International Journal of Thermodynamics(IJoT)
ISSN 1301-9724 / e-ISSN 2146-1511
https://dergipark.org.tr/en/pub/ijot

Vol. 25 (No. 4), pp. 9-22, 2022
doi: 10.5541/ijot.1121062
Published online: December 1, 2022

Research Article

Thermodynamic Properties of Binary Liquid Mixtures Containing Furfural with Chlorobenzene, Nitromethane, Diethylmalonate and 1-Butanol at 308.15K and 318.15K Supported by FTIR Spectral Studies

[1]R. Uthirapathi, [2]U.S. Kishnamoorthy, [3*]R.V. Ambrose

[1,3]Department of Chemistry, St. Joseph's College (Autonomous),
Affiliated to Bharathidasan University, Tiruchirappalli, India.
[2]Department of Chemistry, Cauvery College for Women,
Affiliated to Bharathidasan University, Tiruchirappalli, India.
E-mails: [1]revathiuthirapathi.22@gmail.com, [3*]rosevenis@gmail.com

Received 25 May 2022, Revised 13 July 2022, Accepted 9 August 2022

Abstract

A study on thermodynamic properties of the liquid mixture is used in the industrial process, which often extends to solution chemistry. Density(**ρ**), Viscosity(η), and Ultrasonic velocity(**U**) were determined for binary liquid mixtures of furfural with chlorobenzene, nitromethane, diethyl malonate and 1- butanol at temperature of 308.15K and 318.15K at atmospheric pressure over the whole range of mole fractions. The calculated thermodynamic properties and some excess parameters such as Excess Volume($\mathbf{V^E}$), Deviation in Isentropic Compressibility($\Delta\mathbf{K_S}$), Deviation in Viscosity($\Delta\boldsymbol{\eta}$), Deviation in Intermolecular Free Length($\Delta\mathbf{L_F}$), Deviation in Intermolecular Free Volume($\Delta\mathbf{V_F}$), Deviation in Internal Pressure($\Delta\boldsymbol{\pi}$) and Deviation in Acoustic Impedance($\Delta\mathbf{Z}$) were calculated and applied to the Redlich-Kister type polynomial equation to determine the appropriate coefficients. The effects of composition and temperature on thermodynamic parameters have been studied in terms of molecule interaction in these liquid mixtures. Further, IR spectra of these liquid mixtures were recorded and the data were utilized to examine the mixing behavior of the components.

Keywords: *Furfural; molecular interaction; Redlich-Kister equation; thermodynamic parameters.*

1. Introduction

Furfural is the only unsaturated large-volume organic chemical created from carbohydrate resources and is a critical derivative for producing essential chemicals that cannot be acquired from petroleum, it is an important substance accessible from biomass [1]. The petrochemical, agricultural and polymer industries all employ it as a solvent [2]. The aprotic solvent nitromethane [3] has a strong polarity and is employed in a range of applications. Adhesives, paints, paint removers, polishes, dyes and medications are all made with chlorobenzene as a high boiling solvent. Diethyl malonate is a chemical that is utilized in the production of vitamins B1 and B6, as well as medicines, agrochemicals, flavor, and aroma compounds [4]. 1-Butanol is a useful solvent that is affordable and readily accessible in high purity. It's utilized in chemical and technical operations [5].

We investigated the molecular interaction between binary liquid mixtures of furfural with chlorobenzene, nitromethane, diethyl malonate and 1-butanol. Thermodynamic properties of Density (**ρ**), Viscosity (**η**), and Ultrasonic velocity (**U**) were measured over the entire composition range at temperature of 308.15K 318.15K. Excess Volume ($\mathbf{V^E}$), Deviation in Isentropic Compressibility ($\Delta\mathbf{K_S}$), Deviation in Viscosity ($\Delta\boldsymbol{\eta}$), Deviation in Intermolecular Free Length ($\Delta\mathbf{L_F}$), Deviation in Intermolecular Free Volume ($\Delta\mathbf{V_F}$), Deviation in Internal Pressure ($\Delta\boldsymbol{\pi}$) and Deviation in Acoustic Impedance ($\Delta\mathbf{Z}$) have all been calculated based on the above measured data. The thermodynamic properties of liquid mixtures are needed in many industries, such as medicine, petroleum and chemical engineering [6]. These chemicals prompted the current thermodynamic analysis. Thermodynamic and transport properties of liquid and liquid mixtures are utilized to understand engineering applications such as heat transmission, mass transfer and fluid movement[7-8].Using the data from the aforementioned measurements, to investigate the nature of molecular interactions in liquid mixtures between unlike molecules.

2. Experimental

2.1. Material

Chlorobenzene (Merck, Mumbai, purity > 99%) was dried over anhydrous calcium chloride and distilled. Nitromethane (SRL, Mumbai, purity >99%), 1-butanol (Thermo fisher scientific, Mumbai, Purity >99%), were purified by distillation, and furfural (SRL, Mumbai, Purity >99%), and diethylmalonate (SRL, Mumbai, Purity >99%) were used without further purification. The purity of the pure compounds was also confirmed by comparing the measured density, viscosity, and ultrasonic velocity of the pure compounds at various temperatures with those described in the literature, which showed a fair agreement and is listed in Table 1 [9-15].

*Corresponding Author

2.2. Measurement

For each mixture, a series of nine compositions were prepared, and their physical properties were measured at the relevant compositions on a mole fraction scale ranging from 0.1 to 0.9 in 0.1 increments [16]. Binary liquid mixtures of various compositions were made by combining a predetermined amount of pure liquids in 50ml airtight stopper bottles using an analytical balance with 0.0001g accuracy.

2.2.1. Density(ρ)

Densities of pure liquids and liquid mixtures were measured by specific gravity method [17] with 10 mL relative density bottle and weighed with an exactness of ± 0.001 kg m^{-3}.

$$\rho = \left[\frac{W \times d_0}{W_0} \right] \qquad (1)$$

Where 'w' is the mass of the liquid or liquid mixtures, 'w_0' is the mass of the water, and 'd_0' is the density of the water.

2.2.2. Viscosity (η)

Viscosities were determined by Oswald viscometer 10 mL capability with an accurateness of ± 0.001 cP [18]. From the measured values of density and flow time 't', viscosity 'η' was calculated. The values of constants were occurred by measuring the flow time with distilled water and pure nitrobenzene as standard liquids. The flow time were measured with electronic stop clock.

$$\eta = \left(At - \frac{B}{t} \right) \rho \qquad (2)$$

Where, 'ρ' is the density of a pure liquid or a combination of liquids, 't' is the time flow in seconds, and A and B characteristic constants at the specified temperature.

2.2.3. Ultrasonic Velocity

The ultrasonic velocity pure liquid and liquid mixtures values were measured using an ultrasonic interferometer (Pico, Chennai, India) with a frequency of 2MHz was calibrated [19] using water and nitrobenzene. The overall accuracy in the measurement is ±0.2%. All the measurements were taken using a digital thermostat with a temperature precision of 0.01K at 308.15K and 318.15K. The details of the methods and techniques of the measurements have been described earlier.

2.3. FTIR Study

The FTIR (Fourier transform infrared spectroscopy) spectra were recorded using a Perkin Elmer spectrum RX1 (PerkinElmer, inc., Waltham, MA, USA). FTIR properties have been used to study a specific interaction, such as the formation of a hydrogen bond between molecules that are dissimilar in liquid mixtures.

3. Theoretical approach

3.1. Excess Molar Volume (V^E)

The difference between the volume before and after mixing is called excess volume.

$$V^E = \left[\frac{(X_1 M_1) + (X_2 M_2)}{\rho} \right] - \left[\left(\frac{X_1 M_1}{\rho_1} \right) + \left(\frac{X_2 M_2}{\rho_2} \right) \right] \qquad (3)$$

X_1, M_1 and ρ_1, X_2, M_2 and ρ_2 are mole fraction, molar mass, and density of pure components 1 and 2 respectively [20].

3.2. Isentropic Compressibility (Ks)

Densities and ultrasonic velocities of liquids and liquid mixtures are used to indirectly and directly calculate isentropic compressibility.

$$K_S = \frac{1}{U^2 \rho} \qquad (4)$$

Where, 'U' is the speed of sound and *'ρ'* is the density of the liquid mixtures.

