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Molecular interaction in ternary liquid mixtures at different frequencies

[1]**Vivek Kumar Pandey**

[1]Department of Chemistry,DBS College, Kanpur, U.P (India)

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Abstract

The density, viscosity and ultrasonic velocity are measured in ternary mixtures of N,Ndimethylformamide, toluene and cyclohexane at different frequencies such as 1 MHz, 4 MHz, 6 MHz, and 8 MHz over the entire composition range. From these experimental values various parameters like adiabatic compressibility, free length, free volume, internal pressure, acoustic impedance etc have been evaluated. The different parameters were ploted against the mole fraction of N,N-Dimethylformamide over the whole composition range. The physical parameters were explained on the basis of intermolecular interaction present in the above mixture.

Key words: Ultrasonic velocity, toluene, free volume, acoustic impedance.

Introduction

The The ultrasonic study of liquids plays an important role in understanding the nature and strength of molecular interactions [1,2]. The variations of ultrasonic velocity and related parameters throw some light on the intermolecular interactions and the structural changes associated with the liquid mixtures having weakly interacting components as well as strongly interacting components. The variation of ultrasonic velocity and other acoustic parameters at different frequencies in binary and ternary liquid mixtures has been investigated by various authors [3-10].

In the present study, molecules of Cyclohexane are non-polar, molecules of toluene is polar in nature due to presence of electron releasing methyl group, where as that of N,N-dimethylformamide (DMF) is highly polar. N-N-Dimethyl formamide (DMF), as a polar solvent, is certainly to some extent associated by dipole-dipole interactions. Cyclohexane belongs to alicyclic hydrocarbon (closed chain). It is non-polar, unassociated, inert hydrocarbons and has globular structure. Toluene is aprotic in nature. It is used as an octane booster in fuel, as a solvent for manyorganic compounds, paints, cleaning of polymer surface and electronic materials.

2. Experimental,Materials&Methods

The mixtures of various concentrations in mole fraction were prepared by taking analytical reagent grade and spectroscopic reagent grade chemicals with minimum assay of 99.9% and obtained from E.Merck Ltd (India). All the component liquids were purified by the standard methods [11]. The density, viscosity, and ultrasonic velocity were measured as a function of concentration of the ternary liquid mixture at temperature T = 318K. Ultrasonic velocity was measured by using an ultrasonic interferometer (Model M-84, supplied by M/S Mittal Enterprises, New Delhi) with the accuracy of ±0.1m·s−1. The densities of the mixture were measured using a 10-ml specific gravity bottle by relative measurement method with an accuracy of ±0.01 kg·m−3. An Oswald viscometer (10 ml) with an accuracy of ±0.001 Ns·m−2 was used for the viscosity measurement. The flow time was determined using a digital racer stopwatch with an accuracy of ±0.1s.

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3. Theory

The following thermodynamic parameters were calculated:

(i) Adiabatic Compressibility : $\beta = 1/U2.\rho$

(ii) Intermolecular free length : $Lf = KT\ \beta 1/2$

(iii) Free Volume : $Vf = (Meff.U/K.\eta)3/2$

(iv) Internal Pressure:$\pi i = bRT\ (k\eta/U)1/2\ (\rho 2/3/M7/6)$

(v) Acoustic impedance : $Z = U.\rho$

(vi) Surface tension:$S = 6.3 \times 10\text{-}4.\ (\rho\ .U3/2)$

3. Results and Discussion

The experimental data relating to density, viscosity and velocity of liquid mixtures at 318 K for frequencies 1 MHz, 4 MHz, 6 MHz and 8 MHz are given in table-1..The calculated values of adiabatic compressibility(β), free length(Lf), free volume(Vf), internal pressure(πi), acoustic impedance(Z)and surface tension(S) are reported in table-2-3 and variation of some parameters with molefraction of DMF are shown in Figs.1-2.

It is observed form table-I that, density ρ of ternary mixture increases with the increase in mole fraction of DMF. The increase in density indicates the presence of solvent-solvent interactions in the ternary mixture which may bring a bonding between them. With increase in concentration of DMF, velocity increases which may be due to the structural changes occurring in the mixture resulting in increase of intermolecular forces.

