International Research Journal of Natural and Applied Sciences
Vol. 2, Issue 12, Dec 2015 IF- 2.818 ISSN: (2349-4077)
© Associated Asia Research Foundation (AARF)
Website: www.aarf.asia Email : editor@aarf.asia , editoraarf@gmail.com

STUDY OF INTERMOLECULAR INTERACTIONS IN BINARY MIXTURE OF 3-ACETYL-4,6-DIMETHYLCOUMARIN IN 1-PROPANOL AND 2-PROPANOL AT 300K, 303K AND 307K BY THE MEASUREMENT OF ACOUSTIC PROPERTIES

Harsha V. Burghate and Pravin B. Raghuwanshi
Brijlal Biyani Science College, Amravati – 444605 (M.S.) INDIA

ABSTRACT

Ultrasonic velocity and density measurement of 3-acetyl-4,6-dimethylcoumarin were carried out in two different solvents, 1-propanol and 2-propanol for investigating solute-solvent, solute-solute interactions at 300K, 303K and 307K. Several useful parameters such as adiabatic compressibility (βs), apparent molar compressibility (ϕ_k) and specific acoustic impendence (Z) have been calculated these parameters are used to explain the nature of intermolecular interactions taking place in the binary mixture. The above study is useful in understanding the solute – solvent interactions occurring in different concentrations at 300K, 303K and 307K.

Keywords: Interferometry, Density, Binary mixture, Intermolecular interactions.

INTRODUCTION

Ultrasonic waves, in recent years have acquired the status of an important probe for the study of structure and properties of matter in basic science. In the field of technology, the waves are being used for detection of flows, testing of materials, mechanical cleaning of surface, etc. The study of molecular interaction in liquids provides valuable information regarding internal structure, molecular association, complex formation, etc. Ultrasonic parameters are directly related to a large number of thermodynamic parameters, since various molecular theories of

liquid state are based on thermodynamic considerations. Gopalrao and Jardar[1] formulated the equation a state for a square well fluid and obtained some thermodynamic parameters by extending the Florey's equation to mixture of unrelated type of molecules. Prigogine et al.[2] have shown that the excess parameters such as excess volume V^E gives interaction on the relative strengths of AA, AB and BB interactions in the mixture of A and B liquids.

The study of molecular interaction in liquids provides valuable information regarding internal structure, molecular association, complex formation, etc. Also many attempts have been made to study molecular interaction in pure and binary liquid mixtures[3-5]. The present work deals with the study of several useful parameters such as ultrasonic velocity, density, adiabatic compressibility (βs), apparent molar compressibility (φk) and specific acoustic impedance (Z) which reflects structural interaction by interferometer by 3-acetyl-4,6-dimethylcoumarin at different percentage of 1-propanol-water and 2-propanol-water solvent system at 300K, 303K and 307K are studied.

Experimental

The 3-acetyl-4, 6-dimethylcoumarin used for present ultrasonic measurements.1-Propanol, 2-propanol and distilled water used in analysis was purified[4]. Ultrasonic interferometer from Mittal Enterprises, Model M-81 with accuracy of ± 0.03% and frequency 1 MHz was used for the measurement of ultrasonic velocities of different solutions. The sound velocities of 3-acetyl-4,6-dimethylcoumarin measured at the same concentration (0.01M) in the different percentages of 1-propanol-water and 2-propanol-water mixture in the concentration of 70%, 75%, 80%, 85% and 90% at 300 K 303K and 307K.

The cell of ultrasonic interferometer was filled fully with the solution and the needle of ammeter was adjusted in the range of 20 to 60 with the help of "Adj" knob. It was warmed for 10 minutes so that the range should remain steady. Micrometer reading was noted. Screw was moved anticlockwise to get the maximum deflection of needle. Movement of screw was continued to get five deflections. After returning back of needle to original position, micrometer screw reading was noted. The difference between these two readings gave the distance travelled by the screw for getting five maxima. From this, distance required through which micrometer screw should move for one maxima was calculated just by dividing it by 5 and multiplying by 2. The same procedure was repeated many times.

RESULTS AND DISCUSSION

In present investigation, ultrasonic velocity and density of 3-acetyl-4,6-dimethylcoumarin have been studied at 0.01 M concentration at different concentrations (70%, 75%, 80%, 85% and 90%) in 100% 1-propanol and 2-propanol at 300K, 303K and 307K. From these values, adiabatic compressibility (β_s), apparent molar compressibility (ϕ_k) and specific acoustic impedance (Z) are calculated.

