Chemistry



Studies of Acoustic Properties of Substituted Heterocyclic Drugs in Dioxane & Dioxane-Water Mixture At 29°C.

| KEYWORDS | Acoustical parameters, Ultrasonic Velocity, Density, Dioxane-wate mixture, ultrasonic frequency, adiabatic compressibility, apparent molal volume. | | | | | | | | |
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ABSTRACTThe acoustical properties have been investigated from the ultrasonic velocity and density measurement
of substituted heterocyclic drugs such as Acenocoumarol { 4-Hydroxy-3-[1(4-nitrophenyl)-3-oxobutyl]-2H-
chromen-2-one}, Allopurinal { 1,5 dihydro-4H-pyrazolol(3,4-d)pyrimidin-4-one}, Warfarin {3(-acetonyl benzyl) -4-hydroxy
coumarin} in 10% DMF at 300K. The measurement have been perform to evaluate acoustical parameters such as -Ultrason-
ic Velocity (Us), Density(ds), Adiabatic compressibility (βs), Intermolecular length(Lt), Partial molal compressibility (φok(s)
), Apparent molal volume (φv), Apparent adiabatic compressibility (φk(s)), Relative association(RA), Specific acoustic
impedence (Z), partial molal volume (φov). The behavior of solutions of these compounds in Dioxane and Dioxane-water
mixture.

Introduction:- In the recent years, measurement of the ultrasonic velocity are helpful to interpreted solute-solvent, ion-solvent interaction in aqueous medium and non-aqueous medium[1-4]. Fumio Kawaizumi[5] has been studied the acoustic properties of complex in water. Jahagirdar 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 the different solute-solvent interaction due to their different size, shape and structure[6]. 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] Syal et.al has been studied the ultrasonic velocity of PEG-8000, PEG-study of acoustical properties of substituted hetrocyclic compounds under suitable condition[9]. 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[10]. S. K. Thakur et.al have studied the different acoustical parameters of binary mixture of 1-propanol and water[11]. Tadkalkar et.al. have studied the acoustical and thermodynamic properties of citric acid in water at different temperature[12]. Mishra et.al have investigated ultrasonic velocity and density in non aqueous solution of metal complex and evaluate acoustical properties of metal complex[13]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[14].

After review of literature survey the detail study of substituted heterocyclic drug under identical set of experimental condition is still lacking. It was thought of interest to study the acoustical properties of substituted heterocyclic drug under suitable condition.

Experimental Section:- The substituted heterocyclic

drugs Acenocoumarol, Allopurinal and Warfarin are used in the present study. Dioxane was purified by Vogel's standard method[15]. The double distilled dioxane is used for solution preparation of different drugs. The density was determined by using specific gravity bottle by relative measurement method with accuracy<u>+</u> 1 x 10-5 am/cm3. The ultrasonic velocity was measure by using ultrasonic interferometer having frequency 2 MHz (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), appearent molal volume (ϕ_v), intermolecular free length (L_f), apparent molal compressibility ($\phi_{k(\rho)}$), specific acoustic impedance (Z), relative association (R_A), were studied.

| Adiabatic compressibility (β | $s = 1/U_{s}$ | ²ds(1 |) |
|----------------------------------|-------------------------------------|---|----|
| Adiabatic compressibility (β | o)=1/U ₀ ² d | o(| 2) |
| Apparent molal volume (ϕ_v | $=[M/d_s]x$ | (d ₀ -d _s)x10 ³ /mxd _s xd ₀ | (3 |

Apparent molal compressibility $(\phi_{k(s)}) = 1000 \times [\beta s d0 - \beta ods / Mxd_sxd_0] + \beta s x M / d_s ------(4)$

| Specific acoustic | impedence(Z) = U _s d _s | (5) |
|-------------------|--|-----|
| | | |

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

Relative association (R_A) =(d_s/d_o) x (U_o/U_s)^{1/3} -----(7)

Result and Discussion :- In the present investigation, different thermodynamic parameters, such as adiabatic compressibility (β s), Partial molal volume (ϕ°_{v}), intermolecular free length (L_f), apparent molal compressibility ($\phi_{k(s)}$), specific acoustic impedance (Z), relative association (R_A).

