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NOVEL THERMODYNAMIC PROPERTIES OF BINARY MIXTURES OF TETRAHYDROFURFURYL ALCOHOL WITH SOME ALCOHOLS AT 298.15 K

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ABSTRACT

To understand the nature of molecular aggregation between two solvents, excess properties (e.g. excess molar volume (V_m^E), excess Gibb's free energy of activation viscous flow (ΔG^{*E}) and viscosity deviation of binary mixtures) are therefore needed. Thus, in the current study, the refractive index (n_D), viscosity (η), and density (ρ) of binary mixtures were measured for tetrahydrofurfuryl alcohol (THFA) with ethanol, 2-propanol and 2-butanol at 298.15K. Moreover and based on experimentally obtained results, the V_m^E, the refractive index deviation (Δn_D), excess molar viscosity (η^E) and ΔG^{*E} were calculated. To correct and fit the experimental V_m^E, η^E and Δn_D deviations, Redlich-Kister equation was used. The molecular interaction in binary mixtures was found to explain the variability of physical properties with the composition of the mixtures. In light of obtained results, factors influencing the molecular interactions (e.g. the length of the carbon chain and the position of hydroxyl groups in targeted alcohol) have been also discussed. In all cases the obtained V_m^E, η^E, ΔG^{*E} and Δn_D values were negative at 298.15K except for the binary system (THFA + 2-butanol) where the results indicate the positive deviation in refractive indices.

Keywords: Binary system, tetrahydrofurfuryl alcohol, refractive index, density, viscosity, thermodynamic properties.

INTRODUCTION

In binary liquid solvents mixtures, the excess thermodynamic functions are the key tool for understanding the molecular interactions behavior, they were highly used in the chemical engineering industry for chemical reaction cleaning, extraction and purification[1]. Additionally, physical properties of binary mixtures are essential when heat transfer and mass transfer phenomena involved in industrial processes[2].

A considerable amount of research studying the properties of binary solvent mixtures has been published in the recent decade[3-8]. Hydrogen bond formation, dipole-dipole, and charge transfer interactions have been suggested as the mechanisms of interactions between of solvents[9-11]. For example, Nain[3] studied the densities and volumetric properties of binary mixtures of formamide with alcohols at two temperatures and found that negative V_m^E is attributed to the formation of hydrogen bond interaction. This was confirmed by Kemeakegha[12] when studied the behavior of binary mixtures of organic solvents and amines. Moreover, ρ, η and n_D measurement is expected to shed some light on both solvent-solute interactions[13]. On the other hand, and up to our knowledge, no study was done to investigate the V^E , η^E, Δn_D and ΔG^{*E} at any temperature.Therefore, the objective of this research is to study excess properties including ρ, η and n_D for a range of binary mixtures including (THFA+ Ethanol), (THFA+ 2-propanol) and (THFA + 2-butanol) at 298.15K. From obtained results, another parameter such as V_m^E, viscosity deviation, refractive index deviation and Gibbs free energy (excess molar) were also determined.

EXPERIMENTAL

Chemicals

All solvents used in the study are of high purity (>99%) Tetrahydrofurfuryl alcohol (THFA), 2-propanol, 2-butanol ,and ethanol were purchased from Sigma-Aldrich (UK). The purities of this experiment used

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solvents were checked and results showed high compatibility to those in previous studies (Table-1). Densities, viscosities, and refractive indices were listed for all solvents except THFA where no data available in the literature.

Density and Viscosity Measurements

The average ρ value of three replicates was determined with a precision of ± 10^{-5} $g.cm^{-3}$ using a digital density meter (Anton paar, Model DMA 60/602). For viscosity (η) measurements, a controlled temperature suspended-level ubbelohde viscometer was used under atmospheric pressure at 298.15± 0.01K. The final values represent the average of three measurements.

Refractive Index Measurements

A digital Abbe refractometer (Model:BOE 32400) was used to measure the n_D values for both pure and their binary mixtures solvents. Pure toluene and double distilled water were used for refractometer calibration, at a temperature of 298.15 K.

