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Molecular interaction parameters of binary mixtures of acrylonitrile in polar and non-polar liquids at 298K

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ABSTRACT

The ultrasonic velocity, density and viscosity at 298K have been measured in the binary systems of acrylonitrile with acetone and 1, 4-Dioxane. From the experimental data, various acoustical parameters such as adiabatic compressibility (β_a), intermolecular free length (L_f), free volume (V_f) and internal pressure (Π_i) were calculated. It has been observed that, weak dispersive type intermolecular interactions are confirmed in the systems investigated. Dipole inducement is found to be more predominant in acetone system. The results are interpreted in terms of molecular interaction between the components of the mixtures.

Keywords: Ultrasonic velocity, Acoustical properties, Molecular interactions, Acrylonitrile, Acetone, 1, 4-Dioxane and binary liquid mixtures.

INTRODUCTION

Many approaches and spectroscopic techniques such as X-ray crystallography, chromatography, NMR, EPR, vibration and Raman spectroscopy, neutron & light scattering, circular dichroism (CD), IR and ultrasonic velocity measurements are used to determine the structure - function relationship of biomolecules. Among these techniques, ultrasonic velocity measurements have been found to be most powerful tool in the investigation of structure, the thermodynamic properties and predict the intermolecular interactions in pure liquid [1], liquid mixtures [2-5] and ionic interactions in electrolytic solutions [6, 7]. Though the molecular interactions studies can be best carried out through spectroscopic methods [8, 9] the other non spectroscopic techniques such as dielectric, magnetic, [10-11] Ultrasonic velocity and viscosity [12-18] measurements have been widely used in field of interactions and structural aspect evaluations studies. In the present work an attempt has been made to investigate the behavior of binary solutions of acetone and 1, 4-Dioxane in acrylonitrile with regard to adiabatic compressibility, intermolecular free length, free volume and internal pressure from ultrasonic measurements at 298K. The results are interpreted in terms of molecular interaction between the components of the mixtures.

MATERIALS AND METHODS

Solutions of different concentrations were prepared for each binary system. The ultrasonic velocity (*U*) in liquid mixtures which prepared by taking purified AR grade samples, have been measured at 298K using an ultrasonic interferometer (Mittal type, Model F-81) working at 2 MHz frequency. The accuracy of sound velocity was ±0.1 ms^{-}

[1]. An electronically digital operated constant temperature water bath has been used to circulate water through the double walled measuring cell made up of steel containing the experimental solution at the desire temperature. The density of pure liquids and liquid mixtures was determined using pycknometer by relative measurement method with an accuracy of ±0.1Kgm^{-3}. An Ostwald's viscometer was used for the viscosity measurement of pure liquids and liquid mixtures with an accuracy of ±0.0001NSm^{-2}. The temperature around the viscometer and pycknometer was maintained within ±0.1K in an electronically operated constant temperature water bath. All the precautions were taken to minimize the possible experimental error.

RESULTS AND DISCUSSION

Using the experimental data of ultrasonic sound velocity, density and viscosity, various acoustical parameters such as adiabatic compressibility, free length, free volume and internal pressure, were calculated by the following equations (1-4).

$\beta_a = (U^2 \rho)^{-1}$ ….. (1)
$L_f = K_T \beta a^{1/2}$ ….. (2)
$V_f = (M_{eff}\ U/\eta K)^{3/2}$ ….. (3)
$Ji = bRT(K\eta/U)^{1/2}(\rho^{2/3}/M_{eff}^{7/6})$ ….. (4)

Where, K_T is the temperature dependent constant having a value $205.8336*10^{-8}$ in MKS system at temperature 298 K, K is constant equal to $4.28*10^9$ in MKS system, b is a cubical packing fraction taken as 2 for all the liquids, R is the Universal gas constant, T is the experimental temperature, $M_{eff} = \Sigma\ x_i m_i$, where x_i is the mole fraction and m_i is the molecular weight of the component.