Ligand 1: - Acenocoumarol :- 4-Hydroxy-3-[1(4-nitrophenyl)-3-oxobutyl]-2H-chromen-2-one.(Mol.Wt.:- 353.32)

Ligand2: - Allopurinal :- 1,5 dihydro-4H-pyrazolol(3,4-d) pyrimidin-4-one. (Mol.Wt.:- 136.12)

Ligand3 :- Warfarin :- 3(-acetonyl benzyl) -4-hydroxy coumarin. (Mol.Wt.:- 308.31)

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Table 1 Ultrasonic Velocity in Distilled Water. Temp.:- 29°C ± 0.1 ℃

| Sr. No. | No. of rota- tions of Screw | Mi- crom- eter read- ing (mm) | Differ- ence between Microm- eter reading (mm) | Distance travelled by screw in one rotation (mm) | Ultra- sonic Velocity (U) m/ sec. | Average of Ul- trasonic Veloci- ties (U) m/sec. |
|------------|--------------------------------------|--|--|---|---|--|
| 1 | 5 | 22.234 | | | | |
| 2 | 10 | 18.483 | 3.751 | 0.7502 | 1500.4 | |
| 3 | 15 | 14.733 | 3.750 | 0.7500 | 1500.0 | |
| 4 | 20 | 10.982 | 3.751 | 0.7502 | 1500.4 | 1500.08 |
| 5 | 25 | 7.234 | 3.748 | 0.7496 | 1499.2 | |
| 6 | 30 | 3.483 | 3.751 | 0.7502 | 1500.4 | |

Table 2 System:- L, Ultrasonic Frequency = 2 MHz Medium = Dioxane- Water Temp.:- 29°C

Acoustic properties of different concentrations of Ligand-1 in 70% Dioxane- Water mixture.

| Sr. No. | m.conc. (mole/Lit) x 10 ⁻³ | 7.0 | 7.5 | 8.0 | 8.5 | 9.0 | 9.5 |
|------------|---|----------|---------|---------|---------|---------|---------|
| 1 | Us(cm sec ⁻¹) | 1342 | 1382 | 1437 | 1493 | 1531 | 1582 |
| 2 | ds(g cm ^{-g}) | 1.003 | 0.9947 | 0.9963 | 0.9932 | 0.9921 | 0.9918 |
| 3 | ßs(bar¹) x 10 ⁻⁵ | 5.5509 | 5.2637 | 4.8607 | 4.5169 | 4.3002 | 4.0287 |
| 4 | Lt(A°) x 10 ³ | 4.4814 | 4.3640 | 4.1936 | 4.0426 | 3.9444 | 3.8178 |
| 5 | φ.(cm³mole ⁻¹) x 10 ² | -12.9314 | -8.8098 | -6.8422 | -4.3932 | -1.8761 | 0.4500 |
| 6 | g _{ks)} (cm- 3mole ⁻¹) | 2.3768 | 1.8620 | 1.2497 | 0.7934 | 0.5196 | 0.2159 |
| 7 | R | 1.0787 | 1.0619 | 1.0501 | 1.0336 | 1.0238 | 1.0124 |
| 8 | Z (g cm³ sec ⁻¹) | 1342.48 | 1374.68 | 1431.68 | 1482.85 | 1518.91 | 1569.03 |

Table 3 System:- L₂ Ultrasonic Frequency = 2 MHz Medium = Dioxane- Water Temp.:- 29°C

Acoustic properties of different concentrations of Ligand-2 in 70% Dioxane- Water mixture.

| Sr. No. | m.conc. (mole/Lit) x 10 ⁻³ | 7.0 | 7.5 | 8.0 | 8.5 | 9.0 | 9.5 |
|------------|--|------|------|------|------|------|------|
| 1 | Us(cm sec ⁻¹) | 1437 | 1465 | 1489 | 1518 | 1542 | 1569 |

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| | | - | | | r | 1 | |
|---|--|----------|----------|----------|----------|---------|---------|
| 2 | ds(g cm ^{-j}) | 0.8788 | 0.8667 | 0.8655 | 0.8643 | 0.8638 | 8632 |
| 3 | βs(bar¹) x 10 ⁻⁵ | 5.5106 | 5.3946 | 5.2191 | 5327 | 408350 | 4.7005 |
| 4 | Lt(A°) x 10 ³ | 4.4651 | 4.4179 | 4.3454 | 4.2671 | 4.1825 | 4.1265 |
| 5 | φ _v (cm³mole ⁻¹) x 10 ² | -27.8293 | -21.6818 | -15.9932 | -11.2311 | -4.6882 | 0.1641 |
| 6 | φ _{k(s)} (cm- ³ mole ⁻¹) | 0.8429 | 0.7425 | 0.5533 | 0.3865 | 0.1876 | 0.1149 |
| 7 | R₄ | 1.0547 | 1.0300 | 1.0250 | 1.0162 | 1.0138 | 1.0073 |
| 8 | Z (g cm ³ sec ¹) | 1262.84 | 1265.32 | 1286.79 | 1308.98 | 1341.23 | 1355.93 |

