	1022.81	1276.90	5.97963	4.91807	1.3079
Haloperidol + Dioxane					
1x10 ⁻³	1022.21	1320.64	5.60907	4.76324	1.3500
2x10 ⁻³	1022.27	1314.44	5.66178	4.78557	1.3437
3x10 ⁻³	1022.32	1309.72	5.70238	4.80270	1.3390
4x10 ⁻³	1022.35	1301.84	5.77140	4.83167	1.3309
5x10 ⁻³	1022.37	1296.48	5.81916	4.85163	1.3255
6x10 ⁻³	1022.40	1290.16	5.87614	4.87532	1.3191
7x10 ⁻³	1022.43	1281.72	5.95361	4.90735	1.3105
8x10 ⁻³	1022.44	1270.72	6.05707	4.94981	1.2992
9x10 ⁻³	1022.45	1262.68	6.13439	4.98130	1.2910

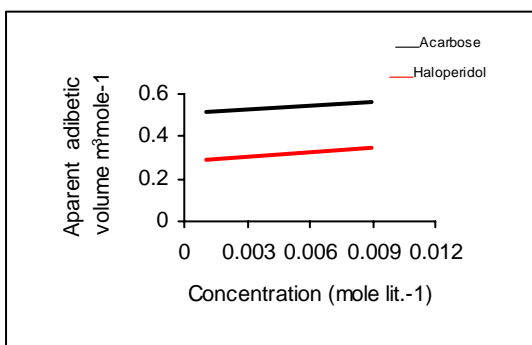


Fig.-1: Apparent molal volume (m³mole⁻¹) Vs Concentration (m²N⁻¹)

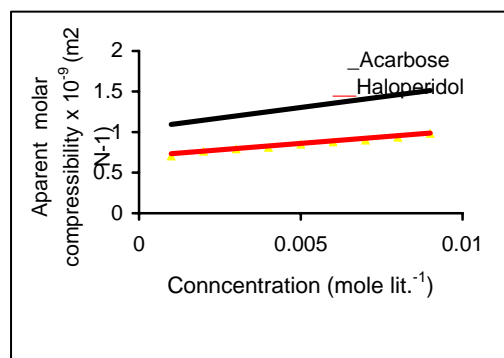


Fig.-2: Apparent molar compressibility 10⁻⁹ (mole lit⁻¹) Vs Concentration (mole lit⁻¹)

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

Concentration(m) moles lit ⁻¹	Apparent molal volume (ϕ_v) m ³ mole ⁻¹	Apparent molar compressibility ($\phi_\kappa \times 10^9$) m ² N ⁻¹	Relative association (R_A)	Solvation number (S_n)
Acarbose + 1,4 Dioxane				
1x10 ⁻³	0.5072	3.5607	1.00166	0.32747
2x10 ⁻³	0.5167	3.5851	1.00352	0.32971
3x10 ⁻³	0.5262	3.6162	1.00582	0.33257
4x10 ⁻³	0.5357	3.6374	1.00739	0.33452
5x10 ⁻³	0.5395	3.6641	1.00935	0.33697
6x10 ⁻³	0.5452	3.6896	1.01190	0.33932
7x10 ⁻³	0.5506	3.7230	1.01354	0.34239
8x10 ⁻³	0.5547	3.7473	1.01525	0.34462
9x10 ⁻³	0.5589	3.7750	1.01718	0.34718
Haloperidol + Dioxane				
1x10 ⁻³	0.2912	2.0627	1.00031	0.32581
2x10 ⁻³	0.3007	2.0821	1.00272	0.32887
3x10 ⁻³	0.3071	2.0970	1.00458	0.33123
4x10 ⁻³	0.3150	2.1225	1.00765	0.33525
5x10 ⁻³	0.3217	2.1401	1.00974	0.33804
6x10 ⁻³	0.3246	2.1612	1.01224	0.34136
7x10 ⁻³	0.3266	2.1898	1.01560	0.34588
8x10 ⁻³	0.3306	2.2281	1.01999	0.35193
9x10 ⁻³	0.3336	2.2567	1.02325	0.35644

Table-3: Limiting Apparent molal compressibility (ϕ_κ^0), Limiting Apparent molal volume (ϕ_v), S_v and S_k

Drugs	Limiting Apparent molal volume (ϕ_v) m ³ mole ⁻¹	Limiting Apparent molal compressibility (ϕ_κ^0) $\times 10^{-9}$ m ² N ⁻¹	S_v m ³ kg ^{1/2} mole ^{-3/2}	S_k m ³ mole ⁻² kg. N ⁻¹
Acarbose	0.5056	1.0429	6.325	51.883
Haloperidol	0.2883	0.6983	6.0214	32.162

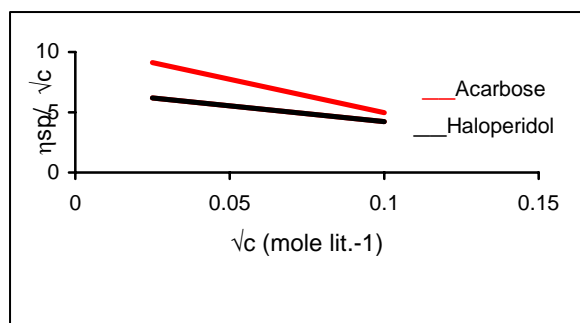


Fig.-3: η_{sp}/\sqrt{c} Vs \sqrt{c} (mole lit.⁻¹)

Table-4: η_r , η_{sp} / \sqrt{c} , Falkenhagen coefficient (A), Jones–Dole coefficient (B) of Acarbose and haloperidol in 1, 4-dioxane Density of solvent (d_0) = 1027.2 kg m⁻³, Flow time for solvent T_0 =137 Sec.

Concentration mole lit ⁻¹	Density kg m ⁻³	Flow time(T) Sec.	η_r	$\frac{\eta_{sp}}{\sqrt{c}}$	A	B
Acarbose + 1,4 Dioxane						
0.01	1030.4	207	1.516	5.5566	10.502	-55.453
0.005	1029.0	198	1.448	6.3327		
0.0025	1028.0	189	1.381	7.6127		
0.00125	1027.5	178	1.300	8.4754		
0.000625	1027.3	169	1.234	9.3479		
Haloperidol +1,4 dioxane						
0.01	1029.1	195	1.426	4.2599	6.8404	-26.281
0.005	1025.1	184	1.344	4.8683		
0.0025	1027.6	175	1.278	5.5574		
0.00125	1027.4	166	1.212	5.9939		
0.000625	1027.3	158	1.153	6.1359		

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