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Molecular Interaction studies of Binary Mixture of Alkanols with O-nitrotolune at 298.15 and 308.15

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Abstract :
The ultrasonic velocities, Viscosities and densities of binary liquid system of 2-Butanol and isodecanol with O nitrotolune have been observed at 298.15 and 308.15 K over entire range of composition. The observed value were use to compute the excess molar volume , deviation in viscosity and isotropic compressibility. The result was interpreted th intermolecular interaction between solution with solvent.

Key Words : Ultrasonic velocity, Density, Viscosity, Excess molar volume, viscosity deviation, Isentropi Compressibility..

Introduction :

The studies of ultrasonic velocity, Viscosity and density are being increasingly used as tools for investigation of properties of pure component and the nature of intermolecular interaction between the binary liquid mixtures constituents.

Earlier we have studied the ultrasonic velocity , density and viscosity of some alkanols with different solvent (1-3). The experimental investigation of excess thermodynamic properties of industrially significant liquid mixtures .

In presence studied measurement of density, visocity and ultrasonic velocities of 2 binary liquid mixtures of 2- Butanol and Isodecanol I with O Nitrotolune as a organic solvent have been observed at two temperatures 298.15 and 308.15 K

The study of ultrasonic velocity, density and viscosity measurement are widely used in characterising the phsico- chemical properties .The alcohols are strongly self associated liquid with three dimensional network of hydrogen bond [5]. The investigation regarding the molecular association in organic binary mixture having one of the alkanol group. Since alkanol group is highly polar and can be association with any other group having some degree of polar attraction

Experimental :

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 use to measured weights of the samples. The Ubbelohd viscometer (20ml) was used to measure the viscosity The efflux time was determined using a digital clock t within ±0.015 sec. The ultrasonic velocities (U) i liquid mixtures were measured using an ultrasoni interferometer (Mittal, F-81, 2 MHz, ±0.1 ms^{-1}).

Theory and Calculation :

Following equations been used to calculat 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_i and V_i are mole fraction and molar volume of i^{th} component in the mixture.

Result and Discussion :

The experimental values of density (ρ) viscosity (η) ultrasonic velocity (U), Excess volume (V^E), viscosity deviations and (Δη), deviation on isentropic compressibility (Δk_S) for binary Systems of 2-Butanol and Isodecanol (1) with o-nitro toluene (2) at 298.15K

and 308.15K are reported in Tables1 and 2 respectively. The variation of excess parameters with mole fraction of alkanols at 298.15K are plotted in Figure 1-4. shows that excess molar volume ,ultrasonic velocity, viscosity deviation and deviation isentropic compressibility are against mole fraction of alkanols at given temperature. In studied work the excess molar volume (V^E) values have been observed negative which attributed strong molecular interaction between the unlike molecules[6]. Generally when two solvents are mixed the molecular interaction held will be depend upon the type and nature of molecules. The positive excess volumes attribute structure breaking interactions while negative excess volumes attribute structure making interactions [7].

The observed V^E values may be analysed in terms of several effects which may be categorised as physical, chemical and geometrical contributions [12].The physical interactions compromise mainly dispersion forces and non specific physical interaction giving positive contribution. The chemical interaction involves the charge transfer complexes, resulting in contraction of volume, geometrical or structural contribution arising from the geometrical fitting of one component into other [4] The negative, viscosity deviation and deviation in isentropic compressibility may be attributed to existence of dispersion dipole forces between unlike molecules and related to the difference in size and shape of molecules [8]. Increase of temperature disturbs hetero and homo association of molecules which increase the fluidity of the liquid. The values of viscosity deviation are more negative for Isodecanol which provides additional evidences for existence of interaction of weak magnitude like dipole –induced dipole type between components of liquid[15]. The magnitude of viscosity deviation and deviation isentropic compressibility the sign and extent of deviation of these properties from idealist depends upon the strength of interaction between unlike molecules. According to fort et. al. the excess viscosity gives the molecular interaction between interacting molecules. For the system where dispersion, induction and dipolar forces which are operated by values of excess viscosity are found to be negative, the large negative values of excess viscosity for the system can be attributed to the presence of dispersion, induction and dipolar forces between the components. The positive isentropic compressibility which indicates loosely packed molecules in the binary system. The Isodecanol has more negative viscosity deviation but less negative isentropic compressibility values this is due to structural differences in these two alcohol molecules.

