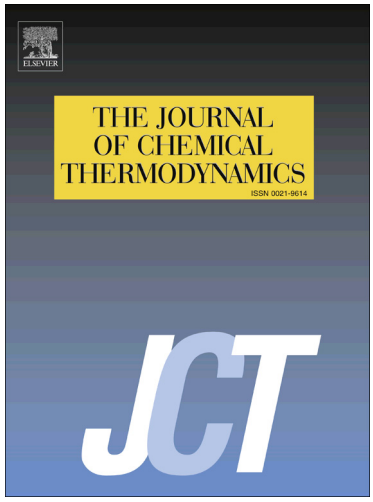

Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures

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Density, speed of sound and refractive index of mixtures containing 2-phenoxyethanol with propanol or butanol at various temperatures

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ABSTRACT

In this work, we reported the new experimental data of densities, speeds of sound, and refractive indices for four binary mixtures: {2-phenoxyethanol (2PhEE) + 1-propanol or 2-propanol or 1-butanol or 2-butanol) over the entire composition range and at temperatures of (293.15, 303.15, 313.15 and 323.15) K and at pressure p = 0.1 MPa. From these experimental data, thermodynamics properties: excess molar volume, isentropic compressibility, deviation in isentropic compressibility and deviation in refractive indices were calculated. Excess molar volume, deviation in isentropic compressibility and deviation in refractive indices data have been correlated using the Redlich−Kister equation**.** From the obtained results, a discussion was carried out in terms of nature of intermolecular interactions and structure factors in these binary mixtures.

Keywords: 2-phenoxyethanol, alcohol, density, speed of sound, refractive index, Redlich-Kister polynomial equation.

1. Introduction

2-Phenoxyethanol (2PhEE) is a member of glycol ether family, it is a colorless liquid with a mildly rosy and also ‘‘metallic’’ odor of poor tenacity, 2PhEE it is widely used in cosmetic industry, it is used as a preservative and antimicrobial agent for personal care products [1, 2], such as shampoos, perfumes, toilet soaps. In perfumes it is used as a fixative and in insect repellant as a solvent [1, 3], in addition it is also used in non-cosmetic products such as household cleaners and detergents [1], furthermore 2PhEE is also used in pharmaceuticals as an ingredient in vaccines [4, 5].

Recently 2PhEE has been classified as emerging contaminants (ECs). ECs are chemicals that are believed to have cause ecological and human health effects [3] ECs chemicals are not very well documented as these chemicals are available in small quantities [3] 2PhEE compound has introduce multiple effects into several species either by affecting it with renal toxicity, hepatotoxicity or hemolysis in different sub chronic and chronic studies [6]. 2-Phenoxyethanol enhance the surface and groundwater contamination and bioaccumulation risk in the trophic chain [7] if water is used without any special treatments, the enhancement of the contamination is due to 2PhEE persistence and stability, furthermore, 2-Phenoxyethanol has been classified as one of the endocrine disrupting compounds (EDCs) [8] according to EPA (environmental agency).

The aim of this work was to study the densities, sound velocities and the refractive index for the binary systems (2PhEE + 1-propanol or 2-propanol or 1-butanol or 2-butanol) over the entire composition range and at(293.15, 303.15, 313.15 and 323.15) K and at p =0.1 MPa. These results were used to calculate the excess molar volumes, isentropic compressibility, and deviation in isentropic compressibility and refractive index respectively, over the entire composition range and at each temperature. The Redlich-Kister polynomial equation was fitted to the excess molar volume and deviation in isentropic compressibility. Four sound velocity

mixing rules were applied to the experimental data. The open literature shows that there are no data available for the binary systems investigated.

2. Experimental procedure

2.1. Chemicals

2PhEE, 1-propanol, 2-propanol, 1-butanol, and 2-butanol were Sigma Aldrich products. The purity of these chemicals was declared to be more than 0.99 on mass fraction basis and have been used without further purification. The Table 1, sum up the source and the purity of all chemicals employed in this work. Table 2 shows the comparison of the measured densities, speed of sound and refractive index with reported literatures [11-68], which are in good accord with literature values except for 2PhEE with literatures [68] at (303.15, 313.15 and 323.15) K for density and speed of sound where noticeable deviation observed. This is may be due to the "lack" purity of the chemicals, as well as the accuracy of the instrument.

2.2. Apparatus and procedure

The binary mixtures containing the 2PhEE with following alcohols: 1-propanol, 2-propanol, 1-butanol, and 2-butanol were prepared by mass, using an OHAUS analytical balance with a precision of ±0.0001 g. The estimated error in the mole fraction was ±0.0005. A digital vibrating-tube densimeter and sound velocity analyzer (Anton Paar DSA 5000M) with an accuracy of ±0.02 K in temperature were used to measure the density and speed of sound for the pure components and their binary mixtures. The speed of sound was measured using a propagation time technique with frequency of 3 MHz. The estimated errors in density and speed of sound velocity were ±0.003 $g.cm^{-3}$ and ±1.2 $m.s^{-1}$, respectively. The refractive indices of the pure liquids used in the present work were measured using an Abbe digital refractometer (Model Abbemat 300, Anton Paar), with an accuracy of ±0.02 K in temperature. The measured

values of the refractive indices using the method and apparatus were estimated to be ±0.005 of their true values.

