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Thermodynamic Properties of Binary Liquid Mixtures of Furfural with Toluene and Nitro Benzene at Varying Temperatures

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ABSTRACT

Binary liquid mixtures of furfural with toluene and nitrobenzene were examined for ultrasonic velocity, viscosity and density at a temperature of 308.15 and 318.15 K in various mole fractions. The calculated thermodynamic properties from density, viscosity, ultrasonic velocity and some excess parameters like 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) and Deviation in Acoustic Impedance(ΔZ) were determined and found the proper coefficients for a polynomial equation of the Redlich-Kister type, from which the theoretical values were calculated. The interaction ability of the binary liquid mixtures was investigated, as well as the deviations of the binary liquid mixtures from their ideal behavior were studied based on the experiment and theoretical values.

Keywords: Binary liquid mixtures, Viscosity, Density, Redlich-Kister equation, Molecular interaction.

INTRODUCTION

Pharmaceutical industries have undergone a major transformation in recent years thanks to ultrasonic analysis of binary liquid mixtures. Utilizing ultrasonic technology is a potent method for understanding the molecular interactions of liquid mixtures[1]. Complex developments in liquid mixtures have been interpreted as excess thermodynamic properties. These discrepancies were explained as being caused by strong or weak interactions. The thermodynamic and transport characteristics of pure liquid and liquid mixtures can be used to investigate the nature of molecular interactions (either intermolecular or intra molecular) between

the mixing liquids as reported by Sekhar *et al.,*[2]. Physical properties like density, viscosity, excess volume, isentropic properties, free length, free volume and acoustic impedance are studied to better understand the environment and strength of intermolecular and intra molecular interactions in multi-component liquid mixtures. Engineering process design and operation also heavily reply on the thermodynamic and transport features of liquid mixtures[3]. For estimating thermodynamic properties, there exist numerous prediction equations. In this study experimental results are used in studying thermodynamic properties of binary liquid mixtures.

The definition of "biomass" includes dedicated energy plants and trees, aquatic plants, animal waste, agricultural food and feed crop residues, timber, wood residues and other waste resource[4]. Furfural is one of the byproducts of the pyrolysis of biomass containing lignocelluloses. It is utilized as a feedstock for the creation of different resins in the pharmaceutical and agrochemical sectors. Furfural is also used or created in the pulp, paper and food sectors as reported by Muhammad *et al.,*[5]. Nitrobenzene is a versatile solvent that is commonly used in synthetic and electrochemical research, a crucial raw material in the production of explosives was reported by Uma *et al.,*[6]. At 308.15K and 318.15K, the transport and thermodynamic properties of prepared liquids of binary mixtures were investigated over the entire range of compositions[7]. Research of their binary liquid mixtures, which gain increasing significance because it more accurately simulates complex real time molecular interaction, is the main objective of this work. Thus the binary liquid mixtures of furfural + toluene, furfural + nitrobenzene and toluene + nitro benzene were measured for ultrasonic velocity, viscosity, density and other estimated excess thermodynamic properties at 308.15K and 318.15K.

Experiment method

Chemical: Furfural (SRL), Toluene (Molychem) and Nitrobenzene (ACS) used were of high purity (<99%). Table 1 shows the thermo physical characteristics of the investigated components.

The purity was further confirmed by comparing the measured values of ultrasonic velocity, viscosity, density with report in the literature, which showed a satisfactory agreement and shown in Table 2. Binary liquid mixtures of various compositions were prepared by volume by weight method, by mixing a constant quantity of pure liquid in airtight stopper bottle[8] of 50 mL capability using an analytical balance with a 0.0001 g precision.

Table 1: Material description

Chemical name	Molecular formula	Molar mass(g.mol^{-1})	Stated purity(mol %)	CAS Number
Furfural	$C_5H_4O_2$	96.08	99	98-01-1
Toluene	C_7H_8	92.14	99.3	108-88-3
Nitrobenzene	$C_6H_5NO_2$	123.11	99	98-95-3

Table 2: Comparison of experimental Ultrasonic velocity (U), Viscosity (η) and Density (ρ) in pure liquids with journalism value by 308.15 and 318.15K

