Study of acoustical parameters in the binary liquid mixtures containing n-alkanes

Dr. Nisha Sharma, Dr. B.P Singh

Department of Physics, Institute of Basic Sciences, Khandari, Agra 282002 (UP) India

E-mail: dr.nishasharma14@gmail.com

Abstract: From the measured value of speed of sound (u), density (ρ) for binary liquid mixtures of n-heptane+ n-hexane, n-hexane+ toluene, n-heptane+ toluene at 298.15K, we calculate some acoustical parameters like inter molecular free length (L_f), acoustic impedance (Z), relative association (R_A). The excess intermolecular free length (L_f^E) and excess acoustic impedance (Z^E) have also been calculated. The excess values are used to understand the molecular interaction between the components of binary mixtures. The deviation in intermolecular free length and acoustic impedance is negative throughout the composition in all three binary mixtures. The theoretical values of ultrasonic speed were calculated using different formulations.

Keywords: Ultrasonic velocity, Molecular interaction, Binary mixtures.

1 Introduction

Study of acoustical properties and their excess parameter are used to understand molecular interaction between components of binary mixtures [1-6]. Ultrasonic study gives the information about physico-chemical properties of the system. Ultrasonic propagation parameters are important in understanding the behavior of liquid system, dipolar interactions, molecular spacing, molecular motion and their strength. With the help of experimental velocity (u) and density (ρ), thermodynamic parameters like intermolecular free length (L_f), acoustic impedance (Z), relative association (R_A) can be calculated. We can also determine some excess parameters like excess intermolecular free length (L_f^E), excess acoustic impedance (Z^E).

It appears from literature survey that the acoustical parameters have been determined by various workers[7-9] on liquid mixtures. Eyring and Kincaid [7] invested that the intermolecular free length (L_f) increases in u and decrease in L_f with molar concentration for acetone + acetophenone and ethyl methyl ketone + acetophenone mixtures. Prabhakar and Rajgopal [8] found that the value of Z increases with molar concentration of acetone + acetophenone and ethyl-methyl ketone + acetophenone mixtures. The relative association R_A increases for acetone + acetophenone and ethyl-methyl ketone+ acetophenone signifies that unlike interactions are relatively strong. Similar reports are available in literature for mixtures of tetrahydrofuran (THF) with 1-butanol and tert butanol given by ALI and AK Nain [9].

Recent investigation shows that very few studies have been done in the case of alkanes. which is used in many petrochemical refining process. Alkanes are almost non-polar molecules and therefore molecules are held by weak Vander wall's force. In the present paper we report ultrasonic velocity, density of binary mixtures of n-heptane + toluene, n-heptane + n-hexane, n-hexane + toluene at 298.15K over entire composition range. The experimental data are used to calculate intermolecular free length (L_f), acoustic impedance(Z), relative association (R_A) and excess intermolecular free length (L_f^E), excess acoustic impedance (Z^E) to understand thermodynamics properties of liquid and their mixtures which is not easily obtained by any other means. Ultrasonic velocity is also calculated theoretically by using Nomoto's relation [10], Van deal and Vangeel's relation [11], Junjie's relation [12] and impedance relation [13]. The theoretical values of ultrasonic velocity obtained various relations [10-13] are compared with experimental ultrasonic velocity binary at various molar concentration.

2 Method of Analysis

By using experimentally measured values of ultrasonic velocity (u) and density (ρ). We have calculated some thermodynamic parameters like intermolecular length (L_f), acoustic impedance (Z) and relative association (R_A) by following relations [14]

$$L_f = \left(\frac{K}{u \rho^{1/2}} \right) \quad \ldots (1)$$

$$Z = \rho u \quad \ldots (2)$$

$$R_A = \left(\frac{\rho}{\rho_0} \right) \left(\frac{u}{u_0} \right)^{1/3} \quad \ldots (3)$$

where K being Jacobson's constant depending on absolute temperature [15].We calculate the excess functions such as excess inter molecular free length (L_f^E) and excess acoustic impedance (Z^E) by using following relationship

$$Y^E = Y_{\exp} - Y_{id} \quad \dots (4)$$

And

$$Y_{id} = \sum X_i Y_i \quad \dots (5)$$

Where X_i is the mole fraction of the component Y_{exp} is the experimental value, Y_{id} is the ideal value, Y^E is the excess property of given parameter.

