Ultrasonic Behaviour and Molecular Relations of Dihydroformazan in DMF at Different Concentrations and in Different Percentages of DMF – Water Mixture

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Abstract **- Ultrasonic velocity and density measurement of Dihydroformazan N'(benzilidene)-3-(pyrid-4-yl) dihydroformazan (S1) in DMF – Water Mixture have been carried out in the concentration range 0.01 to 0.002 mole dm-3 and 85%, 88%, 91%, 94% and 97% DMF –water has been studied in different percentage at 100C (283K). The investigational data have been used to compute several acoustical parameters such as adiabatic compressibility (βs), apparent molar volume(ϕv), apparent molar compressibility(ϕk), intermolecular free length (Lf), specific acoustic impedance (Zs) and relative association (RA). the solute-solute and solute-solvent interaction have been present in the given solutions as well as the significance the molecular interaction in all parameters.**

keywords **- ultrasonic velocity, apparent molar compressibility, specific acoustic impedance, viscosity A and B coefficient.**

I. I.INTRODUCTION

Ion – solvation is the back bone of solution chemistry [1-2]. Ultrasonic velocity studies [3-6] in containing water and some non – aqueous electrolyte solutions have controlled to new intuitions in the solvation method. Acoustic parameters such as velocity (Us), adiabatic compressibility (βs), intermolecular free length (Lf), relative association (RA) and Specific acoustic impedance (Zs), viscous relaxation time (τ), Gibb's free energy (ΔG) apparent molar compressibility (Φk), apparent molar volume (Φv), solvation number (Sn), and internal pressure (π) are useful parameters in explicate ion – solvent interaction [7-10]. Dihydroformazan is the class of compounds which have also promote to contain antimicrobacterial activity, antimicrobial, and antiviral activities against various fungi strains virus, and bacteria. Therefore, it was promoting vital to study their ultrasonic and thermodynamic behaviour which may lead to some new findings in future. Ultrasonic can be feasible skilled technology for the reason that it can be used for various uses in the area comparable pharmaceutical industries, consumer industries, medical industries, and chemical industries etc [11-13]. For the ultrasonic behaviour no reports available in this area of dihydroformazan in DMF – water. In the present attempt ultrasonic behaviour of dihydroformazan at compositions of 85%, 88%, 91%, 94% and 97% DMF –water has been studied [14-16].

II.THEORIES:

Altogether analytical A-grade chemicals and solvents used were gained from Merck, India. The specific conductivity of distilled water was $1x10^{-6}$ $ohm^{-1}cm^{-1}$. Standard solutions of were ready replaced heterocyclic compound in different percentage of DMF-water mixtures. Ultrasonic speed was calculated through single crystal path interferometer (2 MHz) with an accurateness of 0.03%. The density amplitude was implemented at 283K. The apparent molar volumes (Φv) and apparent molar adiabatic compressibility ΦK of Dihydroformazan N'(benzilidene)-3-(pyrid-4-yl) dihydroformazan (S1), in solutions are determined from density (ds) and adiabatic compressibility (βs) of solution. Using following equations.

$$\Phi V = \left\{\frac{(d0-ds)X10^{3}}{m\ ds..d0}\right\} \dagger \frac{M}{ds} \text{----------(1)}$$

II.

Where M is molecular weight of the solute, m is the molality of solution, do is the density of the solvent and ds is the density of the solution.

$$\Phi ks = \left\{\frac{(\beta sd0-\beta 0ds)\ X10^{3}}{m\ ds..d0}\right\} \dagger \frac{\beta sM}{ds} \text{----------(2)}$$

Where βs is the adiabatic compressibility of solution and 0 its is the solvent which can be calculated by

$$\beta s = \underline{100}$$

$$Us^2 X d_s \text{ ----------(3) for solution and}$$
$$\beta 0 = \frac{100}{U0^2 X\, d_0} \text{ ----------(4) for solvent}$$

Where Us &U_0 are the ultrasonic velocities of ultrasound speed in solution and solvent respectively. Knowing β s, β 0 and molecular mass of Dihydroformazan, the values of Φv and $\Phi_K(s)$ are calculated. The values of Φv and $\Phi_K(s)$ are plotted against molality (m) of Dihydroformazan. The curve represented the least square and Φv and ΦK(s) can be given as

$$\Phi v = (\Phi^0 v + Sv\ m) \text{ ----------(5)}$$
$$\Phi ks = (\Phi^0 k(s) + Sk(s)\ m) \text{ ----------(6)}$$

