

# Volumetric, Viscometric, Acoustic and IR Spectroscopic Studies of Binary Mixtures of Tert-butyl Acetate with Isopropylbenzene, Isobutylbenzene and Methoxybenzene at T=298.15 and 308.15 K

Rajashri B Sawant\*

Department of Chemistry, SPH Mahila College, Malegaon Campus, Maharashtra, India

## Abstract

Densities, viscosities, speed of sound and IR spectroscopy of binary mixtures of tert-butyl acetate (tBA) with isopropylbenzene, isobutylbenzene, methoxybenzene have been measured over the entire range of composition, at (298.15 and 308.15) K and at atmospheric pressure. From the experimental values of density, viscosity, speed of sound and IR spectroscopy the excess molar volumes ( $V^E$ ), deviations in viscosity ( $\Delta\eta$ ) and deviation in isentropic compressibility ( $\Delta k_s$ ) and stretching frequency ( $\nu$ ) have been calculated. The excess molar volumes and deviations in isentropic compressibility with tBA are positive for the mixtures of isobutylbenzene and methoxybenzene with tBA and, negative for isopropylbenzene with tBA while deviations in viscosities are negative for the binary mixtures of isobutylbenzene, methoxybenzene and positive for isopropylbenzene. The excess molar volumes, deviations in viscosity and, deviations in isentropic compressibility have been fitted to the Redlich-Kister polynomial equation.

**Keywords:** Benzene; Deviations in viscosity; Deviations in isentropic compressibility; Excess molar volumes; IR; Tert-butyl acetate

## Introduction

Studies on thermodynamic and transport properties of binary liquid mixtures provide information on the nature of interactions in the constituent binaries. Literature provides extensive data on the density and viscosity of liquid mixtures but a combined study of density, viscosity, speed of sound and IR study is quite scarce. In continuation of our earliest studies [1-5] with binary mixtures of esters with normal and branched alcohols, we now report the density, viscosity, speed of sound and spectroscopic studies of tert-butyl acetate (tBA) with isopropylbenzene, isobutylbenzene and methoxybenzene at 298.15 and 308.15K. The effect of chain length and chain branching of alkyl on the solute-solvent interactions were reported earlier [6]. The excess molar volumes were explained on the basis of strong dipole-induced dipole interaction between  $\pi$ -electron cloud of aromatic ring and carbonyl group of tBA. The excess molar volume depends with temperature. The interaction between esters and hydrocarbons were studied [7] for binary mixtures of butyl acetate with aromatic hydrocarbons. The electron withdrawing groups increases IR absorption frequency while electron donating groups lowers IR absorption frequency. In present paper we have studied the physico-chemical properties of the mixtures indicated above, in order to explain the strength and nature of the interactions between the components by deriving various thermodynamic parameters from volumetric, viscometric, acoustic properties of binary mixtures and spectroscopic study.

## Experimental Procedure

Isopropylbenzene (Cumene) (Fluka, purity >99%), isobutylbenzene (SD Fine Chem., purity >99%), methoxybenzene (Anisole) (Sisco Research Lab Pvt Ltd., purity >99.5%), and tert-butyl acetate (tBA) (Spectrochem Pvt. Ltd, purity >99%) were used after single distillation. The purity of the solvents, after purification, was ascertained by comparing their densities, viscosities and speed of sound with the corresponding literature values at 298.15 K and 308.15 K (Table 1). Binary mixtures were prepared by mass in air tight stoppered glass bottles. The masses were recorded on an Adairdutt balance to an accuracy of  $\pm 1 \times 10^{-4}$  g. Care was taken to avoid evaporation and

contamination during mixing. The estimated uncertainty in mole fraction was  $<1 \times 10^{-4}$ .

Densities were determined by using a 15 cm<sup>3</sup> bicapillary pycnometer as described earlier [8-10]. The pycnometer was calibrated using conductivity water with 0.99705 g.cm<sup>-3</sup> as its density [11] at 298.15 K. The pycnometer filled with air bubble free experimental liquids was kept in a transparent walled water bath (maintained constant to  $\pm 0.01$  K) for (10 to 15) min to attain thermal equilibrium. The positions of the liquid levels in the two arms were recorded with the help of a traveling microscope, which could read to 0.01 mm. The estimated uncertainty of density measurements of solvent and binary mixtures was 0.0001 g.cm<sup>-3</sup>. At least three to four measurements were made which had an average deviation of  $\pm 0.0001$  g.cm<sup>-3</sup>.

