

Study of molecular interaction of Pentanol and n-Heptane using ultrasonic technique at different temperatures.

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ABSTRACT

The variation of mole fraction and temperature of the liquid mixture dependence on thermo-acoustic properties are very important parameters for the verification of intermolecular interactions. The thermo-acoustic parameters such as density (ρ), ultrasonic velocity (U) and viscosity (η) have been measured for a binary mixture of Pentanol and n-Heptane system at different mole fraction and at different temperatures. Using the experimental data, some of the acoustical parameters such as, adiabatic compressibility (β_a), free length (L_f), free volume (V_f), internal pressure (π_i), and Gibb's free energy (ΔG) are evaluated at different temperatures. The present paper shows the nonlinear variation of ultrasonic velocity and the thermodynamic properties that lead to dipole-dipole interaction of pure 1- Pentanol stronger than the induced dipole - induced dipole interaction of pure n- Heptane molecule which is responsible for association in the binary liquid mixture. The behavior of these parameters with composition of the mixture has been discussed in terms of molecular interaction between the components of the liquids.

Keywords: Ultrasonic velocity, acoustical parameters, molecular interactions, mole fraction, Pentanol and n-Heptane.

INTRODUCTION

The ultrasonic study of liquid are used to understand the behavior and strength of molecular interactions [1-6].

The studies on the physio-chemical properties of organic liquid like Pentanol in n-Heptane provide useful information, which is used to assess the information of molecular interaction [7-9]. An enormous number of studies have been made on the molecular interaction in liquid systems by various physical methods such as: Raman Effect, Nuclear Magnetic Resonance, and ultra sonic method [10-12]. The ultrasonic velocity data for binary liquid mixtures have been used for by many researchers [13-15]. In this paper the authors report on the ultrasonic velocity, density, and viscosity of Pentanol and n-Heptane at different temperatures over the different composition. From these experimental values, a number of thermodynamics parameters, namely adiabatic compressibility (β_a), free length (L_f), free volume (V_f), internal pressure (π_i) and Gibb's free energy (ΔG) were calculated. The variations of these parameters with concentrations were also useful towards finding the behavior of molecular interactions in the binary liquid mixtures.

METHODOLOGY

The ultrasonic velocity was measured in the binary mixture of Pentanol in n-Heptane using an ultrasonic Pulse overlap technique working at frequency 4 MHz with an overall accuracy of $\pm 0.1 \text{ ms}^{-1}$. The temperature was maintained by a constant temperature water bath using circulated circulate water through the double walled measuring cell made up of a steel containing the experimental solution at the desired temperature. The density of pure liquids and liquid mixtures was determined using a 10ml specific gravity bottle with an accuracy of $\pm 0.1 \text{ Kg m}^{-3}$. An Ostwald's viscometer was used for the viscosity measurement of pure liquids and liquid mixtures with accuracy 0.001 NSm^{-2} . The viscometer was calibrated before used. The time of flow of water (t_w) and time flow of solution (t_s) was measured with digital stop watch having an accuracy $\pm 1 \times 10^{-6} \text{ NSm}^{-2}$.

RESULTS AND DISCUSSION

The experimental values of density, velocity and viscosity of Pentanol with n-Heptane and calculated

acoustic parameters at different composition and temperatures are shown in tables 1-3.

From table 1 it is observed that density increases with increase in molar concentration of 1- Pentanol in n-Heptane. Increase in density decreases the volume, indicating association in component molecules. This makes the liquid medium less compressive. Increasing temperature of the mixture decreases its density (ρ). The decrease in density (ρ) with increase in temperature indicates decrease in cohesive force. Thus increase of temperature favors increase of kinetic energy and volume expansion and hence decrease of density [16]. It is also observed that ultrasonic velocity increases with increase in molar concentration of 1- Pentanol in n-Heptane, indicating the increase in stiffness of the mixture and hence association. The association in the constituent molecules may involve due to dipole-dipole interaction or hydrogen bonding is predominant in case of 1- Pentanol. The association due to stronger dipole-dipole interaction of pure 1- Pentanol than the induced dipole-induced dipole interaction of pure n- Heptane molecule. The process may lead to strong interaction forces [17], [18].

