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MOLECULAR INTERACTION STUDY IN BINARY MIXTURES OF DMSO AND 1-OCTANOL USING ULTRASONIC METHOD AT VARIOUS CONCENTRATIONS AND TEMPERATURES.

[1]R. K. Kolhe, [2]B. B. Bhosale

[1, 2] *Department of physics, K.J. Somaiya College, Kopargaon, Ahmednagar (M.S.)*
*Corresponding Authors- R.K.Kolhe
rangnath_kolhe@rediffmail.com

Abstract— The viscosity **(η),** density (ρ) and ultrasonic velocity (U) of dimethylsulphoxide with 1-Octanol have been measured at different concentrations and temperatures from 303.15K to 318.15K. Above measured data is used to calculate the parameters like adiabatic compressibility (β), acoustic impedance (Z), free length (L_f), free volume (V_f), and available molar volume (V_a). These calculated parameters are helpful to explain the strength of interaction among the molecules of liquid binary mixture under investigation.

Keywords - Density, Viscosity, Acoustic impedance, free volume.

1. INTRODUCTION

The ultrasonic velocity measurement method of binary mixture is very important in understanding the intermolecular interaction among molecules of component. It is found to be applicable in various chemical industries. The works on chemical compounds which are used for medicinal purpose require making the awareness regarding the society with whole characteristics including ultrasonic behaviors. From many years, study of interaction among the molecules in liquid systems has been done with various physical methods like Raman Effect [1], Infrared Radiation (IR) technique [2] [3], NMR technique, Ultraviolet and ultrasonic methods [4].

In present study, an ultrasonic method has an important role which gives valuable information about molecular behavior of liquids.

Technique of measurement of Ultrasonic velocity is one of the active interests, to study the nature of molecular interactions in pure liquids and liquid mixtures. Parameter such as density, viscosity and ultrasonic velocity and their variations with concentrations and with different temperatures of the liquid mixture are important in chemical industries. The study regarding the changes in above parameters of liquids mixtures has been found that, there exist qualitative technique to carry out the information related to structure of molecules and forces among molecules.

Thermal and acoustic properties of binary liquid mixtures are of great importance in obtaining detail information of the molecular interactions. Investigation of binary solution by ultrasonic method, consisting of polar and non-polar components has great significance for finding the molecular interaction among the molecules. This finding has large number of applications in technical and industrial processes [5]. Changes in ultrasonic velocity and other related parameters of liquid binary mixtures have been studied by the researchers to study the interactions among the molecules. They were made focus on change structure related with liquid mixture of strongly as well as weakly interacting compounds [6]. Such study is useful to design engineering process and in chemical and biological industries. The study of molecular interactions in binary mixtures in which, alcohol is one of the components of particular interest, because strong self-association is presented in alcohol. Also, they are having 3-D network of hydrogen bonding and they can easily correlate with any other group with equivalent extent of polar attractions [7], [8], [9], [10].

Since the dimethylsulphoxide is a good non-aqueous solvent because of its use in various chemical and biological interactions and in polymer processing. Hence study of dimethylsulphoxide has become important because of its utilization in wide range of applications in medicine. It easily penetrates the biological membrane as well as facilitating chemical transport in the biological tissue. Also, the use of dimethylsulphoxide is well established, as an anti-inflammatory agent, which is commonly used in arthritic condition. Dimethylsulphoxide also utilized as free radical scavenger in various cancer treatment. Due to unique property of

dimethylsulphoxide, gives rise to its broad use as a solvent as described by Thirumaran *et al.* [11], [12]. Octanol is organic compound having molecular formula $H_3C(H_2C)_7OH$ and synthesized by the Oligomerization of ethylene with the help of triethyl aluminum giving oxidation of alkyl aluminum product. It is transparent liquid having small viscous property and used as a solvent for protective layer, waxes and oils. In the present research work binary liquid system such as dimethyl Sulphoxide with Octanol-1, of whole concentrations of dimethyl Sulphoxide with four different temperatures like 303.15K, 308.15K 313.15K and 318.15K have been taken for the investigation to calculate various acoustic and thermodynamic parameters.

