Journal of Advanced Scientific Research

Available online through http://www.sciensage.info

ISSN
0976-9595
Research Article

EXCESS PROPERTIES &THEORETICAL ASSESSMENT OF ULTRASONIC STUDIES OF TERNARY LIQUID MIXTURES OF 2-BROMOANISOLE + 1-BUTANOL + n-HEXANE AT DIFFERENT TEMPERATURES

J. Edward Jeyakumar[1], S. Chidambara Vinayagam[2], J. Senthil Murugan[3], P. S. Syed Ibrahim[4]
[1]Research scholar, PG & Research Department of Chemistry, Presidency College, Chennai, Tamilnadu, India
[2]PG & Research Department of Chemistry, Presidency College, Chennai, Tamilnadu, India
[3]Department of Chemistry, S.I.V.E.T College, Gowrivakkam, Chennai, Tamilnadu, India
[4]Research scholar, PG & Research Department of Chemistry, Presidency College, Chennai, Tamilnadu, India
*Corresponding author: edwardchemistry@gmail.com

ABSTRACT

Excess properties like Excess Adiabatic Compressibility (β^E), Excess Free Length (L_f^E), Excess Free Volume (V_f^E), Excess Internal Pressure (π_i^E), Excess Ultrasonic Velocity (U^E) and Excess Acoustic Impedance (Z^E) along with molecular interaction parameter and formation constant have been evaluated from the measured values of Ultrasonic Velocity (U), Density (ρ) and Viscosity (η) for a ternary liquid system consisting of 2-Bromoanisole + 1-Butanol in n- Hexane solvent at 303, 308 & 313K at a frequency of 2MHz. The excess properties have been used to discuss and to establish the presence of significant molecular interaction in terms of dipole-dipole, dipole induced-dipole, charge transfer, hydrogen bonded and donor acceptor interactions. The ultrasonic velocity is calculated according to Namoto' s relation, Ideal Mix Relation, Impedance Dependent Relation and Junjies Relation theories and compared with the experimental values and to validate the experimental values with suitable theory for the ternary liquid mixtures containing 2-Bromoanisole +1-Butanol in n-Hexane solvent at 303,308 & 313K.

Keywords: Ultrasonics, Hydrogen Bonded, Excess Properties, Impedance Dependent Relation, Molecular Interaction.

1. INTRODUCTION

The measurement of ultrasonic speed in liquid mixture enables accurate determination of some useful acoustical parameters and their excess values which are highly sensitive to molecular interactions in their mixtures. Acoustic and thermodynamic parameters have been used to understand different kinds of association, the molecular packing, molecular motion and various types of intermolecular interactions and their strength influenced by the size in pure components and in the mixtures [1-5]. Excess parameters play a vital role in assessing the compactness due to molecular arrangement and the extent of molecular interactions in the liquid mixtures through the formation of charge transfer complex, dipole-dipole and dipole-induced dipole interactions [6]. The physical (or) chemical nature and the corresponding strength of the molecular interaction between the components of the ternary liquid mixtures have been successfully investigated by the ultrasonic method [7]. In recent years, the measurements of the ultrasonic velocity have been adequately employed for understanding the nature of molecular systems and physiochemical behavior in liquid mixtures [8-9]. A number of empirical, semi-empirical, and statistical theories have been developed by earlier workers [10]. Several researchers [11-14] carried out ultrasonic investigations on liquid mixtures and correlated the experimental results of ultrasonic velocity with theoretical relations of Nomoto [15], Van dael and Vangeel [16], impedance relation [17] and Junjie [18] relations and the results are interpreted in terms of molecular interactions. This investigation presents the evaluation of ultrasonic velocity using Nomoto's relation, ideal mixture relation, impedance relation and Junjie's relation for 2-Bromoanisole, 1-Butanol in n-Hexane solvent and are compared with the experimental values over the entire range of composition (0.001-0.010 M) at three different temperatures 303K, 308K and 313K.

Alcohols are associated organic liquids and are widely used as basic organic compounds for the synthesis of other organic compounds. Branching of the alkyl group attached to the hydroxyl group results in abnormal behavior of alcohols.

In this present study, the thermodynamic and acoustical parameters such as adiabatic compressibility (β), absorption coefficient (α/f^2), internal pressure (π_i), cohesive energy (CE), free volume (V_f), free length(L_f), acoustic impedance(z), available volume (V_a), viscous relaxation time, ΔG value, Lenard Jones potential, Degree of intermolecular interaction (χ) and K value were calculated from the experimental data of velocity, density & viscosity, various excess parameters like excess ultrasonic velocity, excess acoustic impedance, excess free length, excess free volume and excess intermolecular free length were computed from calculated values for ternary mixture 2- Bromoanisole, 1-Butanol and n hexane at various temperatures viz., 303, 308 and 313K at constant frequency 2MHz. With the aim of analyzing the disruption of self-association in 1-Butanol (having dipole moment value- 1.66 D) and the breaking of the dipole-dipole interactions of 2-Bromoanisole (having dipole moment value- 2.15D) along with the interaction between the hydroxyl group of alcohol molecule in n-hexane is a good non polar solvent. 2-Bromoanisole which is one of the additives used in NCM batteries, while the electrochemical reaction occurring in the NCM batteries, the by-products formed from oxidation-reduction process will influence the total impedance of the NCM batteries [19]. This character of the 2-Bromoanisole simulates the author to probe the current study.

2. MATERIAL AND METHODS

The mixture (2-Bromoanisole +1-Butanol+n-Hexane) of various concentrations of equal ratio 1:1 were prepared by taking analytical reagent grade and spectroscopic reagent grade chemicals with minimum assay of 99.9% and obtained from E. Merck Ltd (India). All the component liquids were purified by the standard methods. The density, viscosity, and ultrasonic velocity were measured for various concentrations as prepared above at different temperatures viz 303, 308 and 313K keeping constant frequency of 2 MHz. Ultrasonic velocity measurements were made using an ultrasonic interferometer (Model F-81, supplied by M/S Mittal Enterprises, New Delhi) with the accuracy of $\pm 0.1 ms^{-1}$. Water at desired temperature is circulated through the outer jacket of the double-walled measuring cell containing the experimental liquid. The densities of the mixture were measured using a 10 ml specific gravity bottle by relative measurement method with an accuracy of $\pm 0.01 Kg{\cdot}m^{-3}$. An Oswald viscometer (10 ml) with an accuracy of $\pm 0.001 Ns{\cdot}m^{-2}$ was used for the viscosity measurement. The flow time was determined using a digital racer stopwatch with an accuracy of ±0.1s.

