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Molecular Interaction Studies in Ternary Liquid Mixtures Containing 2-Nitroanisole and 1- Pentanol in n- Hexane at Different Temperatures using Ultrasonic Techniques

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ABSTRACT

The experimental values of ultrasonic velocity, density and viscosity have been measured for the ternary liquid mixtures containing 2-Nitroanisole and 1-Pentanol in n-Hexane at 303,308 and 313K. To calculate various acoustical parameters like adiabatic compressibility, free volume, internal pressure, acoustical impedance, adsorption co-efficient and molecular interaction parameters have been computed using the experimental data. The linearity of variation in ultrasonic velocity and other parameters are due to the molecular interaction between donor acceptor molecules in liquid-liquid mixture. The various molecular interactions like dipole-dipole, dipole-induced dipole, induced-induced dipole have been discussed for the liquid mixture containing 2-Nitroanisone, 1-Pentanol in n-Hexane at different temperatures and concentration..

Keywords: Acoustical parameters, interaction, complex formation, ternary liquid mixture, ultrasonic techniques, dipole-dipole.

1. INTRODUCTION

The measurement of ultrasonic velocity in liquid-liquid mixtures is used as an effective tool to provide into the properties of liquid mixtures[1]. The ultrasonic studies are extensively used to estimate the thermodynamics properties and predict the intermolecular interaction in pure liquid mixtures[2], ultrasonic velocity and related parameters helps us for characterization thermodynamics and physico-chemical aspects of ternary liquid mixtures such as molecular association and dissociation [3-4]. Pure liquid-liquid mixtures consisting polar and non polar components are considerably importance in analyzing intermolecular interaction between component molecules [5-7]. The ultrasonic investigation of these studies find several applications in industries such as variation in concentration and temperature are useful in insights in to structure and various bonding of associated molecular complexes[8-10] and other related molecular processes. The measurement of ultrasonic velocity has been employed in understanding the nature of the molecular system. It has been widely used in field of interaction structural aspects evaluation studies, the Ultrasonic in liquid mixtures are useful in understanding the nature and strength of molecular interaction.

A large number of studies have been discussed on the intermolecular interaction in ternary liquid system by various methods like ultraviolet, Dielectric constant, infrared , Raman effect, nuclear magnetic resonance and ultrasonic method. In recent year, the method of study of molecular interaction from the knowledge of variation of Acoustic parameters values with change in concentration is common. The increase (or) decrease in ultrasonic velocity have been used in understanding the nature of molecular interaction in pure liquids ternary mixtures. The variation in ultrasonic velocity and relevant parameters shows how much light upon structural changes associated with the liquid mixtures having weekly interaction component as well as strongly interaction components.

In the present study involves the application of ultrasonic velocity measurement to assess the type of molecular interaction in n-Hexane solution containing 2-Nitroanisole ,1-Propanol at various temperature. The ultrasonic velocity, density and viscosity were measured experimentally for the ternary systems namely 2- Nitroanisole and 1- pentanol in n-Hexane at 303,308 and 313K, predicted the possible molecular interaction between unlike molecules. The significant of acoustical studies in mixtures have been used for understanding the intermolecular interaction of different type like dipole- dipole, dipole –induced dipole and induced dipole- induced dipole.

2. MATERIALS AND METHORDS

The liquid mixtures of equal concentration range from 0.001M- 0.010M of 2- Nitroanisole,1-Pentanol in n-Hexane were prepared by taking AR grade chemicals, which were purified by standard methods, ultrasonic velocity have been measured using an ultrasonic interfero meter (Mittal , Model ; F-81) working at frequency of 2MHz with an overall accuracy ± $0.01 ms^{-1}$. A digital constant temperature bath, operating in the temperature range of −10°C to 85°C with an accuracy of ±0.1°C has been used to circulate water through the outer jacket of the double-walled measuring cell containing the experimental liquid. The density and viscosity were measured using a pycko meter (10ml gravity bottle) and an Ostwald's viscometer with an accuracy of ±0.0001 m $Nm^{-2}s$, respectively. All precautions were taken to minimize the possible experimental error, the set up was checked for standard liquids.

