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THEORETICAL EVALUATION OF SOUND VELOCITY IN BINARY LIQUID SYSTEM

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ABSTRACT

Ultrasonic velocity, density and viscosity have been measured using the standard techinques in the binary mixtures ofp-cresol with Carbon tetrachloride. The study of ultrasonic waves through the solution is used for knowing the nature and strength of the intermolecular forces and their interactions in pure liquids and their mixtures. Further theoretically ultrasonic speeds calculated using Nomoto's relation, Ideal mixture relation,Impedance relation, Rao's specific velocity relation,Junjie'srelation and Danusso model. The validity of the theories waschecked by applying the average percentage error (APE).

Keywords: Binary liquid mixtures, Ultrasonic velocity, Theoretical models, APE.

INTRODUCTION

The ultrasonic velocity in liquid is highly sensitive parameter to diagnose the structure and interactions exists in pure liquids and their mixtures and it is essentially related to binding forces between constitutes of liquids. Mixing volume effects are also important from theoretical as well as useful point of view. These properties found many applications in cleaning products, antioxidant agents, paints, varnishes, inks, adhesives, textiles industries and various industries. Where volume effects are also involve in conversion of formulation from gravimetric to volumetric analysis. Properties like molar volume and their deviations from ideality composition of binary mixtures are useful to design engineering processes in chemical and biological industries. Also, volumetric and ultrasonic properties have practical importance in understanding interactions and physicochemical behavior. The impetus of the present investigation is to compare the experimentally determined ultrasonic velocity in binary liquid mixture with the computed ultrasonic velocity using different theoretical relations like Nomoto, Van Dael and Vangael, Impedance relation, Rao's specific velocity, Junjie's relation and Danusso relation.

MATERIAL AND METHODS

P-cresol used in present work is procured from Merck, Mumbai with assay greater than 99% and Carbon tetrachloride from Sdfine Chemical limited, Mumbai with assay of 99.8%. All compounds were of AR/GR grade, used without further purification.The densities of pure and binary mixture were measured using the pre-calibrated standard 10ml specific gravity bottle with Teflon stopper and digital weighing balance with accuracy of 0.1mg. The ultrasonic velocities in pure and binary mixtures were measured using the single-crystal variable-path ultrasonic interferometer operating at 2MHz. The viscosities were measured by using the Ostwald viscometer and digital stop watch with accuracy of 0.01sec.

THEORY AND CALCULATIONS

The adiabatic compressibility is computed using the following relation,

$$\beta_S = 1/U^2\rho$$

The linear free length given by the relation

$$L_f = K/\sqrt{\rho}\,U$$

Where K is the temperature independent Jacobson's constant

$$K = (93.875 + 0.375T) \times 10^{-8}$$

The acoustic impedance (Z) computed by the relation

$$Z = \rho U$$

The molar volume (V_m) computed by the relation

$$V_m = M_{eff}/\rho$$

$$M_{eff} = \sum_i x_i M_i$$

The available volume (V_a) computed by the relation

$$V_a = V_m\left(1 - \frac{U_{exp}}{U_\infty}\right)$$

Where U_∞=1600 m/s

The comparison of theoretical values of ultrasonic velocity in binary mixture those obtained from the experimentally in the binary mixture is expected to interpretation the nature of interaction between components molecules. Such theoretical study is useful in the wide-ranging theoretical model for the liquid mixtures.

Van Dael & Vangel Ideal Mix relation: The ideal mixing theory innovative by Van Deal and Vangael suggested the sound velocity in binary mixture with following relation

$$U_{VV} = \sum_i x_i/m_i u_i^2 \times \sum_i 1/x_i m_i$$

Where x_i is mole fraction, m_i is molecular weight, and u_i is ultrasonic velocity of i^{th} components respectively.

Impedance Relation: The impedance relation based on the interaction molecules based on the forces of resistance for sound velocity is given by

$$U_{IMP} = \sum_i x_i z_i \Big/ \sum_i x_i \rho_i$$

Where x_i is mole fraction, $z_i$is the acoustic impedance and $\rho_i$is the density of the i^{th} components respectively

Nomoto's Relation: The additivity of molar sound velocity R and no volume change on mixing, Nomotoestablished [6] the following relation for the sound velocity of binary liquid mixture is

$$U_{NOM} = \left(\frac{\sum_i R_i}{\sum_i V_i}\right)^3$$

$$R_i = m_i/\rho_i \times u_i^{1/3}$$

$$V_i = m_i/\rho_i$$

Where m_i is molecular weight, $\rho_i$is the density and u_i is ultrasonic velocity of i^{th} components respectively.