The value of these acoustic parameters has been used to discuss an important role in understanding the molecular interaction between the components of the mixtures and provides an insight into the physico-chemical properties of liquid mixtures. Such molecular association and dissociation as well as the strength of interaction between the components.

The values of acoustic parameters (β_s, ϕ_k and Z) in different percentage of 1-propanol-water and 2-propanol-water mixture at 300 K, 303K and 307K are presented in Table 1 and 6 and the graphs are shown in Fig. 1-18.

Acoustic Parameters at different percentages of 1-propanol-water mixture.

Table 1: System: 3-acetyl-4, 6-dimethylcoumarin Temp. = 300 K

Concentration: 0.01 M Ultrasonic Frequencies: 1 MHz

% 1-Propanol	V ($m.\ sec^{-1}$)	$d_s \times 10^3$ ($kg.m^{-3}$)	$\beta_s \times 10^{-7}$ (pa^{-1})	ϕ_k ($m^3\ mol^{-1}\ pa^{-1}$)	Z ($kg\ m^{-2}\ sec^{-1}$)
70	1351.333	0.8746	6.2616	-0.0344	1181.8469
75	1338.266	0.8671	6.4400	-0.0317	1160.3532
80	1307.542	0.8528	6.8591	-0.0255	1115.0360
85	1291.028	0.8457	7.0946	-0.0221	1091.7987
90	1274.857	0.8301	7.4128	-0.0167	1058.2114

Table 2: System: 3-acetyl-4, 6-dimethylcoumarin Temp. = 303 K

Concentration: 0.01 M Ultrasonic Frequency: 1 MHz

% 1-Propanol	V ($m.\ sec^{-1}$)	$d_s \times 10^3$ ($kg.m^{-3}$)	$\beta_s \times 10^{-7}$ (pa^{-1})	ϕ_k ($m^3\ mol^{-1}\ pa^{-1}$)	Z ($kg\ m^{-2}\ sec^{-1}$)
70	1411.800	0.8701	5.7661	-0.0513	1228.4071
75	1325.400	0.8601	6.6184	-0.0406	1139.9765
80	1283.714	0.8505	7.1350	-0.0336	1091.7868
85	1269.733	0.8413	7.3730	-0.0299	1068.1986
90	1256.457	0.8286	7.6453	-0.0252	1041.0530

Table 3: System: 3-acetyl-4, 6-dimethylcoumarin Temp. = 307 K

Concentration: 0.01 M Ultrasonic Frequency: 1 MHz

% 1-Propanol	V ($m.\ sec^{-1}$)	$d_s \times 10^3$ ($kg.m^{-3}$)	$\beta_s \times 10^{-7}$ (pa^{-1})	ϕ_k ($m^3\ mol^{-1}\ pa^{-1}$)	Z ($kg\ m^{-2}\ sec^{-1}$)
70	1334.200	0.8719	6.4430	-0.0426	1163.2889
75	1296.514	0.8646	6.8808	-0.0369	1120.9539
80	1283.200	0.8476	7.1650	-0.0319	1087.6403
85	1274.466	0.8397	7.3327	-0.0291	1070.1136
90	1242.742	0.8279	7.8214	-0.0219	1028.8313

Acoustic Parameters at different percentages of 2-propanol-water mixture.

Table 4: System: 3-acetyl-4, 6-dimethylcoumarin Temp. = 300 K

Concentration: 0.01 M Ultrasonic Frequency: 1 MHz

% 2-Propanol	V ($m.\ sec^{-1}$)	$d_s \times 10^3$ ($kg.m^{-3}$)	$\beta_s \times 10^{-7}$ (pa^{-1})	ϕ_k ($m^3\ mol^{-1}\ pa^{-1}$)	Z ($kg\ m^{-2}\ sec^{-1}$)
70	1352.933	0.9014	6.0610	-0.0487	1219.5040
75	1350.933	0.8796	6.2297	-0.0451	1188.2516
80	1340.857	0.8657	6.4254	-0.0417	1160.7305
85	1290.400	0.8512	7.0553	-0.0330	1098.3884
90	1246.000	0.8335	7.7278	-0.0231	1038.5410