2. EXPERIMENTAL

Ultrasonic interferometer is used to measure ultrasonic velocity through binary mixture (Model No. M-81S). At the time of the temperature was controlled by circulating water around the cell (2MHz) from thermostatically controlled constant temperature bath. Densities and viscosities were measured by 25ml specific gravity bottle and Ostwald's viscometer. In present work, whole chemicals used are of AR grade, whose purity is greater than 99.8%. All these chemicals are distilled by using standard procedure used by John *et al.* [13]. The chemicals were analyzed for the density and viscosity measurement, and the results were compared with the literature values. The various parameters are evaluated by using the following relations.

Formulae:

Ultrasonic velocity,

U = f λ (m sec^{-1})

Density, ρ = $\frac{\text{Mass of solution (M)}}{\text{Volume of the solution (V)}}$

Viscosity, $\eta_S = \frac{\rho_S t_S}{\rho_W t_W}\eta_W$

Adiabatic compressibility, $\beta = \frac{1}{\rho U^2}$ Kg^{-1} ms^2

Free length, $L_f = \frac{K}{\sqrt{\rho U^2}}$

Acoustic impedance, Z = $\frac{P_a}{U}$

Free volume, $V_f = \left[\frac{M_{eff}\,U}{K\eta}\right]^{1/2}$

Available volume, $V_a = \left[1 - \frac{U}{U_\infty}\right]$ m^3 mol^{-1}

3. FIGURES AND TABLES

Table1: Values of ultrasonic velocity (U) of DMSO + 1-octanol at temperatures 303.15, 308.15, 313.15 and 318.15kelvin.

Concentrations of DMSO in mole fraction	Ultrasonic velocity, U (ms^{-1}) (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0	1335.15	1317.05	1300.42	1283.58
0.1808	1340.56	1322.89	1305.47	1291.26
0.3317	1346.58	1328.89	1312.63	1300.58
0.4598	1353	1335.58	1320	1309.79
0.5697	1362.84	1343.79	1328.63	1318.21
0.6651	1372.63	1354.84	1337.68	1327.26
0.7486	1385.58	1368.74	1350.63	1337.32
0.8225	1400.84	1382.11	1366.53	1352.02
0.8882	1418.53	1399.16	1383.37	1368.11
0.947	1442.95	1422	1407.58	1392.79
1	1472.21	1454.95	1436.21	1421.47

Table2: Values of Density (ρ) of DMSO+1-Octanol at temperatures 303.15K, 308.15K, 313.15K and 318.15K

Concentrations of DMSO in mole fraction	Density, ρ (kg m^{-3}) (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0	820.79	816.8	813.3	809.8
0.1434	845.49	840.84	837.83	834.09
0.2736	867.09	862.23	859.8	855.93
0.3923	900.92	896.88	892.15	888.81
0.5011	929.52	925.24	921.41	917.17
0.601	951.67	947.3	942.82	938.12
0.6932	981.39	977.23	973.03	968.26
0.7785	1010.66	1006.34	1002.06	996.79
0.8577	1037.96	1032.98	1028.49	1023.63
0.9313	1062.95	1058.3	1053.48	1048.66
1	1093.29	1086	1082.26	1077.23

Table3: Values of Viscosity (η) of DMSO+1-Octanol at temperatures 303.15, 308.15, 313.15 and 318.15kelvin.

Concentrations of DMSO in mole fraction	Viscosity, η× 10^{-2} ($Nm^{-2}s$) (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0	0.5548	0.4799	0.4152	0.3571
0.1434	0.3428	0.3139	0.2847	0.2646
0.2736	0.2703	0.2464	0.227	0.2061
0.3923	0.2611	0.2408	0.2241	0.2023
0.5011	0.232	0.2139	0.1966	0.1794
0.601	0.1965	0.1784	0.1605	0.143
0.6932	0.1912	0.1732	0.153	0.1405
0.7785	0.1836	0.1635	0.1462	0.1343
0.8577	0.1648	0.1479	0.1328	0.1225
0.9313	0.1497	0.1391	0.126	0.114
1	0.1483	0.1347	0.1225	0.1112

Table4: Values of adiabatic compressibility (β) of DMSO + 1-octanol at temperatures 303.15, 308.15, 313.15 and 318.15kelvin.

