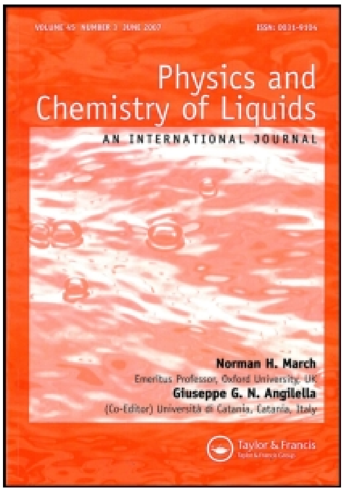

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Study of molecular properties using acoustic non-linearity parameter in the ternary liquid mixtures at different temperatures

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The parameters of non-linearity (B/A) of ternary liquid mixtures, namely phenol and o-cresol with dimethyl sulfoxide (DMSO) in carbon tetrachloride have been evaluated at 293.15, 303.15 and 313.15 K. The non-linearity parameter has been computed by three different methods, namely Tong and Dong's method, Beyer's method and Beyer's method using Tong–Dong coefficients. The excess values of non-linearity parameter $(B/A)^E$ have also been evaluated and discussed in the light of intermolecular interactions present in the liquid mixtures. Sehgal's relations for evaluating molecular properties for pure liquids are extended to ternary liquid mixtures.

Keywords: acoustic non-linearity parameter; temperature and pressure coefficients; molecular properties; ternary liquid mixtures

1. Introduction

Acoustic study provides a deep insight into the molecular structures including intermolecular interaction in multicomponent liquid mixtures [1–3]. The acoustic non-linearity parameter (B/A) plays a significant role in non-linear acoustics and its determination is very important in underwater acoustic, industrial exploitation of acoustical streaming, inhomogeneous materials and multiphase media, medical sciences, sonochemistry and molecular physics, etc. [4].

The B/A is a basic parameter of a fluid, which can be related to the molecular dynamics of the medium and it can be used as a complementary parameter in the characterisation of liquid [5]. The non-linearity parameter has been determined either by the finite amplitude method [6] or by thermodynamic method [7,8]. Analysis of the finite amplitude method carried out by Law *et al.* [9] have shown the total systematic error to be of the order of ±8%. The thermodynamic method requires the experimental determination of sound velocity at different pressures and temperatures, which involve practical difficulties. It has been shown that accuracy for the determination of the non-linearity parameter in liquid by means of the conventional thermodynamic method could be about 5%. Such accuracy of both the finite amplitude and the thermodynamic methods limits the usefulness of direct application of these methods to liquid mixtures investigations [10]. Therefore, theoretical study of non-linearity parameter in ternary liquid mixtures at varying physical conditions

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is important. The main objective of this theoretical study is to develop a new model for ternary liquid system, which is already available for binary systems, and to test its validity.

Kittel [11], assuming that molecules in a liquid are rigid balls and Hartmann [12], taking view of the potential energy between molecules, showed that in an organic liquid the temperature coefficient of ultrasonic velocity is less than zero and the pressure coefficient is greater than zero, but they could not give values of the coefficients quantitatively in view of the molecular parameters. Tong *et al.* [13] calculated the coefficients of ultrasonic velocity together with the non-linearity parameter connected to the molecular radius for pure liquids. Recently, Lu *et al.* [14] have studied the non-linear acoustic parameter along with the coefficient of ultrasonic velocity from Jacobson's theory for pure and binary organic liquid mixtures. We have evaluated and analysed the pressure and temperature coefficients of ultrasonic velocity ($\{(\partial C/\partial P)_T\}$ and $\{(\partial C/\partial T)_P\}$, respectively) using two different methods for ternary mixtures. Singh [15] has evaluated acoustic non-linearity parameter for pure and binary liquid mixtures at elevated pressures.

In condensed physics, the study of the relation between microfeatures and macroparameters in liquid matter has been one of the most difficult but attractive topics. Because the interactions between molecules of the liquid strongly depend on the concrete type of the liquid, the dynamic features of molecules are still far from clear. From this view, it is of special importance to connect the non-linear acoustic parameter with microfeatures in liquid. Sehgal [16] has determined the molecular properties using non-linear ultrasonics for pure liquids. Sehgal's relations for pure liquids have been extended for ternary liquid mixtures to evaluate the molecular properties namely, internal pressure, cohesive energy, effective molecular properties, Van der Waals constants, distance of closest approach of molecules, diffusion coefficient and rotational correlation time.

