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Ultrasonic Velocity Studies Of Molecular Interaction In Binary Liquid Mixtures Of Propan-1-Ol And Propan-2-Ol With P-Anisaldehyde At 298.15 K

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Abstract:

The present paper reports the density, viscosity and ultrasonic velocity over the entire range of composition of propan-1-ol + P-anisaldehyde and Propan-2-ol + P-anisaldehyde at 298.15 K, experiment data were used to calculate acoustical parameters such as acoustic impedance(z), relative association (R_A), internal pressure(π_{int}), intermolecular free length(L_f), Adiabatic compressibility (K_s) and apparent molar volume ($V_{(\phi_1)}$). The results were discussed in term of molecular interaction between the components of system binary liquid mixtures.

Keywords: Density, Ultrasonic velocity, Molecular interaction, viscosity.

Introduction:

The density, viscosity and ultrasonic velocity measurement find wide applications in characterizing the physico-chemical behavior of the binary liquid mixture[1,3]. These studies have been adequately employed in understanding the nature of molecular interaction in pure liquids and binary liquid mixtures[4]. P-anisaldehyde is chemically known as 4-methoxybenzaldehyde and used in perfumes and pharmaceutical industries. These studies find extensive application in chemical engineering design, process simulation, solution theory and molecular dynamics[5,6].

The study of molecular association in binary liquid mixture having alkan-1-ol and alkan-2-ol with p-anisaldehyde. p-anisaldehyde is a protic solvent, strongly associated due to highly polar C = O group in the molecule and large dipole moment.The variation in ultrasonic velocity gives information about the intermolecular attraction between p-anisaldehyde and alcohol molecules and formation of complexes at various mole fractions[7].

An attempt has been made in this paper to elucidate the molecular interaction in binary liquid mixture of Propan- 1-ol and Propan- 2-ol with p-anisaldehyde respectively at 298.15 k with related to adiabaticcompressibility (Ks), acoustic impendance(z), intermolecular free length (L_f), acoustic impendance(z), relative association(R_A) internal pressure (π_{int}) from Ultrasonic velocity measurement.

Material and Methods:

The Chemicals p-anisaldehyde, Propan-1-ol and Propan – 2-ol were commercially available in analytical grade (AR) and spectroscopic regent (SR) grades of minimum assay of 99.9% obtained from Himedia and Sd fine Chemicals, India, which were used as such without any further purification. The binary liquid mixtures of various compositions covering entire mole fraction were prepared in stopper measuring flask. The weight of sample was measured using electronic balance with accuracy of ±0.1mg.

The ultrasonic velocity data were obtained from Ultrasonic interferometer (M-81, Mittal Enterprises, New Delhi) at 2 MHz measuring frequency with accuracy of ±0.1m/s,An electronic digital double walled measuring cell made up of steel containing the experimental solution at the desired temperature with accuracy of ±0.01k. The densities of pure liquid and binary liquid mixtures were determinedpyknometrically, at required temperature ±0.01^{0}c. The viscosities of components were measured by using an Ubbelohde viscometer and efflux time measured using digital clock to within ±0.01s. The experiments were repeated for consistency and the average value was considered.

Results and Discussion:

The acoustic and thermodynamic parameters. Such as adiabatic Compressibility (K_s), intermolecular free length (L_f), acoustic impedance (z), relative association (R_A), internal pressure (π_{int}) and apparent molar volume ($V_{(}\phi_{1)}$) for system 1:p-anisaldehyde + Propan-1-ol and system 2: p-anisaldehyde + Propan–2-ol were investigated using the following relations[8]:

$U = \lambda f$ (1)

$K_s = \frac{1}{\rho U^2}$

$L_f = K\sqrt{(K_s)}$ (3)

Where : K is a Jacoben's Constant it is temperature dependent constant (at 298.15 K, K = 1.976 X 10 $^{-6}$)

$z = \rho U$ (4)

$R_A = (Lf/L'f)^3$ (5)

L*f* – is the free length of the ideal mixture.

