Journal of
Chemistry & Applied Biochemistry

Open Science Publications

Volume 6, Issue 1 - 2022

www.opensciencepublications.com

Study of Acoustical and Physico-Chemical Properties on the Binary Mixture of Cyclopentyl Methyl Ether (Cpme) and Methyl Acrylateat 298.15 K Temperature

Research Article

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Article Information: **Submission:** 07/04/2022; **Accepted:** 08/05/2022; **Published:** 10/06/2022

Abstract

Acoustical and Physico-chemical properties of liquid mixtures and solutions are playing very important role in understanding the nature of intermolecular interactions. Excess function; have been used as a qualitative and quantitative guide to predict the extent of complex formation in binary liquid mixtures. In this paper evaluated experimental densities (ρ) and ultrasonic velocities (U) for the pure liquids and liquid mixture of Cyclopentyl methyl ether and Methyl acrylate using bicapillary pycnometer and single frequency variable path over the different concentration range at 298.15 K Temprature. The observed data had been utilized to calculate various acoustical parameters like isentropic compressibility (K_s), Intermolecular free length (L_f) and acoustic impedance (Z). Excess ultrasonic velocities (U^E), Excess Isentropic compressibility (K_S^E), Excess Intermolecular free length (L_f^E) and Excess acoustic impedance (Z^E) were calculated using the measured values and correlated with the Redlich-Kister polynomial equation. The observed variations of the properties for the above mixture conclude that the interactions between unlike molecules predominate over the dissociation effects in the individual components. It is also evident that the presence of strong interactions between unlike molecules is predominant and characterized by the deviations of Excess acoustical parameters.

Keywords: Acoustic impedance; Density; Inter molecular free-Length; Isentropic compressibility; Ultrasonic velocity

Introduction

Due to recent developments made in the theories of liquid mixtures and experimental techniques, the study of binary liquid mixtures, has attracted several researchers in the field [1]. The prediction of the physicochemical parameters of liquid mixtures is a goal of long standing, with both theoretical and practical importance. A truly fundamental theory would predict the parameters along with other thermodynamic and transport properties from the knowledge of the intermolecular forces and radial distribution function alone. Such a programme has had appreciable success in application to pure simple liquids such as the liquefied rare gases [2], for solutions however although the general theory has been formulated, It has not been reduced successfully to numerical results continuing a study of the effect of molecular structure on refractive index-density relationships [3], mixtures of the three possible combinations of the aromatics compounds were investigated The effect of composition and temperature on refractive index dispersion and density measurement were presented for the mixture at 20, 30 and 40°C. Density measurement provided a satisfactory means for analysing for this system.

In chemical process industries, the materials are normally handled in fluid form and as a consequence, the physical chemical, and transport properties of fluids assume importance. Thus data on some of the properties associated with the liquids and liquid mixtures like density, viscosity and ultrasonic velocity, to find extensive application in solution theory and molecular dynamics [4].

ISSN: 2394-3106

Such results are necessary for interpretation of data obtained from thermo chemical, electrochemical, biochemical and kinetic studies [5]. During the last two decades, ultrasonic study of liquid mixtures has gained much importance in assessing the nature of molecular interactions through the study of the physico chemical properties of such systems. Ultrasonic velocity and related data of liquid mixtures are found to be the most powerful tool in testing the theories of liquid state. In addition, ultrasonic velocity data can be utilized to deduce some useful properties of liquid mixtures which are not easily accessible by other means [6]. The measurement of ultrasonic velocity has been adequately employed as a versatile tool for investigating the physical properties of matter-solid, liquid and gas. These studies are very important because of their extensive use in textile industry, leather industry, and pharmaceutical industry and in many others. Ultrasonic velocity measurement has proved useful in dealing with the problems of liquid structure and molecular interactions in liquid mixtures [7].

The practical importance of liquid mixtures rather than single component liquid systems has gained much importance during the last two decades in assessing the nature of molecular interaction sand investigating the physico-chemical behavior of such systems [8]. Thermodynamic investigation of liquid mixtures consisting of polar and non-polar components are of considerable importance in understanding inter molecular interactions between the component molecules and they find applications in several industrial and technological processes [9]. These studies are very important because of their extensive use in textile industry, leather industry, and pharmaceutical industry and in many others. Acoustical parameters have proved useful in dealing with the problems of liquid structure and molecular interactions in liquid mixtures.