In this study, B/A values of ternary liquid mixtures, namely DMSO + phenol/o-cresol in carbon tetrachloride, have been evaluated using three different approaches at varying temperatures. The variation of excess B/A with mole fraction of one component is also evaluated and discussed in the light of molecular interactions. A comparative study of the non-linearity parameter and its correlation with molecular properties has also been made in the present context.

2. Theory

In the first method, Tong–Dong equation [17] for B/A values of pure liquids has been extended to ternary liquid mixtures. Tong–Dong's equation for B/A values is

$$B/A = J(o) + J(x), \tag{1}$$

where

$$J(o) = \left(1 - \frac{1}{\gamma}\right)\frac{C^2\rho\beta_T}{T\alpha} \quad \text{and} \quad J(x) = \frac{2(3-2x)^2}{3(x-1)(6-5x)},$$

where $x = V/b$.

Here x is the real volume of molecule and b is Van der Waals' constant given by

$$b=\frac{M}{\rho}-\frac{\gamma RT}{\rho C^2}\left\{\left(\sqrt{\frac{MC^2}{\gamma RT}+1}\right)-1\right\}. \tag{2}$$

The second method to calculate B/A, based on Beyer's thermodynamic equation, [18] has been used.

$$B/A=2\rho C\left(\frac{\partial C}{\partial P}\right)_T+\frac{2\alpha TC}{C_p}\left(\frac{\partial C}{\partial T}\right)_P. \tag{3}$$

Here $(\partial C/\partial P)_T$ is the pressure coefficient of ultrasonic velocity and $(\partial C/\partial T)_P$ is the temperature coefficient of ultrasonic velocity for ternary liquid mixtures.

The values of pressure and temperature coefficients have been calculated using the following relations [14]:

$$\left(\frac{\partial C}{\partial P}\right)_T=C\left[\sum_{i=1}^{3}\left\{(l_iV_i/Va_i)-\theta_i/2\right\}\beta_{T_i}\right], \tag{4}$$

where

$$l_i=S_iL_i\Big/\sum_{i=1}^{3}S_iL_i \tag{5}$$

$$\theta_i=X_i\rho_i\Big/\sum_{i=1}^{3}X_i\rho_i \tag{6}$$

and

$$\left(\frac{\partial C}{\partial T}\right)_p=C\left[\tau+\sum_{i=1}^{3}(\theta_i/2-l_iV_i/Va_i)\alpha_i\right]. \tag{7}$$

τ is a constant obtained by linear interpolation method.

The pressure and temperature coefficients of ultrasonic velocity have been theoretically calculated using Tong and Dong's method [19] as follows:

$$\left(\frac{\partial C}{\partial P}\right)_T=\frac{C\beta_T}{2}J(x) \tag{8}$$

and

$$\left(\frac{\partial C}{\partial T}\right)_p=\frac{C\alpha}{2}\left[\frac{1}{T\alpha}-J(x)\right]. \tag{9}$$

These values are substituted in Equation (3) together with other thermo-dynamical parameters using mixtures to get B/A values. This is the third method.

In the study of liquid mixtures, excess properties are important to investigate the molecular interactions between the components of liquid mixtures. The excess non-linearity parameter $(B/A)^{\mathrm{E}}$ for ternary liquid mixtures is defined as

$$(B/A)^E=(B/A)_{\mathrm{mix}}-(B/A)_{\mathrm{ideal}}, \tag{10}$$

where $(B/A)_{\text{mix}}$ is the theoretically calculated value and $(B/A)_{\text{ideal}}$ is that obtained from ideal components defined as

$$(B/A)_{\text{Ideal}} = X_1(B/A)_1 + X_2(B/A)_2 + X_3(B/A)_3. \tag{11}$$

Here, X_1, X_2 and X_3 are the mole fractions and $(B/A)_1$, $(B/A)_2$ and $(B/A)_3$ are the non-linearity parameters of the pure components of the ternary liquid mixture.