3.3. Deviation of Isentropic Compressibility (ΔKs)

$$\Delta K_S = K_S - (\Phi_1 K_{S1} + \Phi_2 K_{S2}) \qquad (5)$$

Where, 'ΔK_S' denotes the mixtures isentropic compressibility, Φ_1, K_1, S_1 and $\Phi_2, K_2 S_2$ denote the volume fraction and isentropic compressibility of pure components 1 and 2, respectively [21].

3.4. Excess viscosity (Δη)

$$\Delta\eta = \eta(X_1\eta_1 + X_2\eta_2') \qquad (6)$$

Where, η_1 and η_2 are the viscosity values of pure component 1 and 2 respectively.

3.5. Free Length

Values of ultrasonic velocity u and density of mixture ρ_{AB} were used to calculate inter molecular Free Length (L_f), Acoustic Impedance (Z) and intermolecular Free Volume (V_f) using the following relation [22] by

$$L_F = \frac{K}{U\rho^{1/2}} \qquad (7)$$

Where, U is ultrasonic velocity of pure liquid and liquid mixtures, and ρ is the density of pure and mixture, where K is Jacobson's constant which is temperature-dependant constant but independent of the nature of the liquid.

3.6. Acoustic Impedance

$$Z = U\rho \qquad (8)$$

Where, U is ultrasonic velocity of pure liquid and liquid mixtures, and ρ is the density of pure and mixture.

3.7. Free Volume

Intermolecular free volume has been calculated using the following relation [23].

$$V_F = \left[\frac{M_{eff} U}{(K\eta)} \right]^{3/2} \qquad (9)$$

Where, K is a temperature independent constant that is equal to 4.28 × 10^9 for all the liquids and M_{eff} is the effective molecular weight of the mixture.

3.8. Presentation of the research findings

The excess properties of Excess Volume ($\mathbf{V^E}$), deviation in Isentropic Compressibility ($\Delta\mathbf{K_S}$), deviation in Viscosity ($\Delta\boldsymbol{\eta}$), deviation in intermolecular Free Length ($\Delta\mathbf{L_F}$), deviation in intermolecular Free Volume ($\Delta\mathbf{V_F}$), deviation in Internal Pressure ($\Delta\boldsymbol{\pi}$) and deviation in Acoustic Impedance ($\Delta\mathbf{Z}$) were fitted to Redlich–Kister type [23] polynomial equation.

$$\Delta A = X_1 X_2 \left[a + b(X_1 - X_2) c(X_1 - X_2) \right] \qquad (10)$$

The least-squares method was used to derive the adjustable parameters a, b and c.

The standard deviations (σ) presented in this work were computed using

$$\sigma = \left(\Sigma (X_{\exp} - X_{cal})^2 \mid N - n \right)^{1/2} \qquad (11)$$

Where, N is the number of data points, and n is the number of co-efficient. Coefficient values of the Redlich-Kister type polynomial equation (Eq.10) and standard deviation (Eq.11) at different temperatures are presented in Table 4.

4. Results and discussion

4.1. Excess thermodynamic parameters

Tables 2 and 3 signify the investigational values of density (ρ), viscosity (η), and ultrasonic velocity (U) and calculated values of excess volume (V^E), deviation in isentropic compressibility (ΔK_S) and deviation in viscosity ($\Delta\eta$) of all the four binary liquid mixtures at 308.15K and 318.15K.

In the pure state, furfural molecules are known to exist as associated molecules [25]. Over the entire range of composition, Excess Volume (V^E) and deviation in Isentropic Compressibility (ΔK_S) values of furfural with nitromethane are low negative (Figure 1 and Figure 2). The oxygen atom of furfural attracts the nitrogen atom of the nitro group, resulting in dipole-dipole interaction. However, there will be less nitro group interaction between the unlike molecules. Over the entire range of composition, Excess Volume (V^E) and deviation in Isentropic Compressibility (ΔK_S) values of furfural + chlorobenzene are negative (Figure 1 and Figure 2). The furfural carbonyl group has a polarity, which allows it to interact with the chlorine atom in chlorobenzene. As a result, it involves a dipole-dipole interaction.

Over the entire range of composition, Excess Volume ($\mathbf{V^E}$) and deviation in isentropic compressibility ($\Delta\mathbf{K_S}$) values of furfural + 1-butanol are large negative (Fig. 1 and 2) values. The presence of substantial interactions between dissimilar molecules is demonstrated by the large negative $\mathbf{V^E}$ values of (furfural + 1-butanol) binary liquid mixtures. These findings suggest that furfural has a stronger interaction with 1-butanol, but alcohols are strongly self-associated by H-bonding, with degrees of association varying depending on chain length and temperature [26]. The presence of a significant dipole-dipole interaction between furfural and 1-butanol is shown by the negative V^E values.

Over the entire range of composition, Excess Volume ($\mathbf{V^E}$) and deviation in Isentropic Compressibility ($\Delta\mathbf{K_S}$) values of furfural + diethyl malonate are negative (Figure1 and Figure 2). Because both esters and aldehydes have a carbonyl group, they become somewhat dipole due to the inductive action. The –O atom of the furfural can attract the –C atom of the ester group, resulting in dipole-dipole interaction [27]. An alkyl group is an electron-donating group, and its ability to do so increases with the length of the ester molecules chain. Furthermore, the negative values found in this study indicate the effective packing effect generated by interstitial accommodation as the chain length of ester molecules rises, increasing intermolecular contact.

Over the entire composition range, the viscosity deviations of all four liquid mixtures are positive show figure 3. Figure 3 depicts the decline in positive values as temperature rises. Furfural + nitromethane have the lowest positive values, indicating that the intermolecular forces are greater than in other mixtures. This backs with the earlier theory that nitromethane interacts with furfural dispersion forces between furfural and 1-butanol and that the deviation from ideality is greater. Because the positive values of deviation in viscosity ($\Delta\boldsymbol{\eta}$) for nitromethane, chlorobenzene, diethylmalonate, and 1-butanol are all greater than nitrobenzene and lower than 1-butanol, the interaction is less than nitromethane and higher than 1-butanol. Deviation in viscosity ($\Delta\boldsymbol{\eta}$) graph's values are in the same order as excess volume ($\mathbf{V^E}$) and deviation in isentropic compressibility ($\Delta\mathbf{K_S}$) values[27].

The observed values of intermolecular free length (ΔL_F), intermolecular free volume (ΔV_F) and intermolecular internal pressure ($\Delta\pi$) (Figures 4, 6 and 7) reflect the same idea as obtained above. For the four liquid mixtures, when the temperature rises, the intermolecular internal pressure ($\Delta\pi$) values of the liquid mixtures decrease and the intermolecular free volume ($\Delta\mathbf{V_F}$) values rise. Due to an increase in the thermal motion of interacting molecules, the nature of interaction for the four liquid mixtures reduces when the temperature is increased. Dispersion forces between mixing liquids cause negative values, while attractive forces like dipole-dipole interaction cause positive values.

Positive and negative deviation of the mixtures shows the level of association or dissociation between the mixing components [28-29], whereas deviation in acoustic impedance ($\Delta\mathbf{Z}$) acts in the opposite direction to intermolecular free length ($\Delta\mathbf{L_F}$). The observed values of deviation in viscosity ($\Delta\boldsymbol{\eta}$) and deviation in acoustic impedance ($\Delta\mathbf{Z}$) are positive throughout the range (Figures 3 and Figures 5), confirming the stated hypothesis. Furfural + nitro methane < furfural + chlorobenzene < furfural + diethylmalonate < furfural + 1-butanol is the order of the interactions between the systems.

4.2. FTIR Results

Figures 8 to 11 show FTIR results for nitromethane, chlorobenzene, diethyl malonate, and 1-butanol in the binary liquid mixtures with furfural in a molar fraction of 0.5.

According to FTIR analysis, a pure furfural molecule shows a peak at 1686.93 cm^{-1} which is due to the C=O bond, while an equimolar mixture of nitromethane, and chlorobenzene (Figure 8, 9) exhibits a peak at 1689.80 cm^{-1}, 1678.78 cm^{-1} and 1679.30 cm^{-1}. Pure nitromethane liquid molecule shows a peak at 1576.88 cm^{-1} which is due to the N=O bond, while an equimolar mixture of furfural + nitro methane (Figure 8) exhibits a peak at 1566.42 cm^{-1}. The change in the frequency and intensity confirms the existence of intermolecular interaction between –C=O and –N=O. Hence, it involves weak dipole-dipole interaction. Pure chlorobenzene liquid molecule shows a peak at 743.20 cm^{-1} which is due to the -C-Cl bond, while an equimolar mixture of furfural + chlorobenzene (Figure 9) exhibits a peak at 751.30 cm^{-1}. The changes in the frequency and intensity confirm the existence of intermolecular interaction between –C=O and –C-Cl, hence, it involves dipole-dipole interaction.

