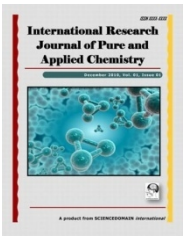

International Research Journal of Pure & Applied Chemistry
4(2): 213-226, 2014

SCIENCEDOMAIN *international*
www.sciencedomain.org

Study of Molecular Interactions in Ternary Mixtures of Quinoline with o-cresol, m-cresol and p-cresol in Methanol at T= 303.15, 308.15, 313.15, and 318.15 K

Ch. Kavitha[1*], A. Ratnakar[1], M. Durga Bhavani[1] and K. Narendra[2]

[1]Department of Chemistry, V.R. Siddhartha Engineering College (Autonomous), Vijayawada, Andhra Pradesh 520 007, India.
[2]Department of Physics, V.R. Siddhartha Engineering College (Autonomous), Vijayawada, Andhra Pradesh 520 007, India.

Authors' contributions

This work was carried out in collaboration between all authors. Author CK performed the experimental part, wrote the protocol, and wrote the first draft of the manuscript. Author AR designed the study, author MDB performed the statistical analyses and Author KN managed the literature searches and modifications in Manuscript. All authors read and approved the final manuscript.

Original Research Article

Received 29th August 2013
Accepted 25th September 2013
Published 16th December 2013

ABSTRACT

Aims: To evaluate the thermodynamical parameters and their excess functions to find the molecular interactions between unlike molecules in ternary liquid mixtures.
Study Design: Ultrasonic velocities, densities and viscosities have been measured for the ternary mixtures of quinoline with cresols in methanol at different temperatures (303.15, 308.15, 313.15 and 318.15K) over the entire range of mole fraction. These measurements are used to evaluate thermodynamical parameters like adiabatic compressibility (β), free length (L_f), free volume (V_f), internal pressure (π), acoustic impedance (Z) and enthalpy (*H*) were calculated. From these values the excess properties such as excess adiabatic compressibility (β^E), excess free length (L_f^E), excess free volume (V_f^E), excess internal pressure (π^E), excess acoustic impedance

**Corresponding author: Email: chkavitha.chem@gmail.com;*

(Z^E) and excess enthalpy (H^E) are calculated.
Place and Duration of Study: Department of Physics and Department of Chemistry, V.R. Siddhartha Engineering College, Vijayawada, between April 2012 and June 2013.
Methodology: The liquids were purified according to the standard procedures. Ultrasonic velocities of pure liquids and liquid mixtures were measured using ultrasonic interferometer, densities and viscosities were measured by using specific gravity bottle and Ostwald's viscometer.
Results: Excess adiabatic compressibility, excess free length and excess free volume exhibit negative values over the entire range of composition. In the first two systems the excess enthalpy values are found to be positive at lower mole fractions and negative for higher mole fraction range and at higher temperatures, whereas for system-3 these values are positive at all mole fractions and at temperatures 303.15, 308.15K and negative at temperatures 313.15 and 318.15K.
Conclusion: These data are required in the development of models for energy efficiency.

Keywords: Ultrasonic velocity; adiabatic compressibility; free length; internal pressure; ternary mixtures; molecular interactions.

1. INTRODUCTION

Study of thermodynamical and transport properties of pure liquids and liquid mixtures have found various applications in chemical, textile, pharmaceutical and many other industries. In predicting the physico-chemical properties of liquid mixtures, the measurements of ultrasonic velocity in pure liquids and liquid mixtures are found to be important [1-4]. Acoustic and thermodynamic parameters have been used to understand different kinds of association like molecular packing, molecular motion and various types of intermolecular interactions and their strengths, influenced by the size in pure components and in the mixtures [5]. Nature of interactions in the systems involving quinoline [6], cresols [7,8,9] and methanol [10,11] have been studied by many researchers. However, no work was reported in ternary mixtures containing quinoline. The liquids used in the present study are important due to their various industrial applications. Quinoline is used in solar cells to increase its efficiency and in dyes. Phenols are widely used for wood preservatives, selective weed killing, cleaning purpose and phonographic record. Alcohols are self-associated organic liquids and are used as basic organic compounds for the synthesis of other organic compounds. The study of ternary mixtures of quinoline with phenols in methanol would be of considerable interest because these mixtures exhibit varying molecular interactions and are important from an industrial point of view.

It is hereby reported that the nature of interactions in ternary liquid mixtures of quinoline with o-cresol or m-cresol or p-cresol and methanol from ultrasonic velocity, density and viscosity measurements at temperatures 303.15, 308.15, 313.15 and 318.15K. From these values adiabatic compressibility, free length, free volume, internal pressure, acoustic impedance and enthalpy were calculated. In order to highlight the presence of interaction between the molecules, it is essential to study the excess parameters [12]. The deviation of physical property of the liquid mixtures from the ideal behaviour is a measure of the interaction between the molecules, which may be due to either adhesive or cohesive forces. The sign and magnitude of these deviations depend on the strength of interaction between unlike-molecules in the mixtures. The experminetal values of u, ρ and η were used to calculate

adiabatic compressibility β, free length L_f, free volume V_f, internal pressure π, acoustic impedance Z and enthalpy H and their excess functions. The sign of excess values plays an important role in assessing the compactness due to molecular rearrangement and extent of molecular interactions in liquid mixtures.

2. EXPERIMENTAL DETAILS

The analytical grade chemicals obtained from SRL Chemicals, Mumbai were used. They were purified by standard procedure [13]. The purity of samples was checked by density and viscosity measurements [14]. To prepare the mixtures in the required proportions, Job's method of continuous variation was used. The mixtures were preserved in well-stoppard conical flasks. After mixing the liquids thoroughly, the flasks were left undisturbed to allow them to attain thermal equilibrium.

Single crystal ultrasonic pulse echo interferometer (Mittal enterprises, India; Model: F-80X) was used for measuring ultrasonic velocities. It consists of a high frequency generator and a measuring cell. The measurements of ultrasonic velocities were made at a fixed frequency of 3MHz. The calibration of the equipment was done by measuring the velocity in benzene and carbon tetrachloride. The results are in good agreement with the literature values [15]. The ultrasonic velocity has an accuracy of ± 0.1 $m.s^{-1}$. The temperature was controlled by circulating water around the liquid cell from thermostatically controlled constant temperature water bath (accuracy ± 0.01K).