The various molecular properties of ternary liquid mixtures are calculated using the following Sehgal's relations:

Internal pressure:

$$P_i = \frac{\rho C^2}{(B/A+1)} \tag{12}$$

Cohesive energy:

$$\Delta A = -\frac{MC^2}{(B/A+1)} \ln\left(\frac{82.051 T\rho}{M}\right) \tag{13}$$

Van der Waals constants:

$$a = \frac{\rho C^2 V_l^2}{(B/A+1)} \tag{14}$$

$$\text{and} \quad b = V_l - \frac{RT}{\rho C^2}(B/A+1) \tag{15}$$

Distance of closest approach of molecules:

$$d = \left\{\frac{3}{2N_0\pi}\left[V_l - \frac{RT}{\rho C^2}(B/A+1)\right]\right\}^{1/3} \tag{16}$$

Diffusion coefficient:

$$D = \left(\frac{2N_0}{3^4\pi^2}\right)^{1/3}\frac{kT}{\eta} \times \frac{1}{\left[V_l - \frac{RT}{\rho C^2}(B/A+1)\right]} \tag{17}$$

Correlation time:

$$\tau = \frac{16\eta}{49N_0}\left[V_l - \frac{RT}{\rho C^2}(B/A+1)\right]. \tag{18}$$

3. Results

The non-linearity parameters for ternary liquid mixtures of phenol and o-cresol with DMSO in carbon tetrachloride have been computed in the concentration range 0.019–0.162 (mole fractions of DMSO) at 293.15, 303.15 and 313.15 K using three different methods and are reported in Tables 1 and 2, respectively. The pressure and temperature coefficients of ultrasonic velocity for both ternary liquid mixtures using two different methods are given in Table 3. Graphical displays of the excess values of B/A, i.e. $(B/A)^E$ as functions of concentration for both liquid mixtures have been presented in Figures 1 and 2. Calculated values of molecular properties using B/A for DMSO-phenol and DMSO-o-cresol systems are reported in Tables 4 and 5, respectively.

Table 1. Non-linearity parameter of DMSO-phenol system.

	B/A		
Mole fraction of DMSO (X_1)	Tong–Dong	Beyer	Tong–Dong and Beyer
$T = 293.15$ K			
0.019	11.38	10.88	12.82
0.029	11.38	10.91	12.80
0.038	11.37	10.94	12.79
0.048	11.37	10.95	12.77
0.057	11.35	10.97	12.74
0.066	11.35	10.99	12.74
0.075	11.35	11.00	12.72
0.084	11.31	10.87	12.69
0.093	11.26	10.71	12.65
0.111	11.19	10.51	12.57
0.128	11.13	10.31	12.51
0.145	11.08	10.09	12.47
0.162	11.01	9.83	12.41
$T = 303.15$ K			
0.019	11.13	10.88	12.44
0.029	11.12	10.91	12.41
0.038	11.11	10.92	12.39
0.048	11.10	10.93	12.38
0.057	11.11	10.97	12.39
0.066	11.07	10.86	12.34
0.075	11.02	10.75	12.28
0.084	10.97	10.55	12.23
0.093	10.93	10.42	12.20
0.111	10.85	10.17	12.11
0.128	10.80	10.00	12.05
0.145	10.74	9.78	12.01
0.162	10.69	9.54	11.97
$T = 313.15$ K			
0.019	10.94	11.09	12.15
0.029	10.94	11.13	12.14
0.038	10.94	11.18	12.12
0.048	10.84	10.86	12.01
0.057	10.80	10.76	11.96
0.066	10.76	10.64	11.91
0.075	10.71	10.51	11.85
0.084	10.67	10.34	11.81
0.093	10.62	10.17	11.77
0.111	10.53	9.88	11.68
0.128	10.46	9.66	11.60
0.145	10.38	9.36	11.52
0.162	10.32	9.11	11.48

4. Discussion

A close perusal of Tables 1 and 2 reveals that the B/A values evaluated by Tong and Dong's method and Beyer's method using Tong–Dong coefficients give a decreasing trend while Beyer's method show a non-linear behaviour with increasing

Table 2. Non-linearity parameter of DMSO-o-Cresol system.