3. THEORY AND CALCULATION

The expression used to determine the ultrasonic velocity is follows,

$$U = f \lambda \ ms^{-1} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (1)$$

The densities of the mixtures were measured by the formula,

$$\rho_2 = (w_2/w_1)\rho_1 \quad \ldots\ldots\ldots\ldots\ldots\ldots (2)$$

Where w_1 = weight of distilled water , w_2 = weight of experimental liquid
ρ_1 = density of water , ρ_2 = density of experimental liquid .
The viscosity was determined using the relation ,

$$\eta_2 = \eta_1 (t_2/t_1) (\rho_2/\rho_1) \quad \ldots\ldots\ldots\ldots\ldots\ldots (3)$$

Using the measured data, the following acoustical parameters can be calculated ,
Adiabatic compressibility (β)

$$K = (1/ U^2\rho) \ kg^{-1} \ ms^{-2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots (4)$$

Free length (L_f)

$$L_f = (K/ U\rho^{1/2}) \text{ m} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots..(5)$$

Where ,K is Jacobson's constant. This constant is a temperature dependent whose value at any temperature (T) is given by (93.875 + 0.3445T) × 10^8

Acoustic Impedance (Z)

$$Z = U\rho \text{ kg m}^{-2} \text{ s}^{-1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

Free Volume (V_f)

$$V_f = (M_{eff} U/ k\eta)^{3/2} \text{ m}^3 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(7)$$

Where, M_{eff} is the effective molecular weight ($M_{eff} = \Sigma m_i x_i$ in which m_i and x_i are the molecular weight and the mole fraction of the individual constituents respectively and k is a temperature independent constant equal to 4.28 × 10^9 for all liquids .

Internal Pressure (π_i)

On the basis of statistical thermodynamics , suryanarayana derived an expression for the determination of internal pressure through use of concept of free volume

$$\Pi_i = bRT (k\eta/U)^{1/2} (\rho^{2/3}/M_{eff})^{7/6} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(8)$$

Where T = is the absolute temperature ρ = is the density and R is the gas constant

M_{eff} = is the effective molecular weight.

Absorption coefficient (α/f^2)

It can be calculated from the viscosity using the relation ,

$$\alpha/f^2 = (8\pi^2\eta/3\rho U^3) \text{ Nps}^2\text{m}^{-1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(9)$$

Viscous Relaxation time (τ) , It is calculated using the following relation,

$$\tau = 4\eta/3\rho u^2 s \ldots\ldots\ldots\ldots\ldots\ldots\ldots..(10)$$

Available Volume (V_a); It is calculated from Schaff's relation

,

$$V_a = V_m (1-U/U_a) \text{ m}^3 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots.(11)$$

Where V_a is the molar volume and U_a = 1600ms^{-1}

Cohesive Energy (CE) ; it is usually given as a product of internal pressure (π_i) and molar volume (Vm)

$$CE = \pi_i \text{ Vm kj mol}^{-1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(12)$$

Free energy of Activation (ΔG^*) = - K_B T ln($h/\tau K_B T$) kjmol^{-1}…….(13)

Where K_B = Boltzman's constant (1.3806×10^{-23} Jk^{-1}) , T = temperature , h= planck's constant (6.626×10^{-34} Js) .

The Lenard Jones Potential exponent is given by LJP = $6V_m/V_a$……(14)

V_m = the molar volume , V_a = the available volume

Formation constant; To calculate the formation constant values of the charge transfer complexes, appreciable to week complexes and in very dilute solution. The stability calculated using the following relation,

$$K = Y/(b-y)^2 \ dm^3 \ mol^{-1} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(15)$$

Where , $Y = (a-k^{1/2}b)/k-k^{1/2})$; $k = x/y$

X = different between U_{cal} and U_{obs} at lower concentration 'a'
Y = different between $U_{cal}$and Uobs at higher concentration 'b' and U_{cal} = the ultrasonic velocity of the mixture , this equation can be used to calculation stability constant values for different combination concentration 'a' and 'b'.

4. RESULTS AND DISCUSSION

Table:1. Velocity ,density and viscosity of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K.