2.1. THEORITICAL ASPECT

2.1.1. Acoustical and Thermodynamical Parameters

The following acoustical and thermodynamics parameters were calculated:

1. Adiabatic compressibility (β) has been calculated from the ultrasonic velocity (U), and the density (ρ) of the medium using the Newton- Laplace equation [20] as follows:

$$\beta = 1/U^2\rho \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(1)$$

2. Intermolecular free length (L_f) has been determined as [21] follows:

$$L_f = K_T\beta^{1/2} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(2)$$

Where, K_T is the temperature dependent constant known as Jacobson's constant ($K_T = 2.131\times10^{-6}$ at 318K), and β is the adiabatic compressibility.

3. Free volume (V_f) in terms of ultrasonic velocity (U) and the viscosity (η) of liquid [22] is as follows:

$$V_f = (\,M_{eff}\,U/\,k\eta)^{3/2} \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots(3)$$

Where, M_{eff} is the effective molecular weight of the mixture ($M_{eff} = \Sigma m_iX_i$, where m_i and X_i are the molecular weight and mole fraction of individual constituents, respectively), k is temperature independent constant which is equal to 4.281×10^9 for all liquids [23].

4. Internal pressure (Π_i) can be calculated using the relation [24] as follows:

$$\Pi_I = bRT(k\eta/U)^{1/2}\,(\,\rho^{2/3}\,/\,M_{eff}^{\;7/6}) \quad \ldots\ldots\ldots\ldots\ldots\ldots(4)$$

Where, b stands for cubic packing, which is assumed to be 2 for all liquids, k is a dimensionless constant independent of temperature and nature of the liquids, its values is 4.281×10^9. T is the absolute temperature in Kelvin, M_{eff} is the effective molar weight, R is the universal gas constant, η is the viscosity of the solution in Nsm^{-2}, U is the ultrasonic velocity in ms^{-2} and ρ is the density in kgm^{-3} of solution.

5. The Gibbs free energy can be determined using the relation as follows:

$$\Delta G = k_{B,}T.\ln(k_B.T.\tau/h) \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(5)$$

Where, τ is viscous relaxation time, T is the absolute temperature, k_B is Boltzmann's constant, and h is Planck's constant.

6. Acoustic impedance (Z) is given as follows:

$$Z = U.\rho \quad \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(6)$$

Where, U and ρ are the ultrasonic velocity and density of the mixture, respectively.

2.1.2. Excess Parameters

In order to study the non-ideality of the liquid mixtures, the difference between the values of acoustic and thermodynamic parameters of real mixtures (A_{exp}) and those corresponding to the ideal mixtures (A_{id}) were computing using the following equation:

$$A^E = A_{exp} - A_{id} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(7)$$

Where, A^E represents Excess parameters, $A_{id} = \Sigma A_i X_i$, i=1 to n, A_i any parameter, X_i mole fraction of the components

2.2. Theoretical Studies

The following theoretical relations were compared with the experimental values of ultrasonic velocity.

Nomoto's Equation:

$$U_{NR} = \sum_{i=1}^{n} \frac{xiRi}{xiVmi} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(8)$$

Van Dael Ideal Mixing Relation:

$$U_{IMR} = \left(\sum_{i=1}^{n} xiMi\right)^{1/2}\left(\sum_{i=1}^{n} \frac{xi}{MiV_{Mi}^2}\right)^{1/2} \ldots\ldots\ldots\ldots(9)$$

Junjie's Relation:

$$U_{JR} = \left(\sum_{i=1}^{n} xiVmi\right)\left(\sum_{i=1}^{n} xiMi\right)^{1/2}\left[\frac{\sum_{i=1}^{n} xiVmi}{\sum_{i=1}^{n} \rho i U_i^2}\right]^{1/2} \ldots(10)$$

Impedance Dependant Relation:

$$U_{IMP} = \frac{\sum_{i=0}^{n} xi\rho iUi}{\sum_{i=0}^{n} xi\rho i} \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(11)$$

Where xi is Mole fraction, Ri is molar sound velocity, ρi is the density and Vmi is the molar volume

Absolute Average Percentage Deviation (AAPD) = $\frac{1}{n}\sum\left[\frac{(Uexp-Uthe)}{Uexp}\right] \times 100 \ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots\ldots(12)$

% Error (PE) = $\{(U_{exp}-U_{the})/U_{exp}\}$X100 ………….(13)

Where, U_{exp} is experimental ultrasonic velocity and U_{the} is theoretical ultrasonic velocity.

3. RESULTS AND DISCUSSION

The present investigation discusses the applications of ultrasonic velocity to study the type of molecular interaction containing 2-Bromoanisole, 1-Butanol in n-hexane ternary liquid mixture; it is the continuation of author's earlier study on 2-Bromoanisole, 1-Propanol in n-Hexane, Edward Jeyakumar J, et al [25]. Ultrasonic velocity along with density and viscosity measurement has been used to determine certain acoustical parameters; a study of excess properties is used to determine more information about the type of interactions. In addition, the ultrasonic velocity has been calculated according to theoretical methods and the experiment values are compared with theoretical value to validate the experimental values.

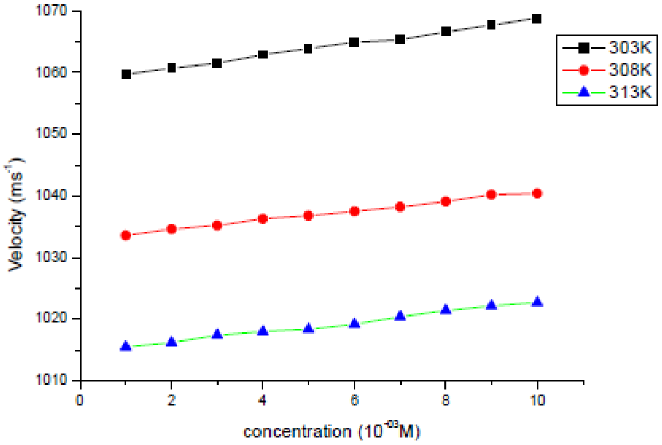

Fig.1: Plot of concentration Verse velocity

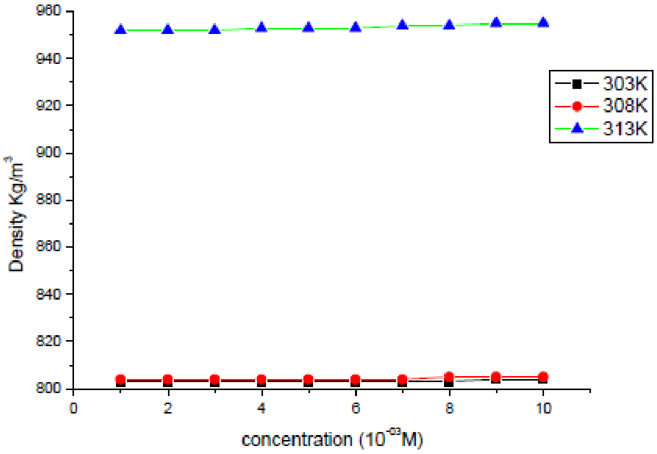

Fig.2: Plot of concentration Verse density

The experimentally measured values of ultrasonic velocity, density, and viscosity for the ternary liquid mixture at various concentrations (0.001-0.010M) and temperatures 303, 308 and 313K are presented in Table-2 and their plots against concentration are depicted in Fig.1, Fig.2 and Fig.3 respectively.