Mole fraction of DMSO (X_1)	B/A Tong–Dong	B/A Beyer	B/A Tong–Dong and Beyer
$T = 293.15$ K			
0.019	11.33	10.78	12.73
0.039	11.32	10.80	12.71
0.048	11.32	10.82	12.71
0.057	11.31	10.83	12.70
0.066	11.32	10.87	12.70
0.076	11.31	10.89	12.69
0.085	11.31	10.91	12.68
0.094	11.31	10.93	12.68
0.102	11.27	10.81	12.64
0.111	11.24	10.69	12.60
0.129	11.19	10.54	12.55
0.146	11.15	10.42	12.51
0.162	11.09	10.22	12.45
$T = 303.15$ K			
0.019	11.05	10.71	12.34
0.039	11.04	10.72	12.31
0.048	11.04	10.73	12.31
0.057	11.04	10.75	12.30
0.066	11.04	10.77	12.30
0.076	11.04	10.80	12.30
0.085	11.00	10.69	12.25
0.094	10.97	10.61	12.21
0.102	10.94	10.53	12.19
0.111	10.92	10.45	12.16
0.129	10.84	10.21	12.08
0.146	10.81	10.10	12.05
0.162	10.76	9.94	12.00
$T = 313.15$ K			
0.019	10.78	10.64	11.95
0.039	10.78	10.68	11.94
0.048	10.78	10.70	11.94
0.057	10.78	10.72	11.94
0.066	10.75	10.64	11.90
0.076	10.71	10.50	11.85
0.085	10.68	10.43	11.81
0.094	10.66	10.36	11.79
0.102	10.64	10.30	11.77
0.111	10.61	10.22	11.74
0.129	10.57	10.10	11.70
0.146	10.52	9.91	11.64
0.162	10.48	9.79	11.61

mole-fractions of DMSO for both the ternary liquid mixtures. The non-monotonous behaviour of B/A values may be due to the presence of molecular interactions between oxygen atom of DMSO molecule and hydrogen atom of phenol/o-cresol molecules [15]. The acoustic non-linearity parameter has been interpreted as the quantity representing the magnitude of hardness of liquids [20].

Table 3. Pressure and temperature coefficients of DMSO-phenol and DMSO-o-cresol systems.

DMSO-phenol system				DMSO-o-cresol system			
Beyer		Tong–Dong		Beyer		Tong–Dong	
$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})	$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})	$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})	$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})
$T = 293.15$ K							
1.17	3.71	4.18	4.37	1.16	3.68	4.13	4.34
1.17	3.70	4.17	4.34	1.15	3.67	4.12	4.31
1.16	3.70	4.17	4.32	1.15	3.66	4.12	4.30
1.16	3.69	4.16	4.30	1.15	3.65	4.12	4.28
1.16	3.68	4.15	4.27	1.15	3.65	4.12	4.27
1.16	3.67	4.15	4.26	1.15	3.65	4.12	4.25
1.15	3.67	4.15	4.24	1.15	3.64	4.12	4.23
1.15	3.64	4.13	4.25	1.15	3.64	4.12	4.22
1.14	3.61	4.10	4.27	1.14	3.61	4.10	4.22
1.12	3.57	4.06	4.27	1.13	3.59	4.08	4.23
1.11	3.53	4.03	4.28	1.12	3.56	4.05	4.23
1.10	3.49	4.00	4.32	1.11	3.53	4.04	4.24
1.09	3.45	3.97	4.35	1.10	3.49	4.00	4.25
$T = 303.15$ K							
1.29	3.81	4.10	4.35	1.28	3.76	4.04	4.34
1.29	3.80	4.09	4.32	1.27	3.75	4.03	4.31
1.29	3.79	4.08	4.30	1.27	3.74	4.03	4.29
1.28	3.78	4.08	4.28	1.27	3.74	4.03	4.28
1.28	3.78	4.08	4.27	1.27	3.73	4.04	4.26
1.27	3.75	4.06	4.26	1.27	3.73	4.04	4.25
1.26	3.72	4.03	4.25	1.26	3.70	4.01	4.24
1.25	3.69	4.00	4.28	1.25	3.68	3.99	4.24
1.25	3.66	3.98	4.29	1.25	3.66	3.98	4.24

(continued)

Table 3. Continued.

