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Acoustic and Volumetric Properties of Digoxin and Thiabendazole in 1, 4 Dioxane at 303 K

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Abstract: Acoustical and volumetric properties have been measured for substituted heterocyclic compounds digoxin and thiabendazole in 1, 4 dioxane at 303 K. The ultrasonic velocity measurement have been performed to evaluate acoustical parameter such as adiabatic compressibility (β_s), 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 (S_n), limiting apparent molal compressibility (ϕ_{κ}^0), limiting apparent molal volume (ϕ_v^0) and their constant (S_{κ}, S_v). The viscosity coefficient (A, B) was evaluated by using john-dole equation. These parameters throw the light on the solute-solvent interaction and solute-solute interaction.

Keywords: Ultrasonic velocity, Viscosity, 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 medium¹⁻⁴. Fumio Kawaizumi⁵ 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 concluded 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 structure⁶. Meshram *et. al.* studies the different acoustical properties of some substituted pyrazolines in binary mixture acetone–water and observed variation of ultrasonic velocity with concentration⁷. Palani have investigated the measurement of ultrasonic velocity and density of amino acid in aqueous magnesium acetate at constant temperature⁸.

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. Thirumaran *e .al.*⁹ has been studied acoustical properties of ternary liquids of substituted benzenes with 1-chlorobutane at different temperature. Syal *et al.* has been studied the ultrasonic velocity and viscosity of PEG-8000, PEG- study of acoustical properties, viscosity coefficient of substituted heterocyclic compounds under suitable condition¹⁰.

Experimental

The substituted heterocyclic compounds digoxin and thiabendazole were used in the present study. Dioxane was purified by Vogel's standard method¹¹. The double distilled dioxane was used for solution preparation of different concentration of drugs. The density was determined by using specific gravity bottle by relative measurement method with accuracy $\pm 1 \times 10^{-5}$ g/cm³. The ultrasonic velocity was measured by using ultrasonic interferometer having frequency 2MHz (Mittal Enterprises, Model No F-81). The constant temperature was mentioned by circulating water through the double wall measuring cell made up of steel. For viscosity measurement Ostwald Viscometer was used. The flow time was measured by using digital clock (0.01 sec).

In the present investigation, different parameters 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_κ , S_v) were studied. Viscosity coefficient (A, B) were evaluated by using following equations.

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

$$\text{Adiabatic compressibility } (\beta_0) = \frac{1}{U_0^2 d_0} \quad (2)$$

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

$$\text{Apparent molal compressibility } (\phi_\kappa) = 1000 \times \frac{\beta_s d_0 - \beta_0 d_s}{M \times ds \times d_0} + \frac{\beta_s \times M}{ds} \quad (4)$$

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

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

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

$$\text{Solvation number } (S_n) = \phi_\kappa / \beta_0 \times (M / d_0) \quad (8)$$

$$\phi_\kappa = \phi_\kappa^0 + S_\kappa C \quad (9)$$

$$\phi_v = \phi_v^0 + S_v C \quad (10)$$

$$\eta_{sp} / \sqrt{c} = A + B \sqrt{c} \quad (11)$$

Results and Discussion

Different thermodynamic parameters, such as adiabatic compressibility (β_s), 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 (S_n), limiting apparent molal compressibility (ϕ_κ^0), limiting apparent molal volume (ϕ_v^0) and their constant (S_κ , S_v) were studied. The viscosity coefficient (A, B) have been calculated at 303 K in 1,4 dioxane.

From Table 1, ultrasonic velocity decreases with increase in concentration for both 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 Kincaid¹². It was found that, intermolecular free length increases linearly on increasing the concentration of substituted heterocyclic compounds (Digoxin and Thiabenzazole) in dioxane. The intermolecular free length increases due to greater force of interaction between solute and solvent by forming hydrogen bonding. Hence, decrease in ultrasonic velocity with increase in concentration of substituted heterocyclic compounds. This was happened because there is significant interaction between ions and solvent molecules suggesting a structure promoting behavior of the added electrolyte. This also may indicate 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 concentration in both substituted heterocyclic compounds in dioxane. When concentration of electrolyte is increases, the thickness of oppositely charged ionic atmosphere may increases due to decrease in ionic strength. This is suggested by decrease in acoustic impedance with increase in concentration in both system investigated. The increase of adiabatic compressibility with increase of concentration of solution may be due to collection of solvent molecule around ions,¹³ this supporting weak ion-solvent interaction. 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.

