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# Thermo-Physical Properties of Heterocyclic Compounds with Aliphatic Alcohols at T = 303.15, 308.15 and 313.15 K

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The densities (ρ), speeds of sound (u), and viscosities (η) have been measured for ternary liquid mixtures of tetrahydrofuran in cyclohexanone with 1-hexanol and 1-octanol at 303.15-313.15 K over the entire range of mole fractions and at atmospheric pressure 0.1 MPa. These experimental data have been used to estimate the thermophysical properties of heterocyclic compounds with aliphatic alcohols at T = 303.15, 308.15 and 313.15 K. Preliminary data was used to assess the excess free volume, internal pressure and free energy of Gibbs, which were discussed in light of the molecular interaction surviving in the mixtures. Analysis of each of the two contributions, namely interaction, free volume $V^E$ showed that the contributions are positive for all systems. The variations of these parameters with the composition and the temperature were discussed with regard to the intermolecular interactions prevailing in these mixtures. These values also indicate the formation of a hydrogen bonding (C=O.....OH) between the hydrogen atom of aliphatic alcohol of 1-hexanol/1-octanol and oxygen atom of heterocyclic compounds tetrahydrofuran in cyclohexanone in the ternary liquid mixtures.

**Keywords: Density, Speed of sound, Viscosity, Tetrahydrofuran, Cyclohexanone, 1-Hexanol, 1-Octanol.**

## INTRODUCTION

Thermodynamic properties of the liquid mixture are widely used in designing calculations of various chemical engineering processes that involve chemical separations, fluid flows and heat transfer, moreover, their use is enormous in many other industrial applications. The study of molecular interactions in liquid mixtures is of great importance in molecular sciences where the results shed light on understanding the structural properties and the molecular environment of liquid mixtures [1-5].

1-Hexanol [$CH_3(CH_2)_5OH$], a colourless liquid is sparingly soluble in water, but miscible with diethyl ether, ethanol and used widely in the perfume industries. 1-Octanol is a fatty alcohol and also used for the synthesis of esters and in perfumes and flavours [6-8]. Octanol esters such as octyl acetate are found as components of essential oils and also utilized to assess the lipophilicity of pharmaceutical products [9,10]. Octanol is manufactured industrially by oligomerizing ethylene using triethylaluminum and then oxidizing the alkyl aluminum products through Ziegler alcohol synthesis route [11,12].

## EXPERIMENTAL

The chemicals used in this study *viz*. tetrahydrofuran (THF), cyclohexanone, 1-hexanol and 1-octanol were purchased from S.D. Fine Chemicals Ltd, India. Tetrahydrofuran was dried with KOH pellets for several hours and then distilled from sodium benzophenone ketyl followed by the addition of 5 g sodium wire and 15 g of benzophenone to 1 L THF in a boiling flask. The reaction mixture was refluxed for several hours until the solvent turn's deep blue in colour (less than 10 ppm). Cyclohexanone dissolved in potassium carbonate, then the aqueous layer was extracted using ether by salting out method and added to the distillate 0.2 g NaCl, washed with 10% NaOH solution to remove the acid and then added 5 g of anhydrous sodium sulfate to remove the drying agent by decantation method and finally washed with excess quantity of water, dried and purified.

1-Hexanol and 1-octanol were stirred on a water bath with 250 mL of 20% NaOH solution, the steam was distilled again as before, then dried with a little anhydrous calcium sulfate [13-18]. The ternary mixtures of all solutions of organic mixtures, THF, cyclohexanone, 1-hexanol and 1-octanol from 0.01 M to 0.09 M in steps of 0.01 M were prepared by weight [8]. All the solutions were left for 2 h and ensured the complete solubility.

**Procedure:** The sound densities and velocities of th pure liquids and their ternary mixtures were measured by digital oscillatory density and sound analyzer with the ability to reproduce ± $1\times10^{-6}$ g $cm^{-3}$ for density and ± $1\times10^{-2}$ m $s^{-1}$ for speed of sound. The speed of sound was measured using 2 MHz propagation time technique. The density meter was calibrated by dry air at atmospheric pressure, distilled water three times, and deionized water [19-25]. After each measurement, distilled water and anhydrous ethanol were used to clean the vibratory tube. Standard uncertainties associated with temperature, density and velocity measurements were estimated within ± 0.01 K, $0.5 \times 10^{-3}$ g $cm^{-3}$ and ± 0.5 m $s^{-1}$, respectively.

The viscosity of pure liquids and their ternary mixtures at atmospheric pressure were determined at T = 303.15-318.15 K by using the Ostwald viscometer, which was calibrated with benzene, carbon tetrachloride, acetonitrile and double distilled water. The viscometer was completely cleaned, dried and filled with sample liquid by installing the viscometer at 30 ºC and its ends were closed with Teflon covers to avoid evaporation. The viscometer was kept in a transparent-walled water bath with a thermal stability ± 0.1 K for 20 min to obtain thermal balance [26-29]. An electronic digital stopwatch with an uncertainty of ± 0.01 s was used for flow time measurements. The experimental uncertainties in viscosity were estimated at ± 1.06% and the uncertainties at ± 0.1 K. The purity of all of these solvents was compared to the measured densities, sound speeds and viscosity of the pure liquids with the literature [30-32].