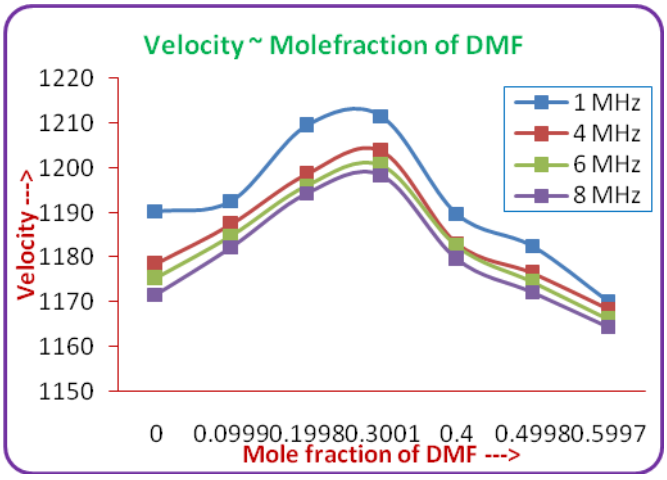

Fig1.Variation of velocity with molefraction of DMF

Adiabatic compressibility decreases with increasing concentration of DMF, which is in conformation with the above fact. Compressibility gives the ease with which a medium can be compressed. In this case the medium appears to be more compact. This is also confirmed by the decreasing trend of free length. Free volume is the average volume in which the centre of a molecule can move due to the repulsion of the surrounding molecules. When concentration of DMF increases and that of toluene

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decreases, ultrasonic velocity (U) increases and viscosity increases, but free volume decreases. This indicates increase in molecular attraction.

Internal pressure is a broader concept and is a measure of the totality of the forces (dispersion + ionic + dipolar) of interaction that contribute to the overall cohesion /adhesion of the liquid system. When concentration of toluene decreases and that of DMF increases, internal pressure increases fast, as the force of cohesion increases. Acoustic impedance (Z) is the ratio of the effective sound pressure at a point to the effective particular velocity at that point. The pressure is measured by the totality of the force of dispersion, repulsion, ionic and dipolar. In our present investigation, acoustic impedance increases slowly with increase in concentration of DMF, showing weak molecular interaction betwwen the components of mixture. Surface tension increases with increase in mole fraction of DMF indicating increase in molecular association.

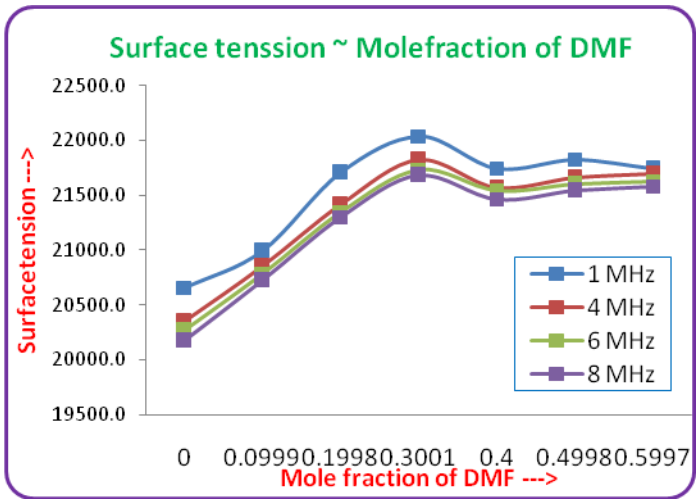

Fig2. Variation of S.T with mole fraction of DMF

It is observed that, for a given concentration and temperature, ultrasonic velocity decreases with increasing frequency of the waves. Such a decrease in velocity is an indication of existence of molecular association between the components of the mixture. Again increasing trend of adiabatic compressibility is observed with increasing frequency. When frequency increases, the interaction between the molecules in the mixture changes causing a structural change and hence increase in adiabatic compressibility. Intermolecular free length depends on 'β' and shows a similar behavior as that of compressibility. Hence free length also increases but at a slower rate. On the basis of a model for sound propagation proposed by Eyring and Kincaid ultrasonic velocity should decrease if the intermolecular free length increases and vice versa.

Acoustic impedance is given by, $Z = U.\rho$. With increase in frequency, acoustic impedance decreases. This factor is governed by the inertial and elastic properties of the medium and hence supports the possibility of molecular interactions. The decreasing nature of 'Z' supports the possibility of weak interaction between unlike molecules.