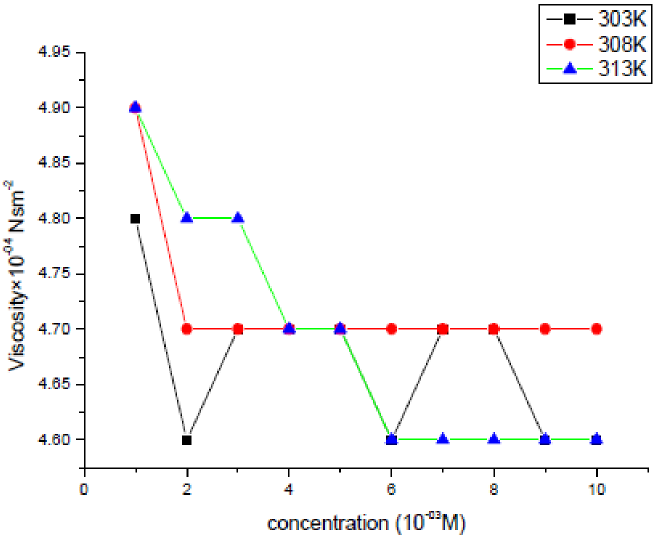

Fig.3: Plot of concentration Verse viscosity

It is observed from Table 2 that ultrasonic velocity increases with increase in concentration. The temperature increases, velocity of ultrasonic wave decreases due to breaking the bond between the associated molecules in their monomers and hence increases in temperature weaker the molecular force which in turn decreases the ultrasonic velocity. The complexation is concentration dependant, increase in viscosity with increase in concentration in all three temperature supports that the extent of complex increases with increase in concentration.

In order to understand the nature of the molecular interaction between the components in the present ternary liquid mixtures it is better to study the excess properties. The positive values of excess properties shows the presence of dispersion forces, while the presence of dipole-dipole, dipole induced dipole, charge transfer interaction and hydrogen bonding between unlike molecules are responsible for possessing negative contribution [26]. They can yield an idea about the linearity of the system as association or other type of interactions [27].

Table 1: Comparison of observed and literature value velocity, density and viscosity of pure substance in the ternary mixture of 2-Bromoanisole, 1-Butanol in n-Hexane at 303, 308 and 313K.

Name of Component in the ternary mixtures		Velocity (ms^{-1})			Density Kg/m^3			Viscosity$\times10^{-04}$ Nsm^{-2}		
		Temperature (K)			Temperature (K)			Temperature (K)		
		303	308	313	303	308	313	303	308	313
n- Hexane	Observed	1065.1	1054.5	1034.6	0.651	0.648	0.64	0.326	0.31	0.302
	Literature	1058.3[35]			0.6540[40]			0.296[41]		
1-Butanol	Observed	1182.5	1180.8	1162.0	0.801	0.798	0.796	1.658	1.516	1.498
	Literature	1198.5[36]		1189.1[37]	0.7951[38]		0.787[39]	1.73[37]		1.3810[37]
2-Bromoanisole	Observed	1267.6	1150.8	1074.9	1.307	1.302	1.30	2.698	2.30	1.994
	Literature	-	-	-	-	-	-	-	-	-

Table 2: Velocity, Density and Viscosity of 2-Bromoanisole, 1-Butanol and n Hexane at 303,308 and 313K

Con. (10^{-03}M)	Velocity (ms^{-1})			Density Kg/m^3			Viscosity$\times10^{-04}$ Nsm^{-2}		
	Temperature (K)			Temperature(K)			Temperature(K)		
	303	308	313	303	308	313	303	308	313
1	1059.7	1033.6	1015.5	803.0	804.0	952.0	4.895	4.492	5.939
2	1060.7	1034.6	1016.2	803.0	804.0	952.0	4.632	4.582	5.327
3	1061.5	1035.2	1017.4	803.0	804.0	952.0	4.636	4.588	5.343
4	1062.9	1036.3	1018.0	803.0	804.0	953.0	4.636	4.592	5.351
5	1063.9	1036.8	1018.4	803.0	804.0	953.0	4.659	4.592	5.355
6	1064.9	1037.5	1019.2	803.0	804.0	953.0	4.663	4.595	5.369
7	1065.3	1038.2	1020.4	803.0	804.0	954.0	4.663	4.603	5.391
8	1066.6	1039.1	1021.4	803.0	805.0	954.0	4.681	4.621	5.401
9	1067.7	1040.2	1022.2	804.0	805.0	955.0	4.686	4.624	5.407
10	1068.8	1040.4	1022.7	804.0	805.0	955.0	4.688	4.628	5.426

Table 3: Comparison of K value with respect to temperature for the system 2-Bromoannisole+1-Butanol in n-Hexane solvent

	Mean K Value
Temperature (K)	K
303K	23.14
308K	22.10
313K	21.04

Table 4: Excess Adiabatic Compressibility, Excess Free Length and Excess Ultrasonic Velocity of 2-Bromoanisole, 1-Butanol, n Hexane at 303,308 and 313K

	Excess Adiabatic Compressibility×10^{-10} $Kg^{-1}ms^{2}$			Excess Free Length×10^{-10} m			Excess Ultrasonic Velocity (m/s)		
Con.×10^{-3}M	Temperature(K)			Temperature(K)			Temperature(K)		
	303	308	313	303	308	313	303	308	313
1	-3.56	-4.14	-6.52	-6.91	-7.13	-7.37	-39.77	-39.50	-34.61
2	-5.57	-6.71	-9.56	-7.14	-7.41	-7.70	-60.46	-55.65	-48.33
3	-7.81	-9.46	-12.81	-7.34	-7.67	-8.00	-79.86	-70.90	-60.49
4	-10.19	-12.52	-16.51	-7.54	-7.92	-8.29	-97.23	-84.65	-72.36
5	-12.85	-15.92	-20.53	-7.73	-8.16	-8.57	-113.68	-97.83	-83.61
6	-15.83	-19.75	-25.05	-7.91	-8.39	-8.83	-129.08	-110.01	-93.68
7	-19.30	-24.17	-30.26	-8.08	-8.61	-9.09	-144.28	-121.55	-102.71
8	-23.14	-29.10	-36.08	-8.25	-8.82	-9.33	-157.24	-132.04	-111.38
9	-27.56	-34.77	-42.78	-8.41	-9.03	-9.57	-169.84	-141.67	-119.59
10	-32.70	-41.36	-50.57	-8.57	-9.22	-9.80	-181.58	-151.58	-125.67