Methyl acrylate is a very important industrial chemical and is widely used commercially for the production of technically important high polymeric and latex compounds. It is polar (dipole moment, μ = 1.77 D at 298.15 K) and strongly associated aprotic solvent due to the presence of polar carbonyl group in the molecule and it is a versatile liquid which finds use as a monomer in the preparation of poly (Methyl acrylate) which has innumerable industrial applications [10].

Cyclopentyl methyl ether (CPME) also known as methoxy cyclopentane, is a totally new hydrophobic ether solvent. It have high boiling point of 106 ˚C (223 ˚F) and preferable characteristics such as low formation of peroxides, relative stability under acidic and basic conditions, formation of azeotropes with water coupled with a narrow explosion range render CPME an alternative to other ethereal solvents such as tetrahydrofuran (THF), 2-methyltetrahydrofuran (2-MeTHF), dioxane, and 1,2-dimethoxyethane (DME). Cyclopentyl methyl ether is used in organic synthesis, mainly as a solvent. However it is also useful in extraction, polymerization, crystallization and surface coating. The utilization of CPME in several organic reactions pertaining to organometallic-, organo-, and biocatalysis. This solvent have favourable physical and chemical characteristics, such as low toxicity and high chemical and thermal stabilities, which make them promising media for a large breadth of synthetic chemistry and triggers development of reactions with green chemistry protocol [11-12]. The objective underlying the present work is to obtain information regarding molecular interactions in mixtures of a highly polar liquid with non-polar or weakly polar liquids [13]. CPME (Cyclopentyl methyl ether) is an important green solvent. Thus, a study of physical properties data on the binary mixture containing CPME has attracted considerable interest in the literature. Thus, Methyl acrylate in CPME mixed solvent would enable us to have a large number of solvents with appropriate physico-chemical properties, which can be used for a particular chemical process. Moreover, literature survey indicates that no study on this binary system has been reported at 298.15 K. Therefore, present study was undertaken in order to have deeper understanding of the intermolecular interaction between the components of the above binary liquid mixture.

Material & Methods

Cyclopentyl methyl etherand Methyl acrylate were purchased from Sd fine chemicals India. Mixture was prepared by mixing weighed amounts of the pure liquids adopting the method of closed system by using Mettler balance with the precision of ± 0.1 mg. Mixture was allowed to stand for some time before every measurement so as to avoid air bubbles. The purities of the liquids were checked by comparing the values of densities and ultrasonic velocities with literature data and are given in Table 1 & 2. The measurements were made with proper care in an AC room to avoid evaporation loss. The densities (ρ) of liquids and their mixture were measured using bicapillary pycnometer having a capillary diameter of 0.85 mm, which was calibrated using double distilled water. The necessary buoyancy corrections were applied. The density values were reproducible within ± 0.2 Kg m-3. The ultrasonic velocity (U) measurements were made by a single frequency (2 MHz) variable path.

Table 1: Comparison of Experimental density (ρ) and ultrasonic velocity (U) of pure liquids with literature at 298.15 K [15-16].

Liquid	Density (ρ) x 10^{-3} Kg m^{-3}		Ultrasonic velocity (U) m s^{-1}	
	Experimental	Literature	Experimental	Literature
Cyclopentyl methyl ether	0.7354	0.7356	1367.4	1368.3
Methyl acrylate	0.9363	0.9356	1142.0	1140.0

Table 2: List of symbols / Notations.

S.No	Symbol / Notation	Description	Unit
1.	X	Mole fraction of liquid	------
2.	P	Density of mixture	Kg m^{-3}
3.	U	Ultrasonic velocity of mixture	m s^{-1}
4.	L_f	intermolecular free-length of mixture	M
5.	K_S	isentropic compressibility for the mixture	m^2 N^{-1}
6.	Z	acoustic impedance for the mixture	Kg $m^{-2}s^{-1}$
7.	U^E	excess ultrasonic velocity for the mixture	m s^{-1}
8.	L_f^E	excess intermolecular free-length for the mixture	M
9.	K_S^E	excess isentropic compressibility for the mixture	m^2 N^{-1}
10.	Z^E	excess acoustic impedance for the mixture	Kg m^{-2} s^{-1}
11.	K_T	Jacobson's constant	------
12.	Y^E	Redlich-Kister Polynomial equation	------
13.	A_i	Where $A_i = A_0, A_1, A_2, A_3, A_4$ are the coefficients obtained from Redlich-Kister polynomial equation	------

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Results & Discussion

From the measured densities (ρ) and ultrasonic velocities (U) the various acoustical parameters such as K_s, Z and L_f were calculated using the following equations 1, 2 & 3 respectively and are incorporated in Table 3, for the binary system under study [14-17].

