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MOLECULAR INTERACTION AND ULTRASONIC VELOCITY STUDIES OF ALKANOLS WITH O-NITRO TOLUENE AT GIVEN TEMPERATURES

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ABSTRACT
*Ultrasonic Velocity (U), Density (ρ) and Viscosity (η) values for the binary mixture system of 1-butanol and 3-methyl, 1-butanol with O-Nitro toluene including those of pure liquids were measured over entire mole fraction range at 298.15 K and 308.15 K .The related parameters of molecular interaction and sound velocity were studied in present work. From experimentally determined values excess molar volume (V E), Viscosity deviation (Δη) and deviation isotropic compressibility (ΔKs), excess free length (LfE), available volume (VaE) and Gibb's free energy (G*E) have been calculated. These results have been explained on the basis of intermolecular interaction between the components in the liquid mixture and correlations among the parameters are discussed.*

Keywords— Ultrasonic Velocity, Density, Viscosity, Excess molar volume, Excess free length, Gibb's free energy.

INTRODUCTION
Ultrasonic velocity investigations along with viscometric and volumetric studies of liquid and liquid mixture are considerable of importance. They play an impotent role in understanding intermolecular interaction among the different component molecules. It also findings extensive application in industrial and technological process [1,2]. Several researchers [3-8] have measured viscosity, Density and Ultrasonic velocity for different binary mixture, containing alcohols as one of the components and these properties were discussed in term of specific and non-specific interaction. Generally alcohols are strongly associated in solution because of its dipole-dipole interaction and hydrogen bonding. They play important role in Chemistry, Biology and Studies in hydrogen bonding in liquid mixture. Alcohols are widely used are solvents. Alcohols play an important role in understanding the behavior of hydrogen bonding with other functional groups.

Aromatic group is highly non-polar and can associate with any other group having same degree of polar attractions. In present work has been reported on alcohols as one of the component in binary mixture of 1-butanol and 3- methyl, 1-btanol with O-Nitro toluene at 298.15 K and 308.15 K. The investigations of thermodynamic properties of multi component liquid mixture and data in term of various models are important for pharmaceutical and industrial application [9]. The excess thermodynamic functions [10, 11] are dependent on difference in intermolecular force and difference in size of the molecules. The magnitude and signs of these excess values can throw light on the strength of intermolecular interactions. So from the experimentally determined values of speed of sound, density and viscosity and other parameters like excess isotropic compressibility, excess molar volume (VE), excess free length (LfE) have been calculated. In present work, is to determine thermodynamics and transport properties of binary mixtures (12-15).

In present investigation we report the result and discuss excess parameter using data at two different temperatures.

MATERIALS AND METHOD
The chemicals 1-butanol, 3- methyl, 1-btanol and O-Nitro toluene used were of analytical grade (A.R) minimum assay of 99.9% obtained from s. d. fine chemicals India. Which are used as such chemical without further purification. The densities of pure components and binary mixtures were measured by using a Bi-capillary pycnometer. The purities of the above chemicals were checked density determination. The binary liquid mixtures of different known concentration were prepared in stopper measuring flask. The weight of the sample was measured using electronic digital balance with an accuracy of ± 0.1mg. The viscosity was measured using Ubbelohde viscometer (20ml) and the efflux time was determined using a digital clock to within ± 0.015. The ultrasonic velocities (U) in liquid mixtures have been measured using an ultrasonic interferometer (Mittal type, model F-81) working at 2 MHz frequency The accuracy of sound velocity was ±0.1 ms-1.

Theory and calculation
Following equations been used to calculate different parameters in binary solutions

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1) The excess molar volume (V^E)

$$V^E = \frac{M_1X_1+M_2X_2}{\rho_{12}} - \frac{M_1X_1}{\rho_1} - \frac{M_2X_2}{\rho_2} \quad (1)$$

(2) The viscosity deviation ($\Delta\eta_m$)

$$\ln\eta_m = X_1\ln\eta_1 + X_2\ln\eta_2 \quad (2)$$

$$\eta_{12} - X_1\eta_1 - X_1\,\eta 2 \quad (3)$$

3) Deviation in isentropic compressibility (Δk_S)

$$\Delta k_S = k_S - \Phi_1 k_{S1} - \Phi_2 k_{S2} \quad (4)$$

Where kS1, kS2 and kS are isentropic compressibility of liquid mixtures and Φ is volume fraction of pure component in the mixture and is defined as

$$\phi = \frac{(Xi\ Vi)}{(\Sigma Xi\ Vi)} \quad (5)$$

Where x1 and Vi are mole fraction and molar volume of ith component in the mixture.