## RESULTS AND DISCUSSION

The experimental densities and viscosity of all ternary systems are used in different combinations to calculate the thermodynamic functions by using the following equations:

$$V^E\ (m^3\ mol^{-1}) = [x_1M_1 + x_2M_2 + x_3M_3]/\rho - [x_1M_1/\rho_1 + x_2M_2/\rho_2 + x_3M_3/\rho_3] \quad (1)$$

$$\Delta\eta\ (mPa\ s) = \eta - (x_1\rho_1 + x_2\rho_2 + x_3\rho_3) \quad (2)$$

$$G^{*E}\ (J\ mol^{-1}) = RT\ [\ln \rho V - (x_1 \ln \eta_1 V_1 + x_2 \ln \eta_2 V_2 + x_3 \ln \eta_3 V_3)] \quad (3)$$

where ρ, η and V are density, viscosity and molar volume of the binary mixture. $x_1$, $M_1$, $\rho_1$, $\eta_1$, $V_1$ and $x_2$, $M_2$, $\rho_2$, $\eta_2$, $V_2$ are the mole fraction, molar mass, density, viscosity and molar volume of pure components 1 and 2, respectively [33-35]; R is the gas constant and T is the absolute temperature.

Experimental data are used to calculate the compressibility ($\kappa_s$) using the following relationship:

$$\kappa_s = (u^2\rho)^{-1} \quad (4)$$

Excess molar volumes, excess compressibility and excess Gibbs energy values to activate the viscous flow are shown in Tables 1-8. The excess molar volume data is affected by (i) dissociation of hydrogen bonds and loss of dipolar bonding, due to differences in the size and shape of the unlike molecules and (ii) intermolecular interactions such as hydrogen bonding or donor interactions between unlike molecules. The previous effect leads to positive excess molar volumes, while the latter effect produces negative values [36-38].

The experimental results indicate that negative values are prevalent in the current research for all ternary mixtures across the entire composition range at T = 303.15-318.15 K. The excess volume has a negative value for all systems studied over the entire composition range and at all studied temperatures (Figs. 1-4). The negative $V^E$ values indicated the presence of specific interactions such as the interaction of the hydrogen bonds between the mixing components, the dipole-dipole or the dipole induced interaction of the dipole leading to electron donor acceptor complexes.

There was a little ability to interact with hydrogen bonds between THF and cyclohexanone derivatives. Moreover, there was a possibility of electronic interactions between the donor and the acceptor between the THF electrolyte oxygen atom and cyclohexanone. In such interactions between donors and electron acceptor, THF acts as an electronic donor and the cyclohexanone act as an electronic donor. In this study, the interactions between THF, cyclohexanone and 1-hexanol can be attributed to the dipole-induced dipole interactions between the mixture components leading to the formation of electron acceptor-donor complexes.

TABLE-1
MEASURED VALUES OF DENSITY (ρ), VISCOSITY (η) AND ULTRASONIC VELOCITY (U) OF TETRAHYDROFURAN + CYCLOHEXANONE + 1-HEXANOL WITH 1-PROPANOL 303.15 K, 308.15 K AND 313.15 K

| Mole fraction | | Density (ρ) (Kg $m^{-3}$) | | | Viscosity (η) × $10^3$ (Ns $m^{-2}$) | | | Ultrasonic velocity (U) (m $s^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8000 | 805.0 | 802.0 | 799.0 | 0.5687 | 0.5687 | 0.5613 | 1243.0 | 1199.3 | 1179.6 |
| 0.0677 | 0.7323 | 811.2 | 808.2 | 805.2 | 0.5665 | 0.5665 | 0.5244 | 1200.4 | 1197.4 | 1181.3 |
| 0.1444 | 0.6556 | 825.0 | 822.0 | 819.0 | 0.5669 | 0.5669 | 0.5276 | 1194.2 | 1195.6 | 1183.4 |
| 0.2119 | 0.5881 | 831.7 | 828.7 | 825.7 | 0.5670 | 0.5670 | 0.5356 | 1198.3 | 1194.2 | 1187.7 |
| 0.3442 | 0.4558 | 838.4 | 835.4 | 832.4 | 0.5679 | 0.5679 | 0.5413 | 1196.3 | 1193.3 | 1191.2 |
| 0.4948 | 0.3052 | 845.2 | 842.2 | 839.2 | 0.6727 | 0.6727 | 0.5832 | 1185.6 | 1182.6 | 1193.3 |
| 0.5484 | 0.2516 | 852.4 | 849.4 | 846.4 | 0.6733 | 0.6733 | 0.6099 | 1175.8 | 1172.8 | 1195.2 |
| 0.6086 | 0.1914 | 859.5 | 856.5 | 853.5 | 0.7564 | 0.7564 | 0.6658 | 1165.0 | 1162.0 | 1197.7 |
| 0.7447 | 0.0553 | 866.7 | 863.7 | 860.7 | 0.7638 | 0.7638 | 0.6774 | 1154.8 | 1151.8 | 1199.2 |
| 0.8000 | 0 | 874.1 | 871.1 | 868.1 | 0.8976 | 0.8976 | 0.8965 | 1144.1 | 1141.1 | 1210.5 |

