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Study Of Molecular Interactions In Binary Liquid Mixtures Of Methyl Benzoate With 1-Octanol And 1-Nonanol At Temperatures 313.15K And 318.15K.

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ABSTRACT

The densities (ρ), viscosities (η) and ultrasonic velocities (U) of binary liquid mixtures of Methyl Benzoate with 1-octanol and 1-Nonanol have been measured at different temperatures 313.15K and 318.15K, over the entire composition range of mole fraction. From the measured values of, density, viscosity and ultrasonic velocity, various acoustic parameters such as adiabatic compressibility (β), internal pressure (π_i), free length (L_f), acoustic impedance (Z), molar volume (V_m) and relaxation time (τ) are estimated using standard relations. The variation of adiabatic compressibility (β), internal pressure (π_i), free length (L_f), acoustic impedance (Z), molar volume (V_m) and relaxation time (τ) with concentration and at different temperatures 313.15K and 318.15K are also studied. The results are interpreted in terms of molecular interactions present in the liquid mixtures.

Keywords: Adiabatic compressibility, Acoustic impedance, Free length, Internal pressure and Molar volume

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INTRODUCTION

The ultrasonic method plays an important role in understanding the intermolecular interactions present in between the component molecules of liquids. The ultrasonic velocity gives very useful information about the bonding between molecules and also about the formation of complex structures at various temperatures through molecular interactions [1]-[2]. Parameters such as densities, viscosities and ultrasonic velocities and their variation with composition and temperature of the binary liquid mixture are useful to design engineering applications and are also useful in various chemical and biological industries [3]-[4]. The study of molecular interactions in binary mixtures having alcohol as one of the component is of particular interest, since alcohols are strongly self-associated liquids having a three dimensional network of hydrogen bonds and can be associated with any other group having same degree of polar attractions [5]-[6]. But a systematic study with primary fatty alcohols in binary liquid mixtures has been very scarcely reported.

Methyl benzoate is an ester, reacts with acids to liberate heat along with alcohols and acids. Methyl benzoate is used in perfumery and also used as pesticide to attract insects. 1- octanol is a straight chain fatty alcohol with 8 carbon atoms. The primary use of 1-octanol is in the manufacture of various esters which are used in the perfumery and flavors.1-nonanol is a straight chain fatty alcohol with 9 carbon atoms. The primary use of 1-nonanol is in the manufacture of artificial lemon oil, perfumery and flavors.

Therefore, in order to understand the intermolecular interactions present in between the component molecules of methyl benzoate and 1-octanol & methyl benzoate and 1-nonanol, a systematic study using ultrasonic velocity data has been performed at temperatures 313.15K and 318.15K and the results are interpreted.

In the present investigation, several acoustic parameters such as adiabatic compressibility (β), internal pressure (π_i), free length (L_f), acoustic impedance (Z), molar volume (V_m) and relaxation time (τ) of binary liquid mixtures , methyl benzoate +1-octanol and methyl benzoate + 1- nonanol at temperatures 313.15K and 318.15K. have been reported using the experimental values of density, viscosity and ultrasonic velocity of the binary liquid mixtures at temperatures 313.15K and 318.15K.

MATERIALS AND METHODS

MATERIALS AND LIQUID MIXTURES

The liquid mixtures of various concentrations in mole fraction were prepared by taking AR grade chemicals (obtained from SDFCL chemicals, Mumbai) Methyl Benzoate + 1-Octanol and Methyl Benzoate + 1-Nonanol (>99%). All the liquids used were further purified by standard procedure [7]. The mixtures were preserved in well-stoppered conical flasks. After the thorough mixing of the liquids, the flasks were left undisturbed to allow them to attain thermal equilibrium. In all the mixtures the mole fraction of 1^{st} compound Methyl Benzoate has been increased from 0 to1.

APPARATUS AND PROCEDURE

The ultrasonic velocities were measured by using single crystal ultrasonic pulse echo interferometer (Mittal enterprises, India; Model: F-80X). It consists of a high frequency generator and a measuring cell. The measurements of ultrasonic velocities were made at a fixed frequency of 3MHz. The temperature was controlled by circulating water around the liquid cell from thermostatically controlled constant temperature water bath. The densities of pure liquids and liquid mixtures were measured by using a specific gravity bottle with an accuracy of ± 0.5%. Weights were measured with an electronic balance (Shimadzu AUY220, Japan) capable of measuring up to 0.1mg. An average of 4-5 measurements was taken for each sample. From the experimentally measured vales of ultrasonic velocity (U), density (ρ) and viscosity (η) various acoustic parameters are calculated using the following relations [8]-[10] and discussed in this investigation.

