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Interferometric Studies of 4-Methyl-7-Hydroxycoumarin in Binary Mixture of Water with 1-Propanol and 2-Propanol

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Abstract

Ultrasonic velocity and density measurement at different concentrations of 4-methyl-7-hydroxycoumarin were carried out in the mixture of water with the solvents 1-propanol and 2-propanol for investigating solute-solvent interactions. The data obtained during the study is used for determining the most significant acoustic parameters like adiabatic compressibility (βs), apparent molar compressibility (□$_k$) and specific acoustic impendence (Z). These parameters have been used to explore the interactions between 4-methyl-7-hydroxycoumarin in different compositions of water-1-propanol and water-2-propanol system at 300K.

Key words: 4-Methyl-7-hydroxycoumarin, 1-Propanol, 2-Propanol.

Introduction

Among naturally occurring heterocyclic compounds, oxygen heterocycles are mostly abundant, importance and interest to various scientists from interdisciplinary fields. Coumarin is the heterocyclic compound containing oxygen as hetero atom. Coumarin and substituted coumarin compounds have their own identity in heterocyclic compound due to its various applications. Mixture containing oxygenated compounds such as coumarin and alkanols (-OH) group are of great importance from a practical point of view due to their increasingly use of additive to gasoline owing to their octane-enhancing and pollution reducing properties. The study of density, viscosity and ultrasonic velocity measurements of coumarin and substituted coumarin are useful in describing the importance, applicability in the field of medicine, industry and analytical chemistry. 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. Also many attempts have been made to study molecular interaction in pure and binary liquid mixtures[1-3]

The present work deals with the study of acoustic parameters i.e. ultrasonic velocity, density, adiabatic compressibility (β_s), apparent molar compressibility (ϕ_k) and specific acoustic impedance (Z) which

reflects structural interaction by interferometer by 4-methyl-7-hydroxycoumarin at different percentage of 1-propanol-water and 2-propanol-water solvent system at 300K are studied.

Experimental

The 4-methyl-7-hydroxycoumarin 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 4-methyl-7-hydroxycoumarin 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.

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 4-methyl-7-hydroxycoumarin 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 300 K. From these values, adiabatic compressibility (β_s), apparent molar compressibility (ϕ_k) and specific acoustic impedance (Z) are calculated.

The values of these acoustic parameters have been used to discuss the interactions of unlike molecule of solvents in presence of solute. These acoustic parameters directly reflect the structural interaction of solvent (water and organic solvent) with solute and explore important and valuable information regarding internal structure, molecular association, internal pressure, complex formation and stability of complexes. Weak molecular interaction can also be detected by this technique. 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 are presented in Table 1 and 2 and the graphs are shown in Fig. 1-6.

Adiabatic Compressibility (βs):

Adiabatic compressibility is one of the important properties during the study of solute-solvent interactions. It may just explain the simple association or closed packing or clinging of molecules. From Table 1 and 2 and Fig. 1 and 2 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.

It is also observed that the values of adiabatic compressibility of 4-methyl-7-hydroxycoumarin 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[5] 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.

Table 1: Acoustic Parameters at different percentages of 1-propanol-water mixture.
System: 4-methyl-7-hydroxycoumarin Temp. = 300 K
Concentration: 0.01 M Ultrasonic Frequencies: 1 MHz

% 1-Propanol	V (m. sec^{-1})	ds x 10^3 ($kg.m^{-3}$)	βs x 10^{-7} (pa^{-1})	ϕ_k (m^3 mol^{-1} pa^{-1})	Z (kg m^{-2} sec^{-1})
70	1364.733	0.8767	6.1245	-0.0362	1196.4324
75	1338.133	0.8639	6.4648	-0.0312	1155.9845
80	1302.666	0.8502	6.9319	-0.0245	1107.4705
85	1294.514	0.8462	7.0521	-0.0227	1095.4059
90	1271.885	0.8303	7.4460	-0.0163	1055.9755