Table 5: System: 3-acetyl-4, 6-dimethylcoumarin Temp. = 303 K

Concentration: 0.01 M Ultrasonic Frequency: 1 MHz

% 2-Propanol	V (m. sec^{-1})	$d_s \times 10^3$ ($kg.m^{-3}$)	$\beta_s \times 10^{-7}$ (pa^{-1})	ϕ_k ($m^3 mol^{-1} pa^{-1}$)	Z ($kg\ m^{-2}\ sec^{-1}$)
70	1380.400	0.8862	5.9218	-0.0627	1223.3104
75	1336.733	0.8733	6.4086	-0.0561	1167.3401
80	1300.733	0.8539	6.9221	-0.0484	1109.8873
85	1244.971	0.8413	7.6697	-0.0383	1047.3343
90	1230.514	0.8227	8.0277	-0.0319	1012.3323

Table 6: System: 3-acetyl-4, 6-dimethylcoumarin Temp. = 307K

Concentration: 0.01 M Ultrasonic Frequency: 1 MHz

% 2-Propanol	V (m. sec^{-1})	$d_s \times 10^3$ ($kg.m^{-3}$)	$\beta_s \times 10^{-7}$ (pa^{-1})	ϕ_k ($m^3 mol^{-1} pa^{-1}$)	Z ($kg\ m^{-2}\ sec^{-1}$)
70	1388.666	0.8740	5.9338	-0.0642	1213.6364
75	1339.333	0.8617	6.4697	-0.0570	1154.0748
80	1263.485	0.8445	7.4185	-0.0442	1066.9413
85	1253.142	0.8295	7.6773	-0.0395	1039.4464
90	1179.428	0.8129	8.8438	-0.0232	958.7342

Adiabatic Compressibility (β_s): Adiabatic compressibility shows a strong correlation with hydrational behaviour of the solute molecule and appears to be sensitive to the structural features of the solute, such as shape, size, branching and presence of aromatic ring. It is argued that these aspects are important in terms of considering the geometrical fit of the solute into the ordered form of the aqueous solvent surrounding these solutes.[6]

From Table 1-6 and Fig. 1-6 it can be noted that the β_s values in 1-propanol medium are considerably and notably smaller than in 2-propanol medium. This may due to nature of solvent of 2-propanol at different temperature. It is also observed that the values of adiabatic compressibility of 3-acetyl-4, 6-dimethylcoumarin is increases with increase in percentage of organic solvent. As the percentage of organic solvent increases, it decreases the number of free ions due to aggregation of solvent molecules around the ions[7] showing the occurrence of ionic association due to strong ion-ion interaction. It may also be due to departure of solvent molecules around the ions. It can also be noted that in both the medium i.e. 1-propanol and 2-propanol the

values of all ligands increases with increase in temperature.