A specific gravity bottle was used for the measurement of densities of pure liquids and liquid mixtures. Weights were measured with an electronic balance (Shimadzu AUY220, Japan) capable of measuring up to 0.1mg. An average of 4-5 measurements were taken for each sample. Ostwald's viscometer was used for measuring viscosities at the desired temperature, which was calibrated using water and benzene. After the mixture had attained bath temperature, flow time has been measured. The flow measurements were made with an electronic stopwatch with a precision of 0.01 s. The viscosity is determined using the relation

$$\eta = k\rho t \tag{1}$$

where k, ρ and t are viscometric constant, density of liquid and time of efflux for a constant volume of liquid, respectively.

From the experimental data of ultrasonic velocity, density and viscosity various thermodynamic parameters are evaluated using standard equations [16]:

Adiabatic compressibility

$$\beta = \frac{1}{\rho u^2} \tag{2}$$

where 'ρ' is the density of liquid and 'u' is the velocity of sound.

Free volume

$$V_f = \left(\frac{M_{eff} u}{K\eta} \right)^{3/2} \quad (3)$$

where M_{eff} is the effective molecular weight, 'u' is the velocity of sound, 'η' is the viscosity of liquid and *K* is proportionality constant, which is sensitive to molecular phenomenon.

Intermolecular free length

$$L_f = K_T \beta^{1/2} \quad (4)$$

where K_T is the temperature dependent constant.

Internal pressure

$$\pi = bRT \left(\frac{k\eta}{u} \right)^{1/2} \left(\frac{\rho^{2/3}}{M^{7/6}} \right) \quad (5)$$

where b is packing factor, *k* is dimensionless constant [17] independent of temperature and nature of liquids and equal to 4.28 x 10^9 and η is the viscosity. The other symbols have their usual meaning.

Acoustic impedance

$$Z = \rho.u \quad (6)$$

where 'u' is the velocity of sound and 'ρ' is the density of liquid.

Enthalpy

$$H = V_{m.}\pi \quad (7)$$

where V_m [$V_m=(x_1M_1+x_2M_2+ x_3M_3)/\rho$] is the molar volume, x_1, x_2 and x_3 are the mole fractions, M_1, M_2 and M_3 are the molar masses of first second and third components and π is the internal pressure.

The strength of interaction between the component molecules of ternary mixtures is well reflected in the deviation of the excess functions from ideality [18]. The excess properties such as β^E, L_f^E, V_f^E, π^E, Z^E and H^E were calculated using the equation

$$Y^E = Y_{mix} - [x_1Y_1+x_2Y_2+ x_3Y_3] \quad (8)$$

where Y^E is β^E or L_f^E or V_f^E or π^E or Z^E or H^E and x represents mole fraction of the component and subscript 1,2 and 3 for the components 1,2 and 3.

3. RESULTS AND DISCUSSION

The experimental values of ultrasonic velocities, densities and viscosities of the pure liquids at 303.15K are presented in Table 1, along with the corresponding literature values [19-23].

Table 1. Comparison of experimental ultrasonic velocities (u), densities (ρ) and viscosities (η) of pure liquids with literature values

Liquid	T (K)	u (ms^{-1})		ρ ($Kg\ m^{-3}$)		η x 10^3 ($Kg\ m^{-1}\ s^{-1}$)	
		Expt.	Literature	Expt.	Literature	Expt.	Literature
Quinoline	303.15	1543.68	1547[19]	1085.45	1085.79[19]	2.928	2.932[21]
o-cresol	303.15	1487.42	1487[20]	1036.20	1036.9[20]	7.477	7.479[22]
m-cresol	303.15	1464.23	1465[20]	1025.80	1026.1[20]	8.922	8.929[22]
p-cresol	303.15	1472	1471[20]	1026.50	1026.3[20]	9.545	9.540[22]
methanol	303.15	1084.34	1084[23]	794.40	795.1[23]	5.064	5.070[23]

The experimental values of ultrasonic velocity, density and viscosity for the three ternary liquid systems (quinoline+methanol+o-cresol, quinoline+methanol+m-cresol, quinoline+methanol+p-cresol) at temperatures 303.15, 308.15, 313.15 and 318.15K are given in Table 2. In all the three systems, it is observed that as the mole fraction of quinoline increases the ultrasonic velocity and density values increase whereas viscosity decreases. It may be due to the fact that quinoline has higher density than those of methanol and cresols. The nonlinear variation of ultrasonic velocity with mole fraction indicates the occurance of complex formation between unlike molecules [24,25]. From Table 2 it is also observed that as the temperature increases, the velocity of ultrasonic wave decreases. With increase in temperature, available thermal energy facilitates breaking of the bonds between the associated molecules into their monomers and hence increase in thermal energy weakens the molecular force which, in turn, decreases the ultrasonic velocity.

Table 2. Ultrasonic velocities (*u*), densities (*ρ*) and viscosities (*η*) for the ternary mixtures of quinoline at T = 303.15, 308.15, 313.15, and 318.15 K

