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Comparative Study of Physicochemical and Acoustic Properties of Binary Liquid Mixtures of Cyclopentyl Methyl Ether with Chlorobenzene and Cyclopentyl Methyl Ether with Methyl Acrylate at 298.15 K Temperature

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Author's contribution

The sole author designed, analysed, interpreted and prepared the manuscript.

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Short Research Article

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ABSTRACT

Physicochemical and acoustic propertie of liquid mixtures give knowlegeble information behaviour and interactions studies of liquids. Ultrasonic studies in liquids and solutions provide some valuable information about the structure and interaction in such systems. Ultrasonic velocity and density have been proved to be important properties to test the validity of liquid state model. The ultrasonic velocity (U) and density (ρ) of the binary liquid mixtures Chlorobenzene (polar)+Cyclopentyl methyl ether (nonpolar) [system I] and Methyl acrylate (polar) +Cyclopentyl methyl ether (nonpolar) [system II] are measured at 298.15 K temp. with pure components. With the help of these measured properties are calculated excess acoustic parameters using standard relations. Excess acoustic parameters are used as a qualitative and quantitative analysis in multicomponent liquid mixtures. The sign and magnitude of excess parameters provided information of different type interactions. Structural chemistry is related to the interactions involved in the liquid systems. structural effects also define nature and bonding of both liquid mixture system I and II.

Keywords: Density; intermolecular interactions; nature; structural; ultrasonic velocity.

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1. INTRODUCTION

The molecules in liquids and liquid mixtures are a state of random motion although the extent of randomness. The molecules are relatively close together. Most of the space in the liquid gets occupied by its molecules and only a small fraction of the space is available to them for their free ovement. This explains the higher density, incompressibility and show diffusion.The average kinetic energy of the molecules in liquids and liquid mixtures are proportional to the absolute temperature increase in temperature would increase the proportion of the energized molecules, lowers the attractive forces between the molecules and consequently. The most of hysicochemical properties of the liquid mixtures arise due to nature and magnitude of the intermolecular forces between the molecules. Appreciable forces of attractions exist between the molecules of a liquid mixtures. These are about 10^6 times as strong. The forces amongst the on stituents of liquid mixtures disallow them from separating spontaneously from each other, but they are not strong enough to hold the molecules in fixed positions. Measurement of physicochemical and acoustic parameters of liquids and liquid mixtures has an advantage, for their are numerous instances where it is impractical to measure product design, optimization various important information. The excess parameters give relative strength of A–A, B–B and A–B in the mixture of A and B liquids [1].

Cyclopentyl methyl ether (CPME), also known as methoxycyclopentane, is a totally new hydrophobic ether solvent. Its Dielectric constant is 4.76. It has a characteristic odour and produces temporary unconsciousness when inhaled. The vapours of CPME are heavier than air and have a tendency to flow along the top of a laboratory bench. It is excellent solvent particularly for oils and fats. It is lighter than water and are slightly soluble in water due to their intermolecular H-bonding with water. It is also used as phase transfer catalyst. May be utilization of CPME formation of new organic compounds [2].

Chlorobenzene is a colourless, pleasant smelling liquid and It have 132^0C B. P. and -45^0C M. P. It have high density and UV spectra show a characteristic band at 225mμ. The orbitals of the carbon atom in C-Cl bond is show sp^3 hybridized. It is insoluble in water but soluble in ethanol and diethyl ether. It is heavier than water, density is 1.112 g/ml at 20^0c. It is steam-volatile. It has dipole moment 1.76 D. Chlorobenzene constitute on of the most versatile synthetic tool in the hands of an organic chemist. It is used for the preparation of phenol, manufacture of azo and sulphur dyes, fungicides, preservatives and DDT [6].

Methyl acrylate It is colourless liquid in pure state and having a pungent smell. It is a very important industrial chemical used for detection of leakage, plastic industry and preparation high polymeric and latex compounds. It is insoluble in water but dissolves in ethanol and ether. It is polar (dipole moment, μ = 1.77 D at 298.15 K). It gives reactions of an alkene and carboxylic acid [7].