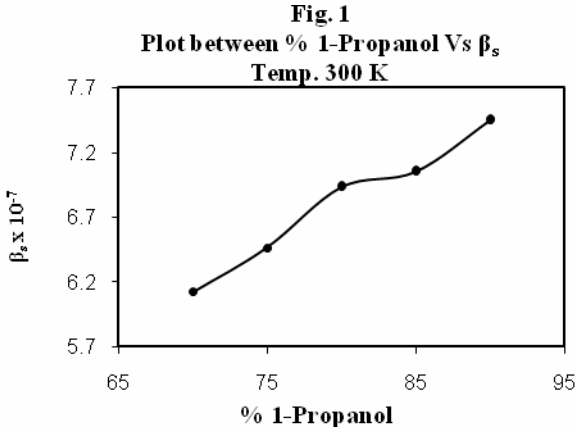
Table 2: Acoustic Parameters at different percentages of 2-propanol-water mixture.
System: 4-methyl-7-hydroxycoumarin Temp. = 300 K
Concentration: 0.01 M Ultrasonic Frequency: 1 MHz

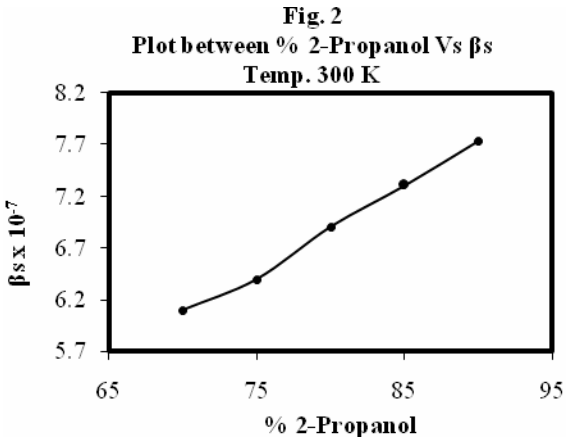
% 2-Propanol	V (m. sec^{-1})	ds x 10^3 ($kg.m^{-3}$)	βs x 10^{-7} (pa^{-1})	ϕ_k (m^3 mol^{-1} pa^{-1})	Z (kg m^{-2} sec^{-1})
70	1365.266	0.8798	6.0985	-0.0466	1201.1029
75	1336.200	0.8757	6.3959	-0.0429	1170.1103
80	1299.828	0.8574	6.9034	-0.0354	1114.4485
85	1273.600	0.8438	7.3062	-0.0293	1074.6636
90	1245.200	0.8333	7.7396	-0.0230	1037.6251

Apparent Molar Compressibility (ϕk): Like adiabatic compressibility (βs) apparent molar compressibility (ϕk) 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 ϕk values.

From Table 1 and 2 and Fig. 3 and 4, it is observed that ϕk values increases with increase in the percentage of 1-propanol and 2-propanol medium at 300K. It could be observed that the ϕk values are negative. A negative compressibility is an indication of strong heteromolecular interaction in the liquid

mixtures which is attributed to charge transfer, dipole-dipole interactions, dipole induced dipole interactions and hydrogen bonding between unlike components.6

