

Remarking An Analisation Investigation of Molecular Interaction in Binary Liquid Mixtures Using Ultrasonic Velocity At 303.15K

Abstract

The ultrasonic velocity (U), the density (ρ) and viscosity (η) of hexane with 1-heptanol have been measured at 303.15K. From the measured data of ultrasonic velocity, density and viscosity acoustic parameters such as – free volume, internal pressure, and Gruneisen parameter have been estimated using standard relation. The variation of free volume, internal pressure, gruneisen parameter with Concentration and temperature have been studied.

Keywords: Ultrasonic Velocity, Density, Viscosity, Internal Pressure, Free Volume, Gruneisen Parameter.

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Introduction

Ultrasonic investigation of binary liquid mixtures using polar and non polar components are of much importance in knowing the intermolecular interaction between the molecules¹⁻³. The density (ρ), viscosity (η) and ultrasonic velocities find broad applications in characterizing the physical and chemical behavior of liquid mixtures and in the study of molecular interactions.

Aim of the Study

The aim of the present investigation is the compare the experimentally determined ultrasonic sound velocity in binary liquid mixtures with those of theoretical relation at 303.15K temperature.

The present investigation is related with the study of the binary system hexane with 1-heptanol at temperature 303.15K, for the entire mole fraction range.

In our research work involving the study of excess properties of binary liquid mixtures, we report the experimental measured values of speed of sound, viscosity and density for the binary mixtures of hexane with 1-heptanol at 303.15K. The experimental values were used to calculate internal pressure and Gruneisen parameter and their excess values.

Material and Methods

All the solvent used are of Merck Indian Limited (A.R. grade). The non polar hydrocarbon used also of Merck India Limited. The purities of the chemicals were checked by densities measurement. The density accurate to $\pm 0.0001 \times 10^3 \text{kgm}^{-3}$ for each sample, determined by Pycnometer after equilibrating in a thermostat (zenith) for half on hour, the measurement are made at a constant temperature $303.15 \pm 0.03\text{K}$ with the help of water thermostat.

The weighing was done using electrical single pan analytical balance with an accuracy of $\pm 1.0 \times 10^{-8} \text{kg}$.

Single crystal ultrasonic pulse echo interferometer (Model M-82) manufactured by Mittal enterprises working at 2MHz. was used to measure the sound velocity of a liquid or liquid mixtures.

To determine the viscosity of a binary liquid mixture, an Ostwald viscometer is used and a stop watch of accuracy in milliseconds is selected to note the time of flow of the liquid mixtures⁴. In the present study the binary mixture prepared is of n-hexane and 1-hexanol with different mole fractions.

Theory and Calculations

Viscosity of binary mixtures is determined by – The ideal viscosity is given by

$$\eta_{\text{ideal}} = \eta_1 X_1 + \eta_2 X_2$$

$$\eta^{\text{e}} = \eta_{\text{mix}} - \eta_{\text{ideal}}$$

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Free volume of binary mixture is given by

$$V_f = (Mv / k\eta)^{3/2}$$

Where η is viscosity of the liquid

k is constant having a value 4.28×10^3 .

M is in gms

V is centimeters / sec.

η is in poise and V_f is in $V_f^E = (V_f)_{mix} -$

$(V_f)_{ideal}$.

On the basis of statistical thermodynamics, Suryanarayan⁵ derived an equation for the calculation of internal pressure of binary mixture

$$P_i = bRT \left(\frac{K\eta}{U} \right)^{1/2} \cdot \left(\frac{\rho^{2/3}}{M_{eff}^{7/6}} \right)$$

b = packing factor ; value = 2

K = temperature independent constant having value 4.28×10^3 for all liquid

R = 0.082 atm dm³ mmol⁻¹ (Universal gas const.)

M_{eff} = effective molecular weight

ρ is the density in kg m⁻³

Gruneisen parameter for the binary liquid, has been computer by using the equation as follows

$$\Gamma_{mix} = \frac{b}{3} \left[\frac{K\eta_{mix}}{U_{mix}} \right]^{1/2} \cdot \left[\frac{V_{mix}^{1/2}}{M_{mix}^{1/2}} \right]$$

$$\Gamma^E = \Gamma^{12} - [\Gamma_1 X_1 + \Gamma_2 X_2]$$

$$\Gamma_{ideal} = [\Gamma_1 X_1 + \Gamma_2 X_2]$$

Where Γ_{ideal} is the geniuses parameter for ideal mixtures.

