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Acoustical properties of molecular interactions in 1-propanol, 1-butanol and 1-pentanol with tetrahydrofuran in cyclohexanone at various temperatures.

Ubagaramary D[1,2*], Muthu Vijayan Enoch IV[3], Mullainathan S[4], Kesavaswamy[5]

[1]R&D Centre, Bharathiyar University, Coimbatore, Tamil Nadu, India

[2]Adhiyamaan College of Engineering, Hosur, India

[3]Department of Chemistry, Karunya University, Coimbatore, Tamil Nadu, India

[4]Department of Physics, Thiru. Vi. Ka. Government Arts College, Thiruvarur, Tamil Nadu, India

[5]Department of Physics, Ramakrishna Engineering College, Coimbatore, Tamil Nadu, India

Abstract

The functions of ultrasonic velocity, density and viscosity for ternary liquid mixtures of 1-proponol, 1-butanol and 1-pentanol with tetra hydro furan are determined by 303.15 K-313.15 K. This data is used to calculate various parameters like the excess free volume, excess internal pressure and Gibb's free energy, which is used to discuss molecular interactions in the ternary liquid mixtures.

Keywords: Ternary mixtures, Ultrasonic velocity, Excess free volume, Viscosity predictive models.

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Introduction

In current years, ultrasonic speeds are effectively used in the energetic environment of molecular interactions in pure liquids and liquid compounds. Ultrasonic technique shows the physical chemical behaviour of liquids as part of a pointer to comfort. The molecular coordination between liquid compounds components is based on analysis concentrations. Mixed compounds are designed for spectroscopic technique. Spectroscopic methods were very common for these exercises. It is responsible for the nature properties of molecular contact in the body environment and liquid compounds. The ultrasonic speed of a fluid is attached.

Attractive forces between polar molecules form from the middle (water), not from direct contact between membrane molecules. Inactive participants in hydrophobic materials hydrophilic events. The liquid hydrocarbon is similar to the hydrocarbon molecules of the molecular interaction of a hydrocarbon with water molecules in aqueous solution.

Hydrophilic effect is an indirect result of strong directional relationships between water molecules and those interactions. The hydrophilic effect consists entirely of water; It is the result of the distinctive molecular structure of water and the unique harmonious properties of water. We can understand molecular and thermodynamic explanations for hydrophobic effect.

The molecular exchanges in liquid water are very complex, surprising and influential, and we have to pay special attention to them. Biology and biochemistry are taking place in complex acupuncture contexts. Living organisms are 80% water weight. The life we know on earth is entirely dependent on water. The main water source of structures and properties of cellular assemblies and argons and biochemical reactions. Water is a reactive chemical and biologic (Hydrolysis and diabetes/ suppression), some of the most direct and critical participants of central and global reactions. Bio-polymers are collected by diabetes/allergy, all of which are broken down by hydrolysis.

Molecular interaction is associated with 1-alkanol hybrids, which are one of the most unique components since the alkonols group is very polar, because it is deeply with other groups that attraction of polar ends. Tetrahydrofuran THF is a heterocyclic organic compound formation ($(CH_2)_4O$). It is a colourless low viscosity fluid with a perfume compared to diethyl ether [1-4]. It is one of the highest polar ethers. THF is the equivalent of the aromatic composite furan entirely hydrogenated. The most widely used industrial process involves the acid-catalysed dehydration of 1, 4 butane diol. Ashland/ISP route is one the biggest producers of this chemical. The method is similar to the production of ethanol. Du developed a process for producing THF by oxidizing n-butane to crude malefic anhydride, followed by catalytic hydrogenation. A third major industrial route of hydroformylation alkyl alcohol followed by hydrogenation to entail the butanediol.

The structure of tetrahydrofuran is given by Figure 1.

Cyclohexanone is heterocyclic compound. It is highly inert towards ordinary temperature at an electrophile or nucleophile. Non-polar being cyclohexanone is not expected to be involved

in any strong interaction with the other components of the mixture [5,6]. However, types of dispersive interactions between them are possible. The structure of cyclohexanone is given by Figure 2.

