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To Study Different Acoustical Properties of Substituted Heterocyclic Drugs in DMF & DMF-Water Mixture at 29^0C.

KEYWORDS Acoustical parameters, Ultrasonic Velocity, Density, DMF-wate mixture, ultrasonic frequency, adiabatic compressibility, apparent molal volume.

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ABSTRACT *The 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 -Ultrasonic 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 DMF and DMF-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 and DMF was purified by Vogel's standard method[15]. The double distilled dioxane is also used for solution preparation of different drugs. In the present study the DMF is used for solution preparation of different drugs. The density was determined by using specific gravity bottle by relative measurement method with accuracy± 1×10^{-5} gm/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($\varphi_{k(s)}$) , specific acoustic impedance(Z), relative association(R_A), were studied.

Adiabatic compressibility (βs) = $1 / U_s^2 d_s$ ------(1)

Adiabatic compressibility (βo)= $1 / U_0^2 d_0$ ------(2)

Apparent molal volume (φ_v) =$[M/d_s] \times (d_0-d_s)\times10^3 / m\times d_s \times d_0$ -----------(3)

Apparent molal compressibility($\varphi_{k(s)}$) =1000 x [βs d0- βods / $M \times d_s \times d_0$] + βs xM / d_s -------(4)

Specific acoustic impedence(Z) = $U_s d_s$ ----------(5)

Intermolecular free length (L_f) =K√ βs ------------(6)

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

Result and Discussion :-
In the present investigation, different thermodynamic parameters, such as adiabatic compressibility(βs), Partial molal volume(φ^o_v), intermolecular free length(L_f), apparent molal compressibility ($\varphi_{k(s)}$), 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)

Volume : 4 | Issue : 7 | July 2014 | ISSN - 2249-555X

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)

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

Sr.No.	No. of rotations of Screw	Micrometer reading (mm)	Difference between Micrometer reading (mm)	Distance travelled by screw in one rotation (mm)	Ultrasonic Velocity (U) m/sec.	Average of Ultrasonic Velocities (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_1
Ultrasonic Frequency = 2 MHz, Medium = DMF, Temp.:- 29°C
Acoustic properties of Ligand-1 in different percentage of DMF .

Sr.No.	% of DMF	75%	80%	85%	90%	95%	100%
1	Us(cm sec^{-1})	1482	1473	1465	1457	1449	1438
2	ds(g cm^{-3})	0.8769	0.8743	0.8737	0.8721	0.8718	0.8712
3	βs(bar^{-1}) x 10^{-5}	5.1922	5.2715	5.3329	5.4015	4.9010	5.5510
4	Lt(A°) x 10^3	4.3342	4.3672	4.3926	4.4207	4.2109	4.4815
5	φ_v($cm^3 mole^{-1}$) x 10^2	-5.9190	-2.5462	-1.1237	0.4352	2.4418	4.0556
6	$\varphi_{k(s)}$ ($cm^3 mole^{-1}$)	-0.3296	-0.2268	-0.1609	-0.0922	-0.9844	0.0225
7	R_A	0.9964	0.9955	0.9967	0.9966	1.1127	1.0000
8	Z (g cm^3 sec^{-1})	1299.57	1287.84	1279.97	1270.64	1408.13	1252.77

Table 3 System:- L_2
Ultrasonic Frequency = 2 MHz Medium = DMF, Temp.:- 29°C
Acoustic properties of Ligand-2 in different percentage of DMF.

Sr.No.	% of DMF	75%	80%	85%	90%	95%	100%
1	Us(cm sec^{-1})	1625	1601	1583	1570	1562	1552
2	ds(g cm^{-3})	0.9834	0.9732	0.9734	0.9749	0.9721	0.9718
3	βs(bar^{-1}) x 10^{-5}	3.8509	4.0088	4.0997	4.1614	4.2163	4.2720
4	Lt(A°) x 10^3	3.7326	3.8084	3.8513	3.8802	3.9057	3.9314
5	φ_v($cm^3 mole^{-1}$) x 10^2	-14.8000	-11.4568	-7.9115	-5.2392	-1.6660	1.4007
6	$\varphi_{k(s)}$ ($cm^3 mole^{-1}$)	-0.5793	-0.3039	-0.1884	-0.1213	-0.0490	0.0059
7	R_A	0.9964	0.9911	0.9946	0.9993	0.9982	1.0000
8	Z (g cm^3 sec^{-1})	1598.03	1558.16	1540.89	1530.60	1518.42	1508.23

Table 4 System:- L_3
Ultrasonic Frequency = 2 MHz, Medium = DMF, Temp.:- 29°C
Acoustic properties of Ligand-3 in different percentage of DMF.