DMSO-phenol system				DMSO-o-cresol system			
Beyer		Tong–Dong		Beyer		Tong–Dong	
$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})	$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})	$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})	$-(\partial C/\partial T)_P$ (m s^{-1}K^{-1})	$(\partial C/\partial P)_T$ ($\times 10^{-6}$ m^3 s^{-1}K^{-1})
1.23	3.61	3.93	4.30	1.24	3.64	3.96	4.24
1.21	3.57	3.90	4.30	1.22	3.59	3.92	4.25
1.20	3.53	3.87	4.33	1.21	3.56	3.90	4.25
1.19	3.49	3.85	4.38	1.20	3.53	3.88	4.26
$T = 313.15$ K							
1.42	3.96	4.07	4.34	1.39	3.86	3.94	4.34
1.42	3.95	4.06	4.31	1.38	3.85	3.95	4.30
1.42	3.95	4.06	4.28	1.38	3.85	3.95	4.29
1.40	3.88	3.99	4.29	1.38	3.84	3.95	4.28
1.39	3.85	3.97	4.28	1.37	3.82	3.93	4.27
1.38	3.82	3.94	4.28	1.36	3.79	3.90	4.27
1.36	3.79	3.90	4.27	1.36	3.77	3.88	4.27
1.35	3.76	3.88	4.29	1.35	3.75	3.87	4.26
1.34	3.73	3.85	4.31	1.35	3.73	3.86	4.26
1.32	3.66	3.80	4.33	1.34	3.71	3.85	4.26
1.30	3.61	3.76	4.34	1.33	3.68	3.82	4.26
1.28	3.55	3.71	4.37	1.31	3.63	3.79	4.27
1.27	3.50	3.69	4.41	1.30	3.60	3.77	4.27

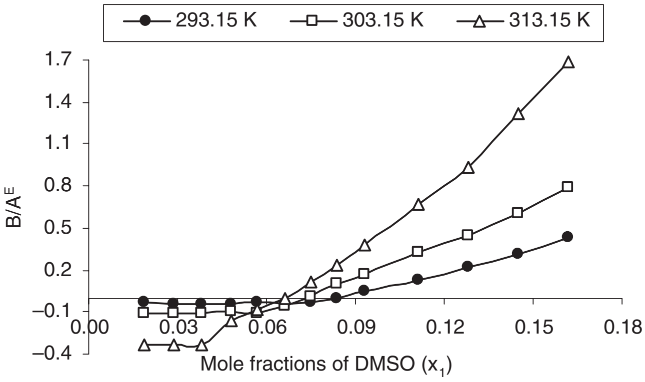


Figure 1. Variation of $(B/A)^E$ with concentration for DMSO-phenol system.

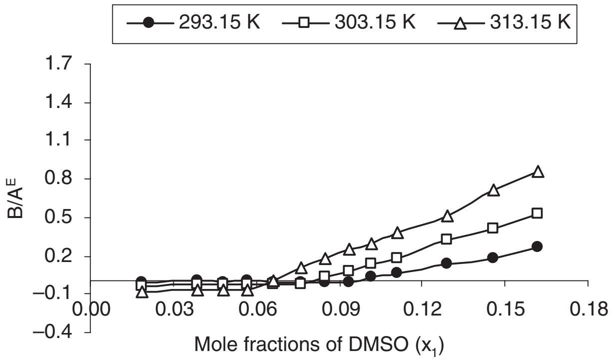


Figure 2. Variation of $(B/A)^E$ with concentration for DMSO-o-cresol system.

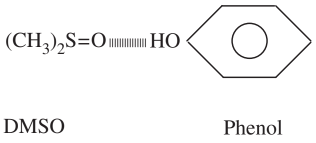
The values of non-linearity parameter have only very slight temperature dependence [8]. It may be seen that the non-linearity parameters computed from Tong and Dong's method, Beyer's method and Beyer's method using Tong–Dong coefficients show similar behaviour with increasing temperature [21].

It is interesting to note that $(B/A)^E$ values show the similar trend as that of the excess adiabatic compressibility $(\beta)^E$ [3,21]. A negative excess value is an indication of strong molecular interaction while a positive sign indicates weak interaction in the liquid mixtures. Also, the magnitude of excess values for liquid mixtures depends on the relative strength of interactions present [22]. It is seen from Figures 1 and 2 that for the DMSO-phenol system, $(B/A)^E$ values are much negative or less positive than for the DMSO-o-cresol system showing stronger molecular interaction in the DMSO-phenol system than the DMSO-o-cresol system. It may be due to the fact that attached methyl group ($-CH_3$) in o-cresol has + I effect as well as hyper conjugative effect. Hence, due to the presence of methyl group, removal of proton in o-cresol is not facilitated as in phenol. Thus, phenol molecules may form hydrogen bonds with DMSO molecules more readily. The excess non-linearity parameters are found to decrease with increasing temperature in both the systems. It may be due to the fact that increase in thermal energy weakens the molecular association and hence decrease in

Table 4. Molecular properties of DMSO-phenol system.