LIQUIDS	T(K)	ρ(g cm^{-3})		η(mPa s^{-1})		U(ms^{-1})	
		Experimental values	Literature values	Experimental values	Literature values	Experimental values	Literature values
Furfural[9,10]	308.15	1.1447	1.1440	1.2616	1.2600	1406.5	1403.77
	318.15	1.1324	1.1330	1.0921	1.0900	1370.5	1367.81
Toluene[11]	308.15	0.8374	0.8378	0.5087	0.5099	1253.5	1250
	318.15	0.8396	-	0.3824	-	1256	-
Nitrobenzene[12]	308.15	0.7980	0.7979	2.0081	2.0080	1218	1209
	318.15	1.1780	1.1773	1.2071	1.2061	1418	1412.5

Densities of pure liquids and liquid mixtures were measured by specific gravity method with 10 mL relative density bottle and weighed with an exactness of ± 0.001 kg m^{-3}. Viscosities were determined by Oswald viscometer 10 mL capability with an accurateness of ± 0.001 cP. From the measured values of density and flow time 't', viscosity 'η' was calculated[12]. 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. The ultrasonic velocity values were measured using an ultrasonic interferometer[13] (Pico, Chennai, India) with a frequency of 2MHz was calibrated using water and nitrobenzene. The overall accuracy in the measurement is ±0.2%. All the measurements were taken at 308.15 and 318.15K with a temperature accuracy of 0.01K using a digital thermostat. A Perkin Elmer spectrum RX1 was used to record the IR spectra (PerkinElmer, inc., Waltham, MA, USA).

RESULT AND DISCUSSION

The following standard formulae are used to calculate the thermodynamic properties based on the investigated data.

Density (ρ)

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

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.

Excess Volume(V^E)

$$V^E=[(X_1 M_1)+(X_2 M_2)/\rho]-[(X_1 M_1)/\rho_1)+(X_2 M_2)/\rho_2)] \quad (2)$$

"ρ"- density of the liquid mixtures and X_1, M_1 and ρ_1, X_2, M_2 and ρ_2-mole fraction, molar mass, and density of pure components 1 & 2 respectively[14].

Isentropic Compressibility(K_S)

$$K_S = 1/(U^2 \rho) \quad (3)$$

Where, "U"-speed of sound and "ρ"- density of the liquid mixtures.

Deviation in Isentropic Compressibility(ΔK_S)

$$\Delta K_S = K_S-(\Phi_1 K_{S1} + \Phi_2 K_{S2}) \quad (4)$$

Where "ΔKS" denotes the mixtures isentropic compressibility, Φ_1, K_1, S_1 and Φ_2, K_2 S_2 denotes the volume fraction and isentropic compressibility of pure components 1 & 2, respectively.

Viscosity (η)

$$\eta = (At-B/t)\rho \quad (5)$$

Where "ρ" denotes the density of a pure liquid or a mixture of liquids, "t" denotes the time flow in seconds and A & B characteristic constants at specified temperature.

Excess Viscosity (Δη)

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

Where, η_1 & η_2 are the corresponding pure component 1 & 2 viscosity values[15].

For binary liquid mixtures

$$\Delta A = X_1 X_2 [a + b(X_1-X_2)c(X_1-X_2)] \quad (7)$$

From this theoretical values were calculated[16]

Using the theoretical values, the relation was used to determine the standard deviation values

$$\sigma = \left(\Sigma(X_{exp} - X_{cal})^2 / N - n\right)^{1/2} \quad (8)$$

Where, the number of data points is N and the number of coefficients is n.

All of the predicted excess parameters were fitted to a polynomial equation of the Redlich-Kister type using[17] the least squares methods to get the adjustment parameters a, b and c.

Table 3: Binary liquid mixtures of furfural, toluene and nitrobenzene with physical and thermodynamic properties at 308.15 and 318.15K

