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Study of Molecular Interaction and Sound Velocity of Alcohols with ONT at Different Temperatures

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Abstract: **The related parameters of molecular interaction and sound velocity studies of 1- butanol and 3- methyl, 1- butanol at 303. 15 and 313.15 K temperatures. The density, ultrasonic velocity and viscosity of binary mixtures were measured at given temperatures. These experimental analysis data have been used to calculate viscosity deviation (Δη) , excess molar volume (V^E), deviation in isentropic compressibility (ΔK_S) , Excess free length(L_f^E), and acoustic impendence (Z^E). The values of excess intermolecular free length and isentropic compressibility are negative over and wide range of mole fraction for a given binary mixtures. These results have been used to explain the nature of interaction between unlike molecules in terms of hydrogen bonding and dipole-dipole interactions.**

Index Terms: **Enter Ultrasonic velocity, Viscosity, Density, Excess molar volume (V^E), Viscosity deviation (Δη), Excess free length (L_f^E).**

I. Introduction

The formation of hydrogen bond in binary mixture solution and its effect on physical properties of mixtures have received much attention. Hydrogen bonding plays an important role in industrial applications and fundamental sciences. Many theoretical and experimental studies have been understanding directing towards the hydrogen bonding. Alcohols are widely used in variety of industrial (Oswal, S. L., et al,1998; Kumar, H., et al.,2011) and consumer applications and hence the knowledge of their physical properties are more importance for practical point of view. Several researchers (Zorebski, E., et al.,2008; Borun, A., et al.,2010; Satry, S. S.et al., 2013; Checoni, R. F. et al.,2010; S. Sreehari S.et al.,2014; Shastry, S. et al.,2014) have measured viscosity, density and ultrasonic velocity for wide range of binary mixtures containing alcohol as one of the components.

In present in investigation the liquid were chosen on the basis of industrial importance alcohols are used as hydraulic fluids in pharmaceutical (Resa, J.M., et al.,2007) and cosmetic. In given work to determine thermodynamics and transport properties of binary liquid mixtures (S. Sharma, S., et al.,2011; Naidu., S., et al.,2005; Narendra K., et al.,2011; Arnett E. M., et al.,1974; Santhi., N., et al.,2013). We report density (ρ), viscosity (η), ultrasonic velocity (U), viscosity deviation (Δη), excess molar volume (V^E), deviation in isentropic compressibility (ΔK_S), Excess free length (L_f^E), and acoustic impendence (Z^E) of the binary mixture of 1- butanol and 3- methyl, 1- butanol with o-nitro tune at 303.15 and 313.15K temperature.

These results have been used to discuss the nature of interaction between unlike molecules in terms of hydrogen bonding dipole interaction and dispersion forces. In given system alcohols are self-associated through hydrogen bonding of their hydroxyl group. The present work was undertaken to determine the effect of position of -OH group of an alcohol molecule that may influence both the sign and magnitude of various thermodynamic functions when they mixed with o-nitro toluene as a solvent.

II. Experimental

In The chemicals used are of A.R. grade with minimum assay of 99.9% obtained from Sigma Aldrich or s. d. fine chemicals India. Bi-capillary pycnometer (10ml) was used to measured densities. An airtight stopper bottles were used to prepare and store the binary liquid mixtures of different known concentrations. The shimatzu electronic digital balance (± 0.1mg.) was used to measured weights of the samples. The Ubbelohde viscometer (20ml) was used to measure the viscosity. The efflux time was determined using a digital clock to within ±0.015sec. The ultrasonic velocities (U) in liquid mixtures were measured using an ultrasonic interferometer (Mittal, F-81, 2 MHz, ±0.1 ms^{-1}).

Table.1. Values of densities viscosities, ultrasonic velocity, excess molar volumes, deviation in viscosity, deviation in isentropic compressibility, acoustic impedance and excess intermolecular free length for binary system of 1-butanol and O-nitro toluene at 303.15 and 313.15 K