$\pi_{int\ 12} = bRT\ [K\eta_{12}/\ U_{12}]\ /\ M_{12}^{7/6}$ (6)

Where 'b' is Constant

K – is an absolute temperature in Kelvin

η_{12} – Viscosity of binary Liquid mixture in Nsm^{-2}

U_{12} – is the Ultrasonic velocity in m/s

M_{12} – is the mean molecular weight of mixture

$M_{12} = x_1 M_1 + x_2 M_2$ (7)

x_1 and x_2 – mole fraction of solute(1) and Solvent

$M_1$and M_2 – molecular weight of Solute (1) and Solvent (2)

$$V_{(\phi 1)} = \frac{X2\ M2\ (\rho 2-\rho 12)}{X1\ \rho 2\ \rho 12} + \frac{M1}{\rho 12} \qquad (8)$$

Where, ρ_2 and ρ_{12} are the densities of p-anisaldehyde and binary liquid mixtures.

The measured parameters viz density (ρ), viscosity(η) and ultrasonic velocity (U) and calculated parameters such as K_s, L_f, z, R_A, π_{int} and $V_{(\phi 1)}$, for the system 1 and system 2 are given in table 1, 2, 3 and 4 respectively.

Density increases with increase in concentration due to increased intermolecular attraction in that solution. This is due to decreases the volume and hence increases density. Table – 1 and Table – 3 indicates that, the increase in density with the increase in concentration of p-anisaldehyde in both systems[9].

Viscosity and Ultrasonic velocity increases with concentration of p-anisaldehyde in both systems this indicates that strong interaction observed at lower concentration of alcohols[10] .

When an solute is added to solvent it attracts certain solvent molecules towards itself by attracting the molecules from bulk of the solvent due to the intermolecular attraction. This is due to the available solvent molecule for the next solute molecule gets decreased. This process is called the compression. Each solvent having a limit of compression called the limiting compressibility value from the Table 2 and Table 4, adiabatic compressibility decreases with increase in

Concentration of solute at a given composition. Therefore increase in structural disorder of p-anisaldehyde may be result in less cohesion and leads to increase in Ks. The increase in Ks results in an decrease in the value of U[11].

The concentration of solute increases leads to decrease in gap between two species which is referred by intermolecular free length (L_f).Thus with the increase in concentration of P-anisaldehyde, intermolecular free length decrease. This indicates that solute and solvent molecules have intermolecular attraction inboth systems[12].

Acoustic impedance (z) is found to be almost reciprocal of adiabatic compressibility (K_s). Table 2 and 4 indicates that acoustic impedance increases with increase the concentration of p-anisaldehyde.Therefore increase the intermolecular forces in between p-anisaldehyde and alcohol molecules. The value of 'z' are higher in system 1: [p-anisaldehyde + Propan-1-ol] then in system 2: [p-anisalehyde + Propan-2-ol]. Thus in system 1, there is high intermolecular attraction[13].

The relative association (R_A) decreases with increase in concentration due to decrease in L_f and increase in electrostatic attraction in both systems.[14] The values of R_A in system 1 are higher than system 2. The internal pressure (π_{int}) decreases with increase the concentration of p-anisaldehyde in propan-1-ol and propan-2-ol in both the systems due to increase in free volume and close association between solute and solvent. Thus a progressive decrease in internal pressure in p-anisaldehyde + propan-2-ol than p-anisaldehyde + propan-1-ol system. It indicates that the existence of solute – solvent interaction is more in system-1, due to structural arrangement is considerably affected; the apparent molar volume is practically available volume of the solute. In both systems, apparent molar volume increases with increase the concentration of solute (p-anisaldehyde) a minimum in apparent molar volume has been observed in system–1 i.e. p-anisaldehyde + propan-1-ol.[15.]

Conclusions:

The density, viscosity and ultrasonic velocity and other related parameter were calculated. These experimental and derived data have been indicated that, the existence of molecular interaction in solute – solvent is favored in system -1 and then system – 2. It is conformed from U, K_s, L_f , z, R_A, π_{int} and $V_{(\phi 1)}$

Table: 1 Densities, Viscosities and Ultrasonic Velocities for the P-anisaldehyde(1) + Propan – 1-ol(2) System at 298.15 K