Fig. 1
Plot between % 1-Propanol Vs β_s
Temp. 300 K

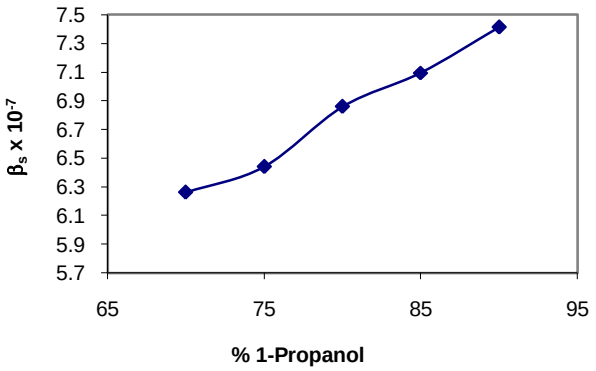


Fig. 2
Plot between % 1-Propanol Vs β_s
Temp. 303 K

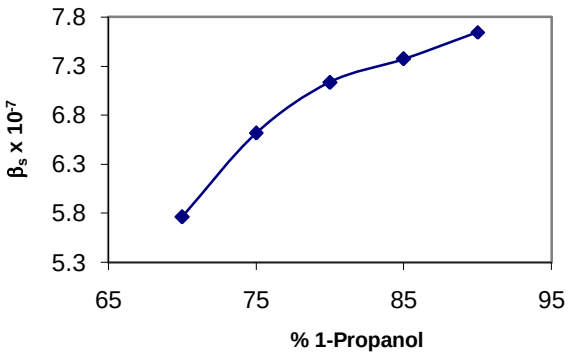


Fig. 3
Plot between % 1-Propanol Vs β_s
Temp. 307 K

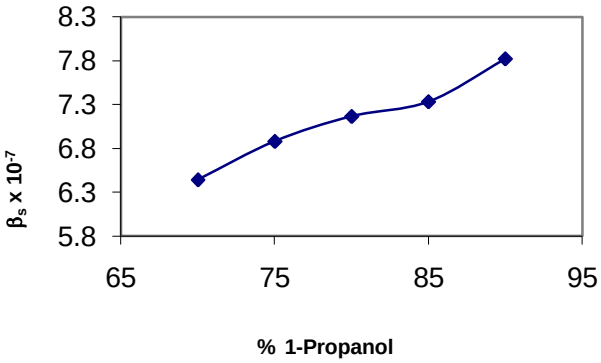


Fig. 4
Plot between % 2-Propanol Vs β_s
Temp. 300 K

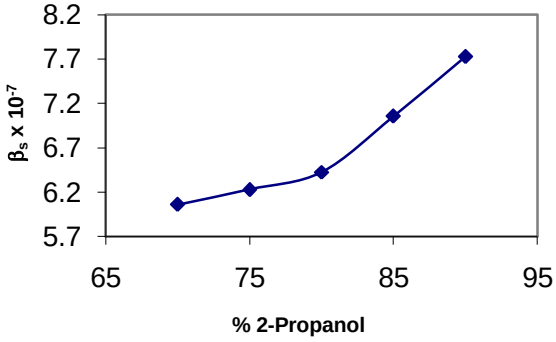


Fig. 5
Plot between % 2-Propanol Vs β_s
Temp. 303 K

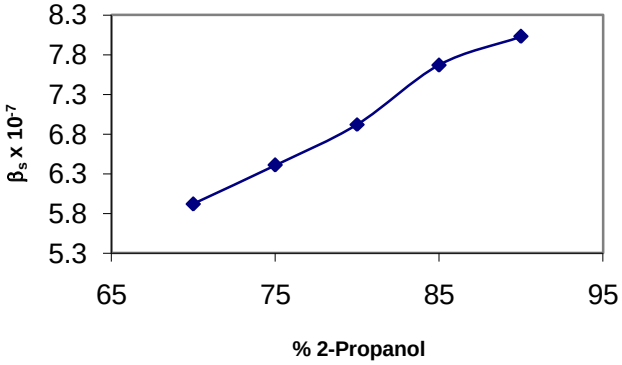
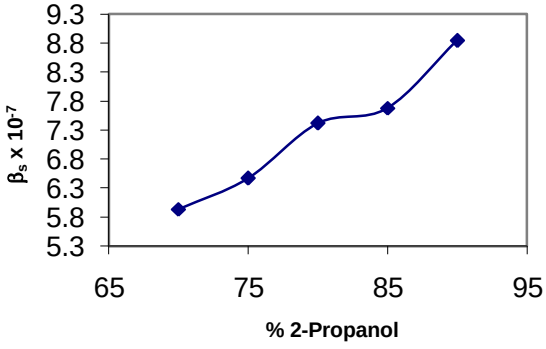


Fig. 6
Plot between % 2-Propanol Vs β_s
Temp. 307 K



Apparent Molar Compressibility (ϕ_k): Like adiabatic compressibility (β_s) apparent molar compressibility (ϕ_k) is another important acoustic parameter, which explains the solute-solvent and solute-solute interactions in solutions. Thus, the structure of solute and the number of atoms present in it will have direct effect on ϕ_k values.

From Table 1-6 and Fig. 7-12, it is observed that ϕ_k values of 3-acetyl-4, 6-dimethylcoumarin increases with increase in the percentage of 1-propanol solvent. Similar results are observed in 2-propanol medium at 300K, 303K and 307K. It could be observed that the ϕ_k values are negative. Negative values of ϕ_k shows that interactions are insensitive to solvent. It could be also explained by postulating the polar –OH groups interact with the surrounding organic solvent through dipole-dipole interaction in such a way that the surrounding solvent molecule looses its own compressibility to a certain extent.