Table 5: Excess Free Volume, Excess Internal Pressure and Excess Acoustic Impedance of 2-Bromoanisole, 1- Butanol in n Hexane at 303,308 and 313K

Con.×10^{-3} M	Excess Free Volume×10^{-07} m^{3}			Excess Internal Pressure×10^{+08} Nm^{-2}			Excess Acoustic Impedance×$10^{05}Kgs^{-1}$		
	Temperature(K)			Temperature(K)			Temperature (K)		
	303	308	313	303	308	313	303	308	313
1	1.06	1.36	0.03	-1.48	-1.47	-1.44	1.51	1.49	3.01
2	0.97	0.97	0.27	-1.96	-1.95	-1.89	1.55	1.54	3.03
3	0.93	0.93	0.23	-2.13	-2.12	-2.04	1.57	1.55	3.07
4	1.04	1.04	0.24	-1.28	-2.28	-2.18	1.59	1.57	3.10
5	0.95	0.96	0.25	-2.43	-2.43	-2.32	1.62	1.60	3.12
6	0.91	0.91	0.26	-2.57	-2.57	-2.45	1.65	1.62	3.14
7	0.98	0.98	0.28	-2.71	-2.71	-2.57	1.67	1.65	3.18
8	1.00	1.01	0.29	-2.84	-2.85	-2.69	1.70	1.67	3.20
9	0.93	0.83	0.23	-2.97	-2.98	-2.81	1.71	1.70	3.24
10	0.93	0.82	0.23	-3.09	-3.10	-2.92	1.73	1.72	3.26

Table 4 represents the excess values of adiabatic compressibility, excess free length and excess ultrasonic velocity. Similarly Table 5 presents the excess values of acoustic impedance, free volume and internal pressure of the ternary liquid mixtures at 303,308 & 313K.

In the present study, the values of excess ultrasonic velocity are negatives at various temperatures. The negative value of excess ultrasonic velocity indicates the presence of dispersive forces between the components in the ternary system. The plots of ultrasonic velocity verses concentration is depicted in Fig. 6. The negative values of excess adiabatic compressibility are the structure forming tendency and positive values is the structure breaking tendency [28]. In the present investigation of ternary liquid mixture, the negative value of excess adiabatic compressibility in Table 4 shows the strong interaction exists between the components in the ternary system. It also indicates tightly packed molecules in the liquid mixtures. The plots of excess adiabatic compressibility verses concentration is illustrated in Fig. 4.

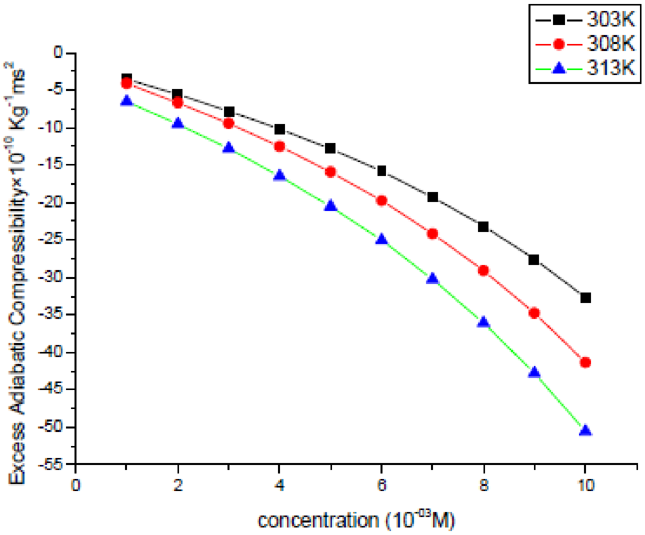

Fig. 4: Plot of concentration Verse excess adiabatic compressibility

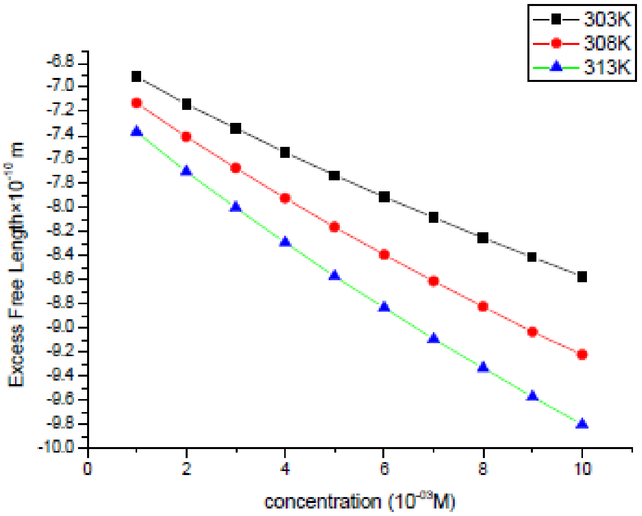

Fig.5: Plot of concentration Verse excess free length

The values of excess free length are negative in the ternary liquid system. Accounting to Fort and Moore [29], the positive excess value of free length due to the dispersive forces, and negative value of excess free length predicts the existence of strong interaction in the ternary liquid mixture due to charge transfer, dipole-dipole, dipole-induced dipole interaction, interstitial accommodation and orientation ordering. In our present study, the negative value of excess free length presented in Table 4, is due hydrogen bonding formation between 2-Bromoanisole, 1-Butanol at various temperature. This observation is further supported by negative values of excess adiabatic compressibility due to structural formation tendency. The polar nature of alcohol and 2-Bromoanisole shows the presence of dipole-dipole types of molecular interaction. This fact is supported by negative values of excess free length, the observed values are tabulated in Table 4 and the graph of excess free length verses concentration is delineated in Fig. 5.