A pure diethyl malonate molecule shows a peak at 1745.13 cm^{-1} which is due to the C=O bond. The equimolar mixture of furfural + diethyl malonate (Figure 10) shows a peak at 1691.24 cm^{-1} and 1740.38 cm^{-1} which is due to the C=O bond. The changes in the frequency and intensity confirm the existence of intermolecular interaction between carbon atom of the ester group and the oxygen atom of furfural, hence it involves dipole-dipole interaction.

A pure 1-butanol molecule has a peak at 3343.65 cm^{-1} which is characteristic of the –OH group. The equimolar mixture of furfural + 1-butanol (Figure 11) shows broad band at 3417.52 cm^{-1}. The change in frequency from 3343.65 to 3417.52 cm^{-1} and changes in intensity confirms the existence of an intermolecular hydrogen bond form between the –OH and –CHO group. These findings suggest that furfural has a stronger interaction with 1-butanol, but alcohols are strongly self-associated by H-bonding, with degrees of association varying depending on chain length and temperature. Hence it involves dipole-dipole interaction.

5. Conclusion

In this study Excess Volume **(V^E)**, Deviation in Isentropic Compressibility **(ΔK_S)** and Deviation in Viscosity **($\Delta\eta$)** for liquid mixtures of furfural with aromatic and aliphatic compounds are studied. The magnitude of Excess Volume **(V^E)**, Deviation in Isentropic Compressibility **(ΔK_S)**, Deviation in Viscosity **($\Delta\eta$),** Deviation in Intermolecular Free Length (ΔL_F), Deviation in Intermolecular Free Volume **(ΔV_F)**, Deviation in Internal Pressure **($\Delta\pi$)** and Deviation in Acoustic Impedance **(ΔZ)** has been interpreted in terms of molecular interactions between these molecules. Both V^E and ΔK_S values are negative and the high positive value of $\Delta\eta$ for furfural + 1-butanol shows more interaction between furfural and 1-butanol. For furfural + nitrometane mixtures the V^E and ΔK_S values are negative and $\Delta\eta$ values are less positive due to less interaction between the mixing liquids. The existence of strong dipole-dipole interaction between furfural + chloro benzene, furfural + diethyl malonate, and furfural + 1-butanol, as well as less dipole-dipole interaction between furfural + nitromethane is proved by the values of excess properties. Because of thermal motion, the intermolecular interaction reduces as the temperature rises. To determine the variable coefficients, the corresponding thermodynamic excess parameters were calculated with the formulas reported earlier and fitted to a Redlich-Kister type polynomial equation. Based on the experimental and calculated results, the behavior of the liquid mixtures and deviation from ideality has been examined. An analysis of FTIR spectroscopy showed the establishment of hydrogen bonds between unlike molecules.

Nomenclature

V^E	Excess volume
K_S	Adiabatic compressibility
K	Jacobson's constant
X_i	Mole fraction of the i^{th} component
A_i	Parameters of the i^{th} component (Redlich–Kister equation Coefficients)
ρ_{mix}	Density of liquid mixture
n	Number of measurements
m	Number of adjustable parameters
t	Flow time

Appendix

Table 1. Comparison of Experimental Density (ρ), Viscosity (η), Ultrasonic Velocity (U) of Pure Liquids with literature Value at 308.15K and 318.15 K.

Liquids	T(K)	$\rho(g\ cm^{-3})$		$\eta(mPa\ s^{-1})$		$U(ms^{-1})$	
		Exp.	Lit.	Exp.	Lit.	Exp.	Lit.
Furfural [9,10]	308.15	1.1447	1.1440	1.2716	1.2600	1406.5	1403.77
	318.15	1.1324	1.1330	1.0921	1.0900	1370.5	1367.81
Chlorobenzene[11,12]	308.15	1.0892	1.0894	0.7002	0.7009	1221.5	1228
	318.15	1.0768	1.0794	0.5630	0.5629	1201.5	1208.5
Nitromethane[13]	308.15	1.1172	1.1176	0.5637	0.5640	1285	1277.1
	318.15	1.1038	1.1042	0.5171	0.5100	1278	-
1-Butanol[14]	308.15	0.7981	0.7979	2.0021	2.0080	1218	1209
	318.15	0.7935	0.7901	1.9022	1.5800	1207	-
Diethylmalonate[15]	308.15	1.0440	1.0418	1.6019	1 .6003	1245	1277.0
	318.15	1.0254	1.0283	1.4200	1.4235	1223	1235.5

Table 2. Physical and Thermodynamic Parameters for Binary liquid Mixtures of Furfural + Chlorobenzene, Furfural + Nitromethane, Furfural + 1-Butanol, and Furfural + Diethylmalonate at 308.15 and 318.15 K.

