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Ultrasonic, Optical and Volumetric Studies of Binary Mixtures of 1-Propanol With Benzonitrile

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Abstract: ***The ultrasonic speed (U), refractive index (n), density (ρ) and viscosity (η) are measured for binary mixtures (Φ = 0.00…1.00) of 1-Propanol (1-PrOH) with Benzonitrile (BN) at temperature 303.15 K. Various acoustical properties such as adiabatic compressibility (β_s), specific acoustic impedance (Z), Rao's molar sound function (R), Molar compressibility (W), intermolecular free length (L_f), relaxation time (τ), classical absorption coefficient (κ_c) and degree of intermolecular attraction (α_i) are calculated. Along with this various optical parameters such as molar volume (V_m), molar refraction (R_m), atomic polarization (P_A),internal pressure (π_i), polarizability (α) and molecular radii (r) of the liquids and their mixtures are calculated. Excess of measured acoustic and optical properties are evaluated and fitted with R-K polynomial. Variations of these parameters are interpreted in terms of intermolecular interactions.***

Keywords: Binary mixtures, Density, Internal pressure, Molecular interaction, Refractive index, Ultrasonic speed, Viscosity

1. Introduction

In the past few years physicochemical properties of pure and binary mixtures are of considerable interest in the fundamental understanding of the nature of interactions between the unlike molecules [1-5]. In recent years, the acoustical properties are also gaining significance in studying the physicochemical behavior and molecular interactions in a variety of liquid mixtures. These data has great significance in applied areas of research [1, 4]. Amongst all the organic liquids, alcohols are undoubtedly the centers of interest. Because of its outstanding role in chemistry and biology, hydrogen bonding in liquid systems has been intensively studied for long and it is still subject to a lively scientific debate. 1-PrOH is associative polar molecule used principally as a solvent inprinting inks, paint, cosmetics, pesticides and insecticides. Benzonitrile (BN) is one the important compound among the nitriles [2]. Derivatives of benzonitrile are widely used inindustry, pharmaceutical and medicinal fields. Because of its wide use and simple structure, a quite good number of studies on benzonitrile (BN) were reported [6, 7]. In view of their industrial importance, the present study reports the experimental values of ultrasonic velocity (U), viscosity (η), refractive index (n) and density (ρ) of pure 1-Propanol (1-PrOH), Benzonitrile (BN) and their binary mixtures over the entire concentration range at 303.15 K. The above experimental data are used to evaluate acoustical parameters such asadiabatic compressibility (β_s), specific acoustic impedance (Z), Rao's molar sound function (R), molar compressibility (W), intermolecular free length (L_f), relaxation time (τ), classical absorption coefficient (κ_c) and degree of intermolecular attraction (α_i) and various optical parameters such as molar volume (V_m), molar refraction (R_m), atomic polarization (P_A),internal pressure (π_i), polarizability (α) and molecular radii (r). All of these excess and deviation quantities have been fitted to Redlich-Kister polynomial equation.

2. Experimental

1-Propanol (1-PrOH) of AR grade and Benzonitrile (BN) of GR grade are procured from Loba Chemie (India). Both the chemicals are used without further purification. Binary mixtures are prepared at different volume percentage and converted into mole fraction [1]. Ultrasonic velocity (U) of the binary mixtures is measured using digital ultrasonic pulse echo velocity meter (Model no. VCT-70A, Vi Microsystems Pvt. Ltd., Chennai India). Refractive index (n) of the binary mixtures are measured at wavelength of 589 nm using an Abbe Refractometer. The temperature of the refractometer is controlled by circulation of water and measured with a thermometer located near the sample holder assembly. Density (ρ) and viscosity (η) of pure liquids and their binary mixtures are measured by using specific gravity bottle and viscometer respectively. All the measurements are carried at 303 K. The experimental values of Ultrasonic velocity (U), density (ρ), refractive index (n) and viscosity (η) of individual compound namely 1-PrOH and BN along with their literature values are presented in Table 1.

Table 1: Comparison of experimental and literature value of pure compounds.