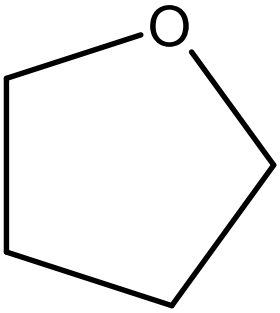

Figure 1. *Structure of tetrahydrofuran.*

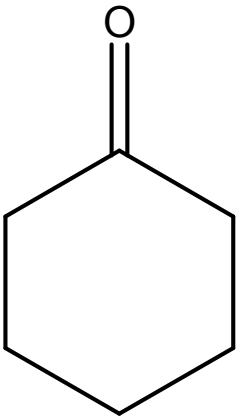

Figure 2. *Structure of cyclohexanone.*

Therefore, tentative studies have been taken by the authors to distinguish between the system of THF+cyclohexanone+1-propanol, 1-butanol and1-pentanol over ultrasonic velocity extents at 303.15 K-313.15 K. The determination of molecular interactions in this study is used to illustrate the effect of these classifications and consequently to regulate the length of the chain 1-alkanols. It says that in all the mixtures mole fraction increase in temperature due to decrease in thermal agitation.

The structure of 1-propanol, 1-butanol and 1-pentanol are given by Figure 3.

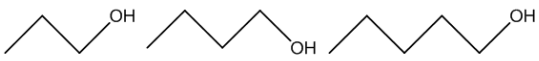

Figure 3. *Structures of 1-propanol, 1-butanol and 1-pentanol.*

Materials and Methods

The mixtures of mole fraction in various concentrations were prepared by taking spectroscopic analytical reagent grade and reagent grade chemicals with minimum assay of 99.9% and obtained from E Merck Ltd. (India). In all the mixtures, the mole fraction of the second component, cyclohexanone (X_2=0.4), was kept fixed while the mole fractions of the remaining two (THF X_1 and 1-propanol X_3) were varied from 0.0 to 0.8, so as to have different concentration of the mixture. There is nothing significant in fixing the mole fraction of the second component at 0.4. The density, viscosity, and ultrasonic velocity were measured as a function of concentration of the liquid ternary mixture at 303.15 K-313.15 K.

Velocity measurement

Ultrasonic velocity measurements were made using an ultrasonic interferometer (Model M-81, supplied by M/S Mittal Enterprises, New Delhi), having the frequency of 3 MHz has been used for velocity measurements at T=303.15 K-313.15 K with the accuracy of ± 0.1 $m.s^{-1}$. The measuring cell is a specially designed interferometer of double-walled vessel with provision for temperature constancy. An electronically operated digital constant temperature bath (Model SSI-03 Spl, supplied by M/S Mittal Enterprises, New Delhi), 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.

$U=n\lambda \rightarrow (1)$

Where n is the frequency of the ultrasonic waves. λ is the wavelength.

Density measurement

The mixture of densities was measured using a 10 ml specific gravity bottle method by measurement with an accuracy of ± relative specific gravity of 0.01 kgm^{-3}. The mixture bottle was immersed in the temperature-controlled experiment with the bath water. The weight of the sample was measured using an electronic digital balance with an accuracy of ± 0.1 mg (model: SHIMADZUAX-200, Kyoto, Japan).

$\rho_s=(W_S/W_w) \times \rho_w \rightarrow (2)$

ρ_w is the density of water.

ρ_s is the density of solution.

W_S is the weight of solution.

W_w is the weight of water.

Viscosity measurement

Measurements Ostwald viscometer 10 ml ± 0.01 Ns^{-1} m^{-2} was used for measuring viscosity of flowing time with the accuracy of ± 0.1 was determined using a digital precision racer stop watch.

$\eta_s \rightarrow (3)$

Where

η_s-Viscosity of the solution,

η_0-Viscosity of water.

ρ-Density of the solution.

ρ_0-Density of water.

t-The time flow for the solution.

t_0-The time flow for water.

Results and Discussion

The density (ρ), viscosity (η) and the ultrasonic velocity (U) of pure liquids and three ternary liquid systems at 303.15 K-313.15 K are tabulated in Table 1 and Figure 1 and the additional standard viscosity, adiabatic compressibility, free length free module, internal pressure, energy, free volume, internal pressure, Gibb's energy free energy and Gruenberg interaction parameter 'd' are also listed in the Table 2.

