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Study of Thermo Physical Properties of Binary Liquid Mixtures of Trichloroethylene with 1-Pentanol at 308 K

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Density and ultrasonic study for the binary mixtures of trichloroethylene and 1-pentanol over the entire concentration range were measured at temperatures 308 K. The experimental data was then used to calculate the compressibility, acoustic impedance, molecular free length, inverse relaxation time, and excess parameters. The values of excess properties further fitted with Redlich–Kister polynomial equation to estimate the binary coefficients. The resulting excess functions were interpreted in terms of the interactions between the molecules in the binary mixtures. Results confirmed that hydrogen-bonded intermolecular interaction took place between trichloroethylene and 1-pentanol.

Key words: Compressibility; acoustic impedance binary mixtures; ultrasonic velocity; excess parameters

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Ultrasonic Study and its analysis for aprotic binary liquid mixtures containing polar-polar components has significant importance in understanding intermolecular interaction and strength between the component molecules as they find application in various industrial and technological processes [1]. Ultrasonic velocity and its derived acoustical parameters like adiabatic compressibility, free length, relaxation time, acoustic impedance with their excess parameters, gives essential information about the molecular interactions and their strengths [1-10]. In the present paper, a variation of various parameters of binary mixtures containing 1-pentanol and trichloroethylene at 2 MHz frequency have been studied for an entire range of concentration range (by adding solute percentage 10% in solvent 0-100%). 1-pentanol is a polar molecule of benzene family different than that of the ketone family of trichloroethylene. When it is mixed with trichloroethylene, the hydrogen bonded interaction dominates. Trichloroethylene is very small, and its linear aliphatic configuration is the important factor which mainly contributes to the volume contraction of the mixture [11-12]. 1-pentanol is relatively a complex molecule. It is highly reactive even if at low temperature. Trichloroethylene being a polar protic solvent is quite expected to be involved in any strong interaction with the other components of the mixture [13-19].

EXPERIMENTAL

Chemicals

In the present system of 1-pentanol with trichloroethylene binary a mixture, the liquid 1-pentanol was used for analytical reagent grade and was obtained from MERCK (99.99), and trichloroethylene was of HPLC grade. Both the liquids were used without further purification.

Solution Preparation

The solutions were prepared at different volume percentages of 1-pentanol in trichloroethylene in steps of 10% at room temperature (droplets of 1-pentanol were mixed in trichloroethylene with increasing volume percentage) (by adding solute percentage 10% in solvent 0-100%). These concentrations were prepared for 5 ml solution samples at room temperature, assuming ideal mixing behaviour, with an accuracy ± 0.0006 ml.

Density Measurement

The Density measurements were carried out by portable digital density meter (DMA-35, Anton Paar) for pure liquids and binary mixture. This digital density meter uses the vibrating U-tube principle to calculate the density of the sample. The required quantity of sample is approximately 2 ml. The accuracy of the instrument used was = 0.0001 g/cm^3.

To reduce error, measurements were done three times, and an average of three readings were taken.

Ultrasonic Velocity Measurements

The ultrasonic velocity measurements were studied using Ultrasonic Interferometer (Model F-05, Mittal Enterprises, New Delhi). It is single crystal interferometer operating at 2 MHz fixed frequency. The sample cell of the instrument is made up of steel and is double walled; the required amount of the sample is approximately 10 cc. To reduce error, measurements were done fifty times and an average of fifty readings were taken.

Viscosity Measurement

Viscosity of the sample in the present study were measured by using Brookfield Viscometer (Brookfield Viscometer, Model: LV DV-II+ Pro, Cone-plate Model with CPE-40 spindle). The accuracy of the instrument is = 0.01 cP. To reduce error, measurements were done three times and an average of three readings were taken.

Theory

The specific acoustic impedance is given by:

$$Z = U.\rho \qquad (1)$$

where, U is the ultrasonic velocity (of the mixture) and ρ is the density of the mixture.

