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Ultrasonic study of molecular interactions in binary mixtures of isopropylbenzene (Cumene) with Benzene, Toluene and Acetone at 303K

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Abstract

The ultrasonic velocity, density and viscosity at 303K have been measured in the binary systems of isopropylbenzene+Benzene, isopropylbenzene + Toluene and isopropyl benzene + Acetone. From the experimental data various acoustical parameters such as adiabatic compressibility (β), free volume(V_f), Shear relaxation time(τ), free length(L_f) and acoustical impedance (Z) ere calculate. The results are interpreted in terms of molecular interaction between the components of the mixtures.

Keywords: Ultrasonic velocity, acoustical properties, molecular interaction.

Introduction

The study of thermodynamic properties of binary liquid mixtures has proved to be a useful tool in elucidating the structural interactions components[1-10]. Many researchers have shown the important and fundamental role of the molecular details of the solvent species to determine the specific interactions which are responsible for macroscopic thermodynamic and other related properties in non-electrolyte solutions. When binary or more complex mixtures are used as solvent media, specific solvent-co solvent interactions can intervene to modify the structural properties and the molecular arrangement of the pure liquids. Thus, the knowledge of the structure of mixed solvent systems becomes an essential prerequisite to interpret and to understand the interaction patterns between ions, ions-pairs and ionic aggregates, and bulking solvent molecules. In principle, the interaction between the molecules can be established from a study of the characteristics abrupt departure from ideal behavior of some physical properties, like volume, compressibility, viscosity etc. Ultrasonic technique has been adequately employed to investigate the properties of any substance to understand the nature of molecular interactions in pure liquid[11], liquid mixtures[12-15] and ionic interactions in electrolytic solutions[16-17]. Though the molecular interactions studies can be best carried out through spectroscopic methods[18-19] the other non spectroscopic techniques such as dielectric10 magnetic11 ultrasonic velocity and viscosity[20-24] 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 isopropylbenzene (cumene) + benzene, isopropylbenzene (cumene) + toluene and isopropylbenzene (cumene) + acetone with regard to adiabatic compressibility, intermolecular free length and specific acoustic impedance from ultrasonic measurements at 303 K.

Material and Methods

Solutions of different molality (m) were prepared for each binary system. The ultrasonic velocity in the mixtures was measured using a variable path fixed frequency ultrasonic interferometer working at 2 MHz frequency (Mittal Enterprises, New Delhi). The accuracy of sound velocity was ±0.1 ms^{-1}. The density and viscosity of the mixture were measured using a specific gravity bottle (5 mL) and Ostwald's viscometer (10 mL) respectively. The accuracy in density measurement was ±0.0001 kg m^{-3} and that in viscosity measurement was ±0.001 $mNsm^{-2}$.

Results and Discussion

Various acoustical parameters such as adiabatic compressibility (β), Intermolecular free length (L_f), free volume (V_f), and specific acoustical impedance (Z), were calculated using the experimental data of ultrasonic sound velocity, density and viscosity by the following equations (1-4).

$$\beta = 1/U^2\rho \quad (1)$$

$$L_f = kT(\beta)^{1/2} \quad (2)$$

$$V_f = (M_{eff}U/\eta k)^{3/2} \quad (3)$$

$$Z = U\rho \quad (4)$$

Where kT is the temperature dependent constant having a value 199.53 x 10^{-8} in MKS system , k is the constant equal to 4.28 x 10^9 in MKS system, independent of temperature of all liquids, and all the notations having the usual meanings.

The measured parameters *viz*., ultrasonic velocity (U), density (p), adiabatic compressibility (β) and viscosity (η) are given in table -1 and table- 2. Tables-1,2 shows that, in all three systems, the velocity increases with concentration of benzene, toluene and acetone. This indicates that strong interaction observed at higher concentrations of X. The viscosity values also same trend with velocity in these three systems. Density decreases in all three systems suggesting thereby more

association between solute and solvent molecules in latter systems.

From the same table- 2, it is observed that adiabatic compressibility (β) increases with increase in concentration of benzene, toluene and acetone. This increase structural order of isopropyl benzene may result in more cohesion, and leads to a increase in (β). The increase in (β) results in an increase in the value of (U). The free length (L_f) is another parameter which is calculated using ultrasonic velocity and adiabatic compressibility. It is observed that L_f, increases with the concentration of benzene, toluene and acetone. It has been observed that intermolecular free length increases with mole fraction. Increase in intermolecular free length leads to positive deviation in sound velocity and negative deviation in compressibility. This indicates that the molecules are nearer in the system.