Γ^E is the excess geniuses parameter X_1 & X_2 and Γ_1 , Γ_2 are the mole fraction and geniuses parameter of the components 1 & 2.

Result and Discussion

The association of alkane and alcohol leads to interaction between the molecules. The experimental values of density, viscosity and ultrasonic velocity for the two liquids at 303.15 K are given in table 1.

The η^E values are negative for all composition range at 303.15K. The negative excess value of η^E demonstrate that there persists some kind of molecular interactions between the molecules of the binary liquid mixtures⁶.

Table-1

S.No.	Mole. Fraction (X_1)	Density(ρ) kgm ⁻³	$\eta_{mix} \times 10^3$ Nsm ⁻²	U ms ⁻¹	Free vol $\times 10^6$ m ³ mol ⁻¹	$P_i \times 10^{-7}$ atm	Γ_{mix}
1.	0.120	807.4	2.4087	1255	0.0426	0.5889	9.7958
2.	0.237	779.7	1.6403	1230	0.716	0.4877	8.2430
3.	0.348	773.0	1.3001	1215	0.0969	0.4556	7.6212
4.	0.452	762.7	1.2164	1190	0.1011	0.4413	7.3583
5.	0.554	745.9	0.9716	1170	0.1345	0.3933	6.5896
6.	0.651	730.2	0.6232	1150	0.2488	0.3249	5.4697
7.	0.740	715.6	0.5118	1130	0.3178	0.2983	5.0738
8.	0.834	692.6	0.4189	1120	0.4134	0.2705	4.6481
9.	0.918	670.2	0.3649	1110	0.4903	0.2524	4.4114

Table-2

The Value of Excess Volume, Viscosity Deviation and other Parameter Given In

S.No.	Mole. Fraction (X_1)	Density(ρ) kgm ⁻³	$\eta_{mix} \times 10^3$ Nsm ⁻²	U ms ⁻¹	$V^E \times 10^6$ m ³ mol ⁻¹	$P_i^E \times 10^{-7}$ atm	Γ_{mix}
1.	0.120	807.4	-0.7784	1255	-0.0426	-0.0480	-0.9814
2.	0.237	779.7	-1.1596	1230	-0.0716	-0.0940	-1.6242
3.	0.348	773.0	-0.1.1330	1215	-0.0969	-0.0739	-1.3827
4.	0.452	762.7	-0.8731	1190	-0.1011	-0.0392	-0.8368
5.	0.554	745.9	-0.7809	1170	-0.1345	-0.0391	-0.8122
6.	0.651	730.2	-0.8179	1150	-0.2488	-0.0618	-1.1776
7.	0.740	715.6	-0.5869	1130	-0.3178	-0.0446	-0.8502
8.	0.834	692.6	-0.-4084	1120	-0.4134	-0.0300	-0.5760
9.	0.918	670.2	-0.1848	1110	-0.4903	-0.0085	-0.1594

The V_f^E values are observed to be negative over the entire mole fraction range. The internal pressure values are negative for all the values of mole fractions at a certain temperature (303.15k)⁷.

The value of gruneisen parameter decreases with the rise in the mole fraction of hydrocarbons. The excess gruneisen parameters for all the system are found to be negative⁸.

Conclusion

From the above data of density, viscosity, speed of sound, some acoustical parameters and excess parameters for the mixture of hexane and 1-heptanol at T = 303.15K are calculated for the entire comparison range.

It is obvious that there exist the strong interaction between the molecules of n-hexane and 1-heptanol⁹.

The negative values of excess free volume suggests that there is specific interactions between unlike molecules¹⁰. The negative values of binary mixtures represents the developments of hydrogen bonds¹¹.

The excess internal pressure and excess gruneisen parameters studies in the present investigations is governed by unlike interaction between the components and there is strong inter molecular interactions between the components of binary system¹².

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