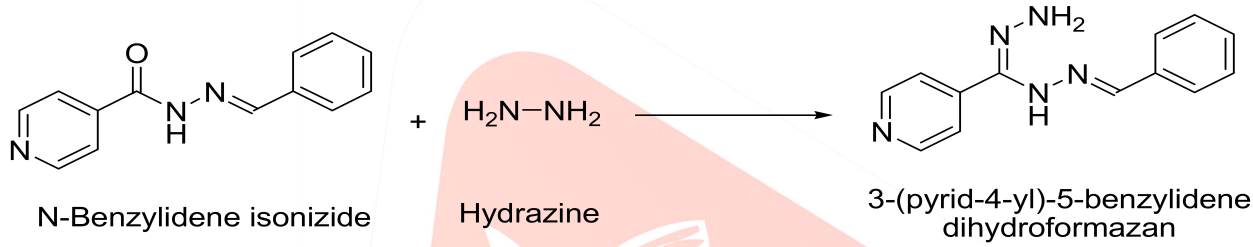
Where $\Phi^0 v = v^o$ and $\Phi^0\ K(s) = K^0$ are the infinite dilution partial molar volumes and adiabatic partial molar compressibilities respectively. Sv and Sk are the experimental slopes. The ΦK and Φv values of in two mixed solvents substituted heterocyclic compound are calculated and given in Table 1 to 3.

The various parameters like intermolecular free length (Lf), specific acoustic impendence (z) and relative association (RA) are computed through using the formulae.

$$Lt = K\ X\ (Bs)^{1/2} \text{ ----------(7)}$$

Where K is Jacobson's constant = 6.0186 X 10^4 and

$$Z = Us\ X\ ds \text{ ----------(8)}$$
$$RA = ds/d_0\ (U_0/Us)^{1/3} \text{ ---------(9)}$$



The dihydroformazan used in the current study were synthesized by standard methods as reported by earlier workers [17]. In this chapter different percentage solvents like 85%, 88%, 91%, 94% and 97% DMF –water have been used. Ultrasonic and thermodynamic parameters have been measured at 100C (283K).

III.EXPERIMENTAL DATA:

Table I :- Velocity (Us), adiabatic compressibility (βs), intermolecular free length (Lf), relative association (RA) and viscous relaxation time (τ), Gibb's free energy (ΔG) of S1 compound in different concentration and different percentage of DMF – Water at 10^0C (283K).

Conc. (kg mol^{-1})	Us (ms^{-1})	βs (m^2N^{-1})	Lf (m)	RA	τ (s)	ΔG ($kJmol^{-1}$)
S1 85% of DMF –Water						
0.01	1622.53	7.6923E-07	52.7864	1.0107	1.114E-06	6.1337E-20
0.008	1621.73	7.7143E-07	52.8620	1.0090	1.053E-06	6.1117E-20
0.006	1618.93	7.7575E-07	53.0081	1.0075	9.498E-07	6.0712E-20
0.004	1617.46	7.8074E-07	53.1787	1.0031	9.296E-07	6.0628E-20
0.002	1611.33	7.8875E-07	53.4508	1.0018	9.279E-07	6.0621E-20
S1 88% of DMF –Water						
0.01	1602.41	7.9524E-07	53.6723	1.0048	9.0261E-07	6.0513E-20
0.008	1595.86	7.9924E-07	53.8057	1.0050	8.8759E-07	6.0448E-20
0.006	1594.42	8.0185E-07	53.8930	1.0054	8.4630E-07	6.0262E-20
0.004	1586.41	8.1043E-07	54.1808	1.0064	8.3993E-07	6.0232E-20
0.002	1582.93	8.1405E-07	54.3021	1.0071	8.1852E-07	6.0131E-20
S1 91% of DMF –Water						
0.01	1588.53	8.0823E-07	54.1084	0.9986	8.8426E-07	6.0433E-20
0.008	1586.26	8.1076E-07	54.1938	0.9988	8.5502E-07	6.0302E-20
0.006	1580.42	8.1396E-07	54.2988	0.9992	8.3417E-07	6.0205E-20
0.004	1576.13	8.4107E-07	55.1968	0.9994	8.3493E-07	6.0209E-20
0.002	1568.93	8.6415E-07	55.9498	0.9997	8.4220E-07	6.0243E-20
S1 94% of DMF –Water						
0.01	1537.73	8.6263E-07	55.8999	1.0069	8.1438E-07	6.0111E-20
0.008	1534.13	8.6825E-07	56.1421	1.0060	7.9343E-07	6.0012E-20
0.006	1532.26	8.7236E-07	56.1473	1.0041	7.7054E-07	5.9895E-20

