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ULTRASONIC STUDIES IN BINARY LIQUID MIXTURES OF TRICHL OR OETHYLENE WITH THREE ALCOHOLS

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ABSTRACT

When conducted in binary liquid mixtures, ultrasonic studies yield extremely useful information regarding the interactions between molecules as well as the thermodynamic properties of the components that are involved. An investigation into the ultrasonic behavior of binary liquid mixes of trichloroethylene (TCE) with three distinct alcohols—methanol, ethanol, and propanol—at a constant temperature of 303.15 K is carried out in this work. Instrumental measurements were taken to determine the ultrasonic velocities, densities, and viscosities of the pure components as well as the mixes of those components. Following the completion of these experiments, significant acoustic and thermodynamic characteristics were computed. These parameters included adiabatic compressibility, intermolecular free length, and excess molar volume. As the proportion of alcohols in the mixes changes, the results show that there are considerable differences in the ultrasonic velocity and the parameters that are calculated; these fluctuations are significant. The presence of complicated molecular interactions between trichloroethylene and the alcohols is suggested by the non-linear fluctuations that are observed in these parameters. To be more specific, the excess molar volume and the excess adiabatic compressibility both displayed both positive and negative deviations from the ideal behavior. These deviations are indicative of the presence of particular interactions, such as hydrogen bonding, dipole-dipole interactions, and dispersion forces. Based on the findings of the study, it was discovered that methanol exhibited the most substantial deviations from ideality. This is because of its smaller molecular size and higher polarity, which indicates that it has stronger interactions with trichloroethylene. On the other hand, propanol, which has a more substantial molecular structure, displayed interactions that were somewhat weaker. Variations in excess intermolecular free length, which provided insights into the compactness of the molecular arrangements within the mixtures, provided additional support for these findings. These findings were further reinforced by the variations they presented. These binary liquid mixtures were subjected to ultrasonic experiments at 303.15 degrees Kelvin, which provided a wealth of information regarding the nature and intensity of the molecular interactions that occur inside these systems. It is possible that the data gathered will be of great assistance in comprehending the dynamics of solvation and in developing mixes that possess the desired qualities for use in industrial applications. Through the provision of a more in-depth

understanding of the interactions that take place in binary liquid mixes containing trichloroethylene and alcohols, this research makes a contribution to the more general subject of solution chemistry and material science.

Keywords: *binary liquid mixtures, trichloroethylene. Ultrasonic velocity, Binary liquid mixtures, Trichloroethylene, Alcohols, Acoustic properties, Molecular interactions, Excess molar volume*

INTRODUCTION

One of the most important areas of research in the field of physical chemistry is the investigation of binary liquid mixtures and the ultrasonic properties of these mixes. This research provides fundamental insights into the molecular interactions and thermodynamic behaviors of mixed liquids. Due to the one-of-a-kind characteristics of trichloroethylene (TCE) and the different molecular structures of alcohols, one such combination, trichloroethylene (TCE) with alcohols, is an intriguing issue. The purpose of this research is to explore the ultrasonic properties of binary liquid mixtures consisting of trichloroethylene, methanol, and propanol, all of which are kept at a constant temperature of 303.15 K. One of the primary reasons for conducting this research is to gain an understanding of the molecular dynamics and interactions that occur inside these mixtures. These interactions are essential for a wide range of scientific and industrial applications.

Background

Trochloroethylene, sometimes known as TCE, is a chlorinated hydrocarbon that is frequently utilized in the industrial sector as a solvent. It can be used for a wide variety of purposes, from cleaning metals to serving as an intermediary in the process of chemical synthesis. Because of its comparatively high density, low viscosity, and strong dipole moment, TCE is a solvent that is of interest for the study of molecular interactions on account of these characteristics. In contrast, alcohols are chemical molecules that include one or more hydroxyl (-OH) groups. Alcohols are a type of phenol. Methanol, ethanol, and propanol are major alcohols that have increasing molecular size and chain length. This provides a gradient of molecular complexity and interaction potential. These alcohols were selected for this study because they demonstrate these characteristics.