308.15K						318.15K					
X_1	ρ ($g\ cm^{-3}$)	η ($mPa\ s^{-1}$)	U (ms^{-1})	ΔV^E (cm^3mol^{-1})	ΔKs (Tpa^{-1})	X_1	ρ ($g\ cm^{-3}$)	η ($mPa\ s^{-1}$)	U (ms^{-1})	ΔV^E (cm^3mol^{-1})	ΔKs (Tpa^{-1})
Furfural+ Chlorobenzene						**Furfural+ Chlorobenzene**					
0.0000	1.0892	0.7002	1221	0.0000	0.0000	0.0000	1.0768	0.5630	1201	0.0000	0.0000
0.1236	1.0958	0.7786	1259	-0.0866	-22.2245	0.1236	1.0833	0.6342	1235	-0.0742	-20.2950
0.1755	1.0987	0.8119	1274	-0.1219	-28.9691	0.1755	1.0860	0.6653	1248	-0.0997	-27.1024
0.2884	1.1049	0.8840	1300	-0.1803	-36.8044	0.2884	1.0923	0.7326	1273	-0.1574	-35.5091
0.4132	1.1121	0.9610	1325	-0.2380	-40.3508	0.4132	1.0995	0.8046	1296	-0.2142	-39.2356
0.5509	1.1200	1.0412	1351	-0.2631	-39.8437	0.5509	1.1072	0.8787	1320	-0.2288	-38.5934
0.6416	1.1252	1.0905	1366	-0.2528	-36.4652	0.6416	1.1124	0.9240	1333	-0.2169	-35.1921
0.7380	1.1305	1.1403	1381	-0.2149	-30.9757	0.7380	1.1177	0.9694	1346	-0.1767	-29.3556
0.8042	1.1341	1.1736	1390	-0.1737	-25.3147	0.8042	1.1213	1.0000	1354	-0.1336	-24.0008
0.9147	1.1401	1.2294	1400	-0.0837	-11.9791	0.9147	1.1275	1.0510	1363	-0.0635	-10.5845
1.0000	1.1447	1.2685	1406	0.0000	0.0000	1.0000	1.1324	1.0921	1375	0.0000	0.0000
Furfural+ Nitromethane						**Furfural+ Nitromethane**					
0.0000	1.1169	0.5635	1266	0.0000	0.0000	0.0000	1.1073	0.5145	1257	0.0000	0.0000
0.0955	1.1216	0.6352	1285	-0.0418	-2.6842	0.0955	1.1114	0.5725	1273	-0.0307	-2.1122
0.1822	1.1254	0.7006	1301	-0.0753	-4.4546	0.1822	1.1148	0.6271	1288	-0.0582	-4.0730
0.2729	1.1289	0.7691	1317	-0.1015	-5.6512	0.2729	1.1180	0.6842	1301	-0.0830	-5.1218
0.3996	1.1333	0.8624	1336	-0.1380	-6.0063	0.3996	1.1220	0.7620	1318	-0.1166	-5.4251
0.4968	1.1362	0.9316	1349	-0.1544	-5.9680	0.4968	1.1247	0.8190	1329	-0.1355	-5.2815
0.5907	1.1382	0.9960	1361	-0.1383	-5.4164	0.5907	1.1265	0.8722	1340	-0.1197	-4.8871
0.6954	1.1403	1.0655	1374	-0.1164	-4.6632	0.6954	1.1283	0.9281	1350	-0.0987	-4.0243
0.7999	1.1420	1.1342	1385	-0.0848	-3.6761	0.7999	1.1299	0.9838	1360	-0.0667	-2.8708
0.8929	1.1434	1.1948	1394	-0.0493	-2.3409	0.8929	1.1311	1.0332	1367	-0.0355	-1.5479
1.0000	1.1447	1.2685	1406	0.0000	0.0000	1.0000	1.1324	1.0921	1375	0.0000	0.0000
Furfural + 1-Butanol						**Furfural + 1-Butanol**					
0.0000	0.7985	1.9466	1201	0.0000	0.0000	0.0000	0.7909	1.8234	1183	0.0000	0.0000
0.0912	0.8292	1.9065	1255	-0.2284	-66.4956	0.0912	0.8210	1.7743	1226	-0.1899	-57.5297
0.1863	0.8621	1.8635	1298	-0.4670	-106.0557	0.1863	0.8534	1.7224	1268	-0.4144	-99.8946
0.2536	0.8857	1.8319	1322	-0.6250	-121.4938	0.2536	0.8768	1.6867	1291	-0.5833	-116.773
0.3530	0.9208	1.7811	1350	-0.7981	-130.9608	0.3530	0.9114	1.6326	1317	-0.7557	-127.415
0.4675	0.9609	1.7113	1374	-0.8883	-127.8928	0.4675	0.9512	1.5584	1340	-0.8489	-125.136
0.5561	0.9920	1.6478	1386	-0.8929	-116.6501	0.5561	0.9820	1.4880	1351	-0.8674	-114.568
0.6619	1.0291	1.5656	1395	-0.8483	-96.2282	0.6619	1.0188	1.3988	1358	-0.8220	-93.2678
0.7833	1.0716	1.4652	1401	-0.7007	-66.5358	0.7833	1.0605	1.2933	1364	-0.6599	-63.5723
0.9015	1.1119	1.3630	1406	-0.4166	-33.2236	0.9015	1.1005	1.1843	1369	-0.3762	-30.4705
1.0000	1.1447	1.2685	1406	0.0000	0.0000	1.0000	1.1324	1.0921	1375	0.0000	0.0000
Furfural + Diethylmalonte						**Furfural + Diethylmalonte**					
0.0000	1.0440	1.6019	1245	0.0000	0.0000	0.0000	1.0254	1.4200	1223	0.0000	0.0000
0.1678	1.0556	1.5726	1303	-0.2250	-43.0370	0.1678	1.0374	1.3865	1273	-0.1977	-39.6491
0.2467	1.0619	1.5554	1327	-0.3393	-56.5555	0.2467	1.0439	1.3692	1296	-0.3021	-54.1231
0.3357	1.0696	1.5329	1350	-0.4662	-66.9954	0.3357	1.0518	1.3475	1317	-0.4240	-65.0450
0.4376	1.0792	1.5027	1372	-0.5845	-73.3277	0.4376	1.0619	1.3175	1338	-0.5491	-71.8324
0.5016	1.0853	1.4827	1382	-0.6116	-73.6144	0.5016	1.0684	1.2973	1348	-0.5845	-72.5150
0.5836	1.0932	1.4535	1393	-0.5740	-70.4455	0.5836	1.0768	1.2683	1357	-0.5481	-68.9323
0.6801	1.1031	1.4157	1401	-0.4792	-62.1206	0.6801	1.0873	1.2303	1364	-0.4462	-60.3671
0.7553	1.1114	1.3849	1404	-0.3812	-51.6762	0.7553	1.0961	1.1992	1367	-0.3389	-49.6422
0.8499	1.1228	1.3425	1405	-0.2291	-34.8472	0.8499	1.1086	1.1582	1370	-0.2077	-34.2550
1.0000	1.1447	1.2685	1406	0.0000	0.0000	1.0000	1.1324	1.0921	1375	0.0000	0.0000

Table 3. Thermodynamic Parameters for binary liquid mixtures of Furfural + Chlorobenzene, Furfural + Nitromethane, Furfural + 1-Butanol and Furfural + Diethylmalonate at 308.15 and 318.15 K.

308.15K					318.15K				
$\Delta\eta$ (mPa.s)	ΔL_F (10^{-10} m)	ΔV_F (10^{-14} m^3mol^{-1})	ΔZ (kg m^{-3} s^{-1})	$\Delta\pi$(Pa)	$\Delta\eta$ (mPa.s)	ΔL_F (10^{-10} m)	ΔV_F(10^{-14} m^3mol^{-1})	ΔZ (kgm^{-3} s^{-1})	$\Delta\pi$(Pa)
Furfural+Chlorobenzene					**Furfural+Chlorobenzene**				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0079	-44.0821	-0.6831	15.2021	-18.5088	0.0059	-39.2563	-1.5300	12.1844	-16.97
0.0115	-57.5586	-0.8664	20.2562	-25.2567	0.0095	-52.7518	-1.9272	16.8683	-23.12
0.0191	-71.6937	-1.1163	25.3895	-37.3985	0.0170	-68.3330	-2.4204	22.2611	-34.22
0.0247	-77.7808	-1.1711	28.1975	-46.6535	0.0230	-74.8265	-2.4944	24.9890	-42.61
0.0263	-76.9120	-1.0451	29.3235	-51.1063	0.0243	-73.3177	-2.1913	25.5580	-46.72
0.0238	-70.4550	-0.8909	27.7817	-50.1193	0.0215	-66.6731	-1.8525	23.9089	-45.90
0.0184	-60.4403	-0.6824	25.0664	-45.0989	0.0158	-55.5401	-1.4112	20.6267	-41.40
0.0140	-49.5817	-0.5236	21.1800	-38.5872	0.0115	-45.4179	-1.0781	17.3416	-35.57
0.0065	-23.0278	-0.2395	9.9586	-20.5165	0.0040	-18.8559	-0.4877	6.8425	-19.07
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.00
Furfural+ Nitromethane					**Furfural+Nitromethane**				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0046	-21.3651	-0.1520	8.9699	-5.4167	0.0029	-18.9283	-0.1479	7.6592	-5.37
0.0092	-35.5900	-0.2339	15.2748	-8.4448	0.0074	-33.0545	-0.2426	13.7694	-8.26
0.0141	-45.5582	-0.2808	19.9551	-10.1756	0.0121	-42.2654	-0.3016	17.9214	-9.87
0.0184	-51.4519	-0.2947	23.0342	-10.8150	0.0167	-47.7103	-0.3270	20.6227	-10.40
0.0193	-51.7365	-0.2756	23.6062	-10.2863	0.0175	-47.7379	-0.3088	20.9569	-9.85
0.0179	-47.7381	-0.2397	22.0683	-9.1640	0.0165	-44.2652	-0.2702	19.6811	-8.75
0.0139	-40.5031	-0.1857	19.0770	-7.3646	0.0119	-36.9853	-0.2060	16.6496	-7.02
0.0092	-30.2718	-0.1247	14.5941	-5.1267	0.0072	-26.6581	-0.1366	12.1316	-4.88
0.0046	-18.1270	-0.0668	8.9392	-2.8594	0.0030	-15.0560	-0.0719	6.8818	-2.72
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Furfural+ 1-Butanol					**Furfural+ 1-Butanol**				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0215	-173.3999	-0.0393	22.1752	-157.5226	0.0176	-151.1061	-0.0741	14.8381	-149.49
0.0429	-282.9059	-0.0896	38.7503	-253.0650	0.0353	-267.5252	-0.1456	30.9964	-247.79
0.0568	-328.3991	-0.1189	46.9876	-290.6030	0.0488	-317.0196	-0.1935	39.1950	-285.10
0.0732	-359.2705	-0.1581	54.4988	-314.6294	0.0674	-350.9433	-0.2592	46.3873	-307.85
0.0808	-354.9281	-0.1931	57.4490	-310.0351	0.0769	-348.5912	-0.3202	49.1777	-302.94
0.0772	-325.8910	-0.2098	54.4753	-287.3289	0.0712	-321.4549	-0.3497	46.8838	-282.17
0.0665	-270.8575	-0.2143	46.6146	-241.3832	0.0594	-263.6740	-0.3616	38.1562	-237.57
0.0483	-188.8896	-0.1895	33.9520	-168.7042	0.0427	-181.0233	-0.3263	26.0477	-166.35
0.0260	-95.2550	-0.1175	19.3192	-81.7851	0.0201	-87.4339	-0.2043	12.7601	-81.34
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Furfural+ Diethylmalonate					**Furfural+ Diethylmalonate**				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0261	-71.9542	0.0598	24.5378	-48.8113	0.0215	-60.4147	0.0674	16.9742	-43.32
0.0350	-93.8008	0.0764	33.3132	-70.3294	0.0301	-83.5236	0.0897	25.1250	-62.42
0.0419	-109.7558	0.0877	40.6589	-92.9290	0.0375	-99.6305	0.1012	31.5104	-82.44
0.0453	-118.1871	0.0938	45.8595	-115.6474	0.0410	-108.4466	0.1093	36.0901	-102.55
0.0465	-116.1241	0.0889	45.9599	-127.4323	0.0417	-107.1919	0.1057	36.4373	-112.99
0.0444	-106.8960	0.0810	43.0712	-138.6472	0.0397	-96.5939	0.0950	32.9721	-122.86
0.0385	-89.1171	0.0679	36.4185	-143.6568	0.0333	-78.2090	0.0818	26.5077	-127.27
0.0325	-69.4722	0.0514	28.2102	-138.2061	0.0268	-58.1819	0.0640	18.8192	-122.47
0.0213	-42.2410	0.0320	16.7363	-113.5611	0.0168	-36.5278	0.0457	11.5587	-100.79
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 4. Coefficient values of Redlich-kister type polynomial equation and standard deviation at different temperatures.