THEORY AND CALCULATIONS

Adiabatic compressibility determined by using the experimentally measured ultrasonic velocity (U) and density (ρ) of the medium by using the equation :

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

Internal pressure is calculated using the formula:

$$\Pi_i = bRT(K\eta/U)^{1/2} (\rho^{2/3}/M_{eff}^{7/6}) \qquad (2)$$

Where b stands for cubic packing factor which is assumed to be 2 for liquids and K is a constant, T is absolute temperature, η is the viscosity in Nsm^{-2}, U is the ultrasonic velocity in ms^{-1}, ρ is the density in kg m^{-3}, M_{eff} is the effective molecular weight and R is universal gas constant.
Intermolecular free length (L_f) has been calculated using the standard relation:

$$L_f = K_r\sqrt{\beta} \qquad (3)$$

Where K_r is a temperature dependant constant known as Jacobson's constant.

The acoustic impedance is the parameter related to elastic properties of the medium and calculated by using the expression :

$$Z = \rho U \qquad (4)$$

Where ρ is the density and U is the ultrasonic velocity.

The molar volumes of the binary liquid mixtures are calculated using the equation :

$$V_m = (x_1V_1 + x_2V_2) / \rho \qquad (5)$$

Relaxation time (τ) can be calculated using viscosity and adiabatic compressibility as:

$$\tau = (3/4)\eta\beta \qquad (6)$$

RESULTS AND DISCUSSION

The experimentally determined values of density (ρ), viscosity (η) and ultrasonic velocity (U) at 303.15K for pure components of Methyl Benzoate , 1-Octanol and 1- Nonanol are listed in Table 1. The experimentally measured values of density (ρ), viscosity (η) and ultrasonic velocity (U) for the binary liquid mixtures Methyl Benzoate +1- Octanol and Methyl Benzoate +1-Nonanol at temperatures 313.15K and 318.15K are presented in Table 2 and Table 3.

From these observed values various acoustic parameters like adiabatic compressibility (β), free length (L_f), molar volume (V_m), internal pressure (π_i), relaxation time (τ) and acoustic impedance (Z) at temperatures 313.15K and 318.15K have been evaluated and are presented in Table 4 and Table 5.

From Table 2 and Table 3, it was observed that the ultrasonic velocity, density decreases with increasing mole fractions of 1-Octanol and 1-Nonanol while the viscosity increases. This may be due to association of a very strong dipole – induced dipole interaction between the component molecules. However the ultrasonic velocity, density, viscosity decreases in all the cases as temperature increases.

In all the binary liquid mixtures, the ultrasonic velocity decreases with increasing concentration of 1-octanol and 1-nonanol. The variation of ultrasonic velocity in a solution depends upon the increase (or) decrease of intermolecular free length after mixing the components. On the basis of a model proposed by Eyring and Kincaid, ultrasonic velocity should decrease, if the intermolecular free length increase and vice-versa [11]. The same result was obtained by Umadevi et al [12].

Here with increase of temperature , due to thermal agitation of component molecules the interaction becomes weak and this is indicated by decrease in ultrasonic velocity values in the present investigation.

Table 1: The values of density (ρ), viscosity (η) and velocity (U) of pure liquids at 303.15K

Liquids	Density ρ (kg/m^3)	Viscosity η ($x10^{-3}Nsm^{-2}$)	Velocity U (m/s)
Methyl Benzoate	1087.5	0.1747	1404
1- Octanol	803.03	0.6306	1365
1- Nonanol	816.45	0.9204	1348.42

Table 2: Density (ρ), viscosity (η) and ultrasonic velocity (U) for the binary mixtures of Methyl Benzoate +1-Octanol at temperatures 313.15K, 318.15K

