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Molecular Interaction between Cyclohexene and Ethyl Methyl Ketone with Cumene at different temperatures by Ultrasonic Measurement

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ABSTRACT

Binary liquid mixtures find practical applications in most physical and chemical processes. Derived parameters from ultrasonic velocity measurement provide qualitative information regarding the nature and strength of interactions in liquid mixtures. The use of Cumene in preparing a large no. of aromatic compounds is well known. Cumene is also used as solvent in various organic synthesis. Thus Cyclohexene and Ethyl Methyl Ketone with cumene mixed solvents would enable us to have a large no. of solvents with appropriate physic-chemical properties. Moreover literature survey indicates that no ultrasonic study on these binary systems has been reported. Therefore present study was undertaken in order have deeper understanding of intermolecular interaction between the compounds of the above binary liquid mixtures.

Keywords:- Ultrasonic velocity, Liquid mixtures, Molecular interactions.

INTRODUCTION

The unique feature of sound wave property is that it gives direct and precise information of adiabatic properties. In the basic sciences, ultrasonic waves have acquired the status of an important probe for the study of structure and properties of matter. The use of ultrasound is one of the well recognized approaches for the study of molecular interactions in fluids [1-4]. Ultrasonic speed plays an important role in the investigation of intermolecular interactions. The structural arrangements are influenced by the shape of the molecules as well as by their mutual interactions [5-9].

Furthermore, in the chemical industry, information on density and viscosity of the liquid mixtures are vital in different applications that include surface facilities, pipeline systems and mass transfer operations [10-11]. In this study, the density, ultrasonic velocity and viscosity, values of pure cyclohexene, ethyl methyl ketone and cumene and those of their binary mixtures over the entire composition range have been measured and reported at 303K and 308K, respectively.

The variation of these properties with composition and temperature of the binary mixtures are studied in terms of molecular interactions between unlike molecules of the mixtures.

RESULTS AND DISCUSSION

Various acoustical parameters such as adiabatic compressibility (β), Intermolecular free length (L_f), free volume (V_f), and specific acoustical impedance (Z), were calculated using the experimental data of ultrasonic sound velocity, density and viscosity by the following equations (1-5).

$$\beta = 1/U^2\rho \quad (1)$$
$$L_f = kT(\beta)^{1/2} \quad (2)$$
$$V_f = (M_{eff}U/\eta k)^{3/2} \quad (3)$$
$$Z = U\rho \quad (4)$$
$$\tau = 4/3\beta\eta \quad (5)$$

Where kT is the temperature dependent constant having a value 199.53 x 10^{-8} in MKS system , k is the constant equal to 4.28 x 10^9 in MKS system, independent of temperature of all liquids, and all the notations having the usual meanings.The experimental and the calculated data for two binary liquids mixtures are listed in table-1 to table-8

System-1:- Cumene + Ethyl Methyl Ketone binary liquid mixture

Table-1:- Value of U, ρ, η and β at 303^0K for Cumene + Ethyl Methyl Ketone binary liquid mixture

Mole fraction (X)	Ultrasound Velocity (U) m/s	Density (ρ)/Kgm^{-3}	Viscosity (η) x 10^3N.s.m^{-2}	Adiabatic compressibility (β)x 10^{10}/m^{2}N^{-1}
0.0000	1141	779.0	0.2918	9.8599
0.0784	1134	778.4	0.3240	9.9901
0.1618	1127	777.8	0.3649	10.0200
0.2497	1122	777.2	0.4058	10.2207
0.3433	1116	776.9	0.4555	10.3348
0.4398	1112	776.5	0.5140	10.4155
0.5382	1109	776.2	0.6108	10.4760
0.6472	1106	775.9	0.8102	10.5363
0.7532	1104	775.7	1.1857	10.5775
0.8729	1103	775.5	1.8807	10.5988
1.0000	1102	775.3	3.3792	10.6202

Table-2:- Value of V_f, L_f, Z, and τ at 303^0K for Cumene + Ethyl Methyl Ketone binary liquid mixture