Jungie's Relation: Jungie has suggested an equation for the determine the velocity of sound in liquid mixtures given as follows

$$U_{JR} = \left[\frac{\sum_i x_i V_i}{\sum_i x_i m_i^{1/2}}\right] \times \left[\frac{\sum_i x_i V_i}{\sum_i \rho_i U_i^2}\right]^{-1/2}$$

Where x_i is mole fraction, V_i is molar volume, m_i is molecular weight, $\rho_i$is the density and u_i is ultrasonic velocityof i^{th} components respectively.

Rao's specific velocity: The Rao's specific sound velocity in liquid mixture is given by

$$U_R = \sum_i (x_i r_i \rho_i)^3$$

Where x_i is mole fraction, $\rho_i$is the density of ith component and r_i is the Rao's specific sound velocity $r_i = U_i^{1/3}/Z_i$ and Z_i is acoustic impedance.

Danusso Model: Danusso model of velocity of sound velocity in liquid mixture is given by

$$U_D = (1/\rho_{mix})\left(1/M_{eff} \times \sum_i x_i m_i/\rho_i^2 U_i^2\right)$$

$$M_{eff} = x_i M_i$$

Where $M_{eff}$is the effective molecular weight of the solute and solvent, x_i is mole fraction, m_i is molecular weight of ith component.

Percentage Error: The percentage deviation in ultrasonic velocity between experimental and computed values can be calculated as

Percentage deviation $\Delta U/U\% = \left[\left(U_{exp} - U_{comp}\right)/U_{exp}\right] \times 100\%$

Molecular Association: The degree of intermolecular interaction or molecular association is given by

$$\alpha = \left(U_{exp} - U_{comp}\right) - 1$$

The measured physical parameters such as ultrasonic velocity, density, viscosities data are recorded sequential in Microsoft Excel 2010 and the various acoustical parameters are computed using the user friendly developed package in VB.NET language running under 64-bit Windows 8 platform.

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RESULT AND DISCUSSIONS

The experimental values of ultrasonic velocity U, density ρ and viscosity η of binary mixtures of p-cresol with Carbon tetrachloride and over the entire composition range (0.0 to 1.0) expressed in terms of mole fraction $x_1$are listed in Table 1.

Table.1.Experimental values of ultrasonic Velocity$U$, density ρ and viscosity η

Mole fraction P-Cresolx_1	Velocity$U$ m/s	Densityρ Kg/m^3	Viscosityη x10^{-3}Ns/m^2
0.0000	980.80	1626	0.9432
0.4398	963.20	1552	1.0939
0.6385	907.20	1521	1.2710
0.7517	1032.00	1462	1.5506
0.8249	1171.20	1399	2.0402
0.8760	1064.00	1344	2.6023
0.9138	1204.80	1287	3.7623
0.9428	1075.20	1252	4.1267
0.9658	1329.60	1177	6.6201
0.9845	1486.40	1120	9.2708
1.0000	1572.80	1069	11.2580

The computed acoustical, thermodynamical parameters listed in Table 2 and Table 3.The change in ultrasonic velocity shows the association between solute and solvent molecules. The decrease in density with increase in mole fraction of component x_1 indicates formation of intermolecular forces between the binary mixtures. Similarly, the variation of compressibility β forp-cresol with CCl_4indicates the molecular association and hydrogen bond formation between unlike molecules.

Table.2.Computed Acoustical Thermodynamical parameters

Mole fraction P-Cresolx_1	Compressibility β x10^{-10} kg^{-1}ms^{-2}	Linear free length L_f x10^{-10} m	Acoustic impedance Z x10^5 kg/m^{2}s
0.0000	6.39320	5.2371	15.9478
0.4398	6.94505	5.4585	14.9488
0.6385	7.98849	5.8542	13.7985
0.7517	6.42234	5.2490	15.0878
0.8249	5.21099	4.7282	16.3850
0.8760	6.57230	5.3100	14.3001
0.9138	5.35293	4.7921	15.5057
0.9428	6.90903	5.4443	13.4615
0.9658	4.80598	4.5407	15.6493
0.9845	4.04120	4.1638	16.6476
1.0000	3.78160	4.0278	16.8132

The variation of intermolecular free length$L_f$decreasing trend with increasing in mole fraction of component x_1 suggests that the specific interactionbetween the components of two system binary mixture molecules. According to Eyring and Kincaid, the ultrasonic velocity increases, if the $L_f$decreases and vice-versa in a result of mixing components. The decrease or increase in values of $L_f$can be explained on the basis of interactions between the solute and solvent molecules. The nonlinear variation of acoustic impedance Z reveals that presence of specific interaction and cluster formation between the mixing components. The molar volume V_m changes in increasing trend and available volume V_a changes non-linearly with concentration of solutions.