Sr.No.	% of DMF	75%	80%	85%	90%	95%	100%
1	Us(cm sec^{-1})	1564	1553	1549	1538	1531	1527
2	ds(g cm^{-3})	1.0021	0.9937	0.9847	0.9797	0.9743	0.9737
3	βs(bar^{-1}) x 10^{-5}	4.0796	4.1726	4.2325	4.3151	4.3788	4.4050
4	Lt(A°) x 10^3	3.8419	3.8854	3.9132	3.9512	3.9803	3.9922
5	φ_v($cm^3 mole^{-1}$) x 10^2	-35.7313	-24.7354	-17.3662	-13.8416	2.4987	3.1664
6	$\varphi_{k(s)}$ ($cm^3 mole^{-1}$)	-0.5618	-0.3667	-0.2303	-0.1067	-0.0138	0.0139
7	R_A	1.0209	1.0149	1.0064	1.0038	0.9997	1.0000
8	Z (g cm^3 sec^{-1})	1567.28	1543.22	1525.30	1506.78	1491.65	1486.84

Volume : 4 | Issue : 7 | July 2014 | ISSN - 2249-555X

Table 5 System:- L_1
Ultrasonic Frequency = 2 MHz, Medium = DMF- Water, Temp.:- 29°C
Acoustic properties of different concentrations of Ligand-1 in 70% DMF-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})	1462	1465	1482	1542	1592	1639
2	ds(g cm^{-3})	1.0680	1.0400	1.0020	0.9938	0.9727	0.9835
3	βs(bar^{-1}) x 10^{-5}	4.3806	4.4801	4.5439	4.2319	4.0563	3.6834
4	Lt(A°) x 10^3	3.9811	4.0261	4.0546	3.9129	3.8309	3.6834
5	φ_v(cm^3mole^{-1}) x 10^2	-11.1616	-10.4254	-9.9398	-8.426	-7.3761	-6.3599
6	$\varphi_{k(s)}$ (cm^3mole^{-1})	0.7402	0.9450	1.1008	0.7085	0.5526	0.1501
7	R_A	1.1387	1.1081	1.0634	1.0409	1.0079	1.0186
8	Z (g cm^3 sec^{-1})	1561.42	1523.60	1484.96	1532.44	1548.54	1627.04

Table 6 System:- L_2
Ultrasonic Frequency = 2 MHz, Medium = DMF- Water, Temp.:- 29°C
Acoustic properties of different concentrations of Ligand-2 in 70% DMF-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})	1471	1485	1512	1565	1599.1	1645
2	ds(g cm^{-3})	1.0032	0.9938	0.9933	0.9921	0.9881	0.9903
3	βs(bar^{-1}) x 10^{-5}	4.6067	4.5629	4.4037	4.1154	3.9578	3.7316
4	Lt(A°) x 10^3	4.0825	4.0631	3.9916	3.8587	3.7841	3.6743
5	φ_v(cm^3mole^{-1}) x 10^2	-9.8832	-7.1897	-6.0209	-4.6519	-3.3944	-1.6394
6	$\varphi_{k(s)}$ (cm^3mole^{-1})	1.4471	1.3253	1.0513	0.6650	0.4721	0.2104
7	R_A	1.0653	1.0519	1.0451	1.0319	1.0204	1.0132
8	Z (g cm^3 sec^{-1})	1475.71	1475.80	1501.87	1552.64	1580.07	1329.04

Table 7 System:- L_3
Ultrasonic Frequency = 2 MHz, Medium = DMF- Water, Temp.:- 29°C
Acoustic properties of different concentrations of Ligand-3 in 70% DMF-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})	1432	1437	1467	1482	1517	1542
2	ds(g cm^{-3})	0.9998	0.9967	0.9971	0.9952	0.9937	0.9941
3	βs(bar^{-1}) x 10^{-5}	4.8775	4.8587	4.6602	4.5750	4.3729	4.2337
4	Lt(A°) x 10^3	4.2008	4.1927	4.1062	4.0685	3.9776	3.9135
5	φ_v(cm^3mole^{-1}) x 10^2	-5.9770	-3.7155	-1.4506	0.0752	1.8775	3.1033
6	$\varphi_{k(s)}$ (cm^3mole^{-1})	1.2071	1.1159	0.8006	0.6632	0.4119	0.2470
7	R_A	1.0410	1.0365	1.0298	1.0246	1.0149	1.0092
8	Z (g cm^3 sec^{-1})	1431.7136	1432.25	1462.746	1474.89	1507.44	1531.98

From Table 1, the ultrasonic velocity in distilled water at the temperature $29^0C\pm 0.1^0C$. 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 apparent molal volume increases with increases in the percentage of the DMF in all system such as ligand L_1,L_2 & L_3. The value of the apparent adiabatic compressibility is increases with increase in the percentage of the DMF for all the system. 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 is increases with increase in the percentage of DMF in all systems. It is found that there is weak interaction between solute and solvent.

From Table 5,6 & 7 , it is found that the ultrasonic velocity increases with increase in the concentration of the ligand L_1,L_2 & L_3 in 70% DMF-water mixture at 29^0C 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 increases at some interval then decreases linearly on increasing the concentration ligand L_1,L_2 &L_3 in 70% DMF-water mixture at 29^0C temperature. 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 behavior 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 ligandL_1,L_2 &L_3 in 70% DMF-water mixture. The value of adiabatic compressibility isincrease first then again decreases with the increase in the concentration of the ligand L_1,L_2 &L_3 in 70% DMF-water mixture at 29^0C temperature and at ultrasonic frequency is 2 MHz is given in table. Also the increase of adiabatic compressibility with increase in the percentage of DMF 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 weakening intermolecular interaction.

Conclusion :-

In the present study mentions the experimental data for ultrasonic velocity, density and at 29^0C for all substituted heterocyclic drugs in DMF and DMF-water mixture. 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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