Free Volume (V_f) x 10^7/m^3.mol^{-1}	Free Length (L_f) x 10^{11}/m	Acoustic impedance (Z) x 10^{-6}/Kg.m^2.s^{-1}	Shear's relaxation time (τ) x 10^{-7}sec.
1.1658	6.5164	8.8899	3.8553
1.1482	6.5580	8.8302	4.3373
1.1278	6.5983	8.7728	4.8994
1.1037	6.6355	8.7202	5.5577
1.0756	6.6692	8.6734	6.3080
1.0439	6.6973	8.6348	7.1737
1.0067	6.7157	8.6108	8.5743
0.9664	6.7317	8.5884	11.4389
0.9279	6.7448	8.5707	16.8059
0.8844	6.7542	8.5576	26.7104
0.8407	6.7624	8.5461	48.0896

From the experimental data, it is observed that density decreases with concentration of ethyl methyl ketone. The viscosity of the mixture increasing with increasing mole fraction of ethyl methyl ketone. The increase in viscosity indicates that their dipole- induced dipole interaction between component molecules. From the calculated data, it is evident that adiabatic compressibility (β) increases with increase in concentration of ethyl methyl ketone as expected. The increase in β results in decrease in the value of velocity. It is also noted that the free volume (V_f) decreases as concentration of ethyl methyl ketone increases. This decrease is due to the various degree of dispersive interaction.

The acoustical impedance (Z) decreases with increasing mole fraction of ethyl methyl ketone. The decrease of Z indicates significant interaction between the component molecules.

Table-3:- Value of U, ρ, η and β at 308^0K for Cumene + Ethyl Methyl Ketone binary liquid mixture

Mole fraction (X)	Ultrasound Velocity (U) m/s	Density (ρ)/Kgm^{-3}	Viscosity (η) x 10^3N.s.m^{-2}	Adiabatic compressibility (β)x 10^{10}/m^{2}N^{-1}
0.0000	1121	773.5	0.2809	10.2870
0.0784	1116	772.8	0.3158	10.3896
0.1618	1110	772.2	0.3535	10.5108
0.2497	1104	771.6	0.3941	10.6337
0.3433	1099	771.1	0.4405	10.7365
0.4398	1095	770.7	0.4928	10.8213
0.5382	1092	770.5	0.5830	10.8837
0.6472	1089	770.4	0.7695	10.9457
0.7532	1087	770.3	1.0725	10.9878
0.8729	1085	770.2	1.6319	11.0290
1.0000	1082	770.1	2.6427	11.0913

Table-4:- Value of V_f, L_f, Z, and τ at 308^0K for Cumene + Ethyl Methyl Ketone binary liquid mixture

Free Volume (V_f) x 10^7/m^3.mol^{-1}	Free Length (L_f) x 10^{11}/m	Acoustic impedance (Z) x 10^{-6}/Kg.m^2.s^{-1}	Shear's relaxation time (τ) x 10^{-7}sec.
1.2496	6.7151	8.6740	3.8720
1.2246	6.7506	8.6244	4.3959
1.1990	6.7873	8.5745	4.9788
1.1729	6.8250	8.5239	5.6156
1.1434	6.8601	8.4775	6.3374
1.1096	6.8888	8.4399	7.1458
1.0716	6.9093	8.4139	8.5025
1.0287	6.9262	8.3927	11.2864
0.9889	6.9413	8.3739	15.7911
0.9452	6.9552	8.3567	24.1176
0.9023	6.9698	8.3386	39.2831

Also from the data it is evident that Shear's relaxation time (τ) increases with increasing mole fraction of ethyl methyl ketone. This increase is due to structural relaxation process, which shows the presence of molecular interaction between the component molecules.