Parameters	1-Propanol		Benzonitrile	
	Experimental	Literature	Experimental	Literature
U (cm/s)	1.1842×10^5	1.1890×10^5 (a)	1.3911×10^5	1.4027×10^5 (d)
ρ(gm/cc)	0.7963	0.7956 a	0.9960	0.9954 (c)
η (P)	1.6914×10^{-3}	1.6100×10^{-3} (b)	1.1354×10^{-3}	1.4800×10^{-3} (c)
n	1.3820	1.3820 (a)	1.5230	1.5189 (c)

***** (a)-Ref 10, (b)- Ref. 11, (c)-Ref 6, (d)- Ref. 7

3. Results and Discussion

From the table 1 it is clear that the experimental values of ultrasonic velocity (U), density (ρ), viscosity (η) and refractive index (n) of individual component namely 1-PrOH and BN found in the present investigation are in good agreement with the literature values. The acoustic parameters determined from the ultrasonic velocity of the binary mixtures viz. adiabatic compressibility (β_s), specific acoustic impedance (Z), Rao's molar sound function (R), Molar compressibility (W), intermolecular free length (L_f), relaxation time (τ), classical absorption coefficient (κ_c) and degree of intermolecular attraction (α_i) are obtained using the formulas reported elsewhere in the literature [4]. Correspondingly the optical parameters determined using the refractive index (n) namely molar volume (V_m), molar refraction (R_m), atomic polarization (P_A), internal pressure (π_i), polarizability (α) and molecular radii (r) are obtained using the equations reported elsewhere in the literature [2]. The acoustic and optical parameters of pure components and their binary mixtures are presented in Table 2 and Table 3 respectively.

Table 2: Variation of ultrasonic velocity (U), density (ρ), viscosity (η) and refractive index (n) with change in concentration (X) of 1-PrOH in BN.

X	U ($x10^5$) cm s^{-1}	ρ gm/cm^3	η ($x10^{-3}$) P	n
0.0000	1.3911	0.9960	1.1354	1.5230
0.1323	1.3763	0.9757	1.0750	1.5130
0.2554	1.3578	0.9568	1.0539	1.5019
0.3703	1.3399	0.9380	1.0607	1.4867
0.4777	1.3201	0.9182	1.0868	1.4751
0.5784	1.3063	0.8994	1.1286	1.4581
0.6730	1.2813	0.8788	1.1868	1.4441
0.7620	1.2611	0.8569	1.2650	1.4291
0.8459	1.2353	0.8390	1.3703	1.4155
0.9251	1.2071	0.8175	1.5096	1.3980
1.0000	1.1842	0.7963	1.6914	1.3820

A close perusal of table 2, indicate that ultrasonic velocity (U), refractive index (n) and density (ρ) of each binary mixtures decreases as the concentration of 1-PrOH increases, while an exactly opposite trend is observed for viscosity (η).

Table 3: Acoustic parameters viz. adiabatic compressibility (β_s) cm^2/dyn, specific acoustic impedance (Z) gm/cm^2s, Rao's molar sound function (R), molar compressibility (W), intermolecular free length (L_f) Å, relaxation time (τ) s and degree of intermolecular interaction (α_i).

X	β ($x10^{-11}$)	Z ($x10^5$)	W ($x10^3$)	L_f	τ ($x10^{-13}$)	α_i
0.0000	5.1884	1.3856	3.0503	0.4381	7.7442	0.0000
0.1323	5.4111	1.3428	2.9245	0.4474	7.6467	0.0921
0.2554	5.6690	1.2991	2.8015	0.4579	7.8542	0.1486
0.3703	5.9386	1.2567	2.6865	0.4687	8.2805	0.1817
0.4777	6.2497	1.2121	2.5800	0.4808	8.9291	0.1921
0.5784	6.5157	1.1749	2.4809	0.4909	9.6672	0.1982
0.6730	6.9312	1.1260	2.3859	0.5063	10.8140	0.1718
0.7620	7.3383	1.0806	2.3017	0.5210	12.2035	0.1447
0.8459	7.8099	1.0365	2.2103	0.5375	14.0689	0.1006
0.9251	8.3951	0.9868	2.1306	0.5572	16.6605	0.0473
1.0000	8.9543	0.9430	2.0569	0.5755	19.9101	0.0000

Table 4: Refractometric parameters viz. molar volume (V_m) cm^3/mol, molar refraction (R_m) cm^3/mol, atomic polarization (P_A), polarizability (α) and molecular radii (r) Å.

X	V_m	R_m	P_A	π_i	α ($x10^{-23}$)	r ($x10^{-8}$)
0.0000	103.5295	31.6262	2.4355	95.2659	1.2544	2.3235
0.1323	99.8570	30.0134	2.4036	97.2408	1.1904	2.2833
0.2554	96.2966	28.4136	2.3685	99.1001	1.1270	2.2420
0.3703	92.9592	26.7219	2.3208	100.2357	1.0599	2.1966
0.4777	89.9252	25.3225	2.2847	101.7385	1.0044	2.1576
0.5784	86.9877	23.7401	2.2324	102.3764	0.9416	2.1117
0.6730	84.3997	22.4235	2.1897	103.1848	0.8894	2.0719
0.7620	82.0879	21.1666	2.1444	103.5664	0.8395	2.0324
0.8459	79.5316	19.9371	2.1038	104.5715	0.7908	1.9923
0.9251	77.4609	18.6954	2.0521	104.3502	0.7415	1.9500
1.0000	75.4725	17.5641	2.0054	104.3199	0.6967	1.9099