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})	ΔVE (cm^3mol^{-1})	ΔKs (Tpa^{-1})
Furfural + toluene						Furfural + toluene					
0.0000	0.8539	0.5093	1268	0.0000	0.0000	0.0000	0.8407	0.3771	1255	0.0000	0.0000
0.1365	0.8866	0.6374	1304	-0.0928	-33.6016	0.1365	0.8731	0.4868	1286	-0.0784	-31.9250
0.1941	0.9009	0.6893	1318	-0.1296	-44.1411	0.1941	0.8875	0.5354	1298	-0.1119	-42.0773
0.2999	0.9285	0.7815	1341	-0.2020	-57.7428	0.2999	0.9150	0.6220	1318	-0.1879	-55.8189
0.4302	0.9642	0.8895	1365	-0.2730	-65.6184	0.4302	0.9508	0.7235	1339	-0.2557	-64.0679
0.5172	0.9891	0.9580	1378	-0.2879	-65.5631	0.5172	0.9756	0.7880	1349	-0.2684	-64.1010
0.6013	1.0138	1.0198	1387	-0.2718	-61.2051	0.6013	1.0005	0.8453	1356	-0.2572	-59.7283
0.7133	1.0481	1.0973	1397	-0.2171	-50.4220	0.7133	1.0349	0.9183	1362	-0.1974	-48.6961
0.7895	1.0725	1.1468	1401	-0.1670	-40.0863	0.7895	1.0594	0.9669	1365	-0.1466	-38.4659
0.8917	1.1066	1.2098	1405	-0.0927	-22.5566	0.8917	1.0938	1.0282	1366	-0.0783	-21.5308
1.0000	1.1447	1.2685	1406	0.0000	0.0000	1.0000	1.1324	1.0921	1366	0.0000	0.0000
Furfural + nitro benzene						Furfural + nitro benzene					
0.0000	1.1863	1.6194	1439	0.0000	0.0000	0.0000	1.1780	1.2071	1418	0.0000	0.0000
0.1247	1.1818	1.5642	1430	0.0228	2.5496	0.1247	1.1731	1.1859	1408	0.0137	2.1643
0.1915	1.1792	1.5361	1426	0.0340	3.8905	0.1915	1.1704	1.1747	1403	0.0230	3.2813
0.2797	1.1758	1.5011	1420	0.0480	5.4050	0.2797	1.1667	1.1603	1396	0.0350	5.0073
0.3983	1.1711	1.4564	1414	0.0613	6.8765	0.3983	1.1615	1.1429	1388	0.0486	6.4193
0.5048	1.1667	1.4187	1410	0.0674	7.0300	0.5048	1.1567	1.1298	1383	0.0558	6.5400
0.5958	1.1629	1.3879	1407	0.0639	6.5103	0.5958	1.1525	1.1199	1379	0.0513	6.0733
0.6835	1.1592	1.3604	1406	0.0536	5.3596	0.6835	1.1485	1.1121	1376	0.0409	4.9573
0.7911	1.1544	1.3274	1404	0.0377	3.6358	0.7911	1.1433	1.1039	1372	0.0251	3.3456
0.8793	1.1504	1.3018	1403	0.0225	2.3018	0.8793	1.1389	1.0983	1369	0.0122	2.0129
1.0000	1.1447	1.2685	1401	0.0000	0.0000	1.0000	1.1324	1.0912	1365	0.0000	0.0000
Toluene + Nitro benzene						Toluene + Nitro benzene					
0.0000	1.1863	1.6216	1439	0.0000	0.0000	0.0000	1.1780	1.2071	1418	0.0000	0.0000
0.1379	1.1403	1.5431	1436	-0.1422	-27.0357	0.1379	1.1304	1.1521	1408	-0.1186	-24.4083
0.2540	1.1019	1.4673	1430	-0.2661	-46.2203	0.2540	1.0910	1.1085	1400	-0.2404	-42.6919
0.3655	1.0650	1.3959	1420	-0.3596	-60.2163	0.3655	1.0533	1.0674	1390	-0.3374	-57.2814
0.4608	1.0333	1.3262	1409	-0.4025	-68.8240	0.4608	1.0210	1.0301	1380	-0.3804	-66.1278
0.5797	0.9937	1.2131	1391	-0.4176	-73.8138	0.5797	0.9807	0.9491	1363	-0.3978	-71.6304
0.6612	0.9665	1.1100	1375	-0.3961	-72.2344	0.6612	0.9530	0.8705	1348	-0.3711	-69.9959
0.7477	0.9375	0.9828	1354	-0.3335	-65.0348	0.7477	0.9236	0.7562	1329	-0.3063	-62.3279
0.8382	0.9070	0.8213	1329	-0.2269	-50.2404	0.8382	0.8927	0.6161	1304	-0.1933	-46.4829
0.9234	0.8785	0.6568	1303	-0.1142	-30.1785	0.9234	0.8640	0.4819	1281	-0.0843	-26.8109
1.0000	0.8530	0.5087	1272	0.0000	0.0000	1.0000	0.8385	0.3728	1255	0.0000	0.0000