The computed other parameters like free volume (V_f) and shear's relaxation time(r) are given in table-3. The variation in free volume (V_f) decreases with increases in molality of benzene, toluene and acetone in all three systems. The free volume is the space available for the molecule to move in an imaginary unit cell. This increases shear's relaxation time (r). The variations in shear's relaxation time are given in the same table-3. As stated above the shear's relaxation time increases with increase in molality of benzene, toluene and acetone. The acoustic impedance (Z) is the product of ultrasonic velocity and density of the solution. The value of acoustic impedance also decreases with increase in concentration of benzene, toluene and acetone. Increase in L_f and decrease of Z with the concentration of benzene, toluene and acetone, suggest presence of solvent-solute interactions in three systems. The value of acoustic impedance (Z) is listed in table- 4.

Table -1
Values of ultrasonic velocity(U) and density(ρ) at 303K

Mole fraction of isopropylbenzene	Ultasonic velocity(U) m/sec.			Density(ρ) gm/mol		
(X)	Benzene	Toluene	Acetone	Benzene	Toluene	Acetone
0.0000	1261	1282	1138	0.8748	0.8448	0.7714
0.1623	1273	1305	1212	0.8756	0.8140	0.7480
0.3036	1285	1327	1260	0.8388	0.7829	0.7334
0.5376	1309	1347	1308	0.8028	0.7524	0.7182
0.7234	1333	1367	1332	0.7668	0.7213	0.7106
0.9401	1369	1376	1356	0.7128	0.7062	0.7030
1.0000	1381	1381	1381	0.6948	0.6948	0.6948

Table-2
Values of viscosity(η) and adiabatic compressibility(β) at 303K

Viscosity(η) $\eta \times 10^3/Nsm^{-2}$			Adiabatic compressibility(β) $\beta \times 10^{10}/m^2N^{-1}$		
Benzene	Toluene	Acetone	Benzene	Toluene	Acetone
0.5976	0.5394	0.2818	7.189	7.202	7.001
0.6991	0.7714	0.6826	7.247	7.252	7.056
0.8006	1.0034	0.9498	7.297	7.309	7.273
1.0036	1.2354	1.2147	7.381	7.376	7.357
1.2066	1.4674	1.3506	7.448	7.454	7.457
1.5111	1.5714	1.4842	7.525	7.498	7.515
1.6121	1.6126	1.6126	7.547	7.547	7.547

Table-3
Values of free volume(V_f) and shear's relaxation time(r) at 303K

Free Volume(V_f) $V_f \times 10^7/m^3mol^{-1}$			Shear's relaxation time(τ) ($\tau \times 10^{-11}$)		
Benzene	Toluene	Acetone	Benzene	Toluene	Acetone
2.3902	3.6587	4.0609	0.5700	0.518	0.3761
2.2332	3.3355	3.6532	0.6700	0.7419	0.8277
2.0966	2.9642	3.2722	0.7700	0.9704	1.0876
1.8704	2.5331	2.7451	0.9700	1.2066	1.3206
1.6907	2.0267	2.3990	1.1800	1.4516	1.4283
1.4812	1.7388	1.9683	1.5100	1.567	1.5309
1.4233	1.4233	1.4233	1.6200	1.6226	1.6226

Table-4
Values of free length(L_f) and acoustical impedance (Z) at 303K

Free length (L_f) (L_f x 10^{11}/m)			**Acoustic impedance(Z)** (**Kg/** $m^2.sec^{-1}$)		
Benzene	**Toluene**	**Acetone**	**Benzene**	**Toluene**	**Acetone**
5.831	5.899	5.976	1.1031	1.0830	0.8775
6.067	5.957	6.006	1.0907	1.0629	0.9073
6.146	6.019	6.016	1.0778	1.0389	0.9240
6.208	6.125	6.120	1.0508	1.0134	0.9394
6.265	6.224	6.225	1.0237	0.9861	0.9465
6.310	6.295	6.291	0.9758	0.9717	0.9532
6.370	6.371	6.371	0.9595	0.9598	0.9591