Table-1: This study and literature obtained density (ρ), viscosity (η) and refractive index (n_D) values for solvents at 298.15 K.

Compound	ρ ($g.cm^{-1}$)		η (mpa.s)		n_D	Literature
	Measured	Literature	Measured	Literature	Measured	
THFA	1.04761		4.89883		1.45322	
Ethanol	0.78522	0.78730[14] 0.78493[15] 0.78510[16]	1.10221	1.0826[17]	1.36003	1.3593[14] 1.35941[15] 1.3592[16]
2-Propanol	0.78084	0.78088[18] 0.78089[19] 0.78126[20]	2.12112	2.0436[22]	1.37521	1.37444[19] 1.3752[20,21]
2-Butanol	0.80252	0.802487[23] 0.80237[24] 0.80241[20]	3.51542	3.1150[25]	1.39523	1.39488[24] 1.39530[20]

RESULTS AND DISCUSSION

In the current study, measured density (ρ) values were used to estimate the V_m^E of the binary mixtures following the equation (1)[26]:

$$V_m^E = \frac{X_1M_1+X_2M_2}{\rho_m} - \frac{X_1M_1}{\rho_1} - \frac{X_2M_2}{\rho_2} \qquad (1)$$

Where M_1, X_1, and ρ_1 are the molecular weight (M_{wt}), mole fraction, and density of the pure THFA, respectively; while M_2, X_2 and ρ_2 are the M_{wt}, mole fraction and density of alcohols, ρ_m is the density of the binary mixtures, respectively.Table -2 lists the density and V_m^E of the binary mixtures at the various mole fractions of THFA and (ethanol, 2-propanol and 2-butanol). The V_m^E plotted against (X_1) mole fraction for THFA is shown in Fig. -1.

Table-2: Experimentally obtained density, viscosity and refractive index values and their corresponding parameters values in binary solvents Mixtures.

X_1 THFA + X_2 Ethanol at 298.15 K

X_1	ρ(g cm^3)	$V^E cm^3mol^{-1}$	n_D	Δn_D	η	η^E mpa.s	ΔG^{*E} $J.mol^{-1}$
0.0000	0.78522	0.0000	1.36003	0.0000	1.10221	0.0000	0.0000
0.0556	0.81012	-0.11407	1.36505	-0.55088	1.10534	-0.08011	-178.99553
0.2003	0.86480	-0.18979	1.37553	-1.66105	1.31196	-0.12458	-252.46773

0.2717	0.88824	-0.20756	1.38417	-1.89185	1.43335	-0.14260	-285.66860
0.4115	0.92906	-0.22680	1.39508	-2.25869	1.72669	-0.16493	-329.93131
0.5054	0.95301	-0.21833	1.40398	-2.24400	1.99616	-0.16551	-351.24693
0.6219	0.97940	-0.17580	1.41302	-2.11791	2.41119	-0.14481	-287.69246
0.7334	1.00195	-0.12520	1.42197	-1.81120	2.93841	-0.11345	-223.83736
0.8055	1.01378	-0.09323	1.42880	-1.48260	3.33886	-0.09324	-186.08495
0.9278	1.036461	-0.05379	1.43914	-0.84900	4.16206	-0.05529	-118.46276
1.0000	1.04761	0.0000	1.45322	0.0000	4.89883	0.0000	0.0000