x_1	x_3	u ($m\ s^{-1}$)	ρ ($kg\ m^{-3}$)	η x 10^3 ($Kg.m^{-1}.s^{-1}$)	x_1	x_3	u ($m\ s^{-1}$)	ρ ($kg\ m^{-3}$)	η x 10^3 ($Kg.m^{-1}.s^{-1}$)
quinoline (1) + methanol (2) + o-cresol (3)									
T = 303.15 K									
0.0000	0.7765	1482.16	1030.46	6.7070	0.3996	0.3645	1504.52	1063.35	4.7409
0.0765	0.6977	1487.78	1037.46	6.4127	0.4849	0.2764	1509.00	1068.87	4.2840
0.1546	0.6171	1491.16	1045.16	5.9417	0.5722	0.1864	1515.30	1072.80	3.6529
0.2345	0.5347	1495.52	1051.22	5.5147	0.6615	0.0943	1520.26	1078.08	3.0764
0.3161	0.4505	1500.52	1058.30	5.2090	0.7530	0.0000	1527.10	1082.54	2.5834
T = 308.15 K									
0.0000	0.7765	1460.00	1021.66	5.5977	0.3996	0.3645	1499.31	1054.66	3.8353
0.0765	0.6977	1469.70	1029.44	5.3276	0.4849	0.2764	1504.31	1058.72	3.5192
0.1546	0.6171	1478.05	1037.08	4.9588	0.5722	0.1864	1510.60	1063.56	3.0119
0.2345	0.5347	1485.68	1042.75	4.5740	0.6615	0.0943	1515.89	1068.24	2.5174
0.3161	0.4505	1492.89	1048.99	4.1273	0.7530	0.0000	1520.94	1072.32	2.0114
T = 313.15 K									
0.0000	0.7765	1443.15	1016.90	3.9098	0.3996	0.3645	1488.00	1050.40	2.6320
0.0765	0.6977	1453.50	1022.86	3.6617	0.4849	0.2764	1495.43	1054.40	2.4641
0.1546	0.6171	1464.05	1030.72	3.3695	0.5722	0.1864	1500.47	1059.28	2.0456
0.2345	0.5347	1474.16	1037.98	3.1722	0.6615	0.0943	1505.78	1062.52	1.7551
0.3161	0.4505	1481.52	1043.94	2.9141	0.7530	0.0000	1511.47	1066.08	1.4592
T = 318.15 K									
0.0000	0.7765	1421.05	1011.86	2.3176	0.3996	0.3645	1479.15	1044.31	1.6801
0.0765	0.6977	1434.50	1017.53	2.2703	0.4849	0.2764	1488.31	1049.75	1.5922
0.1546	0.6171	1449.05	1025.29	2.1257	0.5722	0.1864	1494.30	1054.28	1.4256
0.2345	0.5347	1460.68	1031.87	2.0064	0.6615	0.0943	1500.78	1057.90	1.2614
0.3161	0.4505	1469.36	1038.49	1.8341	0.7530	0.0000	1505.10	1061.86	1.0698

quinoline (1) + methanol (2) + m-cresol (3)									
T = 303.15 K									
0.0000	0.7769	1460.32	1023.94	7.2862	0.4019	0.3633	1495.21	1057.45	4.8669
0.0772	0.6975	1469.09	1031.69	6.7052	0.4874	0.2754	1502.37	1063.38	4.3087
0.1559	0.6165	1476.54	1038.05	6.2833	0.5747	0.1855	1509.71	1069.60	3.7283
0.2362	0.5338	1482.67	1045.00	5.7997	0.6639	0.0938	1519.42	1075.85	3.1825
0.3182	0.4495	1489.00	1051.67	5.2968	0.7550	0.0000	1527.10	1082.54	2.5834
T = 308.15 K									
0.0000	0.7769	1444.32	1017.94	6.7614	0.4019	0.3633	1485.47	1048.58	4.3968
0.0772	0.6975	1455.28	1025.39	6.3549	0.4874	0.2754	1494.31	1054.84	3.8336
0.1559	0.6165	1463.66	1031.16	5.8696	0.5747	0.1855	1502.12	1060.65	3.2729
0.2362	0.5338	1470.94	1037.73	5.4038	0.6639	0.0938	1510.30	1065.91	2.6781
0.3182	0.4495	1478.58	1043.32	4.8428	0.7550	0.0000	1520.94	1072.32	2.0114
T = 313.15 K									
0.0000	0.7769	1433.46	1012.57	5.0748	0.4019	0.3633	1478.84	1043.13	3.1958
0.0772	0.6975	1446.17	1018.81	4.6565	0.4874	0.2754	1486.16	1048.11	2.8040
0.1559	0.6165	1455.32	1025.73	4.2961	0.5747	0.1855	1495.15	1054.35	2.3578
0.2362	0.5338	1463.41	1031.42	3.9499	0.6639	0.0938	1502.28	1059.55	1.9521
0.3182	0.4495	1470.52	1037.87	3.5887	0.7550	0.0000	1511.47	1066.08	1.4592
T = 318.15 K									
0.0000	0.7769	1416.25	1007.63	4.3075	0.4019	0.3633	1468.15	1037.42	2.5022
0.0772	0.6975	1427.19	1013.77	3.9387	0.4874	0.2754	1476.68	1042.97	2.1756
0.1559	0.6165	1440.27	1019.90	3.5688	0.5747	0.1855	1485.67	1049.18	1.8232
0.2362	0.5338	1450.37	1026.39	3.2080	0.6639	0.0938	1494.06	1055.06	1.3956
0.3182	0.4495	1460.21	1032.05	2.8562	0.7550	0.0000	1505.10	1061.86	1.0698
quinoline (1) + methanol (2) + p-cresol (3)									
T = 303.15 K									
0.0000	0.7756	1475.32	1024.76	6.9880	0.4030	0.3616	1501.15	1060.41	4.9919
0.0776	0.6960	1481.15	1034.10	6.6442	0.4884	0.2739	1506.69	1065.37	4.5224
0.1566	0.6148	1486.80	1040.95	6.1827	0.5755	0.1844	1512.56	1071.35	3.8995
0.2371	0.5320	1491.30	1048.06	5.7814	0.6643	0.0931	1518.58	1075.81	3.3819
0.3193	0.4476	1496.47	1054.81	5.3935	0.7550	0.0000	1527.10	1082.54	2.5834
T = 308.15 K									
0.0000	0.7756	1451.21	1019.60	5.8979	0.4030	0.3616	1493.42	1051.34	4.0080
0.0776	0.6960	1462.44	1027.33	5.5675	0.4884	0.2739	1499.84	1056.84	3.5814
0.1566	0.6148	1470.89	1033.98	5.1697	0.5755	0.1844	1506.12	1061.32	3.1633
0.2371	0.5320	1478.31	1039.65	4.7147	0.6643	0.0931	1513.29	1066.11	2.6592
0.3193	0.4476	1486.05	1045.83	4.3531	0.7550	0.0000	1520.94	1072.32	2.0114
T = 313.15 K									
0.0000	0.7756	1440.15	1015.20	4.1748	0.4030	0.3616	1486.48	1045.87	2.8418
0.0776	0.6960	1450.19	1021.30	3.8981	0.4884	0.2739	1492.48	1050.80	2.5630
0.1566	0.6148	1460.89	1028.24	3.6093	0.5755	0.1844	1499.31	1055.84	2.2463
0.2371	0.5320	1470.83	1034.58	3.3408	0.6643	0.0931	1504.38	1060.19	1.9253
0.3193	0.4476	1479.15	1040.79	3.0784	0.7550	0.0000	1511.47	1066.08	1.4592
T = 318.15 K									
0.0000	0.7756	1418.58	1009.35	2.5837	0.4030	0.3616	1476.63	1040.50	1.9821
0.0776	0.6960	1430.98	1015.22	2.4877	0.4884	0.2739	1484.84	1045.06	1.8313
0.1566	0.6148	1444.69	1021.61	2.3858	0.5755	0.1844	1491.82	1050.80	1.6034
0.2371	0.5320	1457.15	1028.50	2.2945	0.6643	0.0931	1498.22	1055.79	1.4104
0.3193	0.4476	1466.99	1034.74	2.1767	0.7550	0.0000	1505.10	1061.86	1.0698