Con. 10^{-03}M	Velocity (ms^{-1})		
	Temperature (K)		
	303	***308***	***313***
1	1058.03	1037.16	1012.16
2	1058.18	1037.56	1012.58
3	1058.18	1038.01	1013.10
4	1059.08	1038.20	1014.20
5	1059.52	1038.24	1014.56
6	1060.06	1038.76	1014.76
7	1060.34	1039.10	1014.98
8	1060.98	1039.56	1015.10
9	1061.02	1040.20	1015.36
10	1061.12	1040.72	1015.76

Plot of velocity Vs concentration

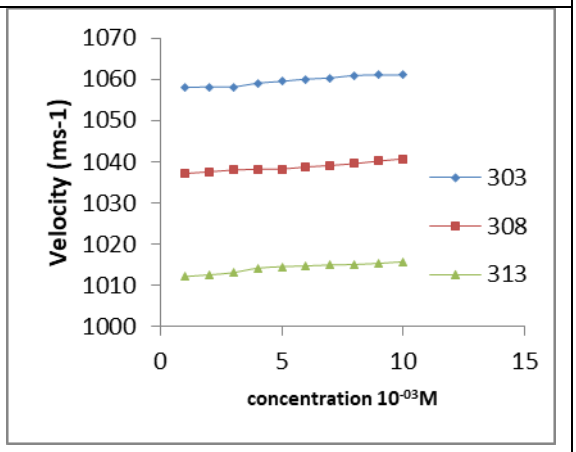


Table:2. Viscosity of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K

Con.10^{-03}M	Density Kg/m^3		
	Temperature(K)		
	303	***308***	***313***
1	802.0	790.0	795.0
2	802.0	796.0	801.0
3	801.0	796.0	801.0
4	801.0	796.0	801.0
5	801.0	796.0	801.0
6	801.0	796.0	801.0
7	802.0	796.0	801.0
8	802.0	796.0	801.0
9	803.0	796.0	802.0
10	803.0	797.0	802.0

Plot of density Vs concentration

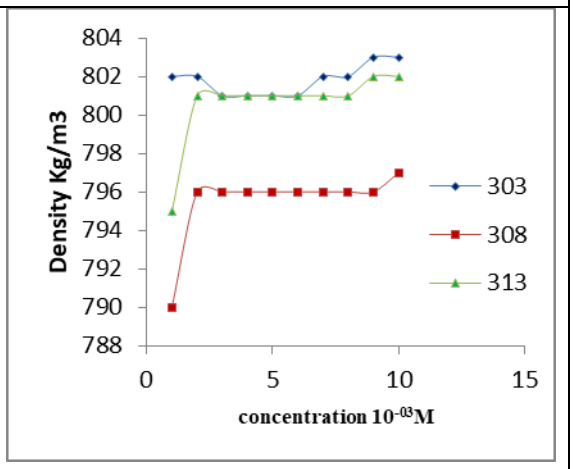


Table:3. Viscosity of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K

Con. 10^{-03}M	Viscosity×10^{-04} Nsm^{-2}			Plot of viscosity Vs concentration
	Temperature(K)			
	303	*308*	*313*	
1	4.753	4.795	4.921	
2	4.590	4.548	4.850	
3	4.561	4.532	4.872	
4	4.515	4.573	4.955	
5	4.576	4.521	4.991	
6	4.584	4.502	4.991	
7	4.654	4.548	4.989	
8	4.661	4.588	4.918	
9	4.688	4.600	4.941	
10	4.756	4.638	4.985	

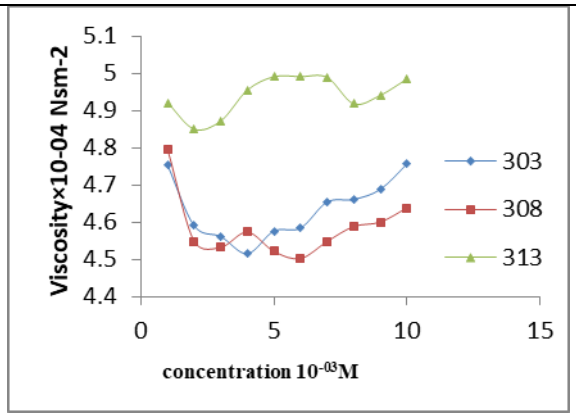


Table:4. Adiabatic compressibility of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K

Adiabatic compressibility×10^{-09} Kg^{-1} ms^2				Plot of adiabatic compressibility Vs concentration
Temperature(K)				
Con.× 10^{-3} M	*303K*	*308K*	*313K*	
1	1.11	1.18	1.23	
2	1.11	1.17	1.22	
3	1.11	1.17	1.22	
4	1.11	1.17	1.21	
5	1.11	1.17	1.21	
6	1.11	1.16	1.21	
7	1.11	1.16	1.21	
8	1.11	1.16	1.21	
9	1.11	1.16	1.21	
10	1.11	1.16	1.21	

