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Speed of Sound, Density and Refractive Index Data of 5-chloro-3H-Benzooxazol-2-one in Acetonitrile-Water Mixt ures at 37^{o}C

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Abstract

The experimental speed of sound (u), density (ρ) and refractive index (n) studies on soluti ons of muscle relaxant 5-chloro-3H-benzooxazol-2-one (chlorzoxazone) have been carried out in binary acetonitrile (AN)-w ater mixtures of different vol% at 37^{o}C. From experimental results, va rious acoustical properties like isentropic compres sibility (κ_s), intermolecular free length (L_f), specific acoustic impedance (Z), relative association (R_A), apparent molar ise ntropic compressibility (κ_φ) and relaxation strength (r) have been calcu lated. Apparent molar volume (V_φ) of drug has been calculated from density data and fitted to modified Massons relation to obtain partial molar volume (V^0_φ) for the evaluation of drug-solvent interactions. The experimental and derived properties h ave been used to throw the light on drug-drug and drug-solvent interactions.

Keywords: Drug, Acoustical properties, Isentropic compressibility, Relative association, M lecular interactions.

Introduction

A drug-solvent interaction is of great th eoretical and practical importance. The volumetric, acoustic and optical properties give significant information regarding molecular interactions in drug solutions. The acoustic and thermodynamic properties which give qualitative information about intermolecular forces in solutions are calculated from speed of s ound and density[1-3]. Studies on speeds of sound and densities of pharmaceutically important drugs solutions are of interest [4-6]. The 5-chloro-3H-benzooxazol-2-one is a centrally acting muscle relaxant. No reports are available in the literature on the ultrasonic studies of 5-chloro-3 H-benzooxazol-2-one in binary aqueous + non-aqueous solvent systems like aceton itrile-water mixtures. Therefore, in continuation with our earlier work[7-8], here we report, density, refractive, speed of sound and derived thermophysical properties of this drug in acetonitrile-water mixtures of three different compositions at 37^{o}C.

Materials and Methods

The 5-chloro-3H-benzooxazol-2-one (Chlorzoxazone, $C_7H_4ClNO_2$) was supplied as a gift samp le by Cipla Pvt. Ltd. Mumbai. Double distilled water and a cetonitrile (AN) (AR grade, Fisher Scientific, 99.8%) were us ed for perpetration of solutions. Density measurements were p erformed using single capillary pycnometer (Borosil, 10 cm^3, 20×46 mm, ±0.3 ml). Pycnometer was calibrated at using d ouble distilled water. Weighing was done on single pan electro nic balance (±0.001g). Speed of sound (u) was measured u sing thermostatically controlled ultrasonic interferometer (Mo del-F05, Mittal, 2 ± 0.0001 MHz). Refractive index measure ments were performed on thermostatically controlled Cyber LAB-Cyber Abbe refractometer (Amkette Analytics, ±0.0002). Refractometer was calibrated using standard specimen (n=1.5167). Averages of three readings of density and refractive index are reported.

Results and Discussion

From density and speeds of sound, various acoustical properties like κ_s, L_f, Z, V , R_A, κ a nd r are calculated using standard relations[9-12] and reported in Table-1.

The speed of sound (u) in creases by increase in the solute concentration which is attributed to decrease in the intermolecular free length d ue to solute-solvent interactions and structure promoting nature of drug. The decrease in the speed of sound with increase in the c ontent of AN is due to increase in the intermolecular free len gth. The density (ρ) increases by increase in the solute concentration due to increase in the compactness of the system due to attractive type of solute-solvent interactions. The de nsity decreases by increase in the volume % of AN.

The properties κ_s and L_f are related with packing phenomenon and structural effects. The decrease in κ_s as well as L_f with solute concentration signifies the structural compactness and aggregation of solvent a round solute molecule due to predominance of solute-solvent interactions. The L_f values shows increasing trend with increase in the content of AN which is in agreement with the earlier work[13]. However, with increase in solute concentration, L_f v alues shows decreasing trend which suggests strong drug-solvent interaction.