From these data various parameters like adiabatic compressibility, free volume, free length, internal pressure, acoustic impedance and enthalpy are evaluated.

Plots of respective excess parameters against mole fraction of quinoline are shown in Figs. 1(a) – 6(a) in case of system-1, in Figs. 1(b) – 6(b) for system-2 and in Figs. 1(c) – 6(c) for system-3. It is observed from the calculated values of adiabatic compressibility, free volume and free length that as the concentration of quinoline increases, adiabatic compressibility and free length decrease whereas the free volume increases. The decrease in free length is due to the close packing of the molecules inside the shield, which may be brought by strengthening of molecular interactions. From the calculated values of internal pressure,

enthalpy and acoustic impedance it is observed that as the mole fraction of quinoline increases, internal pressure and enthalpy values decrease while acoustic impedance values increase. This suggests close packing of the molecules inside the shield, which may be brought about by the increasing magnitude of interactions [26, 27]. However, in all the systems under study, the free volume increases and internal pressure decreases as temperature is increased.

To confirm the existence of interactions in the systems, it is customary to calculate the excess values of the parameters considered in the present work [28]. Any non-zero value in the excess parameter is a measure of non-linearity and is the confirmation for the existence of interaction among the components of the systems. For mixtures in which strong attractive interactions are likely to occur between the components, the excess volumes and excess adiabatic compressibilities are negative [29], while for mixtures with only weak London type interactions between the components, both excess volumes and excess adiabatic compressibilities are positive. But, however, in some systems there is no simple correlation between the strength of the interactions and the observed properties. In the present investigations, from Figs. 1(a-c) to 3(a-c) it is observed that the excess adiabatic compressibility (β^E), excess free length (L_f^E) and excess free volume (V_f^E) exhibit negative values over the entire range of composition clearly indicating the presence of strong interactions between unlike-molecules [30].

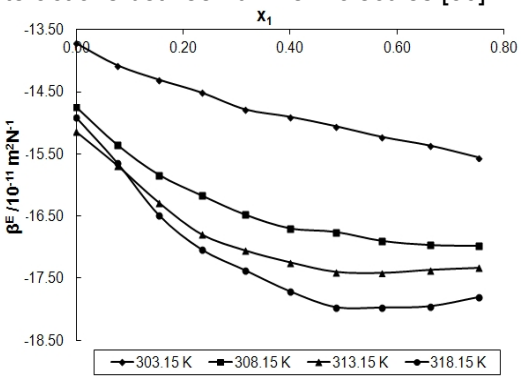

Fig. 1(a). Variation of excess adiabatic compressibility, β^E, with mole fraction, x_1, for Quinoline+ methanol+o-cresol mixtures

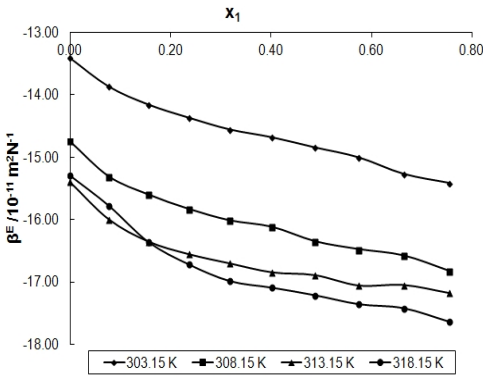

Fig. 1(b). Variation of excess adiabatic compressibility, β^E, with mole fraction, x_1, for Quinoline+ methanol+m-cresol mixtures

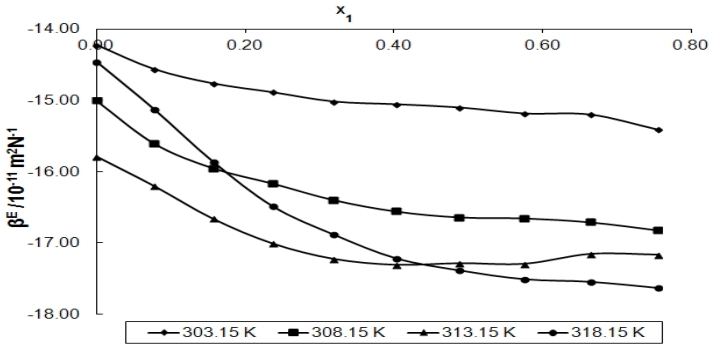

Fig. 1(c). Variation of excess adiabatic compressibility, β^E, with mole fraction, x_1, for Quinoline+ methanol+p-cresol mixtures

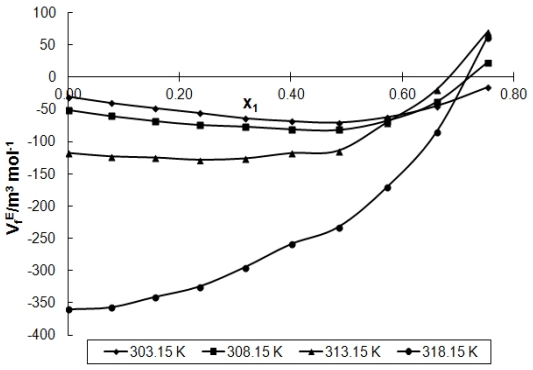

Fig. 2(a). Variation of excess free volume, V_f^E, with mole fraction, x_1, for Quinoline+ methanol+o-cresol mixtures.

