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Ultrasonic Study of Acoustical Parameters of Binary Liquid Mixtures of Methyl Benzoate with 1-Octanol at 303.15K, 308.15K, 313.15K and 318.15K

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Abstract

The ultrasonic velocity (U), the density (ρ) and viscosity (η) of methyl benzoate with 1-Octanol have been measured at 303.15K, 308.15K, 313.15K and 318.15K over the entire range of composition. From the measured data of ultrasonic velocity, density and viscosity, acoustic parameters such as adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π_i), relaxation time (τ) and acoustic impedance (Z) have been estimated using standard relations. The variation of adiabatic compressibility (β), free length (L_f), free volume (V_f) internal pressure (π_i), relaxation time (τ) and acoustic impedance (Z) with concentration and temperature have been studied. Acoustic parameters provide important information in understanding the solute-solvent interaction in a polymer solution.

Keywords: Adiabatic compressibility, free length, free volume, internal pressure, relaxation time, acoustic impedance, binary liquid mixture.

Introduction

Ultrasonic investigations of liquid mixtures consisting of polar and non polar components are of considerable importance in understanding intermolecular interactions between the component molecules and find applications in several industrial and technological processes[1-3]. The variation of ultrasonic velocity and other ultrasonic parameters of binary liquid mixtures have been studied by many researchers and they have shed light upon structural changes associated with liquid mixtures of weakly or strongly interacting compounds[4-10]. The study of molecular association 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[11-15]. But a systematic study with primary fatty alcohols in binary systems has been 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. Octanol is a straight chain fatty alcohol with 8 carbon atoms. The primary use of octanol is in the manufacture of various esters which are used in the perfumery and flavors.

Therefore in order to have a clear understanding of the intermolecular interactions between the component molecules, a thorough study on the binary liquid mixtures (methyl benzoate +1-octanol) using ultrasonic velocity data has been performed at temperatures 303.15K, 308.15K, 313.15K and 318.15K.

In the present study several acoustic parameters such as adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π_i), relaxation time (τ) and acoustic impedance (Z) of a binary system methyl benzoate +1-octanol have been reported using the experimental values of density, viscosity and ultrasonic velocity of the binary liquid mixtures at temperatures 303.15K, 308.15K, 313.15K and 318.15K.

Material 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 (>99%). All the liquids used were further purified by standard procedure[16]. 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 fractions of 1st compound Methyl Benzoate has been increased from 0 to1.

Apparatus and Procedure: The ultrasonic velocities were measured by using a 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 3 MHz. 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 0.1 mg. An average of 4-5 measurements was taken for each sample. From the experimentally measured values of ultrasonic velocity (U), density (ρ) and viscosity (η) , various acoustic parameters are calculated using the following relations[17-21] and discussed in this investigation.

Theory and Calculations: Adiabatic compressibility has been calculated from the speed of sound (U) and density (ρ) of the medium using the equation as:

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

Intermolecular free length (L_f) has been determined using the standard relation as:

$$L_f = K_r\sqrt{\beta} \quad (2)$$

Where K_r is a temperature dependant constant known as Jacobson's constant. The relation for free volume in terms of ultrasonic velocity (U) and viscosity (η) of the liquid as:

$$V_f = (M_{eff}\, U/\eta K)^{3/2} \quad (3)$$

Where M_{eff} is the effective molecular weight ($M_{eff} = \Sigma m_i x_i$ in which m_i and x_i are the molecular weight and mole fraction of the individual components respectively). K is a temperature independent constant which is equal to 4.28×10^9 for all liquids.

On the basis of statistical thermodynamics, Suryanarayana[22] derived an expression for determination of internal pressure by the use of free volume concept as:

$$\Pi_i = bRT(K\eta/U)^{1/2} (\rho^{2/3}/M_{eff}^{7/6}) \quad (4)$$

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.

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

$$\tau = (3/4)\eta\beta \quad (5)$$

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

$$Z = \rho U \quad (6)$$

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

Results and Discussion

The experimentally determined values of density (ρ), viscosity (η), and ultrasonic velocity (U) at 303.15K for pure components of the system Methyl Benzoate +1-Octanol are listed in Table-1. The same values for the binary liquid mixture Methyl Benzoate +1-Octanol at temperatures 303.15K, 308.15K, 313.15K and 318.15K are presented in table-2.