Table 4: Binary liquid mixtures of furfural, toluene and nitrobenzene with thermodynamic parameters at 308.15 and 318.15K

308.15K					318.15K				
Δη (mPa.s)	ΔL_F (10^{-10}m)	ΔV_F (10^{-14} m^3mol^{-1})	ΔZ (kgm^{-3} s^{-1})	Δπ(Pa)	Δη (mPa.s)	ΔL_F (10^{-10}m)	ΔV_F (10^{-14} m^3mol^{-1})	ΔZ (kgm^{-3} s^{-1})	Δπ(Pa)
Furfural + toluene					Furfural + toluene				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0245	-69.3918	-2.0867	1.3139	-16.7556	0.0121	-65.8607	-2.9049	0.6505	-42.45
0.0326	-91.2414	-2.7789	2.3241	-24.8084	0.0195	-86.8810	-4.2192	1.4168	-51.33
0.0444	-119.3095	-3.0015	4.1727	-38.0188	0.0305	-115.6168	-5.1773	3.4251	-65.79
0.0536	-135.2528	-2.8141	6.5523	-49.1167	0.0388	-132.4920	-5.0490	5.9304	-78.96
0.0561	-134.3648	-2.5303	7.4868	-52.5884	0.0411	-131.6366	-4.5624	6.7039	-83.04
0.0540	-123.8933	-2.1773	6.9154	-54.8138	0.0383	-120.9535	-3.9004	5.9345	-87.40
0.0465	-100.0258	-1.6306	5.4095	-51.6059	0.0312	-95.9066	-2.8593	3.6993	-83.95
0.0382	-78.3005	-1.2233	4.0633	-44.2965	0.0252	-74.1736	-2.0826	2.1980	-71.93
0.0236	-43.0051	-0.6473	1.8829	-24.0848	0.0135	-40.2638	-0.9713	0.5555	-47.06
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Furfural + nitro benzene					Furfural + nitro benzene				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
-0.0115	4.3217	0.0115	-3.7922	-1.8701	-0.0067	2.2743	0.0077	-2.5937	-183.24
-0.0161	6.8553	0.0157	-5.8448	-2.7514	-0.0102	3.7780	0.0122	-4.0110	-270.70
-0.0202	9.8032	0.0191	-8.1359	-3.7620	-0.0144	6.9153	0.0159	-6.4559	-372.14
-0.0232	12.7522	0.0213	-10.2851	-4.8025	-0.0181	9.3357	0.0194	-8.2624	-478.70
-0.0236	12.7193	0.0227	-10.2038	-5.3640	-0.0188	9.0775	0.0197	-8.0838	-537.57
-0.0224	11.3152	0.0229	-9.1052	-5.4983	-0.0181	7.8316	0.0187	-7.1332	-553.30
-0.0192	8.5729	0.0209	-7.0509	-5.2508	-0.0158	5.3490	0.0157	-5.3099	-530.94
-0.0144	5.0568	0.0173	-4.3512	-4.3523	-0.0115	2.5552	0.0104	-3.0851	-441.46
-0.0090	3.0487	0.0111	-2.6407	-2.9897	-0.0068	1.0952	0.0045	-1.6378	-303.99
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
Toluene + nitro benzene					Toluene + nitro benzene				
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000
0.0750	-85.8255	-0.9309	16.0737	0.5906	0.0600	-77.8833	-2.3346	6.9317	52.66
0.1284	-146.2334	-1.7002	26.5000	1.1784	0.1134	-135.8125	-4.3140	13.8556	110.57
0.1810	-189.6352	-2.4431	32.4099	1.8984	0.1652	-181.2138	-6.2184	19.9261	179.03
0.2174	-215.3029	-3.0599	35.3079	2.5604	0.2074	-207.8299	-7.8437	23.1242	247.74
0.2367	-228.5513	-3.7575	35.5711	3.2726	0.2257	-222.9055	-9.6586	24.8186	313.77
0.2243	-221.8295	-4.1340	32.9354	3.5144	0.2151	-216.1674	-10.6917	23.1399	336.81
0.1932	-197.6301	-4.3798	27.5709	3.4791	0.1729	-190.8078	-11.2770	18.8687	314.22
0.1326	-150.5973	-4.2016	19.4525	2.8194	0.1083	-140.8855	-10.7332	11.9111	236.66
0.0628	-88.5151	-3.0689	11.6661	1.5761	0.0453	-79.7547	-7.6340	6.7243	120.52
0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000	0.0000