T/K	a	b	c	σ
Furfural+ Chlorobenzene				
		V^E(cm^3mol^{-1})		
308.15	-1.0337	-0.0300	0.0214	0.0018
318.15	-0.8987	-0.8987	0.0329	0.0031
		η (mPa.s)		
308.15	4.0455	0.2869	0.9811	0.1026
318.15	3.4041	0.2654	0.8203	0.0856
		ΔK_S(Tpa^{-1})		
308.15	-160.6080	8.0902	-4.5168	0.6174
318.15	-155.6480	7.9220	-2.5607	0.4235
		Δη(mPa.s)		
308.15	4.0455	0.2869	0.9811	0.0005
318.15	3.4041	0.2654	0.8203	0.0007
		ΔZ (kg m^{-3} s^{-1})		
308.15	120.4250	-0.5614	3.5045	0.3478
318.15	105.3910	-1.0116	0.5962	0.0483
		ΔL_F (10^{-12} m)		
308.15	-3.1776	0.0860	-0.0914	0.0082
318.15	0.0989	0.1264	-0.2291	0.0217
		ΔV_F (10^{-14} m^3mol^{-1})		
308.15	-4.3863	0.2856	-0.0995	0.0053
318.15	-9.2586	0.6909	-0.2810	0.6780
		Δπ(10^{-05} Nm^{-2})		
308.15	-204.4740	-7.4226	-0.9531	0.1846
318.15	-186.9700	-6.9596	-1.1874	0.2027
Furfural+ Nitromethane				
		V^E(cm^3mol^{-1})		
308.15	-0.5755	-0.0023	0.0160	0.0016
318.15	-0.4946	-0.4946	0.0255	0.0025
		η (mPa.s)		
308.15	3.7323	0.3501	0.9192	0.0863
318.15	3.2806	0.2880	0.7972	0.0757
		ΔK_S(Tpa^{-1})		
308.15	-24.3693	-0.5687	-0.3952	0.0428
318.15	-22.2040	-0.4114	0.3189	0.0375
		Δη(mPa.s)		
308.15	3.7323	0.3501	0.9102	0.0004
318.15	3.2807	0.2880	0.7972	0.0006
		ΔZ (kg m^{-3} s^{-1})		
308.15	94.0036	-1.1537	0.7473	0.0801
318.15	83.9778	-1.6584	-0.4472	0.0328
		ΔL_F (10^{-10} m)		
308.15	-2.0647	0.0517	-0.0179	0.0021
318.15	0.0692	0.0564	-0.1191	0.0119
		ΔV_F (10^{-14} m^3mol^{-1})		
308.15	-1.1049	0.0841	-0.0151	0.0016
318.15	-1.2319	0.0822	0.0046	0.0912
		Δπ(10^{-04} Nm^{-2})		
308.15	-414.0070	25.8787	-6.7420	0.8219
318.15	-396.8830	26.2209	-7.7625	0.9232

Table 4. Coefficient values of Redlich-kister type polynomial equation and standard deviation at different temperatures (Continued).

Furfural+1-Butanol				
		V^E(cm^3mol^{-1})		
308.15	-3.5997	-0.1167	-0.0219	0.0001
318.15	-3.4603	-3.4603	0.0256	0.0048
		η (mPa.s)		
308.15	6.7471	-0.3380	1.6016	0.1633
318.15	6.1194	-0.3654	1.4453	0.1498
		ΔK_S(Tpa^{-1})		
308.15	-495.3510	38.1970	-112.4146	0.8741
318.15	-485.6340	35.4538	-114.8937	0.1754
		Δη(mPa.s)		
308.15	6.7471	-0.3380	1.6016	0.0007
318.15	6.1195	-0.3654	1.4454	0.0012
		ΔZ (kg m^{-3} s^{-1})		
308.15	225.1470	-5.1840	1.8690	0.2817
318.15	192.2600	-4.9386	-4.6036	0.3568
		ΔL_F (10^{-10} m)		
308.15	-13.9677	0.7926	-0.2574	0.0403
318.15	0.6291	0.4396	-0.9361	0.1000
		ΔV_F (10^{-14} m^3mol^{-1})		
308.15	-0.9385	-0.0608	0.0257	0.0082
318.15	-1.4682	-0.1074	0.0008	0.1082
		Δπ(10^{-05} Nm^{-2})		
308.15	-122.9580	7.1849	-2.6324	0.3945
318.15	-120.7240	6.8046	-2.3832	0.3629
Furfural+ Diethylmalonate				
		V^E(cm^3mol^{-1})		
308.15	-2.3454	-0.0364	0.2180	0.0141
318.15	-2.2077	-2.2077	0.2422	0.0157
		η (mPa.s)		
308.15	5.9313	-0.1673	s1.4348	0.0934
318.15	5.1895	-0.1665	1.2493	0.0812
		ΔK_S(Tpa^{-1})		
308.15	-274.3760	33.9457	-67.8867	0.6873
318.15	-268.7230	33.5111	-66.2114	0.5818
		Δη(mPa.s)		
308.15	5.9313	-0.1673	1.4349	0.0001
318.15	5.1896	-0.1665	1.2493	0.0004
		ΔZ (kg m^{-3} s^{-1})		
308.15	181.6370	-4.2740	-8.5935	0.5842
318.15	140.8350	-4.0531	-11.2746	0.7592
		ΔL_F (10^{-10} m)		
308.15	-4.6094	0.2074	0.1029	0.0077
318.15	0.1865	0.2522	-0.5622	0.0357
		ΔV_F (10^{-14} m^3mol^{-1})		
308.15	0.3389	-0.0214	0.0081	0.0008
318.15	0.4023	-0.0189	0.0121	0.0333
		Δπ(10^{-03} Nm^{-2})		
308.15	5.1216	-0.6018	-0.2647	0.8672
318.15	-4.5666	-0.5331	-0.2364	0.0180