The dynamic viscosities were measured using an Ubbelohde suspended level viscometer [9], calibrated with conductivity water. An electronic digital stop watch with readability of  $\pm 0.01$  s was used for the flow time measurements. At least three repetitions of each data reproducible to  $\pm 0.05$  s were obtained, and the results were averaged. The uncertainties in dynamic viscosities are of the order  $\pm 0.003$  mPa.s. The speed of sound ( $u$ ) were measured at a frequency of 2 MHz in these solutions through interferometric method (using Mittal's F-81 model) at (298.15 and 308.15) K ( $\pm 0.05$  K). The uncertainty in speed measurements is estimated to be  $\pm 0.1\%$ . The other experimental details are the same as reported earlier [4,12]. FTIR spectra of the above were recorded on FTIR spectrometer model Shimadzu 8400S PC.

\*Corresponding author: Rajashri B Sawant, Department of Chemistry, SPH Mahila College, Malegaon Campus, Maharashtra-423 105, India, Tel: +919890856562; E-mail: [rajashriahire@gmail.com](mailto:rajashriahire@gmail.com)

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Liquid	Temp	$\rho \times 10^{-3} \text{ (kg.m}^{-3}\text{)}$		$\eta \text{ (mPa.s)}$		$u \text{ (m.s}^{-1}\text{)}$	
	K	Expt	Lit	Expt.	Lit	Expt.	Lit.
tert-butyl acetate	298.15	0.8611	0.86057 <sup>a</sup>	0.683	-	1092	1092.76 <sup>b</sup>
	308.15	0.8494	0.84938 <sup>a</sup>	0.596	-	1055	1049.71 <sup>b</sup>
isopropylbenzene	298.15	0.8570	0.85752 <sup>c</sup> 0.8571 <sup>d</sup>	0.735	0.739 <sup>d</sup> 0.731 <sup>c</sup>	1330	1338 <sup>d</sup>
	308.15	0.8485	0.84924 <sup>c</sup> 0.84915 <sup>f</sup>	0.656	0.636 <sup>c</sup>	1280	1266.5 <sup>e</sup> 1264 <sup>k</sup>
isobutylbenzene	298.15	0.8488	0.84891 <sup>f</sup>	0.979	-	1296	1296.7 <sup>e</sup>
	308.15	0.8404	0.84082 <sup>f</sup>	0.844	0.848 <sup>k</sup>	1260	1257.5 <sup>e</sup> 1252 <sup>k</sup>
methoxybenzene	298.15	0.9892	0.9893 <sup>l</sup> 0.9889 <sup>g</sup> 0.98932 <sup>h</sup> 0.98915 <sup>j</sup>	1.017	1.0023 <sup>g</sup> 1.017 <sup>j</sup> 0.991 <sup>i</sup>	1404	1410 <sup>g</sup> 1408.02 <sup>j</sup>
	308.15	0.9791	0.9788 <sup>l</sup> 0.9796 <sup>h</sup>	0.890	0.8896 <sup>g</sup>	1376	-

<sup>a</sup>Ref. [6]; <sup>b</sup>Ref. [19]; <sup>c</sup>Ref. [20]; <sup>d</sup>Ref. [21]; <sup>e</sup>Ref. [22]; <sup>f</sup>Ref. [7]; <sup>g</sup>Ref. [23]; <sup>h</sup>Ref. [24]; <sup>i</sup>Ref. [25]; <sup>j</sup>Ref. [26]; <sup>k</sup>Ref. [27]; <sup>l</sup>Ref. [28].

**Table 1:** Comparison of experimental density, viscosity and speed of sound pure liquids with literature values at 298.15 and 308.15K.

## Results and Discussion

Experimental values of densities  $\rho$ , viscosities  $\eta$  and speed of sound  $u$  of mixtures at (298.15 and 308.15) K are listed as a function of mole fraction in Table 2. The density values have been used to calculate excess molar volumes  $V^E$  using the following equation

$$V^E / \text{cm}^3 \cdot \text{mol}^{-1} = \left( \frac{x_1 M_1 + x_2 M_2}{\rho_{12}} \right) - \left( \frac{x_1 M_1}{\rho_1} \right) - \left( \frac{x_2 M_2}{\rho_2} \right) \quad (1)$$

where  $\rho_{12}$  is the density of the mixture and  $x_1, M_1, \rho_1$ , and  $x_2, M_2, \rho_2$  are the mole fraction, the molecular weight, and the density of pure components 1 and 2, respectively.