The *Z* increases by increase in the solute concentration due to effective solute-solvent interactions [12]. There is a decrease in the *Z* values with increase in the content of AN in AN + water mixtures which supports the decrease in *u* and *ρ* values with increase in the content of AN. This is due to weakening of solute-solvent interactions and strengthening of solvent-solvent interactions.

Table-1

Molality (*m*, mol·kg^{-1}), density (ρ,g·cm^{-3}), speed of sound (*u*, m·s^{-1}), refractive index (*n*) and derived isentropic compressibility (κ_s, × 10^{-10} m^2· N^{-1}), intermolecular free length (L_f, x 10^{-10} m), specific acoustic impedance (Z, × 10^6 kg·m^{-2}·s^{-1}), relative association (R_A), apparent molar isentropic compressibility (κ_φ × 10^{-10} m^3·mol^{-1}·Pa^{-1}) and relaxation strength (*r*) of 5-chloro-3H-benzooxazol-2-one in AN-W mixtures at 37^{o}C

m	*ρ*	*u*	*n*	κ_s	L_f	*Z*	R_A	κ_ϕ	*r*
50 vol % AN									
0.0000	804.43	1506.15	1.3404	5.480	0.4920	1.212	1.0000	-	0.1139
0.0125	804.79	1416.71	1.3407	6.191	0.5230	1.140	1.0211	0.0717	0.2160
0.0375	806.06	1417.25	1.3414	6.176	0.5224	1.142	1.0226	0.0240	0.2154
0.0625	807.87	1419.23	1.3421	6.145	0.5210	1.147	1.0244	0.0140	0.2132
0.0878	809.58	1420.00	1.3429	6.126	0.5202	1.150	1.0264	0.0099	0.2123
0.1131	811.21	1420.17	1.3437	6.112	0.5196	1.152	1.0284	0.0077	0.2122
60 vol % AN									
0.0000	787.25	1470.50	1.3395	5.874	0.5094	1.158	1.0000	-	0.1553
0.0127	787.43	1385.35	1.3400	6.617	0.5407	1.091	1.0203	0.0756	0.2503
0.0383	788.07	1387.53	1.3408	6.591	0.5396	1.093	1.0206	0.0250	0.2480
0.0640	789.24	1391.20	1.3416	6.547	0.5378	1.098	1.0212	0.0144	0.2440
0.0899	790.78	1393.88	1.3424	6.509	0.5362	1.102	1.0226	0.0100	0.2411
0.1158	792.22	1395.09	1.3433	6.486	0.5353	1.105	1.0241	0.0077	0.2397
70 vol % AN									
0.0000	752.26	1415.23	1.3385	6.637	0.5415	1.065	1.0000	-	0.2176
0.0133	752.44	1331.95	1.3392	7.491	0.5753	1.002	1.0207	0.0869	0.3070
0.0401	752.98	1336.21	1.3401	7.438	0.5732	1.006	1.0203	0.0280	0.3026
0.0671	753.89	1340.63	1.3410	7.380	0.5710	1.011	1.0204	0.0161	0.2979
0.0942	755.15	1343.12	1.3419	7.341	0.5695	1.014	1.0215	0.0112	0.2953
0.1214	756.42	1346.52	1.3429	7.291	0.5675	1.019	1.0223	0.0084	0.2918

It is clear from Figure-1a that *V* decreases by increase in solute concentration which suggests strengthen ing of solute-solvent interactions and it increases by increase in the content of AN due to weakening of these interactions.

The R_A values increase with increase in drug concentration in all studied mixtures which is due to solute-solvent interactions dominates over solvent-solvent interacti ons because of close association between drug and solvent. The R_A decrease slightly with increase in the content of AN for given solute concentration. The κ_φ values are small positive due to weak solute-solute interactions and relatively loose attachments of solvent molecules to drug at low molalities[14].

The κ_φ values decreases by increases in solute concentration which is due to aggregation of solvent around solute due to strengthening of solute-solvent interactions and weakening of solute-solute interactions. The κ_φ values increases with increase in the content of AN is due to dominating solute-solute interactions. Similarly, decrease in the *r* values by increases in solute concentration supports solute-solvent intractions[15]. The *r* values increase with increase in the content of AN.