The adiabatic compressibility is given by:

$$\beta = 1/(U^2.\rho) \qquad (2)$$

where, U and ° are the velocity and density of the liquid mixture.

The general formula for calculating the excess parameters is given below:

$$A^E = A_m - (x_1 M_1 + (1 - x_1)M_2) \qquad (3)$$

where, A^E is the excess parameter such as excess density x_1 mole fraction.

The excess parameters are fitted to the Redlich-Kister polynomial equation [8], of third order and this equation is given by:

$$A^E = x_1 x_2 \sum_{i=0}^{n} A_i (1 - 2x_2)^i \qquad (4)$$

Where, x_i is the mole fraction of pure component 1 and 2.

RESULT AND DISCUSSION

Table 1 depicts the value of densities increases as the concentration of TCE increases in contrast values of viscosities, and ultrasonic velocity decreases as the concentration of TCE decreases.

Table 2 depicts the RK coefficients and values of standard error prove the correctness of data.

Table 1. Density, ultrasonic velocity of trichloroethylene + 1-pentanol.

Volume farction of TCE	Density (g/cm^3)	Viscosity (cP)	Velocity (m/s)
0	0.803	3.50	1227
0.1	0.866	3.28	1204
0.2	0.930	3.07	1181
0.3	0.993	2.45	1158
0.4	1.056	2.23	1136
0.5	1.120	2.02	1113
0.6	1.183	1.70	1090
0.7	1.246	1.38	1067
0.8	1.309	1.06	1045
0.9	1.373	0.75	1022
1.0	1.436	0.50	1000

Table 2. RK coefficients and standard deviation (error) of excess parameters.

Parameter	a_0	a_1	a_2	a_3	Sandard error
Excess molar volume	-10.3293	2.9189	-0.86258	0.2478	5.11E-04
Excess velocity	39.4849	-4.9558	-3.85637	-5.6184	5.73E-02
Excess compressibility	2.17E+08	-1.6E+07	-1.2E+07	-160074	0.1646
Excess acoustic impedance	59831.51	5680.411	-6704.56	-7961.980	0. 0823
Excess molecular free length	3.51E+11	2.15E+09	-2.4E+10	-2.338E+10	0. 2469

Table 3 depicts values of excess parameters (i.e. excess molar volume, excess velocity, excess viscosity, excess compressibility, excess acoustic impedance and excess inverse relaxation time).

Figure 1 gives an excess molar volume of trichloroethylene+1-pentanol. As the concentration of trichloroethylene increases, excess molar volume becomes negative. Negative values indicate that volume contraction takes place upon mixing due to the cross association between dissimilar molecules. This contraction gave more compactness, i.e. molecules came close to each other. This attributed the strong hydrogen bonded interaction between unlike molecules [20].

As shown in Figure 2 excess velocity becomes positive as the concentration of trichloroethylene increases. Positive deviation and non-linear dependence suggests the presence of strong interaction between the components of the mixture. Positive excess velocity can be concluded as the formation of the structure [18-20]. Strong interaction arise among the components of the mixture leading to the formation of molecular aggregates and less compact structure then sound will travel faster through the mixture by means of longitudinal waves and hence the speed of sound concerning linear behaviour will be positive [18-20].

Table 3. Values of excess parameters.

Mole fraction TCE	Excess molar volume	Excess velocity	Excess viscosity	Excess compressibility	Excess acoustic impedance	Excess inverse relaxation time
0	0	0	0	0	0	0
0.1176	-1.20158906	3.902864	0.135858	20551477	4892.74698	-9.742E-11
0.2307	-1.990699183	6.781614	0.258166	36089238	8940.04441	-1.888E-10
0.3396	-2.446220237	8.69413	-0.03231	46752029	12026.7864	-2.42E-10
0.4444	-2.628130033	9.694013	0.065137	52682893	14046.381	-3.161E-10
0.5454	-2.582841057	9.830972	0.151166	54028778	14899.977	-3.819E-10
0.6428	-2.346830352	9.151167	0.126388	50940191	14495.7739	-4.206E-10
0.7368	-1.949163047	7.697528	0.091372	43570883	12748.4046	-4.338E-10
0.8275	-1.413283916	5.510024	0.046645	32077575	9578.38104	-4.017E-10
0.9152	-0.758313253	2.62592	-0.0073	16619702	4911.59697	-2.706E-10
1.0	0	0	0	0	0	0