X_1 THFA + X_2 2- propanol at 298.15

X_1	ρ(g. cm^{-3})	V ^{E}cm^{3}mol^{-1}	n_D	Δ n_D	Ƞ	η^E mpa.s	ΔG*^{E} J.mol^{-1}
0.0000	0.78084	0.0000	1.37521	0.0000	2.12112	0.0000	0.0000
0.1101	0.82262	-0.54309	1.38772	-0.12789	2.18949	-0.06044	-142.59655
0.2240	0.86442	-1.14715	1.40052	-0.17011	2.35137	-0.08445	-196.76866
0.3408	0.90885	-2.07105	1.41189	-0.19689	2.54123	-0.10456	-243.27626
0.4539	0.94311	-2.32896	1.42105	-0.22405	2.74769	-0.12113	-282.99355
0.5534	0.96779	-2.19084	1.42811	-0.23356	2.96293	-0.12899	-302.81608
0.6497	0.98765	-1.80049	1.43439	-0.21909	3.24407	-0.11895	-279.48010
0.7472	1.00770	-1.49545	1.43999	-0.19451	3.59524	-0.09778	-229.82004
0.8353	1.02229	-0.97714	1.44435	-0.16946	3.96494	-0.07448	-173.51734
0.9249	1.03612	-0.42426	1.44555	-0.11083	4.36632	-0.05221	-124.93248
1.0000	1.04761	0.0000	1.45322	0.0000	4.89883	0.0000	0.0000

X_1 THFA + X_2 2- butanol at 298.15 K

X_1	ρ(g.cm^{-3})	V ^{E}cm^{3}mol^{-1}	n_D	Δ n_D	Ƞ	η^E mpa.s	ΔG*^{E} J.mol^{-1}
0.0000	0.80252	0.0000	1.39523	0.0000	3.51542	0.0000	0.0000
0.0940	0.83401	-0.81245	1.40329	0.10142	3.52793	-0.02765	-68.213775
0.2027	0.86405	-1.04580	1.41112	0.21055	3.57309	-0.05099	-115.61921
0.2978	0.88871	-1.09891	1.42019	0.31392	3.60972	-0.07235	-178.57860
0.4044	0.91574	-1.12394	1.42833	0.40165	0.68238	-0.08779	-216.76150
0.4993	0.93852	-1.04328	1.43429	0.42228	3.79225	-0.0889	-221.91290
0.5946	0.96038	-0.88946	1.43745	0.36444	3.94820	-0.08121	-200.4288
0.6958	0.98330	-0.72903	1.44266	0.28581	4.15021	-0.06489	-160.08807
0.8040	1.00733	-0.54637	1.44738	0.22631	4.39545	-0.04338	-101.70914
0.9059	1.02899	-0.31478	1.45081	0.12573	4.64281	-0.02245	-55.34835
1.0000	1.04761	0.0000	1.45322	0.0000	4.89883	0.0000	0.0000

Excess molar volume (V^E), refractive index deviation (Δn_D), excess molar viscosities (η^E) and excess molar Gibbs free energy (ΔG^{*E}).

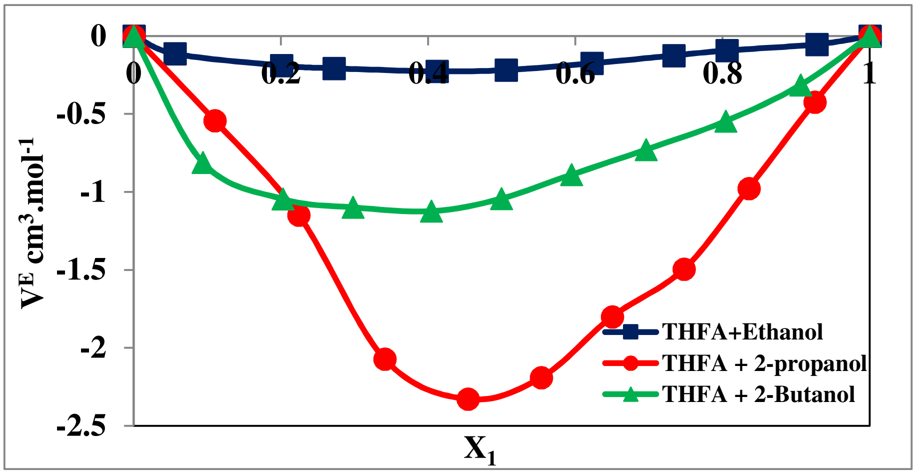

Fig.-1: Plots (V^E) excess molar volume against X_1 for (X_1THFA+ X_2-Mono alcohols) at 298.15 K.