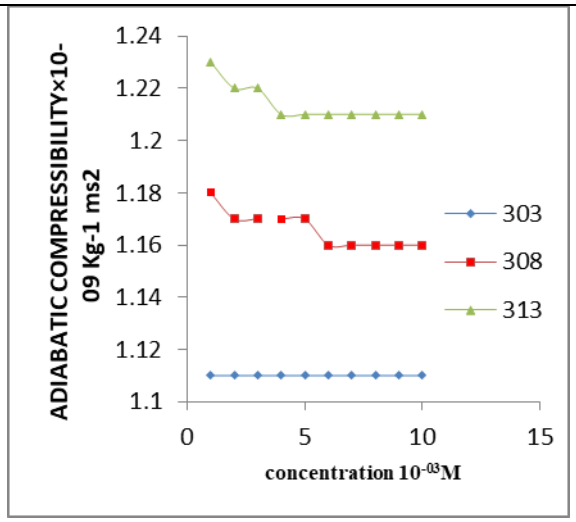


Table:5. Free length of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K

Con. 10^{-03}M	FREE LENGTH×10^{-11} m			Plot of free length Vs concentration
	Temperature(K)			
	303K	*308K*	*313K*	
1	6.56	6.81	6.95	
2	6.56	6.72	6.86	
3	6.56	6.72	6.86	
4	6.55	6.72	6.85	
5	6.55	6.72	6.85	
6	6.55	6.71	6.85	
7	6.55	6.71	6.85	
8	6.54	6.70	6.85	
9	6.55	6.70	6.85	
10	6.54	6.70	6.85	

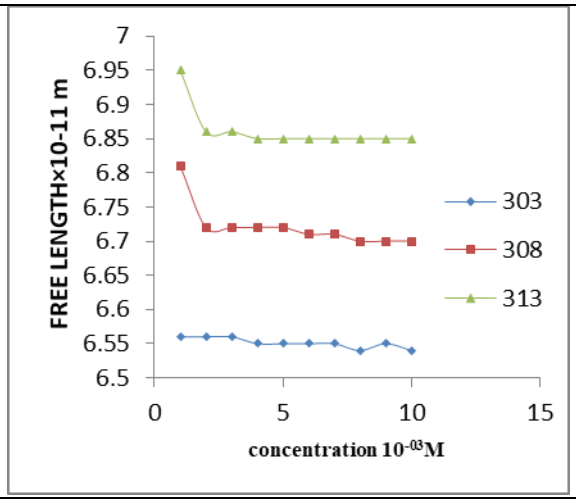


Table:6. Free volume of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K

FREE VOLUME $\times 10^{-07}$ m^3			
Temperature(K)			
Con $\times 10^{-03}$ M	303K	308K	313K
1	3.859	3.696	3.427
2	3.052	3.005	2.630
3	3.081	3.022	2.615
4	3.123	2.983	2.553
5	3.072	3.023	2.527
6	3.066	3.053	2.528
7	2.998	3.011	2.530
8	2.994	2.974	2.586
9	2.969	2.965	2.568
10	2.906	2.931	2.536

Plot of free volume Vs concentration

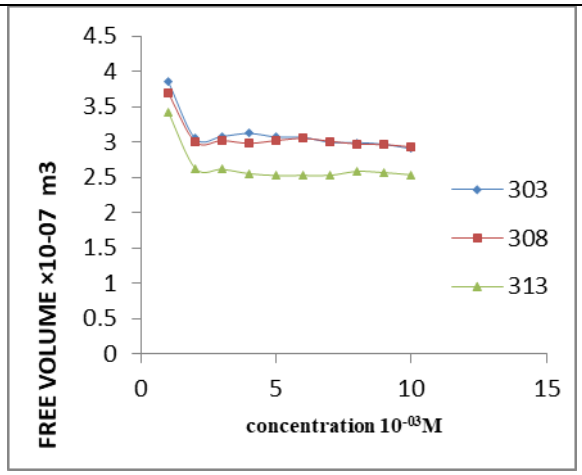


Table7. Internal pressure of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K