Temp K	**X_1**	**ρ (gm /cm^3)**	**η10^3 (Nsm^{-2})**	**U(MS^{-1})**	**V^Ex10^6 (m^3/mole)**	**Δ ηx10^3 (Kg m^{-1}s^{-1})**	**Δksx10^{11} (m^{2}N^{-1})**	Z^E xKg s^{-1} m^{-3}	**L_f^E x 10^{-10} m**
303.15	0.0000	0.80320	3.19400	1559.0	0.0000	0.000	0.000	0.000	0.000
	0.1066	0.83170	2.94090	1467.2	-1.1001	-15.697	-18.58	-14.41	-0.005
	0.2138	0.86050	2.41230	1519.2	-2.0718	-58.234	-20.47	-22.06	-0.007
	0.3212	0.88510	2.26620	1540.6	-2.3077	-61.583	-22.70	-26.46	-0.020
	0.4301	0.94880	1.68600	1602.2	-3.0652	-97.489	-34.41	-42.39	-0.024
	0.5091	0.95680	2.01510	1604.3	-5.0404	-81.412	-37.73	-63.03	-0.029
	0.6149	0.99120	1.84900	1622.2	-5.9088	-63.641	-34.37	-61.70	-0.023
	0.7159	1.08010	1.84460	1635.3	-6.3641	-48.373	-33.57	-52.34	-0.022
	0.8203	1.09620	1.76970	1675.7	-5.8733	-38.465	-27.78	-32.57	-0.013
	0.9128	1.11430	1.75290	1680.1	-4.4019	-21.015	-15.55	-22.60	-0.012
	1.0000	1.06470	1.75020	1631.2	0.0000	0.000	0.000	0.000	0.000
313.15	0.0000	0.79520	2.52550	1417.7	0.0000	0.000	0.000	0.000	0.000
	0.1066	0.82370	2.39760	1449.6	-0.5131	-4.699	-25.23	-14.05	-0.010
	0.2138	0.85240	1.96540	1503.1	-1.8367	-39.232	-29.68	-25.04	-0.025
	0.3212	0.87670	1.85750	1528.2	-2.3237	-40.545	-36.59	-32.25	-0.027
	0.4301	0.94000	1.39600	1584.1	-4.3521	-76.501	-38.59	-45.57	-0.045
	0.5091	0.94710	1.67140	1596.1	-5.3420	-57.880	-48.61	-66.48	-0.036
	0.6149	0.98210	1.53800	1604.0	-6.3806	-39.119	-46.67	-61.79	-0.030
	0.7159	1.07070	1.68650	1625.8	-7.9138	-11.050	-37.16	-41.71	-0.026
	0.8203	1.08650	1.65640	1656.2	-6.2481	-8.581	-25.04	-40.69	-0.022
	0.9128	1.10450	1.55620	1668.4	-5.5105	-6.660	-12.59	-34.80	-0.014
	1.0000	1.13740	1.31050	1682.4	0.0000	0.000	0.000	0.000	0.000

Table.2. Values of densities viscosities, ultrasonic velocity, excess molar volumes, deviation in viscosity, deviation in isentropic compressibility, acoustic impedance and excess intermolecular free length for binary system of 3-methyl, 1-butanol and O-nitro toluene at 303.15 and 313.15 K

Temp K	**X_1**	**ρ (gm /cm^3)**	**η10^3 (Nsm^{-2})**	**U(MS^{-1})**	**V^Ex10^6 (m^3/mole)**	**Δ ηx10^3 (Kg m^{-1}s^{-1})**	**Δksx10^{11} (m^{2}N^{-1})**	Z^E xKg s^{-1} m^{-3}	**L_f^E x 10^{-10} m**
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	0.3212	0.88510	2.26620	1540.6	-2.3077	-61.583	-22.70	-26.46	-0.020
	0.4301	0.94880	1.68600	1602.2	-3.0652	-97.489	-34.41	-42.39	-0.024
	0.5091	0.95680	2.01510	1604.3	-5.0404	-81.412	-37.73	-63.03	-0.029
	0.6149	0.99120	1.84900	1622.2	-5.9088	-63.641	-34.37	-61.70	-0.023
	0.7159	1.08010	1.84460	1635.3	-6.3641	-48.373	-33.57	-52.34	-0.022
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	1.0000	1.06470	1.75020	1631.2	0.0000	0.000	0.000	0.000	0.000
313.15	0.0000	0.79520	2.52550	1417.7	0.0000	0.000	0.000	0.000	0.000
	0.1066	0.82370	2.39760	1449.6	-0.5131	-4.699	-25.23	-14.05	-0.010
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	0.9128	1.10450	1.55620	1668.4	-5.5105	-6.660	-12.59	-34.80	-0.014
	1.0000	1.13740	1.31050	1682.4	0.0000	0.000	0.000	0.000	0.000