The viscosity deviations  $\Delta\eta$  were calculated using

$$\Delta\eta / \text{mPa.s} = \eta_{12} - X_1 \eta_1 - X_2 \eta_2 \quad (2)$$

where  $\eta_{12}$  is the viscosity of the mixture and  $x_1, x_2$  and  $\eta_1, \eta_2$  are the mole fraction and the viscosity of pure components 1 and 2, respectively.

The speed of sound  $u$  was used to calculate the isentropic compressibility  $\kappa_s$  by the equation

$$\kappa_s = \frac{1}{u^2 \times \rho} \quad (3)$$

The deviation from isentropic compressibility, ( $\Delta\kappa_s$ ), was obtained using the relation,

$$\Delta\kappa_s = \kappa_{s12} - X_1 \kappa_{s1} - X_2 \kappa_{s2} \quad (4)$$

where  $\kappa_{s12}$  is the experimental isentropic compressibility of the mixture,  $x_1, x_2$  and  $\kappa_{s1}, \kappa_{s2}$  are the mole fraction and isentropic compressibility of pure components.

The excess molar volumes and deviations in viscosity and isentropic compressibility were fitted to Redlich Kister [13] equation of the type

$$Y = X_1 X_2 \sum_{i=0}^n a_i (x_1 - x_2)^i \quad (5)$$

Where  $Y$  is either  $V^E$ , or  $\Delta\eta$ , or  $\Delta\kappa_s$ , and  $n$  is the degree of polynomial. Coefficients  $a_i$  were obtained by fitting eq 5 to experimental results

using a least-squares regression method. In each case, the optimum number of coefficients is ascertained from an examination of the variation in standard deviation  $\sigma$ .

$\sigma$  was calculated using the relation

$$\sigma(Y) = \left[ \frac{\sum (Y_{\text{exp}i} - Y_{\text{calc}})^2}{N - n} \right]^{1/2} \quad (6)$$

where  $N$  is the number of data points and  $n$  is the number of coefficients. The calculated values of the coefficients  $a_i$  along with the standard deviations  $\sigma$  are given in Table 3. The variation of  $V^E$  with the mole fraction  $x_1$  of tBA for isopropylbenzene, isobutylbenzene and methoxybenzene is represented in Figure 1 at 298.15K. The values of  $V^E$  are positive for the binary mixtures of tBA with isobutylbenzene and methoxybenzene while these are negative for the binary mixtures of tBA with isopropylbenzene. If the interaction between molecules of two mixed components is weaker than in the pure component, the excess volume will be positive. This usually occurs when one component has polar groups and the other a non-polar or weakly polar behaviour. tBA is weakly polar and aromatic hydrocarbons are nearly non-polar. When the pure compounds are mixed, the non-polar hydrocarbon molecules intersperse among the tBA molecules resulting in a decreased interaction among the dipoles of the acetate and the destructions of dispersive interactions among benzenic rings. The new interaction among unlike molecules is less strong and produces expansion [7].

Figure 2 depicts the variation of  $\Delta\eta$  with the mole fraction  $x_1$  of tBA. The  $\Delta\eta$  values are positive for isopropylbenzene and negative for isobutylbenzene and methoxybenzene systems. The methoxybenzene is more negative than isobutylbenzene.

The viscosities of binary mixtures are fitted to Grunberg and Nissan [14] viscosity model.

$$\ln \eta = X_1 \ln \eta_1 + X_2 \ln \eta_2 + X_1 X_2 G_{12} \quad (7)$$

where  $G_{12}$  is an interaction parameter which is a function of the components 1 and 2 as well as temperature. Table 4 includes the different parameters for Grunberg - Nissan, Hind et al., Heric - Brewer and percentage standard deviations.