Con $\times 10^{-3}$ M	Internal pressure $\times 10^{+08}$ Nm^{-2}		
	Temperature(K)		
	303K	308K	313K
1	2.748	2.760	2.842
2	3.376	3.376	3.544
3	3.362	3.370	3.551
4	3.344	3.385	3.579
5	3.365	3.365	3.592
6	3.368	3.357	3.591
7	3.396	3.377	3.590
8	3.398	3.388	3.565
9	3.409	3.394	3.575
10	3.434	3.407	3.591

Plot of internal pressure Vs concentration

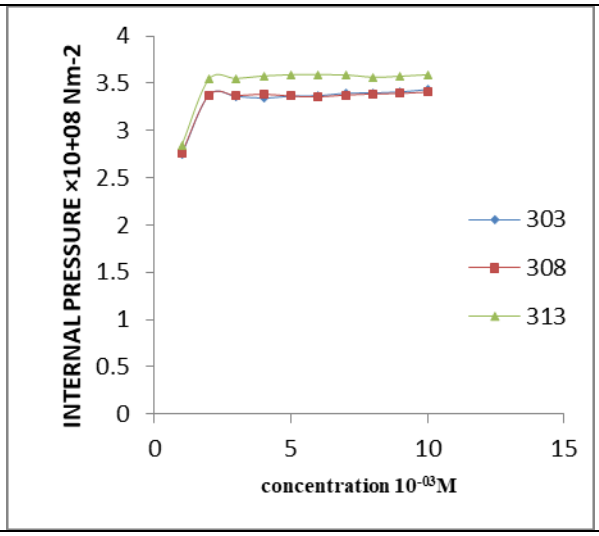
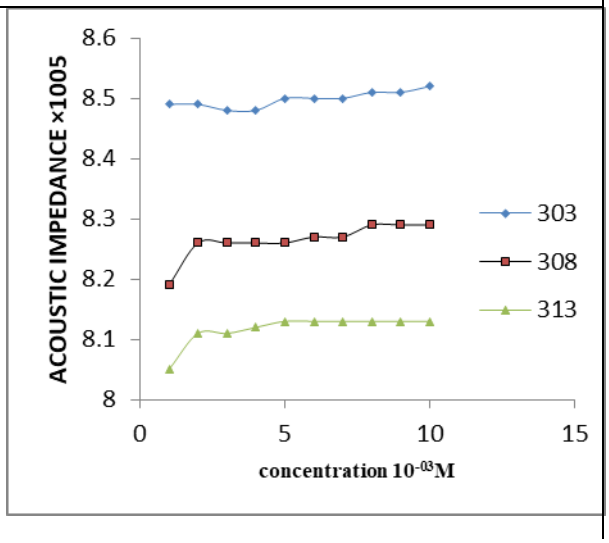


Table8. Acoustic impedance of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K.

Acoustic Impedance $\times 10^{05}$ Kg m^2 s^{-1}			
Temperature(K)			
Con. $\times 10^{-3}$M	303K	308K	313K
1	8.49	8.19	8.05
2	8.49	8.26	8.11
3	8.48	8.26	8.11
4	8.48	8.26	8.12
5	8.50	8.26	8.13
6	8.50	8.27	8.13
7	8.50	8.27	8.13
8	8.51	8.29	8.13
9	8.51	8.29	8.13

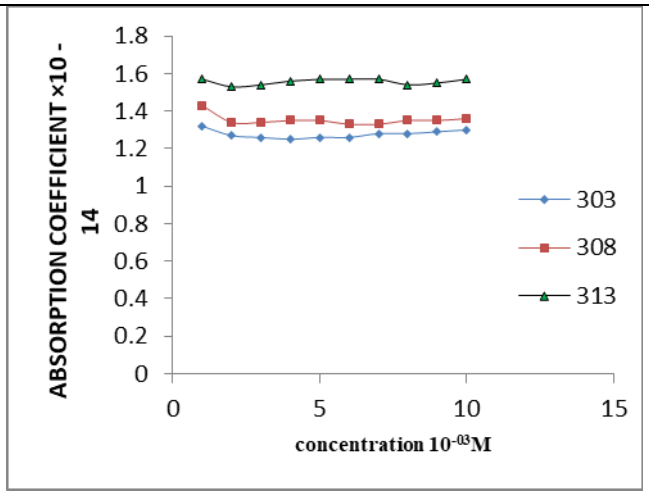
Plot of acoustic impedance Vs concentration



10	8.52	8.29	8.13	

Table9. Absorption coefficient of 2-nitroanisole ,1-pentanol in n-hexane at 303,308 and 313K.