4) The excess free length (LfE)

$$LfE=Lfmix-x1Lf1-x2Lf2 \quad (6)$$

$$AE=Aexp-Aid \quad (7)$$

Where Aid = $\sum$ Ai Xi, Ai is any acoustical parameters and Xi the mole fraction of the liquid component.

5) Available volume (Va)

$$Va = (Vm-V0) = Vm\,(1-U/Um) \quad (8)$$

Where Vm = M/ρ, is the molar volume, U=Velocity, V0=M/ρ0 = molar volume at absolute zero temperature and Um = Schaaf's limiting value taken as 1600m/s for liquids.

6) The excess Gibbs free energy of flow (G*E)

$$G^*E=RT[In(\eta V) - x1In(\eta 1V1) - x2In(\eta 2V2) \quad (9)$$

Where Vi is the molar volume of ith component.

7) Internal pressure (πi)

$$\pi i = bRT\,(K\,\square / U)1/2\,(\square\square\ 2/3 / M7/6) \quad (10)$$

Where b is packing factor, K is a constant independent of temperature having value of 4.28 x 109, R is gas constant and M is molecular weight the other symbols have their usual meaning.

RESULT AND DISCUSSION

In pure state , the self association of alcohols decreases with increasing chain length , when alcohols mixed with O-Nitro toluene then there is interaction between their individual functional groups (-OH and -NO2) . The presence of electron withdrawing group on benzene ring decreases electron densities. The polarity of alcohols is less hence there is a degree of self association is less than compare to O-Nitro toluene.

The measured volumes of ultrasonic velocity, density, viscosity, excess molar volume (VE), viscosity deviation (Δn) and deviation in isentropic compressibility (ΔKs) parameters for the binary liquid mixtures 1-butanol and 3- methyl, 1-btanol with O-Nitro toluene including those of pure liquids were measured over entire mole fraction range at 298.15 K and 308.15 K are reported in table 1 and table 2 respectively while Excess free length(LfE), Internal pressure (πE) ,available volume (VaE) and Gibbs free energy(G*E) are given in Table-3 and Table-4 respectively. Figure :- 1, A,and B shows Excess molar volume (VE), Viscosity deviation (Δ) against mole fraction for binary system of 1-butanol and 3- methyl, 1-butanol at 298.15 K respectively. All these parameters shows negative deviations with minima at about X2= 0.4 for excess molar volume and X2 = 0.6-0.8 for deviation in viscosity. And Figure:-2, A and B shows available volume (VaE) and Gibbs free energy(G*E) against mole fraction for binary system of 1-butanol and 3- methyl, 1-butanol at 298.15 K respectively The parameters Gibb's free energy are negative but available volume was positive this may be due to presence of stronger solute solvent interactions in between highly polar functional groups Nitro and -OH.

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Ultrasonic velocity and viscosity measurement of alcohols with O-Nitro toluene gives reliable information about molecular interaction between the components of mixtures. Alcohols in pure state get associated. The association of alcohols decreases with increase in chain length and substituent.

The excess parameters of alcohols become less negative with increased of temperature. The negative values of excess parameters shows that the existence of dispersion and dipole-dipole interaction between unlike molecules.

V. RESULT AND DISCUSSION

The experimental data of ultrasonic velocity, density and viscosity are reported for binary system of 1-butanol and 3- methyl, 1-butanol with O-Nitro toluene including those of pure liquids were measured over entire mole fraction range at 298.15 K and 308.15 K. Calculated excess molar volume deviation in viscosity and deviation in isentropic compressibility shows large negative deviation for most of binary mixtures these concluded that the existence of molecular interaction exist in above binary mixture which may be due to presence of more chain length and methyl substituent. It is well notified that most of values are negative due presence of polar functional group on aromatic ring alcoholic –OH group which increases salvation effect in solution so it shows that structure making interaction between solvent and solute.

TABLE-I: Values of densities viscosities, ultrasonic velocity, excess molar volumes and deviation in viscosity and deviation in isentropic compressibility for binary system of 1-butanol and O-Nitro toluene at 298.15 and 308.15 K.