TABLE-2
CALCULATED VALUES OF ADIABATIC COMPRESSIBILITY (β), ACOUSTIC IMPEDANCE (Z) AND FREE LENGTH ($L_F$) OF TETRAHYDROFURAN + CYCLOHEXANONE + 1-HEXANOL AT 303.15 K, 308.15 K AND 313.15 K

| Mole fraction | | Adiabatic compressibility (β) × $10^{10}$ ($Pa^{-1}$) | | | Acoustic impedance (Z) × $10^{-7}$ (Kg $m^{-2}s^{-1}$) | | | Free length (LF) × $10^{11}$ (m) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8000 | 8.0401 | 8.6690 | 8.9946 | 0.1001 | 0.0962 | 0.0943 | 2.6144 | 2.5178 | 2.4718 |
| 0.0677 | 0.7323 | 8.5550 | 8.6298 | 8.8997 | 0.0974 | 0.0968 | 0.0951 | 2.5345 | 2.5235 | 2.4849 |
| 0.1444 | 0.6556 | 8.4995 | 8.5105 | 8.7187 | 0.0985 | 0.0983 | 0.0969 | 2.5428 | 2.5411 | 2.5106 |
| 0.2119 | 0.5881 | 8.3734 | 8.4615 | 8.5855 | 0.0997 | 0.0990 | 0.0981 | 2.5618 | 2.5485 | 2.5300 |
| 0.3442 | 0.4558 | 8.3343 | 8.4063 | 8.4664 | 0.1003 | 0.0997 | 0.0992 | 2.5679 | 2.5568 | 2.5477 |
| 0.4948 | 0.3052 | 8.4171 | 8.4900 | 8.3683 | 0.1002 | 0.0996 | 0.1001 | 2.5552 | 2.5442 | 2.5626 |
| 0.5484 | 0.2516 | 8.4857 | 8.5593 | 8.2707 | 0.1002 | 0.0996 | 0.1012 | 2.5448 | 2.5339 | 2.5777 |
| 0.6086 | 0.1914 | 8.5724 | 8.6469 | 8.1677 | 0.1001 | 0.0995 | 0.1022 | 2.5319 | 2.5210 | 2.5939 |
| 0.7447 | 0.0553 | 8.652 | 8.7274 | 8.0791 | 0.1001 | 0.0995 | 0.1032 | 2.5203 | 2.5094 | 2.6081 |
| 0.8000 | 0 | 8.7400 | 8.8163 | 7.8614 | 0.1000 | 0.0994 | 0.1051 | 2.5075 | 2.4967 | 2.6440 |

TABLE-3
EXCESS VALUES OF ADIABATIC COMPRESSIBILITY ($\beta^E$), FREE LENGTH (LFE) AND FREE VOLUME (VFE) OF TETRAHYDROFURAN + CYCLOHEXANONE + 1-HEXANOL AT 303.15 K, 308.15 K AND 313.15 K

| Mole fraction | | $\beta^E \times 10^{10}$ ($Pa^{-1}$) | | | $L_F^E \times 10^{10}$ (m) | | | $V_F^E \times 10^7$ ($m^3$ $mol^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0.0677 | 0.7323 | 3.8829 | 4.4378 | 4.3209 | -1.2627 | -1.2477 | -1.2627 | 10.4391 | 7.9033 | 8.2310 |
| 0.1444 | 0.6556 | 4.1527 | 4.7312 | 4.5494 | -1.2308 | -1.2089 | -1.2308 | 9.6376 | 6.3331 | 7.0318 |
| 0.2119 | 0.5881 | 4.4674 | 4.9333 | 4.7244 | -1.206 | -1.1829 | -1.2060 | 9.1928 | 4.9306 | 6.2664 |
| 0.3442 | 0.4558 | 4.8762 | 5.2887 | 4.9253 | -1.1775 | -1.1380 | -1.1775 | 7.7104 | 2.1691 | 4.2197 |
| 0.4948 | 0.3052 | 5.2142 | 5.5467 | 5.1165 | -1.1505 | -1.1090 | -1.1505 | 6.0263 | 4.7096 | 4.2879 |
| 0.5484 | 0.2516 | 5.2954 | 5.5990 | 5.2472 | -1.1311 | -1.1045 | -1.1311 | 6.6711 | 3.8843 | 4.8733 |
| 0.6086 | 0.1914 | 5.3769 | 5.6480 | 5.3875 | -1.1100 | -1.1007 | -1.1100 | 6.7356 | 5.9428 | 6.6053 |
| 0.7447 | 0.0553 | 5.6776 | 5.8764 | 5.5602 | -1.0848 | -1.0748 | -1.0848 | 5.5143 | 3.7297 | 4.8860 |
| 0.8000 | 0 | 5.9365 | 6.0691 | 5.8547 | -1.0389 | -1.0532 | -1.0389 | 7.4707 | 4.9870 | 9.7863 |