Table 5: Standard deviation and coefficients of the Redlich-Kister polynomial equation at various temperatures

T/K	a	b	c	σ
		Furfural + Toluene		
		VE (cm^3mol^{-1})		
308.15	-1.1077	-0.0211	0.0607	0.0052
318.15	-1.0365	-1.0365	0.0749	0.0064
		η(mPa.s)		
308.15	3.7769	0.3818	0.8864	0.0803
318.15	3.0976	0.3608	0.7262	0.0657
		$\Delta K_S(Tpa^{-1})$		
308.15	-256.2960	14.3467	1.4753	0.4308
318.15	-249.5330	13.8062	1.0171	0.2795
		Δη(mPa.s)		
308.15	-3.7770	0.3818	0.8864	0.0339
318.15	3.0977	0.3608	0.0000	0.0007
		$\Delta Z(kg\ m^{-3}\ s^{-1})$		
308.15	27.5603	1.1563	-2.8911	0.2467
318.15	23.7754	0.5017	-4.2782	0.3723
		ΔL_F(10-10m)		
308.15	5.3507	0.1338	0.0242	0.8156
318.15	-0.1712	0.2266	-0.4349	0.0106
		$\Delta V_F(10^{-14}\ m^3mol^{-1})$		
308.15	1.0478	1.1510	-0.6172	0.9227
318.15	1.8818	1.6216	-0.1046	0.1436
		Δπ(10-05 Nm^{-2})		
308.15	215.1630	-1.1856	0.3749	0.1808
318.15	-341.1850	-1.2568	-1.5414	0.2334
		Furfural + nitro benzene		
		$V^E(cm^3mol^{-1})$		
308.15	0.2603	0.0008	-0.0119	0.0011
318.15	0.2045	0.2045	-0.0544	0.0009
		η(mPa.s)		
308.15	5.6814	-0.1735	1.4437	0.1278
318.15	4.8017	-1.3069	3.0813	0.0507
		$\Delta K_S(Tpa^{-1})$		
308.15	27.0760	-1.2965	-1.2180	0.0746
318.15	24.7860	-2.8112	0.8736	0.0995
		Δη(mPa.s)		
308.15	5.6814	-0.1735	1.4438	0.0001
318.15	4.8018	-1.3070	3.0813	0.0002
		$\Delta Z(kg\ m^{-3}\ s^{-1})$		
308.15	-39.5562	1.2791	2.3476	0.2014
318.15	-30.4981	1.5467	2.3128	0.1832
		$\Delta L_F(10^{-10}\ m)$		
308.15	0.4894	-0.0150	-0.0358	0.0031
318.15	0.0018	-0.0252	0.0371	0.0003
		$\Delta V_F(10^{-14}\ m^3mol^{-1})$		
308.15	0.2177	-0.0006	-0.0491	0.0084
318.15	0.0629	-0.0436	0.0659	0.0058
		$\Delta\pi(10^{-05}\ Nm^{-2})$		
308.15	-215.3550	-10.3025	-2.1602	0.1470
318.15	-215.6990	-36.1059	32.0132	0.6720
		Toluene + nitro benzene		
		$V^E(cm^3mol^{-1})$		
308.15	-1.6605	-0.0509	0.0586	0.0032
318.15	-1.5761	-1.5761	0.0908	0.0068
		η(mPa.s)		
308.15	5.1702	-0.5147	1.0276	0.0773
318.15	4.0199	-0.3777	0.7297	0.0526
		$\Delta K_S(Tpa^{-1})$		
308.15	-288.9300	-16.2319	-0.2111	0.6829
318.15	-278.3900	-16.6389	3.6765	0.3346
		Δη(mPa.s)		
308.15	5.1702	-0.5147	1.0277	0.0019
318.15	4.0200	-0.3777	0.7297	0.0042
		$\Delta Z(kg\ m^{-3}\ s^{-1})$		
308.15	143.1650	1.3677	-0.0900	0.0438
318.15	95.5696	3.8653	-5.0718	0.3308
		$\Delta L_F(10^{-10}\ m)$		
308.15	-9.0176	-0.0399	0.0102	0.0158
318.15	0.1733	0.3654	-0.5878	0.0415
		$\Delta V_F(10\text{-}14\ m^3mol^{-1})$		
308.15	-13.9947	-2.1795	-1.0539	0.1903
318.15	-3.6067	-5.5960	-2.4651	0.3295
		$\Delta\pi(10\text{-}04\ Nm^{-2})$		
308.15	120.0240	16.1399	-1.8502	0.4417
318.15	115.1310	13.9889	-5.0257	0.0602