The measured parameters *viz*., ultrasonic velocity (U), density (ρ) and viscosity (η) for the **system-I: Acrylonitrile**+ **Acetone** and **system-II: Acrylonitrile+ 1,4-dioxane** at temperature 298K are given in Table-1. Table-2 shows, calculated parameters such as adiabatic compressibility (β_a), intermolecular free length (L_f), free volume (V_f) and internal pressure (JI_i) for the **system-I: Acrylonitrile**+ **Acetone** and **system-II: Acrylonitrile+ 1, 4-dioxane** at temperature 298K. Table-1 shows that, in both the system-I and system-II, velocity increases with concentration of **A**crylonitrile in acetone and 1, 4- Dioxane. This indicates that strong interaction observed at higher concentrations of x. The density values also have the same trend with velocity in the system-I and reverse trend in system-II. Viscosity increases in system-I and decreases in system-II, suggesting thereby more association between solute and solvent molecules. It is observed that for a given concentration as the number of CH- group or chain length increases, the sound velocity increases.

From the Table-2 it is observed that, the adiabatic compressibility and free length decreases with increase of mole fraction of the solute in system I and increases in system II. This may lead to the presence of specific molecular interaction between the molecules of the liquid mixture. The adiabatic compressibility and free length are the deciding factors of the ultrasonic velocity in liquid systems. Decrease in intermolecular free length in system I leads to positive deviation in sound velocity and negative deviation in compressibility. This indicates that the molecules are nearer in the system.

The internal pressure and free volume increases with increasing mole fraction of the solute in system-I and decreases in system-II. The internal pressure may give information regarding the nature and strength of forces existing between the molecules. The decrease in free volume in system-II shows that the strength of interaction decreases gradually with the increase in solute concentration. It represents that there is weak interaction between the solute and solvent molecules.

The free volume is the space available for the molecule to move in an imaginary unit cell. This reduces internal pressure. The variations in internal pressure are given in the same Table-2. As stated above the internal pressure (JI_i) decreases with increase in concentration of Acrylonitrile in the systems-II. Same trend, as expected, is seen in the free volume changes in the systems-II. The observed decreases values of V_f in system II are due to close association between solute and solvent. Thus, a progressive decrease in free volume and internal pressure in Acrylonitrile +1, 4-dioxane mixtures clearly indicates the existence of ion-solvent interaction, due to which the structural arrangement is considerably affected.

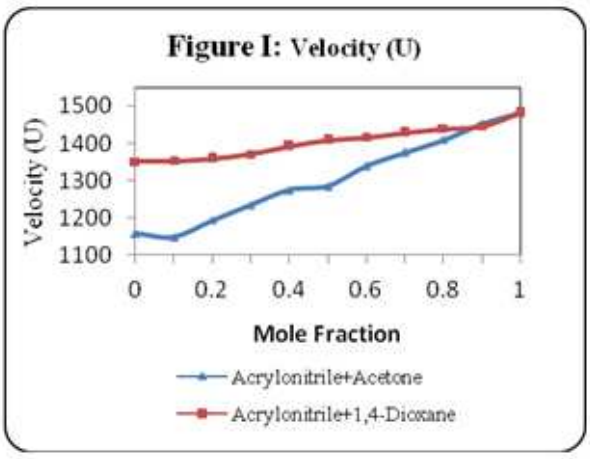
The variations of Velocity (U), Density (ρ), Viscosity (η), Adiabatic compressibility (β_a), Intermolecular free length (L_f), and free volume (V_f) with respect to compositions (x) of Acrylonitrile+ Acetone & Acrylonitrile+ 1,4-dioxane binary systems are shown in Fig.: 1(A), 1(B), 1(C), 1(D), 1(E), and 1(F) respectively.

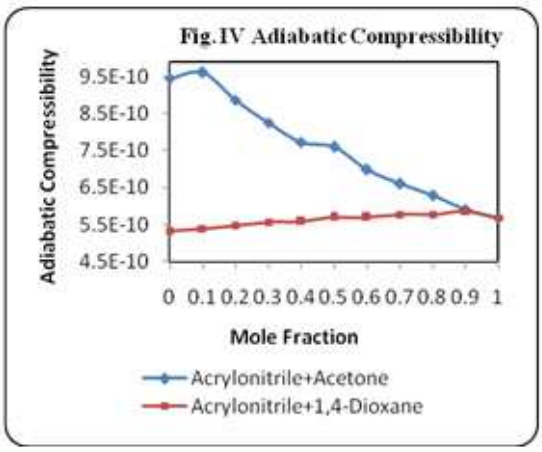
Table: 1 - Velocity (U), Density (ρ) and Viscosity (η) of Acrylonitrile+ Acetone & Acrylonitrile+ 1, 4-dioxane at 298K.