Table 1. *Measured values of density (ρ) of the pure liquids at 303.15 K.*

	Density (ρ) kgm^{-3}		Reference
Components	**Observed values**	**Literature values**	
Tetrahydrofuran (THF)	870	877.1	Rathnam et al. (2013)
Cyclohexanone	946.4	940	Nayeem et al. (2014)
1-propanol	798	801.1	Palani et al. (2008)
1-butanol	800	805	Nayeem et al. (2014)
1-pentanol	802	809	Palani et al. (2008)

Table 2. *Values of density (ρ) viscosity (η) and ultrasonic velocity (U) for THF (X_1)+cyclohexanone (X_2)+1-propanol (X_3) and THF (X_1)+cyclohexanone (X_2)+1-pentanol (X_3) at THF (X_1)+cyclohexanone (X_2)+1-pentanol (X_3) at 303.15 K-313.15 K.*

Mole fraction (X_3)	Density (ρ) Kgm^{-3}			Viscosity (η) × 10^3 Nsm^{-2}			Ultrasonic velocity (U) ms^{-1}		
	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**
THF (X_1)+cyclohexanone (X_2)+1-propanol (X_3) at 303.15-313.15 K.									
0	758.8	755.7	752.6	0.6174	0.5687	0.5613	1202.3	1192.4	0.5613
0.1444	751	755.6	749.1	0.6477	0.5665	0.5244	1200.4	1194.3	0.5244
0.2119	750.5	740.6	748.8	0.6534	0.5669	0.5276	1198.6	1196	0.5276
0.3442	739.3	738.4	735.9	0.67	0.567	0.5356	1197.2	1197.2	0.5356
0.4948	730.3	734.1	730.4	0.6823	0.5679	0.5413	1196.3	1199.7	0.5413
0.5484	729.9	732.6	729.9	0.6914	0.6727	0.5832	1195.6	1200.7	0.5832
0.6086	725.2	731.6	724.7	0.7245	0.6733	0.6099	1195.8	1202.2	0.6099
0.7447	723.1	730.3	713.1	0.7459	0.7564	0.6658	1195	1209.3	0.6658
0.8	722.3	729.8	704.7	0.7632	0.7638	0.6774	1194.8	1218.2	0.6774
THF (X_1)+cyclohexanone (X_2)+1-butanol (X_3) at 303.15 K-313.15 K.									
0	758.8	755.7	752.6	0.6174	0.5687	0.5613	1202.3	1192.4	1182.6
0.1444	756.6	755.6	750.3	0.6346	0.5672	0.5543	1202.7	1194.3	1184.3
0.2119	755.9	750.3	748.8	0.6583	0.5669	0.5413	1204.2	1196	1186.4
0.3442	748.1	745.8	743	0.6845	0.5658	0.5348	1209.5	1197.9	1193.6
0.4948	746	740.6	740.7	0.7076	0.5649	0.5244	1210.3	1199.7	1194.2
0.5484	743.8	739.1	738.4	0.7133	0.6724	0.5689	1214.9	1200.6	1195.4
0.6086	740.9	738.4	735.9	0.7272	0.6733	0.6099	1218.2	1202.2	1196.3
0.7447	736.5	730.5	723.7	0.9528	0.7865	0.6321	1220.8	1210.4	1198.2
0.8	732.8	729.3	725.1	1.0138	0.7638	0.6774	1224.6	1218.2	1202.2

THF (X_1)+cyclohexanone (X_2)+1-pentnol (X_3) at 303.15 K-313.15 K.									
0	758.8	755.7	752.6	0.6174	0.5687	0.5613	1202.3	1192.4	1182.6
0.1444	751	755.6	749.1	0.6477	0.5665	0.5244	1200.4	1194.3	1184.3
0.2119	750.5	740.6	748.8	0.6534	0.5669	0.5276	1198.6	1196	1186.4
0.3442	739.3	738.4	735.9	0.67	0.567	0.5356	1197.2	1197.2	1190.7
0.4948	730.3	734.1	730.4	0.6823	0.5679	0.5413	1196.3	1199.7	1194.2
0.5484	729.9	732.6	729.9	0.6914	0.6727	0.5832	1195.6	1200.7	1196.3
0.6086	725.2	731.6	724.7	0.7245	0.6733	0.6099	1195.8	1202.2	1198.2
0.7447	723.1	730.3	713.1	0.7459	0.7564	0.6658	1195	1209.3	1200.7
0.8	722.3	729.8	704.7	0.7632	0.7638	0.6774	1194.8	1218.2	1202.2

1-propanol and as THF and cyclohexanone at 303.15 K-313.15 K 1-butanol in the mixture having a mole fraction dissimilarity additional acoustic parameters [7,8]. Higher thermodynamic properties of liquid mixtures of the molecular interaction between molecules in the direction established to be the most elegant. Depending on the strength of the interaction between different molecules identified and due to the high level of sign and size of irregularity of excess of parameters.