Con×10^{-3}M	**Absorption coefficient ×10 $^{-14}$**			**Plot of absorption co efficient Vs concentration**
		Temperature(K)		
	303K	308K	313K	
1	1.32	1.43	1.57	
2	1.27	1.34	1.53	
3	1.26	1.34	1.54	
4	1.25	1.35	1.56	
5	1.26	1.35	1.57	
6	1.26	1.33	1.57	
7	1.28	1.33	1.57	
8	1.28	1.35	1.54	
9	1.29	1.35	1.55	
10	1.30	1.36	1.57	



The study of molecular association in organic ternary liquid mixture with alcohols as one of the component in the mixture, since alcohols are strongly self associated liquid having a three dimensional network of hydrogen bond and can be associated with any other group having polar attraction. Methoxy group(-OCH_3) present in 2-Nitroanisole is donating electron easily due to its mesomeric effect to interact with 1-Pentanol in n-Hexane solution. Due to the non polar nature of n-Hexane a weak dispersive type of interaction occurs between 1-Pentanol and n-Hexane.

From Table 1,2 and 3, it is observed that as temperature increases ultrasonic velocity, density and viscosity of the liquid mixture increases with respect to concentration, the variation in ultrasonic velocity with increases in concentration and temperature is mainly due to interaction between donor and acceptor molecules, whereas viscosity and density found to be decreases with increasing concentration of the mixture, however ultrasonic velocity, density and viscosity decreases in all cases as temperature is increased as shown in Table 1,2 and 3. The variation ultrasonic velocity, density and viscosity is plotted vs concentration presented in Table 1,2 and 3. On the basis of Kincaid and Erying models (1938) proposed for propagation , free length is the distance between the surfaces of the neighboring molecules, free length decreases when ultrasonic velocity increases the result of mixing the components. The decrease in free volume shows that the strength of interaction increases gradually with the increase in concentration.

It represents that there is a weak interaction between the molecules in the mixture.The variation in ultrasonic velocity depends on increases (or) decreases of intermolecular free length in the liquid mixture as shown in Table-5 that free length decreases as concentration increases and free length increases as temperature increases.

Adiabatic compressibility which is indicated in Table-4 observed a reverse trend to that of ultrasonic velocity which indicates the extent of complex formation. Internal pressure tabulated in Table-7 gives information regarding nature and strength of force existing between the molecules. Internal pressure gradually increases as concentration of liquid mixture increases as represented in Table-7 shows the formation of donor acceptor complexes.

The increases values of acoustic impedance with concentration supports the possibility of molecules interaction between the unlike molecules 2- Nitroanisole and 1-Pentanol in n-Hexane mixture. The positive values of acoustical parameters shows the interaction between the liquid mixture presents in the component. From the above ,its confirmed that a weaker molecular interaction in the form of dipole-dipole, dipole-induced dipole or induced-induced dipole interaction in the liquid-liquid ternary mixture is possible.

5. CONCLUSION

- The increase in temperature due to thermal agitation, resulting in a decrease in ultrasonic velocity. An increase in viscosity with increase in concentration suggests that molecular interactions are increasing in thickness of the liquid mixture and molecular size and shape of the elements that play an equally important role.
- The adiabatic compressibility suggests that the lack of interaction between unlike molecules that have the minimum declarations.
- From the magnitude of velocity, there is molecular interactions in the mixture, which are linked to the phenolic group of oxygen atoms, resulting in a weak link between them.
- The solute- solute molecular association arise due to dipole-dipole interaction and the polar nature of different molecular entities in the mixture. The solute solvent association arise due to slightly polar solute and non polar nature of the solvent (n hexane). In this system, solute – solute molecular association is proposed for nearly equal in ratio of 2-Nitroanisole and 1-Pentanol.
- Due to the non polar nature of n-hexane a weak dispersive type of interaction occurs between 1-pentanol and n-hexane.

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Conflict of Interest

None of the authors have any conflicts of interest to declare.