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

Table-2
Density (ρ), viscosity (η) and ultrasonic velocity (U) for the binary mixtures of Methyl Benzoate +1-Octanol at temperatures 303.15K, 308.15K, 313.15K and 318.15K

X_1	T=303.15K			T=308.15K		
	ρ (kg/m^3)	η($10^{-3}Nsm^{-2}$)	U (m/s)	ρ (kg/m^3)	η$x10^{-3}$(Nsm^{-2})	U (m/s)
0.0000	803.03	0.6306	1365.00	801.60	0.6171	1326.31
0.1258	836.40	0.4667	1370.52	835.00	0.4380	1329.47
0.2446	859.20	0.4344	1371.80	857.30	0.3969	1333.33
0.3570	902.50	0.2949	1376.84	900.10	0.2737	1343.33
0.4634	908.90	0.2793	1380.00	905.90	0.2484	1348.42
0.5643	938.00	0.2567	1383.52	935.50	0.2361	1351.76
0.6602	986.00	0.2237	1387.05	983.80	0.2071	1354.66
0.7514	986.30	0.2057	1390.00	984.00	0.1811	1357.89
0.8382	1011.80	0.1914	1396.66	1010.40	0.1764	1369.41
0.9210	1059.10	0.1515	1400.00	1056.00	0.1396	1373.68
1.0000	1087.50	0.1747	1404.00	1085.90	0.1546	1376.84
0.0000	800.00	0.5890	1303.33	798.10	0.6408	1291.57
0.1258	833.40	0.3781	1306.66	831.70	0.3678	1301.05
0.2446	854.80	0.3680	1312.94	853.40	0.3627	1302.35
0.3570	897.80	0.2471	1320.00	895.10	0.2468	1310.52
0.4634	904.00	0.2372	1332.63	902.00	0.2442	1312.94
0.5643	933.80	0.2134	1335.78	931.50	0.2151	1314.86
0.6602	981.80	0.1893	1335.78	979.90	0.1828	1320.00
0.7514	982.10	0.1653	1338.94	980.20	0.1622	1323.00
0.8382	1008.30	0.1622	1346.66	1003.80	0.1619	1326.00
0.9210	1054.80	0.1284	1354.73	1054.40	0.1263	1330.00
1.0000	1084.10	0.1313	1367.36	1083.80	0.1279	1348.42

Table-3
Adiabatic compressibility (β), free length (L_f) and free volume (V_f) of Methyl Benzoate and 1-Octanol at temperatures 303.15K, 308.15K, 313.15K and 318.15K

X_1	Adiabatic compressibility β (x 10^{-11} m^2/N)				Free length L_f (A°)				Free volume V_f (x10^{-7} m^3 mol^{-1})			
	303.15K	308.15K	313.15K	318.15K	303.15K	308.15K	313.15 K	318.15 K	303.15K	308.15K	313.15K	318.15K
0.0000	66.8348	70.9173	73.587	75.1116	0.0162	0.0168	0.0173	0.0176	5.3449	5.2881	5.5247	4.803
0.1258	63.6525	67.7574	70.2783	71.0306	0.0158	0.0164	0.0169	0.0171	8.5187	8.9514	10.8738	11.2617
0.2446	61.8478	65.6133	67.865	69.0863	0.0156	0.0162	0.0166	0.0168	9.5775	10.5093	11.4987	11.6116
0.3570	58.4502	61.5664	63.9253	65.0491	0.0152	0.0157	0.0161	0.0163	17.3443	18.6919	21.2282	21.042
0.4634	57.7731	60.7113	62.2891	64.3137	0.0151	0.0156	0.0159	0.0162	19.0172	21.9011	23.0622	21.5902
0.5643	55.6963	58.5002	60.0173	62.0952	0.0148	0.0153	0.0156	0.016	21.8194	23.8825	27.3089	26.3525
0.6602	52.7156	55.3902	57.083	58.5693	0.0144	0.0149	0.0152	0.0155	27.0933	29.3564	32.8778	34.0456
0.7514	52.4761	55.1157	56.7966	58.2862	0.0144	0.0148	0.0152	0.0155	30.9996	36.229	40.6961	41.1078
0.8382	50.6669	52.7764	54.6883	56.6586	0.0141	0.0145	0.0149	0.0152	35.0071	38.3953	42.4534	41.6071
0.9210	48.1734	50.1841	51.6564	53.6156	0.0138	0.0141	0.0145	0.0148	50.1558	55.0899	61.1789	60.9802
1.0000	46.6484	48.5784	49.3361	50.7458	0.0135	0.0139	0.0141	0.0144	40.8834	47.7024	60.289	61.4248