The viscosity is a physical property in understanding the structure as well as molecular interaction occurring in the aqueous system. Entropy measures the disorder of medium. It also depends on the temperature. Higher the disorder more will be entropy. It is observed that viscosity increases with increase in molar concentration of 1- Pentanol in n-Heptane indicating strong molecular interaction. The viscosity gives the strength of molecular interaction between interacting molecules. Increase in temperature of the mixture increases disorder of the medium and hence entropy increases. As entropy increases, viscosity of the binary mixture decreases.

From table 2 it is found that adiabatic compressibility decreases with increase in molar concentration of 1- Pentanol in n-Heptane indicating strong intermolecular interaction between 1- Pentanol and n-Heptane. This also shows associating tendency of the component molecules. This is because of the fact that dipole-dipole interaction of pure 1- Pentanol stronger than the induced dipole - induced dipole interaction of pure n- Heptane molecule. The decrease in free

length is a result of dipole-dipole and induced dipole - induced dipole interaction between 1- Pentanol and n-Heptane indicating association.

Free volume decreases (V_f) and internal pressure (Π_i) increases with increase in molar concentration of 1- Butanol in n-Heptane, indicating association in the molecules of the component liquids. In the present system, it is observed that free volume decreases and internal pressure increases. Further, the decrease in free volume and increase in internal pressure with increase in clearly show the increasing magnitude of interactions. This suggests that both solute- solute and solute solvent interaction exist in the system. In the present case relaxation time, which is in the order of

10^{-12} s is due to structural relaxation process[19]and in such situation it is suggested that the molecules get rearranged due to co-operative process[20]. It is observed that relaxation time increases with increase in molar concentration of 1- Butanol in n-Heptane, indicating high stability. Therefore relaxation time increases.

Gibb's free energy measures mobility of the medium. Higher the mobility of the medium, higher will be the entropy lower will be the free energy. Gibb's free energy increases with increase in molar concentration of 1- Pentanol in n-Heptane, indicating the mobility of the molecule is low i.e. highly ordered, due to outstanding salvation.

TABLE-1: - Density (ρ), Velocity (U) and Viscosity (η) of the binary mixture of Pentanol + n-Heptane at different temperatures.

Mole Fraction		ρ (Kgm ⁻³)			U (ms ⁻¹)			η *10 ⁻³ (NSm ⁻²)		
X ₁	X ₂	298K	303K	308K	298K	303K	308K	298K	303K	308K
0.0	1.0	657.98	655.43	650.61	1112	1100	1092	0.342	0.315	0.282
0.1	0.9	668.11	664.54	657.68	1116	1110	1100	0.383	0.346	0.299
0.2	0.8	687.34	681.50	677.68	1118	1112	1104	0.430	0.370	0.322
0.3	0.7	695.44	693.87	683.94	1124	1120	1108	0.474	0.433	0.387
0.4	0.6	704.55	698.25	695.06	1136	1128	1124	0.603	0.471	0.453
0.5	0.5	718.72	714.10	707.18	1156	1140	1136	0.658	0.597	0.529
0.6	0.4	732.89	727.25	721.32	1180	1156	1148	0.794	0.704	0.626
0.7	0.3	750.10	745.46	739.51	1204	1180	1168	1.020	0.908	0.807
0.8	0.2	766.30	762.65	759.71	1216	1188	1176	1.330	1.190	1.060
0.9	0.1	773.51	767.87	764.87	1248	1230	1216	1.730	1.550	1.370
1.0	0.0	779.30	774.22	770.23	1268	1252	1240	2.220	1.980	1.750

TABLE-2: - Adiabatic compressibility (β_a), free length (L_f) and free volume (V_f) of the binary mixture of Pentanol + n-Heptane at different temperatures.

