International Journal of Science and Research (IJSR)
ISSN (Online): 2319-7064, Impact Factor (2013): 4.438
www.ijsr.net

Acoustic and Thermodynamical Studies of Ternary Mixture of 2-Aminothiazole with Acetonitrile in Water at Varying Temperatures

P. B. Morey[1], A. B. Naik[2]

[1]Department of Chemistry, Vidya Bharti College, Karanja (Lad), Dist. Washim (M.S.) India

[2]Department of Chemical Technology, SGBAU Amravati, (M.S.) India

Abstract: ***Thiazole moiety is present in large number of biologically active compounds which find wide applications in pharmaceuticals and agrochemical industries. 2-Aminothiazole has great synthetic and structural versatility due to the potential of number of substitution position. In addition to substituent's hetero atom S and N offer several possible modes of interaction. Thus ultrasonic study of substituted thiazole was undertaken. The densities (ρ) and ultrasonic velocities (u) in a ternary liquid mixture of 2-aminothiazole with acetonitrile (AN) in water have been measured at (303.15, 305.15 and 313.15) K respectively, over the entire composition range by using an ultrasonic interferometer at 2MHz frequency. From the experimental data various acoustic and thermo dynamical parameters such as; adiabatic compressibility (β_s), Intermolecular free length (L_f), Specific acoustic Impedance (Z), relative association (R_A) and molar sound velocity have been computed using the standard relations. The results have been analyzed on the basis of variation in thermodynamic parameters. These parameters are found to be very sensitive in exploring the interaction between the component molecules, which enable to have better understanding of the liquid mixtures. The variation in densities and ultrasonic velocities with concentrations in the system show similar trends for evaluated parameters of the constituents in ternary mixture at different temperatures. The results have been interpreted in term of solute-solvent and solvent-solvent interaction.***

Keywords: ultrasonic velocity, density, acoustic parameter, aminothiazole.

1. Introduction

In recent year's concentration and temperature dependent measurements of ultrasonic velocities along with related thermo acoustic parameters has been used to study nature of intermolecular interactions in pure liquids and liquid mixtures[1]. Although AN liquid mixture has been extensively studied. However, literature survey shows that no ultrasonic and thermo dynamical studies have been conducted for ternary mixture of 2-aminothiazole with AN. Thus, in present attempt we reported the results of our study on the ternary mixture of 2-aminothiazole with AN in water covering the entire composition range, at (303.15, 308.15 and 313.15) K. The 2-aminothiazole is a heterocyclic organic compound, it is used as an intermediate for dyestuff, in photographic chemicals; its ring structure is also useful in medicinal chemistry[2]. This molecule has found application in drug development for treatment of allergies, hypertension,[3] anti-inflammatory activity,[4] schizophrenia and HIV infections. Its derivatives can also find application for making biologically active agents such as antibacterial and antifungal agents[5, 6]. AN molecule is a aprotic and highly polar, non-hydrogen bonded liquid. Acetonitrile is used to make pharmaceuticals, perfumes rubber products, pesticides, acrylic nail removers and batteries. It is also used to extract fatty acids from animals and vegetable oils. It has strongly ordered structure due to dipole-dipole interactions[7,8]. The various thermo acoustical parameters such as adiabatic compressibility (β_s), intermolecular free length (L_f), specific acoustic impedance (Z), relative association (R_A) and molar sound velocity (R_m) have been estimated by using experimental values of ultrasonic velocity (u) and density (ρ). The results are interpreted in terms of molecular association between the components of the liquid mixtures.

2. Materials and Methods

2.1 Materials

In present study, the used solute is 2-aminothiazole (Hi-media) and solvent AN (Fisher scientific) were analytical (AR) and spectroscopic reagent (SR) grade respectively. They were used without further purification.

2.2 Method

The solvent AN-water was prepared using double distilled water. The mass of 2-aminothiazole was measured on an electronic balance (Model SHIMADZU AUY-220, Japan,) with precision of ± 0.01 mg. The required ternary mixtures were prepared over the entire range of compositions acetonitrile-water solvent.

2.3 Density Measurements

The densities of pure liquids and ternary mixtures were measured with portable digital densitometer (Anton Paar, Austria, DMA-35) at (303.15, 308.15 and 313.15) K. The average uncertainty in measurement in the measured density is ± 0.05 kgm^{-3}. The values are agreed closely with given literature values (Expt. Distilled water = 991.5 $kg.m^{-3}$ AN=765[9] Lit. = 996 $kg.m^{-3}$ 07728$kg.m^{-3}$) respectively.