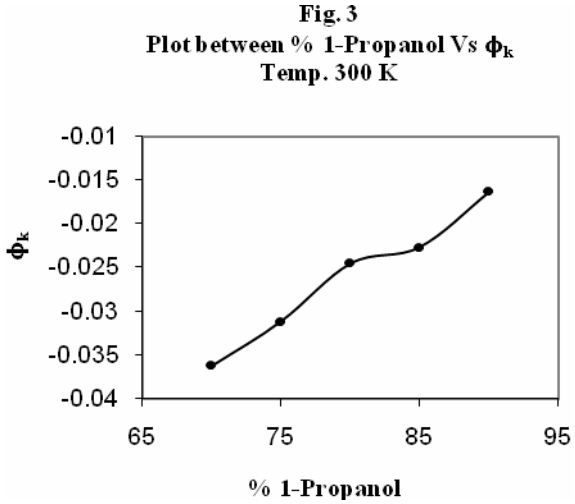


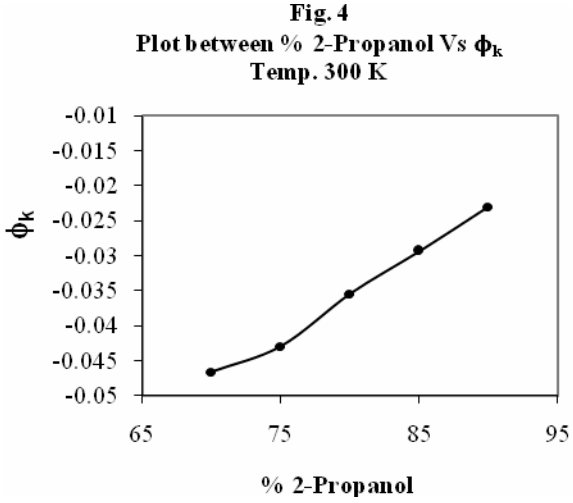


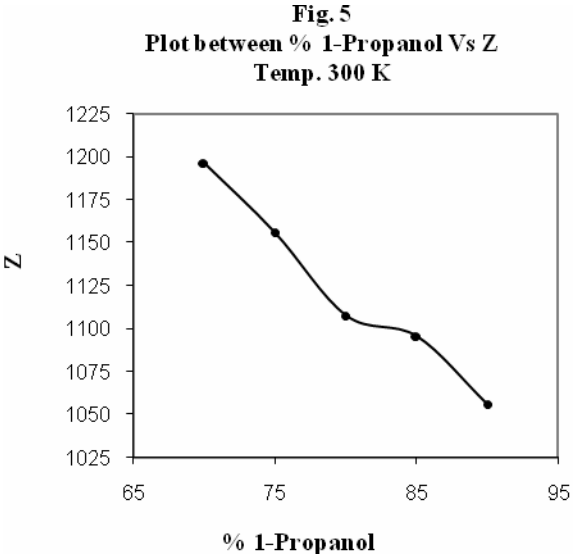
The ϕ_k values of 2-propanol are lower than 1-propanol solvent. This appears to be reverse trend than which is observed for β_s. Here the difference between the two properties can be clearly seen. The adiabatic compressibility may just explain the simple association or close packing or clinging of molecules. 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. Apparent molar compressibility property fairly sensitive to structural changes especially like water/ethanol and is hence expected to throw interesting light.[7]

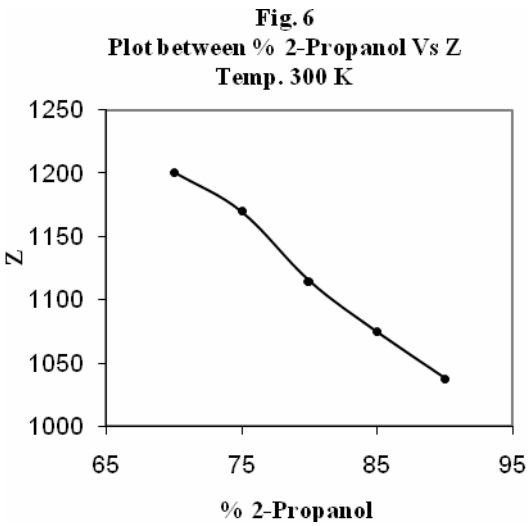
From the difference in the trends in two compressibilities, adiabatic and apparent molar, it may be predicted that adiabatic compressibility can detect gross changes in interaction but minute changes due to change in structure may only be noticed by apparent molar compressibility.

Specific Acoustic Impedance (Z): Specific acoustic impedance also makes the contribution in explaining molecular interactions. The values of specific acoustic impedance (Z) of 4-methyl-7-hydroxycoumarin are decreases with increase in percentage of 1-propanol and 2-propanol at 300 K (Fig. 5 and 6). It is also observed that the Z values of 4-methyl-7-hydroxycoumarin at 300 K in 2-propanol solvents are higher than in 1-propanol solvent. This can happen only when the effective particle velocity increases, this turn 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 interactions such as hydrogen bonding etc









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 by taking constant concentration of 4-methyl-7-hydroxycoumarin (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.

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