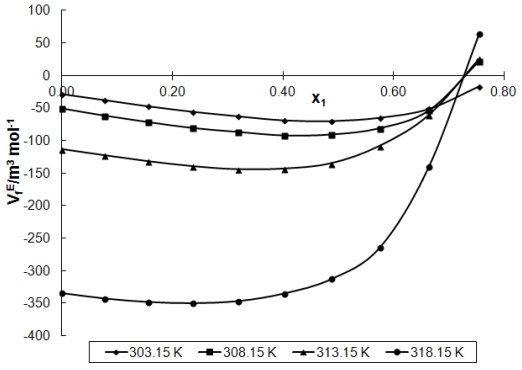

Fig. 2(b). Variation of excess free volume, V_f^E, with mole fraction, x_1, for Quinoline+methanol+m-cresol mixtures.

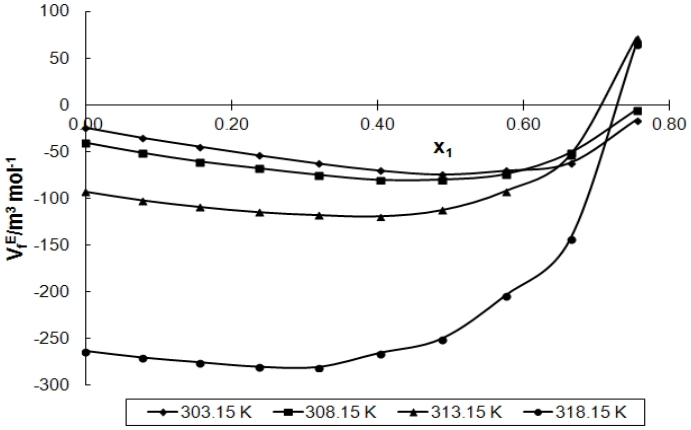

Fig. 2(c). Variation of excess free volume, V_f^E, with mole fraction, x_1, for Quinoline+ methanol+p-cresol mixtures

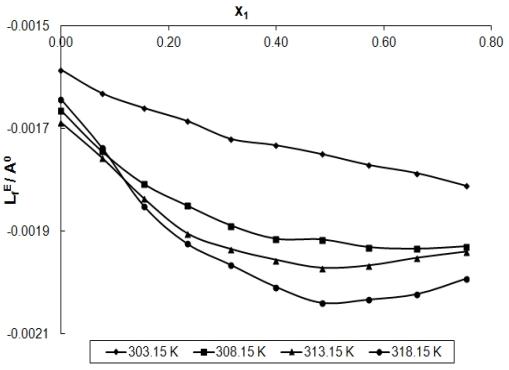

Fig. 3(a). Variation of excess intermolecular freelength, L_f^E, with mole fraction, x_1, for Quinoline+ methanol+o-cresol mixtures

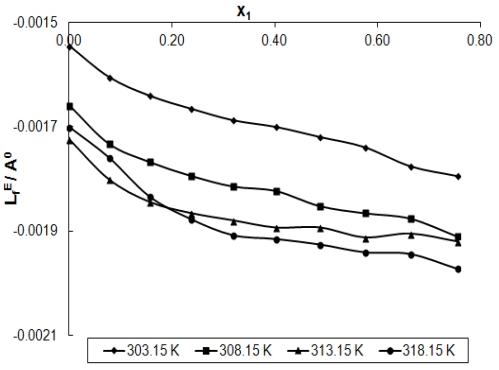

Fig. 3(b). Variation of excess intermolecular freelength, L_f^E, with mole fraction, x_1, for Quinoline+ methanol+m-cresol mixtures

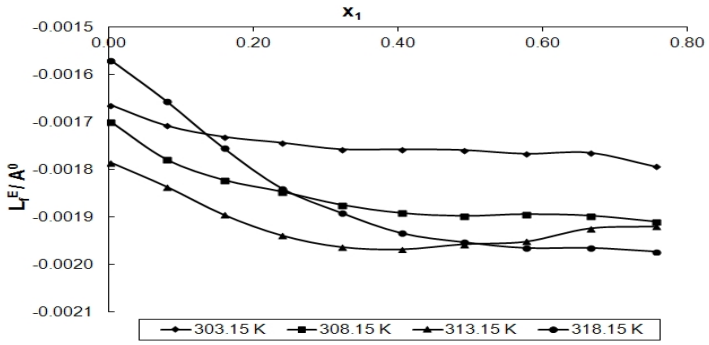

Fig. 3(c). Variation of excess intermolecular freelength, L_f^E, with mole fraction, x_1, for Quinoline+ methanol+p-cresol mixtures.

The internal pressure is the result of the forces of attraction or repulsion between the molecules in a liquid. From Fig. 4(a-c) it is observed that in all the three systems π^E values are positive at lower mole fraction and negative at higher mole fraction. It supports the increasing molecular interactions at higher concentration of quinoline [31].