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

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

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

Where 'K_T' is Jacobson's constant. It is temperature-dependent empirical constant, proposed by Jacobson in 1952 and given as $K_T = (93.87\ 5 + 0.375 \times T) \times 10^{-8}$ at temperature T [18]. The excess functions Y^E are calculated using the relation:

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

Where Y denotes U, Z, K_S and L_f respectively, X is the mole fraction and suffixes 1 & 2 denote the components 1 & 2 in binary liquid mixture and the values are given in Table 4. The dependence of U^E, Z^E, K_S^E and L_s^E on the mole fraction of Cyclopentyl methyl ether for liquid mixture was fitted to the following Redlich-Kister equation by the least-squares method and the values are given in Table 5 [19].

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

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 5 together with the standard deviations (σ) values. From Table 3, it is observed that the values of U, Z, K_s and L_f varied linearly with the mole fraction of Cyclopentyl methyl ether. This indicates the presence of interactions between the components in this binary liquid mixture.

With this view in mind, the variations in excess acoustical parameters, like the excess ultrasonic velocity (U^E), excess Acoustic impedance (Z^E), excess isentropic compressibility (K_S^E) and excess intermolecular free-length (L_f^E) with the mole fraction of Cyclopentyl methyl ether are examined from the Table 4. It is observed that the positive deviations in U^E and Z^E for in the system standby are observed over the entire range of composition due to orientation of liquids. The negative deviations 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 [20-21]. The mole fraction of Cyclopentyl methyl ether is increased with decreased density due to size and shape of molecules more hindered. The interactions are minor intensity of Cyclopentyl methyl ether and Methyl acrylate molecules; they can lead to in the term of short range forces exist while the long range forces are negligible. Cyclopentyl methylether and Methyl acrylate liquid mixture is more compressible due to structural effects and dispersive type interaction. This study helps to understand the effect of the molecular interaction on behavior of liquid mixtures of polar and nonpolar liquids clearly and concisely.

Table 3: Values of density (ρ), ultrasonic velocity (U), acoustic impedance (Z), isentropic compressibility (K_S) and inter molecular free-length (L_f) for the binary liquid mixture of Cyclopentyl methyl ether with Methyl acrylate at 298.15 K.

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 4: Values of excess ultrasonic velocity (U^E), excess acoustic impedance (Z^E), excess isentropic compressibility (K_S^E) and excess intermolecular free-length (L_f^E) for the binary liquid mixture of Cyclopentyl methyl ether with Methyl acrylate at 298.15 K.

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

Table 5: Parameters of Equation 5 and Standard deviations.

Excess Property	A_0	A_1	A_2	A_3	A_4	σ
K_S^E x 10^{-11} m^2 N^{-1}	-0.00215	-2.02142	3.25142	1.36250	0.68572	0.05884
L_f^E x 10^{-11} m	-0.00217	-1.02587	1.45874	-0.32655	-1.25482	0.00478
Z^E x 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

Conclusion

In the present research workcalculated various excess parameters like Ultrasonic velocity (U^E), Isentropic compressibility (K_S^E), Intermolecular free length (L_f^E), acoustic impedance (Z^E) of Cyclopentyl methyl ether and Methyl acrylate liquid mixture and investigation on the acoustical and physico-chemical Properties. It is observed from the measured data that the values of U^E, Z^E are positive deviations and K_S^E, L_f^E, are negative deviations in the mixture and the variation of the properties of the mixture studied supports the view that the strong interactions between molecules predominate over the dissociation effects in the individual components and nature, molecular geometry, concentration of mixture.

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Future Aspects

The purpose of the present work should focus on future the Theoretical values of acoustical and physico-chemical parameters of this binary liquid mixture have been compared with experimental data to verify the applicability studied.

Acknowledgment

The author is thankful to the authorities of D. B. S. (P. G.) College, Dehradun, Uttarakhand for providing research facilities to carry out this work. This research did not receive any specific grant from any funding agencies.

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