X_1	ρ (kg/m^3)		η($10^{-3}Nsm^{-2}$)		U (m/s)	
	T=313.15K	T=318.15K	T=313.15K	T=318.15K	T=313.15K	T=318.15K
0.0000	800.00	798.10	0.5890	0.6408	1303.33	1291.57
0.1258	833.40	831.70	0.3781	0.3678	1306.66	1301.05
0.2446	854.80	853.40	0.3680	0.3627	1312.94	1302.35
0.3570	897.80	895.10	0.2471	0.2468	1320.00	1310.52
0.4634	904.00	902.00	0.2372	0.2442	1332.63	1312.94
0.5643	933.80	931.50	0.2134	0.2151	1335.78	1314.86
0.6602	981.80	979.90	0.1893	0.1828	1335.78	1320.00
0.7514	982.10	980.20	0.1653	0.1622	1338.94	1323.00
0.8382	1008.30	1003.80	0.1622	0.1619	1346.66	1326.00
0.9210	1054.80	1054.40	0.1284	0.1263	1354.73	1330.00
1.0000	1084.10	1083.80	0.1313	0.1279	1367.36	1348.42

Table 3: Density (ρ), viscosity (η) and ultrasonic velocity (U) for the binary mixtures of Methyl Benzoate +1-Nonanol at temperatures 313.15K, 318.15K

X_1	ρ (kg/m^3)		η($10^{-3}Nsm^{-2}$)		U (m/s)	
	T=313.15K	T=318.15K	T=313.15K	T=318.15K	T=313.15K	T=318.15K
0.0000	813.76	812.32	0.77071	0.7654	1338.00	1329.47
0.1355	839.65	838.27	0.70755	0.6876	1340.00	1330.00
0.2608	876.47	874.84	0.64915	0.6448	1340.00	1332.30
0.3769	890.79	889.04	0.5981	0.5832	1341.70	1333.40
0.4848	940.31	938.48	0.55291	0.5522	1343.33	1334.11
0.5853	945.11	943.59	0.54232	0.5428	1344.70	1336.66
0.6792	954.83	952.58	0.5061	0.5033	1346.66	1338.00
0.7671	995.24	993.34	0.46202	0.4253	1348.42	1342.10
0.8495	1014.47	1012.85	0.31356	0.3123	1353.33	1343.33
0.9270	1032.68	1030.93	0.3166	0.3115	1360.80	1344.70
1.0000	1084.10	1083.80	0.13131	0.1279	1367.36	1348.42

Table 4: Adiabatic compressibility (β), Internal pressure (π_i), free length (L_f) ,acoustical impedance (Z), molar volume (V_m) and relaxation time (τ) of Methyl Benzoate and 1-Octanol at temperatures 313.15K and 318.15K.

	Adiabatic Compressibility β ($x 10^{-11}m^2/N$)		Internal pressure π_i ($x10^6 N/m^2$)		Free length L_f (A°)		Acoustical impedance Z($x10^4$ kg $m^{-2}sec^{-1}$)		Molar volume V_m ($x10^{-5}m^3 mol^{-1}$)		Relaxation time τ ($x10^{-12}$ sec)	
X_1	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K
0.0000	73.5870	75.1116	212.86	226.23	0.0173	0.0176	104.27	103.08	16.2788	16.3175	0.5779	0.6417
0.1258	70.2783	71.0306	173.88	174.37	0.0169	0.0171	108.90	108.21	15.7157	15.7478	0.3543	0.3484
0.2446	67.8650	69.0863	172.97	174.96	0.0166	0.0168	112.23	111.14	15.4046	15.4298	0.3330	0.3341
0.3570	63.9253	65.0491	145.20	147.65	0.0161	0.0163	118.51	117.30	14.7408	14.7853	0.2106	0.2140

0.4634	62.2891	64.3137	141.44	146.68	0.0159	0.0162	120.47	118.43	14.7094	14.7421	0.1970	0.2094
0.5643	60.0173	62.0952	136.21	139.81	0.0156	0.0160	124.74	122.48	14.3040	14.3393	0.1707	0.1781
0.6602	57.0830	58.5693	132.01	132.40	0.0152	0.0155	131.15	129.35	13.6625	13.6890	0.1441	0.1428
0.7514	56.7966	58.2862	122.65	124.03	0.0152	0.0155	131.50	129.68	13.7133	13.7399	0.1252	0.1261
0.8382	54.6883	56.6586	122.76	125.19	0.0149	0.0152	135.78	133.10	13.4079	13.4681	0.1183	0.1223
0.9210	51.6564	53.6156	111.73	113.61	0.0145	0.0148	142.90	140.24	12.8633	12.8682	0.0884	0.0903
1.0000	49.3361	50.7458	114.09	115.17	0.0141	0.0144	148.24	146.14	12.5588	12.5623	0.0864	0.0865