Conclusion :

The experimental data of density, viscosity and ultrasonic velocity are reported for binary mixtures of 2-Butanol and Isodecanol with O-nitro toluene over entire range of mole fractions at 298.15K and 308.15K. Calculated, viscosity deviation, excess molar volume and deviation in isentropic compressibility shows large negative deviations for most investigated binary system. This reveals the existence of molecular interaction in binary system. The present investigation shows that greater molecular interaction exist in Isodecanol and O-nitrotolune binary mixture which may be due to presence of more carbon –carbon linkage than 2-Butanol.

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Table 1: Values of density (ρ) viscosity (η) ultrasonic velocity (U), Excess volume (V^E), viscosity deviations and ($\Delta\eta$), deviation on isentropic compressibility (Δk_s) for Binary System of 2-Butanol (1) with O-nitrotolune(2) at 298.15K and 308.15K.

Temp. (K)	x_1	ρ (gm/cm^3)	η10^3 (Nsm^{-2})	U (MS^{-1})	V^E x 10^6(m^3 mole^{-1})	$\Delta\eta$ x 10^3 (Kg m^{-1} s^{-1})	Δk_s x 10^{11}(m^2 N^{-1})
298.15	0.0000	0.80210	2.95470	1451.0	0.0000	0.000	592.2
	0.0568	0.83140	2.37190	1483.9	-0.9900	-52.487	546.3
	0.1192	0.85680	2.08440	1500.7	-1.4098	-74.839	518.2
	0.1881	0.89150	1.97480	1517.3	-2.7197	-78.736	487.2
	0.2651	0.92200	1.83930	1565.2	-3.4087	-84.392	442.7
	0.3514	0.93510	1.55420	1625.0	-2.0673	-104.054	418.3
	0.4480	0.96870	1.63930	1650.5	-4.9552	-85.641	364.2
	0.5579	1.01290	1.60790	1700.7	-4.5311	-77.514	341.3
	0.6840	1.04240	1.51270	1714.3	-4.4814	-74.106	326.4
	0.8293	1.05410	1.43650	1730.5	-2.2514	-66.830	316.8
	1.0000	1.06920	1.92950	1932.0	0.0000	0.000	250.6
308.15	0.0000	0.79380	2.09760	1401.4	0.0000	0.000	641.5
	0.0568	0.82260	1.75580	1448.9	-0.9627	-31.418	579.1
	0.1192	0.84780	1.57690	1456.0	-1.3778	-46.250	556.4
	0.1881	0.88260	1.50860	1500.5	-2.7343	-49.704	503.2
	0.2651	0.91280	1.43760	1520.8	-3.4114	-53.031	473.7
	0.3514	0.92660	1.35960	1549.9	-2.1281	-56.602	449.3
	0.4480	0.97890	1.32270	1558.5	-4.9346	-55.559	420.6
	0.5579	1.00320	1.30330	1665.4	-4.5158	-52.114	359.4
	0.6840	1.04280	1.24830	1669.2	-5.5663	-51.435	344.2
	0.8293	1.05430	1.14580	1672.3	-3.3319	-54.565	339.2
	1.0000	1.06030	1.60760	1719.2	0.0000	0.000	319.1

Table 2 : Values of density (ρ) viscosity (η) ultrasonic velocity (U), Excess volume (V^E), viscosity deviations and ($\Delta\eta$), deviation on isentropic compressibility (Δk_s) for Binary System of Isodecanol () with O-nitrotolune(2) at 298.15K and 308.15K .

Temp. (K)	x_1	ρ (gm/cm^3)	η10^3 (Nsm^{-2})	U (MS^{-1})	V^E x 10^6(m^3 mole^{-1})	$\Delta\eta$ x 10^3 (Kg m^{-1} s^{-1})	Δk_s x 10^{11}(m^2 N^{-1})
298.15	0.0000	0.85750	12.80620	1584.5	0.0000	0.000	464.5
	0.1142	0.88060	10.73480	1629.2	-1.1496	-83.056	427.8
	0.2254	0.91160	8.62750	1649.2	-3.4823	-172.837	403.3
	0.3309	0.92810	6.75690	1661.6	-2.9375	-245.148	390.3
	0.4344	0.95120	5.04190	1664.4	-3.3671	-304.074	379.5
	0.5355	0.98540	3.67280	1664.7	-5.2820	-331.021	366.2
	0.6338	1.01590	3.39130	1668.1	-6.2695	-252.253	353.8
	0.7291	1.03970	2.51920	1699.7	-6.1060	-235.808	332.9
	0.8221	1.07590	2.43480	1814.5	-7.3206	-143.095	282.3
	0.9128	1.15260	2.18490	1847.6	-12.5922	-69.433	254.2
	1.0000	1.06920	1.92950	1932.8	0.0000	0.000	250.4
308.15	0.0000	0.84560	7.89520	1546.7	0.0000	0.000	494.3
	0.1142	0.87300	7.66480	1596.0	-2.0320	48.686	449.7
	0.2254	0.90400	5.84110	1597.7	-4.3208	-63.567	433.4
	0.3309	0.92040	4.67200	1598.4	-3.6676	-114.342	425.3
	0.4344	0.94380	3.69300	1600.2	-4.0746	-147.166	413.8
	0.5355	0.97680	2.80820	1601.2	-5.7517	-172.078	399.3
	0.6338	1.00710	2.66070	1629.9	-6.6567	-125.021	373.8
	0.7291	1.03150	2.08260	1633.8	-6.5022	-122.910	363.2
	0.8221	1.06710	1.99230	1647.3	-7.5878	-73.465	345.3
	0.9128	0.14250	1.85440	1683.0	840.7976	-30.227	2477.5
	1.0000	1.06030	1.60760	1719.2	0.0000	0.000	319.1