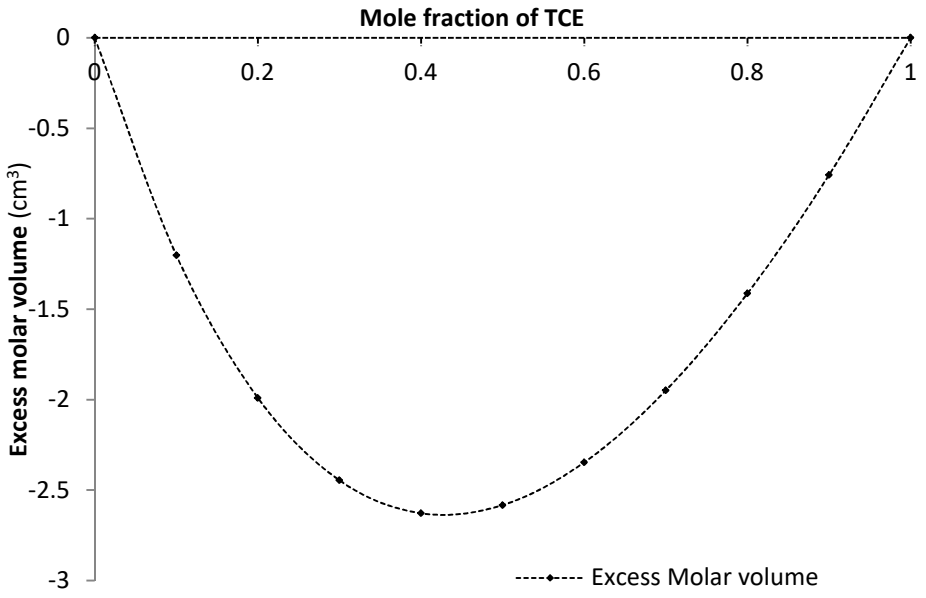

Figure 1. Excess molar volume of trichloroethylene + 1-pentanol.

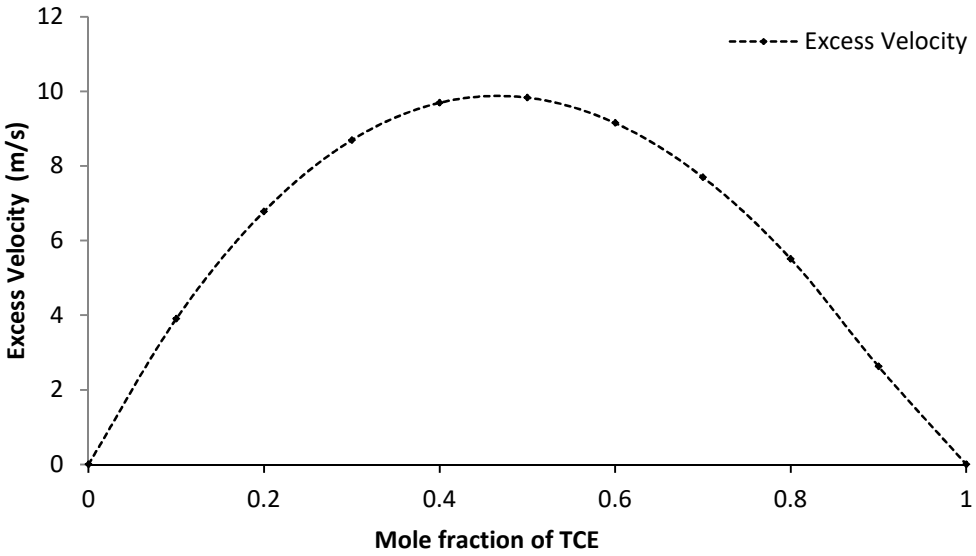

Figure 2. Excess Velocity of trichloroethylene+1-pentanol.