Mole Fraction		β_a *10 ⁻¹⁰ (m ² N ⁻¹)			L_f *10 ⁻¹⁰ (m)			V_f *10 ⁻⁷ (m ³ mol ⁻¹)		
X ₁	X ₂	298K	303K	308K	298K	303K	308K	298K	303K	308K
0.0	1.0	12.29	12.60	12.88	0.6941	0.7101	0.7216	6.622	7.383	8.615
0.1	0.9	12.01	12.25	12.56	0.6864	0.7002	0.7125	5.522	6.364	7.823
0.2	0.8	11.68	12.22	12.10	0.6767	0.6992	0.6993	4.567	5.693	6.917
0.3	0.7	11.38	11.48	11.90	0.6679	0.6779	0.6936	3.924	4.474	5.201
0.4	0.6	10.99	11.25	11.38	0.6566	0.6709	0.6782	2.719	3.892	4.099
0.5	0.5	10.41	10.77	10.95	0.6388	0.6565	0.6653	2.396	2.719	3.240
0.6	0.4	9.790	10.28	10.51	0.6198	0.6415	0.6519	1.131	2.124	2.509
0.7	0.3	9.190	9.630	9.910	0.6004	0.6207	0.6328	1.266	1.468	1.725
0.8	0.2	8.820	762.65	759.71	1216	1188	1176	1.330	1.190	1.060
0.9	0.1	8.300	767.87	764.87	1248	1230	1216	1.730	1.550	1.370
1.0	0.0	7.980	774.22	770.23	1268	1252	1240	2.220	1.980	1.750

TABLE-3: - Internal pressure (Π_i), relaxation time (τ) and Gibb's free energy of the binary mixture of Pentanol + n-Heptane at different temperatures.

Mole fraction		$\Pi_i * 10^6$ (Nm ⁻²)			$\tau * 10^{-12}$ (Sec.)			$\Delta G * 10^{-20}$ (KJ/mol)		
X ₁	X ₂	298K	303K	308K	298K	303K	308K	298K	303K	308K
0.0	1.0	199.34	194.96	187.32	0.561	0.530	0.485	0.4152	0.4068	0.3863
0.1	0.9	215.70	208.43	196.43	0.614	0.566	0.502	0.4482	0.4314	0.3992
0.2	0.8	235.92	217.27	210.34	0.670	0.603	0.521	0.4801	0.4552	0.4134
0.3	0.7	251.78	244.69	234.27	0.720	0.664	0.616	0.5067	0.4909	0.4767
0.4	0.6	290.10	260.16	259.14	0.884	0.707	0.689	0.5817	0.5145	0.5192
0.5	0.5	309.42	300.33	286.10	0.914	0.857	0.773	0.5940	0.5863	0.5630
0.6	0.4	345.71	332.91	318.37	1.037	0.966	0.878	0.6402	0.6309	0.6111
0.7	0.3	400.61	386.09	369.93	1.254	1.166	1.066	0.7098	0.7009	0.6848
0.8	0.2	468.82	453.29	437.25	1.569	1.468	1.348	0.7919	0.7867	0.7734
0.9	0.1	539.17	519.74	498.40	1.917	1.782	1.616	0.8654	0.8587	0.8421
1.0	0.0	618.41	594.34	569.03	2.367	2.175	0.882	0.9426	0.9331	0.9175

CONCLUSION

- The decrease in adiabatic compressibility and free length for the binary system, 1- Pentanol in n-Heptane is due to strong association in the constituent molecules.
- The dipole-dipole interaction of pure 1- Pentanol stronger than the induced dipole - induced dipole interaction of pure n- Heptane molecule which is responsible for association in the binary liquid mixture.
- The non-linear variation of ultrasonic velocity and adiabatic compressibility with concentration in the liquid mixture is due formation of hydrogen bond or due to London desperation forces in the constituent molecules.
- In the present study the dipole-dipole interaction of pure 1- Pentanol molecule is stronger than induced dipole -induced dipole interaction of pure- Heptane molecule.

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