Hind et al. [15] suggested an equation for the viscosity of binary liquid mixtures as

$x_1$	$\rho \times 10^{-3}$ (kg. m <sup>-3</sup> )	$V^E \times 10^6$ (m <sup>3</sup> .mol <sup>-1</sup> )	$\eta$ (mPa.s)	$\Delta\eta$ (mPa.s)	$u$ (m.s <sup>-1</sup> )	$\kappa_s$ (TPa <sup>-1</sup> )	$\Delta\kappa_s$ (TPa <sup>-1</sup> )
tBA (1)+isopropylbenzene (2) at 298.15K							
0.0000	0.8570	0.000	0.735	0.000	1330	660	0
0.0991	0.8574	-0.001	0.732	0.002	1302	688	-3
0.1972	0.8578	-0.003	0.729	0.004	1276	716	-6
0.2970	0.8583	-0.019	0.724	0.004	1250	746	-7
0.3962	0.8587	-0.018	0.719	0.005	1225	776	-8
0.4965	0.8591	-0.017	0.713	0.004	1201	807	-9
0.5963	0.8596	-0.031	0.707	0.003	1177	840	-7
0.6973	0.8600	-0.028	0.701	0.002	1154	873	-6
0.7976	0.8604	-0.025	0.695	0.001	1132	907	-3
0.8992	0.8608	-0.020	0.689	0.001	1111	941	-1
1.0000	0.8611	0.000	0.683	0.000	1092	974	0
tBA (1)+isopropylbenzene (2) at 308.15K							
0.0000	0.8485	0.000	0.656	0.000	1280	719	0
0.0991	0.8486	-0.002	0.652	0.002	1254	749	-4
0.1972	0.8487	-0.005	0.647	0.003	1230	779	-7
0.2970	0.8488	-0.006	0.642	0.004	1205	811	-9
0.3962	0.8489	-0.008	0.636	0.004	1181	845	-8
0.4965	0.8491	-0.026	0.629	0.003	1157	880	-7
0.5963	0.8492	-0.028	0.623	0.003	1135	914	-7
0.6973	0.8493	-0.029	0.616	0.002	1114	949	-6
0.7976	0.8493	-0.014	0.609	0.001	1093	986	-3
0.8992	0.8494	-0.015	0.602	0.000	1074	1021	-3
1.0000	0.8494	0.000	0.596	0.000	1055	1058	0
tBA (1)+isobutylbenzene (2) at 298.15K							
0.0000	0.8488	0.000	0.979	0.000	1296	701	0
0.0980	0.8496	0.045	0.948	-0.002	1273	726	-2
0.1980	0.8501	0.152	0.916	-0.004	1250	753	-2
0.2973	0.8506	0.260	0.883	-0.008	1228	780	-2
0.3981	0.8511	0.374	0.850	-0.011	1207	807	-3
0.4980	0.8517	0.471	0.818	-0.014	1186	835	-2
0.5972	0.8526	0.519	0.787	-0.015	1167	861	-3
0.6974	0.8539	0.507	0.758	-0.015	1148	889	-2
0.7983	0.8556	0.439	0.730	-0.013	1129	917	-2
0.8980	0.8579	0.281	0.705	-0.008	1110	946	0
1.0000	0.8611	0.000	0.683	0.000	1092	974	0
tBA (1)+isobutylbenzene (2) at 308.15K							
0.0000	0.8404	0.000	0.844	0.000	1260	750	0
0.0980	0.8410	0.031	0.819	-0.001	1237	777	-3
0.1980	0.8414	0.105	0.792	-0.003	1214	806	-5
0.2973	0.8417	0.199	0.765	-0.005	1192	836	-6
0.3981	0.8421	0.278	0.737	-0.008	1171	866	-7
0.4980	0.8425	0.358	0.710	-0.010	1151	896	-7
0.5972	0.8431	0.404	0.684	-0.012	1131	927	-7
0.6974	0.8440	0.404	0.600	-0.071	1111	960	-5
0.7983	0.8453	0.343	0.636	-0.010	1092	992	-4
0.8980	0.8470	0.221	0.615	-0.006	1074	1024	-3
1.0000	0.8494	0.000	0.596	0.000	1055	1058	0
tBA (1)+methoxybenzene (2) at 298.15K							
0.0000	0.9892	0.000	1.017	0.000	1404	513	0
0.0974	0.9736	0.063	0.966	-0.018	1339	573	15
0.1983	0.9581	0.137	0.921	-0.030	1284	633	29