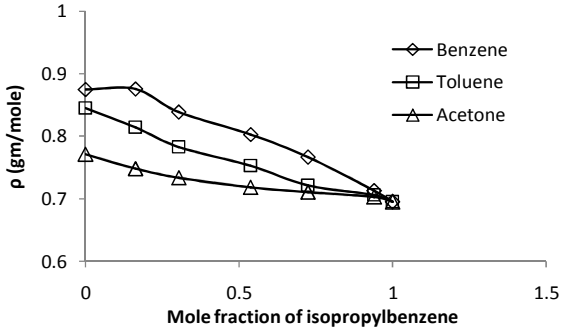

Figure-1:- Mole fraction versus density at 303K

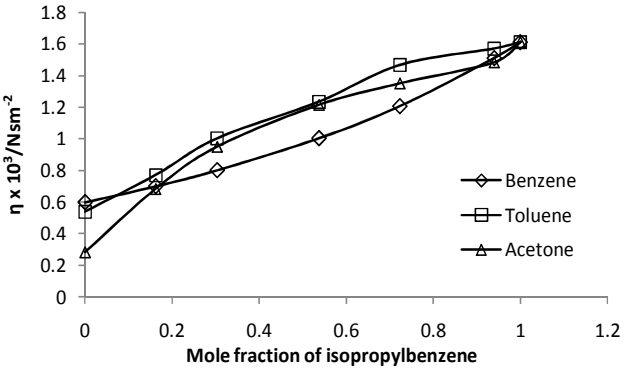

Figure-2:- Mole fraction versus viscosity at 303K

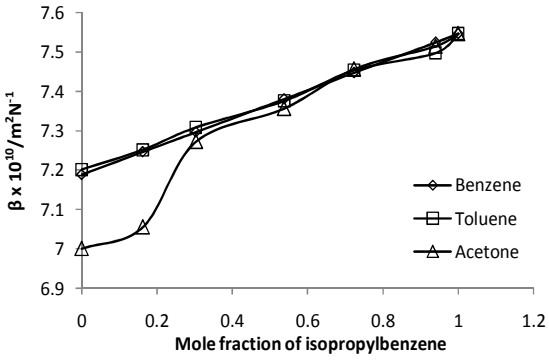

Figure-3:- Mole fraction versus Adiabatic compressibility at 303K

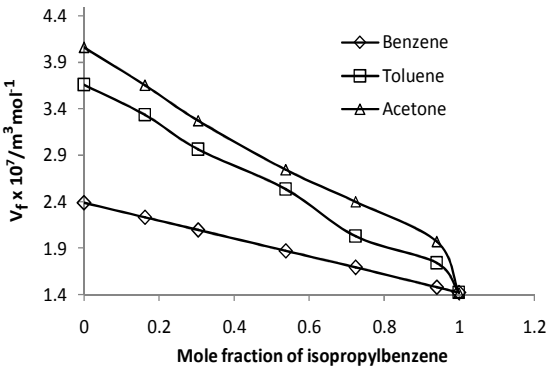

Figure-4:-Mole fraction versus free volume at 303K

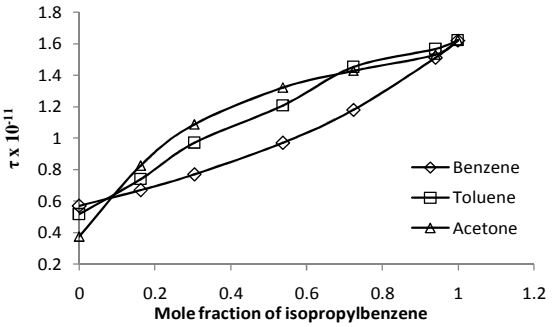

Figure-5:- Mole fraction versus Shear relaxation time at 303K

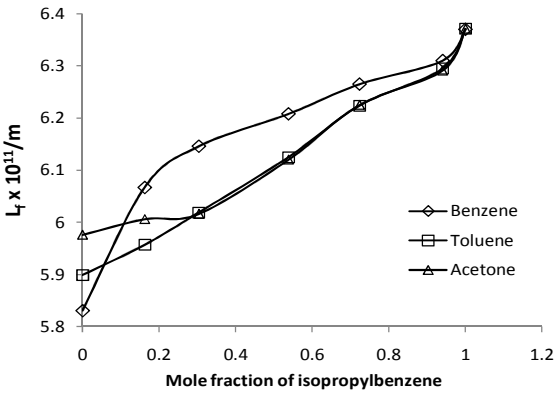

Figure- 6:- Mole fraction versus free length at 303K

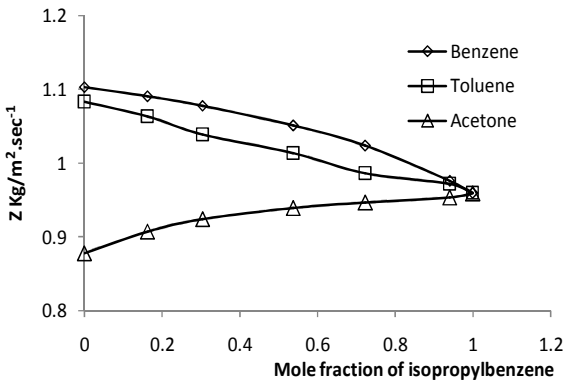

Figure- 7:- Mole fraction versus acoustic impedance at 303K

Conclusion

The ultrasonic velocity, density, viscosity and other related parameters were calculated. The observed increase of ultrasonic velocity indicates the solute-solvent interaction. The existence of type of molecular interaction is solute-solvent is favored in all these three systems, confirmed from the Z, U and η etc., the existence of solute-solvent interaction is in the order: Acetone >Toluene> Benzene.

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