0.004	1528.83	8.8284E-07	56.5488	0.9974	7.7042E-07	5.9895E-20
0.002	1525.73	8.7493E-07	56.2941	1.0112	7.6278E-07	5.9856E-20
S1 97% of DMF –Water						
0.01	1533.73	8.7082E-07	56.1650	1.0012	6.2727E-07	6.2720E-20
0.008	1531.24	8.7494E-07	56.2950	1.0004	6.0267E-07	6.2517E-20
0.006	1528.53	8.7882E-07	56.4197	1.0001	6.0499E-07	6.2341E-20
0.004	1526.43	8.8142E-07	56.5051	1.0003	6.0644E-07	6.2227E-20
0.002	1525.24	8.8314E-07	56.5597	1.0002	6.0734E-07	6.2155E-20

Table II: - Apparent molar compressibility (Φk), apparent molar volume (Φv), solvation number (Sn), internal pressure (π) and specific acoustic impedance (Zs) of S1 compound in different percentage of DMF – Water at 10^0C (283K).

Conc. (kg mol^{-1})	Φk* 10^{-3} $(kmol)^{-1}$	Φv (m^3mol^{-1})	Zs $(kgm^{-2}s^{-1})$	Sn	Π (Nm^{-2})
S1 - 85% of DMF -Water					
0.01	-2.1731	254.2969	8012.21	3.2802E+08	9.9673E+19
0.008	-1.6929	252.6953	7993.28	2.5543E+08	9.9334E+19
0.006	-0.0093	257.6062	7963.01	1.3971E+08	9.8625E+19
0.004	4.9694	419.6478	7919.19	-7.1235E+08	9.7984E+19
0.002	21.6426	664.9109	7868.60	-3.2345E+08	9.6533E+19
S1 - 88% of DMF -Water					
0.01	-0.8734	381.7743	7857.06	1.2753E+08	9.5089E+19
0.008	0.1440	371.4974	7835.50	-2.1031E+08	9.4409E+19
0.006	1.1784	339.3797	7822.19	-1.7208E+08	9.3959E+19
0.004	7.0338	301.1723	7778.32	-1.0273E+08	9.2497E+19
0.002	18.2010	126.4777	7760.59	-2.6582E+08	9.1883E+19
S1 - 91% of DMF -Water					
0.01	-7.6949	389.4487	7788.70	1.0675E+08	9.2869E+19
0.008	-8.8613	373.7498	7775.29	1.2285E+08	9.2444E+19
0.006	-10.5799	346.3641	7759.23	1.4673E+08	9.1921E+19
0.004	2.3950	542.9468	7615.94	-3.3191E+08	8.7703E+19
0.002	35.6624	1032.104	7499.75	-4.9441E+08	8.4363E+19
S1 - 94% of DMF -Water					
0.01	1.7654	389.1993	7538.55	-2.4087E+08	8.4229E+19
0.008	4.7715	415.5879	7508.09	-6.5111E+08	8.3497E+19
0.006	6.9007	481.2136	7482.07	-9.4150E+08	8.3004E+19
0.004	18.7827	922.1224	7409.55	-2.5633E+08	8.1829E+19
0.002	35.3579	-197.258	7491.80	-4.8244E+08	8.2406E+19
S1 - 97% of DMF -Water					
0.01	1.6273	484.3428	7487.04	-2.1848E+08	8.3219E+19
0.008	3.4979	522.9386	7464.79	-4.6962E+08	8.2698E+19
0.006	6.4180	571.7275	7444.82	-8.6168E+08	8.2190E+19
0.004	11.1746	627.8174	7432.69	-1.5034E+08	8.1827E+19
0.002	24.4262	810.4858	7421.42	-3.2793E+08	8.1605E+19

Table III: - Values of A, B, $Φ^0$k, Sk, $Φ^0$v, Sv of S1 - compound in different percentages DMF – Water at 10^0C(283K).