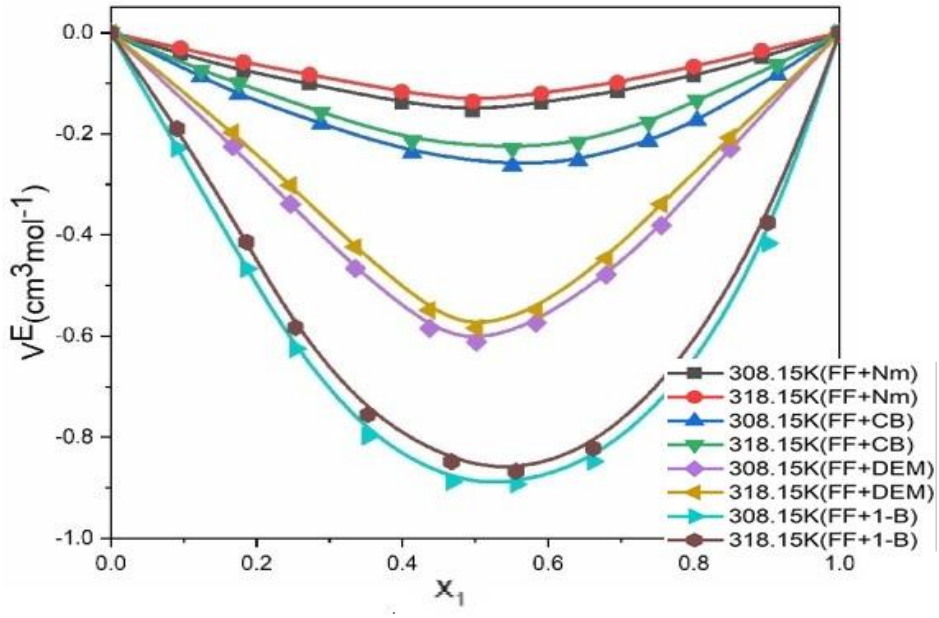

Figure 1. Excess volume (V^E) against the mole fraction (X_1) of Furfural at 308.15K and 318.15 K for the binary liquid mixtures of Furfural with Nitromethane, Cholobenzene, Diethylmalonate and 1-Butanol.

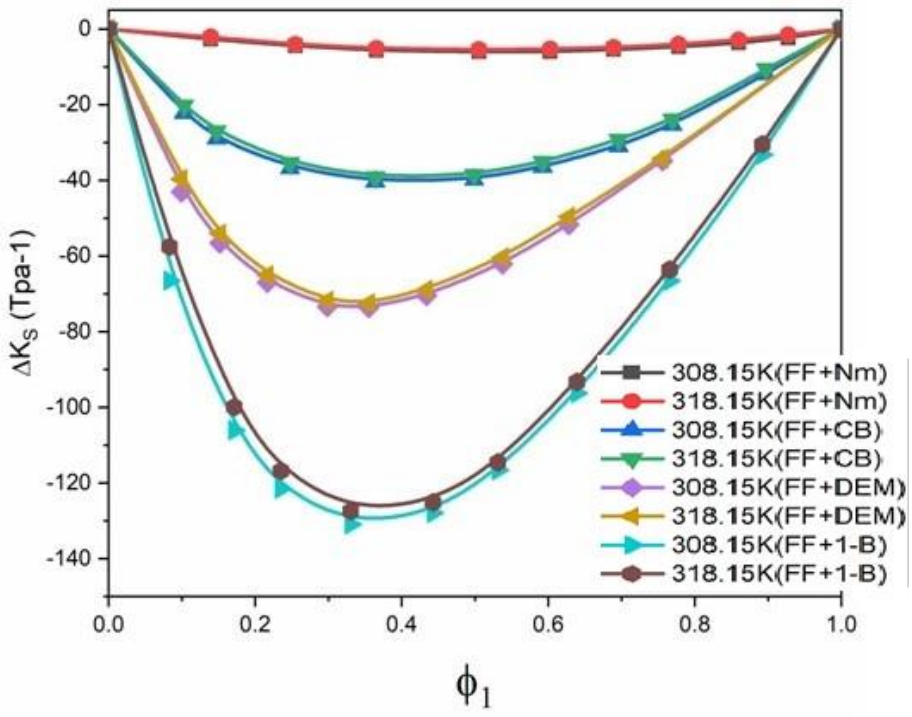

Figure 2. Deviation in isentropic compressibility (ΔK_S) against the Volume fraction (Φ_1) of Furfural at 308.15K and 318.15 K for the binary liquid mixtures of Furfural with Nitromethane, Cholobenzene, Diethyl malonate and 1-Butanol.

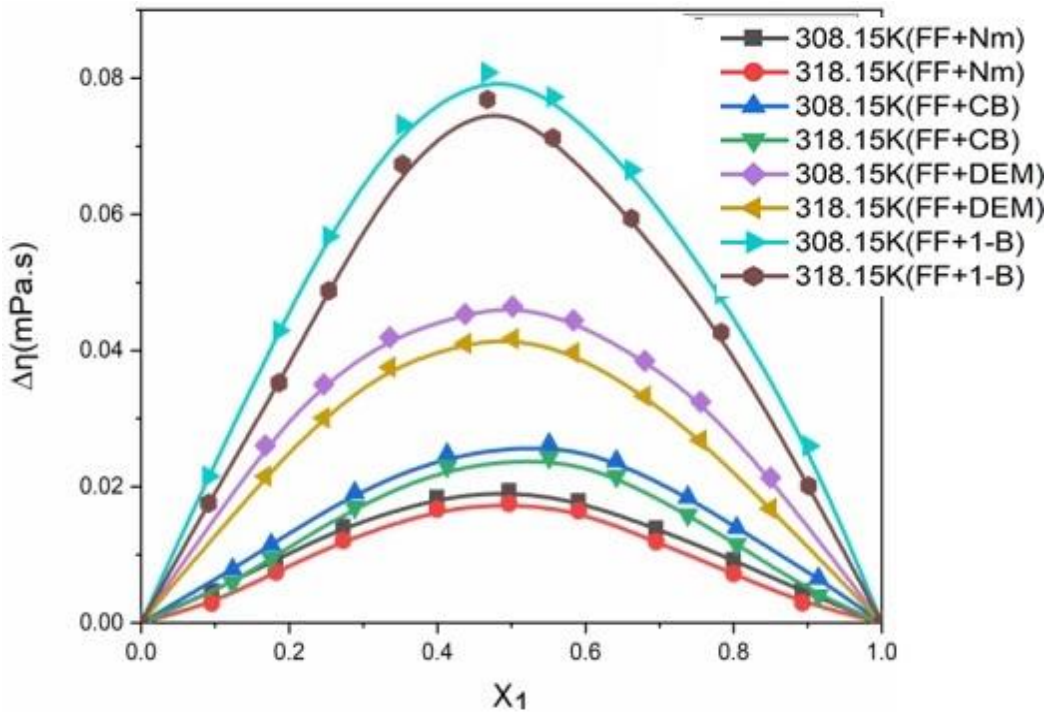

Figure 3. Deviation in viscosity (Δη) against the mole fraction (X_1) of Furfural at 308.15K and 318.15 K for the binary liquid mixtures of Furfural with Nitromethane, Cholobenzene, Diethyl malonate and 1-Butanol.

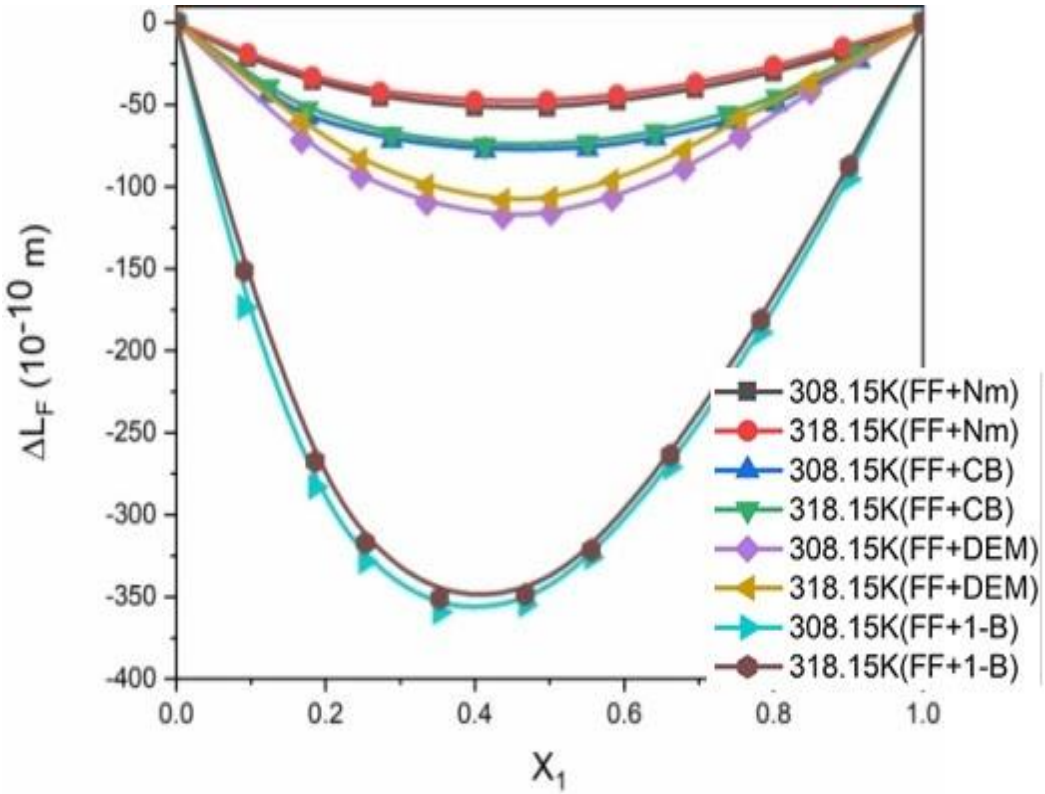

Figure 4. Intermolecular free length (ΔL_F) against the mole fraction of Furfural at 308.15K and 318.15 K for the binary liquid mixtures of Furfural with Nitromethane, Cholobenzene, Diethyl malonate and 1-Butanol.