TABLE-4
EXCESS VALUES OF INTERNAL PRESSURE (πiE), VISCOUS RELAXATION TIME (τE) AND CHANGE IN GIBB'S FREE ENERGY (ΔG) OF 4-TETRAHYDROFURAN + CYCLOHEXANONE + 1-HEXANOL AT 303.15 K, 308.15 K AND 313.15 K

| Mole fraction | | $\beta^E \times 10^{10}$ ($Pa^{-1}$) | | | $L_F^E \times 10^{10}$ (m) | | | $V_F^E \times 10^7$ ($m^3$ $mol^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8000 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0.0677 | 0.7323 | 3.8829 | 4.4378 | 4.3209 | -1.2627 | -1.2477 | -1.2627 | 10.4391 | 7.9033 | 8.2310 |
| 0.1444 | 0.6556 | 4.1527 | 4.7312 | 4.5494 | -1.2308 | -1.2089 | -1.2308 | 9.6376 | 6.3331 | 7.0318 |
| 0.2119 | 0.5881 | 4.4674 | 4.9333 | 4.7244 | -1.206 | -1.1829 | -1.2060 | 9.1928 | 4.9306 | 6.2664 |
| 0.3442 | 0.4558 | 4.8762 | 5.2887 | 4.9253 | -1.1775 | -1.1380 | -1.1775 | 7.7104 | 2.1691 | 4.2197 |
| 0.4948 | 0.3052 | 5.2142 | 5.5467 | 5.1165 | -1.1505 | -1.1090 | -1.1505 | 6.0263 | 4.7096 | 4.2879 |
| 0.5484 | 0.2516 | 5.2954 | 5.5990 | 5.2472 | -1.1311 | -1.1045 | -1.1311 | 6.6711 | 3.8843 | 4.8733 |
| 0.6086 | 0.1914 | 5.3769 | 5.6480 | 5.3875 | -1.1100 | -1.1007 | -1.1100 | 6.7356 | 5.9428 | 6.6053 |
| 0.7447 | 0.0553 | 5.6776 | 5.8764 | 5.5602 | -1.0848 | -1.0748 | -1.0848 | 5.5143 | 3.7297 | 4.8860 |
| 0.8000 | 0 | 5.9365 | 6.0691 | 5.8547 | -1.0389 | -1.0532 | -1.0389 | 7.4707 | 4.9870 | 9.7863 |

TABLE-5
MEASURED VALUES OF DENSITY (ρ), VISCOSITY (η), ULTRASONIC VELOCITY (U) OF TETRAHYDROFURAN + CYCLOHEXANONE + 1-OCTANOL AT 303.15 K, 308.15 K AND 313.15K

| Mole fraction | | Density (ρ) (Kg $m^{-3}$) | | | Viscosity (η) × $10^3$ (Ns $m^{-2}$) | | | Ultrasonic velocity (U) (m $s^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8000 | 801.0 | 797.0 | 783.0 | 0.6214 | 0.5693 | 0.5653 | 1202.3 | 1172.6 | 1162.6 |
| 0.0677 | 0.7323 | 807.2 | 801.2 | 787.2 | 0.6517 | 0.5324 | 0.5284 | 1200.4 | 1174.3 | 1164.3 |
| 0.1444 | 0.6556 | 821.0 | 815.0 | 801.0 | 0.6574 | 0.5356 | 0.5316 | 1198.6 | 1176.4 | 1166.4 |
| 0.2119 | 0.5881 | 827.7 | 821.7 | 807.7 | 0.6740 | 0.5436 | 0.5396 | 1197.2 | 1180.7 | 1170.7 |
| 0.3442 | 0.4558 | 834.4 | 828.4 | 814.4 | 0.6863 | 0.5493 | 0.5453 | 1196.3 | 1184.2 | 1174.2 |
| 0.4948 | 0.3052 | 841.2 | 835.2 | 821.2 | 0.6954 | 0.5912 | 0.5872 | 1195.6 | 1186.3 | 1176.3 |
| 0.5484 | 0.2516 | 848.4 | 842.4 | 828.4 | 0.7285 | 0.6179 | 0.6139 | 1195.8 | 1188.2 | 1178.2 |
| 0.6086 | 0.1914 | 855.5 | 849.5 | 835.5 | 0.7499 | 0.6738 | 0.6698 | 1195.0 | 1190.7 | 1180.7 |
| 0.7447 | 0.0553 | 862.7 | 856.7 | 842.7 | 0.7672 | 0.6854 | 0.6814 | 1194.8 | 1192.2 | 1182.2 |
| 0.8000 | 0 | 870.1 | 864.1 | 850.1 | 0.9041 | 0.9045 | 0.9005 | 1194.1 | 1203.5 | 1193.5 |

