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Ultrasonic Behaviour of 1-Propanethiol in Benzene, Carbon Tetrachloride, Cyclohexane and n-Hexane

KEYWORDS: propanethiol, ultrasonic velocity, adiabatic compressibility, acoustic impedance,

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ABSTRACT *Ultrasonic velocity (U) and density (ρ) for the binary liquid mixtures of 1-Propanethiol with Benzene, Carbon tetrachloride, Cyclo hexane, n-Hexane have been measured for 2MHz ultrasonic frequency at 300C. The experimental data have been used to calculate acoustic parameters such as adiabatic compressibility (βad), acoustic impedance (z), relative association (RA) and intermolecular free length (Lf). The results are interpreted in terms of molecular interaction between the components of the mixture.*

Introduction:
1-Propanethiol is an organic compound with the molecular formula C_3H_8S. It is cabourless liquid with a strong, offensive odour ($C_3H_7H_S$) it is moderately toxic. [1] It is used as flavoring agent, chemical intermediate, herbicide and fungicide and as an odorant in odorless gases.[2] Study of the intermolecular interaction between 1-propanethiol with different solvents plays important role in the selection of modifier / diluents. Hence author feels the necessity to study the binary mixture of these compounds.

In the present study, the measurements of ultrasonic velocity and density has been taken and used to determine the acoustic parameters; adiabatic compressibility (β_{ad}) acoustic impedance (Z) relative association and intermolecular free length (L_f) of 1-Propanethiol with Benzene, carbon tetrachloride, cyclohexane and n-hexane in order to explain the intermolecular interactions in these mixtures.[3]

Experimental:
In the present work, chemicals used are obtained from E-Merk, Germany and S.P. Find chemicals, India. A pyknometer employed to determine the density of mixture [4] and Ultrasonic sound velocities were measured using multifrequency ultrasonic interferometer at 2MHz for the systems (Benzene + 1-Propanethiol),(Carbon tetrachloride + 1-Propanethiol),(Cyclohexane + 1-Propanethiol),(n-hexane + 1-Propanethiol) [5].

From the measured values of density (ρ) and ultrasonic velocity (U), acoustic parameters like adiabatic compressibility (β_{ad}), intermolecular free length (L_f), Acoustic impedance (Z) and relative association (R_A) were calculated using the following relations.

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

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

$$Z = U\rho U\rho \quad \ldots (3)$$

$$R_A = \frac{\rho_s}{\rho_0}\left(\frac{U_0}{U_s}\right)^{1/3} \quad \ldots (4)$$

Where, K is temperature – dependent constant

Results and discussions:
Values of density (ρ), Ultrasonic velocity (U), adiabatic compressibility (β_{ad}), intermolecular free length (L_f), acoustic impedance (Z) and relative association (R_A). along with mole fraction of 1-propanethiol in Benzene, carbon tetrachloride, cyclo hexane and n-hexane are listed in table No. 1, 2, 3 and 4 respectively. Also the graphical representation for above said parameters against mole fraction (X) of 1-propanethiol is depicted in Fig. 1, 2, 3, 4 and 5 respectively.

From the above values it is clear that in the system Benzene + 1-Butane thiol and cyclo hexane + 1-Propanethiol, the ultrasonic velocity decreases with increasing mole fraction of 1-propanethiol.

Decrease in ultrasonic velocity may be attributed to the solute-solvent interaction and also due to increase in the mobility of solutes. The decrease in velocity and increase in compressibility were attributed to the formation of hydrogen bonds between solute and solvent molecules [2].

Whereas in the systems carbon tetrachloride + 1-propanethiol and n-hexane + 1-propanethiol, the ultrasonic velocity increases with increase in mole fraction of 1-propanethiol. Increases with increase in mole fraction of 1-propanethiol. Increase in ultrasonic velocity indicates that interaction in the mixture is not strong and hence increases with mole fraction [6].

Fig. (1), indicate variation of ultrasonic velocity (U) for all the four systems, it is clear that the systems Benzene + 1-propanethiol and carbon tetrachloride + 1-propanethiol, the maxima occur at mole fraction 0.14775 and 0.053 respectively. This indicates maximum intermolecular interaction resulting in complex formation [7,8].