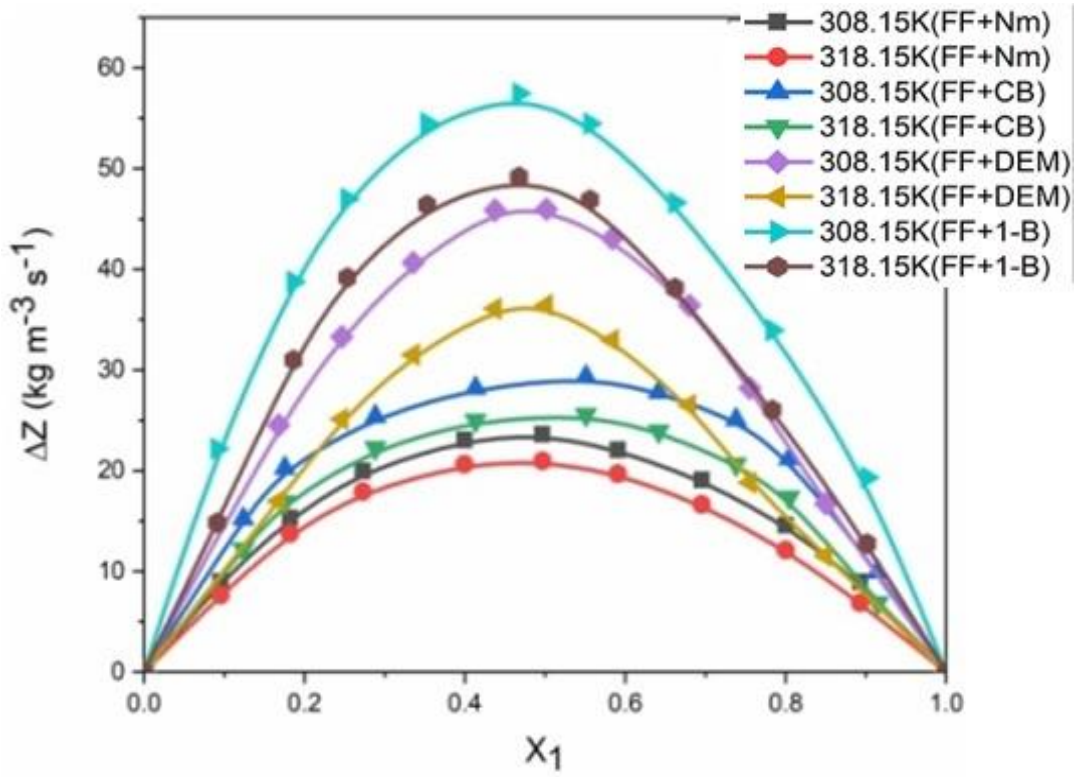

Figure 5. Deviation of acoustic impedance (ΔZ) against the mole fraction (X_1) of Furfural at 308.15K and 318.15 K for the binary liquid mixtures of Furfural with Nitromethane, Cholobenzene, Diethyl malonate and 1-Butanol.

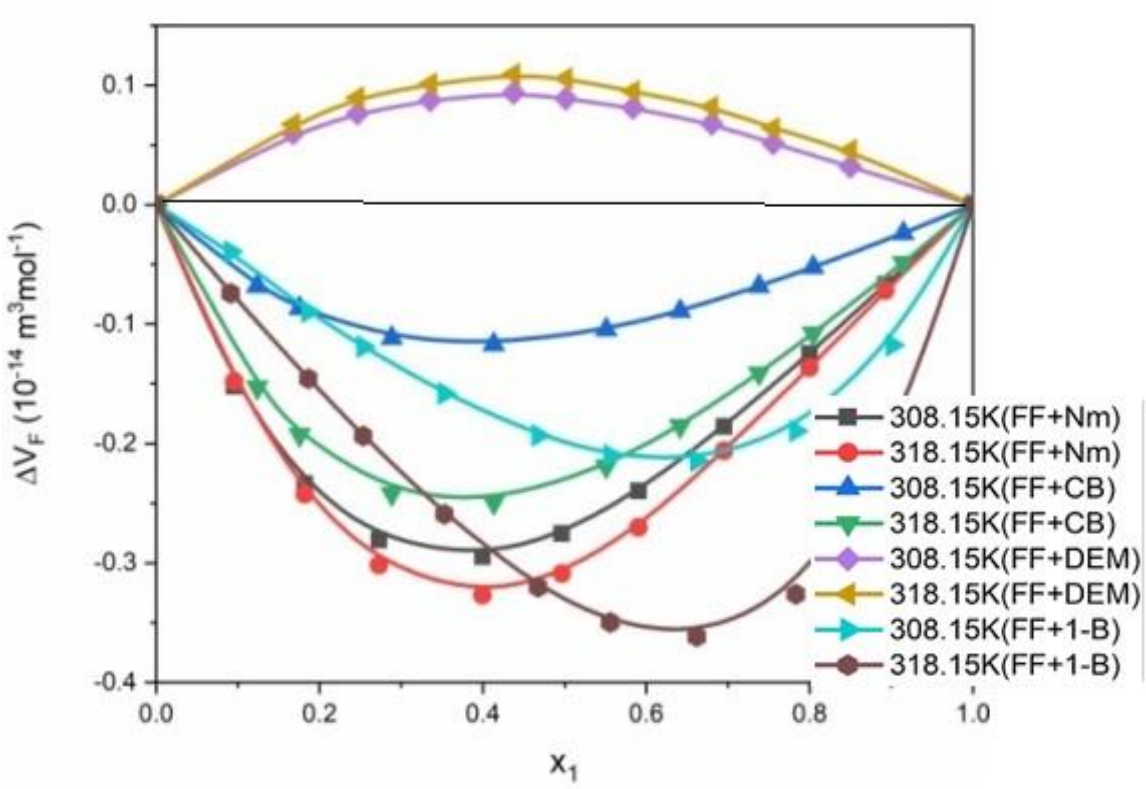

Figure 6. ΔV_F against the mole fraction of Furfural at 308.15K and 318.15 K for the binary liquid mixtures of Furfural with Nitromethane, Cholobenzene, Diethyl malonate and 1-Butanol

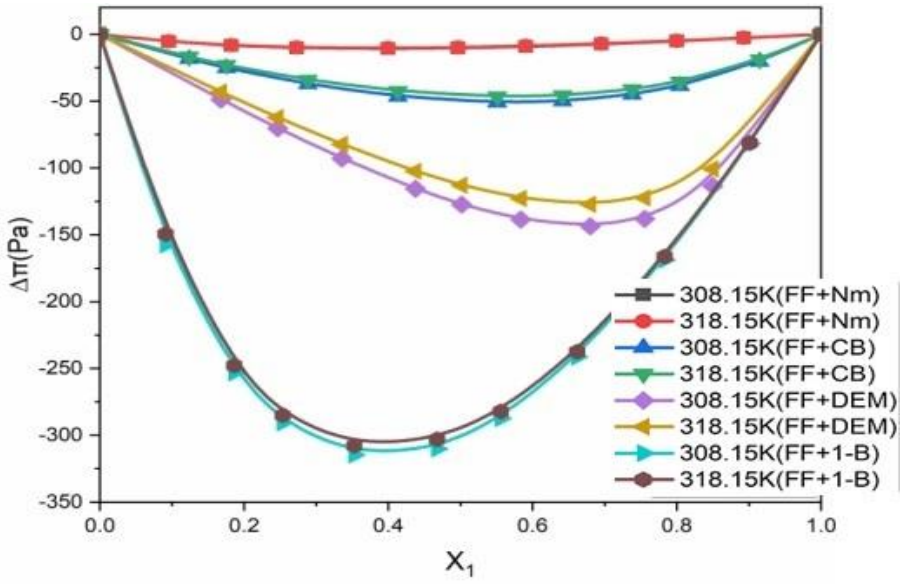

Figure 7. Intermolecular internal pressure ($\Delta\pi$) against the mole fraction (X_1) of Furfural at 308.15K and 318.15 K for the binary liquid mixtures of Furfural with Nitromethane, Cholobenzene, Diethyl malonate and 1-Butanol.

