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The Physico-Chemical and Solvolytic Study of Alprazolam Drug in Ethanol at 303 K

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ABSTRACT

The physico-chemical and solute –solvent interaction of Alprazolam in ethanol were reported at 303 K. The solute solvent interaction have been carriedout by computing various acoustic parameters, Specific acoustic impedance(z),Intermolecular freelength (L_f), Isentropic compressibility (β_s), Apparent molal adiabatic compressibility (ϕ_k), Shear's relaxation (τ_s), and Solvation number (Sn).These parameters have been evaluated by using ultrasound velocity, density and viscosity data.These results are interpreted in terms of solute-solvent interaction between the molecules.

Key words: Solute-solvent interaction, Ultrasound velocity, Alprazolam.

INTRODUCTION

Alprazolam is a triazolobenzodiazepine compound with antianxiety and sedative-hypnotic actions, that is efficacious in the treatment of panic disorders, with or without agoraphobia and in generalized anxiety disorders.It is marketed under the trade name xanax.

In the present study, we are reported the ultrasound velocity, density and viscosity measurements at 303K have been used to calculate Intermolecular freelength(L_f)[1] , Specific acoustic impedance(z)[2], Apparent molal adiabatic compressibility (ϕ_k)[3], Shear's relaxation(τ_s), and Solvation number (Sn)[4] of Alprazolam compound in ethanol at 303 K. Several investigators have reported the results on ultrasound studies of liquid mixtures[4-12].

EXPERIMENTAL

The solutions were prepared by dissolving the accurately known weight of Alprazolam in ethanol and kept for some time. A continuous interferometer technique was employed for measurement of ultrasound velocity at 2Mhz. The density and viscosity were determined using vibrating densitometer DMA 48 fitted with a Hook G thermostat and viscometer.The experiment were reported atleast twice and results were reproducible with experimental error 0.00002 Kgm^3 and 0.001 cm/ sec respectively.

Computation of different physical parameters:
Ultrasound Velocity (V)

$$V=2d\times10^5 \text{ cm/sec. or } V=2d\times10^3 \text{ m/sec.}$$

Density : $$\rho = \frac{M}{V + \pi r^2 (h_1 + h_2)}$$

where 'M': is the weight of the liquid filled in pyknometer used.
'r'is radius of capillaries
'h_1'& 'h_2'are the heights of the liquid in capillaries

Viscosity (h):

$$\eta = \rho\left[at - \frac{b}{t}\right]$$

where
'η' is the viscosity of liquid
'ρ' is the density of liquid.
'τ' is the time flow of liquid
'a'&'b' are viscometeric constants.

Specific Acoustic Impedance

$$Z=Vr.$$

Where, V and '*r*' are the ultrasonic velocity and density respectively.

Isentropic Compressibility : $$\beta_s = \frac{1}{V^2\rho}$$

where 'V' is the ultrasound velocity and 'ρ' is the density of liquid mixtures.

Intermolecular Free Length: $$L_f = K\sqrt{\beta_s}$$

where,
'K' is temperature dependent constant.
Molal Adiabatic Compressibility

$$\phi_k = \frac{1000}{C\rho^0}(\rho^0 \beta_s - \beta_{s0}\rho) + \beta_{s^0}\frac{M}{\rho^0}$$

where 'ρ^0' and 'β_s^0' are compressibility and density of pure solvent and 'β_s' & '*r*' are the compressibility and density of the solution respectively.
'C' is the concentration in mole/liter of solute.
'M' is the molecular weight of solute.

Solvation Number :

$$S_n = \frac{n_1}{n_2}\left[1 - \frac{\beta_s}{\beta_{s_0}}\right]$$

Where ' n_1 ' moles of solvent and ' n_2 ' moles of solute

Shear's Relaxation Time (τ)

$$\tau_s = \frac{4}{3}.\eta\beta_s$$

RESULT AND DISCUSSION

The ultrasound velocity of the solution of Alprazolam drug in ethanol increases with increasing concentration Alprazolam drug which is shown in above table.

The variation of velocity with concentration (C) can be expressed by the following relationship.