Refractive index deviation

Refractive index deviation (Δn_{D}) was calculated using equation (2)[27]:

$$\Delta n_D = n_D - X_1 n_{D1} - X_2 n_{D2} \qquad (2)$$

Where n_D is the refractive index of the mixture and (n_{D1}, n_{D2}) are pure component refractive index.

Lorentz-Lorenz equation (3,4,and 5) [28] were used to calculate ($n_{D1,}$ n_{D2} and n_{D}) as follows:

$$n_D = \left(\frac{n_m^2-1}{n_m^2+2}\right)\frac{X1M1+X2M2}{\rho_m} \qquad (3)$$

$$n_{D1} = \left(\frac{n_1^2-1}{n_1^2+2}\right)\frac{X1M1}{\rho_1} \qquad (4)$$

$$n_{D2} = \left(\frac{n_2^2-1}{n_2^2+2}\right)\frac{X2M2}{\rho_2} \qquad (5)$$

Table -2 lists the experimental ($n_{D,}$ and Δn_D) values of the binary mixtures, while Fig-2 illustrates the relation between Δn_D against mole fraction (X_1) for the THFA .

Excess molar viscosities (η^E)

Excess molar viscosities (η^E) were obtained by using equation (6)[29]:

$$(\eta^E) = (\eta_m) - (X_1\eta_1 + X_2\eta_2) \qquad (6)$$

Where X_1, X_2, $\eta 1$, $\eta 2$ are the mole fraction and the viscosity of the components 1 and 2; while η_m is the viscosity of the mixture, as listed in Table -2 . The relation between the η^E against mole fraction (X_1) for THFA is shown in Fig-3.

Excess molar Gibbs free energy

Excess molar Gibbs free energy (ΔG^{*E}) of activation of viscous flow was estimated by using equation (7)[30]:

$$\Delta G^{*E} = RT\,[\ln(\eta_m V_m) - (X_1 \ln\eta_1 V_1) - (X_2 \ln\eta_2 V_2)] \qquad (7)$$

Where R is the universal constant for gases and T is the absolute temperature (K). The V_1, V_2 and V_m represent the molar volumes of solvent 1, solvent 2, and binary mixture solvents, respectively. V_m was obtained from equation (8)[31]:

$$V_m = (X_1V_1 + X_2V_2)\ /\rho_m \qquad (8)$$

Table-2 lists the ΔG^{*E} while Fig- 4 shows the relation between ΔG^{*E} and the mole fraction (X_1) for THFA. The Redlich-Kister [32] (Eq. 9) was used to calculate the excess functions of the binary systems:

$$Y = X_1X_2\sum_{k=0}^{p} A_k(X_1 - X_2)^k \qquad (9)$$

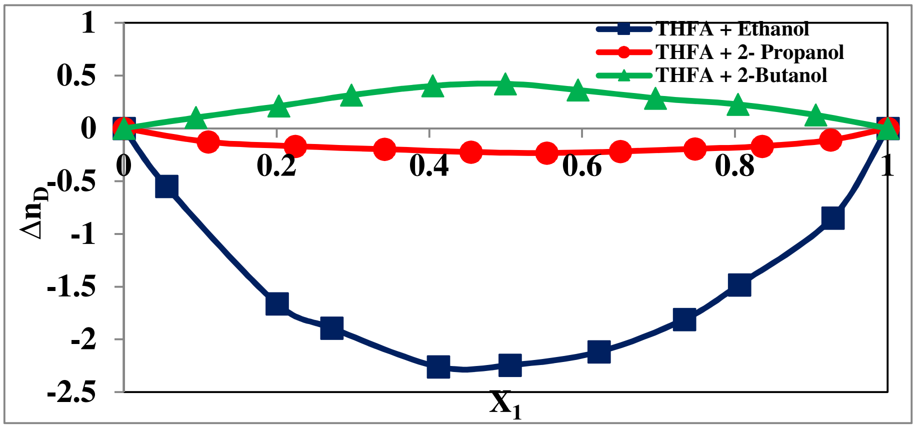

Fig.-2: Plots (Δn_D) refractive index deviation against X_1 For (X_1THFA + X_2- Mono alcohols) 298.15K.