Compound	A $(dm^3mol^{-1})^{1/2}$	B (dm^3mol^{-1})	$Φ^0$k $(kmol)^{-1}$	Sk	$Φ^0$v (m^3mol^{-1})	Sv
S1- 85% of DMF -Water	0.6789	2.7599	35.8857	-417.991	938.736	-7588.05
S1 - 88% of DMF –Water	0.6672	0.7900	30.8573	-343.060	-28.925	4441.35
S1 - 91% of DMF -Water	0.6505	0.6074	59.7244	-767.470	1390.759	-1138.38
S1 - 94% of DMF -Water	0.6014	-0.0468	59.4029	-612.044	-76.733	6387.64
S1 - 97% of DMF -Water	0.3569	-0.1358	39.6115	-402.576	1029.803	-5686.52

IV.FIGURES:

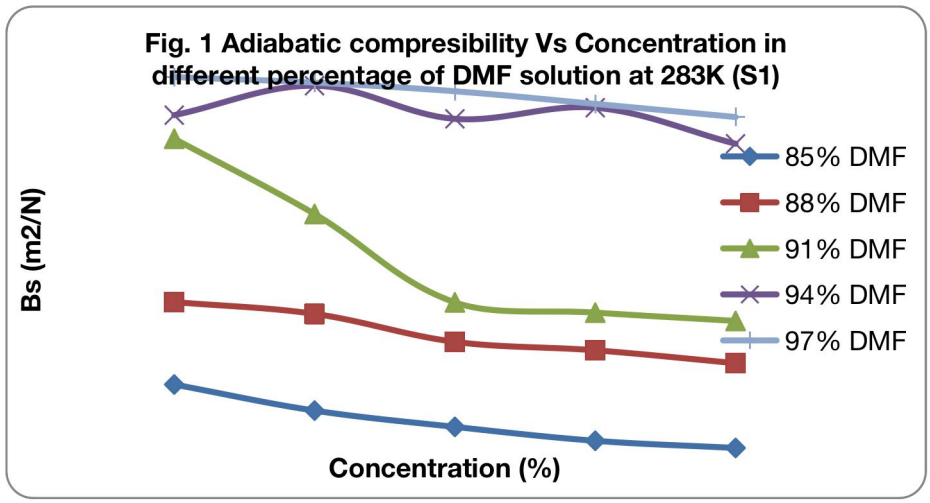


Fig. 1 Adiabatic compresibility Vs Concentration in different percentage of DMF solution at 283K (S1)
Bs (m2/N)
Concentration (%)
85% DMF
88% DMF
91% DMF
94% DMF
97% DMF

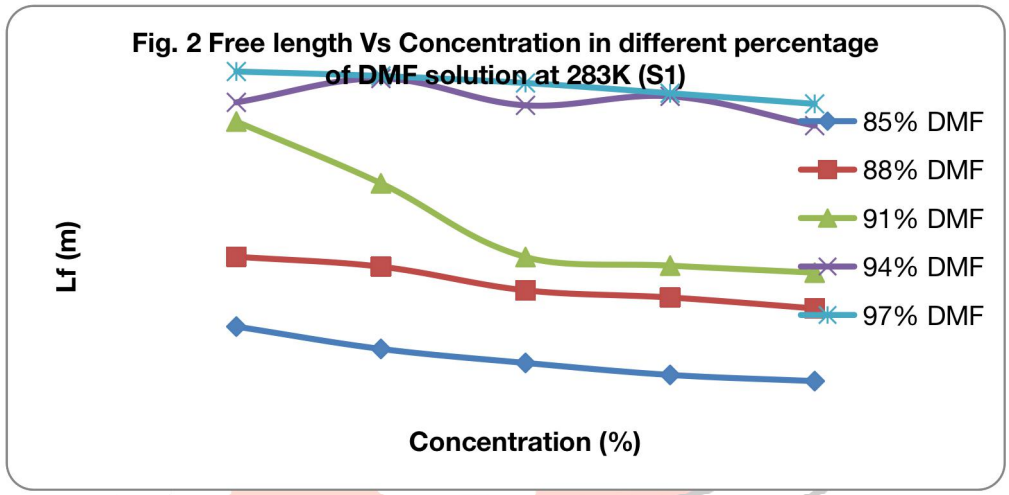


Fig. 2 Free length Vs Concentration in different percentage of DMF solution at 283K (S1)
Lf (m)
Concentration (%)
85% DMF
88% DMF
91% DMF
94% DMF
97% DMF