The value of free volume decreases whereas internal pressure increases with increase in frequency. This is due to the various dispersive interactions and the columbic interaction between the components of mixture.

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TABLE–1: Measured Values of Density (ρ), Viscosity (η) and velocity (U) of ternary mixture.

Mole fraction		Density(ρ) $Kg.m^{-3}$	Viscosity (η) 10^{-3} $N.s.m^{-2}$	Velocity (U) $m.s^{-1}$			
X_1	X_3			1 MHz	4 MHz	6 MHz	8 MHz
0.0000	0.6000	798.41	0.468	1190.35	1178.41	1175.23	1171.62
0.0999	0.4999	808.95	0.486	1192.65	1187.26	1184.84	1182.36
0.1998	0.4001	819.16	0.520	1209.35	119.46	1196.12	1194.35
0.3001	0.3000	829.44	0.548	1211.55	1203.63	1200.45	1198.42
0.4000	0.1999	841.02	0.574	1189.8	1183.2	1182.42	1179.52
0.4998	0.1001	851.86	0.636	1182.54	1176.45	1174.38	1172.24
0.5997	0.0000	861.98	0.701	1170.23	1168.56	1166.14	1164.51

TABLE–2: Calculated values of adiabatic compressibility, free length and free volume.

Mole fraction		Adia. compressibility (β) $(10^{-10}\ N^{-1}.m^2)$				Free length (L_f) $(10^{-10}$ m)				Free volume (V_f) $(10^{-7}\ m^3.mol^{-1})$			
X_1	X_3	1MHz	4MHz	6MHz	8MHz	1MHz	4MHz	6MHz	8MHz	1MHz	4MHz	6MHz	8MHz
0.0000	0.6000	8.839	9.019	9.068	9.124	0.604	0.610	0.612	0.613	3.841	3.783	3.768	3.750
0.0999	0.4999	8.691	8.769	8.806	8.843	0.599	0.601	0.603	0.604	3.524	3.500	3.489	3.478
0.1998	0.4001	8.347	8.499	8.533	8.558	0.587	0.592	0.593	0.594	3.145	3.103	3.094	3.087
0.3001	0.3000	8.214	8.322	8.366	8.394	0.582	0.586	0.587	0.588	2.816	2.789	2.778	2.771
0.4000	0.1999	8.399	8.493	8.504	8.546	0.589	0.592	0.592	0.594	2.470	2.449	2.447	2.438
0.4998	0.1001	8.395	8.482	8.512	8.543	0.589	0.591	0.592	0.594	2.027	2.011	2.006	2.000
0.5997	0.0000	8.471	8.496	8.531	8.555	0.591	0.592	0.593	0.594	1.661	1.658	1.653	1.649

TABLE-3: Calculated Excess values of Internal pressure, Acoustic impedance and Surface tension.

Mole fraction	Internal pressure (π_i) (x 10^6 N.m-^{2})	Acoustic impedance (Z) (x 10^6 $Kg.m^2.s^{-1}$)	Surface tension (S) ($N.m^{-1}$)

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X_1	X_3	1MHz	4MHz	6MHz	8MHz	1MHz	4MHz	6MHz	8MHz	1MHz	4MHz	6MHz	8MHz
0.0000	0.6000	314.2	315.8	316.2	316.7	0.950	0.941	0.938	0.935	20658	20348	20265	20172
0.0999	0.4999	331.0	331.7	332.1	332.4	0.965	0.960	0.958	0.956	20991	20849	20785	20720
0.1998	0.4001	351.8	353.4	353.7	354.0	0.991	0.982	0.980	0.978	21704	21411	21349	21301
0.3001	0.3000	373.6	374.8	375.3	375.6	1.005	0.998	0.996	0.994	22036	21821	21734	21679
0.4000	0.1999	400.1	401.2	401.3	401.8	1.001	0.995	0.994	0.992	21745	21564	21543	21464
0.4998	0.1001	437.8	439.0	439.4	439.8	1.007	1.002	1.000	0.999	21824	21656	21598	21539
0.5997	0.0000	479.3	479.7	480.2	480.5	1.009	1.007	1.005	1.004	21739	21693	21625	21580

CONCLUSION-

It is obvious that, there exist a molecular interaction between the components of the mixture. In specific weak molecular interaction (like dipole-dipole, dipole-induced dipole and dispersive forces) are found to exist between components of the mixtures.

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