0.2988	0.9433	0.218	0.883	-0.034	1240	689	38
0.3987	0.9293	0.290	0.850	-0.034	1203	744	47
0.4982	0.9161	0.342	0.820	-0.031	1173	793	50
0.5990	0.9034	0.380	0.792	-0.025	1149	838	49
0.6992	0.8916	0.373	0.766	-0.017	1128	881	46
0.7984	0.8807	0.318	0.739	-0.011	1113	917	36
0.8975	0.8707	0.190	0.713	-0.004	1100	949	22
1.0000	0.8611	0.000	0.683	0.000	1092	974	0
tBA (1)+methoxybenzene (2) at 308.15K							
0.0000	0.9791	0.000	0.890	0.000	1376	539	0
0.0974	0.9635	0.037	0.847	-0.014	1309	606	16
0.1983	0.9479	0.096	0.810	-0.022	1255	670	28
0.2988	0.9331	0.153	0.776	-0.026	1211	731	37
0.3987	0.9191	0.201	0.747	-0.026	1174	789	43
0.4982	0.9058	0.243	0.720	-0.024	1144	844	46
0.5990	0.8930	0.271	0.695	-0.019	1119	894	44
0.6992	0.8811	0.255	0.671	-0.013	1098	941	39
0.7984	0.8699	0.222	0.647	-0.008	1081	984	31
0.8975	0.8594	0.149	0.623	-0.003	1067	1022	17
1.0000	0.8494	0.000	0.596	0.000	1055	1058	0

**Table 2:** Density ( $\rho$ ), viscosity ( $\eta$ ), excess molar volume ( $V^E$ ), deviation in viscosity ( $\Delta\eta$ ), speed of Sound ( $u$ ), isentropic compressibility ( $\kappa_s$ ) and deviation in isentropic compressibility ( $\Delta\kappa_s$ ).

Standard deviations	T/K	$a_0$	$a_1$	$a_2$	$a_3$	$a_4$	$\sigma$
tBA (1)+isopropylbenzene (2)							
$V^E/(\text{cm}^3.\text{mol}^{-1})$	298.15	-0.0931	-0.1154	-0.0287			0.0042
	308.15	-0.0804	-0.0866	-0.0028			0.005
$\Delta\eta/(\text{mPa.s})$	298.15	0.0162	-0.0197	-0.0082	0.0187	0.0145	0.0004
	308.15	0.0141	-0.0127	-0.0043			0.0003
$\Delta\kappa_s/(\text{TPa}^{-1})$	298.15	-33.5391	13.6785	17.0287	0	0	0.4448
	308.15	-30.4397	13.0323	-11.732	0	0	0.707
tBA (1)+isobutylbenzene (2)							
$V^E/(\text{cm}^3.\text{mol}^{-1})$	298.15	1.8709	1.3876	-0.1099	0.3165		0.0052
	308.15	1.4375	1.2575	-0.0811			0.0039
$\Delta\eta/(\text{mPa.s})$	298.15	-0.0547	-0.0423	0.0005			0.0003
	308.15	-0.089	-0.0818	0.0652			0.0186
$\Delta\kappa_s/(\text{TPa}^{-1})$	298.15	-10.59	-8.0089	-1.5468	33.0352		0.5755
	308.15	-28.7762	7.8474	16.3418	-10.7753	-37.0481	0.3528
tBA (1)+methoxybenzene (2)							
$V^E/(\text{cm}^3.\text{mol}^{-1})$	298.15	1.3823	0.9712	0.2266	-0.1930	-0.3255	0.0032
	308.15	0.9717	0.5746	0.0767	0.2622		0.0053
$\Delta\eta/(\text{mPa.s})$	298.15	-0.123	0.1006	-0.0035			0.0005
	308.15	-0.0935	0.0772	-0.0024			0.0004
$\Delta\kappa_s/(\text{TPa}^{-1})$	298.15	199.596	40.0968	8.6513	0	0	0.6392
	308.15	181.8703	6.8637	3.1048	0	0	0.5049

**Table 3:** Parameters and standard deviation  $\sigma$  of equations (5) and (6) for tBA + isopropylbenzene, + isobutylbenzene, + methoxybenzene at temp. 298.15 and 308.15 K.

System	T/K	$G_{12}$	$\sigma$	$H_{12}$	$\sigma$	Heric- Brewer		$\sigma$
						$\alpha_{12}$	$\alpha_{21}$	
tBA (1) + isopropylbenzene (2)	298.15	0.025	0.17	0.717	0.17	0.026	-0.017	0.08
	308.15	0.024	0.10	0.631	0.08	0.024	-0.020	0.05
tBA (1) + isobutylbenzene (2)	298.15	-0.003	0.44	0.804	0.41	0.021	-0.044	0.07
	308.15	-0.056	2.33	0.681	2.25	-0.028	-0.120	2.06
tBA (1) + methoxybenzene (2)	298.15	-0.066	0.85	0.788	1.01	-0.032	0.107	0.08
	308.15	-0.045	0.48	0.695	0.67	-0.014	0.094	0.06

**Table 4:** Interaction parameters of Grunberg-Nissan, Hind et al., Heric-Brewer model and standard deviations  $\sigma$  at temp. 298.15 and 308.15 K.