Table 3 shows that the Gibbs's free energy values may be worthy of significant interactions such as hydrogen bonding, which can lead to negative irregularities [9,10].

Table 3. *Excess values of internal pressure (π_i^E), Gibb's free energy (ΔG) and Gruenberg interaction parameter for THF+cyclohexanone (X_1)+ 1-propanol (X_2), THF (X_1)+cyclohexanone+1-butanol (X_2) and THF (X_1)+cyclohexanone (X_2)+ 1-pentanol (X_3) at 303.15 K-313.15 K.*

Mole fraction	**$\pi_i^E \times 10^7$ Nm^{-2}**			**$\Delta G \times 10^{-23}$ kJ mol^{-1}**			**d**		
	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**
THF (X_1)+cyclohexanone (X_2)+1-propanol (X_3) at 303.15 K-313.15 K.									
0	0	0	0	0	0	0	0	0	0
0.1444	-0.0344	-0.3697	-0.367	-2.0695	-2.1185	-2.1428	-0.0135	-0.0155	-0.0167
0.2119	-0.0344	-0.4044	-0.3817	-2.0768	-2.1292	-2.1526	-0.0063	-0.0073	-0.0078
0.3442	-0.0355	-0.4281	-0.3995	-2.0774	-2.1415	-2.1562	-0.0042	-0.005	-0.0052
0.4948	-0.0366	-0.4737	-0.427	-2.0874	-2.1652	-2.1718	-0.0025	-0.003	-0.0032
0.5484	-0.0389	-0.4668	-0.4337	-2.1025	-2.162	-2.1793	-0.0017	-0.0018	-0.0021
0.6086	-0.0412	-0.4849	-0.4333	-2.0991	-2.1718	-2.1772	-0.0015	-0.0016	-0.0018
0.7447	-0.0408	-0.4667	-0.424	-2.1003	-2.1614	-2.1664	-0.0013	-0.0013	-0.0015
0.8	-0.041	-0.5104	-0.451	-2.1119	-2.1852	-2.1805	-0.001	-0.001	-0.0012
THF (X_1)+cyclohexanone (X_2)+1-butanol (X_3) at 303.15 K-313.15 K.									
0	0	0	0	0	0	0	0	0	0
0.1444	-0.3687	-0.3713	-0.3458	-2.0757	-2.1175	-2.2696	-0.0138	-0.0155	-0.0158
0.2119	-0.3861	-0.4005	-0.3717	-2.0779	-2.1308	-2.2737	-0.0062	-0.0073	-0.0076
0.3442	-0.4045	-0.4266	-0.3951	-2.076	-2.1428	-2.2745	-0.0041	-0.005	-0.0052
0.4948	-0.4444	-0.4735	-0.4298	-2.0857	-2.1669	-2.2776	-0.0024	-0.0031	-0.0033
0.5484	-0.501	-0.4648	-0.4351	-2.1014	-2.1629	-2.2617	-0.0017	-0.0018	-0.0021
0.6086	-0.5172	-0.4827	-0.4246	-2.1034	-2.1726	-2.2482	-0.0015	-0.0016	-0.0018
0.7447	-0.4415	-0.4547	-0.4327	-2.0603	-2.1533	-2.2382	-0.0009	-0.0012	-0.0015

0.8	-0.471	-0.5127	-0.4369	-2.064	-2.1843	-2.2255	-0.0006	-0.001	-0.0012
THF (X_1)+cyclohexanone (X_2)+1-pentnol (X_3) at 303.15 K-313.15 K.									
0	0	0	0	0	0	0	0	0	0
0.1444	4.7215	4.7724	4.7777	0.1026	8.0776	8.262	-0.0135	-0.0155	-0.0167
0.2119	4.7477	4.6226	4.8167	9.4812	6.4764	7.0583	-0.0063	-0.0073	-0.0078
0.3442	4.6381	4.6233	4.7281	9.276	5.0575	6.2902	-0.0042	-0.005	-0.0052
0.4948	4.6112	4.627	4.7283	7.9892	2.3085	4.2359	-0.0025	-0.003	-0.0032
0.5484	4.7129	4.6455	4.7734	6.326	4.7393	4.3042	-0.0017	-0.0018	-0.0021
0.6086	4.6961	4.6641	4.7417	6.8568	3.6837	4.8919	-0.0015	-0.0016	-0.0018
0.7447	4.7024	4.767	4.6332	6.8257	5.533	6.6304	-0.0013	-0.0013	-0.0015
0.8	4.7952	4.9169	4.5581	5.6272	3.026	4.9046	-0.001	-0.001	-0.0012