Further, the κ_s ($\times 10^{-10}$ $m^2 \cdot N^{-1}$), κ_ϕ ($\times 10^{-10}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$) and V_ϕ ($m^3 \cdot mol^{-1}$) data are fitted to equations (1) to (3)[16-17], Bachem's, modified Massons and Gucker's relation respectively.

$$V_\phi = V_\phi^0 + S_v m \quad (1)$$

$$\left(\frac{\kappa_s - \kappa_0}{m}\right) = A + Bm^{1/2} \quad (2)$$

$$\kappa_\phi = \kappa_\phi^0 + S_k m^{1/2} \quad (3)$$

Where: V_ϕ^0 is partial molar volume of drug, κ_ϕ^0 is limiting apparent molar isentropic compressibility, S_v, *B* and S_k are slope. From plots of i) V_ϕ versus *m* (Figure-1a), V_ϕ^0 and S_v, ii) κ_s-κ_ϕ/m versus $m^{1/2}$ (Figure-1b), *A* and *B* and iii) κ_ϕ versus $m^{1/2}$, κ_ϕ^0 and S_k are determined as an intercept and slope respectively. Graphical parameters are reported in Table-2.

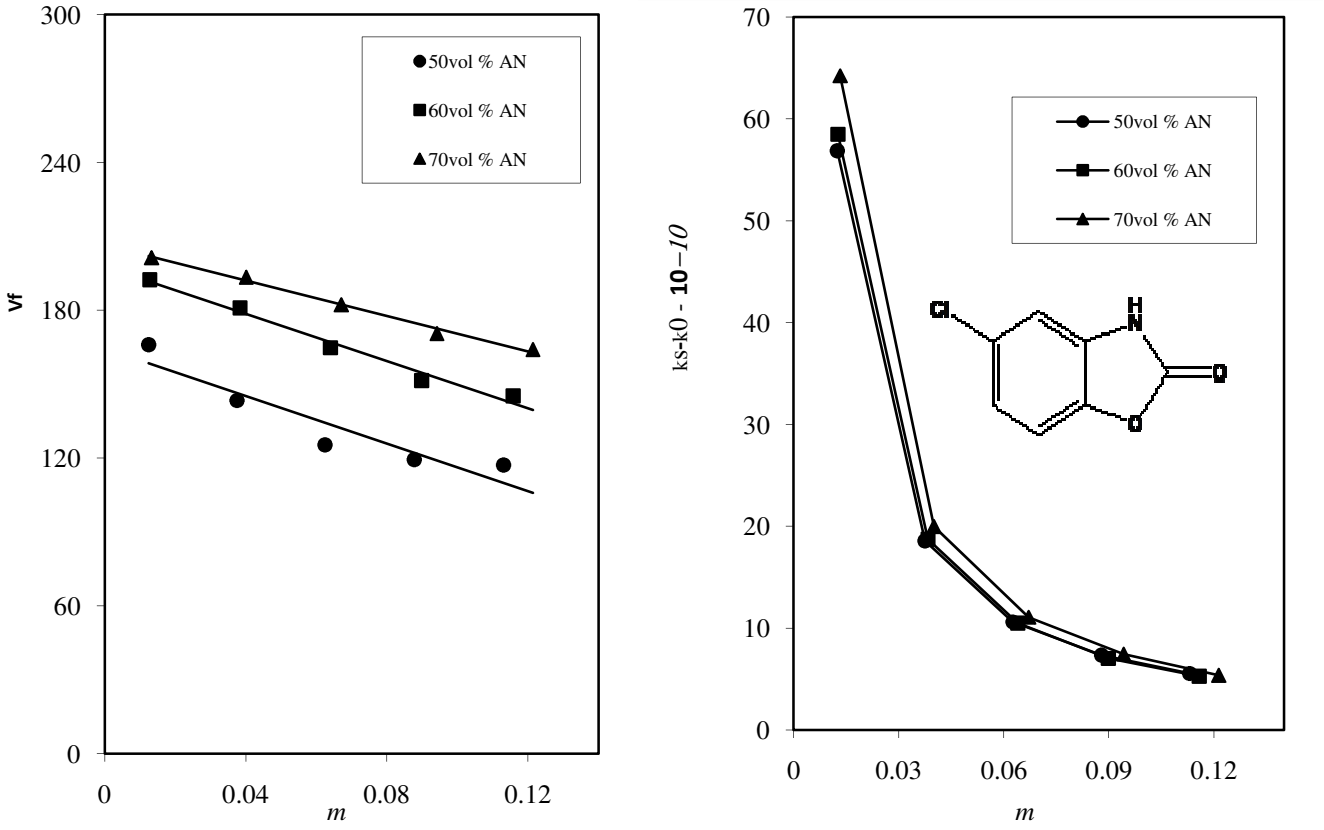

Figure 1a-b
Plots of κ_s-κ_0/m versus $m^{1/2}$ and V_ϕ versus *m* for equation (1) and (2)

Table-2
Graphical parameters obtained for equations (1)-(3) for respective plots

Graphical parameters	50vol % AN	60vol % AN	70vol % AN
A, $\times 10^{-10}$ $m^2 \cdot N^{-1}$ $mol \cdot kg^{-1}$	48.118	49.358	53.946
B, $\times 10^{-10}$ $m^2 \cdot N^{-1}$ $mol^{1/2} \cdot kg^{-1/2}$	-451.67	-457.47	-480.77
V_ϕ^0, $m^3 \cdot mol^{-1}$	164.57	197.76	206.52
S_v, $kg \cdot cm^3 \cdot mol^{-2}$	-483.53	-480.08	-360.70
κ_ϕ^0, $\times 10^{-10}$ $m^3 \cdot mol^{-1} \cdot Pa^{-1}$	0.0909	0.0958	0.1099
S_k,$\times 10^{-10}$ $m^3 \cdot mol^{-3/2} \cdot Pa^{-1} \cdot kg^{1/2}$	-0.2753	-0.2882	-0.3245
n^0	1.3403	1.3396	1.3387
K, $kg \cdot mol^{-1}$	0.0298	0.0318	0.0340

The V_ϕ^0 and κ_ϕ^0 values provide information about solute-solvent interactions and S_v and S_k provide information regarding solute-solute interactions. Positive values of V_ϕ^0 indicates strong solute-solvent interactions. These values increases with the content of AN which is attributed to weakening of solute-solvent interactions and strengthening of solvent–solvent interactions in solutions containing higher content of AN. Negative values of S_v indicate