Importance of Ultrasonic Studies

Researchers are able to investigate the acoustic and thermodynamic features of a medium through the use of ultrasonic investigations, which entail the transmission of high-frequency sound waves through the medium. In a liquid mixture, the speed of sound can be used to determine critical characteristics such as adiabatic compressibility, intermolecular free length, and excess molar volumes. This can be done in conjunction with measurements of density and viscosity. These parameters are illustrative of the molecular interactions that take place inside the mixture, and they offer vital information regarding the structural and dynamic properties of the mixture.

Objectives

At a temperature of 303.15 degrees Kelvin, the major purpose of this investigation is to obtain a better understanding of the molecular interactions that take place between trichloroethylene and the three alcohols (methanol, ethanol, and propanol) through the examination of their ultrasonic characteristics. These are some specific goals:

1. Measuring the ultrasonic velocities, densities, and viscosities of pure TCE, the three alcohols, and their binary mixes at various concentrations.

2. Calculating acoustic and thermodynamic characteristics, such as the adiabatic compressibility, the intermolecular free length, and the excess molar volume of the substance.

3. The third step involves analyzing the deviations of these parameters from their ideal behavior in order to deduce the nature and strength of the interactions between molecules.

Methodology

The Merck Company, Inc. in Germany provided the samples that were used in this investigation. These samples were of a high purity and AR grade. The liquids were distilled before to their use, and then they were mixed in the required proportions using a burette. After that, they were allowed to remain for five or six hours in order to achieve temperature equilibrium before the experimental observations were obtained. It is common for bubbles to occur in organic liquids due to the presence of dissolved gases, which can lead to inaccurate readings of density. A degassing procedure was performed on each and every liquid before the readings were taken in order to circumvent the challenge. A variable path ultrasonic interferometer with a gold-plated x-cut quartz crystal, a natural frequency of 2 MHz, and an accuracy of +0.1 ms-1 was utilized in the experiment. This instrument was supplied by M/s Mittal enterprises (model-05 F), which is located in New Delhi, India. The temperature was controlled by a digitally operated constant temperature bath that circulated water through a double-walled measuring cell made of steel. The thermostat was regulated with an accuracy of + 0.05%, and the cell was heated to a temperature that was constant. A specific gravity container with a capacity of 10 milliliters was utilized in order to determine the densities of all of the liquids and liquid combinations. A chemical balance was utilized in order to accurately determine the weight of the solution, which was found to be 0.1 mg. Ostwald's viscometer, which has an accuracy of 0.001Nm-2s, was utilized in order to ascertain the viscosities. Prior to their use, the viscometer underwent calibration. At 303.15 degrees Kelvin, the densities, viscosities, and velocities of each of the mixtures were measured according to their respective values. The use of a digital stopwatch allowed for the measurement of both the time of flow of water and the time of flow of solution. Throughout the entirety of the experimental procedure, measurements were taken five times, and the average values were taken into consideration in order to minimize the possibility of

experimental error. An inaccuracy of 0.1% is considered to be within the range of the measurements' fluctuation.

Theory

V_E stands for "excess volume." In the event that V represents the average molar volume of a binary liquid mixture. The relation that is used to compute excess molar volume is as follows:

$$V^E = V - (V_1X_1 + \bar{V}_2X_2) \quad (1)$$

Where V_1 and V_2 represent the molar volumes of the binary liquid mixture, and X_1 and X_2 represent the mole fractions of the mixture, respectively.

βad stands for adiabatic compressibility. It is possible to calculate adiabatic compressibility by using the relation between the density and velocity of ultrasonic sound. This is done under the assumption that ultrasonic absorption is completely insignificant.

$$\beta_{ad} = 1/\rho U^2 \quad (2)$$

Za stands for acoustic impedance.

The particular acoustic impedance is as follows:

$$Z_a = U_\rho \quad (3)$$

The formula for calculating the deviation in adiabatic compressibility ($\Delta\beta_{ad}$) at a specific mole fraction is as follows:

$$\Delta\beta_{ad} = \beta_{ad} - (\beta_{ad\,1}X_1 + \beta_{ad\,2}X_2) \quad (4)$$

At the temperature in question, the values of $\beta_{ad\,1}$ and $\beta_{ad\,2}$ represent the individual adiabatic compressibility values of pure liquids that are contained within the binary clusters.

The formula that is used to calculate the intermolecular free length (Lf) is as follows:

$$L_f = K(\beta_{ad})^{1/2} \quad (5)$$

The constant K represents Jacobson's constant.