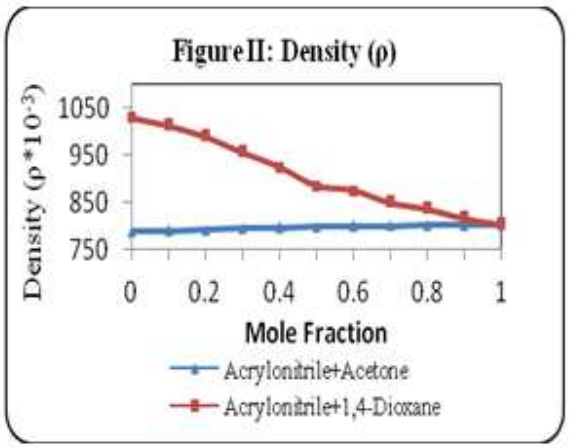
X	U (m/s)		ρ*10^{-3} (kg/m^{-3})		η*10^{-3} (Ns/m^2)	
	Acetone	1, 4-dioxane	Acetone	1, 4-dioxane	Acetone	1, 4-dioxane
0.0	1158.57	1350.00	788.00	1030.00	0.3642	0.500
0.1	1148.00	1338.66	789.23	1012.38	0.3651	0.484
0.2	1193.66	1358.66	791.14	989.27	0.3659	0.477
0.3	1235.00	1370.00	794.10	956.00	0.3662	0.448
0.4	1274.66	1392.00	796.16	925.16	0.3669	0.445
0.5	1284.57	1408.00	798.10	885.10	0.3673	0.431
0.6	1338.66	1416.00	799.23	875.66	0.3679	0.421
0.7	1375.33	1428.00	800.10	849.19	0.3688	0.407
0.8	1408.85	1439.10	801.10	835.78	0.3697	0.395
0.9	1452.00	1446.00	801.96	815.96	0.3705	0.382
1.0	1481.00	1481.00	803.00	803.00	0.3715	0.371

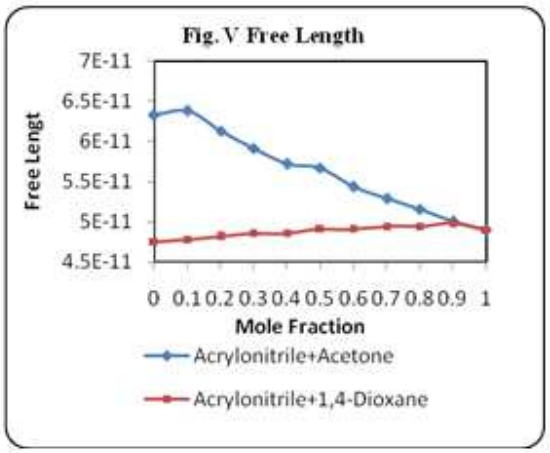
Table 2: Adiabatic compressibility (β_a), free length (L_f), free volume (V_f) and internal pressure (Ji) of system-I and system-II at 298K.