2. 4 Velocity measurements

The ultrasonic velocity of pure and liquid mixtures was measured using ultrasonic interferometer (Mittal Enterprises, New Delhi F-81s) at 2 MHz with accuracy of ± 2 m/s. The temperature was controlled through the water circulating around the liquid cell using thermostatically controlled High

Precision water bath (Macro scientific work Delhi MSW-274) with an uncertainty of ± 0.3^0C.The data of density (ρ) and ultrasonic velocity (u) has been used to determine other thermodynamic and acoustical properties by using the following expressions;

2.5 Adiabatic compressibility (β_s)

When acoustical waves are passes through a liquid medium, adiabatic compression and refraction take place. This results a change in pressure and corresponding change in volume. Hence, the adiabatic compressibility is the fractional decrease of volume per unit increase of pressure when no heat flows in or out. The adiabatic compressibility (β_s) was calculated from Newton-Laplace equation:

$$\beta = \frac{1}{\rho_s \times u_s^{\,2}} \text{--------(1)}$$

Where, ρ_s = density of solution, u_s = Speed of sound

2.6 Intermolecular free length (L_f)

In the liquid state of matter, molecules are loosely packed; leaving free unoccupied space among them[10].The free length is the distance between the surfaces of the adjacent molecules. The intermolecular free length (L_f) is calculated by using the standard expression;

$$L_f = K\sqrt{\beta} \text{------(2)}$$

Where 'K' is a temperature dependent constant known as Jacobson constant K= 93.875+ 0.375Tx10^{-8}.

2.7 Specific acoustic impedance (Z)

When the sound wave travels through a solution under the influence of sound pressure, certain part of acoustic travels through the medium and rest of gets reflected by the ions[11].The character that decreases this backward movement of sound waves is known as acoustic impedance. The specific acoustic impedance (Z) is obtained by;

$$Z = u_s \times \rho_s \text{-------(3)}$$

2.8 Molar sound velocity (Rao's constant) (R_m)

The molar sound velocity was calculated by the equation;

$$R_m = \frac{M}{\rho_s} \times u_s \text{-------(4)}$$

Where 'M' molar mass

2.9 Relative association (R_A)

It denotes magnitude of association between two interacting species. This association or dissociation is influenced by polarization of the solvent by solute or that of solute by solvent molecules[12]. The relative association (R_A) was calculated by the following equation;

$$R_A = \left(\frac{\rho_s}{\rho}\right)\left(\frac{u}{u_s}\right)^{1/3} \text{------(5)}$$

Where ρ, u and ρ_s, u_s = density and ultrasonic velocity of solvent and solution respectively.

3. Results and Discussion

The experimental determined values of density and ultrasonic velocity for the pure AN liquid and mixtures at (303.15, 308.15 and 313.15) K are presented in Table 1. From the experimental data, various acoustic and thermo dynamical parameters such as; adiabatic compressibility (β_s), Inter-molecular free length (L_f), acoustic impedance (Z), relative association (R_A) and molar sound velocity(R_m)have been computed and are presented in Table 1.

3.1 Ultrasonic velocity (u)

From the Fig. a and b, noted that density and ultrasonic velocity increases with increase in concentration of solute, which suggest powerful dipole-dipole interaction between the component molecules[13]. It is also observed decrease in ultrasonic velocity and density with increase in temperature show molecular forces are weaken, thus interaction become weak at high temperature. The change in ultrasonic velocity can be explained by a model presented by Eyring and Kincaid[14]. According to this model, variation of ultrasonic velocity in solution depends upon the increase or decrease of intermolecular free length after mixing the components. The increase in ultrasonic velocity is structure making type[15].

3.2 Adiabatic Compressibility (β_s)

From Fig. c. the adiabatic compressibility decreases with increase in concentrations of solute, It reveals that the medium can be compressed is higher in lower concentration. This shows more available space due to density of medium. Decreasing trend supports strong solute-solvent interaction, due to which aggregation of solvent molecules around solute molecule may takes place[16]. Due to which structural arrangements are considerably affected. It is also observed that adiabatic compressibility increases with increase in temperature, it clearly reveal that interaction become weaker at higher temperature.