The excess functions are used to study the interaction between the like and unlike molecules[16,17] depending on the sign and extent of deviation. Theoretical the ultrasonic velocity can be determined using the following relations.

Nomoto's relation

$$u = \left[\frac{\sum X_i R_i}{\sum X_i V_i} \right]^3 \quad \dots (6)$$

Impedance relation

$$u = \left[\frac{\sum X_i Z_i}{\sum X_i \rho_i} \right] \quad \dots (7)$$

Vandeal and Vangeal relation

$$u = \left[\frac{1}{\sum X_i M_i}\right]^{1/2} \left[\frac{\sum X_i}{\sum M_i u_i^2}\right]^{-1/2} \quad \ldots(8)$$

Junjie's relation

$$u = \frac{\sum X_i V_i}{\left[\sum X_i M_i \sum X_i V_i / \sum \rho_i u_i^2\right]^{1/2}} \quad \ldots(9)$$

where R_i is the molar sound velocity, X_i is the mole fraction of ith component. M_i is the molecular weight, ρ_i is the density, Z_i is the acoustic impedance of the component of binary mixture.

Table – 1

Experimental values of sound velocity (u), density (ρ) for pure liquids.

Liquids	**Ultrasonic velocity (m/s)**	**Density (kg/m^3)**
Toluene	1304.3	862.6
n-heptane	1131.0	679.0
n-hexane	1075.8	654.8

Table - 2

Density (ρ), speed of sound (u), inter molecular free length (L_f), excess inter molecular free length (L_f^E), acoustic impedance (Z), excess acoustic impedance (Z^E) and relative association (R_A) of binary liquid mixture of n-heptane + toluene

n –heptane + toluene									
X	ρ (kg/m^3)	u (m/s)	$L_f \times 10^{-12}$ (m)		$Z \times 10^{-7}$ (Kg/m^3/s)		$L_f^E \times 10^{-12}$ (m)	$Z^E \times 10^{-7}$ (kg/m^3/s)	R_A
			Eq. (1)	Eq. (5)	Eq. (2)	Eq. (5)			
0.0	862..6	1304.3	53.723	53.723	11.240	11.240	0	0	1.000
0.1	843.2	1286.9	55.085	55.329	10.840	10.883	-0.244	-0.043	0.982
0.2	825.8	1269.6	56.429	56.936	10.469	10.527	-0.507	-0.058	0.965
0.3	807.5	1252.3	57.830	58.542	10.103	10.171	-0.712	-0.068	0.948
0.4	788.1	1234.9	59.376	60.149	9.723	9.815	-0.773	-0.092	0.930
0.5	770.8	1217.6	60.905	61.756	9.370	9.459	-0.851	-0.089	0.913
0.6	752.4	1200.3	62.503	63.362	9.024	9.103	-0.859	-0.079	0.896
0.7	733.1	1182.9	64.272	64.969	8.664	8.747	-0.697	-0.083	0.878
0.8	715.7	1165.6	66.026	66.575	8.324	8.391	-0.549	-0.062	0.860
0.9	697.3	1148.3	67.863	68..124	8.001	8.035	-0.261	-0.034	0.843
1.0	679.0	1131.0	69.789	69.789	7.679	7.679	0	0	0.825