TABLE-6
CALCULATED VALUES OF ADIABATIC COMPRESSIBILITY (β), ACOUSTIC IMPEDANCE (Z) AND FREE LENGTH (LF) OF TETRAHYDROFURAN + CYCLOHEXANONE + 1-OCTANOL AT 303.15 K, 308.15 K AND 313.15 K

| Mole fraction | | Adiabatic compressibility (β) × $10^{10}$ ($Pa^{-1}$) | | | Acoustic impedance (Z) ×$10^{-7}$ (Kg $m^{-2}$ $s^{-1}$) | | | Free length ($L_F$) × $10^{11}$ (m) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8000 | 8.6366 | 9.1252 | 9.4488 | 0.9630 | 0.9346 | 0.9103 | 2.5225 | 2.4541 | 2.4117 |
| 0.0677 | 0.7323 | 8.5974 | 9.0511 | 9.3710 | 0.9690 | 0.9408 | 0.9165 | 2.5283 | 2.4641 | 2.4217 |
| 0.1444 | 0.6556 | 8.4783 | 8.8661 | 9.1764 | 0.9841 | 0.9588 | 0.9343 | 2.5460 | 2.4896 | 2.4472 |
| 0.2119 | 0.5881 | 8.4293 | 8.7299 | 9.0336 | 0.9909 | 0.9702 | 0.9456 | 2.5533 | 2.5090 | 2.4665 |
| 0.3442 | 0.4558 | 8.3742 | 8.6081 | 8.9059 | 0.9982 | 0.9810 | 0.9563 | 2.5617 | 2.5267 | 2.4841 |
| 0.4948 | 0.3052 | 8.3163 | 8.5079 | 8.8007 | 1.0057 | 0.9908 | 0.9660 | 2.5706 | 2.5415 | 2.4989 |
| 0.5484 | 0.2516 | 8.2429 | 8.4082 | 8.6960 | 1.0145 | 1.0009 | 0.9760 | 2.5820 | 2.5565 | 2.5139 |
| 0.6086 | 0.1914 | 8.1855 | 8.3029 | 8.5857 | 1.0223 | 1.0115 | 0.9865 | 2.5911 | 2.5727 | 2.5300 |
| 0.7447 | 0.0553 | 8.1199 | 8.2125 | 8.4907 | 1.0308 | 1.0214 | 0.9962 | 2.6015 | 2.5868 | 2.5441 |
| 0.8000 | 0 | 8.0603 | 7.9899 | 8.2582 | 1.0390 | 1.0399 | 1.0146 | 2.6111 | 2.6226 | 2.5797 |

TABLE-7
EXCESS VALUES OF ADIABATIC COMPRESSIBILITY ($\beta^E$), FREE LENGTH ($L_F^E$) AND FREE VOLUME ($V_F^E$) OF TETRAHYDROFURAN + CYCLOHEXANONE + 1-OCTANOL AT 303.15 K, 308.15 K AND 313.15 K

| Mole fraction | | $\beta^E \times 10^{10}$ ($Pa^{-1}$) | | | $L_F^E \times 10^{10}$ (m) | | | $V_F^E \times 10^7$ ($m^3$ $mol^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8000 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0.0677 | 0.7323 | 4.292 | 4.3779 | 4.523 | -1.2678 | -1.2551 | -1.2342 | 9.5752 | 8.0394 | 8.4120 |
| 0.1444 | 0.6556 | 4.5123 | 4.6128 | 4.7675 | -1.2369 | -1.2231 | -1.2027 | 8.8089 | 6.8808 | 7.2532 |
| 0.2119 | 0.5881 | 4.6504 | 4.7929 | 4.9542 | -1.2178 | -1.1981 | -1.1782 | 8.6048 | 6.1364 | 6.5101 |
| 0.3442 | 0.4558 | 4.8801 | 5.0006 | 5.1678 | -1.1865 | -1.1694 | -1.1503 | 7.3332 | 4.1588 | 4.5323 |
| 0.4948 | 0.3052 | 5.1369 | 5.1988 | 5.3710 | -1.1515 | -1.1419 | -1.1238 | 5.6901 | 4.2035 | 4.5878 |
| 0.8000 | 0 | 8.0603 | 7.9899 | 8.2582 | 1.0390 | 1.0399 | 1.0146 | 2.6111 | 2.6226 | 2.5797 |

TABLE-8
EXCESS VALUES OF INTERNAL PRESSURE ($\pi_i^E$), VISCOUS RELAXATION TIME ($\tau^E$) AND CHANGE IN GIBB'S FREE ENERGY (ΔG) OF TETRAHYDROFURAN + CYCLOHEXANONE + 1-OCTANOL AT 303.15 K, 308.15 K AND 313.15 K