3.3 Acoustic impedance (Z)

From Fig. d, the increase in Z with increase in concentration is due to increase ρ and u with concentration. Decrease in Z value with rise in temperature again attribute to corresponding decrease in ρ and u with temperature[17], such increasing trend of acoustic impedance further support the possibility of molecular interaction due to H-bonding between solute-solvents and solvent-solvent molecules[18] which restrict the free flow of sound waves.

3.4 Intermolecular free length (L_f)

It denotes the magnitude of either solute-solute or solute-solvent interaction or both of system. Free length depends upon adiabatic compressibility. Table no.1 and Fig. e, shows decreasing trends with increasing the concentration of 2-aminothiazole in AN-water solvent due to compression of liquid[19]. The magnitude of L_f increases with increase in temperature[20] with increase in concentration; number of solute in a given volume increases, thus free length decreases, this is agreements with model of Eyring and Kincaid. This indicates significant molecular interaction

between solute and solvent molecules suggesting a structure promoting behavior of added solute.

3.5 Molar sound velocity (R_m)

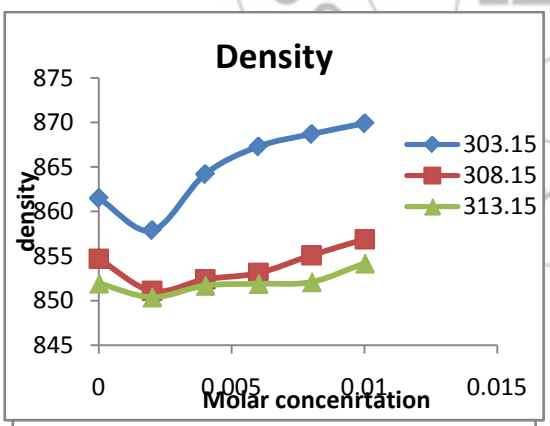
Molar sound velocity or Rao's constant decreases with increase in concentration which indicate interaction between solute-solvent molecule increases. From Fig. f, this increasing trends of Rao's constant reveals that availability of more number of components in a given regions of space. This leads to tight packing of the medium and there by increases the interactions[21].

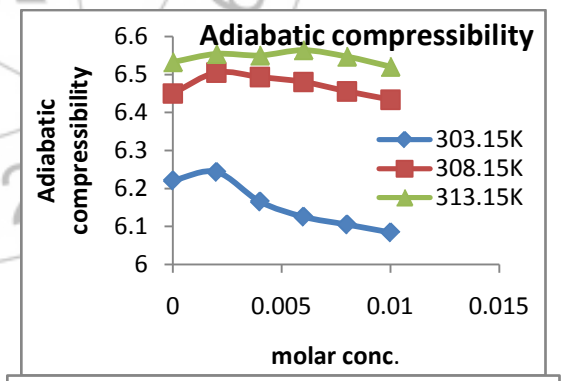
3.6 Relative association (R_A)

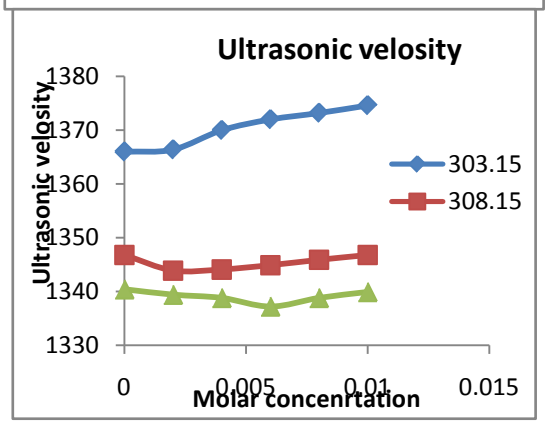
It is the measure of extent of association of components in the medium. The relative association is depends on either breaking up of the solvent molecules on addition of solute to it or the salvation of present ions. From Fig. g, the relative association decreases with increase in concentration. The decreasing trend indicates the breaking up of the solvent molecules on addition of solute[22].