Fig. (2) represents the variation of the adiabatic compress-

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ibility (β_{ad}) for all the four systems. From fig. (2), it is clear that the adiabatic compressibility increases with increase in mole fraction of 1-propanethiol in the systems benzene + 1-propanethiol, carbon tetrachloride + 1-propanethiol and on further addition of 1-propanethiol the solvent-solvent association breakdown and thereby $_{ad}$ and L_f increases [9].

The decrease in adiabatic compressibility in the system n-hexane + 1-propanethiol can be seen in fig. (2), mixing of 1-propanethil with n-hexane tends to break the n-hexane – n-hexane association relating several 1-propanethiol dipoles. Consequently free dipoles would induce moments in the neighbouring molecules (h-hexane) resulting in dipolar – induced dipolar interaction leading to contraction in volume. This leads to subsequent decrease in adiabatic compressibilities (β_{ad}) and as well as intermolecular free length (L_f) [10].

Since the adiabatic compressibility (β_{ad}) has an inverse relationship with the velocity, it decreases as the concentration of solute increases and reaches minimum and then again increases. The mixtures studied Benzene + 1-propanethiol and carbon tetrachloride + 1-propanethiol show compressibility minima in the same region of concentration where the velocity maxima occurs as expected. The hydrogen bond formation strengthens the intermolecular forces resulting in a decrease in β_{ad} and an increase in U at or near the concentration where complex formation occurs. In case of liquid mixtures showing minima in β_{ad}, there is a definite contraction on mixing and the variation observed is due to complex formation [11]

Fig. (3) depicts the intermolecular free length (L_f) for all four systems. In systems Benzene + 1-propanethiol, Corban Tetrachloride + 1-propane thiol and cyclohexane + 1+propanethiol, the free length (L_f) increases with increasing concentration of 1-propanethiol. This increase in free length is due to loose packing of the molecules inside the shield which may be brought by weakening of molecular interactions [12]

In System n-hexane + 1-propanethiol, the free length decreases with increasing concentration of 1-propanethiol. The intermolecular free length depends on the intermolecular attractive and repulsive forces. It could also be seen that intermolecular free length (L_f) decreases linearly on increasing the concentration of solute. As concentration increases, number of ions or particles increases in a given volume, leading to the decrease in the gap between two species. This indicates that there is a strong interaction between ion and solvent molecules, suggesting a structure promoting behavior of the added solute [13].

Fig. (4) depicts the graphical representation of acoustic impedance of all four systems. In systems Benzene + 1-propanethiol and carbon tetrachloride + 1-propanethiol. The acoustic impedance decreases with increase in concentration of 1-propanethiol. The decrease in specific acoustic impedance indicates significant interaction between the mixing components[13].

In systems cyclohexane + 1-propanethiol and n-hexane + 1-propanethiol, the acoustic impedance (Z) increase with increase in concentration of 1-propanethiol. This increase of Z with concentration suggests the presence of solvent – solute interactions [14].

Fig.(5) depicts the graphical representation of relative association (R_A) with concentration of 1-propanethiol of all four systems. In system Benzene + 1-propanethiol and carbon tetrachloride + 1-propanethiol, the relative association decreases with increase in concentration of 1-propanethiol. It is found that there is weak interaction between solute and solvent [15].

In systems cyclohexane + 1-propanethiol and n-hexane + 1-propanethiol, the relative association increases with increase in concentration of 1-propanethiol. This indicates significant solute-solvent interaction [16].

Benzene + 1-Propanethiol

Table No.1 : The values of density (ρ), ultrasonic velocity (U), adiabatic compressibility (β_{ad}), intermolecular free length (L_f), Acoustic impedance (Z) and relative association (R_A) of the binary liquid mixture of Benzene + 1-Propanethiol at 30°C.