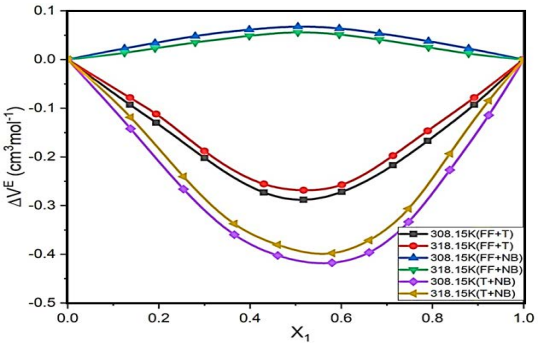

Fig. 1. Excess Volume(V^E) relative to the mole fraction(X_1) of furfural at 308.15K &318.15K for the binary liquid mixtures of furfural (FF) with Toluene (T) and Nitro benzene(NB)

V^E and ΔK_S values of Furfural + Toluene are negative (Fig. 1 and 2) and Toluene + Nitro benzene are more negative (Fig. 1 & 2) across the entire composition range. The methyl (electron-donating) group in toluene releases electron toward the benzene ring mainly due to hyper conjugation and partly due to inductive effect[18]. In toluene hyper conjugation overcomes the inductive effect. As a result, the negative charge on the toluene molecules $-CH_3$ groups is stabilized, allowing the hydrogen atom to have a positive charge. Due to the hyper conjugation nature of the toluene molecule, there may be a contact between the positive charge on the hydrogen atom of the toluene molecule and the negative charge on the O atom of furfural molecule and nitrobenzene molecule in the two liquid mixtures, resulting in a partial H- bond. Two liquid mixtures are excess volume increases the temperature increase. As the temperature increases, molecules gain thermal energy, which affects the breakdown of intermolecular interaction between dissimilar molecules.

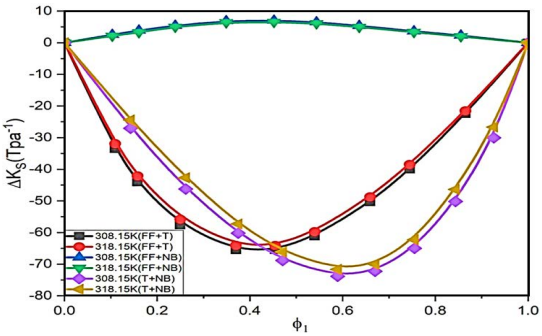

Fig. 2. Deviation in Isentropic Compressibility(ΔK_S) relative to the volume fraction(Φ_1) of furfural at 308.15K & 318.15K for the binary liquid mixtures of furfural (FF) with Toluene (T) and Nitro benzene(NB)

V^E and ΔK_S values of Furfural + Nitro benzene are positive (Fig. 1 & 2), indicating reduced interaction across the entire composition range. Observed excess volume may be broken down into physical, chemical and geometrical effects[19]. Dispersion forces and non-specific physical interactions make up the majority of physical interaction that contributes positively. Furfural's oxygen atom deviates from the nitro group's oxygen atom, involving the forces of Vander Waals in the process. Dispersive forces, which show a weak chemical contact between dissimilar molecules, have been linked in this study to positive excess volume deviations. VE decreases with temperature increases, showing the interaction increases with temperature increases. The molecules are activated by thermal energy, which also speeds up the connection of molecules that are dissimilar to one another. As a result, interacting molecules have more incredible energy when approaching components at higher temperatures.