The excess intermolecular free length, often known as L_f^E, has been calculated as follows:

$$L_f^E = L_f - (L_{f1}X_1 + L_{f2}X_2) \quad (6)$$

In this context, the values of L_{f1} and L_{f2} represent the intermolecular free lengths of pure liquids that are extracted from the binary mixes.

The calculation of the deviation in viscosity ($\Delta\eta$) is found by:

$$L_f^E = L_f - (L_{f1}X_1 + L_{f2}X_2) \quad (7)$$

Where η_{mix}, η_1, and η_2 represent the viscosities of the liquid mixture and the independent values of pure liquids, respectively, the viscosity of the mixture is η_{mix}.

The following formula is being utilized in order to determine the molar sound velocity, also known as Rao's constant (R):

$$R = VU^{1/3} \quad (8)$$

Using the following formula, the molar compressibility, often known as Wada's constant (W), has been determined:

$$W = M/\rho \; X \; \hat{\beta}_{ad}^{-1/7} \quad (9)$$

Table-1: Comparison of experimental values of Density (ρ), Viscosity (η) and Ultrasonic Velocity (U) Values of pure liquids with literature values

Component	Density (g/cc)		Viscosity(centipoise)		Velocity (m/s)	
	Literature	Experimental	Literature	Experimental	Literature	Experimental
Trichloroethylene (HCIC=CCICI):	1.4556	1.4559	0.5362	0.5365	1015	1016
1-Pentanol	0.8086	0.8087	3.73	3.7309	1264	1264.5
1-Hexanol	0.81165	0.8117	4.683	4.6834	1273	1275.5
1-Heptanol	0.8149	0.8088	6.188	6.1778	1312	1316

Results and discussion

The measured values of ultrasonic velocity (U), density (ρ), viscosity (η) and computed values of deviation in viscosity (Δ_η), molar volume (V), excess molar volume (V_E), adiabatic compressibility (β_{ad}), acoustic impedance (Z), deviation in adiabatic compressibility ($\Delta\beta_{ad}$), intermolecular free length (L_f), excess intermolecular free length (L_f^E), excess velocity (U_E), excess acoustic impedance(Z_E), Rao's constant (R) and Wada's constant (W) for the three binary liquid systems are presented in Tables2,3,4,5, and 6 respectively.

As illustrated in Figure 1, the divergence in ultrasonic velocity with the mole fraction of trichloroethylene for each of the three systems demonstrates that there is a non-linear drop in velocity without any minimum. This is the case regardless of whatever system is being considered. At any intermediate concentration of trichloroethylene with 1-pentanol, 1-hexanol, and 1-heptanol, the absence of maximum or dip can be interpreted as evidence that there is no complex formation between the components. The overall tendencies of the ultrasonic velocity fluctuations in binary liquids are also consistent with these observations, which are in agreement with those trends.

In the presence of species in solution that have different structures, it is inevitable that these variations will have an impact on the other different physical properties. It was necessary to

compute the extra volumes of the cluster as a function of composition in order to investigate the possibility of such occurrences. It was discovered that the surplus volumes for all three systems were negative across the full compositional range at 303.15K, as can be seen in Figure 2.

Approximately 0.5 mole fraction of trichloroethylene is the point at which the negative surplus volumes reach their minimal value, as seen by the data, which suggests that there is a volume contraction that occurs during mixing. Due to the high interaction, the three results imply that molecules that are not similar are becoming closer to one another. It is dependent on the proportionate amount of expansion and contraction that occurs when two liquids are mixed together that the indication of excess volume (V_E) of a system is determined. In order for the VE to become positive, it must first become negative, which causes expansion, and then it must dominate the forces that cause contraction. If, on the other side, the contractive variables are more prevalent than the expansive factors, then the value of V_E will be seen as negative.