Table-4
Internal pressure (πi), relaxation time (τ) and acoustical impedance (Z) of Methyl Benzoate and 1- Octanol at temperatures 303.15K, 308.15K, 313.15K and 318.15K

X_1	Internal pressure π_i (x10^6 N/m^2)				Relaxation time τ (x10^{-12} sec)				Acoustical impedance Z (x10^4 kg $m^{-2}$$sec^{-1}$)			
	303.15K	308.15K	313.15K	318.15K	303.15K	308.15K	313.15K	318.15K	303.15K	308.15K	313.15K	318.15 K
0.0000	208.87	212.82	212.86	226.23	0.5620	0.5835	0.5779	0.6417	109.61	106.32	104.27	103.08
0.1258	183.04	182.80	173.88	174.37	0.3961	0.3957	0.3543	0.3484	114.63	111.01	108.90	108.21
0.2446	178.57	175.73	172.97	174.96	0.3582	0.3472	0.3330	0.3341	117.87	114.31	112.23	111.14
0.3570	150.88	149.32	145.20	147.65	0.2298	0.2247	0.2106	0.2140	124.26	120.91	118.51	117.30
0.4634	146.54	141.80	141.44	146.68	0.2152	0.2011	0.1970	0.2094	125.43	122.15	120.47	118.43
0.5643	142.53	140.33	136.21	139.81	0.1906	0.1842	0.1707	0.1781	129.77	126.46	124.74	122.48
0.6602	136.70	135.09	132.01	132.40	0.1572	0.1529	0.1441	0.1428	136.76	133.27	131.15	129.35
0.7514	130.38	125.62	122.65	124.03	0.1439	0.1331	0.1252	0.1261	137.10	133.62	131.50	129.68
0.8382	127.03	125.09	122.76	125.19	0.1293	0.1241	0.1183	0.1223	141.31	138.37	135.78	133.10
0.9210	115.88	113.94	111.73	113.61	0.0973	0.0934	0.0884	0.0903	148.27	145.06	142.90	140.24
1.0000	125.97	121.51	114.09	115.17	0.1086	0.1001	0.0864	0.0865	152.69	149.51	148.24	146.14

Figure-1
Variation of Adiabatic compressibility with Mole fraction of Methyl Benzoate at temperatures 303.15K, 308.15K, 313.15K and 318.15K

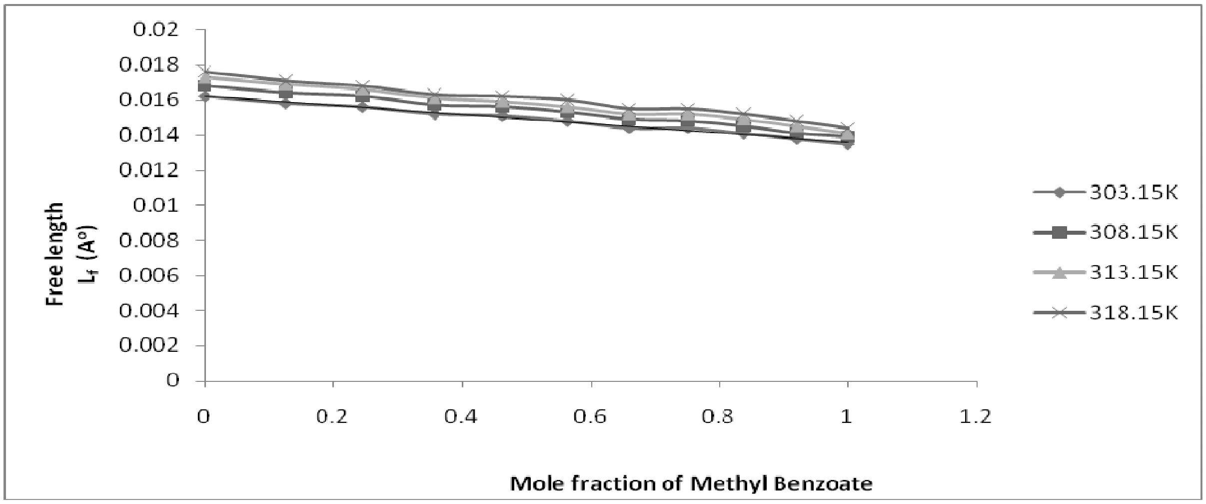

Figure-2
Variation of Free length with Mole fraction of Methyl Benzoate at temperatures 303.15K, 308.15K, 313.15K and 318.15K