The ϕ_k values of 2-propanol are lower than 1-propanol solvent. This appears to be reverse trend than which is observed for β_s. The adiabatic compressibility may just explain the simple association or close packing or clinging of molecules. But on the contrary, apparent molar compressibility is a property with difference, which may explain the molecular interactions like structure making and structure breaking nature of solute.

Fig. 7
Plot between % 1-Propanol Vs ϕ_k
Temp. 300 K

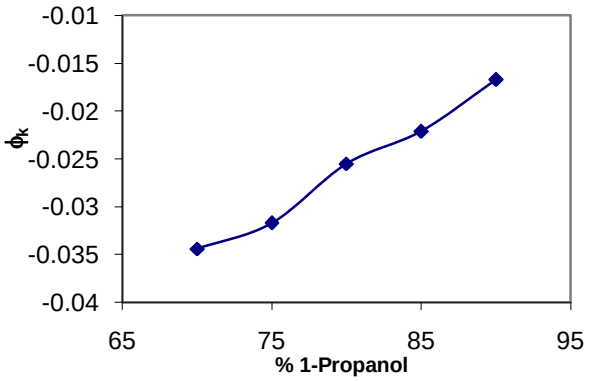


Fig. 8
Plot between % 1-Propanol Vs ϕ_k
Temp. 303 K

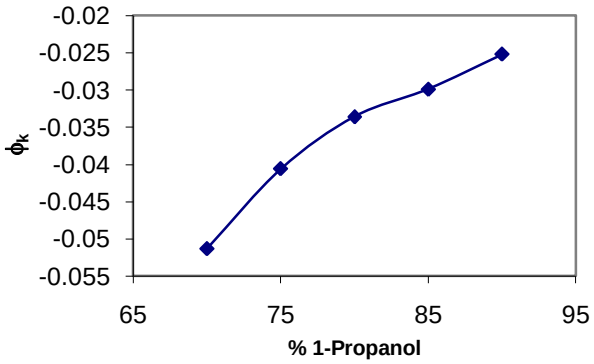


Fig. 9
Plot between % 1-Propanol Vs ϕ_k
Temp. 307 K

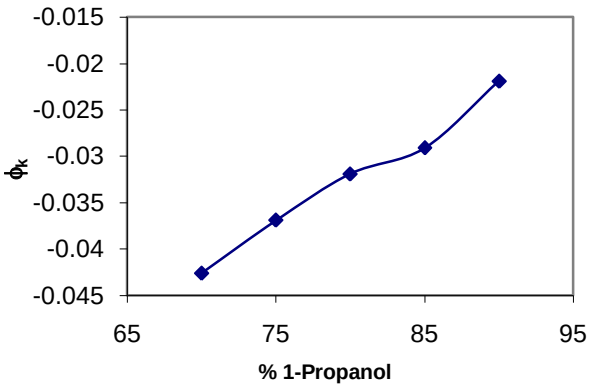


Fig. 10
Plot between % 2-Propanol Vs ϕ_k
Temp. 300 K

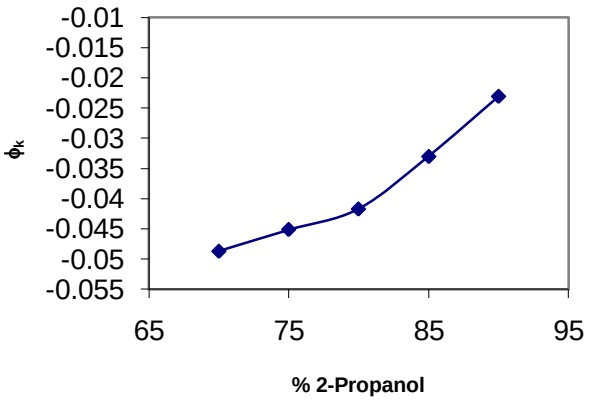


Fig. 11
Plot between % 2-Propanol Vs ϕ_k
Temp. 303 K

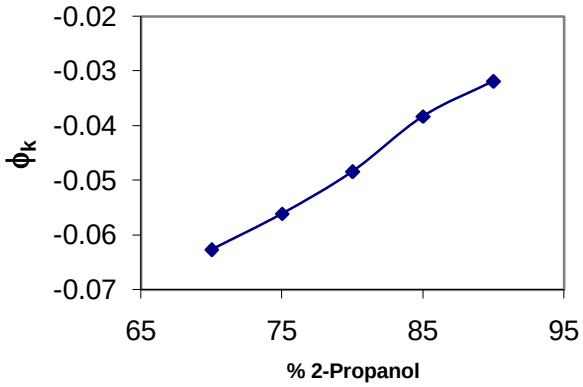
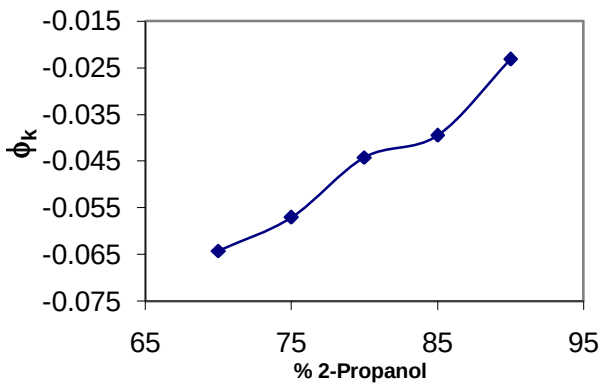


Fig. 12
Plot between % 2-Propanol Vs ϕ_k
Temp. 307 K



Specific Acoustic Impedance (Z): Literature survey shows that the impedance approach to explain the molecular interactions in liquid mixtures has been rather less commonly employed. This is one of the reasons why the impedance approach has been adopted here, to examine the behaviour of the solutions regarding molecular interactions. The mathematical relation for specific acoustic impedance Z = V.d and adiabatic compressibility $\beta = 1/V^2.d$ shows that their behaviour is opposite

The values of specific acoustic impedance (Z) of 3-acetyl-4, 6-dimethylcoumarin is decreases with increase in percentage of 1-propanol and 2-propanol at different temperature (Fig. 13-18). It is also observed that the Z values of 3-acetyl-4, 6-dimethylcoumarin at 300 K, 303 K

and 307 K in 2-propanol solvents are higher than in 1-propanol solvent. This can happen only when the effective particle velocity increases, this means that dispersion forces should be active in mixtures, a result anticipated in the absence of any specific interactions such as hydrogen bonding etc. On the contrary, the Z values in 1-propanol are lower indicating hydrogen bonding.