Figure 3 indicates Excess compressibility of trichloroethylene+1-pentanol**.** Positive excess compressibility of values are due to the closed packed molecules which accounts for the existence of strong molecular interaction between unlike molecules [21]. The sign of compressibility plays a vital role in assessing the compactness due to molecular interaction in the liquid mixture through hydrogen bonded interactions, leading to less compact structure making positive excess compressibility [21].

Positive values of acoustic impudence as shown in Figure 4 hint to the possibility of the presence of strong attractive forces between the reacting components of the mixture [19-21]. Positive deviation also suggests that trichloroethylene molecules do not cooperate with 1-pentanol molecules hence strong intermolecular interactions occurs between them [21].

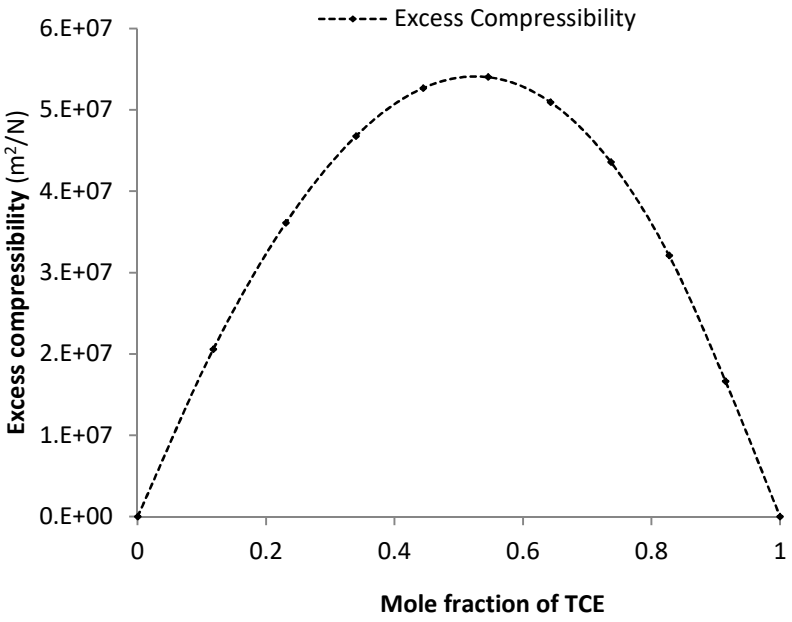

Figure 3. Excess compressibility of trichloroethylene+1-pentanol.