Mole fraction of DMSO (X_1)	P_i (MPa)	ΔA (KJ mol^{-1})	a (l^2 atm mol^{-2})	b (l mol^{-1})	d (Å)	D (m^2 s^{-1})	τ (ps)
$T = 293.15$ K							
0.019	139.97	−163.24	12.97	0.098	4.26	8.41E–10	1.20
0.039	140.78	−163.09	12.86	0.097	4.25	8.40E–10	1.20
0.048	141.52	−162.87	12.75	0.096	4.24	8.40E–10	1.19
0.057	142.20	−162.49	12.61	0.096	4.23	8.39E–10	1.19
0.066	142.80	−161.89	12.46	0.095	4.22	8.38E–10	1.18
0.076	143.60	−161.92	12.38	0.094	4.21	8.37E–10	1.18
0.085	144.15	−161.57	12.27	0.094	4.20	8.36E–10	1.17
0.094	142.35	−159.30	12.07	0.093	4.20	8.34E–10	1.17
0.102	139.92	−156.35	11.83	0.093	4.20	8.32E–10	1.18
0.111	137.20	−152.03	11.40	0.092	4.18	8.29E–10	1.17
0.129	134.37	−148.10	11.04	0.092	4.18	8.26E–10	1.17
0.146	131.10	−144.43	10.75	0.092	4.17	8.21E–10	1.18
0.162	127.19	−139.89	10.39	0.092	4.17	8.17E–10	1.18
$T = 303.15$ K							
0.019	131.93	−155.37	12.43	0.098	4.27	9.41E–10	1.08
0.039	132.67	−154.99	12.29	0.098	4.26	9.40E–10	1.07
0.048	133.23	−154.51	12.15	0.097	4.25	9.39E−10	1.07
0.057	133.68	−154.13	12.04	0.096	4.24	9.37E–10	1.07
0.066	134.74	−154.65	12.01	0.096	4.23	9.35E–10	1.07
0.076	133.21	−152.00	11.74	0.095	4.22	9.33E–10	1.06
0.085	131.52	−149.20	11.45	0.095	4.22	9.31E–10	1.06
0.094	128.42	−145.51	11.16	0.095	4.22	9.29E–10	1.06
0.102	126.50	−143.06	10.95	0.094	4.21	9.26E–10	1.07
0.111	122.50	−137.43	10.43	0.094	4.20	9.21E–10	1.07
0.129	119.93	−133.67	10.07	0.093	4.19	9.17E–10	1.07
0.146	116.50	−129.54	9.73	0.093	4.19	9.12E–10	1.07
0.162	112.56	−125.21	9.40	0.093	4.19	9.05E–10	1.08
$T = 313.15$ K							
0.019	126.48	−150.82	12.17	0.099	4.29	1.05E–09	0.97
0.039	127.29	−150.66	12.06	0.099	4.28	1.05E–09	0.97
0.048	128.45	−150.84	11.97	0.098	4.26	1.05E–09	0.96
0.057	123.16	−143.70	11.34	0.097	4.26	1.04E–09	0.96
0.066	121.70	−141.18	11.08	0.097	4.25	1.04E–09	0.96
0.076	119.82	−138.19	10.78	0.096	4.24	1.04E–09	0.96
0.085	117.50	−134.71	10.45	0.096	4.23	1.04E–09	0.96
0.094	114.78	−131.46	10.18	0.096	4.23	1.03E–09	0.96
0.102	111.87	−127.85	9.88	0.095	4.23	1.03E–09	0.96
0.111	106.77	−121.12	9.30	0.095	4.22	1.02E–09	0.96
0.129	102.73	−115.67	8.81	0.094	4.21	1.02E–09	0.97
0.146	97.06	−108.84	8.26	0.094	4.20	1.01E–09	0.97
0.162	92.48	−103.62	7.85	0.093	4.20	1.01E–09	0.98

$(B/A)^E$ values is expected.