Table 1. The values of ultrasonic velocity, density, adiabatic compressibility (β_s), specific acoustic impedance (Z), intermolecular free length (L_f), digoxin, thiabendazole in 1,4 dioxane at 303 K.

Concentration moles lit ⁻¹ (M) $\times 10^3$	Density (ds) kg m ⁻³	Ultrasonic velocity (Us) m s ⁻¹	Adiabatic compressibility (β_s) $\times 10^{-10}$ m ² N ⁻¹	Intermolecular free length (L_f) $\times 10^{-11}$ m	Specific acoustic impedance ($Z \times 10^6$) kg m ⁻² s ⁻¹
Digoxin + Dioxane					
1	1022.28	1309.72	5.7026	4.8028	1.3389
2	1022.42	1301.23	5.7765	4.8338	1.3304
3	1022.55	1292.56	5.8535	4.8659	1.3217
4	1022.67	1285.11	5.9209	4.8938	1.3142
5	1022.78	1278.59	5.9807	4.9185	1.3077
6	1022.87	1271.95	6.0428	4.9439	1.3010
7	1022.96	1262.85	6.12 97	4.9793	1.2918
8	1023.04	1255.01	6.2060	5.0103	1.2839
9	1023.10	1246.23	6 .2934	5.0454	1.2750
Thiabendazole + Dioxane					
1	1022.17	1314.36	5.6630	4.7861	1.3435
2	1022.20	1311.95	5.6837	4.7948	1.3411
3	1022.22	1310.06	5.6999	4.8017	1.3392
4	1022.23	1308.15	5.7166	4.8087	1.3372
5	1022.24	1305.85	5.7367	4.8171	1.3349
6	1022.25	1303.24	5.7596	4.8267	1.3322
7	1022.26	1299.21	5.8954	4.8417	1.3281
8	1022.27	1296.85	5.8164	4.8505	1.3257
9	1022.28	1294.21	5.8401	4.8604	1.3230

From Table 2, it is observed that apparent molal volume increases with concentration in both system indicates the existence of strange ion-solvent interaction. The value of apparent molal compressibility is increase with increase in concentration of both system in dioxane. It shows strong electrostatic attractive force in the vicinity of ions. It can be concluded that strong molecular association is found in Digoxin than thiabendazole. The value of relative association increases with increase in concentration in both systems. It is found that there is strong interaction between solute and solvent.

Table 2. The values of concentration (m), relative association (R_A), apparent molal compressibility (ϕ_k), apparent molal volume (ϕ_v), solvation number (S_n)-digoxin, thiabendazole in 1,4 dioxane at 303 K.

Concentration (M) moles lit ⁻¹ x10 ³	Apparent molal volume (ϕ_v) m ³ mole ⁻¹	Apparent molal compressibility (ϕ_k)x10 ⁻¹⁰ m ² N ⁻¹	Relative association (R_A)	Solvation number (S_n)
Digoxin + 1,4 Dioxane				
1	0.6204	4.3566	1.0045	0.3312
2	0.6251	4.4124	1.0079	0.3354
3	0.6298	4.4707	1.0115	0.3399
4	0.6345	4.5217	1.01145	0.3438
5	0.6392	4.5670	1.0172	0.3472
6	0.6455	4.6141	1.0199	0.3508
7	0.6500	4.6801	1.0237	0.3558
8	0.6546	4.7381	1.0270	0.3602
9	0.6602	4.8047	1.0306	0.3653
Thiabendazole +1,4 Dioxane				
1	0.1586	1.1154	1.0027	0.3290
2	0.1634	1.1192	1.0036	0.3301
3	0.1682	1.1225	1.0044	0.3310
4	0.1730	1.1257	1.0051	0.3320
5	0.1759	1.1296	1.0060	0.3332
6	0.1778	1.1341	1.0070	0.3345
7	0.1791	1.1412	1.0086	0.3366
8	0.1802	1.1454	1.0095	0.3378
9	0.1810	1.1500	1.0105	0.3392