Figure-3
Variation of Free volume with Mole fraction of Methyl Benzoate at temperatures 303.15K, 308.15K, 313.15K and 318.15K

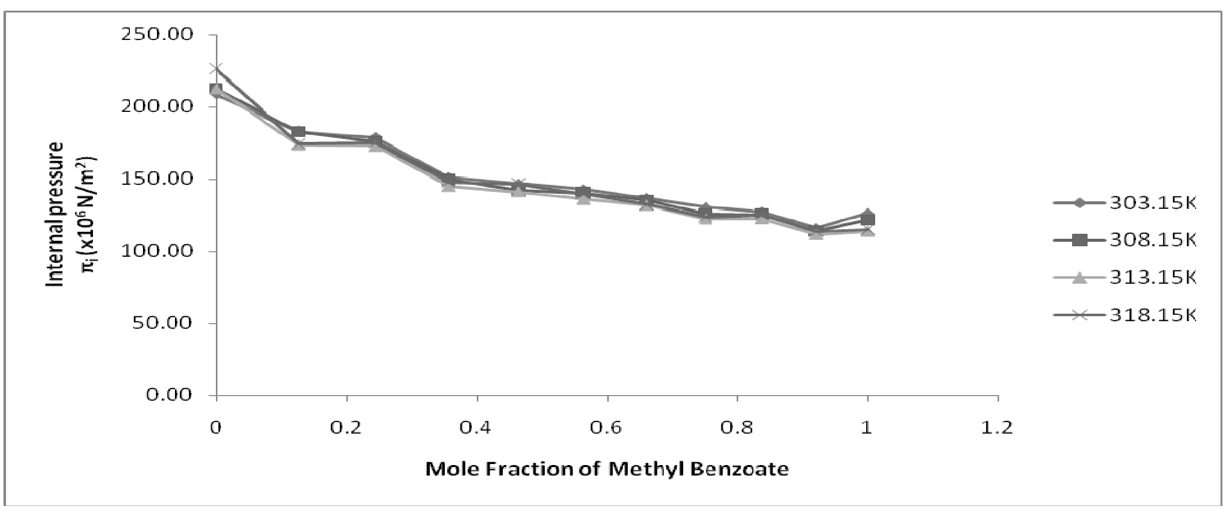

Figure-4
Variation of Internal Pressure with Mole fraction of Methyl Benzoate at temperatures 303.15K, 308.15K, 313.15K and 318.15K

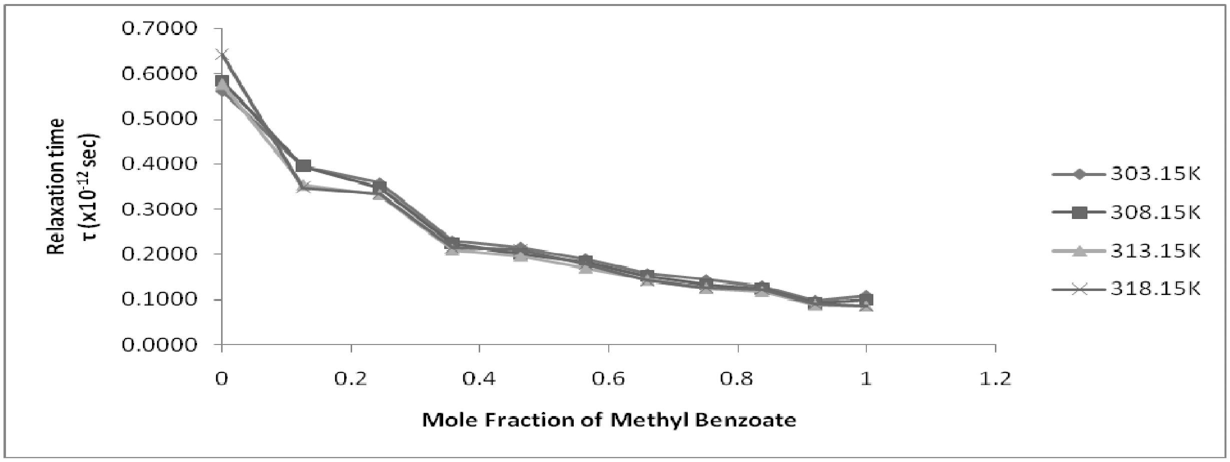

Figure-5
Variation of Relaxation time with Mole fraction of Methyl Benzoate at temperatures 303.15K, 308.15K, 313.15K and 318.15K