weak solute-solute interactions compared to solute-solvent interactions. The κ_ϕ^0 values are positive and increases with increase in the content of AN which indicates the solvation effect of solute. The negative values of S_v and S_k indicates the dominance of solute-solvent interactions over solute-solute interactions[18].

Refractive index is an important optical parameter which is directly related with molecular interactions in solution[19]. Refractive index data are fitted to $n=n^0 + K \times m$.

The n^0 is infinite dilution refractive index and K is a constant which depends on chemical and physical properties of solute. From the n versus m plots (R^2>0.999), the n^0 and K are determined as an intercept and slope. Graphical values of the n^0 and K are reported in Table-2.

The n increased with increase in drug concentration in each mixture which is assigned to the tighter packing of molecules and overall structural reorganization in solution and it is decreased by increase in the content of AN in mixture due to relatively loose packing of the molecules. Density-refractive index relationship is found to be linear with R^2>0.9804 for all the studied systems. It is seen that the n^0 decreased and the constant K increased with increase in the content of AN in AN + water mixtures.

Conclusion

It is concluded from results, that the solute-solvent interactions strengthens with increase in concentration of solute that signifies structural compactness and aggregation of solvent around solute which is supported by decrease in apparent molar volume and compressibility. There exists hydrogen bonding interactions between drug (>=O, -O-, -NH) and water molecules which is supported by the properties like ρ, u, κ_s, L_f, V_ϕ and V_ϕ^0 and κ_ϕ^0 values. As the content of increases from 50 vol% to 70 vol%, the solute-solvent interactions weaken and strong AN-water interactions exists which is supported by values of experimental and derived properties. Presence of weak solute-solute interactions is supported by S_v and S_k values.

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