X	ρ	v	β_{ad}	L_f	Z	R_A
0	877	1309.6	6.64849	5.34065	1148519	1
0.04912	875.15	1276	7.01845	5.48723	1116628	1.00651
0.098419	873.3	1272.8	7.06832	5.50669	1111536	1.00528
0.14775	871.45	1295.2	6.84083	5.41735	1128637	0.99728
0.19718	869.6	1267.2	7.16127	5.54278	1101957	1.00250
0.39576	862.2	1255.2	7.3615	5.61973	1082233	0.99712
0.59574	854.8	1233.6	7.68753	5.74283	1054481	0.99430
0.79715	847.4	1214.4	8.00181	5.85904	1029083	0.99086
1	840	1212.8	8.09361	5.89256	1018752	-

CTC +1-Propanethiol

Table No.2 : The values of density (ρ), ultrasonic velocity (U), adiabatic compressibility (β_{ad}), intermolecular free length (L_f), Acoustic impedance (Z) and relative association (R_A) of the binary liquid mixture of Carbon tetrachloride + 1-Propanethiol at 30°C.

X	ρ	v	β_{ad}	L_f	Z	R_A
0	1594	914.4	7.5125	5.67708	1455725	1
0.05305	1556.3	968	6.85734	5.423889	1506498	0.95798
0.10576	1518.6	957.6	7.18106	5.55043	1454211	0.93815
0.15814	1480.9	971.2	7.15908	5.54193	1438250	0.91056
0.21018	1443.2	984.8	7.14459	5.53632	1421263	0.88328
0.41508	1292.4	1016.8	7.48397	5.66629	1314112	0.78260
0.61489	1141.6	1076	7.56592	5.69722	1228362	0.67837
0.80983	990.8	1120.8	8.03448	5.87099	1110489	0.58080
1	840	1212.8	8.09361	5.89256	1018752	-

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Cyclohexane+1-Propanethiol

Table No.3 : The values of density (ρ), ultrasonic velocity (U), adiabatic compressibility (β_{ad}), intermolecular free length (L_f), Acoustic impedance (Z) and relative association (R_A) of the binary liquid mixture of Cyclo-hexane + 1-Propanethiol at 30°C.

X	ρ	v	β_{ad}	L_f	Z	R_A
0	777	1282	7.83074	5.79607	996114	1
0.05916	780.15	1237.6	8.36876	5.99188	965514	1.01592
0.11719	783.3	1236	8.3567	5.98756	968159	1.02046
0.17413	786.45	1228	8.43257	6.01468	965699	1.02672
0.22999	789.6	1211.2	8.63299	6.08574	956364	1.03564
0.44337	802.2	1208.8	8.53117	6.04974	969699	1.05286
0.64185	814.8	1189.6	8.67256	6.09967	969286	1.07512
0.82696	827.4	1187.2	8.57505	6.06528	982289	1.09248
1	840	1212.8	8.09361	5.89256	1018752	-

n-hexane+1-Propanehiol

Table No.4 : The values of density (ρ), ultrasonic velocity (U), adiabatic compressibility (β_{ad}), intermolecular free length (L_f), Acoustic impedance (Z) and relative association (R_A) of the binary liquid mixture of n-hexane + 1-Propanethiol at 30°C.

X	ρ	v	β_{ad}	L_f	Z	R_A
0	658	1086	1.28859	7.43515	714588	1
0.07033	667.1	1089.6	1.26263	7.35987	726872	1.01271
0.13832	676.2	1091.2	1.24198	7.29946	737869	1.02602
0.20315	685.3	1092	1.2237	7.24552	748348	1.03957
0.26534	694.4	1103.2	1.18326	7.12481	766062	1.04980
0.49061	730.8	1102.4	1.12596	6.95015	805634	1.10510
0.68425	767.2	1145.6	9.93174	6.52748	878904	1.14537
0.85248	803.6	1168	9.12167	6.25561	938605	1.19200
1	840	1212.8	8.09361	5.89256	1018752	-

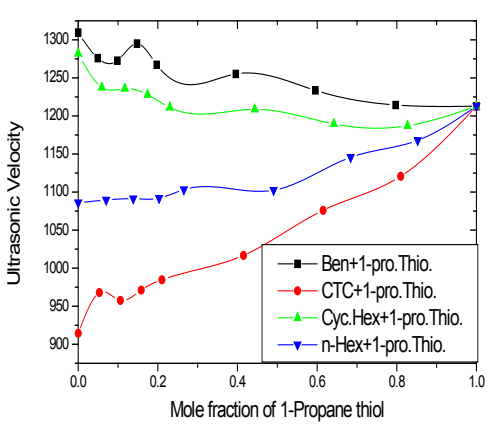

Fig.1 : The ultrasonic velocity for binary mixtures of 1-propanethiol with benzene, carbon tetrachloride, cyclohexane and n-hexane