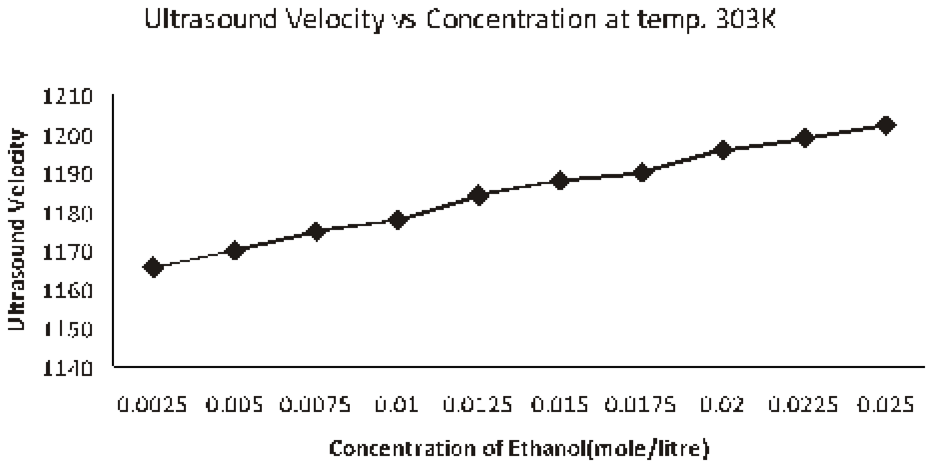
$$\frac{dv}{dc} = -\frac{V}{2}\left[\frac{1}{\rho}\left[\frac{dp}{dc}\right] + \frac{1}{\beta_s}\left[\frac{d\beta_s}{dc}\right]\right]$$

The result shows that while the density increases, the isentropic compressibility decreases with increasing concentration of the solute and quantity (dp/dc) is positive while (db_s/dc) is negative. Since the value of $\frac{1}{\beta_s}\left[\frac{d\beta_s}{dc}\right]$ are larger than the value of $\frac{1}{\rho}\left[\frac{dp}{dc}\right]$ for the system . The concentration derivatives of velocity(dv/dc) is positive. i.e. the ultrasonic velocity increases with increasing the concentration of solute[13-16].

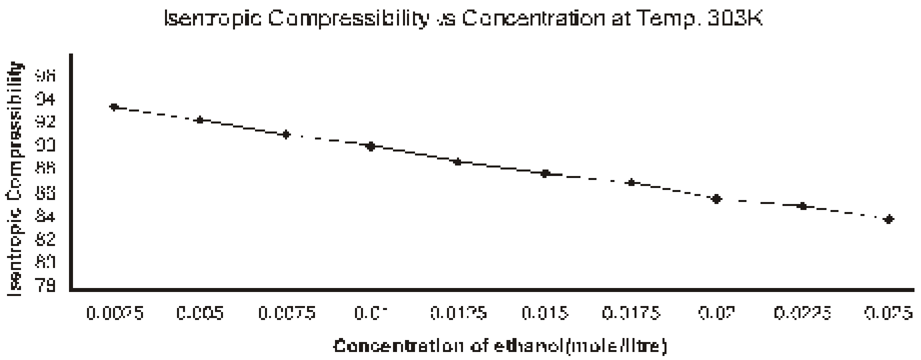
Intermolecular free length and isentropic compressibility (β_s) of Alprazolam drug solution decreases with increase in molar concentration of