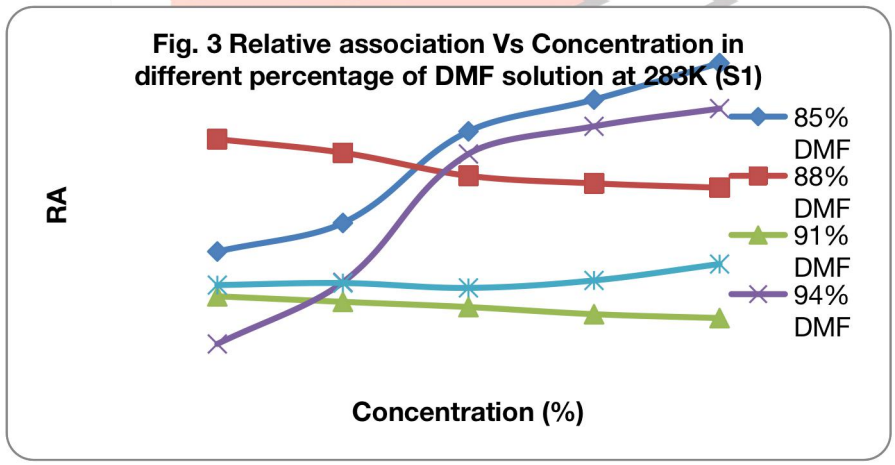
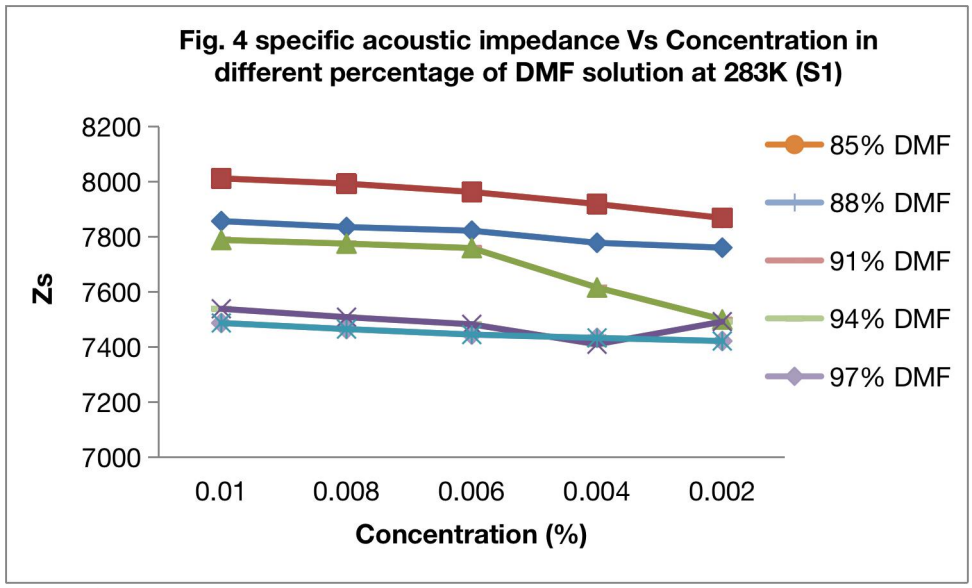
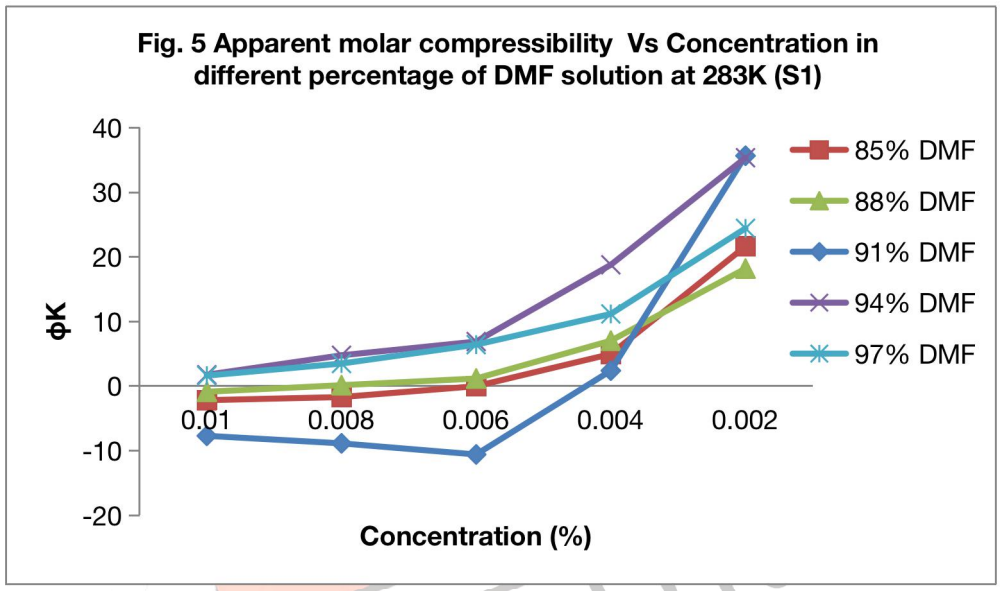
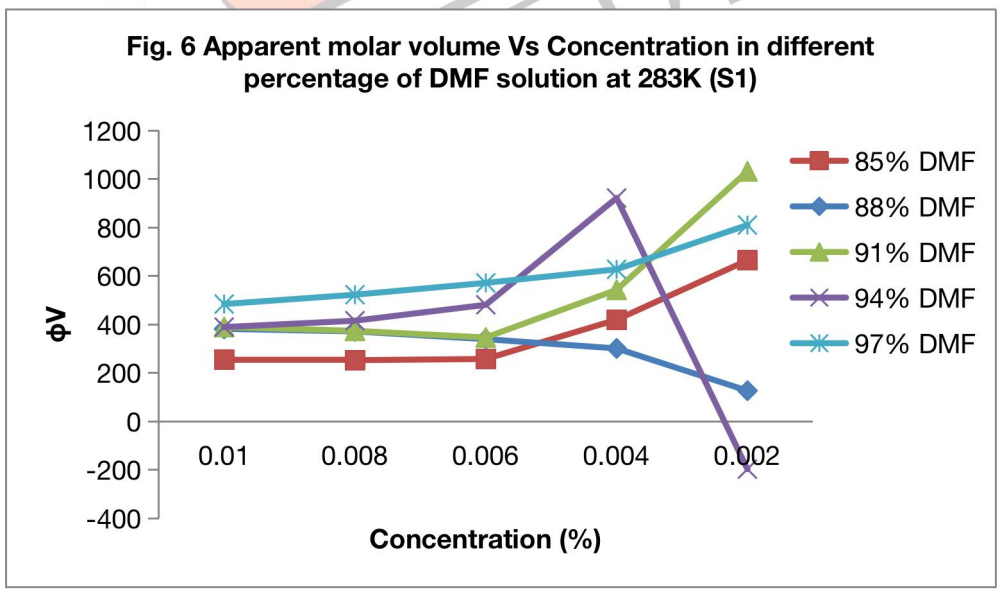