In this research paper is to study the excess acoustic and physicochemical properties, which are the measures of different type interactions involved between molecules in the liquid mixtures. It is obvious that the study of these parameters gives details on molecules of liquids are held together by different intermolecular forces in the liquid mixtures.

2. MATERIALS AND METHODS

In this work take three liquids are Cyclopentyl methyl ether, Chlorobenzene and Methyl acrylate in pure state and determine ultrasonic velocity and density with the help of interferometer and pyknometer. The uncertainty in mole fraction is 0.0001. A multi frequency digital micrometer reading ultrasonic interferometer operating at a single frequency (2 MHz) variable path was used to measure the ultrasonic velocity of the liquids and binary liquid mixtures at a constant temperature of 298.15 K. Pyknometer is an apparatus for measuring the density of liquids and liquid mixtures. It consists of a U tube having a cylindrical bulb and two capillary arms. The pyknometer was thoroughly cleaned first with chromic acid and then successively with distilled water and alcohol. It was then dried in electric oven. It was suspended from the beam of the balance with a hook of a wire. The pyknometer was then filled with distilled water up to the mark and weighed again. It was then made empty, dried with a cloth and filled with liquid and liquid mixture and carefully weihed at a constant temperature of 298.15 K.

3. RESULTS AND DISCUSSION

A precise prediction of the systems depends largely on the extent of interaction involved in the liquid mixtures. In this work measured densities

and ultrasonic velocities with checked their validity and calculated various acoustical parameters such as K_S, Z and L_f were using the following equations 1, 2 & 3 respectively and are incorporated in Table 2 for the binary system under study [8-11].

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

$$Z = \rho U \quad \ldots (2)$$

$$L_f = K_T (K_s)^{1/2} \quad \ldots (3)$$

Where 'K_T' is Jacobson's constant [12]. The excess functions Y^E are calculated using the relation:

$$Y^E = Y_{mix} - (X_1Y_1 + X_2Y_2) \quad \ldots (4)$$

Where Y denotes U, Z, $K_S$and $L_f$respectively, X is the mole fraction and suffixes 1 & 2 denotes the components 1 & 2 in binary liquid mixture and the values are given in Table 3. The dependence of U^E, Z^E, $K_S{}^E$ and $L_f{}^E$ on the mole fraction of Chlorobenzene for liquid mixture were fitted to the following Redlich-Kisterequation [14] by the least-squares method and the values are given in Table 4.

$$Y^E = x(1- X) \sum i\, A_i(2x - 1)^i \quad \ldots (5)$$

Where Y^E is U^E, Z^E, $K_S{}^E$ and $L_f{}^E$ parameters. The parameters A_i, obtained by a nonlinear least squares polynomial fitting procedure, are also given in Table 4. together with the standard deviations (σ) values. From Table 2, it is observed that the values of U, Z, K_s and L_f varied linearly with the mole fraction of Cyclopentyl methyl ether. Cyclopentyl methyl ether, Chlorobenzene and Methyl acrylate were chosen because they can directly bonded due to strained configuration. The variations in excess acoustical parameters with the mole fraction of Cyclopentyl methyl ether are examined.

In binary liquid mixtures system I(Cyclopentyl methyl ether and Chlorobenzene) It is observed that the estimated data show positive values of excess ultrasonic velocity and negative values of excess acoustic impedance (Table 3) due to difference in size and shape of unlike molecules and interstitial accommodation between molecules of liquid. Furthermore both $K_S{}^E$ and $L_f{}^E$ are show negative values due to CPME have great angular strain since its bond angles is much smaller and show high reactivity and the

Table 1. Comparison of experimental density (ρ) and ultrasonic velocity (U) of pure liquids with literature at298.15 K [3-5]

S. No.	Liquid	Density (ρ) x 10^{-3} Kg m^{-3}		Ultrasonic velocity (U) m s^{-1}	
		Experimental	Literature	Experimental	Literature
1.	Cyclopentyl methyl ether	0.7354	0.7356	1367.4	1368.3
2.	Chlorobenzene	1.1011	1.1009	1270.2	1271.0
3.	Methyl acrylate	0.9363	0.9356	1142.0	1140.0