Table 4 System:- L₃ Ultrasonic Frequency = 2 MHz Medium = Dioxane- Water Temp.:- $29^{\circ}C$

Acoustic properties of different concentrations of Ligand-3 in 70% Dioxane- Water mixture.

| Sr. No. | m.conc. (mole/Lit) x 10 ⁻³ | 7.0 | 7.5 | 8.0 | 8.5 | 9.0 | 9.5 |
|------------|---|----------|---------|---------|---------|---------|---------|
| 1 | Us(cm sec ⁻¹) | 1378 | 1387 | 1405 | 1423 | 1439 | 1456 |
| 2 | ds(g cm ^{-j}) | 0.9834 | 0.9812 | 0.9797 | 0.9783 | 0.9764 | 1.9748 |
| 3 | βs(bar ¹) x 10 ⁻⁵ | 5.3555 | 5.2977 | 5.1708 | 5.0480 | 4.9459 | 4.8391 |
| 4 | Lt(A°) x 10 ³ x | 4.4019 | 4.3789 | 4.3253 | 4.2736 | 4.2302 | 4.1843 |
| 5 | $\varphi_v(cm^3mole^{-1}) \propto 10^2$ | -12.8449 | -9.4325 | -7.0350 | -4.7719 | -1.9432 | 0.8315 |
| 6 | g _{k(s)} (cm- ³ mole ⁻¹) | 0.8105 | 0.6979 | 0.5153 | 0.3586 | 0.2313 | 0.1344 |
| 7 | R | 1.0349 | 1.0303 | 1.0243 | 1.0169 | 1.0128 | 1.0072 |
| 8 | Z (g cm³ sec ¹) | 1355.13 | 1360.92 | 1376.48 | 1392.12 | 1405.04 | 1419.31 |

Table 5 System:- L₁ **Ultrasonic Frequency = 2 MHz Medium = Dioxane Temp.:- 29°C** Acoustic properties of Ligand-1 in different percentage of 1,4 Dioxane.

| Sr.No. | % of 1,4 Dioxane | 75% | 80% | 85% | 90% | 95% | 100% |
|--------|---------------------------|------|------|------|------|------|------|
| 1 | Us(cm sec ⁻¹) | 1632 | 1597 | 1572 | 1549 | 1517 | 1482 |

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| 2 | ds(g cm ⁻³) | 0.9787 | 0.9767 | 0.9748 | 0.9732 | 0.9717 | 0.9701 |
|---|---|---------|---------|---------|---------|---------|---------|
| 3 | βs(bar-1) x 10-5 | 3.8362 | 4.0144 | 4.1513 | 4.2825 | 4.4720 | 4.6930 |
| 4 | Lt(A°) x 10 ³ | 3.7255 | 3.8111 | 3.8755 | 3.9363 | 4.0224 | 4.1206 |
| 5 | φ_v (cm ³ mole ⁻¹) x 10 ² | -8.4672 | -5.0897 | -3.2226 | -0.0179 | 1.8494 | 3.6421 |
| 6 | φ _{k(s)} (cm³mole ⁻¹) | -1.0898 | -0.8022 | -0.5946 | -0.4179 | -0.2044 | 0.0171 |
| 7 | R _A | 0.9769 | 0.9820 | 0.9901 | 0.9884 | 0.9938 | 1.0000 |
| 8 | Z (g cm ³ sec ⁻¹) | 1597.23 | 1559.79 | 1532.39 | 1507.49 | 1474.70 | 1437.69 |

Table 6 System:- L_2 Ultrasonic Frequency = 2 MHz

Acoustic properties of Ligand-2 in different percentage of 1,4 Dioxane .