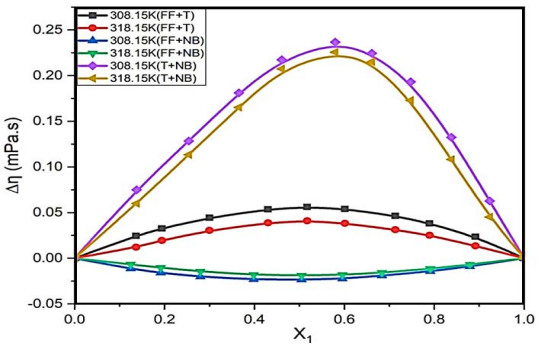

Fig. 3. Deviation in Viscosity($\Delta\eta$) relative to the mole fraction(X_1) of furfural at 308.15K & 318.15K for the binary liquid mixtures of furfural (FF) with Toluene (T) and Nitro benzene(NB)

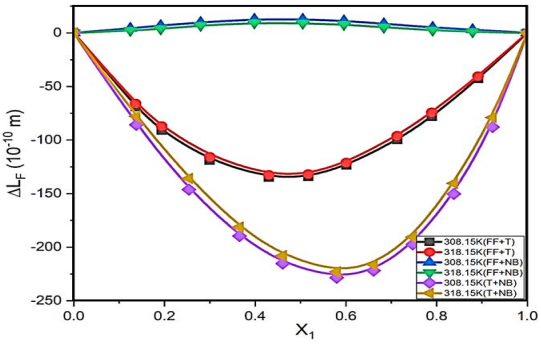

Fig. 4. Deviation in Intermolecular Free Length(ΔL_F) relative to the Mole Fraction(X_1) of furfural at 308.15K & 318.15K for the binary liquid mixtures of furfural (FF) with Toluene (T) and Nitro benzene(NB)

$\Delta\eta$ values of Furfural + Toluene and Toluene + Nitro benzene are positive (Fig. 3) and furfural + Nitro benzene are negative (Fig. 3) over the entire range of composition. Toluene + nitrobenzene liquid mixtures have a higher intermolecular interaction than furfural + toluene liquid mixtures, as indicated by the positive value[20]. The negative value of deviates more from ideality, indicating that there is a dispersion forces between furfural and nitrobenzene. The positive values of binary liquid mixtures are greater than furfural + toluene and lower than toluene + nitro benzene. The graph's values are in the same order as the VE and ΔK_S values.

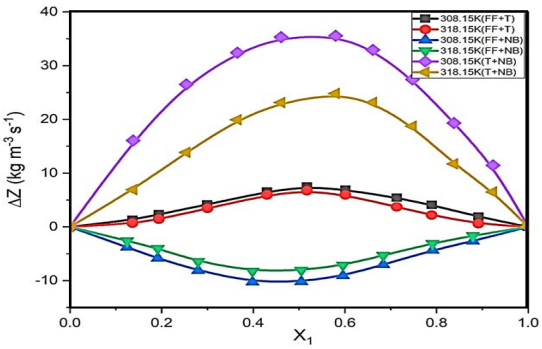

Fig. 5. Deviation in Acoustic Impedance(ΔZ) relative to the mole fraction(X_1) of furfural at 308.15K & 318.15K for the binary liquid mixtures of furfural (FF) with Toluene (T) and Nitro benzene(NB)

The observed value of ΔL_F, ΔV_F, $\Delta\pi$ reflect the same ideal as obtained above. Due to an increase in the thermal movements of interacting molecules, the nature of interaction for the three liquid mixtures changes as the temperature rises. Dispersion forces between the mixed liquids cause negative values, whereas attractive forces like dipole–dipole interaction. ΔZ be haves in a manner opposed to ΔL_F, the positive and negative deflection of mixtures indicates the degree of association or dissociation between the mixing components[21]. The measured values of $\Delta\eta$ and ΔZ are positive and negative across the whole composition range (Fig.3 & 5), which both strongly and weakly support the aforementioned concept. The systems interact in the following order: furfural + nitro benzene < furfural + toluene < toluene + nitro benzene.

There is excellent agreement between experimental and anticipated results for the degree polynomial solution. Table 5 displays the outcomes in terms of the parameters a, b, c & σ. The degree

polynomial solution produced using VE, ΔK_S, η, Δη, ΔZ, ΔL_F, ΔV_F and Δπ was found to be in good agreement with the Redlich-Kister parameters.

FT-IR Results

Figures 6 to 8 show FTIR results for toluene and nitro benzene in the binary liquid mixtures with furfural in a molar fraction of 0.5.