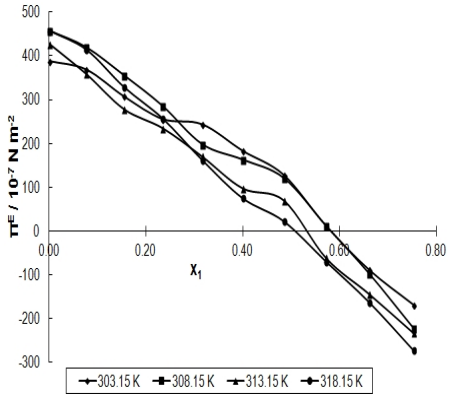

Fig. 4(a). Variation of excess internal pressure, π^E, with mole fraction, x_1, for Quinoline+ methanol+o-cresol mixtures

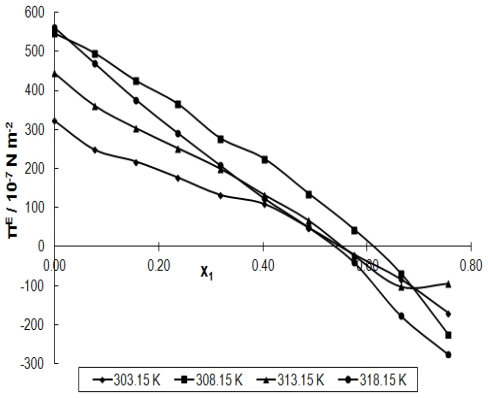

Fig. 4(b). Variation of excess internal pressure, π^E, with mole fraction, x_1, for Quinoline+ methanol+m-cresol mixtures

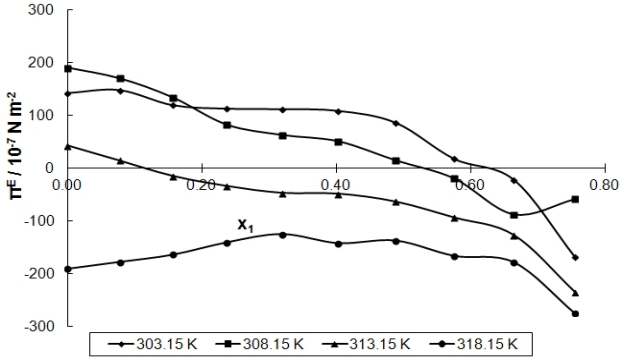

Fig. 4(c). Variation of excess internal pressure, π^E, with mole fraction, x_1, for Quinoline+ methanol+p-cresol mixtures

The variation of excess acoustic impedance (Z^E), with respect to mole fraction, x_1, is given in Fig. 5(a-c) over the entire composition range and at T= 303.15, 308.15, 313.15 and 318.15 K. It is observed from the figures that the values of Z^E are positive in all the three systems. Such positive values of Z^E suggest the presence of strong interactions between the molecules of the mixture [32].

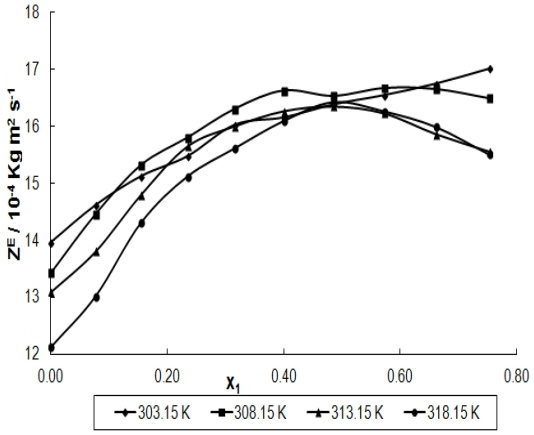

Fig. 5(a). Variation of excess acoustic impedance, Z^E, with mole fraction, x_1, for Quinoline+ methanol+o-cresol mixtures

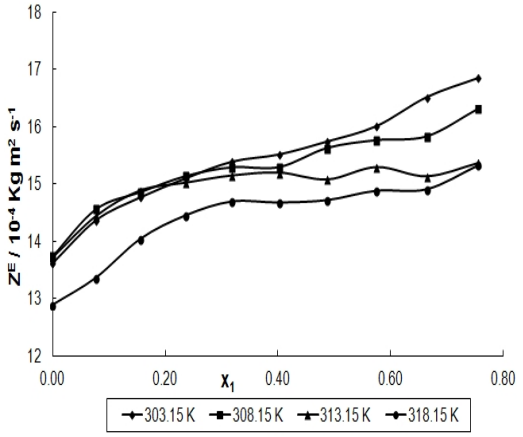

Fig. 5(b). Variation of excess acoustic impedance, Z^E, with mole fraction, x_1, for Quinoline+ methanol+m-cresol mixtures

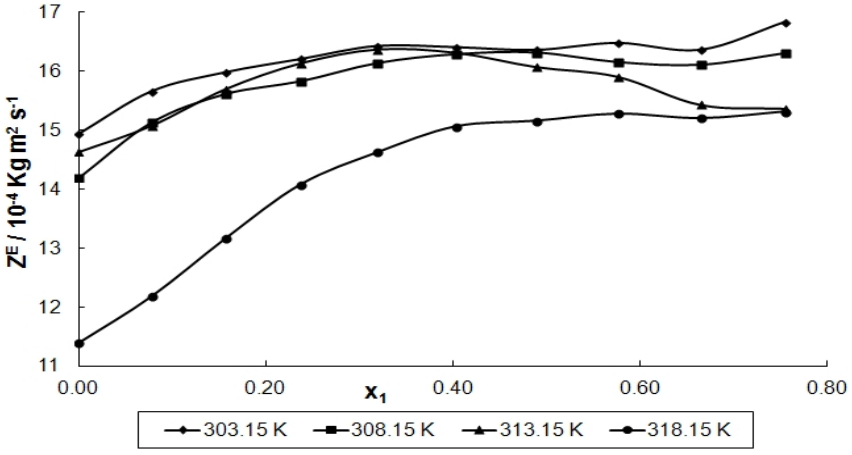

Fig. 5(c). Variation of excess acoustic impedance, Z^E, with mole fraction, x_1, for Quinoline+ methanol+p-cresol mixtures

In the first two systems (Fig. 6(a,b)), the H^E values are found to be positive at lower mole fractions and negative for higher mole fraction range and at higher temperatures, whereas for system-3 (Fig. 6(c)) the H^E values are positive at all mole fractions for temperatures 303.15, 308.15K and negative for temperatures 313.15 and 318.15K. The negative values of H^E in the mixtures indicate the presence of strong interactions between unlike molecules.