In the current study, all structures attained high negative dispersion force ΔGE Gibb shows the apparent power. In recent years, characteristics of the accumulation of positive ΔGE in some ternary liquid mixture, different molecules of hydrogen bond formation in tetrahydrofuran (THF) +cyclohexanone+1-propanol, tetrahydrofuran (THF) +cyclohexanone+1-butanol and tetrahydrofuran (THF) +cyclohexanone+1-pentanol at 303.15 K-313.15 K.

The corresponding values are tabulated in the Table 2 and the increasingly negative as the quality of the system of 1-propanol, 1-butanol and 1-pentanol is lacking these standard due to increasing of temperature [11-14]. Table 3 shows that the magnitude of Gruenberg and Nissan equivalent parameter (*d*) is in the strong interaction between the components. Standards specify different types of interactions were added. Strong interaction indicates a large positive values and small positive values for the weak interaction and no interaction refers to the large negative values. Negative values should be recognized widely, depending on the strength of the forces. The anti-hydrogen bonds present in the additional component of mixtures. In the current study, no specific interactions between unlike molecules in ternary structures, the negative values of '*d*' may be attributed [15,16]. The decreasing values of '*d*' with increasing of temperature through the interaction between the components of mixtures shows weakening.

As a measure of deviation from the ideal behaviour and the combination of excess parameters are found to be strong intermolecular interactions between molecules of the mixture.

The higher values of unlike molecules are positive for the weak interaction between molecules. Whereas, the negative excess parameters in unlike molecules may be due to the presence of dipole-dipole, dipole-induced dipole, charge transfer and hydrogen bonding whereas those of dipole-dipole, dipole-induced dipole, charge transfer and hydrogen bonding between unlike molecules gives negative excess parameters. Ultrasonic velocity dispersion in the system that causes dispersion should contain information about the relaxation time τ. Due to the structural relaxation process of relaxation time 10-12 s, it is said that it would molecules rearranged due to the co-operative process [16-18].

The excess values of internal pressure, adiabatic compressibility and Gibbs free energy indicate that the strength of the interaction between molecules with changing temperatures do not vary much and mole fraction in the case of THF+cyclohexanone+1-propanol mixture, while change clearly is able to detect in THF+cycloxanone+1-butanol and 1-pentanol mixture [19].

This is due to the fact that THF+cycloxanone+1-propanol there may be a large dipole in comparison to THF+cycloxanone+1-butanol mixture. Hence, in combination with the larger substrate interaction of THF+cycloxanone+1-propanol intermolecular interaction in the mixture containing 1-propanol in cycloexanone is large compared to that containing 1-butanol and 1-pentanol in ternary liquid mixture.

Conclusion

The validity paper which presents and conclusions drawn:

1. The net increase in the mole fraction of THF increases the strong interactions. If the medium also becomes more compact, the speed increases and the continued observance of the two systems (THF+cyclohexanone+1-butanol and THF +cyclohexanone+1-pentanol).

2. The increase in temperature due to thermal agitation, resulting in a decrease in velocity of ultrasonic mutual decreases at higher temperatures. An increase in viscosity with increase in mole fraction of THF 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.

3. The VFE negative values over the full range of mole fraction may be due to the difference in size and the shape of the molecules.

4. The adiabatic compressibility suggests that the lack of interaction between unlike molecules that have the minimum declarations.

5. Unlike molecules, weak interactions provide positive higher values, while the dipole-dipole, dipole-induced dipole, charge transfer and hydrogen bonding are unlike the molecules of negative ones [19]. From the magnitude of velocity, there is molecular interactions in the combination of THF and cyclohexanone mixture, which are linked to the keto group of oxygen atoms, resulting in a weak link between them. However, the mixture is more reactive with 1-propanool. 1-propaneol hydroxyl group is bound to the sp3 hybrid carbon atom and easily removed. This shows that the reaction rate with 1-propanool is faster than 1-butanol and 1-pentanol. As the magnitude of VFE, the survival of molecular connections in the mixture is increasing:

THF+cyclohexanone+1-propanol>1-butanol>1-pentanol.

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*Correspondence to

Ubagaramary D

R&D Centre

Bharathiyar University

Tamil Nadu

India