From the various computed acoustical, thermodynamical parameters for the binary mixtures imply that the specific chemical interactions directed towards the weak molecular interaction prevailing in the present systems of the binary mixtures. Such interactions are due to weak dipole-dipole and dipole-induced dipole forces. Dispersive forces are also found to exist between the components of the mixtures.

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Table.3.Computed Acoustical Thermodynamical parameters

Mole fraction P-Cresol x_1	molar volume V_m x10^{-2} m^3	available volume V_f x10^{-2} m^3
0.0000	9.4600	3.6610
0.4398	16.8788	6.7177
0.6385	17.2228	7.4575
0.7517	17.9179	6.3608
0.8249	18.7248	5.0182
0.8760	19.4910	6.5295
0.9138	20.3543	5.0275
0.9428	20.9233	6.8628
0.9658	22.2565	3.7613
0.9845	23.3892	1.6606
1.0000	10.1159	0.1719

The computed theoretical ultrasonic theoretical velocities are listed in Table 4

Table.4.Experimental velocities and computed theoretical velocities for P-Cresol with Carbon tetra chloridebinary system in m/s

Mole fraction P-Cresol x_1	U_{EXP}	U_{NOM}	U_{JR}	U_{VV}	U_R	U_{IMP}	U_D
0.4398	0.4398	1228.040	1183.888	1173.542	1218.404	1182.369	1464.554
0.6385	0.6385	1346.736	1300.564	1288.825	1337.261	1298.926	1564.072
0.7517	0.7517	1416.180	1376.333	1365.648	1408.313	1374.892	1673.309
0.8249	0.8249	1461.710	1429.504	1420.540	1455.519	1428.325	1782.059
0.8760	0.8760	1493.849	1468.876	1461.731	1489.140	1467.953	1880.509
0.9138	0.9138	1517.746	1499.208	1493.790	1514.302	1498.518	1984.201
0.9428	0.9428	1536.207	1523.290	1519.451	1533.834	1522.806	2056.248
0.9658	0.9658	1550.897	1542.875	1540.459	1549.437	1542.574	2201.563
0.9845	0.9845	1562.863	1559.115	1557.973	1562.186	1558.973	2326.020

Table.5.Percentage deviation for P-Cresol with Carbon tetra chloride binary system

Mole fraction P-Cresol x_1	$\%U_{NOM}$	$\%U_{JR}$	$\%U_{VV}$	$\%U_R$	$\%U_{IMP}$	$\%U_D$	α
0.4398	-27.4958	-22.9119	-21.8378	-26.4954	-22.7542	-52.0508	-0.3263
0.6385	-48.4496	-43.3601	-42.0661	-47.4053	-43.1797	-72.4065	-0.5045
0.7517	-37.2267	-33.3655	-32.3302	-36.4644	-33.2259	-62.1423	-0.4289
0.8249	-24.8044	-22.0546	-21.2893	-24.2758	-21.9539	-52.1567	-0.3202
0.8760	-40.3993	-38.0522	-37.3807	-39.9568	-37.9654	-76.7395	-0.4701
0.9138	-25.9749	-24.4362	-23.9865	-25.6890	-24.3789	-64.6913	-0.3494
0.9428	-42.8763	-41.6750	-41.3180	-42.6557	-41.6300	-91.2432	-0.4992
0.9658	-16.6438	-16.0405	-15.8588	-16.5340	-16.0178	-65.5808	-0.2550
0.9845	-5.1441	-4.8920	-4.8151	-5.0986	-4.8824	-56.4868	-0.0897

For the binary system p-cresol with carbon tetra chloride, the corresponding percentage of deviation and interaction parameters (α) are listed in Table 5. The observed deviations of the theoretical ultrasonic velocity from the experimental values are attributed to the presence of intermolecular interactions between the component molecules of the mixture. The observed deviationsfollowing all theories illustratemolecular interaction between unlike molecules in the liquid mixtures. The suitability ofthese theories based on percentage deviation.

CONCLUSION

In the present work, the investigational densities, viscosities and ultrasonic velocities of binary mixtures forthe p-cresol with carbon tetra chloride determined as function of composition at temperature 302.15K. Using these data, various acoustical and thermodynamicalparameters were computed with the standard relations obtained from the literature survey. All these parameters indicate the presence of specific interactions between the subjected system componentof molecules. Again, the computed ultrasonic velocities from different theories have been correlated with the experimentally measured values.

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