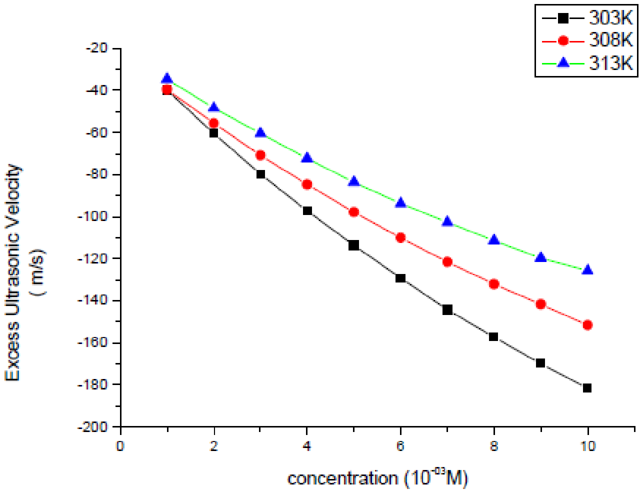

Fig. 6: Plot of concentration Verse excess ultrasonic velocity

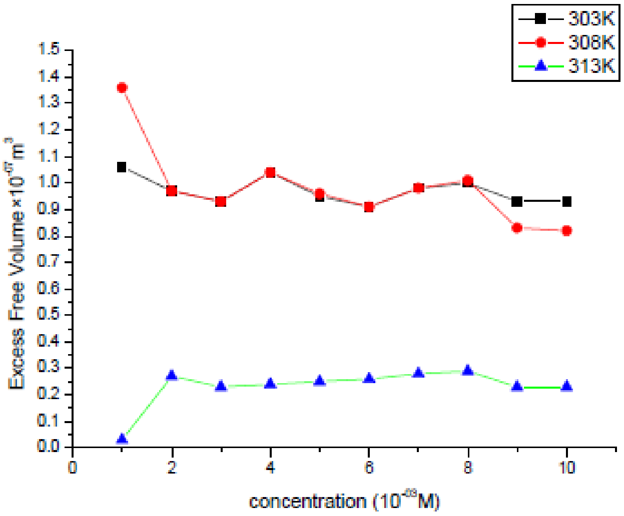

Fig.7: Plot of concentration Verse excess free volume

The excess free volume is positive in the ternary system at different temperatures. Adgaonkar et al [30] shows the positive values of excess free volume indicates the presence of weak molecular interaction and negative values shows the strong molecular interaction between the component in the ternary liquid mixtures. In the present study of liquid mixture the values of excess free volume is positive and increases with the increase of concentration and decreases with increases of temperature. It shows that the interaction decreases with increases of temperature and increase with increase of temperature. The values of excess free volume and plot of excess free volume verses concentration are outlined in Table 5 and Fig. 7. The study of excess internal pressure plays a vital role in the interaction of the components in the liquid mixtures. A positive value of excess internal pressure indicates the existence of weak interaction between the components in the liquid mixture and negative value shows the existence of strong interaction in the liquid mixture [31]. In the present investigation, the value of excess internal pressure is negative and the values are increasing with increase of concentration and decreases with increase of temperature. This shows that all the system exhibits strong interaction which has been observed from Table 5, and plot of excess internal pressure verses concentration is in Fig. 8.

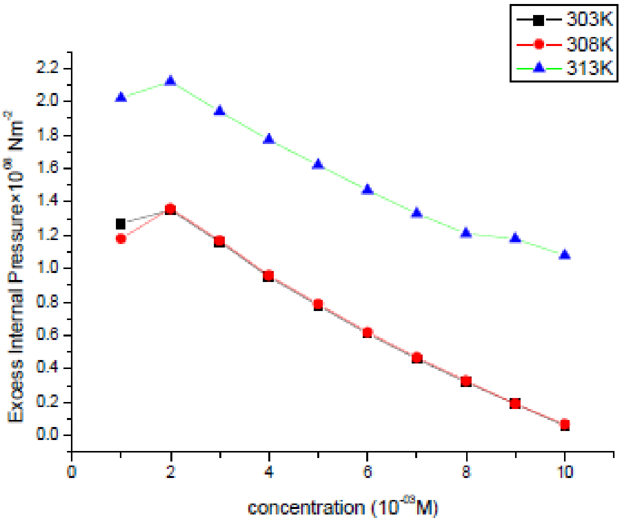

Fig.8: Plot of concentration Verse excess internal pressure

The variation of excess acoustic impedance at various concentration and temperatures which are tabulated in Table 5, and the plot against concentration in Fig. 9, the positive excess value of acoustic impedance indicates the presence of strong interaction in the liquid mixtures. In the present study, values of excess acoustic impedance increase with increase of concentration and decrease with increase of temperature. The values of excess acoustic impedance also prove the presence of strong molecular interaction in the ternary liquid mixture of 2-Bromoanisole, 1-Butanol 303, 308 & 313K.

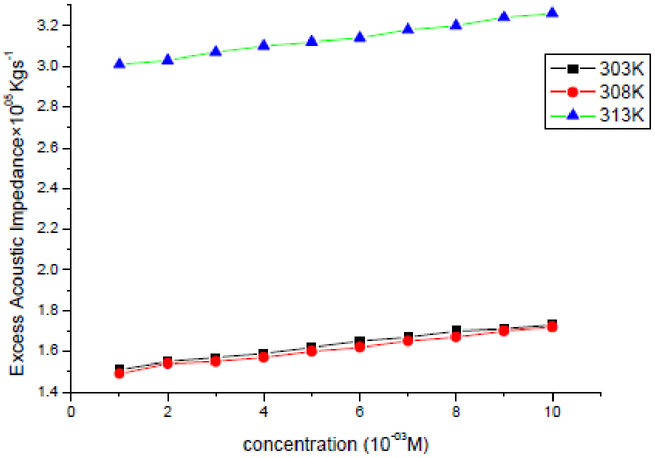

Fig.9: Plot of concentration Verse excess acoustic impedance

Molecular interaction parameter term used to measure the extent of deviation from ideal behavior caused by complexation. It is also used to measure the strength of interaction between donor and acceptor in non- polar medium. Both positive and negative is an indicative of corresponding positive and negative deviation from ideal behavior [32]. The present investigation shows negative values of all the system for all concentration and temperatures confirm the negative deviation from ideal behavior. The observed negative values of molecular interaction are represented in Tables 6-9.

The formation constant values for the ternary liquid system, 2-Bromoanisole, 1-Butanol in n-Hexane solvent, can be calculated by kannappan [33, 34] et al. The formation constant is a measure of strength of interaction between donor and acceptor molecules, that comes together to form a complex. In the present investigation the formation constant is high at 303K than other temperatures 308, 313K. The observed values of formation constants represented in Table 3.

The theoretical studies estimate the nature of molecular interactions in the ternary liquid mixtures of Bromo substituted anisole with 1-Butanol in n-hexane solvent which is under investigation. The theoretical values of ultrasonic speed using the relations such as Van Dael Ideal Mixing Relation, Impedance Dependant Relation, Junjie's and Nomoto's relation along with the experimental ultrasonic velocities and the corresponding Average Percentage Error (APE) are calculated and tabulated in Tables 6-9.