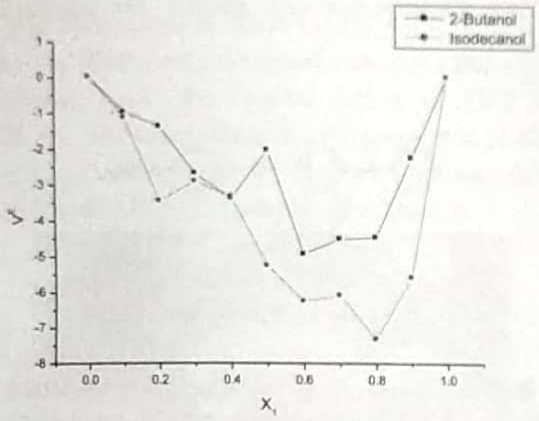
Figure 1.

(a) V^E against mole fraction for 2-Butanol and Isodecanol with O-nitrotolune at 298.15 K

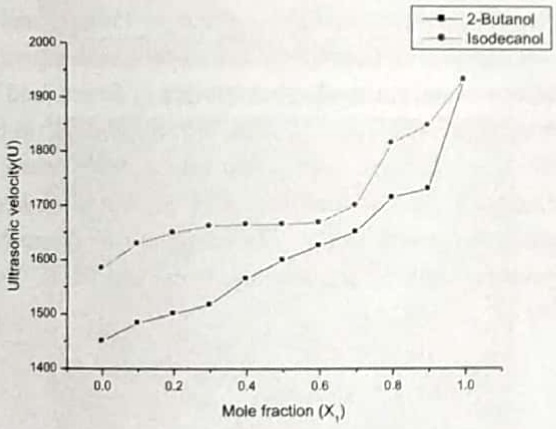
(b) Ultrasonic velocity against mole fraction for 2-Butanol and Isodecanol with O-nitrotolune at 298.15 K

(c) Δn against mole fraction for 2-Butanol and Isodecanol with O-nitrotolune at 298.15 K

(d) ΔKs against mole fraction for 2-Butanol and Isodecanol with O-nitrotolune at 298.15 K



(a)



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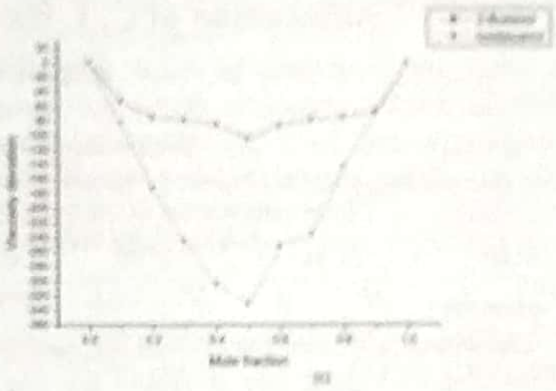

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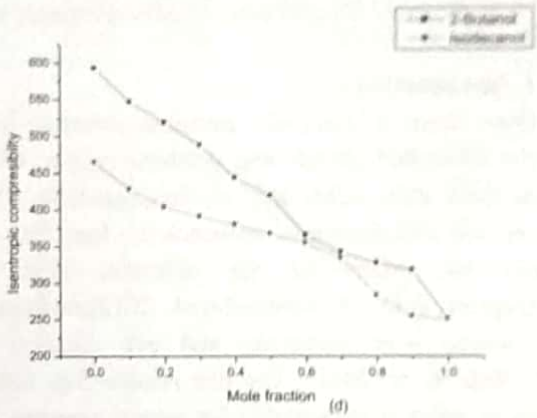

(d)