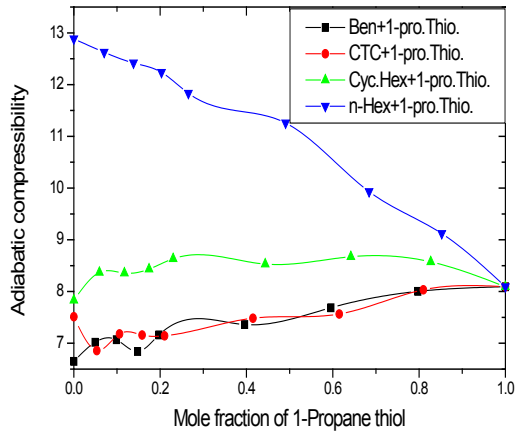

Fig.2 : The Adiabatic compressibility for binary mixtures of 1-propanethiol with benzene, carbon tetrachloride, cyclohexane and n-hexane

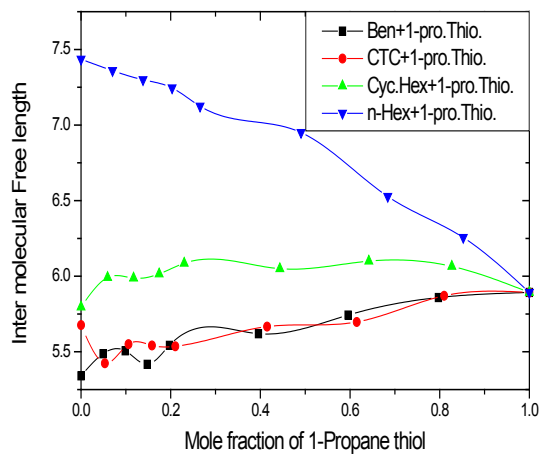

Fig.3 : The intermolecular free length for binary mixtures of 1-propanethiol with benzene, carbon tetrachloride, cyclohexane and n-hexane

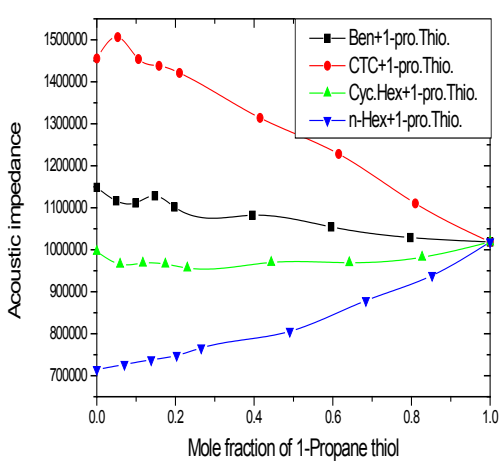

Fig.4 : The Acoustic impedance for binary mixtures of 1-propanethiol with benzene, carbon tetrachloride, cyclohexane and n-hexane

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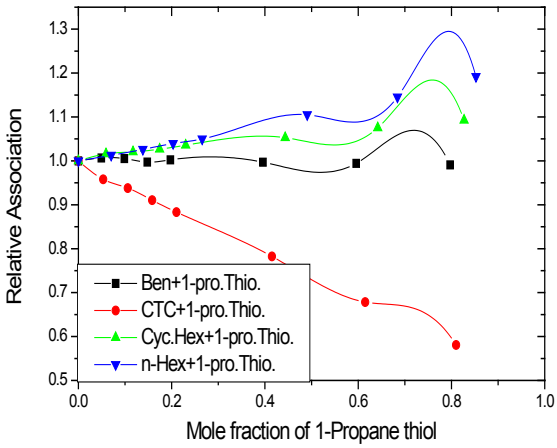

Fig.5 : The relative association for binary mixtures of 1-propanethiol with benzene, carbon tetrachloride, cyclohexane and n-hexane

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