III. THEORY AND CALCULATION

Following equations been used to calculate different parameters in binary solutions

a) The molar excess volume

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

b) The viscosity deviation

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

$$\Delta\eta_m = \eta_{12} - X_1\eta_1 - X_1\,\eta_2 \quad (3)$$

c) Deviation in isentropic compressibility

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

Where k_{S1}, k_{S2} and k_S are isentropic compressibility of liquid mixtures and Φ is volume fraction of pure i^{th} component in the mixture and is defined as

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

Where x_1 and V_i are mole fraction and molar volume of i^{th} component in the mixture.

a) The excess free length

$$L_f^E = L_{fmix} - x_1L_{f1} - x_2L_{f2} \quad (6)$$

$$A^E = A_{exp} - A_{id} \quad (7)$$

Where $A_{id} = \sum Ai\ Xi$, Ai is any acoustical parameters and Xi

IV. RESULT AND DISCUSSION

The measured values such as density (ρ), viscosity (η), The measured values such as density (ρ), viscosity (η), ultrasonic velocity (U), viscosity deviation (Δη), excess molar volume (V^E), deviation in isentropic compressibility (ΔK_S), Excess free length (L_f^E), and acoustic impendence (Z^E) are given in Table-1 and Table-2 respectively. Figure: - (A) and (B) shows Excess molar volume (V^E), and Deviation in isentropic compressibility (ΔK_S) against mole fraction for binary system of 1-butanol and 3-methyl, 1-butanol with O-nitro toluene at 303.15 K.

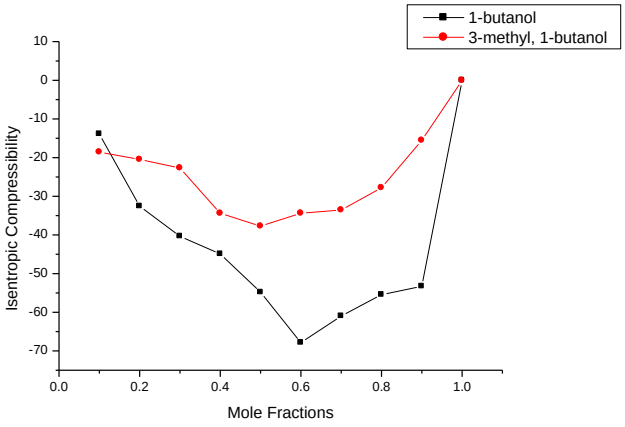

Fig.1. (A) Excess molar volume (V^E) against mole fraction for 1-butnol and 3- methyl, 1-butanol with o-nitro toluene at 303.15 K.

All these parameters show negative deviations with minima at about X_2= 0.6-0.8 this may be due to presence of stronger solute solvent interactions in between highly polar functional groups Nitro and -OH. This causes fitting of alkanol molecules in the avoids of self-associated solvent molecules resulting volume contraction than ideal. With increase in temperature all these parameters become less negative showing less salvation effect at higher temperature.

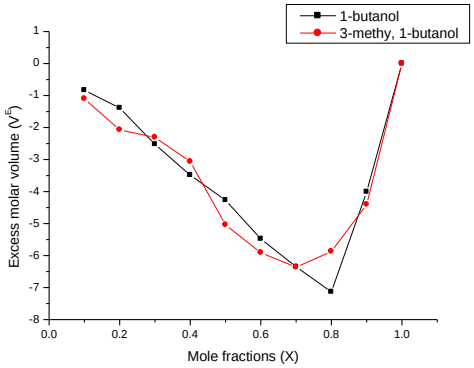

Fig.1. (B) Deviation in isentropic compressibility (ΔKs) against mole fraction for 1-butnol and 3- methyl, 1-butanol with o-nitro toluene at 303.15 K.

CONCLUSION

From experimental data ultrasonic velocity (U), density (ρ) and viscosity (η) have been measured for binary system at 303.15 and 313.15 K. The data have been used to compute the parameters $\Delta\eta$,V^E, ΔK_S, L_f^E, and Z^E . It is a well justified that most of values are negative due to presence of polar functional groups on aromatic ring and alkanols which increases salvation effect in solution so it shows structure making interactions between solvent and solute.

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