Table-3

Density (ρ), speed of sound (u), inter molecular free length (L_f), excess inter molecular free length (L_f^E) acoustic impedance (Z), excess acoustic impedance (Z^E) and relative association (R_A) of binary liquid mixture n- heptane +n-hexane

n -heptane + n -hexane									
X	ρ (kg/m^3)	u (m/s)	$L_f \times 10^{-12}$ (m)		$Z \times 10^{-7}$ ($kg/m^3/s$)		$L_f^E \times 10^{-12}$ (m)	$Z^E \times 10^{-7}$ ($kg/m^3/s$)	R_A
			Eq. (1)	Eq. (5)	Eq. (2)	Eq. (5)			
0.0	654.8	1075.8	74.715	74.715	7.044	7.044	0	0	1.000
0.1	656.5	1081.3	74.222	74.238	7.098	7.104	-0.016	-0.005	1.001
0.2	659.6	1086.8	73.687	73.730	7.168	7.174	-0.043	-0.006	1.003
0.3	662.0	1092.3	73.181	73.237	7.231	7.236	-0.056	-0.005	1.006
0.4	664.4	1097.8	72.682	72.745	7.294	7.299	-0.063	-0.005	1.007
0.5	669.9	1103.4	72.182	72.224	7.358	7.363	-0.065	-0.005	1.011
0.6	669.3	1108.9	71.695	71.760	7.421	7.426	-0.065	-0.005	1.012
0.7	671.7	1114.4	71.214	71.267	7.485	7.489	-0.053	-0.004	1.013
0.8	674.1	1119.9	70.738	70.775	7.549	7.552	-0.037	-0.003	1.015
0.9	676.5	1125.4	70.267	70.294	7.613	7.615	-0.027	-0.002	1.017
1.0	679.0	1131.0	69.790	69.790	7.679	7.679	0	0	1.019

© 2025 IJRTI | Volume 10, Issue 6 June 2025 | ISSN: 2456-3315

Table - 4

Density (ρ), speed of sound (u), inter molecular free length (L_f), excess inter molecular free length (L_f^E), acoustic impedance (Z), excess acoustic impedance (Z^E) and relative association (R_A) of binary liquid mixture of n-hexane + toluene

n –hexane +toluene									
X	ρ (kg/m^3)	u (m/s)	$L_f \times 10^{-12}$ (m)		$Z \times 10^{-7}$ (kg/m^3/s)		$L_f^E \times 10^{-12}$ (m)	$Z^E \times 10^{-7}$ (kg/m^3/s)	R_A
			Eq. (1)	Eq. (5)	Eq. (2)	Eq. (5)			
0.0	862.6	1304.3	53.692	53.692	11.250	11.25	0	0	1.000
0.1	841.8	1281.4	55.322	55.794	10.786	10.829	-0.472	-0.043	0.981
0.2	821.0	1258.4	57.043	57.896	10.331	10.408	-0.853	-0.077	0.963
0.3	800.2	1235.7	58.841	59.998	9.883	9.988	-1.157	-0.105	0.944
0.4	779.4	1212.9	60.742	62.101	9.453	9.567	-1.359	-0.114	0.919
0.5	758.7	1190.1	62.747	64.203	9.028	9.147	-1.456	-0.119	0.901
0.6	737.9	1167.2	64.871	66.305	8.612	8.726	-1.434	-0.114	0.882
0.7	717.1	114.35	67.119	68.408	8.206	8.305	-1.289	-0.099	0.868
0.8	696.3	1121.5	69.501	70.510	7.809	7.885	-1.009	-0.076	0.848
0.9	675.5	1098.6	72.034	72.612	7.421	7.464	-0.577	-0.043	0.829
1.0	654.8	1075.8	74.715	74.715	7.044	7.044	0	0	0.809