Mole Fraction x_1	**Density** ρx10 $^{-3}$(kgm^{-3})	**Viscosity** η (mPas)	**Ultrasonic velocity** U(ms^{-1})
0.0000	0.7996	1.9449	1206.3
0.0359	0.8199	1.9876	1220.4
0.0839	0.8451	2.0393	1236.0
0.1200	0.8629	2.8050	1245.8
0.1741	0.8887	2.1554	1264.2
0.2415	0.9176	2.2461	1287.2
0.3181	0.9478	2.3652	1314.2
0.4149	0.9813	2.5606	1340.4
0.5673	1.0267	2.9162	1384.2
0.7374	1.0687	3.3978	1440.0
1.0000	1.1159	4.2025	1526.2

Table: 2 Calculate Parameter for the P-anisaldehyde(1) + Propan – 1-ol at 298.15 k

Mole Fraction x_1	Adiabatic compressibility K_s X 10^{11}(M^{2}N^{-1})	Acoustic impedance z X10^{-3} (kgs^{-1}m^{-3})	Intermolecular Free Legnth L_f X 10^{11}(m)	Relative association R_A	Internal Pressure π_{int}(atm)	Apparent molar volume $V_{(\phi_1)}$X 10^6 (m^{3}mol^{-1})
0.0000	859.44	964.6	0.5793	1.0000	93092.1	
0.0359	818.91	1000.6	0.5655	0.9396	90324.6	116.34
0.0839	774.56	1044.5	0.5499	0.8776	86851.5	116.12
0.1200	746.69	1075.0	0.5400	0.8415	84607.4	117.35
0.1741	704.07	1123.5	0.5243	0.7887	81417.0	117.45
0.2415	657.74	1181.1	0.5068	0.7360	77766.0	118.02
0.3181	610.89	1245.6	0.4884	0.6895	74232.5	118.45
0.4149	567.79	1315.3	0.4706	0.6615	70987.2	119.12
0.5673	508.35	1421.12	0.4455	0.6500	66865.3	119.93
0.7374	451.25	1538.9	0.4198	0.6878	63329.9	120.66
1.0000	384.42	1703.8	0.3874	1.0000	58509.0	122.01

Table: 3 Densities, Viscosities and apparent molar volume for P-anisaldehyde(1)+Propan – 2-ol(2) system at 298.15 k

Mole Fraction x_1	**Density** ρx10 $^{-3}$(kgm^{-3})	**Viscosity** η (mPas)	**Ultrasonic velocity** U(ms^{-1})
0.0000	0.7813	2.0629	1153.2
0.0559	0.8144	2.1363	1172.6
0.1546	0.8601	2.2850	1204.6
0.2203	0.8898	2.3877	1228.6
0.3048	0.9252	2.5083	1260.4
0.3955	0.9601	2.6479	1296.2
0.4962	0.9951	2.8329	1332.4
0.5706	1.0181	2.9871	1364.2
0.7086	1.0551	3.3003	1412.0
0.8466	1.0855	3.7080	1464.4
1.0000	1.1159	4.2025	1526.8

Table: 4 Calculated parameter for the P-anisaldehyde(1) +Propan – 2-ol system at 298.15 k.

Mole Fraction x_1	Adiabatic compressibility K_s X $10^{11}(M^2N^{-1})$	Acoustic impedance z X10^{-3} ($kgs^{-1}m^{-3}$)	Intermolecular Free Legnth L_f X 10^{11}(m)	Relative association R_A	Internal Pressure π_{int}(atm)	Apparent molar volume $V_{(\phi_1)}$X 10^6 (m^3mol^{-1})
0.0000	962.44	901.0	0.6130	1.0000	96541.1	
0.0557	896.92	951.4	0.5916	0.9152	92296.2	119.42
0.1546	801.25	1036.1	0.5593	0.8068	86051.7	119.76
0.2203	744.54	1093.2	0.5392	0.7490	82374.7	119.81
0.3048	680.37	1166.1	0.5154	0.6921	77903.2	119.86
0.3955	619.93	1244.5	0.4920	0.6483	73729.2	119.91
0.4962	566.06	1325.9	0.4701	0.6259	70047.6	120.04
0.5706	527.78	1388.9	0.4540	0.6159	67594.6	120.26
0.7086	475.38	1489.8	0.4308	0.6473	63897.7	120.83
0.8466	429.59	1589.6	0.4096	0.7377	61159.9	121.52
1.0000	384.42	1703.8	0.3874	1.0000	58509.0	122.01

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