Temp K	X1	ρ (gm /cm3)	η103 (Nsm-2)	U(MS-1)	VEx106 (m3/mole)	Δ ηx103 (Kg m-1s-1)	Δksx1011 (m2N-1)
298.15	0.0000	0.80540	2.52940	1499.6	0.0000	0.000	0.000
	0.1156	0.83310	2.35250	1515.8	-0.8195	-14.302	-6.34
	0.2019	0.85980	2.11890	1548.9	-1.4049	-33.919	-19.52
	0.3188	0.89320	2.00670	1531.8	-2.5991	-41.017	-25.48
	0.4265	0.92540	1.93240	1566.9	-3.4923	-43.822	-31.19
	0.5251	0.95760	1.87980	1599.5	-4.2497	-43.923	-44.38
	0.6048	1.05690	1.82200	1662.4	-6.4269	-43.890	-49.80
	0.7257	1.07230	1.73500	1682.9	-6.3425	-46.003	-30.72
	0.8283	1.11090	1.78750	1682.7	-7.2998	-33.194	-27.89
	0.9129	1.14890	1.83100	1715.1	-3.0733	-20.098	-16.53
	1.0000	1.06920	1.92950	1932.0	0.0000	0.000	0.000
308.15	0.0000	0.79800	1.99670	1401.4	0.0000	0.000	0.000
	0.1156	0.82500	1.84770	1441.1	-0.7698	-12.706	-31.44
	0.2019	0.85150	1.70580	1467.2	-1.3594	-24.468	-45.34
	0.3188	0.88360	1.60400	1516.5	-2.4488	-31.975	-50.40
	0.4265	0.91660	1.55200	1517.4	-3.4626	-34.175	-64.69
	0.5251	0.94880	1.53910	1532.5	-4.2493	-32.119	-65.27
	0.6048	1.04710	1.49980	1566.6	-5.4740	-32.278	-80.87
	0.7257	1.06250	1.40870	1598.2	-6.3805	-29.116	-69.71
	0.8283	1.10080	1.47670	1603.4	-8.3379	-25.413	-60.98
	0.9129	1.13800	1.51100	1633.3	-8.0581	-16.310	-48.90
	1.0000	1.06030	1.60760	1665.8	0.0000	0.000	0.000

Table2. Values Of Densities Viscosities, Ultrasonic Velocity, Excess Molar Volumes And Deviation In Viscosity And Deviation In Isentropic Compressibility For Binary System Of 3-Methyl,1-Butanol And O-Nitro Toluene At 298.15 And 308.15 K.

Temp K	X1	ρ (gm /cm3)	η103 (Nsm-2)	U(MS-1)	VEx106 (m3/mole)	Δ ηx103 (Kg m-1s-1)	Δksx1011 (m2N-1)
298.15	0.0000	0.80660	3.74590	1488.6	0.0000	0.000	0.000
	0.1066	0.83550	3.36850	1499.7	-1.1321	-25.644	-13.44
	0.2138	0.86450	2.82450	1525.5	-2.1086	-67.057	-23.52
	0.3212	0.88920	2.60070	1545.6	-2.3422	-75.269	-33.18
	0.4301	0.95330	1.95640	1601.2	-3.0904	-104.459	-46.97

Temp K	X1	ρ (gm /cm3)	η103 (Nsm-2)	U(MS-1)	VEx106 (m3/mole)	Δ ηx103 (Kg m-1s-1)
	0.5091	0.96100	2.32250	1610.0	-5.0368	-91.284
	0.6149	0.99590	2.13420	1630.7	-5.9413	-72.022
	0.7159	1.08460	2.08160	1642.0	-6.3053	-57.520
	0.8203	1.10090	1.96870	1687.8	-5.8342	-46.922
	0.9128	1.11900	1.92200	1694.5	-4.3612	-27.525
	1.0000	1.06920	1.92950	1832.0	0.0000	0.000
308.15	0.0000	0.79940	2.79410	1449.2	0.0000	0.000
	0.1066	0.82790	2.59620	1450.2	-1.1181	-11.892
	0.2138	0.85640	2.16230	1516.7	-2.0672	-46.799
	0.3212	0.88090	2.03580	1538.3	-2.3002	-85.194
	0.4301	0.94430	1.49470	1597.0	-4.0742	-94.349
	0.5091	0.95230	1.79070	1600.2	-5.0371	-73.928
	0.6149	0.98660	1.64660	1619.2	-5.9090	-56.521
	0.7159	1.07570	1.70020	1633.0	-12.4484	-38.252
	0.8203	1.09120	1.67040	1667.9	-10.8883	-26.934
	0.9128	1.10940	1.61370	1678.3	-9.4195	-16.883
	1.0000	1.06030	1.60760	1719.2	0.0000	0.000