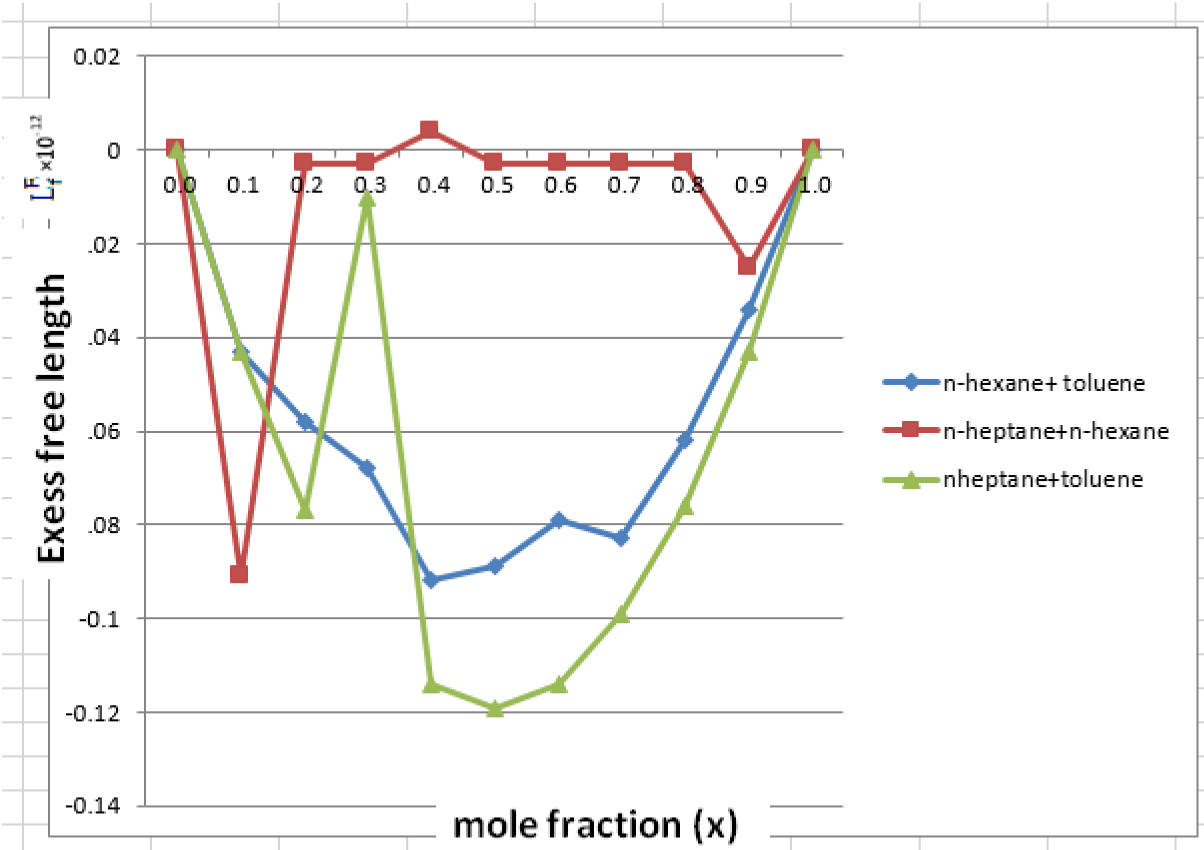
0.02
0
.02
.04
.06
.08
-0.1
-0.12
-0.14
0.0 0.1 0.2 0.3 0.4 0.5 0.6 0.7 0.8 0.9 1.0
Exess free length
mole fraction (x)
n-hexane+ toluene
n-heptane+n-hexane
nheptane+toluene