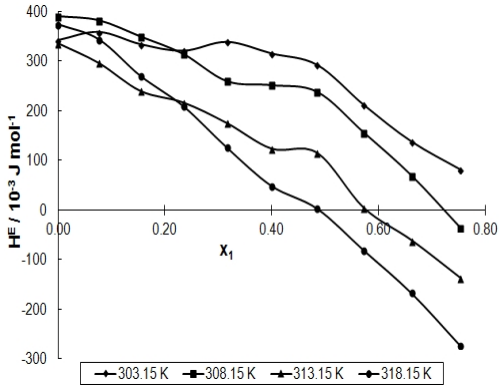

Fig. 6(a). Variation of excess enthalphy, H^E, with mole fraction, x_1, for Quinoline+ methanol+o-cresol mixtures

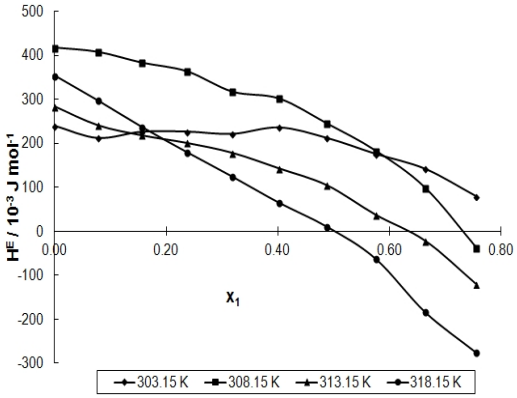

Fig. 6(b). Variation of excess enthalphy, H^E, with mole fraction, x_1, for Quinoline+ methanol+m-cresol mixtures

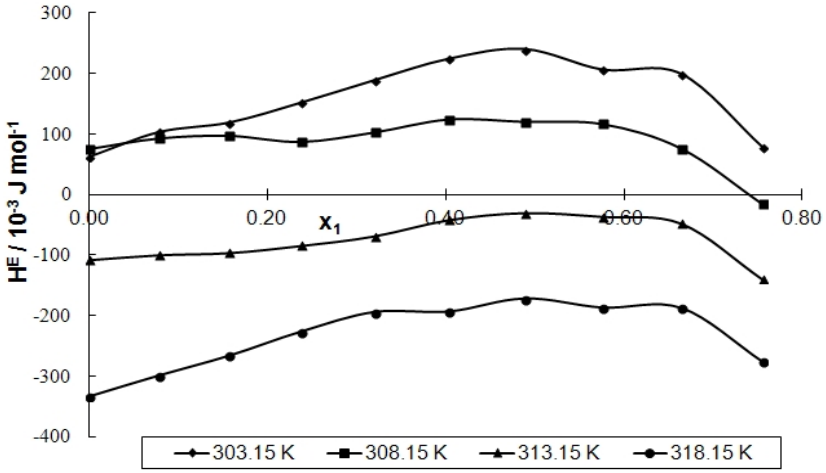

Fig. 6(c). Variation of excess enthalphy, H^E, with mole fraction, x_1, for Quinoline+ methanol+p-cresol mixtures

Based on all the above results, it can be inferred that all the three components of the ternary systems are involved in more than one type of interactions among themselves. Quinoline contains a heteroatom, nitrogen on which a lone pair of electron is available. It is an aromatic compound with delocalised π-electron cloud. Cresols also pocesses aromaticity along with alcoholic–OH group. Based on these structural features, it is possible to assess the presence of inter molecular hydrogen bonding among the component molecules: For example, hydrogen bonding may be possible between nitrogen of quinoline and –OH group of cresols.

Apart from hydrogen bonding, significant interactions of π-electron cloud of aromatic molecule and hydroxyl group are also possible. For instance, π-electron cloud of quinoline can interact with –OH group of cresols. Similar interactions can occur between π-electron cloud of cresols with methanoic –OH group. Along with hydrogen bonding and interactions

involving π-electron clouds the ternary mixtures are expected to be involved in other molecular interactions, which are generally weak compared with the above two.

4. CONCLUSION

The excess adiabatic compressibility, excess free length and excess free volume exhibit negative values over the entire range of composition and at all the temperatures considered in the present study for all the three ternary systems. It clearly indicates the presence of strong interactions between unlike-molecules. Further excess acoustic impedance, which is usually discussed in terms of molecular interactions, having positive values for all the systems under study, supports strong molecular associations between the unlike molecules of the mixtures. The strength of interactions between unlike molecules is in the order of (quinoline+methanol+p-cresol) > (quinoline+methanol+o-cresol) > (quinoline+methanol+m-cresol).

ACKNOWLEDGEMENTS

The authors acknowledge the Siddhartha Academy of General and Technical Education, Vijayawada for providing financial assistance.

COMPETING INTERESTS

Authors have declared that no competing interests exist.

REFERENCES

1. Goralski P, Wasiak M, Bald A. Heat capacities, Speeds of Sound, and Isothermal Compressibilities of Some n-Amines and Tri-n-amines at 298.15 K. J Chem. Eng. Data. 2002;47(1):83-86. DOI**:** 10.1021/je010206v
2. Litovitz TA, Davis CM. Structural and shear relation in liquids, in Physical acoustics edited by Mason WP vol.II (Part-A); Academic Press, New York. 1965;282.
3. Moha-Ouchane M, Boned C, Xans P. Variations with pressure, temperature and composition of the excess volume V^E of the ternary system water + diacetone alcohol+2-propanol. Physica B. 1999;265(1-4):287-290.
4. Palaniappan Lakshmanan. Ultrasonic analysis in the ternary system of pyridine+benzene+2-butanol. Physica B. 2008;403(21-22):3887-3891.
5. Gokhan S, Ertunc A. Excess isentropic compressibility and speed of sound of the ternary mixture 2-propanol+diethyl ether+n-hexane and the constituent binary mixtures at 298.15 K. Indian academy of Sciences. 2006;66(2):435-446.
6. Bhawana S, Tripathi, Anjali A, Aashees A. Estimation of acoustic nonlinearity parameter and molecular characteristic of ternary liquid mixtures at different temperatures. Canadian J. Physics. 2010;88(4):283-292. DOI: 10.11 39/P10-001.
7. Kammerer K, Oswald G, Rezanova E, Silkenbaumer D, Lichtenthaler RN. Thermodynamic excess properties and vapor-liquid equilibria of binary and ternary mixtures containing methanol, tert-amyl methyl ether and an alkane. Fluid Phase Equilib. 2000;167(2):223-241.
8. Nayakulu SVR, Venkateswar S, Reddy CS, Reddy DL. Ultrasonic and sonochemical reaction studies of o-cresols in different solvent mixtures. Phys. Chem. Liquids 2006;44(3):269-273.