$x_1$	vC=O	vC-H	vC=C	vC-O
tBA( $x_1$ )+isopropylbenzene (1- $x_1$ )				
0.0	-	2955(s) and many peaks within 2886 to 3023	1466 (m)	-
0.4	1736 (s)	2963 (s) 3053 (shoulder)	1452 (m) 1373 (m)	1262 (s) 1169 (s)
0.5	1734 (s)	2957 (s)	1468 (m) 1381 (m)	1263 (s) 1167 (s)
0.6	1734 (s)	2963 (m)	1464 (m) 1373 (m)	1262 (s) 1169 (s)
0.7	1732 (s)	2961 (m)	1470 (m) 1377 (m)	1263 (s) 1165 (s)
0.8	1736 (s)	2974 (m) and many peaks within 2882 to 3065	1458 (m) 1368 (m)	1262 (s) 1171 (s)
1.0	1732 (s)	2982 (m)	-	1262 (s) 1169 (s)
tBA( $x_1$ ) + isobutylbenzene (1- $x_1$ )				
0.0	-	2957 (s) and many Shoulders 2878 to 3071	1458 (m) 1377 (m)	-
0.4	1732 (s)	2947 (s) 3038 (shoulder)	1464 (m) 1373 (m)	1260 (s) 1169 (s)
0.5	1732 (s)	2947 (s) 3042 (shoulder)	1462 (m) 1375 (m)	1260 (s) 1165 (s)
0.6	1736 (s)	2967 (m) and many Shoulders 2876 to 3065	1460 (m) 1370 (s)	1260 (s) 1169 (s)
0.7	1732 (s)	2955 (s) 2920(shoulder) 2874(shoulder)	1460 (m) 1377 (m)	1263 (s) 1171 (s)
1.0	1732 (s)	2982 (m)	-	1262 (s) 1169 (s)

$x_1$	vC=O	vC-H	vC=C	vC-O
tBA( $x_1$ )+methoxybenzene (1- $x_1$ )				
0.0	-	2945 (m) 2837 (m) 3052 (m)	1483 (s) 1593 (s)	-
0.4	1728 (s)	2967 (m)	1478 (s) 1591 (m)	1263 (s) 1169 (m) 1040 (m)
0.5	1728 (s)	2969 (m)	1476 (m) 1593 (m)	1262 (s) 1169 (m) 1038 (m)
0.6	1728 (s)	2971 (m)	1478 (m) 1594 (m)	1262 (s) 1169 (m) 1038 (m)
0.7	1730 (s)	2980 (m) 2859 (shoulder) 3050 (shoulder)	1481 (m) 1595 (m)	1260 (s) 1169 (m) 1032 (m)
0.8	1732 (s)	2980 (m)	1478 (m) 1601 (m)	1260 (s) 1169 (m) 1030 (m)
1.0	1732 (s)	2982 (m)	-	1262 (s) 1169 (s) 1028 (m)

**Table 5:** FTIR stretching frequency ( $\text{cm}^{-1}$ ) of tBA( $x_1$ ) and isopropylbenzene, isobutylbenzene, methoxybenzene (1- $x_1$ ).

$$\eta = X_1^2 \eta_1 + X_2^2 \eta_2 + 2X_1X_2H_{12} \quad (8)$$

where  $H_{12}$  is an interaction parameter and is attribute to unlike pair interactions.

The two parameter Heric and Brewer [16] equation is of the form

$$\ln v = x_1 \ln v_1 + x_2 \ln v_2 + x_1 \ln M_1 + x_2 \ln M_2 - \ln \left[ \frac{M_1 + x_2 M_2}{M_1 + x_1 M_2} \right] + x_1 x_2 [\alpha_2 + \alpha_3 (x_1 - x_2)] \quad (9)$$

where  $M_1$  and  $M_2$  are molecular weights of components 1 and 2 and  $\alpha_{12}$ ,  $\alpha_{21}$  are interaction parameters.