| Mole fraction | | $\pi_i^E \times 10^7$ $Nm^{-2}$ | | | $\tau^E \times 10^{-5}$ (S) | | | $\Delta G \times 10^{-23}$ (KJ $mol^{-1}$) | | |
|---|---|---|---|---|---|---|---|---|---|---|
| $X_1$ | $X_2$ | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K | 303.15 K | 308.15 K | 313.15 K |
| 0 | 0.8000 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 0 |
| 0.0677 | 0.7323 | -0.3682 | -0.3899 | -0.3925 | 0.5802 | 0.6195 | 0.6264 | -2.0612 | -2.1045 | -2.1419 |
| 0.1444 | 0.6556 | -0.3684 | -0.3944 | -0.3971 | 0.6696 | 0.7213 | 0.7295 | -2.0725 | -2.1181 | -2.1555 |
| 0.2119 | 0.5881 | -0.3654 | -0.3989 | -0.4016 | 0.7225 | 0.7964 | 0.8055 | -2.0781 | -2.1271 | -2.1644 |
| 0.3442 | 0.4558 | -0.3756 | -0.4161 | -0.4193 | 0.8506 | 0.953 | 0.9639 | -2.0931 | -2.1466 | -2.1838 |
| 0.4948 | 0.3052 | -0.3903 | -0.4137 | -0.4171 | 1.0033 | 1.0739 | 1.0859 | -2.1114 | -2.1572 | -2.1940 |
| 0.5484 | 0.2516 | -0.3767 | -0.4038 | -0.4071 | 1.0169 | 1.1040 | 1.1162 | -2.1113 | -2.1587 | -2.1953 |
| 0.6086 | 0.1914 | -0.3705 | -0.3793 | -0.3824 | 1.0564 | 1.0967 | 1.1084 | -2.1152 | -2.1533 | -2.1895 |
| 0.7447 | 0.0553 | -0.3787 | -0.3936 | -0.3971 | 1.1824 | 1.2507 | 1.2642 | -2.1300 | -2.1722 | -2.2083 |
| 0.8000 | 0 | -0.3272 | -0.3053 | -0.3080 | 1.1131 | 1.0706 | 1.0804 | -2.1175 | -2.1412 | -2.1762 |

When the hydrogen atoms of THF and cyclohexanone were replaced by an oxygen atoms, the charge in the bond away from the loop was transferred to the oxygen atom (-I effect) -OH group in 1-hexanol (+I effect) leaving a positive charge. However, the oxygen atom/-OH group has acted as a hydrogen bond acceptor as well as donor in case of 1-hexanol for the donor-acceptor association [39-42]. As a result of these two opposite effects, there may be a net transfer of a negative charge from the ring to the -OH to enhance the acceptor's ability of the hydrocarbons. Therefore, the interaction between the heterocyclic rings increased when oxygen is attached to the ring.

The $V^E$ data (Table-3) of ternary systems of THF and cyclohexanone systems showed more positive $V^E$ values than before. A oxygen atom in THF (-I effect) of an electron pulls an atom, and tries to attract the σ-electrons of the heterocyclic ring and thus the electron density of the heterocyclic ring decreases. As a result, the heterocyclic ring in THF and cyclohexanone becomes a relatively electronic donor towards an electron seeking a proton from any group. Thus, THF and cyclohexanone reacts strongly with 1-hexanol which leads to more positive $V^E$ values. The experimental results in the current investigation also supported this claim.

The $V^E$ data exhibit the positive values for a THF ternary system with cyclohexanone with 1-hexanol mixtures due to high dipole moment and dielectric constant. The THF and cyclohexanone are assumed to be a relatively complex molecule and its non-idealization arises because the oxygen group rotates freely along the C-O axis, so it gives more flexibility to the reaction created by two highly polar -OH bond. Further-more, the most positive $V^E$ value of the 1-hexanol and 1-octanol mixture with THF and cyclohexanone when compared to other

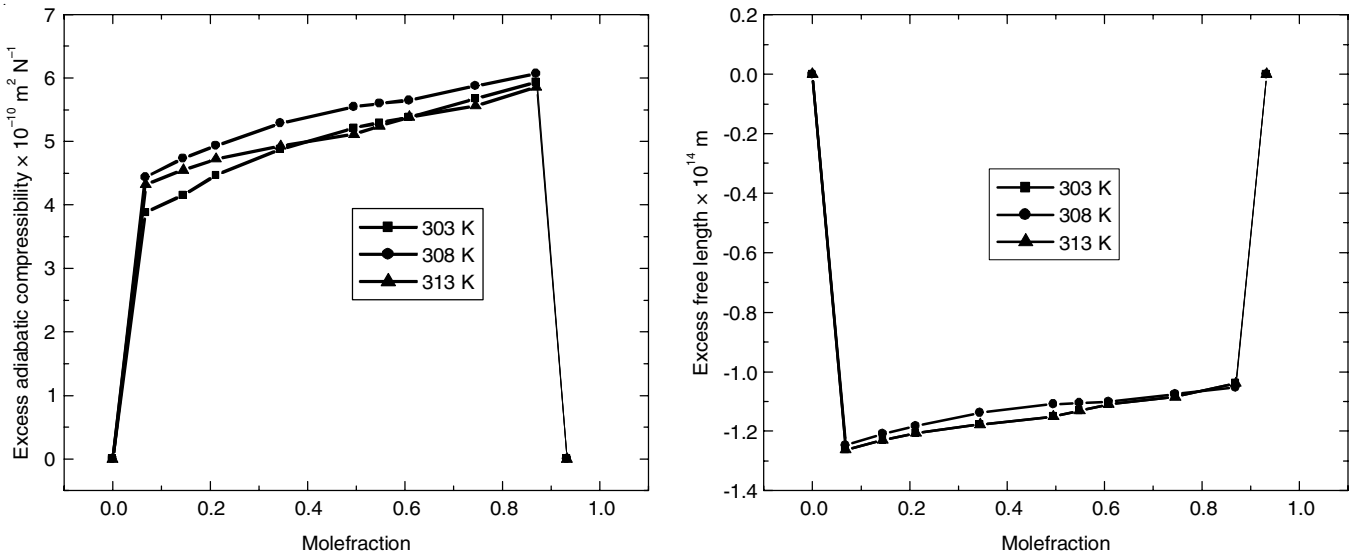


Fig. 1. Plots of excess values of adiabatic compressibility ($\beta^E$), free length ($L_F^E$) for various mole fraction (X) of tetrahydrofuran + cyclohexanone + 1-hexanol at 303.15 K, 308.15 K and 313.15 K