The solvation number increase with increase in concentration due to strong solute-solvent interaction. There is regular increase in solvation number with increase in concentration indicates the increase in size of secondary layer of solvation. The solvation number in digoxin -1, 4 dioxane system increases with concentration indicates the solvent molecule forms strong coordination bond in primary layer. The solvation number in primary layer corresponds to coordination number and it is concentration independent. The solvation number in secondary layer is concentration dependent. The concentration increases, solvation number increases indicates the solvent molecules are also strongly attached in secondary layer.

The limiting molal compressibility is positive in digoxin indicates existence of weak solute-solvent interaction in solution. The limiting molal compressibility is negative in thiabendazole indicates existence of strong solute-solvent interaction in solution. The value of S_k exhibits negative in thiabendazole. It indicates the weak existence of ion-ion or solute-solute interactions in thiabendazole system. The value of S_k exhibits positive in thiabendazole

-1, 4 dioxane system, it indicates the existence of ion-ion or solute-solute interactions in thiabendazole system. From Table 3 it is found that the value of limiting apparent molal volume is positive in both systems. It indicates that the ion-dipolar interaction in thiabendazole, digoxin and 1, 4 dioxane. The positive value of S_v indicates the strong solute-solvent interaction. These value indicates induced effect of 1, 4 dioxane on solute-solvent interaction.

From Table 4 it is observed that the value of 'A' (Falkenhagen coefficient) are positive in both system studied. 'A' is measure of ionic interaction. It indicates that there is a strong solute-solute interaction in solute molecules. 'B' is Jones–Dole coefficient measures solute – solvent interaction. The value of 'B' coefficient is negative in both drugs. Solute with negative 'B' coefficient is characterized as 'Surface breaker' indicating weak solute-solvent interactions.

Table 3. Results of limiting apparent molal compressibility (ϕ_{κ}^0), limiting apparent molal volume (ϕ_v^0), S_v and S_{κ} .

Drugs	Limiting Apparent molal volume (ϕ_v^0) $m^3 mole^{-1}$	Limiting Apparent molal compressibility (ϕ_{κ}^0) $\times 10^{-8} m^2 N^{-1}$	S_v $M^3 kg^{1/2} mole^{-3/2}$	S_{κ} $M^3 mole^{-2} kg. Pa^{-1}$
Digoxin	0.6150	4.3005	4.9850	54.685
Thiabendazole	0.1592	1.1096	2.7700	4.3800

Table 4. The values of η_r , A, B of digoxin +1, 4 dioxane and Thiabendazole in 1, 4 dioxane. Density of solvent (d_0) = 1027.2 Kg/M^3 , Flow time for solvent T_0 =137 Sec.

Concentration mole /kg	Density $kg m^{-3}$	Flow time (T), sec.	η_r	$\frac{\eta_{sp}}{\sqrt{c}}$	A	B
Digoxin + 1,4 dioxane						
0.01	1031.1	202	1.48	4.80051	6.7775	-20.964
0.005	1029.0	187	1.367	5.19519		
0.0025	1028.1	175	1.278	5.56983		
0.00125	1027.5	166	1.212	5.99719		
0.000625	1027.4	159	1.161	6.43240		
Thiabendazole + 1,4 dioxane						
0.01	1027.28	150	1.1030	1.03027	1.6385	-5.9289
0.005	1027.24	148	1.0883	1.24843		
0.0025	1027.21	145	1.0662	1.32374		
0.00125	1027.17	143	1.0514	1.45494		
0.000625	1027.15	141	1.0367	1.46857		

Conclusion

Acoustic and volumetric properties of digoxin and thiabendazole in 1, 4 dioxane at 303 K was studied and the experimental data was presented. From the experimental data solute-solvent interaction and ion-ion / solute-solute interaction was discussed and it's existing between drugs and 1, 4 dioxane was also explained. From experimental data it can be conclude that, there is a weak solute-solvent interaction in digoxin-1, 4 dioxane systems and strong solute solvent interaction in thiabendazole-dioxane system.

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