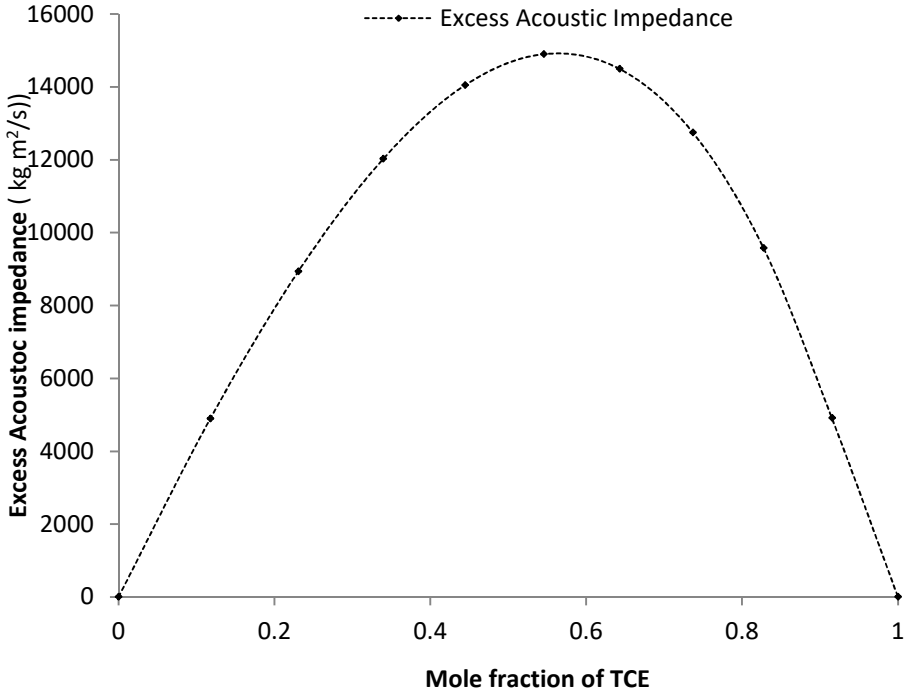

Figure 4. Excess acoustic impedance of trichloroethylene+1-pentanol.

Positive values exhibit a strong interaction. Increase in values of free length with concentration can be concluded as there is significant interaction between two liquids. Positive values also suggests that as trichloroethylene molecules are mixed with 1-pentanol molecules, and their intermolecular distance increases and give rise to hydrogen bonded interaction between them [19-21].

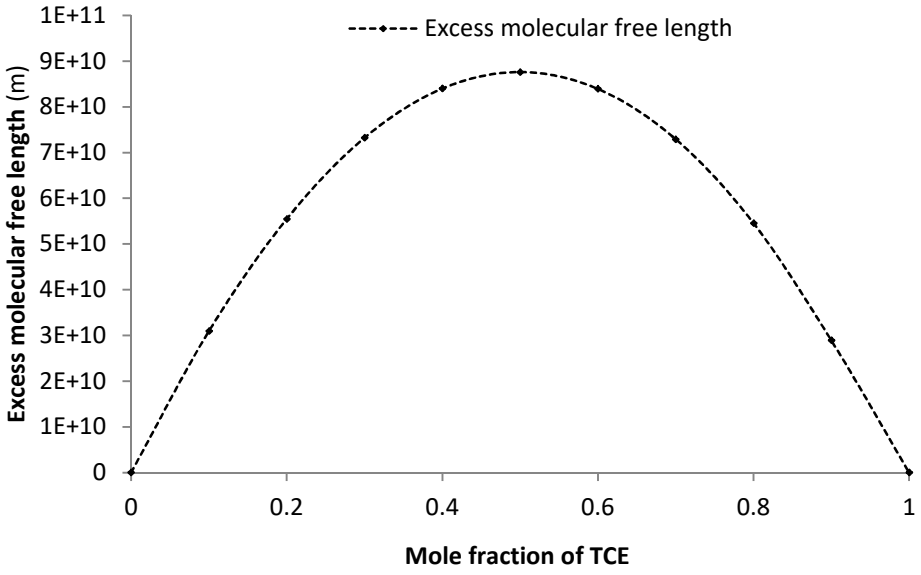

Figure 5. Excess molecular free length of trichloroethylene+1-pentanol.

CONCLUSION

In this work, the measurement of density, ultrasonic velocity and other acoustical parameters of trichloroethylene in 1-pentanol solution was studied in different concentrations at 308 K. Negative excess molar volume V_m^E values indicated the presence of strong hydrogen bonded interactions. It was observed that the excess velocity values became more positive with the rise in the concentration of trichloroethylene. The experimental ultrasonic velocity data and other acoustical parameters contain valuable information regarding the solute-solvent interactions in the measurements; it could be concluded that the concentration of trichloroethylene affected and gave rise to the strong hydrogen bonded interaction. Our volumetric and ultrasonic study suggested that trichloroethylene acted as the structure breaker. Increase in concentration of trichloroethylene played an important role in forming hydrogen bonded interactions in the solutions.

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