Concentrations of DMSO in mole fraction	Adiabatic compressibility, β (X 10^{-10} ms^2 kg^{-1}) (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0	6.835	7.058	7.271	7.495
0.1434	6.581	6.796	7.003	7.191
0.2736	6.36	6.567	6.75	6.907
0.3923	6.063	6.251	6.433	6.558
0.5011	5.792	5.985	6.148	6.275
0.601	5.577	5.751	5.927	6.051
0.6932	5.308	5.462	5.634	5.775
0.7785	5.042	5.202	5.344	5.488
0.8577	4.788	4.945	5.081	5.219
0.9313	4.518	4.673	4.791	4.916
1	4.22	4.35	4.48	4.594

Table5: Values of acoustic impedance (Z) of DMSO + 1-octanol at temperatures 303.15, 308.15, 313.15 and 318.15kelvin.

Concentrations of DMSO in mole fraction	Adiabatic compressibility, β (×10^{-10} ms^2 kg^{-1}) (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0.0000	6.835	7.058	7.271	7.495
0.1434	6.581	6.796	7.003	7.191
0.2736	6.360	6.567	6.750	6.907
0.3923	6.063	6.251	6.433	6.558
0.5011	5.792	5.985	6.148	6.275
0.6010	5.577	5.751	5.927	6.051
0.6932	5.308	5.462	5.634	5.775
0.7785	5.042	5.202	5.344	5.488
0.8577	4.788	4.945	5.081	5.219
0.9313	4.518	4.673	4.791	4.916
1.0000	4.220	4.350	4.480	4.594

Table6: Values of linear free length (L_f) of DMSO + 1-octanol at temperatures 303.15, 308.15, 313.15 and 318.15kelvin.

Concentrations of DMSO in mole fraction	Linear free length, L_f A^0 (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0.0000	0.538	0.551	0.565	0.578
0.1434	0.528	0.541	0.554	0.567
0.2736	0.519	0.532	0.544	0.555
0.3923	0.506	0.519	0.531	0.541
0.5011	0.495	0.508	0.519	0.529
0.6010	0.486	0.498	0.510	0.520
0.6932	0.474	0.485	0.497	0.508
0.7785	0.462	0.473	0.484	0.495
0.8577	0.450	0.462	0.472	0.483
0.9313	0.437	0.449	0.458	0.468
1.0000	0.423	0.433	0.443	0.453

Table7: Values of linear free volume (V_f) of DMSO + 1-octanol at temperatures 303.15, 308.15, 313.15 and 318.15kelvin.

Concentrations of DMSO in mole fraction	Free volume, V_f ($\times 10^{-8}$ ml) (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0.0000	1.1031	1.3434	1.6378	2.0136
0.1434	2.2222	2.4835	2.8084	3.0798
0.2736	3.1621	3.5561	3.9286	4.3710
0.3923	3.3458	3.6979	4.0264	4.6311
0.5011	4.0345	4.4530	4.9446	5.5949
0.6010	5.2147	5.8995	6.7539	7.5224
0.6932	5.4643	6.2112	7.3068	8.1672
0.7785	5.8118	6.7668	7.8452	8.7568
0.8577	6.7925	7.8168	9.0134	9.9952
0.9313	7.7612	8.4711	9.6657	11.0481
1.0000	7.9417	8.7524	9.8976	11.2683

Table8: Values of available volume (Va) of DMSO + 1-octanol at temperatures 303.15, 308.15, 313.15 and 318.15kelvin.

Concentrations of DMSO in mole fraction	Available volume, V_a ($\times 10^{-8}$ ml) (All temperatures are in Kelvin scale)			
	303.15	308.15	313.15	318.15
0.0000	1.7777	1.9085	2.0294	2.1527
0.1434	1.6594	1.7811	1.8952	1.9940
0.2736	1.5697	1.6869	1.7872	1.8684
0.3923	1.4699	1.5786	1.6748	1.7401
0.5011	1.3670	1.4817	1.5708	1.6366
0.6010	1.2773	1.3818	1.4813	1.5460
0.6932	1.1616	1.2566	1.3576	1.4355
0.7785	1.0368	1.1380	1.2223	1.3039
0.8577	0.9047	1.0053	1.0876	1.1689
0.9313	0.7462	0.8491	0.9214	0.9964
1.0000	0.5708	0.6522	0.7390	0.8157