Table-2: System-1; Trichloroethylene + 1- Pentanol; Temperature – 303.15

Mole fraction X	(U) m/s	ρ x 10^{-3} kg/m^3	η Cp	V_m cm^{-3} mol^{-1}	β_{ad} 10^{12} m^2 N^{-2}	L_f 10^{-10} m	R	W	Z
0.0000	1264.50	0.8087	3.7309	109.0021	77.3348	0.5514	5471	3034	1022.60
0.1183	1235.20	0.8762	3.3869	106.4439	74.8034	0.5423	5301	2976	1082.28
0.2319	1206.06	0.9435	3.0494	104.0522	72.8611	0.5352	5141	2921	1137.98
0.3411	1178.31	1.0104	2.7161	101.8379	71.2828	0.5294	4993	2867	1190.58
0.4460	1152.00	1.0774	2.3886	99.7162	69.9369	0.5243	4852	2815	1241.20
0.5471	1127.35	1.1440	2.0684	97.7316	68.7792	0.5200	4721	2766	1289.69
0.6443	1104.00	1.2088	1.7516	95.9690	67.8721	0.5166	4604	2721	1334.56
0.7381	1082.28	1.2726	1.4384	94.3487	67.0869	0.5136	4496	2680	1377.28
0.8285	1061.74	1.3357	1.1303	92.8129	66.4109	0.5110	4395	2640	1418.22
0.9158	1041.09	1.3969	0.8292	91.4526	66.0491	0.5096	4302	2603	1454.27
1.0000	1016.00	1.4559	0.5365	90.2466	66.5397	0.5115	4211	2566	1479.19

Table-3: System-1; Trichloroethylene + 1- Pentanol; Temperature – 303.15k

Mole fraction X	V_m^E Cm^3 mol^{-1}	β_{ad}^E 10^{10} m^2 N^{-1}	η^E Cp	L_f^E 10^{-10}m	U^E	Z^E
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.1183	-0.3390	-1.2541	0.0340	-0.0044	0.1034	5.6590
0.2319	-0.6000	-1.9700	0.0594	-0.0069	-0.8046	9.4847
0.3411	-0.7670	-2.3700	0.0748	-0.0084	-1.4349	12.2415
0.4460	-0.9200	-2.5828	0.0826	-0.0093	-1.6566	14.9370
0.5471	-1.0100	-2.6500	0.0850	-0.0096	-1.2056	17.3038
0.6443	-0.9480	-2.5069	0.0790	-0.0091	-0.3795	17.7612
0.7381	-0.8100	-2.2800	0.0653	-0.0084	1.1985	17.6707
0.8285	-0.6500	-1.9800	0.0460	-0.0074	3.1240	17.3269
0.9158	-0.3740	-1.4000	0.0236	-0.0053	4.1565	13.5422
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table-4: System-2; Trichloroethylene +1- Hexanol; Temperature – 303.15K

Mole fraction X	(U) m/s	ρ x 10^{-3} kg/m^3	η Cp	V_m cm^{-3} mol^{-1}	β_{ad} 10^{12} m^2 N^{-2}	L_f 10^{-10} m	R	W	Z
0.0000	1275.5	0.8117	4.6834	125.8839	75.7257	0.5456	6337	3514	1035.32
0.1342	1248.31	0.8792	4.1688	120.6817	72.9930	0.5357	6031	3386	1097.48
0.2586	1219.40	0.9464	3.6798	115.9456	71.0606	0.5285	5750	3266	1154.05
0.3741	1190.40	1.0135	3.2179	111.6024	69.6288	0.5232	5490	3153	1206.47
0.4818	1163.12	1.0801	2.7812	107.6382	68.4395	0.5187	5254	3048	1256.23
0.5824	1137.27	1.1460	2.3671	104.0072	67.4654	0.5150	5039	2952	1303.33
0.6766	1112.52	1.2111	1.9695	100.6860	66.7103	0.5121	4843	2862	1347.41
0.7650	1089.06	1.2752	1.5900	97.6525	66.1187	0.5098	4663	2779	1388.75
0.8480	1066.64	1.3379	1.2258	94.8880	65.6958	0.5082	4500	2703	1427.06
0.9262	1044.25	1.3988	0.8755	92.3869	65.5574	0.5077	4351	2633	1460.74
1.0000	1016.00	1.4559	0.5365	90.2466	66.5397	0.5115	4211	2566	1479.19