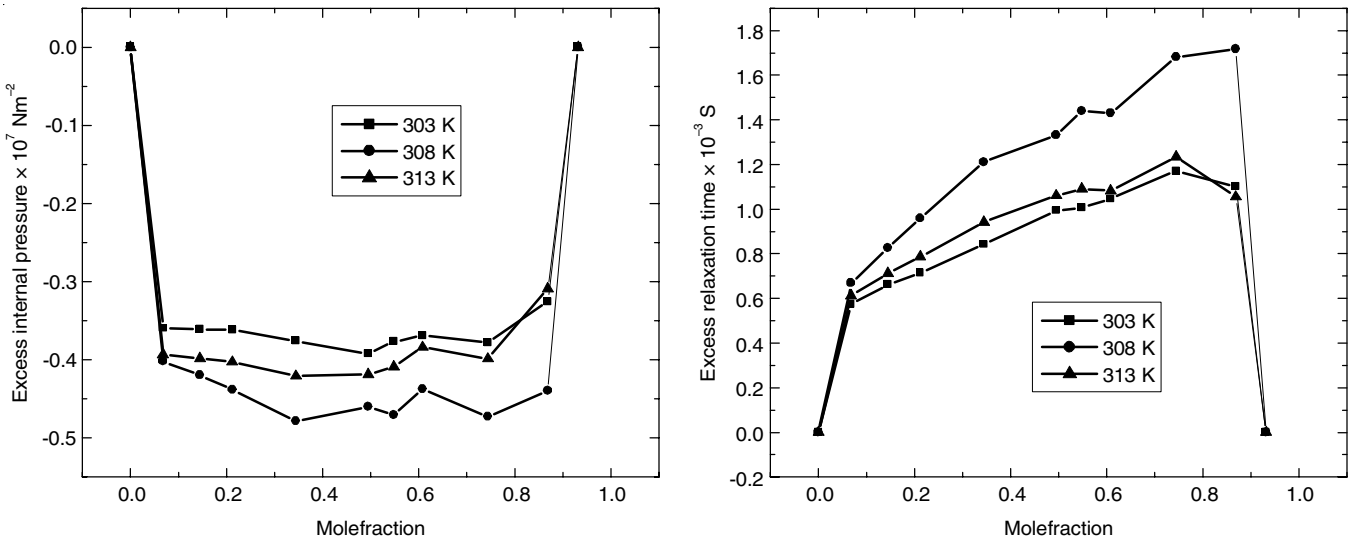


Fig. 2. Plots of internal pressure ($\pi_i^E$), relaxation time ($\tau^E$) for various mole fraction (X) of tetrahydrofuran + cyclohexanone + 1-hexanol at 303.15 K, 308.15 K and 313.15 K

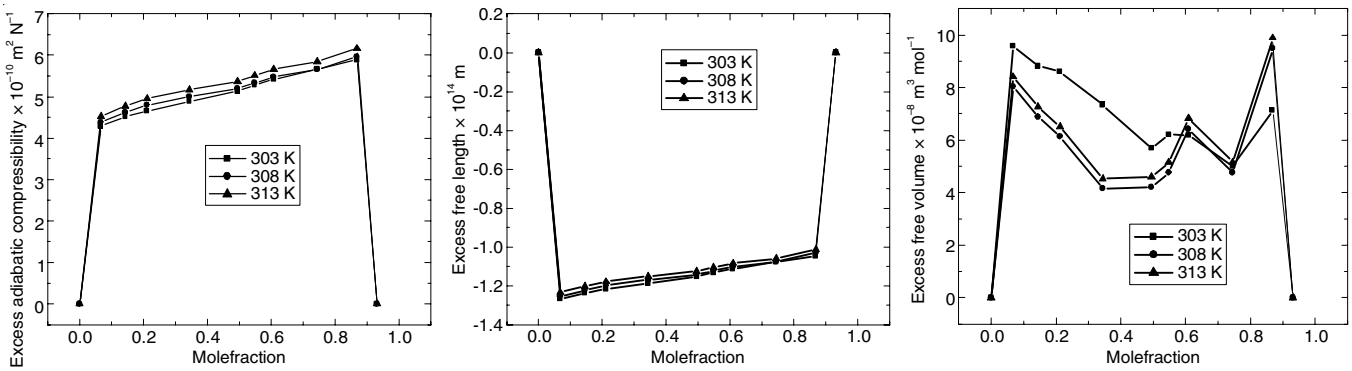


Fig. 3. Plots of excess values of adiabatic compressibility ($\beta^E$), free length ($L_F^E$) and free volume ($V_F^E$) for various mole fraction (X) of tetrahydrofuran + cyclohexanone + 1-octanol at 303.15 K, 308.15 K and 313.15 K

mixtures, which may also be due to (i) medium positive and positive electromechanical effects; (ii) the sticky nature of THF and cyclohexanone.