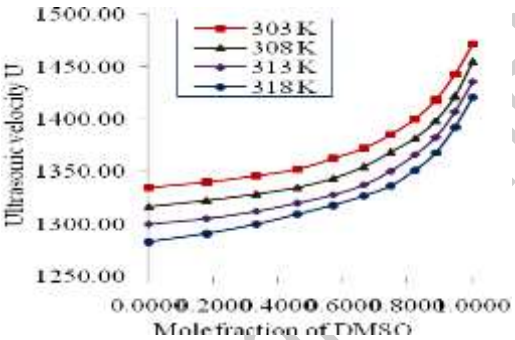

Figure-1: Mole fraction of DMSO evolution graph of ultrasonic velocity

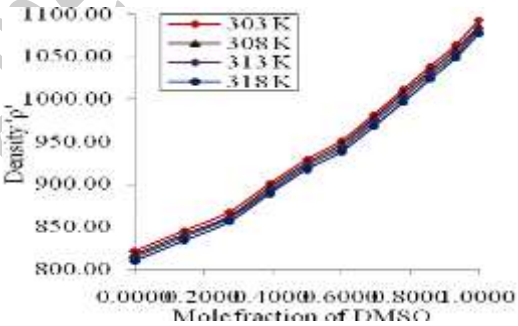

Figure-2: Mole fraction of DMSO evolution graph of density

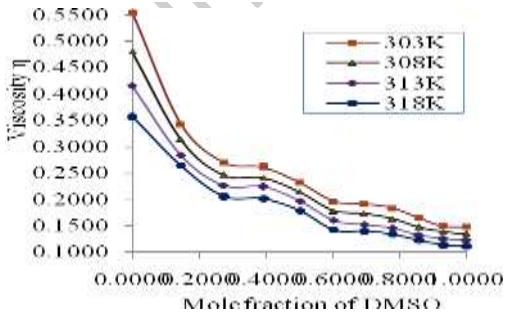

Figure-3: Mole fraction of DMSO evolution graph of Viscosity

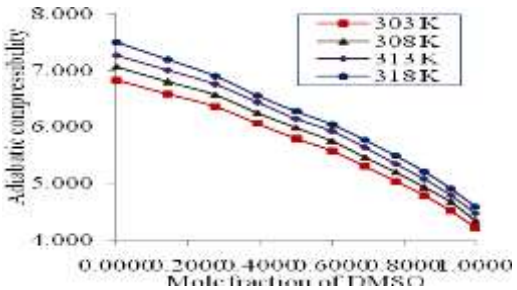

Figure-4: Mole fraction of DMSO evolution graph of Adiabatic Compressibility

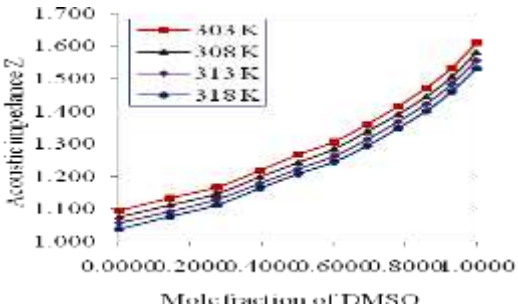

Figure-5: Mole fraction of DMSO evolution graph of Acoustic Impedance

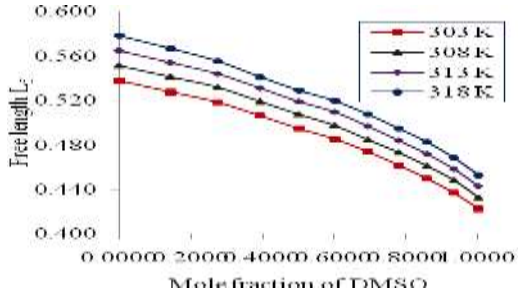

Figure-6: Mole fraction of DMSO evolution graph of Free Length

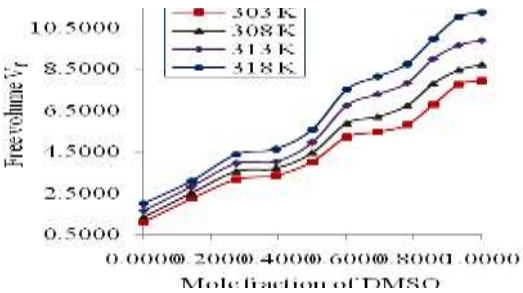

Figure-7: Mole fraction of DMSO evolution graph of Free Volume

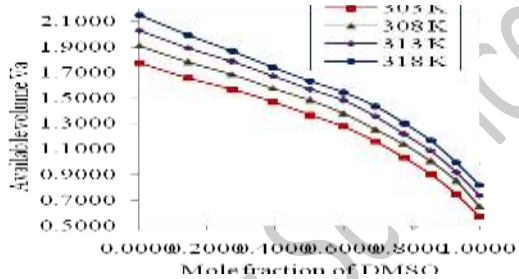

Figure-8: Mole fraction of DMSO evolution graph of Available Volume

4. RESULT AND DISCUSSION

Tables: 1–3 represents the practical values of ultrasonic speed of sound (ultrasonic velocity), density and viscosity for the liquid mixture of dimethylsulphoxide + 1-Octanol at various temperatures. The close perusal of Table: 1-2 and Fig.1-2 shows**,** there is increase in the values of ultrasonic speed of sound as well as density with rise in mole fractions of dimethylsulphoxide with 1-Octanol.

Table-3 and Fig.3 shows that, the values of viscosities decreases with increase in mole fractions of dimethylsulphoxide. This may be due to the dissociations of the extremely weak dipole-induced-dipole interaction among the molecules. Conversely, the values of the ultrasonic velocities, densities and viscosities decrease in every case with increase in temperature. The same results were derived by Thirumaran *et al.* [14] and Umadevi *et al.* [15]. In this case, there is increase in temperature and interaction becomes weak, due to thermal anxiety of molecules of the component. In the present investigation, this is indicating by decrease in the values of ultrasonic velocities. The variations in the values of adiabatic compressibility (β), acoustic impedance (Z), linear free length (L_f), free volume (V_f), available volume(Va), with composition of DMSO in 1-Octanol are tabulated in table 4 to 8.