The correlating ability of equations (7) to (9) was tested by calculating the percentage standard deviation ( $\sigma$  %) between the experimental and calculated viscosity as

$$\sigma \% = \left[ \frac{1}{(n-m) - \sum \left\{ \left( \frac{100(i_{\text{exptl}} - i_{\text{calcd}})}{i_{\text{exptl}}} \right)^2 \right\}^{1/2}} \right] \quad (10)$$

where  $n$  represents the number of experimental points and  $m$  represents the number of coefficients. From Table 4, it is seen that the values of  $G_{12}$  are positive for the binary mixtures of tBA with isopropylbenzene and negative for methoxybenzene. Also for isobutylbenzene  $G_{12}$  negative at 298.15K and positive at 308.15K. The values of  $H_{12}$  are positive for all the binary mixtures while  $\alpha_{12}$  is positive for isopropylbenzene and isobutylbenzene and for methoxybenzene it is negative at 298.15K and positive at 308.15K. Also  $\alpha_{21}$  is negative for isopropylbenzene and isobutylbenzene and positive for methoxybenzene.

The variation of  $\Delta\kappa_s$  with mole fraction of tBA,  $x_1$ , is represented in Figure 3. The values of  $\Delta\kappa_s$  for mixtures of tBA with isobutylbenzene and methoxybenzene are positive and negative for isopropylbenzene. The trend is observation is methoxybenzene more positive than isobutylbenzene.

Kiyohara and Benson [17] have suggested that  $\Delta\kappa_s$  is the resultant of several opposing effects. The positive values may be attributed to the size of these molecules that allow relative molecular interactions between acetate molecules [18]. The trend signify decreasing dipole-dipole interactions due to decreasing proton donating abilities with increasing chain length of aromatic hydrocarbons. From Table 5, the  $\nu\text{C}=\text{O}$  of tBA+isopropylbenzene decreased slightly from  $x_1=0.4$  onwards. Irregular trend in  $\nu\text{C}=\text{C}$  and alkyl  $\nu\text{C}-\text{H}$  is observed. There is no drastic change in  $\nu\text{C}-\text{O}$  stretching frequencies. From observation of  $\nu\text{C}=\text{C}$  of system it is concluded that the magnitude of interaction are more for tBA+isopropylbenzene.

The  $\nu\text{C}=\text{O}$  of TBA+Isobutylbenzene remains same within  $x_1=0.4-0.7$  except at  $x_1=0.6$ . Trend of  $\nu\text{C}-\text{H}$  was irregular with remarkable changes.  $\nu\text{C}=\text{C}$  increased from  $x_1=0.0$  to 0.4 and decreased  $x_1=0.5$  onwards. There are equal intense bands for  $\nu\text{C}-\text{O}$  in  $x_1=0.4-0.6$ . Presence of extra  $\text{CH}_2$  group in isobutylbenzene as compared to isopropyl benzene affects  $\nu\text{C}=\text{C}$  and  $\nu\text{C}-\text{H}$ . More changes in  $\nu\text{C}=\text{C}$  are observed in isobutylbenzene. The  $\nu\text{C}=\text{O}$  almost remain same for tBA+methoxybenzene from  $x_1=0.4$  to 0.6 and then slightly increases.  $\nu\text{C}-\text{H}$  sharply increased from  $x_1=0.4$  onwards. An irregular trend in  $\nu\text{C}=\text{C}$  is observed for this system. The aromatic  $\nu\text{C}-\text{O}$  decreased with increase in  $x_1$ . This suggests dipole-induced dipole interaction between carbonyl of tBA and aryl C-O.

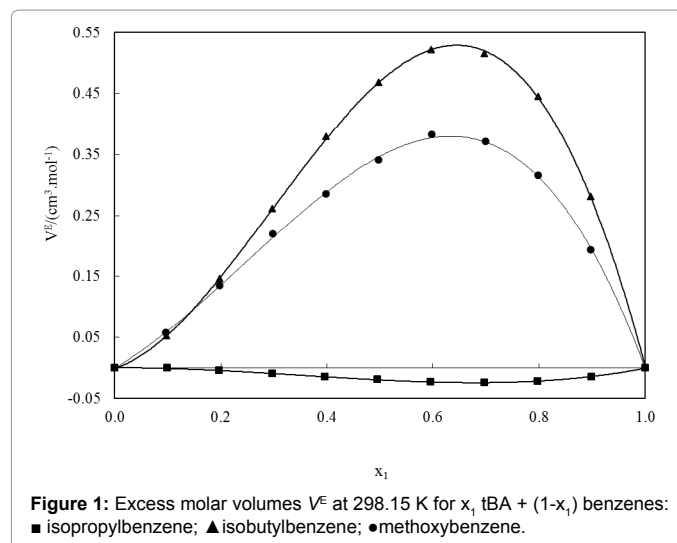


Figure 1: Excess molar volumes  $V^E$  at 298.15 K for  $x_1$  tBA +  $(1-x_1)$  benzenes: ■ isopropylbenzene; ▲ isobutylbenzene; ● methoxybenzene.