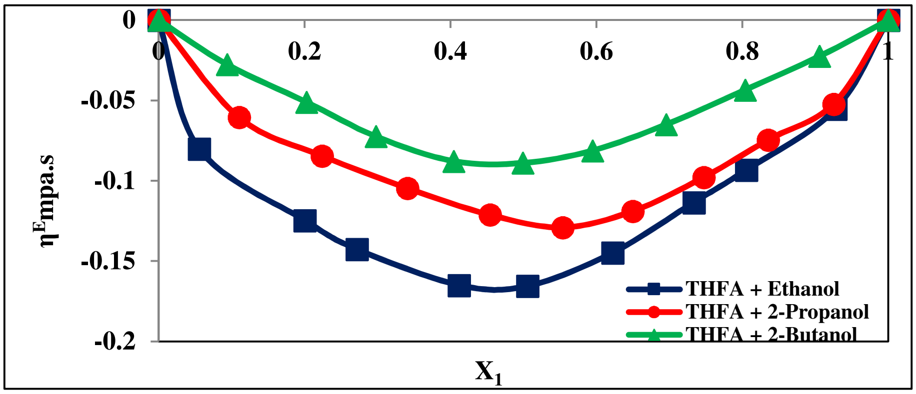

Fig.-3: Plots (η^E) excess Molar viscosities against X_1 for (X_1-THFA+ X_2-Mono alcohols) at 298.15K.

Where Y is V^E, Δn_D, and η^E, p is the degree of polynomial expansion, X_1 and X_2 are the mole fractions of the components 1 and 2, respectively, and A_k denotes the polynomial coefficients. The standard deviation was calculated by the following equation[26]:

$$\sigma = [\sum \frac{(X^E_{Cal} - X^E_{exp})^2}{m - n}]^{0.5} \tag{10}$$

Where, m and n are the number of data points and the estimated parameters, respectively. The values of these coefficients and the standard deviation are given in Table-3. The standard deviation values agreed satisfactorily with the experimental values.

The obtained negative values of V^E_m , are believed to be attributable mainly to the association between THFA and alcohols compound through between the –OH groups in mono-alcohols and the –OH group in the THFA via the formation of hydrogen bonds. The strength of the associations arising from the interactions between the unlike molecules was stronger than the strength of the associations between like molecules [33]. THFA as a highly polar, an aprotic solvent has the capability of destroying the self-associated molecules of alcohols compound and orienting its molecules to interact strongly with it and forming new complexes have smaller volume. Fig.- 2 is shown refractive index deviation (Δn_D) of mixtures (THFA + mono-alcohols) against mole fraction (X_1) for THFA.

For ethanol-THFA and 2-propanol-THFA mixtures, over the range of mole fractions, Δn was found to have negative values. This behavior suggests that the molecular interaction between the -OH of alcohols compound and the oxygen atom of (THFA) (non-associated molecule) is greater than the molecule interaction between ethanol and 2-propanol molecules (self-associated). This leads to destroying the self-associated structure of alcohols compound and giving the highest negative values of Δn_D.

As the count of carbon atoms increases in the alcohol chain, Δn_D becomes positive for mixture of (2-butanol-THFA), such behavior is a result of lower electronic perturbation of the molecular orbital of the mixing liquids and the enhanced structure of THFA as dipolar and aprotic solvent[34-35]. The η^E, Fig.-3 and ΔG^{*E}, Fig. -4 found to be negative along the range of mole fraction, at 298.15 K.