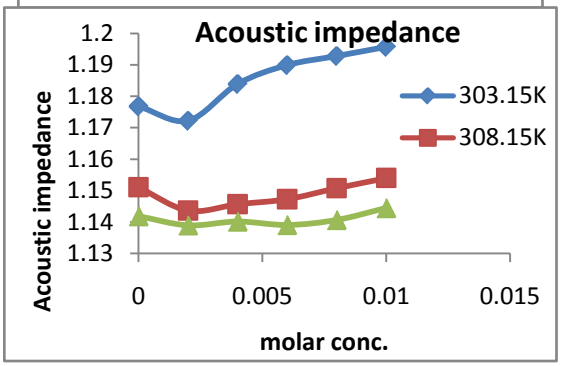
Table 1: The values of density (ρ), ultrasonic velocity (u) and acoustical values of ternary mixtures at (303. 15,308.15 and 313.15)K.

Temp (K)	Conc.	ρ kg.m^{-3}	u ms^{-1}	β_sx10^{-10}N^{-1}m^{-2}	Zx10^{6} kgm^{-2} s^{-1}	L_f x10^{-15}m	R_m	R_A
303.15	0.000	861.5	1366	6.2207	1.1768	5.18	1.5949	0.9957
	0.002	857.9	1366	6.2432	1.1722	5.19	1.5875	0.9957
	0.004	864.2	1370	6.1651	1.1839	5.15	1.5841	1.0034
	0.006	867.3	1372	6.1252	1.1899	5.14	1.5829	1.0030
	0.008	868.7	1373	6.1046	1.1928	5.13	1.5823	1.0013
	0.010	869.9	1374	6.0838	1.1957	5.12	1.5949	1.0010
308.15	0.000	854.7	1346	6.4503	1.1511	5.36	1.5812	0.9965
	0.002	851.1	1343	6.5056	1.1437	5.38	1.5812	0.9965
	0.004	852.4	1344	6.4937	1.1457	5.38	1.5790	1.0014
	0.006	853.1	1344	6.4807	1.1473	5.365	1.5786	1.0006
	0.008	855.1	1345	6.4559	1.1508	5.36	1.5617	1.0021
	0.010	856.9	1346	6.4337	1.1540	5.35	1.5739	1.0018
313.15	0.000	851.9	1340	6.5330	1.1419	5.39	1.5772	0.9984
	0.002	850.4	1339	6.5547	1.1390	5.42	1.5772	0.9984
	0.004	851.7	1338	6.5506	1.1402	5.41	1.5741	1.0016
	0.006	851.9	1337	6.5647	1.1391	5.41	1.5718	1.0006
	0.008	852.1	1338	6.5475	1.1407	5.40	1.5720	0.9998
	0.010	854.2	1339	6.5207	1.1445	5.39	1.5708	1.0029









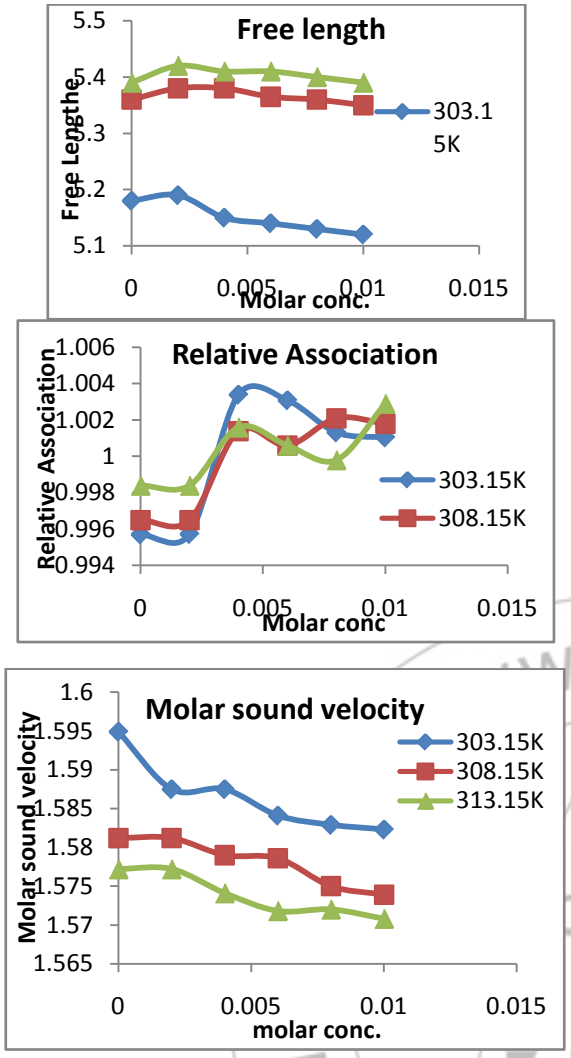


Figure:- a) density (ρ), b) ultrasonic velocity (u), c) adiabatic compressibility, d) acoustic impedance, e) free length, f) molar sound velocity and g) relative association of ternary mixtures at (303.15,308.15 and 313.15) K.