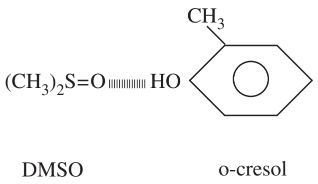


Table 5. Molecular properties of DMSO- o-cresol system.

Mole fraction of DMSO (X_1)	P_i (MPa)	ΔA (KJ mol^{-1})	a (l^2 atm mol^{-2})	b (l mol^{-1})	d (Å)	D (m^2 s^{-1})	τ (ps)
$T = 293.15$ K							
0.019	138.03	−159.89	12.64	0.097	4.25	8.40E–10	1.20
0.039	139.19	−159.57	12.46	0.096	4.24	8.37E–10	1.19
0.048	139.86	−159.49	12.38	0.095	4.23	8.36E–10	1.19
0.057	140.49	−159.36	12.29	0.095	4.22	8.35E–10	1.19
0.066	141.47	−159.64	12.23	0.094	4.21	8.34E–10	1.18
0.076	142.17	−159.55	12.14	0.094	4.20	8.33E–10	1.18
0.085	142.96	−159.58	12.07	0.093	4.19	8.32E–10	1.18
0.094	143.68	−159.52	11.98	0.093	4.19	8.31E–10	1.17
0.102	142.00	−157.21	11.78	0.092	4.18	8.30E–10	1.17
0.111	140.37	−155.00	11.58	0.092	4.18	8.28E–10	1.17
0.129	138.41	−151.77	11.24	0.091	4.17	8.24E–10	1.17
0.146	137.07	−149.44	10.99	0.091	4.16	8.21E–10	1.17
0.162	134.10	−145.51	10.65	0.090	4.15	8.18E–10	1.17
$T = 303.15$ K							
0.019	128.78	−150.79	12.03	0.098	4.27	9.39E–10	1.08
0.039	129.68	−150.18	11.82	0.097	4.25	9.36E–10	1.07
0.048	130.23	−150.01	11.73	0.096	4.24	9.34E–10	1.07
0.057	130.96	−150.16	11.68	0.096	4.23	9.32E–10	1.07
0.066	131.65	−150.25	11.62	0.095	4.23	9.30E–10	1.07
0.076	132.48	−150.36	11.55	0.095	4.22	9.29E–10	1.06
0.085	130.83	−147.72	11.28	0.094	4.21	9.27E–10	1.06
0.094	129.74	−145.75	11.07	0.094	4.20	9.25E–10	1.06
0.102	128.55	−143.93	10.89	0.093	4.20	9.23E–10	1.06
0.111	127.50	−142.31	10.73	0.093	4.19	9.20E–10	1.06
0.129	123.77	−137.14	10.26	0.092	4.18	9.16E–10	1.06
0.146	122.31	−134.66	10.00	0.092	4.17	9.11E–10	1.06
0.162	119.87	−131.19	9.68	0.091	4.16	9.08E–10	1.06
$T = 313.15$ K							
0.019	118.27	−139.77	11.23	0.099	4.28	1.05E–09	0.97
0.039	119.61	−139.90	11.10	0.098	4.26	1.04E–09	0.97
0.048	120.27	−140.03	11.05	0.097	4.25	1.04E–09	0.97
0.057	120.80	−139.99	10.98	0.097	4.25	1.04E–09	0.97
0.066	119.63	−137.94	10.76	0.096	4.24	1.04E–09	0.96
0.076	117.42	−134.65	10.45	0.096	4.23	1.03E-09	0.96
0.085	116.24	−132.63	10.24	0.095	4.22	1.03E–09	0.96
0.094	115.26	−130.93	10.06	0.095	4.22	1.03E–09	0.96
0.102	114.48	−129.63	9.92	0.094	4.21	1.03E–09	0.96
0.111	113.28	−127.78	9.73	0.094	4.21	1.02E–09	0.96
0.129	111.47	−124.80	9.42	0.093	4.20	1.02E–09	0.96
0.146	108.38	−120.46	9.02	0.093	4.18	1.01E–09	0.96
0.162	106.34	−117.51	8.74	0.092	4.18	1.01E–09	0.96

It is seen from Table 3 that the pressure coefficient $(\partial C/\partial P)_T$ is positive and the temperature coefficient $(\partial C/\partial T)_P$ is negative [8,14]. From the literature we know that under atmospheric pressure and room temperature, for most organic liquids α is in the range 0.5–1.7 × $10^{-3}\,\mathrm{K}^{-1}$, β_T is of the magnitude $10^{-10}\,\mathrm{m}^2\,\mathrm{N}^{-1}$ and γ is about 1–1.5 [23–25]. So, we can conclude easily that

$$(\partial C/\partial T)P < 0, \quad (\partial C/\partial P)T > 0 \quad \text{and} \quad B/A > 8.$$

The value of pressure coefficient computed from Beyer's method and Tong and Dong's method is almost the same but the value of temperature coefficient computed from Tong and Dong's method is much negative than those computed from Beyer's method.