Table 1: Alprazolam + ethanol At 303K

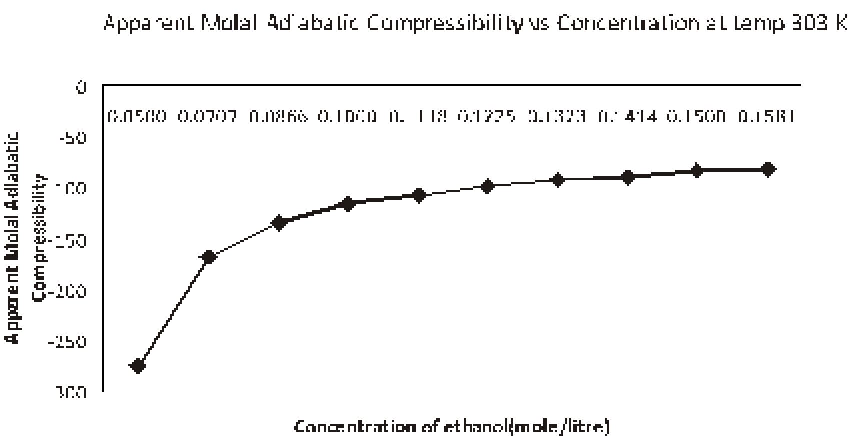
Conc. of ethanol mol/litre	Ultrasound velocity m/sec.	Density gm/mol . (Exp.)	Specific Acoustic Impedance (C.G.S.) z×10^{-5}	Isentropic compressib-ility (Exp.) cm^2/ dyne.10^{12}	Lowering Isentropic compressibility cm^2/ deyne.10^{12}	Intermole cular free length (A°)	Viscosity (Exp.) (C.P.)	Apparent molal Adiabatic compressibility cm^2/dyne.10^9	Solvatio n number	Shear's Relaxati on time
0.0025	1166	0.7883	0.0919	93.31	-6.76	0.6095	1.2546	-274.1037	46.2196	156.0890
0.0050	1170	0.7923	0.0927	92.20	-7.87	0.6059	1.2960	-167.4630	53.8089	159.3216
0.0075	1175	0.7965	0.0936	90.94	-9.13	0.6017	1.3374	-134.2552	62.4238	162.1642
0.0100	1178	0.8010	0.0944	89.97	-10.10	0.5985	1.3786	-115.1329	69.0559	165.3769
0.0125	1184	0.8052	0.0953	88.59	-11.48	0.5939	1.4201	-106.6343	78.4912	167.7422
0.0150	1188	0.8091	0.0961	87.57	-12.50	0.5905	1.4515	-98.3142	85.4652	169.4771
0.0175	1190	0.8137	0.0968	86.78	-13.29	0.5878	1.5026	-91.5657	90.8666	173.8608
0.0200	1196	0.8178	0.0978	85.49	-14.59	0.5834	1.5442	-88.7363	99.6866	176.0182
0.0225	1199	0.8199	0.0983	84.84	-15.23	0.5812	1.5853	-82.4719	104.1308	179.3291
0.0250	1202	0.8263	0.0993	83.76	-16.31	0.5775	1.6271	-81.4079	111.5150	181.7145


Ultrasound Velocity vs Concentration at temp. 303K
Ultrasound Velocity
1210
1200
1190
1180
1170
1160
1150
1140
0.0025 0.005 0.0075 0.01 0.0125 0.015 0.0175 0.02 0.0225 0.025
Concentration of Ethanol(mole/litre)

1(a)


Isentropic Compressibility vs Concentration at Temp. 303K
Isentropic Compressibility
Concentration of ethanol(mole/litre)

1(b)


Apparent Molal Adiabatic Compressibility vs Concentration at temp 303 K
Apparent Molal Adiabatic Compressibility
0
-50
-150
-250
Concentration of ethanol(mole/litre)

1(c)

solute (Fig.1-b) .The complementary use of isentropic compressibility data can provide interesting information of of solute- solvent interaction.

Apparent molal adiabatic compressibility (ϕ_k) varies linearly s the square root of concentration.The value of apparent molal adiabatic compressibilities are negative with the increase in molar concentration. The values of apparent molal adiabatic compressibility as shown in figure 1 (c) . The values of for the solutions of Alprazolam drug were tabulated in table. These results are in agreement with the result reported by Masson[17] for electrolytic solution.

The value of specific acoustic impedance (z) increases with increasing the concentration of Alprazolam drug can be explained on the basis of lyophobic interaction between solute and solvent molecules which increase the intermolecular distance making relatively under gaps between the molecules and becoming the main cause of impedance in the propagation of ultrasound waves are tabulated.

The increase with the concentration suggest a significant interaction between the solute solvent molecules and the values are in agreement with the reported for solution of cobalt carboxylates[18].

From the above discussion it is concluded that solvolytic study of Alprazolam in ethanol at 303 K shows specific ion – solvent interaction. Alprazolam drug shows significant solvolysis in ethanol.

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