Fig. 13
Plot between % 1-Propanol Vs Z
Temp. 300 K

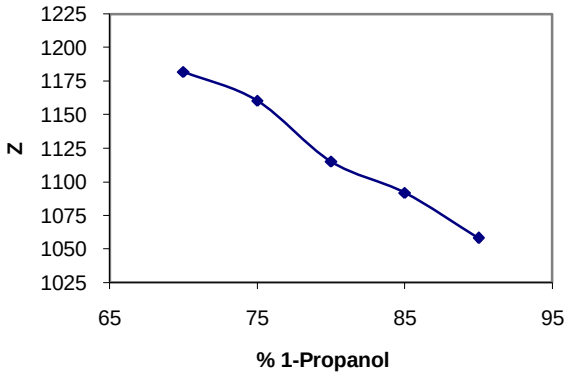


Fig. 14
Plot between % 1-Propanol Vs Z
Temp. 303 K

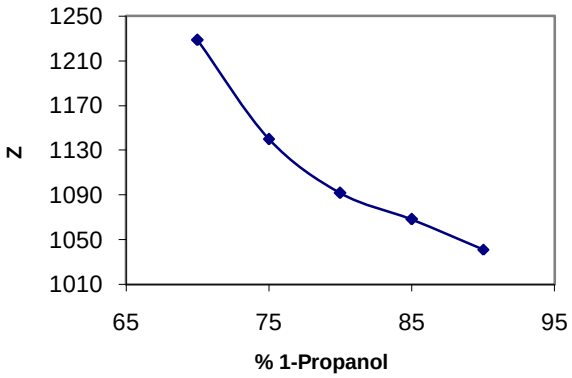


Fig. 15
Plot between % 1-Propanol Vs Z
Temp. 307 K

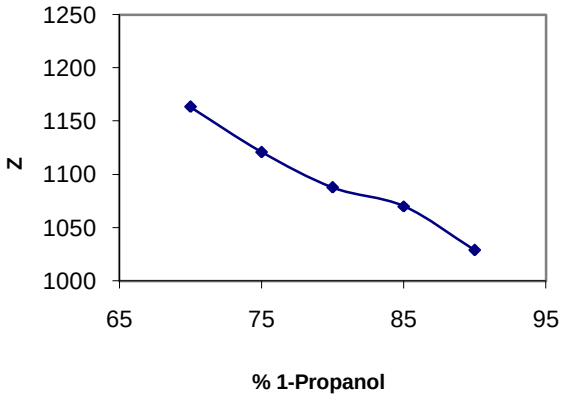


Fig. 16
Plot between % 2-Propanol Vs Z
Temp. 300 K

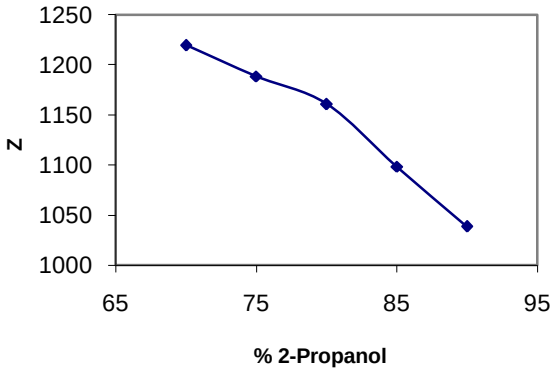


Fig. 17
Plot between % 2-Propanol Vs Z
Temp. 303 K

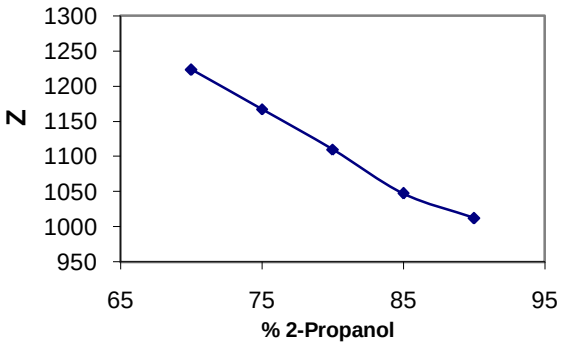
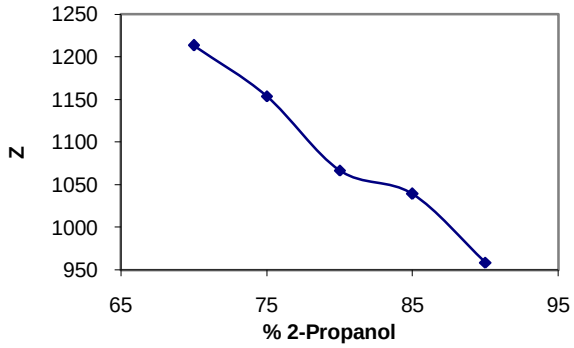


Fig. 18
Plot between % 2-Propanol Vs Z
Temp. 307 K



CONCLUSION

The present studies investigated that with increasing the concentration of 1-propanol and 2-propanol β_s and ϕ_k increases while Z decreases at 300 k, 303K and 307K by taking constant concentration of 3-acetyl-4, 6-dimethylcoumarin (0.01M). From this study it is clear that properties, which are directly or indirectly responsible for this are protic nature of solvent, dielectric constant, polarity, density, tendency of forming hydrogen bonding, surface tension, viscosity of solvent etc.

REFERENCES

[1] Gopalrao R.V. and Jardar R.N., Ind. J. Pure & Appl. Phys., **26**, (1988), 340.

[2] Prigogine I., Bellemans A. and Englertchowless, J. Chem. Phys., **24**, (1956), 518.

[3] Grace Sahaya Sheba S. and Omegala Priakumari R., International Journal of Physical, Nuclear Science and Engineering, 8(2), (2014).

[4] Chandra Sekhar G., Lee Ming-Jer and Lin Ho-Mu, Int. J. Res. Chem. Environ., 4(2), (2014), 126-129.

[5] Rajavelu S., International Journal of Science and Research, 3(4), (2014), 845-848.

[6] Mohammad Iqbal and Verrall R.Z. Can. J. Chem., **67**, (1989), 727-735.

[7] Pandey J.D., Shukla A., Rai D.D. and Mishra K.J. J. Chem. Eng. Data, 34, (1989), 29.