From Table 4 & 6 and Fig.4 & Fig.6, it is observe that, there is Increase in the values of adiabatic compressibility and free length as temperature increases. On the other hand, values of adiabatic compressibility and free length decrease with respect to increase in concentrations of DMSO.

The decrease in the values of adiabatic compressibility indicates that, the bond strength enhancing at this concentration. Such a decrease in adiabatic compressibility with respect to compositions attributes the effect of hydrogen bonding or dipole-dipole interaction.

Table 5 and Fig.5 shows the variation in acoustic impedance with temperatures and concentrations. It has been observed that, there is decrease in the values of acoustic impedance as temperature increases. Also, the values of acoustic impedance increases with increase in compositions of dimethylsulphoxide. This is in good agreement with the requirement because both ultrasonic velocity as well as density increases with increase in compositions of the solute. This is also effective due to solute-solvent interactions [16].

Table-7 and Fig.7 shows increase in the values of free volume with increase in

concentrations of dimethylsulphoxide. Values of the free volume also increase with increase in temperature. This rise in the values of free volume with increase in compositions indicates the decrease in magnitude of interaction. From table-8 and Fig.8, it has been observed that, there is increase in values of available volume as temperature increases. There is decrease in values of available volume with increase in concentration of dimethylsulphoxide with 1-Octanol.

CONCLUSION

From observed values of ultrasonic speed, viscosity and density of mixture, other parameters such as adiabatic compressibility, acoustic impedance, free length, free volume and available volume for binary mixtures of dimethylsulphoxide with 1-Octanol at various temperatures, it is found that, molecular association is present among the molecules of liquid combinations. Particularly, very less interaction between molecules is remarked in present system.

It is observed that, interaction among dissimilar molecules is higher as compared to intra-molecular interactions, which lead to reduction of interaction. Thus in present study weak interaction is observed.

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