Fig. 3 Relative association Vs Concentration in different percentage of DMF solution at 283K (S1)
RA
Concentration (%)
85% DMF
88% DMF
91% DMF
94% DMF







V.RESULTS AND DISCUSSION

In the present research dissimilar acoustic parameters such as Ultrasonic velocities (U), adiabatic compressibility (βs), apparent molar volume (ϕv), apparent molar compressibility (ϕk) and acoustic impedance (Zs), relative association (R_A) and

intermolecular free length (Lf) of the solutions in different DMF-water mixture and at different concentrations and different percentage of solute are determined at temperature 283 K and presented in Table 1.

The Ultrasonic velocity signifies the magnitude of movement of sound velocity in the respective medium. It decreased with increase in volume of DMF in DMF- water solvent system. Probably this increased in concentration of DMF is not allowing the sound wave to travel freely in solution and hence it decreases. Sound velocity increased with increase in concentration of solute.

Adiabatic compressibility is a measured of intermolecular association or repulsion calculated from the measured ultrasonic velocity (U) and density (d). Ultrasonic velocity increases through increase in concentration of solute for all composition of DMF solution. As more and more solute molecules are added; it fascinates more solvent molecules towards itself and less number of solvent molecules are available for incoming species and hence, with increase in concentration; adiabatic compressibility decreases. Also, as the percentage of DMF increased in solvent system, the intestinal species of water get completely filled and more and more solvent molecules will be available to solute. It reflects in increase in the value of adiabatic compressibility with increase in percentage composition of DMF in solvent system.

The R_A values decreases with decrease in percentage of dioxane. .The values of ϕv, Lf decreases with increase in concentrations of solute. This may be due to decreasing intermolecular interactions with addition of solute forming aggregate of solvent.

Specific acoustic impedance (Zs) increases with increase in concentration of solute indicating the presence of bulkier solute due to solute – solvent as well as solvent – solvent interactions. These interactions oppose the free flow of sound waves. As percentage of DMF goes on increasing, specific acoustic impedance (Zs) values decrease. This means, now at increased percentage of DMF; sound waves has no restrictions and it can flow smoothly.

As we increase the percentage of non aqueous solvent, solvent gets separated by the ion pair and therefore the solvation number decreases.

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