9. Thirumaran S, Deepesh George. Ultrasonic study of intermolecular association through hydrogen bonding in ternary liquid mixtures. ARPN J. Eng. App. Sci. 2009;4(4):1-11.
10. Taghreid AS, Abeer KS. Thermodynamic properties of the binary and ternary systems containing N-Formylmorpholine, methanol, benzene and toluene at 298.15 K. J.Al-Nahrain University. 2011;14(4):1-10.
11. Zoran PV, Abel GMF, Isabel MAF. Densities and Viscosities of the Ternary Mixtures Water + Butyl Acetate + methanol and Water + Ethyl Propionate + Methanol at 303.15 K. J. Chem.Eng.Data. 2000;45(5):926-931. DOI: 10.1021/je000085j
12. Narendra K, Srinivasu Ch, Fakruddin Sk, Narayanamurthy P. Excess parameters of binary mixtures of anisaldehyde with o-cresol, m-cresol and p-cresol at T=(303.15, 308.15, 313.15, and 318.15) K. J. Chem. Thermodyn. 2011;43:1604-1611. DOI: 10.1016/j.jct.2011.05.018
13. Pandey JD, Rai RD, Shukla RK, Sukhla AK, Mishra N. Ultrasonic and thermodynamic properties of quaternary liquid system at 298.15K. Indian J Pure Appl Phys. 1993;31:54.
14. Perrin DD, Armarego WLF. Purification of laboratory chemistry. Oxford: Pregamon press; 1988.
15. Das D, Hazra DK. Molecular interaction study in binary mixtures of N, N-dimethylacetamide with 2-ethoxyethanol at three different temperatures. Indian J Phys. 2003;77B(5):519-523.
16. Sumathi T, Uma Maheswari J. Ultrasonic and theoretical studies of some ternary liquid mixtures at various temperatures. Indian J Pure Appl Phys. 2009;47:782-786.
17. Pandey JD, Sukhla BP, Dubey SN. Study of variation of internal pressure with temperature. Indian J Pure Appl Ultrason. 1993;15:33-39.
18. Lide DR, CRC hand book of chemistry and physics. Florida: CRC Press; 1995;6.
19. Jagan Nath. Ultrasonic velocities, relative permittivities and refractive indices for binary liquid mixtures of trichloroethene with pyridine and quinoline. Fluid Phase. Equilib. 1995;109(1):39-51.
20. Bhatia SC, Rani R, Bhatia R. Densities, Speeds of Sound, and Refractive Indices of Binary Mixtures of Decan-1-ol with Anisole, o-cresol, m-cresol, and p-cresol at T= (298.15, 303.15, and 308.15)K. J. Chem. Eng. Data. 2011;56(4):1669-1674. DOI: 10.1021/je100362p
21. Fakruddin Sk, Narendra K, Srinivasu Ch. Excess parameters of binary mixtures of quinoline with o-cresol, m-cresol and p-cresol at T=(303.15, 308.15, 313.15, and 318.15)K. RJPBCS. 2012;3(4):578-588.
22. Raosal R, Medina I, Forster E, Maclnnes J. Viscosities and densities for binary mixtures of cresols. Fluid Phase Equilib. 2003;211(2):143-150.
23. Praveen S, Shukla D, Singh S, Singh KP, Gupta M, Shukla JP. Ultrasonic velocity, density, viscosity and their excess parameters of the binary mixtures of tetrahydrofuran with methanol and o-cresol at varying temperatures. Applied Acoust. 2009;70(3):507-513.
24. Awasthi A, Rastogi M, Gupta M, Shukla JP. Ultrasonic investigation of molecular association in ternary mixtures. J. Mol. Liqs. 1999;80(1):77-88.
25. Palaniappan L. Ultrasonic study of 2-butanol in cyclohexane with toluene. Indian J Phys. 2001;75B(6):515-518.
26. Govindarajan S, Venu Kannappan, Naresh MD, Venkataboopathy K, Lokanadam B. Ultrasonic studies on the molecular interaction of gallic acid in aqueous methanol and acetone solutions and the role of gallic acid as viscosity reducer. J. Mol. Liqs. 2003;107(1-3):289-316.

27. Ali A, Abida Hyder S, Nain AK. Ultrasonic, volumetric and viscometric study of molecular interactions in binary mixtures of 2,3,4-trimethylpentane with n-hexane and cyclohexane at 308 K. Indian J Phy. 2002;76B(15):661-667.
28. Sreehari Sastry S, Shaik Babu, Vishwam T, Parvateesam K, Sie Tiong Ha. Excess parameters for binary mixtures of ethyl benzoate with 1-propanol, 1-butanol and 1-pentanol at T=303,308,313,318, and 323 K. Physica B. 2013;420:40-48.
29. Fort RJ, Moore WR. Adiabatic compressibilities of binary liquid mixtures. J. Trans. Faraday Soc. 1965;61:2102-2111.
30. Rai RD, Shukla RK, Shukla AK, Pandey JD. Ultrasonic speeds and isentropic compressibilities of ternary liquid mixtures at (298.15±0.01) K. J. Chem. Thermodynamics. 1989;21(2):125-129.
31. Narendra K, Srinivas Ch, Kalpana Ch, Narayanamurthy P. Excess thermo dynamical parameters of binary mixtures of toluene and mesitylene with anisaldehyde using ultrasonic technique at different temperatures. J Therm Anal Calorim. 2012;107(1):25-30.
32. Ali A, Nain AK. Study of molecular interactions in non-aqueous binary liquid mixtures through ultrasonic measurements. J Pure Appl Ultrason. 2000;22:10.

Peer-review history:
The peer review history for this paper can be accessed here:
http://www.sciencedomain.org/review-history.php?iid=318&id=7&aid=2757