Table-5: System-2; Trichloroethylene +1- Hexanol; Temperature – 303.15K

Mole fraction X	V_m^E Cm^3 mol^{-1}	β_{ad}^E 10^{10} m^2 N^{-1}	η^E cp	L_f^E 10^{-10}m	U^E	Z^E
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0033
0.1342	-0.4200	-1.5000	0.0419	-0.0053	7.6339	2.5945
0.2586	-0.7240	-2.2900	0.0686	-0.0082	10.9928	3.9678
0.3741	-0.9480	-2.6600	0.0860	-0.0096	11.9939	5.0795
0.4818	-1.0740	-2.8600	0.0960	-0.0105	12.6593	7.0319
0.5824	-1.1200	-2.9100	0.0990	-0.0107	12.9191	9.4783
0.6766	-1.0850	-2.8000	0.0920	-0.0104	12.6029	11.7578
0.7650	-0.9700	-2.5800	0.0788	-0.0097	12.0691	13.8832
0.8480	-0.7750	-2.2400	0.0590	-0.0085	11.2035	15.3334
0.9262	-0.4890	-1.6600	0.0330	-0.0063	9.1038	14.3012
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044

Table-6: System-3: Trichloroethylene + 1- Heptanol; Temperature – 303.15K

Mole fraction X	V_m^E Cm^3 mol^{-1}	β_{ad}^E 10^{10} m^2 N^{-1}	η^E cp	L_f^E 10^{-10}m	U^E	Z^E
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0008
0.1503	-0.5520	-1.8000	0.0550	-0.0067	15.8262	1.8443
0.2847	-0.9290	-2.6700	0.0875	-0.0101	22.9343	2.1806
0.4056	-1.1800	-3.1300	0.1063	-0.0119	26.1131	3.3609
0.5149	-1.3120	-3.3500	0.1156	-0.0128	27.1178	5.6000
0.614	-1.3700	-3.4400	0.1188	-0.0132	26.8954	9.2466
0.7048	-1.3400	-3.3500	0.1100	-0.0129	25.2217	12.9630
0.7879	-1.2310	-3.0600	0.0956	-0.0118	22.0408	15.9046
0.8643	-1.0400	-2.6200	0.0739	-0.0101	17.9595	18.0171
0.9348	-0.6800	-1.9200	0.0425	-0.0074	12.7193	16.9029
1.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0044

The following is a list of the factors that are responsible for the increase in volume:

1. Loss of dipolar association (also known as the breaking apart of associates held by weaker forces or the rupturing of H-bonding of a component by the other, namely dipole-dipole or dipole-induced dipole interactions or by Van der Waals forces).

2. The inherent characteristics of the molecular structure, which do not permit the incorporation of particular components into other components.

3. In addition, the steric barrier works against the close proximity of the constituent molecules. The prevailing influence of the following elements is responsible for the prevalence of negative VE values:

    I. Strong specific interaction refers to the chemical contact that occurs between constituent molecules. This type of interaction includes hetero molecular connections that are formed by the establishment of H-bonds.

    II. Accommodation of one kind of molecule component into the other interstitials of molecules with each other component.

    III. The nature of the molecular structure that is favorable to the fitting of the component molecules with each other is the third point.

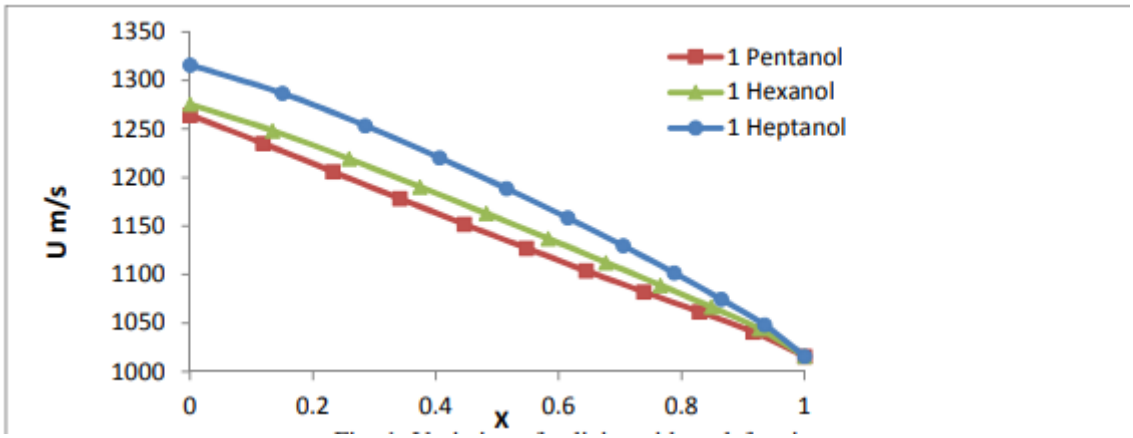

Fig.-1: Variation of velocity with molefraction

The fact that the excess volumes of all three systems were found to be negative at the temperature that was investigated is evidence that there are powerful dipole-dipole interactions between the components. This can be attributed to the preponderance of the elements that were described earlier that are responsible for the reduction in volume.