The $V^E$ values with respect to the unshared component are in the order: THF + cyclohexanone + 1-hexanol < 1-octanol. This arrangement indicates that the electron acceptance ability

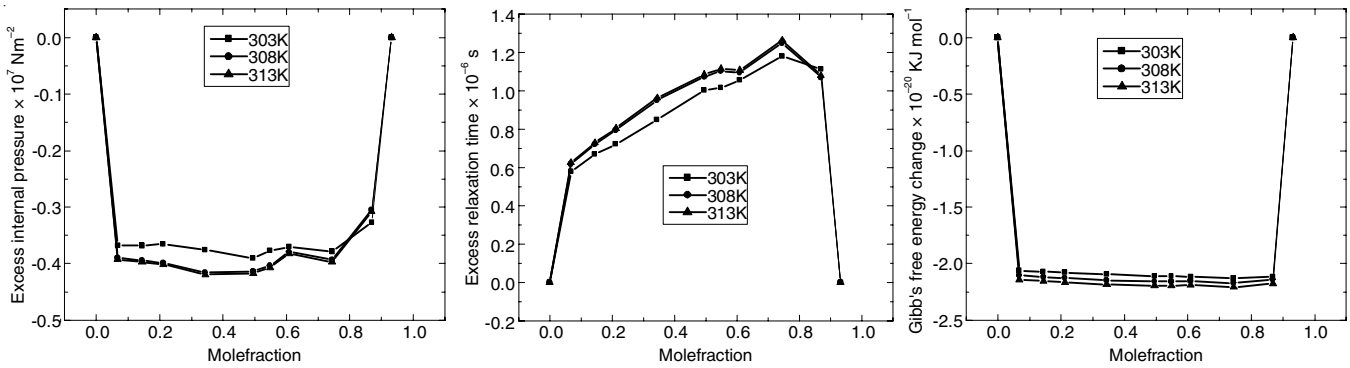


Fig. 4. Excess values of internal pressure ($\pi_i^E$), viscous relaxation time ($\tau^E$) and change in Gibb's free energy ($\Delta G$) for various mole fraction (X) of tetrahydrofuran + cyclohexanone + 1-octanol at 303.15 K, 308.15 K and 313.15 K

decreases with increasing hydroxyl/electron acceptor group in the heterocyclic derivatives. An increase in $V^E$ values with an increase in temperature may be due to factors (i) components being blocked at a higher temperature, (ii) weak bipolar dipole reactions due to a decrease in polarizations and (iii) an increase in kinetic energy at higher temperatures.

The excess isentropic compressibility data (Table-3) indicates that the excess isentropic compressibility data for all ternary systems are positive across the entire temperature range (T = 303.15-318.15 K). The observed values can be interpreted qualitatively as (i) disruption of associated structures/ molecular arrangement in pure liquids, (ii) formation of weak bonds through dipole-induced dipole interaction between reverse molecules and (iii) change in the different sizes of mixing components. The first factor contributes to positive values, while the remaining two factors lead to negative values. The resulting positive values of the ternary systems indicated that the ternary systems are more compressive than the ideal mixtures.

Excess isentropic compressibility values for all ternary systems are in order: THF + cyclohexanone + 1-hexanol < 1-octanol. The above arrangement indicates that the extent of the interaction between the molecules in contrast increases with the polarization value and the appropriate dipole alignment of the components. The increase in the positive values with the increasing temperature indicates a decrease in specific reactions due to the enhanced thermal energy.

The observed negative opposite behaviour in $\beta^E$ curves over the entire composition range of the systems strengthened the view that the structure breaking effect and weak interactions between unlike molecules dominates in all the ternary systems. Molecular association, which is a measure of non-ideality of the system, shows positive deviation from zero for all the two systems under study [41]. This suggests that the non-ideality in these systems varies in order: THF + cyclohexanone + 1-hexanol < 1-octanol.

## Conclusion

In this work, the density, speed of sound and viscosity data was reported for ternary liquid mixtures of THF + cyclohexanone +1-hexanol and 1-octanol at different temperatures. The excess parameter studies such as $V^E$, $\beta$ indicate that the rupture of hydrogen bonded chain of the dipolar interaction between like molecules exceed the intermolecular interaction through dipole-dipole and hydrogen bonding between THF, cyclohexanone, 1-hexanol and 1-octanol. Moreover, the $V^E$ values showed that the interactional contribution is the factor for positive values of excess molar quantities. The results were analyzed in terms of molecular interactions through dipole-dipole interactions between the components of the mixtures, which leads to the formation of acceptor-donating electron complexes.

## CONFLICT OF INTEREST

The authors declare that there is no conflict of interests regarding the publication of this article.

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