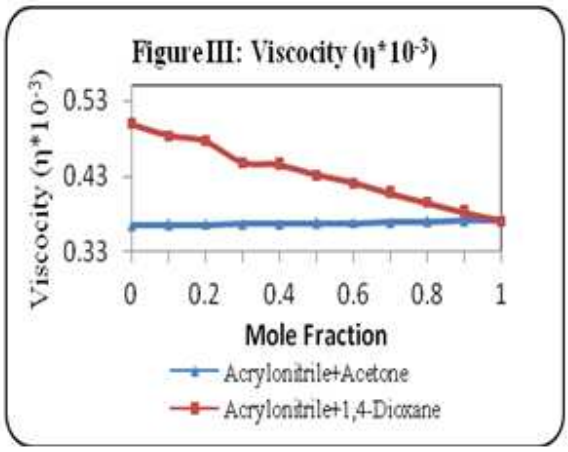
X	β_a *10^{-10} (Pa^{-1})		L_f *10^{-10} (m)		V_f*10^{-7} (m^{3}mol^{-1})		Ji *10^8 (P_a)	
	Acetone	1,4-Dioxane	Acetone	1, 4-dioxane	Acetone	1,4-Dioxane	Acetone	1, 4-dioxane
0.0	9.454	5.327	0.6329	0.4751	2.836	4.144	4.2903	3.4235
0.1	9.614	5.399	0.6382	0.4783	2.751	4.106	4.3638	3.4879
0.2	8.871	5.476	0.6131	0.4817	2.869	3.965	4.3352	3.5743
0.3	8.256	5.573	0.5914	0.4859	2.976	4.128	4.3187	3.5501
0.4	7.731	5.578	0.5723	0.4861	3.071	3.985	4.3070	3.6245
0.5	7.593	5.699	0.5672	0.4914	3.06	3.954	4.3450	3.6439
0.6	6.982	5.696	0.5439	0.4912	3.203	3.827	4.3092	3.7839
0.7	6.608	5.775	0.5291	0.4946	3.278	3.762	4.3054	3.8643
0.8	6.289	5.777	0.5162	0.4947	3.34	3.656	4.3088	4.0088
0.9	5.914	5.861	0.5006	0.4983	3.435	3.538	4.2984	4.1516
1.0	5.678	5.678	0.4905	0.4905	3.474	3.481	4.3127	4.3098











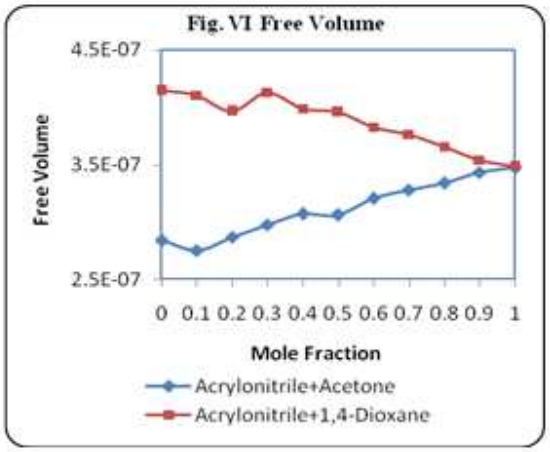


Fig.-I-VI : The variations of Velocity (U), Density (ρ), Viscosity (η), Adiabatic compressibility (β_a), free length (L_f), and free Volume (V_f) w. r. to compositions (x) of Acrylonitrile+ Acetone & Acrylonitrile+ 1, 4-dioxane at 298K are shown in Fig.: I, II, III, IV, V and VI respectively.

CONCLUSION

The ultrasonic velocity (U), density (ρ) and viscosity (η) and other related thermodynamic parameters such as adiabatic compressibility (β_a), intermolecular free length ($L_{f)}$ and free Volume (V_f) at various concentrations and at the temperature 298K for the binary mixture of 1 Acrylonitrile + Acetone & Acrylonitrile + 1, 4-dioxane were calculated. The observed increase of ultrasonic velocity indicates the solute-solvent interaction. The existence of type of molecular interaction in solute-solvent is favored in system I and II, confirmed from the U, ρ, η, βa, $L_{f,}$ and V_f data. The variation in ultrasonic velocity (U), density (ρ) and viscosity (η) and other related thermodynamic parameters is non-linear. Consequently ultrasonic velocity of system increases depending on concentration of Acrylonitrile. It is known that electrostriction leads to decrease in the compressibility of the solution. The non linear behavior confirms the presence of solute-solvent, solvent-solvent, and dipole-dipole interactions. For the observed molecular interaction, hydrogen bond formations are responsible for the heteromolecular interaction in the liquid mixture. This provides useful information about inter and intra molecular interactions of the mixture as existing in the liquid systems.

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