Fig-1

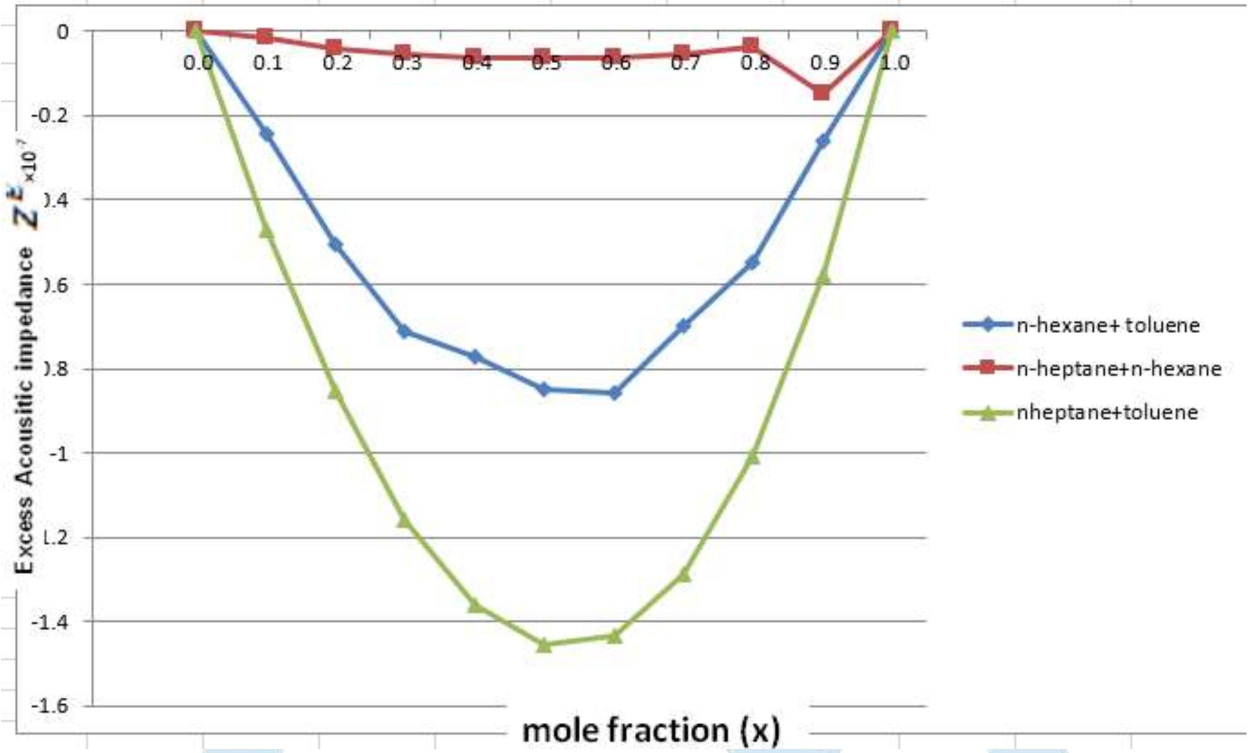

Fig-2

3 Results and Discussion

In the present investigation we consider three binary liquid mixtures viz. n-heptane + toluene, n-heptane + n-hexane, n-hexane + toluene. In Table1, we reported the experimental values of ultrasonic velocity and density for pure liquids at 298.15K. The experimental values of ultrasonic velocity and density are used to calculate various thermoacoustic parameters like intermolecular free length, acoustic impedance and relative association by using Eqs (1-3) for all the binary mixtures. We also calculate the excess thermodynamic parameters like excess intermolecular free length and excess acoustic impedance in all three binary liquid mixtures using the Eq (4). The experimental ultrasonic velocity, density and derived parameters like intermolecular free length, acoustic impedance, relative association along with excess intermolecular free length and excess acoustic impedance at 298.15 K are reported in Tables 2-4 for all three liquid mixtures.

The intermolecular free length affects the sound velocity. The increase or decrease of molecular free length depends on the variation of ultrasonic after mixing the components, The variation in Table 2 and 4 represent increasing trend with increasing increasing mole fraction which shows a strong intermolecular interaction between liquids while showing reverse trend in Table 3. The value of z shows decreasing trend in n-heptane + toluene and n-hexane + toluene whereas showing the increasing trend in n- heptane + n-hexane. This decrease in specific acoustic impedance indicates significant interaction between component of molecules.The relative association (R_A) is found is increase with mole concentration of n-heptane + n-hexane showing that unlike interaction are relatively strong compared to like interaction while showing decreasing trend in n-heptane + toluene and n-hexane + toluene. Same fact was given in literature for binary mixture of polyethene and 1- propanol[15].