Table 6: Theoritical evolution of Nomotos Relation of ultrasonic studies of 2-Bromoanisole and 1-Butanol in n- Hexane at 303, 308 & 313

	Ultrasonic Velocity(U)			Namotos Relation (U_{NOM})			Degree of Molecular Interaction (α)			Average Percentage Error (APE)		
Con.×10^{-3} M	Temperature(K)			Temperature(K)			Temperature (K)			Temperature (K)		
	303	308	313	303	308	313	303	308	313	303	308	313
1	1059.7	1033.6	1015.5	1150.2	1094.8	1054.4	-0.151	-0.108	-0.072	-8.54	-5.59	-3.83
2	1060.7	1034.6	1016.2	1188.1	1115.1	1064.3	-0.202	-0.139	-0.088	-12.0	-7.78	-4.73
3	1061.5	1035.2	1017.4	1211.1	1127.3	1070.3	-0.231	-0.156	-0.096	-14.0	-8.89	-5.19
4	1062.9	1036.3	1018.0	1226.4	1131.5	1074.3	-0.248	-0.161	-0.102	-15.38	-9.18	-5.53
5	1063.9	1036.8	1018.4	1237.4	1141.1	1074.1	-0.260	-0.174	-0.101	-16.30	-10.05	-5.46
6	1064.9	1037.5	1019.2	1245.8	1145.7	1078.2	-0.269	-0.179	-0.106	-16.98	-10.42	-5.78
7	1065.3	1038.2	1020.4	1252.3	1149.1	1080.6	-0.276	-0.183	-0.108	-17.55	-10.68	-5.89
8	1066.6	1039.1	1021.4	1257.5	1151.8	1082.2	-0.280	-0.186	-0.109	-17.87	-10.84	-5.95
9	1067.7	1040.2	1022.2	1261.8	1154.1	1083.3	-0.283	-0.188	-0.110	-18.17	-10.94	-5.97
10	1068.8	1040.4	1022.7	1265.3	1156.1	1084.2	-0.286	-0.190	-0.111	-18.37	-11.12	-6.01
										=-155.1	=-95.49	=-54.34
					Average					X=-15.5	X=-9.54	X=-5.43

Table 7: Theoretical (Ideal Mix Relationship) studies of 2- Bromoanisole, 1- Butanol in n-Hexane at 303,308 & 313K

	Ultrasonic Velocity(U)			Ideal Mix Relation (U_{IMR})			Degree of Molecular Interaction (α)			Average Percentage Error (APE)		
Con.×10^{-3} M	Temperature(K)			Temperature(K)			Temperature (K)			Temperature (K)		
	303	308	313	303	308	313	303	308	313	303	308	313
1	1059.7	1033.6	1015.5	1237.3	1214.1	1192.2	-0.266	-0.275	-0.274	-16.75	-17.46	-17.40
2	1060.7	1034.6	1016.2	1238.6	1215.3	1194.2	-0.264	-0.274	-0.273	-16.77	-17.46	-17.51
3	1061.5	1035.2	1017.4	1239.1	1215.7	1194.6	-0.263	-0.272	-0.272	-16.73	-17.43	-17.41
4	1062.9	1036.3	1018.0	1239.2	1215.9	1194.8	-0.262	-0.270	-0.270	-16.58	-17.33	-17.36
5	1063.9	1036.8	1018.4	1239.4	1216.1	1194.9	-0.260	-0.269	-0.268	-16.48	-17.29	-17.33
6	1064.9	1037.5	1019.2	1239.5	1216.1	1195.1	-0.259	-0.268	-0.267	-16.39	-17.21	-17.25
7	1065.3	1038.2	1020.4	1239.5	1216.2	1195.1	-0.258	-0.266	-0.265	-16.35	-17.14	-17.12
8	1066.6	1039.1	1021.4	1239.6	1216.3	1195.2	-0.257	-0.265	-0.263	-16.21	-17.05	-17.11
9	1067.7	1040.2	1022.2	1239.6	1216.3	1195.2	-0.255	-0.264	-0.262	-16.10	-16.92	-16.92
10	1068.8	1040.4	1022.7	1239.7	1216.3	1195.2	-0.254	-0.262	-0.261	-15.98	-16.90	-16.86
										=-164.3	=-172.1	=-172.2
						Average				X=-16.4	X=-17.2	X=-17.22

The plots of concentration verses ultrasonic velocity and it is corresponding theoretical velocity like Namotos relation, Ideal Mix relation, Impedance dependant relation and Junjies relation are represented in Fig.10, Fig.11, Fig.12 and Fig.13 respectively. The order of theoretical relation with respect to the experimental value with equidistant temperature 303, 308, 313K is predicted in Table 10.

2-Bromoanisole, 1-Butanol in n-Hexane: UJUN<UIMP<UIMR<UNOM

It is observed from the table 10 that the AAPD values for the system 2-Bromoanisole+1 Butanol+n Hexane is in good agreement with Junjie Relation values i.e. least percentage of deviation when compare with the rest of the other theory among all the four relations which are considered for this study. An important reason for the high deviation for the systems of other theory is due to weak or weakest molecular associations between the components.

Table 8: Theoretical studies of Impedance dependent relation 2-Bromoanisole 1-Butanol in N-Hexane at 303,308 & 313 K

	Ultrasonic Velocity(U)			Impedance dependant Relation (U_{IDR})			Degree of Molecular Interaction (α)			Average Percentage Error (APE)		
Con.×10^{-3} M	Temperature(K)			Temperature(K)			Temperature (K)			Temperature (K)		
	303	308	313	303	308	313	303	308	313	303	308	313
1	1059.7	1033.6	1015.5	1092.4	1069.7	1049.1	-0.058	-0.066	-0.063	-3.08	-3.49	-3.30
2	1060.7	1034.6	1016.2	1108.8	1085.1	1063.7	-0.084	-0.090	-0.087	-4.53	-4.88	-4.67
3	1061.5	1035.2	1017.4	1125.3	1100.3	1078.4	-0.110	-0.114	-0.109	-6.01	-6.28	-5.99
4	1062.9	1036.3	1018.0	1141.8	1115.7	1093.1	-0.133	-0.137	-0.132	-7.42	-7.66	-7.37
5	1063.9	1036.8	1018.4	1158.5	1131.2	1107.9	-0.156	-0.159	-0.155	-8.89	-9.10	-8.78
6	1064.9	1037.5	1019.2	1175.2	1146.8	1112.7	-0.178	-0.181	-0.161	-10.35	-10.53	-9.17
7	1065.3	1038.2	1020.4	1192.1	1162.4	1137.6	-0.201	-0.202	-0.195	-11.90	-11.96	-11.48
8	1066.6	1039.1	1021.4	1208.9	1178.1	1152.6	-0.221	-0.222	-0.214	-13.34	-13.37	-12.84
9	1067.7	1040.2	1022.2	1225.9	1193.9	1167.6	-0.241	-0.240	-0.233	-14.81	-14.77	-14.22
10	1068.8	1040.4	1022.7	1243.1	1209.7	1182.7	-0.260	-0.260	-0.252	-16.30	-16.27	-15.64
										=-9.66	=-9.83	=-9.36
				Average						X=-9.66	X=-9.83	X=9.36

Table 9: Theoretical studies of Junjies relation of 2-Bromoanisole, 1-Butanol in n-Hexane at 303.308 & 313K