Medium = Dioxane Temp.:- 29°C

| | | 1 | 0 | | | | |
|--------|--|---------|---------|---------|---------|---------|---------|
| Sr.No. | % of 1,4 Dioxane | 75% | 80% | 85% | 90% | 95% | 100% |
| 1 | Us(cm sec ⁻¹) | 1652 | 1608 | 1569 | 1532 | 1498 | 1457 |
| 2 | ds(g cm ⁻³) | 0.8834 | 0.8821 | 0.8817 | 0.8812 | 0.8807 | 0.8805 |
| 3 | βs(bar ⁻¹) x 10 ⁻⁵ | 4.1479 | 4.3844 | 4.6072 | 4.8351 | 5.0600 | 5.3500 |
| 4 | Lt(A°) x 10 ³ | 3.8739 | 3.9828 | 4.0828 | 4.1825 | 4.2787 | 4.3996 |
| 5 | φ _v (cm ³ mole ⁻¹) x 10 ² | -3.4302 | -2.3319 | -1.2747 | -0.5423 | 1.2741 | 1.5459 |
| 6 | φ _{k(s)} (cm³mole ⁻¹) | -1.1075 | -0.8269 | -0.5961 | -0.3866 | -0.2015 | 0.0082 |
| 7 | R _A | 0.9622 | 0.9694 | 0.9770 | 0.9841 | 0.9910 | 1.0000 |
| 8 | Z (g cm ³ sec ⁻¹) | 1459.38 | 1418.42 | 1383.39 | 1350.00 | 1319.29 | 1282.89 |

Table 7 System:- L₃ Ultrasonic Frequency = 2 MHz Medium = Dioxane Temp.:- 29°C

Acoustic properties of Ligand-3 in different percentage of 1,4 Dioxane .

| Sr.No. | % of 1,4 Dioxane | 75% | 80% | 85% | 90% | 95% | 100% |
|--------|---|---------|---------|---------|---------|---------|---------|
| 1 | Us(cm sec ⁻¹) | 1498 | 1473 | 1457 | 1439 | 1423 | 1417 |
| 2 | ds(g cm ⁻³) | 0.9891 | 0.9887 | 0.9879 | 0.9871 | 0.9865 | 0.9861 |
| 3 | βs(bar-1) x 10-5 | 4.5054 | 4.6616 | 4.7722 | 4.8924 | 5.0060 | 5.0500 |
| 4 | Lt(A°) x 10 ³ | 4.0374 | 4.1068 | 4.1552 | 4.2072 | 4.2558 | 4.2745 |
| 5 | φ_v (cm ³ mole ⁻¹) x 10 ² | -0.9840 | -0.2151 | 0.9147 | 1.6819 | 2.3925 | 3.1266 |
| 6 | $\phi_{k(s)}$ (cm ³ mole ⁻¹) | -0.7047 | -0.4689 | -0.3052 | -0.1589 | -0.0314 | 0.0158 |
| 7 | R _A | 0.9845 | 0.9898 | 0.9918 | 0.9959 | 0.9991 | 1.0000 |
| 8 | Z (g cm³ sec⁻¹) | 1481.67 | 1456.36 | 1438.20 | 1420.44 | 1403.79 | 1397.30 |

From Table 1, the ultrasonic velocity in distilled water at the temperature $29^{\circ}C\pm 0.1^{\circ}C$. The ultrasonic velocity(Us) in distilled water is nearly same with neglizible difference with the no. of relations of screw is incresease. The average ultrasonic velocity(U) in distilled water also given in table 1.

From Table 2, 3 & 4 , it is found that the ultrasonic velocity increases with increase in the concentration of the ligand L_1, L_2 & L_3 in 70% Dioxane-water mixture at 29°C temperature. 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 propogation proposed by Erying and Kincaid[16]. It was found that, intermolecular free length decreases linearly on increasing the concentration ligand L_1, L_2 & L_3 . The intermolecular free length increases 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 bahaviour 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) increases with increase in the concentration of ligandL₁,L₂ &L₃ in 70% Dioxane-water mixture. The decrease of adiabatic compressibility with increase in the percentage of dioxane in solution may be due to the collection of solvent molecule around ions, this supporting weak ion-solvent interaction[17]. This indicate that there is significant solute-solvent interaction. The increase in adiabatic compressibility following a decrease in ultrasonic velocity showing there by weaking intermolecular interaction.

From Table 5, 6 & 7, it is found that apparent molal volume increases with increases in he percentage of the 1,4 Dioxane in all system indicate the existence of weak ion-solvent interaction. The value of the apparent molal compressibility is increases with increases in the percentage of the dioxane 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 the relative association increases with increase in the percentage of dioxane in all systems. It is found that there is weak interaction

between solute and solvent.

Conclusion :- In the present study mentions the experimental data for ultrasonic velocity, density and at 29°C for all substituted heterocyclic drugs in 1,4 dioxane-water mixture and dioxane. 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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