4. Conclusions

From the observed experimental values of density, ultrasonic velocity and related acoustic parameter values indicate that thermodynamic parameter are sensitive to molecular interaction for ternary liquid mixtures of 2-Aminothiazole with AN in water at different concentrations and at varying temperatures. We can find general conclusion that the increase in intermolecular free length and decreasing in adiabatic compressibility indicate strong interaction between solute-solvent molecules.

5. Acknowledgments

The author thanks Head, Department of Chemical Technology, SGB Amravati University, Amravati India, for providing necessary facilities and also thanks Principal Dr. G. P. Patil, Vidya Bharti College, Karanja (Lad) for their constant support.

References

[1] A. G. Shankarwar, V. A. Shelke, S.G. Shankarwar, Adv. in Appl. Sci. Res., 2(4), (2011), 426.
[2] D. W. Young, Heterocyclic chemistry,1st ed. London: Longmann group Ltd.,1975.
[3] W. C. Patt, H. W. Hammilton, M. D. Taylor, M. J. Ryan, J. Med. Chem., 35(14), (1992), 2562.
[4] R. N. Sharma, F. P. Xavier, K. Vasu, S. Chaturvedi, S. S. Pancholi, J. Enzyme inhibi. and Med. Chem., 24(3), (2009), 890.
[5] P. Bhattacharya, J.T. Leonard, and K. Roy. Bioorg. and Med. Chem.,13 (4), (2005),1159.
[6] B. Narayana, Vijay Raj, K. K. Ashalata, B.V. Sarojini, B.K., Eur. J. Med. Chem.,39,(2004), 867.
[7] H. Othaki, T. Itoh, Yamaguchi, S. Bratos, Bull. Chem. Soc. Japan., 56, (1983), 3406.
[8] A. B. Naik, M. L. Narwade, P. S. Bodakhe, and G. G. Muley, Russ. J. Physical Chem., 88(1), (2014), 37.
[9] A. U. Mandakmare, M. L. Narwade, D. T. Tayade and A. B. Naik, Russ. J. Physical Chem. 88(13), (2014), 2334.
[10] V. N. Maurya, K. Arora, A. K. Maurya, Int. J. of Engg. Res. and Tech., 1(8), (2012), 1.
[11] T. Sumathi, U. Maheshwari, Ind. J. of Pure & Appl. Phys., 47 (2009), 782.
[12] J. G. Dawber, J. Chem. Soc. FarTrans., 78, (1982), 1127.
[13] R. Kumar, S. Jaykumar, and V. Kannappan, Ind. J. Pure Appl. Phys.,46, (2008), 169.
[14] H. Eyring, and J. F. Kincaid, J. Chem. Phys., 6, (1938), 6620.
[15] M. S. Wagh, S. S. Kharkale, P. S. Agrawal, L. J. Paliwal, Der Chemica., 2(6),(2011). 273.
[16] R. Ezhil Pavai, S. Renuka, Int. J. Res. Pure and Appl. Phys. 2 (2), (2011). 6.
[17] A. B. Dikkar, A. S. Aswar, J. Ind. Chem. Soc., 89,(2012), 1507.
[18] J. Asgar, F. Liakath Ali Khan and K. Subramani., RASAYAN J. Chem. 3(4), (2010), 697.
[19] S. Nithiyanantham, and L. Palaniappan, Acta Cinica Indica., 22, (2006), 392.
[20] V. K. Syal, R. Gautam, and S. Chauhan, Ind. J Pure Appl. Phys., 36, (1998),108.
[21] S. Nithiyanantham, and L. Palaniappan., Chem. Sci. Trans., 2(1), (2013), 35.
[22] M. R. Ingle, A. B. Naik and M. L. Narwade, Bionano Frontier, Special Issue, (2011), 61.