Con.×10^{-3} M	Ultrasonic Velocity(U)			Junjies Relation (U_{JUR})			Degree of Molecular Interaction (α)			Average Percentage Error (APE)		
	Temperature(K)			Temperature(K)			Temperature (K)			Temperature (K)		
	303	308	313	303	308	313	303	308	313	303	308	313
1	1059.7	1033.6	1015.5	849.26	796.22	805.95	0.556	0.685	0.587	11.78	17.83	20.63
2	1060.7	1034.6	1016.2	844.39	777.83	796.06	0.577	0.769	0.629	13.46	18.38	21.66
3	1061.5	1035.2	1017.4	863.51	790.57	811.66	0.511	0.714	0.571	11.17	16.58	20.22
4	1062.9	1036.3	1018.0	887.02	811.04	832.32	0.435	0.632	0.495	8.64	14.40	18.23
5	1063.9	1036.8	1018.4	910.33	833.26	853.24	0.365	0.548	0.424	6.18	12.19	16.21
6	1064.9	1037.5	1019.2	932.19	855.24	873.03	0.304	0.471	0.362	3.91	10.15	14.34
7	1065.3	1038.2	1020.4	952.27	876.27	891.31	0.251	0.403	0.310	1.80	8.27	12.65
8	1066.6	1039.1	1021.4	970.61	896.10	908.05	0.207	0.344	0.265	-0.02	6.59	11.09
9	1067.7	1040.2	1022.2	987.33	914.69	923.36	0.169	0.293	0.225	-1.70	5.08	9.66
10	1068.8	1040.4	1022.7	1002.6	932.07	937.35	0.136	0.245	0.190	-3.20	3.63	8.34
										=52.0	=113.1	=153.0
							Average			X=5.20	X=11.3	X=15.3

From the above order, it is inferred that a Junjie Relation gives the least deviation among the theories taken up for validation of sound velocity. This is because of hydrogen bond and charge transfer complex formation between the components present in the ternary system in addition to dipole-dipole, dipole-induced dipole interactions. Furthermore the values of excess adiabatic compressibility parameter yielded excellent comparison with the validation of Junjie theory towards experimental ultrasonic velocities for this system 2-Bromoanisole with

1-Butanol in n-Hexane. The stability constant K value is also supported this fact.

The value implies linearity of the system whereas uneven increase/decrease in values predicts the non-linearity of the system. In present study, the systems with respect to all the theoretical relations the values are found to be decreases gradually. Hence, 2-Bromoanisole+1-Butanol+n hexane is believed to be linear.

Table1 reveals the comparison of experimental values with literature values of viscosity, density and velocity at 303, 308 & 313K for pure substance which are used in the entire investigation that is 2-Bromoanisole, 1-Butanol and n-Hexane.

Table 10: Comparison of mean value of average percentage error for theoretical studies for the system 2-Bromoanisole, 1-Butanol in n-Hexane at 303,308 & 313K

Temperature(K)	Namoto's Relation	Ideal Real Mix Relation	Impedance Dependent Relation	Junjie Relation
303K	15.5	16.4	9.6	5.2
308K	9.5	17.2	9.8	11.1
313K	5.4	17.2	9.3	15.3

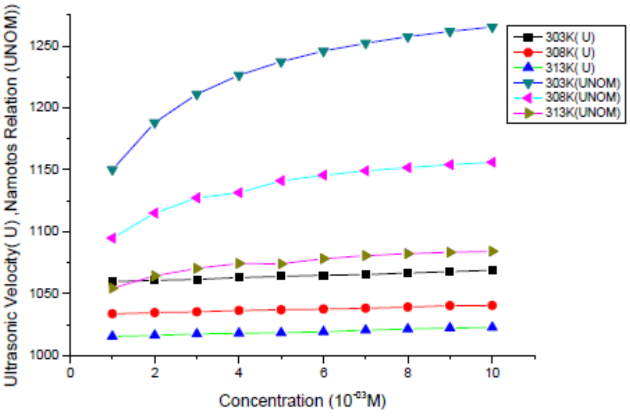

Fig. 10: plot of concentration Verse, With respect to ultrasonic velocity and Namotos relation

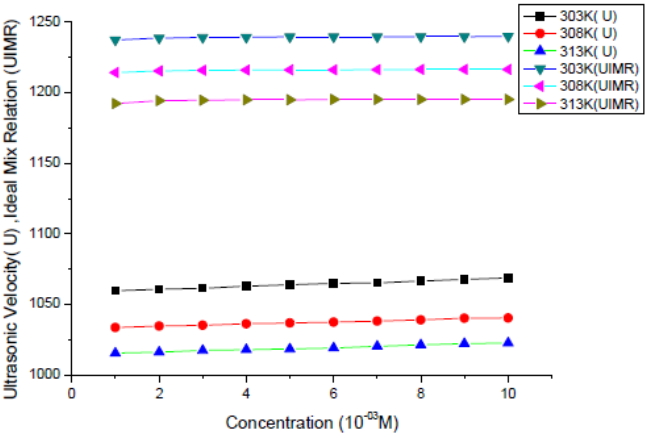

Fig 11: plot of concentration Verse, With respect to ultrasonic velocity and Ideal Mix Relation (U_{IMR})

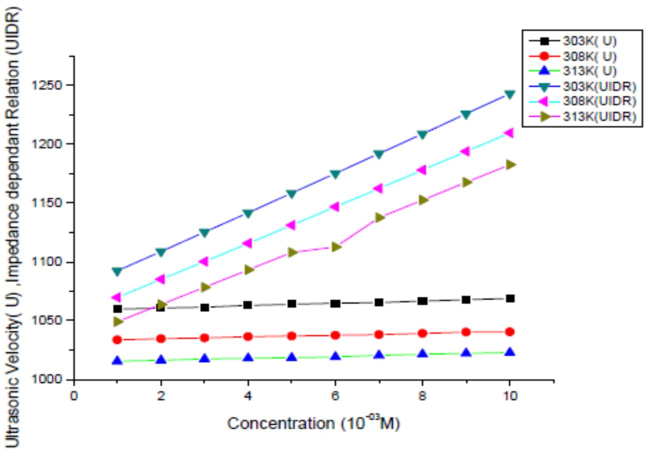

Fig. 12: plot of concentration Verse, With respect to ultrasonic velocity and Impedance dependant Relation (U_{IDR})

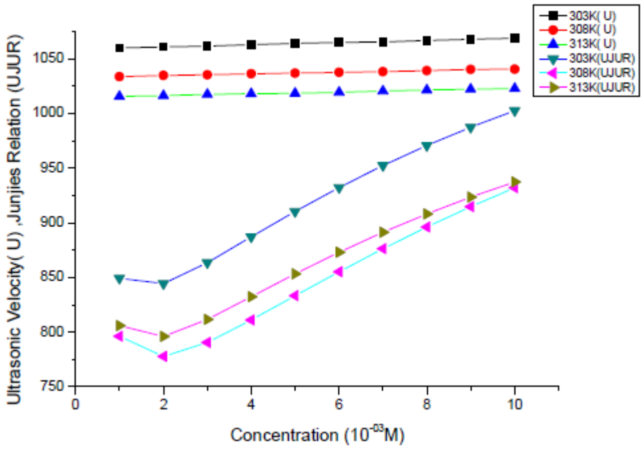

Fig 13: Plot of concentration Verse, With respect to ultrasonic velocity and Junjies Relation (U_{JUR})