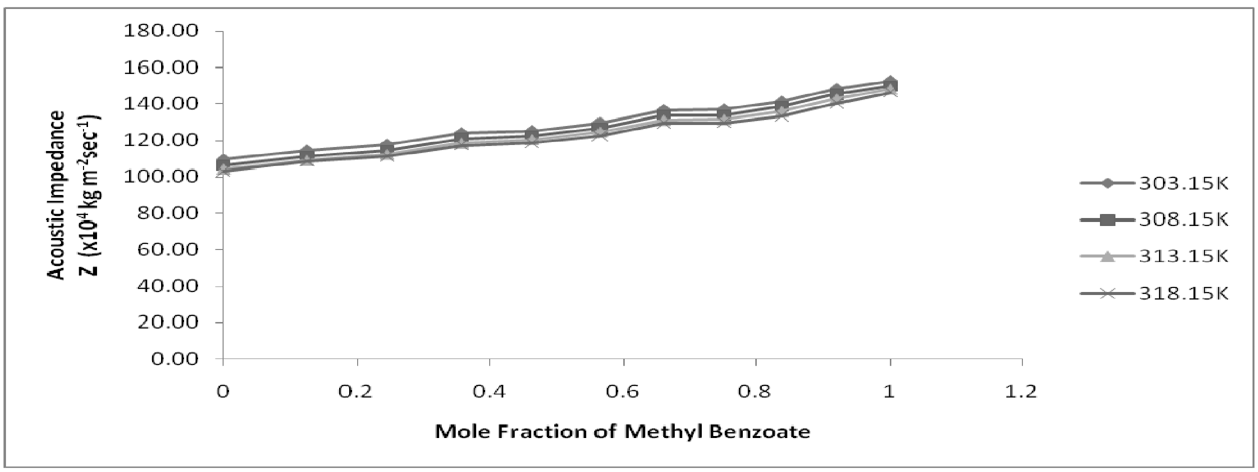

Figure-6
Variation of Acoustic Impedance with Mole fraction of Methyl Benzoate at temperatures 303.15K, 308.15K, 313.15K and 318.15K

From these observed values various acoustic parameters like adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π_i), relaxation time (τ) and acoustic impedance (Z) at temperatures 303.15K, 308.15K, 313.15K and 318.15K have been evaluated and are presented in table-3 and table-4.

The variation of β, L_f, V_f, π_i, τ and Z with mole fraction of Methyl Benzoate at different temperatures are shown in figures-1-6.

From table-2, it was observed that the ultrasonic velocityand density decrease with increasing mole fraction of Octanol 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. The same result was obtained by S.Thirumaran et al[23] and M.Umadevi et al[24].

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-3, 4 and figures-1-6 show the variation of adiabatic compressibility, free length, free volume, internal pressure, relaxation time and acoustic impedance with temperature and concentration respectively. From table-3 and figures-1 and 2, it is observed that adiabatic compressibility and free length increase with increase in temperature and decrease with increase in concentration of Methyl Benzoate. The decrease in adiabatic compressibility indicates the enhancement of the bond strength at this concentration. From table-3 and figure-3, it is also observed that the values of free volume increase with increase in concentration of Methyl Benzoate.

It is seen from table-4 and figures-4 and 5 that internal pressure (π_i) and relaxation time (τ) decrease with increase in concentration of Methyl Benzoate. 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 figure-6. It is observed 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.

Conclusion

From the observed experimental values of density, viscosity and ultrasonic velocity and related acoustical parameters values for the binary liquid mixtures of methyl benzoate and 1-octanol system at temperatures 303.15K, 308.15K, 313.15K and 318.15K, it is clear that there exists a strong intermolecular association between the component molecules of the liquid mixtures. In the present system when the temperature increases, the interaction between the component molecules decreases.

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