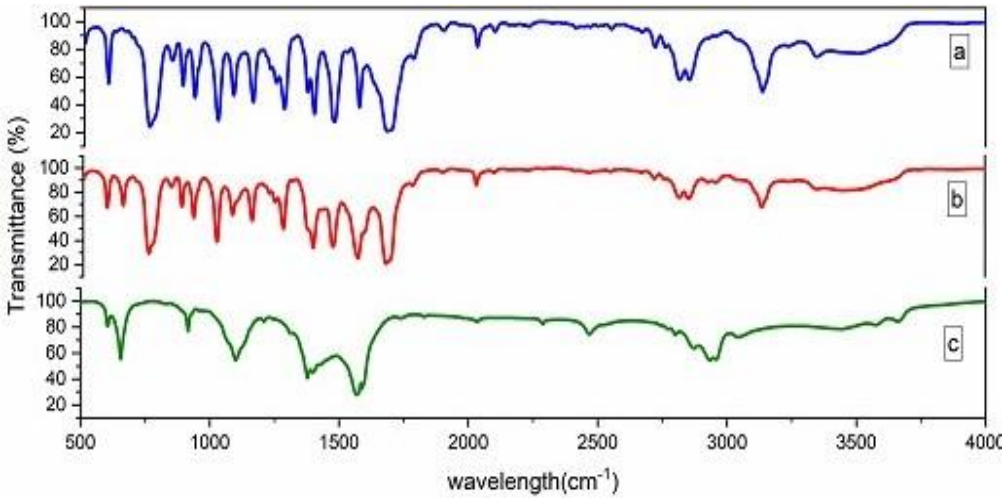

Figure 8. FTIR spectrum. (a) Pure furfural liquid, (b) equimolar mixture of furfural + nitromethane, (c) Pure nitromethane liquid.

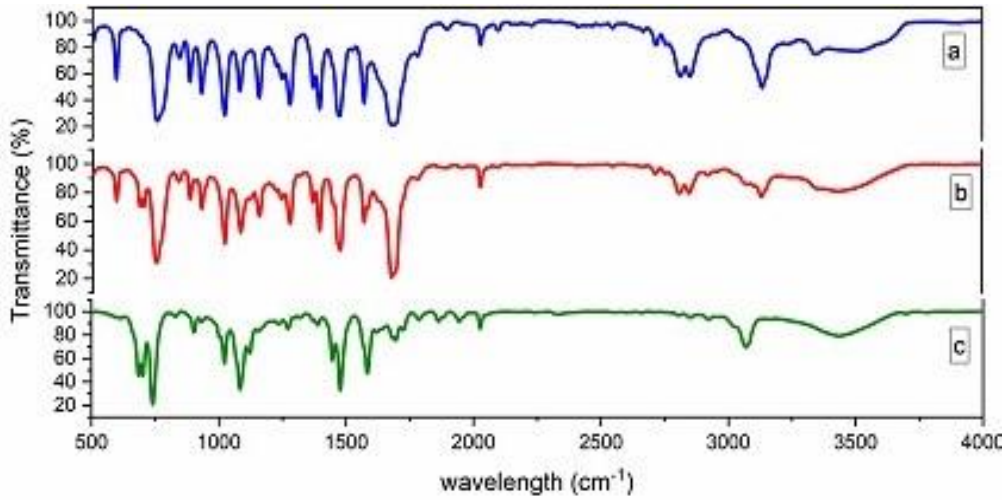

Figure 9. FTIR spectrum. (a) Pure furfural liquid, (b) equimolar mixture of furfural + chlorobenzene, (c) Pure chlorobenzene liquid.

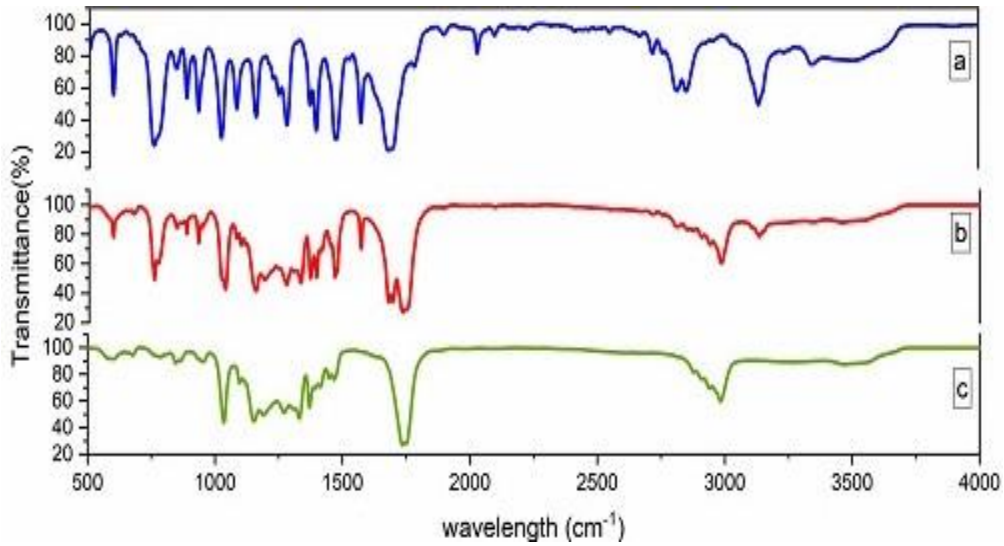

Figure 10. FTIR spectrum. (a) Pure furfural liquid, (b) equimolar mixture of furfural + diethylmalonate, (c) Pure diethylmalonate liquid.

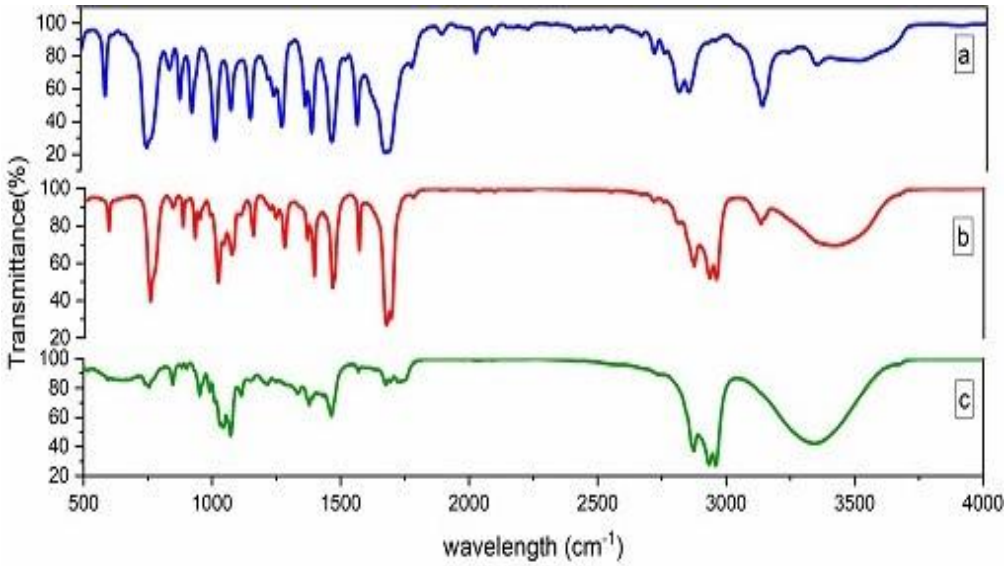

Figure 11. FTIR spectrum. (a) Pure furfural liquid, (b) equimolar mixture of furfural + 1-butanol, (c) Pure 1-butanol liquid.

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