The excess functions are very sensitive towards mutual interactions between component molecules of liquid mixtures. The extent of deviation and sign of these functions depend on the strength of interaction between unlike molecules [16-17]. The excess functions like excess intermolecular free length, excess acoustic impedance was estimated by the Eqs (4-5). According to Fort and Moore[1], the excess values are negative in system having unequal molecular size in which dispersion forces are dominant. The excess properties depend on various contributions [18].The negative values of L_f^E and Z^E involves physical contribution allowing the fitting of molecules of two different size into each other structures [16].The deviation in excess intermolecular free length and excess acoustic impedance is negative over the whole range of composition for all the binary mixtures.

The excess function (L_f^E) showing the same trend for all these liquid mixtures. The negative values of (L_f^E) is obtain due to strong dipole–dipole interaction between component molecule[19]. The excessive acoustic impedance (Z^E) first increase and then decrease for liquid mixture n-heptane + toluene and n-hexane + toluene.

We plot a graph between mole fraction and excess intermolecular free length and mole fraction and excess acoustic impedance. Figure 1 shows that (L_f^E) is more negative in n- heptane +toluene than in n-heptane +n- hexane and n-hexane + toluene. The negative value of (L_f^E) suggest the presence of significant dipole-dipole interaction between the component molecules of these mixtures. Similar negative value are reported in literature [20]. Fig 2 shows that deviation is more negative in n-hexane + toluene than n-heptane+ n-hexane and n- heptane + toluene. Theoretical values of ultrasonic velocity for binary mixtures were estimated using various models given by Eqs (6-9) and then compared with the experimental values. All the theoretical models are reasonably close to experimental values for all three binary mixtures, showing the validity of these theoretical models for binary mixtures.

4 Conclusions

We study some acoustical parameters in binary liquids using Eqs (1-3) and their excess parameters from Eq (4) and Eq (5). The deviation is due to interaction between molecules of system. Ultrasonic velocity can be theoretically calculated using Eqs (6-9). The result shows that theoretical value agree well with experimental values.

References

[1] Fort R Jand Moore W R ,*Trans faraday soc* 61 (1965) 2102.

[2] Ali A, Nain A K and Mohmmed Ibrahim, *Acoustics letters* **2A** (2001) 218.

[3] NikamP S, Mahall T A and Mehdihasan , *Acoustica Acta Acoustica* **8A** (1986) 360.

[4] Aminabhavi T M and Kanalika Banerje , *Indian J Chem.* **40A (**2001) 53.

[5] Agnihotri S C and Om Prakash , *Acustica* **63** (1987) 290.

[6] Kanappan A N and Rajendran V, *Indian J. Pure and Appl. Phys.* **30** (1992) 240.

[7] Eyring H and Kincaid J F, *J. Chem. Phys.* **6 (**1938) 620.

[8] Pabakar S and Rajagopal K , *J Pure Appl. Ulrtason* **27** (2005)41.

[9] Ali A and Nain A K, *Pramana –J. Phys.* **4** (2002) 695.

[10] Nomoto O , *J. Phys. Soc Jap.* **13** (1959) 1529.

[11] Van Deal W and Vangeel E , *Proc. First International conference on calorimetry and Thermodynamics* (Warsaw,1969) 556.

[12] Junjie Z J, *China Univ. Sci Tech* **14** (1984) 298 .

[13] Vogel A J , *Text Book of organic chemistry 5th Edition* (John Wiley, N.Y.1989)

[14] Thakur K P and Gupta N K , *Acustica* **53** (1983) 591.

[15] Jocobson B, *J. Chem. Phys* **20** (1952) 927.

[16] Redlich O and Kister A T , *Ind. Eng. Chem.* **40** (1948) 345.

[17] Ali A and Nain A K , *International Conference and Exhibition on Ultrasonic* (ICEU-99) Dec 2-A, New Delhi, 1999.

[18] Assarson P and Eirich F R, *J. Phys. Chem*. **72** (1968) 2710.

[19] Ali A and Nain A K, *J. Pure. Appl. Ultrason.* **21** (1999) 31.

[20] Yanadi Reddy N , Subramanyam Naidu P, and Ravindra Prasad K, *Ind J. Pure Appl. Phys*. **32** (1994) 958.