Table 2. Calculated data of ρ, U, Z, K_S, L_f for the liquid mixtures of Cyclopentyl methyl ether withChlorobenzene and Cyclopentyl methyl ether with Methyl acrylate at 298.15 K

System-I (Cyclopentyl methyl ether with Chlorobenzene)

Mole fraction of Cyclopentyl methyl ether (X)	ρ x 10^{-3} Kg m^{-3}	U m s^{-1}	Z x 10^4 Kg $m^{-2}s^{-1}$	K_S x 10^{-11} m^2 N^{-1}	L_f x 10^{-11} m
0.0000	0.7872	1482.3	0.1166	57.8152	7.8650
0.1047	0.7836	1470.2	0.1152	59.0406	7.9142
0.2021	0.7778	1456.4	0.1132	60.6136	8.0190
0.3056	0.7689	1432.3	0.1101	63.3960	8.2010
0.4058	0.7602	1418.8	0.1078	65.3476	8.3262
0.5124	0.7565	1401.5	0.1060	67.2984	8.4496
0.6020	0.7421	1389.3	0.1030	69.8144	8.6061
0.7201	0.7388	1376.8	0.1017	71.4054	8.7036
0.8087	0.7324	1368.5	0.1002	72.9057	8.7946
0.9098	0.7301	1359.7	0.0992	74.9057	8.9144
1.0000	0.7258	1347.8	0.0978	75.8459	8.9702

System-II (Cyclopentyl methyl ether with Methyl acrylate)

Mole fraction of Cyclopentyl methyl ether (X)	ρ x 10^{-3} Kg m^{-3}	U m s^{-1}	Z x 10^{4} Kg $m^{-2}s^{-1}$	K_S x 10^{-11} m^2 N^{-1}	L_f x 10^{-11} m
0.0000	0.9363	1142.0	0.1069	81.8941	1.8612
0.1047	0.9101	1174.2	0.1068	79.6942	1.8361
0.2021	0.8902	1198.4	0.1066	78.2183	1.8190
0.3056	0.8697	1217.6	0.1058	77.5570	1.8113
0.4058	0.8453	1234.2	0.1043	77.4310	1.8098
0.5124	0.8214	1258.8	0.1033	76.8301	1.8284
0.6020	0.8006	1273.4	0.1019	76.1877	1.7952
0.7201	0.7798	1295.9	0.1010	76.0671	1.7938
0.8087	0.7601	1322.7	0.1005	75.1980	1.7835
0.9098	0.7496	1339.5	0.1004	74.3506	1.7750
1.0000	0.7354	1367.4	0.1002	72.7252	1.7540

Table 3. Calculated data of U^E, Z^E, K_S^E, L_f^E for the liquid mixtures of Cyclopentyl methyl ether with Chlorobenzene and Cyclopentyl methyl ether with Methyl acrylate at 298.15 K

System-I(Cyclopentyl methyl ether with Chlorobenzene)

Mole fraction of Cyclopentyl methyl ether (X)	U^E m s^{-1}	Z^E x 10^{4} Kg m^{-2} s^{-1}	K_S^E x 10^{-11} m^2 N^{-1}	L_f^E x 10^{-11} m
0.0000	0.0000	0.0000	0.0000	0.0000
0.1024	6.2358	-1.0245	-4.2358	-1.5485
0.2085	6.8752	-1.2875	-4.8548	-1.7855
0.3088	7.0254	-1.4412	-5.0215	-1.9020
0.4102	7.6982	-1.5689	-5.6254	-2.0321
0.5069	8.0012	-1.7750	-5.9645	-2.3210
0.6124	8.7582	-1.8521	-6.1241	-2.5854
0.7154	8.9882	-1.9689	-6.4325	-2.7878
0.8107	9.2547	-2.0350	-6.9960	-2.8788
0.9059	9.7483	-2.2145	-7.2231	-3.0020
1.0000	0.0000	0.0000	0.0000	0.0000

System-II(Cyclopentyl methyl ether with Methyl acrylate)