4. CONCLUSION

The results obtained in the ultrasonic study of molecular interaction in the ternary liquid mixture are summarized, a halogen substituted anisole, 2-Bromoanisole is taken as electron donor and 1-Butanol as electron acceptor in a non-polar solvent n-Hexane at three equidistant temperatures 303, 308 & 313K. The experimental investigations compared with theoretical value to pick the suitable theory which correlate with it. Methoxy group (-OCH_3) present in the in 2-Bromoanisole, an electron releasing group, releases electron to 1-Butanol due to mesomeric effect. Formation constant values reported that electron donor-acceptor complex formation made easier.

Increase of temperature affects the stability of complex formation; therefore the molecular interaction parameters and formation constant were more at low temperature (303K). Excess studies were determined for confirmation and theoretical comparison to validate the experimental values to pick suitable theory. From the present investigation, it is concluded that the experimental values are validated to Junjie theory at 303K and Nomoto's theory at 308K & 313K with least average percentage error.

5. REFERENCES

1. Sumathi T, Uma Maheswari J. *Indian J of Pure and Appl.Phys.,* 2009; **47(11):**782-786.
2. Rama Rao GV. *Indian J of Pure and Appl. Phys.*, 2004; **42:**820-826.
3. Narendra K. *e-Journal of Chem.,* 2010; **7(3):**927-934.
4. Ali A, Nain AK. *Ind. J. Pure & Appl. Phys.,* 2001; **39:**421-427.
5. Anwar. *Journal of the Chinese Chemical Society,* 2004; **51:**477-485.
6. Tadkalkar Alka P. *Archives of Physics Research,* 2012; **3(4):**287-291.
7. Arul G, and Palaniappan L, *Ind. J Pure. Appl. Phys.* 2005; **43:**755-758.
8. Aralaguppi MI, Barragi JC. *J. Chem. Therm.* 2006; **38:**434-442.
9. Furniss BS, Hannaford AJ, Smith PWG and Tatchell AR. Vogal's Text book of practical organic chemistry. 5th Ed. Addison Wesley Longman Ltd. 1941, p.1442.
10. Morrison RT and Nelson BR, Organic Chemistry. Prentice Hall of India Pvt. Ltd., New Delhi. 6th Ed.2001, p.1071.
11. Ali A, Yasmin A, Nain AK. *Indian J Pure &Appl. Phys.,* 2002; **40:** 315.
12. Anwar Ali A, Anil Kumar Nain, Soghra Hyder. *J. Pure &Appl. Ultrason.*, 2001; **23:**73.
13. Shipra Baluja, Swathi Oza. *J. Pure & Appl.Ultrason.*, 2002; **54:**580.
14. Sk Faktuddin, Ch Srinivasu, Narendra K. *J. Chem. Pharm. Res.*, 2012; **4(3):**1799.
15. Nomoto O. *J. Phys. Soc. Jpn.*, 1958; **13:**1528.
16. Van Dael W, Vangeel E, *Proc. Int. Conf. On. Calorimetry and Thermodynamics,* Warasa**,** 1955; 555.
17. Baluja S, Parsania PH, *Asian J. Chem.*, 1995; **7:**417.
18. Junjie Z. *J. China. Univ. Sci. Techn*, 1984; **14:**298.
19. Zhian Zhang. *Acta Chimica Sinica-Chinese edition*, 2013; **71(5):**798-802.
20. Rao, Krishnaiah DN, Naidu A. *Acta Chim Acad. Sci. Hung* 1981; **107(1):**49-55.
21. Nikam PS, Hasan M, *Asian J of Chem,* 1993; **5(2):**319-321.
22. Prasad N. *J. Pure App.Ultrasonic,* 2003; **25:**25-30.
23. Palani R, Balakrishnan S. *Ind J, Pure &App Phy,* 2010; **48:**544-650.
24. Varada R, Sreenivasulu A, Raghuraman G. *Ind J of Che.Tech.*1994; **1**:302-304.
25. Edward Jeyakumar J, Chidambara Vinayagam S, Senthil Murugan J, Syed Ibrahim PS. *International Journal of Scientific Research and Review*, 2019; **8:(6)**338-400.
26. Thirumaran S, Priya D. *Indian Journal of Pure and Applied Physics*, 2013; **5(6):**413-420.
27. Surjit Singh Bhatti, Devinder Pal Singh. *Ind. J. Pure Appl. Phys.*, 1983; **21:**506-509.
28. Thirumaran S, Rajeshwari M. *Scholar research library*, 2011; **2(2):**149-156.
29. Fort RJ, Moore WR. *Trans Faraday Soc*, 1965; **61:**2102.
30. Adgaonkar CS, Agnihtri. *Ultrasonics*, 1989; **27:**248-251.
31. Manojku, Praharaj, Prativaranni Mishra, Sarmistha Mishra, Abhiram Sahapathy. *Advances in Applied Science Research*, 2012; **3(3):**1515-1530.
32. Shubhajit Halder, Shivani Tomar, Pratibha S Agrawal and Lalit Mohan. *Der, Pharma Chemica*, 2013; **5(6)**:282-287.
33. Kannappan V, Kothai S. *Adv. of Ultrasonics,* 2001; 124.
34. Kannappan V, Kothai S. *J. Acous. Soc., Ind.,* 2001; **29:**169.

35. Kannappan V, Kothai S. *Indian J. Pure Appl. Phys*, 2004; **40**:17-23.
36. Thirumaran S, Murugan R, Prakash N, *J. Chem, Res*, 2010; **2(1):**53-61.
37. Chintan M, Trivedi VA. *International Symposium on Ultrasonics*, 2015; *(IJSR)* (**1):**22-24.
38. Ezekiel D, Dikio, M. Simphiwe M, Nelana David A, Isabirye, Eno E, Ebenso. *Int. J. Electrochem, Sci,* 2012; **7**:11101-11122.
39. J Liu C, Zhu, Y Ma. *J. Chem. Eng, Data*, 2012; **56:**2095-2099.
40. Riddick JA, Bunger WB, Sakano T. *Organic solvents , Techniques of Chemistry*, 4th edn, Vol.I, John Wiley, New York, 1986.
41. TRC. Thermodynamics tables: Hydrocarbons Thermodynamic Research Centre: The Texas, A & M, University System, College Station, Texas 1989.