Table.3. Values Of Excess Free Length (Lfe), Internal Pressure (Πe) ,Available Volume (Vae) And G Free Energy(G*E) For Binary System Of 1-Butanol And O-Nitro Toluene At 298.15 And 308.15

Temp. K	X1	LfE x 10-10 m	VaEx10-6 m3mol-1	πE x 106 Nm-1	G*E Jmol-1
298.15	0.0000	0.000	0.000	0.000	0.000
	0.1156	-0.004	0.977	-3036.9	-156.3
	0.2019	-0.011	1.118	-7074.8	-380.9
	0.3188	-0.014	4.416	-7717.9	-492.6
	0.4265	-0.016	4.840	-8921.1	-549.4
	0.5251	-0.021	5.627	-9789.3	-572.0
	0.6048	-0.022	11.955	-8895.1	-756.3
	0.7257	-0.021	10.008	-7003.6	-767.9
	0.8283	-0.018	8.915	-3755.8	-626.9
	0.9129	-0.010	5.176	-2429.4	-485.7
	1.0000	0.000	0.000	0.000	0.000
303.15	0.0000	0.000	0.000	0.000	0.000
	0.1156	-0.014	0.222	-3746.6	-180.7
	0.2019	-0.022	0.566	-6786.0	-358.3
	0.3188	-0.026	1.290	-9023.3	-498.6
	0.4265	-0.034	1.953	-9226.4	-558.8
	0.5251	-0.044	2.337	-8805.3	-645.3
	0.6048	-0.050	4.946	-6729.4	-735.0
	0.7257	-0.045	3.021	-7609.6	-797.5
	0.8283	-0.036	2.239	-4549.2	-624.6
	0.9129	-0.029	1.133	-1789.2	-500.2
	1.0000	0.000	0.000	0.000	0.000

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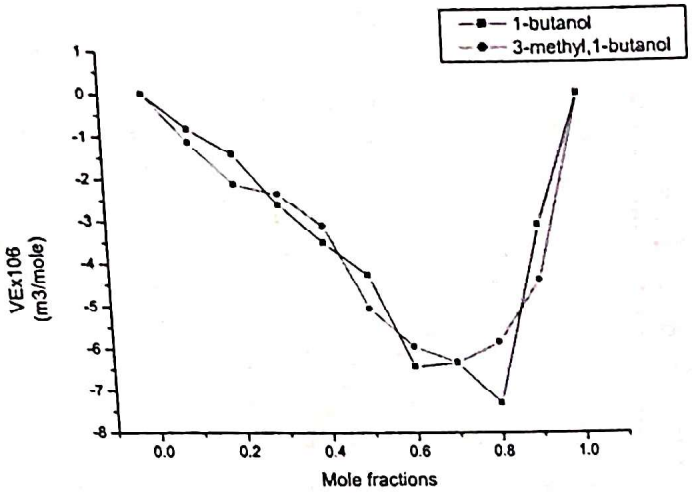


A)

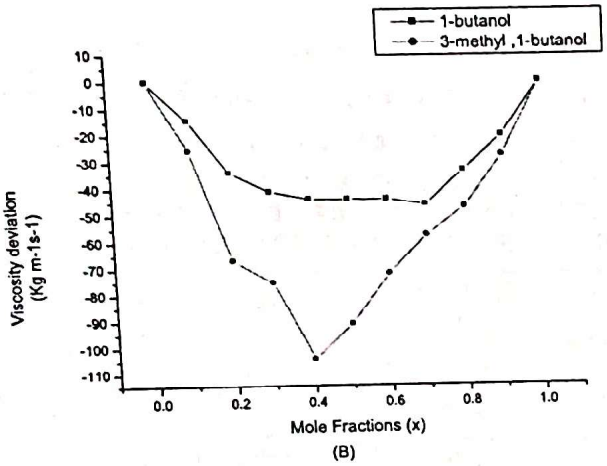
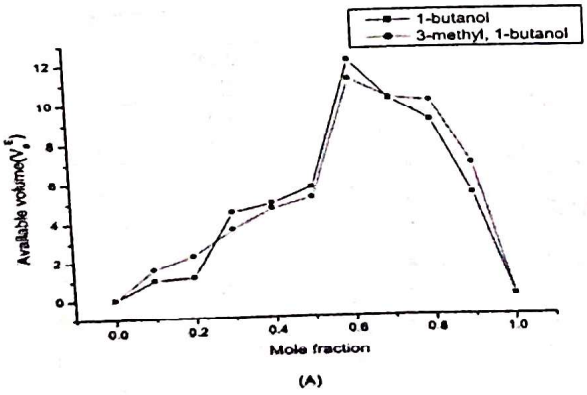