Mole fraction of Cyclopentyl methyl ether (X)	U^E m s^{-1}	Z^E x 10^{4} Kg m^{-2} s^{-1}	K_S^E x 10^{-11} m^2 N^{-1}	L_f^E x 10^{-11} m
0.0000	0.0000	0.0000	0.0000	0.0000
0.1024	1.2514	0.1245	-0.2145	-0.0985
0.2085	1.4758	0.2548	-0.3754	-1.0212
0.3088	1.7212	0.2875	-0.5214	-1.2542
0.4102	1.9254	0.2968	-0.6325	-1.3524
0.5069	2.1254	0.3124	-0.7548	-1.4524
0.6124	2.3254	0.3451	-0.7625	-1.5245
0.7154	2.4575	0.3545	-0.7772	-1.6326
0.8107	2.6254	0.3754	-0.7854	-1.7457
0.9059	2.5243	0.3654	-0.7685	-1.7325
1.0000	0.0000	0.0000	0.0000	0.0000

phenomena between molecules of two liquids Cyclopentyl methyl ether and Chlorobenzene represent interaction analysis between chlorine atom of Chlorobenzene with the maximal inductive effect of cyclopentyl cation of Cyclopentyl methyl ether.

Table 4. Parameters of Eq. (5) and Standard deviations

System-I(Cyclopentyl methyl ether with Chlorobenzene)

Excess Property	A_0	A_1	A_2	A_3	A_4	σ
$K_S^E \times 10^{-11}$ m^2 N^{-1}	0 .08548	-3.2312	1.2358	2.0254	0.9857	1.0254
$L_f^E \times 10^{-11}$ m	-0.10254	-4.0030	1.8587	-0.8458	-3.0214	1.3654
$Z^E \times 10^4$ Kg m^{-2} s^{-1}	0.12100	2.3654	-3.2654	-3.6584	0.9689	1.8502
U^E m s^{-1}	-0.14545	5.3650	-7.0254	4.3258	3.2545	3.2654

System-II(Cyclopentyl methyl ether with Methyl acrylate)

Excess Property	A_0	A_1	A_2	A_3	A_4	σ
$K_S^E \times 10^{-11}$ m^2 N^{-1}	-0.00215	-2.02142	3.25142	1.36250	0.68572	0.05884
$L_f^E \times 10^{-11}$ m	-0.00217	-1.02587	1.45874	-0.32655	-1.25482	0.00478
$Z^E \times 10^4$ Kg m^{-2} s^{-1}	0.01452	2.36581	-2.30268	-2.98547	-1.08865	0.0014
U^E m s^{-1}	-0.00253	6.58742	-8.98752	6.32562	-1.65245	2.52482

In binary liquid mixtures system II (Cyclopentyl methyl ether and Methyl acrylate) It is observed that The positive deviations in U^E and Z^E (Table 3) for in the system standby are observed over the entire range of composition due to orientation of liquids. The negative values observed of K_S^E and L_f^E due to little dipolar association between their molecules anticipated dipole moment of Cyclopentyl methyl ether indicate significant interactions between Methyl acrylate and Cyclopentyl methyl ether molecules forming dipole dipole interaction. In contrast, there is possibility of the electron donor acceptor (charge-transfer) type interactions [13-14].

4. CONCLUSIONS

The variation of excess acoustic parameters and physiochemical properties represents analysis of molecular interactions between the components of the mixtures. There is an opposite trend for the systemsI and II. In system I, the positive values are observed due to the strong attractive bonding, while the negative values are observed due to the weak interaction between unlike molecules. Simultaneously great angular strain of Cyclopentyl methyl ether and Inductive effect, electron density of Chlorobenzene make the system less compressible. In system II, the positive values are observed due orientation and lower value of x_1, while the negative values are observed due to the dipole dipole interaction dominates, electron-donor–acceptor interaction are accountable for conduct of the system. As compared to system II, system I has size and shape of molecules difference, intermolecular forces tend to decrease as the distance between the molecules surrounding them, but afford those provide with tightly packed design System II is more compressible ascribable to scatter essence interlinkage and structural effects .

COMPETING INTERESTS

Author has declared that no competing interests exist.

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