Internal pressure is the resultant of the forces of attraction and of repulsion between the molecules in a liquid medium, and is a measure of the totality of force of dispersion, repulsion, ionic and dipolar interactions. It is seen from Tables 4 and 5 that at specific temperature, the internal pressure (P_i) increases with increasing mole fraction of DMSO, attains a maximum value and then decreases with further increase in mole fraction of DMSO. The values of internal pressure for DMSO-phenol system are larger than for changes in DMSO-o-cresol system. This suggests the presence of stronger intermolecular interactions in DMSO-phenol system. The cohesive energy (ΔA) almost decreases with increasing mole fraction. The cohesive energy is the measure of total molecular cohesion in contrast to the internal pressure, which is a measure of the change in internal energy of a liquid as it experiences a small isothermal expansion. It also represents the total strength or stiffness of the solvent structure [26]. The decrease in cohesive energy with increase in mole fraction of DMSO for both the systems shows the presence of intermolecular interaction. The values of cohesive energy for DMSO-phenol system are larger than for the changes in DMSO-o-cresol system. This is because the appearance of hydrogen bonding in a solvent substantially increases the cohesive energy. When temperature increases, the hydrogen bonds break up due to thermal vibrations in solute and solvent molecules. As a result, the weakened intermolecular forces lead to a decrease in internal pressure and cohesive energy [27].

The effective Van der Waals' constant a represents a measure of the attractive forces between molecules and b represents the effective volume of a molecule. It is observed that the constant a shows almost decreasing trend while effective volume b is constant for both the systems (Tables 4 and 5). The effective volume is almost independent of temperature [13]. The distance of closest approach of molecules (d) decreases with the increase in mole fraction of DMSO for both systems. It is found that as temperature increases the distance of closest approach slightly increases. The distance of closest approach is not only dependent upon how close the neighbouring molecules are, but also on how efficiently they are packed together.

The proportionality constant between the flux and potential is the diffusion coefficient or diffusivity. The diffusion coefficient (D) decreases with increasing mole fraction of DMSO in both ternary liquid mixtures. The rotational correlation time (τ) is almost constant as mole fraction of DMSO increases in both the systems. The rotational correlation time is the average time between molecular collisions and is the length of time that the molecule can be considered to be in a particular state of motion [28]. The correlation time (τ) decreases as temperature increases. It is because at higher temperature the hydrogen bonds become weak due to the thermal vibrations and structure-breaking effect predominates over the formation through hydrogen bonding [29].

5. Conclusions

The coefficients of ultrasonic velocity and the non-linear acoustic parameters with its excess value for both the ternary liquid mixtures are determined. The results of this study illustrates that the non-linearity parameter is an important quantity similar to other thermodynamic properties that are useful in explaining the molecular interactions in ternary liquid mixtures. The non-linear ultrasonics also offers an independent means to determine the molecular properties of ternary liquid mixtures.

List of symbols

M	molecular weight of mixture
C	ultrasonic velocity of mixture
V	volume of mixture
X_i	mole fraction of *i*th component
T	absolute temperature
R	universal gas constant
b	Van der Waals constant
C_p	specific heat at constant pressure
L	intermolecular length of mixture
L_i	intermolecular free length of *i*th component
$V\mathrm{a}$	available volume of mixture
$V\mathrm{a}_i$	available volume of *i*th component
Y	surface area
Y_i	surface area of *i*th component
S	surface fraction of component in mixture
N_0	Avogadro number
k	Boltzmann constant

Greek letters

ρ	density of mixture
ρ_i	density of *i*th component
α	thermal expansion coefficient of mixture
β_T	adiabatic compressibility of mixture
γ	specific heat ratio
η	viscosity of mixture

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