Figure1.

(A) Excess molar volume (VE) against mole fraction for 1-butanol and 3-methyl, 1-butanol at 298.15 K

(B) Deviation in viscosity (Δn) against mole fraction for 1-butanol and 3-methyl, 1-butanol at 298.15 K



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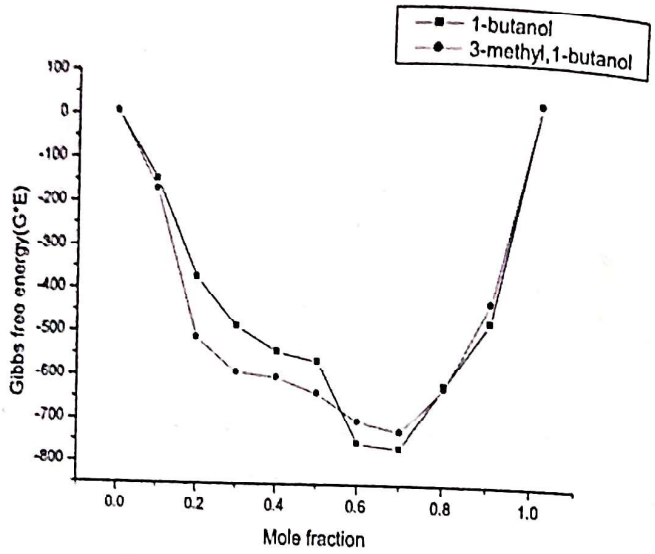

(B)

Figure :-2

(A) Available volume (VaE) against mole fraction for 1-butanol and 3-methyl, 1-butanol at 298.15 K

(B) Gibbs free energy (G*E) against mole fraction for 1-butanol and 3-methyl, 1-butanol at 298.15 K

TABLE.4. VALUES OF EXCESS FREE LENGTH (LFE), INTERNAL PRESSURE (ΠE) ,AVAILABLE VOLUME (VAE) AND GIBBS FREE ENERGY(G*E) FOR BINARY SYSTEM OF 3-METHYL, 1-BUTANOL AND O-NITRO TOLUENE AT 298.15 AND 308.15 K.

Temp. K	X1	LfE x 10-10 m	VaEx10-6 m3mol-1	πE x 106 Nm-1	G*E Jmol-1
298.15	0.0000	0.000	0.000	0.000	0.000
	0.0668	-0.001	1.536	-2751.6	-178.1
	0.1383	-0.011	2.236	-7530.4	-516.9
	0.2163	-0.022	3.567	-8801.9	-596.3
	0.3002	-0.021	4.582	-13887.0	-608.7
	0.3914	-0.025	5.085	-13935.0	-644.3
	0.4910	-0.018	11.030	-12903.9	-707.8
	0.5998	-0.015	10.070	-9072.6	-730.4
	0.7203	-0.014	9.885	-7082.3	-633.8
	0.8528	-0.010	6.714	-4249.0	-441.4
	1.0000	0.000	0.000	0.000	0.000
303.15	0.0000	0.000	0.000	0.000	0.000
	0.0668	-0.004	1.283	-1454.8	-118.5
	0.1383	-0.020	1.853	-7098.5	-505.4
	0.2163	-0.022	2.739	-7952.1	-552.5
	0.3002	-0.042	3.178	-13479.8	-633.1
	0.3914	-0.032	4.570	-8392.9	-691.0
	0.4910	-0.031	7.926	-8011.6	-782.3
	0.5998	-0.026	5.635	-4112.7	-693.3
	0.7203	-0.023	4.769	-2869.1	-528.3
	0.8528	-0.019	3.954	-2121.1	-394.3
	1.0000	0.000	0.000	0.000	0.000

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