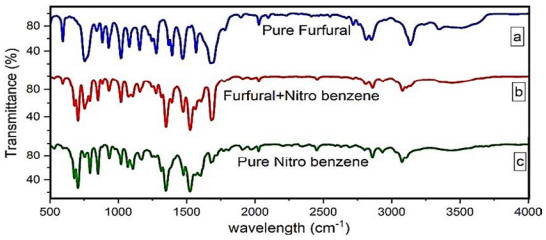

Fig. 6. FT-IR spectra for the following substances: (a) Pure Furfural liquid, (b) equimolar mixture of Furfural + Nitrobenzene, (c) Pure Nitro benzene liquid

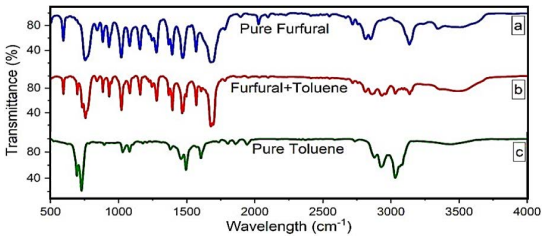

Fig. 7. FT-IR spectra for the following substances: (a) Pure Furfural liquid, (b) equimolar mixture of Furfural + Toluene, (c) Pure Toluene liquid

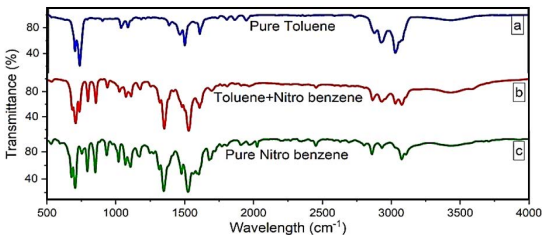

Fig. 8. FT-IR spectra for the following substances: (a) Pure Furfural liquid, (b) equimolar mixture of Furfural + Toluene, (c) Pure Toluene liquid

Pure furfural molecule shows a peak at 1686.93 cm^{-1} which is due to the C=O bond, pure nitrobenzene liquid molecule has a peak at 1523.72 cm^{-1} due to the N=O bond, and pure toluene molecule has a peak at 3032.58 cm^{-1} due to the C-H bond, according to FT-IR study.

Figure 6 shows a peak at 1680.18 cm^{-1} in equimolar composition of furfural with toluene. The change in frequency and intensity indicates the existence of an intermolecular partial H-bond between hydrogen atom of the toluene molecule and oxygen atom of the furfural. Fig. 7 shows a frequency and intensity of the equimolar combination of furfural + nitrobenzene do not change, indicating that dispersion forces exist between –C=O and –N=O. Fig. 8 shows a peak at 3078.38 cm^{-1} in equimolar composition of toluene with nitro benzene. The alteration in frequency and intensity is evidence that there is a partial H-bond between hydrogen atom of the toluene molecule and oxygen atom of the nitro benzene.

CONCLUSION

The mixing characteristics of binary liquid mixtures of furfural + toluene, furfural + nitrobenzene, and toluene + nitrobenzene were investigated in the current study. The magnitude of the chemical interactions between the molecules excess volume, deviation in isentropic compressibility, deviation in intermolecular free length, deviation in intermolecular free volume, deviation in internal pressure, deviation in viscosity and deviation in acoustic impedance has been used to interpret their magnitude.

VE and ΔK_S values are negative of toluene + nitrobenzene shows more interaction than furfural + toluene interaction and VE and ΔK_S values are positive of furfural + nitrobenzene is the mixing liquids interact less frequently. The –O atom of furfural deviates from the intermolecular H- bond form between the toluene molecules hydrogen atom, the hydrogen atom toluene molecules from the intermolecular H- bond form between the nitrobenzene molecules oxygen atom and the furfural molecules oxygen atom and the nitro benzene molecule's oxygen atom consequently, Vander Waals forces are involved. To determine the variable coefficients, the corresponding thermodynamic excess parameters were calculated using the techniques previously mentioned and adapted to the Redlich- Kister polynomial equation. On the basis of experimental and calculated results, the behavior of the liquid mixtures and the deviation from ideality has been examined. An analysis of FT-IR spectroscopy showed the establishment of H-bond between unlike molecules.

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