From table 3, it is seen that the adiabatic compressibility (β_s), intermolecular free length (L_f) and relaxation time (τ) increases as the concentration of 1-PrOH increases in the binary mixtures whereas other acoustic parameter namely specific acoustic impedance (Z) and molar compressibility (W) show opposite trend. Molar refraction is a measure of volume occupied with an atom or molecule and depends on the refractive index. It is noticed that the molar refraction (R_m) of the studied binary mixtures decreases as the molar volume and refractive index. These reflect in decrease in atomic polarization (P_A), polarizability (α) and molecular radii (r) of binary mixtures as the concentration of 1-PrOH increases in the mixtures whereas the internal pressure increases with increase in concentration of 1-PrOH. The internal pressure is defined as the energy required to vaporize a unitvolume of a substance. Many researchers have suggested that molecules with similarinternal pressures would interact with each other [12,13]. The deviation of the experimental values from the ideal values for ultrasonic velocity (U) density (ρ), viscosity (η), refractive index (n), adiabatic compressibility (β_s), and intermolecular free length (L_f) of the binary mixtures are evaluated and fitted to Redlich–Kister polynomial [2]. The values of coefficients (a_0, a_1, a_2, a_3) and correlation coefficient (δ) are listed in Table 5.

Table 5: Values of coefficients of Redlich-Kister coefficients (a_0, a_1, a_2, a_3) and correlation coefficient (σ).

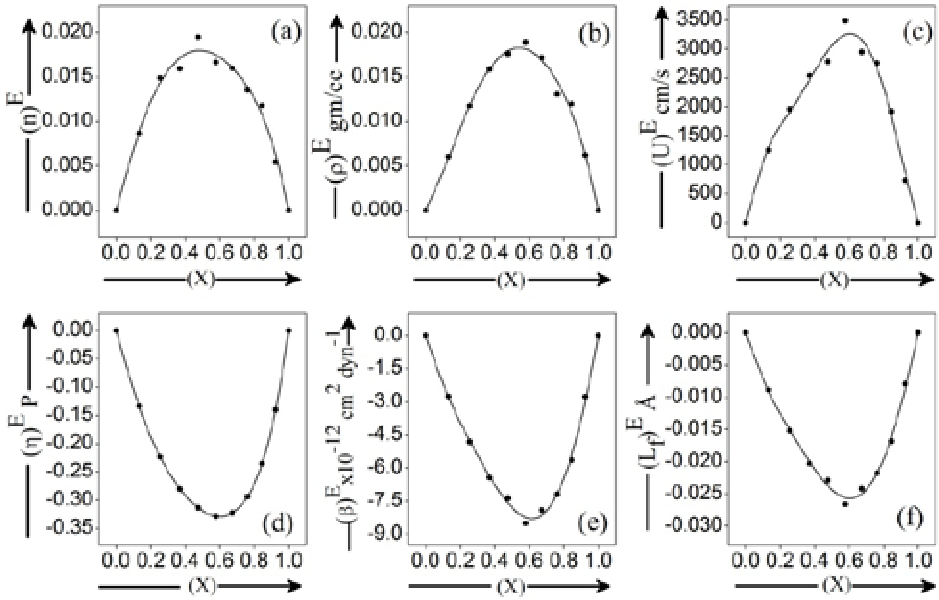

Figure 1: Variation of excess parameters against mole farctopn of 1-PrOH in binary mixtures ((●) solid geometrical shape and smooth line shows experimental points and Redlich- Kister fitting respectively).

Figure 1(a-f) show the deviation of excess parameters ($(n)^E$, $(\rho)^E$, $(\eta)^E$, $(U)^E$, $(\beta_s)^E$ and $(L_f)^E$) from their linear behavior against mole fraction of 1-PrOH in binary mixtures. The sign (positive/negative) and magnitude depend on the strength of hetero interaction between the molecular species in the mixtures. A close perusal of fig. 1 (a-c) [$(n)^E$, $(\rho)^E$, $(U)^E$] show positive deviation against mole fraction of 1-PrOH. The positive deviation suggests significant specific interaction between molecular species. The negative deviation (fig. 1 (d-f)) ($(\eta)^E$, $(\beta_s)^E$ and $(L_f)^E$) suggests chemical/specific interaction which include charge transfer, hydrogen bond formation and other complex forming interactions in the binary mixtures [6, 8-11].

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