System-2:- Cumene + Cyclhexene binary liquid mixture:-

Table-5:- Value of U, ρ, η and β at 303^0K for Cumene + Cyclohexene binary liquid mixture

Mole fraction (X)	Ultrasound Velocity (U) m/s	Density (ρ)/Kgm^{-3}	Viscosity (η) x 10^3N.s.m^{-2}	Adiabatic compressibility (β)x 10^{10}/m^{2}N^{-1}
0.0000	1130	780.50	0.985	10.033
0.1000	1133	777.20	0.898	10.001
0.1980	1136	775.10	0.880	9.989
0.3001	1145	772.50	0.858	9.860
0.3970	1154	770.80	0.835	9.731
0.5001	1163	764.50	0.820	9.684
0.5891	1173	755.70	0.804	9.620
0.7070	1184	750.80	0.788	9.491
0.8050	1191	742.70	0.772	9.463
0.9004	1209	738.70	0.749	9.250
1.0000	1230	727.20	0.702	8.605

Table-6:- Value of V_f, L_f, Z, and τ at 303^0K for Cumene + Cyclohexene binary liquid mixture

Free Volume (V_f) x $10^7/m^3.mol^{-1}$	Free Length (L_f) x 10^{11}/m	Acoustic impedance (Z) x 10^{-6}/Kg.$m^2.s^{-1}$	Shear's relaxation time (τ) x 10^{-7}sec.
0.435	6.370	0.8819	13.2425
0.565	6.310	0.8805	12.0344
0.648	6.306	0.8804	11.7790
0.774	6.265	0.8845	11.7362
0.878	6.224	0.8895	10.8880
1.004	6.208	0.8891	10.6407
1.137	6.188	0.8864	10.3642
1.298	6.146	0.8889	10.0217
1.454	6.137	0.8845	9.7892
1.552	6.067	0.8931	9.0382
1.662	5.853	0.8944	8.0945

Table-7:- Value of U, ρ, η and β at 308^0K for Cumene + Cyclohexene binary liquid mixture

Mole fraction (X)	Ultrasound Velocity (U) m/s	Density (ρ)/Kgm^{-3}	Viscosity (η) x 10^3N.$s.m^{-2}$	Adiabatic compressibility (β)x $10^{10}/m^2N^{-1}$
0.0000	1182	795.60	1.643	8.831
0.1000	1185	791.70	1.579	8.963
0.1980	1187	786.90	1.482	9.097
0.3001	1191	782.60	1.353	9.099
0.3970	1193	778.80	1.226	9.104
0.5001	1195	775.30	1.153	9.060
0.5891	1198	771.00	1.035	9.103
0.7070	1212	767.50	0.942	9.124
0.8050	1216	754.40	0.902	9.106
0.9004	1222	742.70	0.826	8.922
1.0000	1230	727.20	0.702	8.605

Table-8:- Value of V_f, L_f, Z, and τ at 308^0K for Cumene + Cyclohexene binary liquid mixture

Free Volume (V_f) x $10^7/m^3.mol^{-1}$	Free Length (L_f) x 10^{11}/m	Acoustic impedance (Z) x 10^{-6}/Kg.$m^2.s^{-1}$	Shear's relaxation time (τ) x 10^{-7}sec.
0.328	5.976	0.9403	19.4425
0.401	5.973	0.9381	18.9644
0.467	6.006	0.9340	18.0655
0.572	6.016	0.9320	16.4564
0.785	6.020	0.9291	14.9567
0.983	6.012	0.9264	14.038
1.107	6.015	0.9236	12.1294
1.109	6.025	0.9202	11.5170
1.372	6.019	0.9174	11.0064
1.488	6.067	0.9076	9.8752
1.662	5.899	0.8945	8.0945`

From the experimental data, it is observed that velocity of sound increases with increase in mole fraction of cyclohexene whereas the density and viscosity decreases with the mole fraction of cyclohexene. The increase in velocity indicates that there is a dipole-induced dipole interaction between the component molecules. The decrease in density and in viscosity suggesting thereby more association between solute and solvent molecules in this binary liquid mixture.

It is observed from the data that adiabatic compressibility and the free length decreases with increase in mole fraction of cyclohexene. The adiabatic compressibility is a powerful thermodynamic parameter in sensing the molecular interaction in liqui9d mixture. The addition of cyclohexene with cumene leads to a compact structure due the presence of dipolar i9ntewraction, which contributes a decrease in free length (L_f). The regular fall in free length with the mole fraction of cyclohexene may be attributed to close approach of the molecules. The acoustic impedance

decreases with mole fraction of cyclohexene whereas the free volume increases. The relaxation time also decreases with the increase of mole fraction of cyclohexene.

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