Table 5: Adiabatic compressibility (β), Internal pressure (π_i), free length (L_f), acoustical impedance (Z), molar volume (V_m) and relaxation time (τ) of Methyl Benzoate and 1-Nonanol at temperatures 313.15K and 318.15K

	Adiabatic Compressibility		Internal pressure		Free length		Acoustical impedance		Molar volume		Relaxation time	
	β (x $10^{-11}m^2/N$)		π_i (x10^6 N/m^2)		L_f (A°)		Z (x10^4 kg $m^{-2}sec^{-1}$)		V_m (x$10^{-5}m^3$ mol^{-1})		τ (x10^{-12} sec)	
X_1	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K	313.15K	318.15K
0.0000	68.6415	69.6488	215.73	218.86	0.0167	0.0169	108.88	108.00	17.7262	17.7577	0.7054	0.7108
0.1355	66.3273	67.4392	212.79	213.69	0.0164	0.0166	112.51	111.49	17.0490	17.0771	0.6257	0.6183
0.2608	63.5404	64.3971	211.49	214.49	0.0160	0.0163	117.45	116.56	16.2169	16.2472	0.5500	0.5536
0.3769	62.3605	63.2641	206.67	207.71	0.0159	0.0161	119.52	118.54	15.8507	15.8820	0.4973	0.4919
0.4848	58.9337	59.8674	207.38	211.00	0.0154	0.0157	126.31	125.20	14.9231	14.9522	0.4345	0.4408
0.5853	58.5145	59.3163	207.38	211.19	0.0154	0.0156	127.09	126.13	14.7610	14.7849	0.4231	0.4293
0.6792	57.7504	58.6390	202.85	205.86	0.0153	0.0155	128.58	127.46	14.5312	14.5656	0.3897	0.3935
0.7671	55.2612	55.8898	200.31	195.46	0.0150	0.0151	134.20	133.32	13.8697	13.8962	0.3404	0.3169
0.8495	53.8209	54.7128	167.78	170.56	0.0148	0.0150	137.29	136.06	13.5409	13.5626	0.2250	0.2278
0.9270	52.2930	53.6438	171.05	173.20	0.0145	0.0148	140.53	138.63	13.2413	13.2638	0.2207	0.2228
1.0000	49.3361	50.7458	114.09	115.17	0.0141	0.0144	148.24	146.14	12.5588	12.5623	0.0864	0.0865

Table 4 and Table 5 show the variation of adiabatic compressibility, internal pressure, free length, acoustic impedance, molar volume and relaxation time with temperature and concentration respectively for both the systems. From Table 4 and Table 5, it is observed that adiabatic compressibility, internal pressure, free length and molar volume increase with increase in temperature and decrease with increase in concentration of Methyl Benzoate for both the binary mixtures. The increase in adiabatic compressibility and intermolecular free length with increasing mole fractions of 1-octanol and 1-nonanol indicates significant interactions between methyl benzoate and 1-octanol and methyl benzoate and 1- nonanol molecules forming hydrogen bonding through dipole-dipole interaction. Similar results were observed by earlier workers in their mixtures.

Further, the increase in molar volume and internal pressure with rise in concentration of 1-octanol and 1-nonanol in both the systems clearly show the increasing magnitude of interactions. It is seen from Table 4 and Table 5 that relaxation time (τ) decrease with increase in concentration of Methyl Benzoate and increase with increase in temperature. This is similar to the change found in viscosity, showing that viscous forces play a dominant role in the relaxation process. The variation of acoustic impedance with temperature and concentration is shown in Table 4 and Table 5. It is observed that the acoustic impedance decreases with increase in temperature and it increases with increase in concentration. This is in agreement with requirement as both ultrasonic velocity and density increase with increase in concentration of the solute and also effective due to solute-solvent interactions.

CONCLUSIONS

From the experimental data of density, viscosity and ultrasonic velocity, some thermo acoustical parameters for the binary liquid mixtures of Methyl Benzoate and 1- Octanol & Methyl Benzoate and 1-Nonanol are measured at temperatures 313.15K and 318.15K. The observed results suggest the existence of a strong dipole-dipole molecular interaction between the component molecules of the binary liquid mixture. From the experimental evidence, it is also concluded that the interaction between the component molecules decreases with increase in temperature in both the binary liquid mixtures.

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