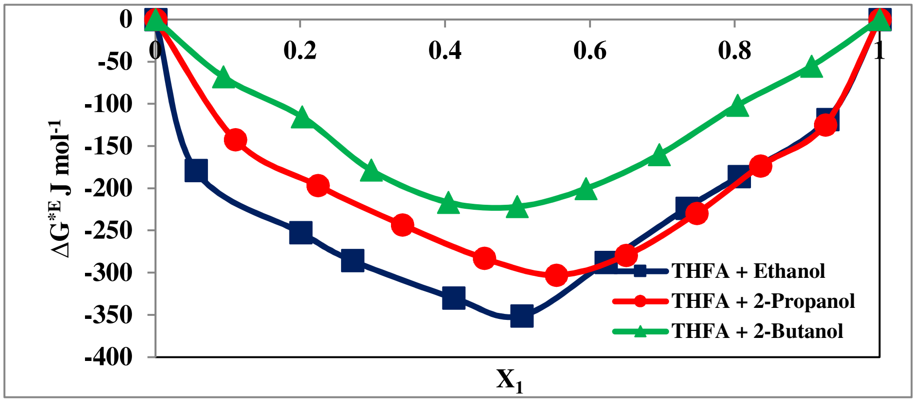

Fig.-4: Plots of (ΔG^{*E}) excess molar Gibbs free energy of activation of viscous flow against (X_1) for (X_1-THFA+ X_2-Mono alcohols) at 298.15.

These results may be related to the formation of hydrogen bonding between unlike molecules through. This study results suggest that the formation of the mixture leads to the structure of the alcohol to be broken since the (–OH) group is located at the end of the molecular chain which means the formation of hydrogen bonds with THFA is highly expected[36].

Table- 3: Fitting Coefficient (Ak) and Standard Deviations (σ) for All Binary Mixtures at 298.15K.

Function	System	A_0	A_1	A_2	σ
V^E ($cm^3.mol^{-1}$)	THFA + Ethanol	-0.82916	0.49235	-0.33529	0.01894
V^E ($cm^3.mol^{-1}$)	THFA + 2- propanol	-9.10026	-0.07495	5.49486	0.02098
V^E ($cm^3.mol^{-1}$)	THFA + 2- butanol	-1.52662	0.451045	-9.34118	0.09010

Function	System	A_0	A_1	A_2	σ
Δn_D ($cm^3.mol^{-1}$)	THFA + Ethanol	-0.62798	0.17401	-0.29913	0.01692
Δn_D ($cm^3.mol^{-1}$)	THFA + 2- propanol	-0.88270	-0.10255	-0.64391	0.03180
Δn_D ($cm^3.mol^{-1}$)	THFA + 2- butanol	1.60546	-0.01332	-0.62052	0.03339

Function	System	A_0	A_1	A_2	σ
η^E (mPa.s)	THFA + Ethanol	-8.96561	0.36658	-2.85256	0.02086
η^E (mPa.s	THFA + 2- propanol	-0.48809	-0.04308	-0.14539	0.02559
η^E (mPa.s)	THFA + 2- butanol	-0.35173	0.04250	0.12705	0.01351

Function	System	A_0	A_1	A_2	σ
ΔG^{*E} $J.mol^{-1}$	THFA + Ethanol	-1269.934	376.455	-639.646	0.86779
ΔG^{*E} $J.mol^{-1}$	THFA + 2-propanol	-1141.320	-108.683	-350.962	1.28422
ΔG^{*E} $J.mol^{-1}$	THFA + 2- butanol	-872.512	95.157	385.575	0.84470

CONCLUSION

New values of ρ, η and n_D of binary mixtures of THFA with ethanol, 2-propanol and 2-butanol at 298.15K were experimentally obtained. The V_m^E, Δn_D, η^E and ΔG^{*E} were correlated using the Redlich-Kister polynomial equation. The deviations in refractive indices were negative for the systems THFA + ethanol and THFA + 2-propanol due to the abolishing the self-associated structure of alcohols compound. On the other hand, the results indicate the positive deviation for THFA + 2-butanol mixture which may relate to the increase number of carbon atoms in alcohol chain. The values of V_m^E, η^E and ΔG^{*E} resulted in from this study, showed to be negative over the range of mole fractions at 298.15K.

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