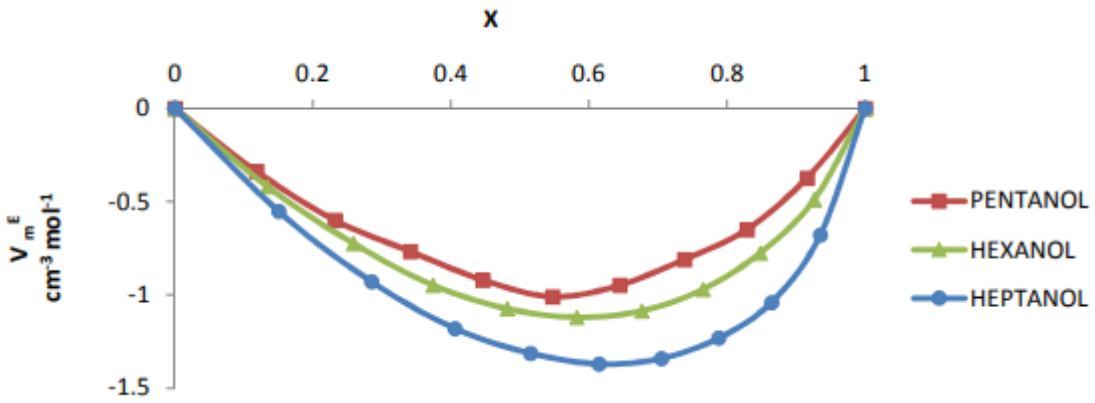

Fig.-2: Variation of Excess Molar volume with Molefraction

Several employees noticed the same patterns that emerged. Specifically, this phenomenon can be linked to the interactions that occur between molecules that are not similar to one another in the systems.

The intermolecular free length is an additional crucial metric that must be understood in order to comprehend the structural adjustment that occurs in solution as a result of molecular interactions.

Conclusion

Significant insights into the molecular interactions and thermodynamic behaviors of these systems have been offered as a result of this research project on the ultrasonic characteristics of binary liquid mixes of trichloroethylene (TCE) with methanol, ethanol, and propanol at 303.15 degrees Kelvin. By calculating crucial characteristics such as adiabatic compressibility, intermolecular free length, and excess molar volume, as well as monitoring ultrasonic velocities, densities, and viscosities, we have obtained a comprehensive understanding of the nature of the interactions that occur inside these mixes. The findings imply that the ultrasonic velocity and the parameters that were obtained from it display non-linear fluctuations with changing alcohol concentrations. This suggests that there are complicated molecular interactions between TCE and the alcohols. The presence of certain interactions, such as hydrogen bonding, dipole-dipole interactions, and dispersion forces, is brought to light by the departures in excess molar volume and adiabatic compressibility from the ideal behavior of the system. Methanol, which has a smaller molecular size and a higher polarity than the other alcohols that were investigated, caused the most substantial deviations, which indicates that it interacts with TCE more strongly than the other alcohols. When compared to other molecules, propanol, which has a bigger molecular structure, exhibited interactions that were somewhat weaker. These findings are further supported by the changes in excess intermolecular free length, which are a reflection of the compactness of the molecular configurations that are present within the mixtures. The research highlights the significance of temperature control, since it was determined that the observed differences were mostly caused by changes in mixture composition rather than thermal impacts. This was accomplished by keeping a constant temperature of 303.15 K throughout the experiment. In

conclusion, the findings of this research contribute to a better knowledge of the molecular dynamics that occur in binary liquid mixes of TCE coupled with various alcohols. The information that was gathered can be used to contribute to the larger fields of solution chemistry and material science, as well as make a contribution to the design of solvent systems that have the qualities that are required for commercial applications. The insights that were gathered from this work are significant for both the advancement of fundamental understanding in the field of molecular interactions in liquid mixtures as well as for practical applications.

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