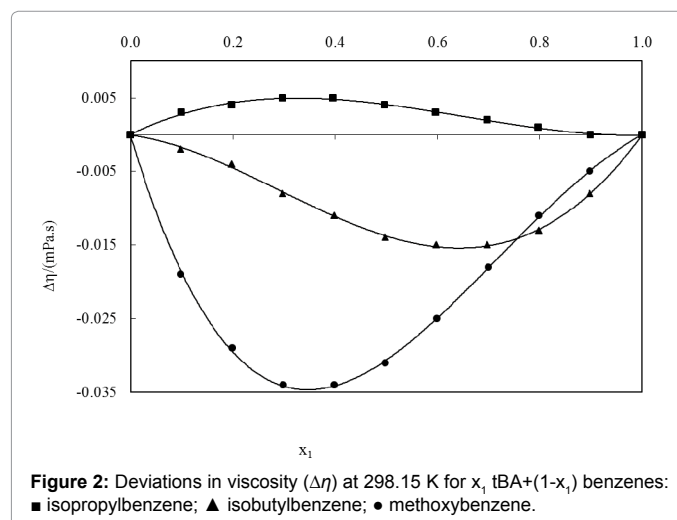


Figure 2: Deviations in viscosity ( $\Delta\eta$ ) at 298.15 K for  $x_1$  tBA+( $1-x_1$ ) benzenes: ■ isopropylbenzene; ▲ isobutylbenzene; ● methoxybenzene.

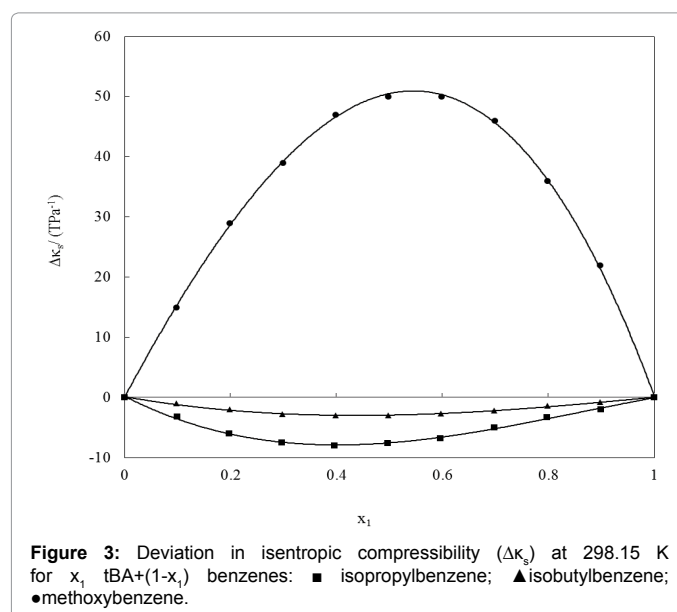


Figure 3: Deviation in isentropic compressibility ( $\Delta\kappa_s$ ) at 298.15 K for  $x_1$  tBA+( $1-x_1$ ) benzenes: ■ isopropylbenzene; ▲ isobutylbenzene; ● methoxybenzene.

## Conclusion

The excess molar volumes and deviations in isentropic compressibility with tBA are positive for the mixtures of isobutylbenzene and methoxybenzene with tBA and, negative for isopropylbenzene with tBA while deviations in viscosities are negative for the binary mixtures of isobutylbenzene, methoxybenzene and positive for isopropylbenzene. The excess molar volumes, deviations in viscosity and, deviations in isentropic compressibility have been fitted to the Redlich-Kister polynomial equation. In FTIR spectra, presence of extra CH<sub>2</sub> group in isobutylbenzene as compare to isopropylbenzene affects  $\nu_C = C$  and  $\nu_{C-H}$ . More changes in  $\nu_{C=C}$  are observed in isobutylbenzene. The aromatic  $\nu_{C-O}$  decreased with increase in  $x_1$ . This suggests dipole-induced dipole interaction between carbonyl of tBA and aryl C-O.

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