3. Results and discussion

3.1. Density, speed of sound and refractive indices

Thermophysical properties are important parameters to understand nature of molecular interactions between mixtures such as speed of sound has been extensively employed to understand the nature of intermolecular interactions of pure liquids, binary, ternary and quaternary mixtures and refractive indices, measurements are expected to shed some light on both solute-solute and solute-solvent interactions. In this regards, the values of density ρ, speed of sound u and refractive indices n_D were measured at (293.15, 303.15, 313.15 and 323.15) K, and pressure p = 0.1 MPa for the binary systems (2PhEE + 1-propanol or 2-propanol or 1-butanol or 2-butanol) and are given in Table 3. It can be seen from Table 3 that the values of ρ, u and n_D decreases with an increase in temperature, and increases with an increase in concentration x_1 for all investigated binary systems.

3.2. Excess molar volumes

The excess molar volumes, V_m^E, were calculated using equation (1) for systems studied:

$$V_m^E = \frac{x_1M_1 + x_2M_2}{\rho} - \frac{x_1M_1}{\rho_1} - \frac{x_2M_2}{\rho_2} \quad (1)$$

where x_1 and x_2 are mole fractions; M_1 and M_2 denote molar masses; ρ_1 and ρ_2 are the densities; where 1 refers to 2PhEE and 2 refers 1-propanol or 2-propanol or 1-butanol or 2-butanol, and ρ is the density of the binary mixtures. Table 1S represent the results of excess molar volume, V_m^E, for the studied system and are also plotted in Figure 1 (a-d). The V_m^E values are negative for all the systems (2PhEE + 1-propanol, or 2-propanol, 2PhEE + 1-butanol, or 2-butanol). To

the best of our knowledge there are no data available in the literature for any of the mixtures considered here to compare our results. The negative values of V_m^E for the studied binary systems indicate that the presence of stronger unlike interaction in the mixtures as well as intermolecular hydrogen bond formation in the phenoxyethanol and alcohol molecules. The factor contributes to decrease in volume were caused by contraction in volume. The experimental results suggested that the factors responsible for decrease in volume are dominant over the composition range. As can been seen the results in Table 1S, the V_m^E values for (2PhEE + 2-butanol) > (2PhEE + 1-butanol) > (2PhEE + 1-propanol) > (2PhEE + 2-propanol). Therefore, it is clear that 2-propanol interacts more strongly with 2PhEE than with 1-propanol than with 1-butanol than with 2-butanol. The V_m^E values decrease with an increase in temperature for all systems.

3.3. Isentropic compressibility, and deviation in isentropic compressibility

The Newton–Laplace equation was used to calculate the isentropic compressibility, κ_s,

$$\kappa_s = \frac{1}{\rho u^2} \tag{2}$$

The deviations in isentropic compressibility, $\Delta\kappa_s$, were calculated using the equation given below:

$$\Delta\kappa_s(x) = \kappa_s - \sum_i^2 x_i \kappa_{s,i} \tag{3}$$

where $\kappa_{s,i}$ and x_i are the isentropic compressibility and mole fractions of the pure component i, respectively. The results of isentropic compressibility, κ_s, for studied systems at (293.15, 303.15, 313.15 and 323.15) K are given in Table 3. The isentropic compressibility, κ_s, values increases with an increase in temperature and decreases with an increase in concentration at a fixed composition for all systems. The calculated $\Delta\kappa_s$ values for studied system at (293.15,

303.15, 313.15 and 323.15) K are also given in Table 1S and are graphically presented in Figures 2 (a-d). It is observed from Figures 2(a-d), the values of $\Delta\kappa_s$ are negative over the entire mole fraction for all systems suggesting that structure–making effect would lead to decrease in free-space for mixing the 2PhEE with 1-propanol, or 2-propanol, 2PhEE + 1-butanol, or 2-butanol molecules lead to negative deviation in isentropic compressibility [9].

3.4. Deviation in refractive index

The deviation in refractive index, Δn_D, was calculated using equation given below:

$$\Delta n_D = n_D - x_1 n_1 - x_2 n_2 \quad (4)$$

where n_1 and n_2 are the refractive index of pure components and n is the refractive index of the mixtures. The results of deviation in refractive index, Δn_D, for the binary systems (2PhEE + 1-propanol or 2-propanol or 1-butanol or 2-butanol) at (293.15, 303.15, 313.15 and 323.15) K are given in Table 1S and graphically presented in Figures 3 (a-d). The values of Δn_D are positive for the all binary systems at each temperature. In general the Δn_D values increase with an increase in temperature at fixed composition for all systems.

3.7. Correlation of derived properties

Experimental excess/deviation properties of the (2PhEE +1-propanol or 2-propanol or 1-butanol or 2-butanol) at (293.15, 303.15, 313.15 and 323.15) K were correlated by Redlich–Kister equation [10]:

$$X = x_1 x_2 \sum_{i=1}^{k} A_i \left(1 - 2x_1\right)^{i-1} \quad (5)$$

where X is excess molar volumes, V_m^E, deviation in isentropic compressibility, $\Delta\kappa_S$ and deviation in refractive indices Δn_D. The values of the fitting parameters A_i have been evaluated

using a least-square method. These results are summarized in Table 4, together with the corresponding standard deviations, σ, for the correlation as determined using equation (6):

$$\sigma(X) = \left[\frac{\sum_{i=1}^{N} \left(X_{\text{exp t}} - X_{\text{calc}} \right)^2}{(N - k)} \right]^{1/2} \quad (6)$$

where N is the number of experimental points and k is the number of coefficients used in the Redlich-Kister equation. The values of V_m^E, $\Delta\kappa_S$ and Δn_D as well as the plots of the Redlich-Kister model are displayed in Figures 1 (a-d), 2 (a-d) and 3 (a-d), respectively. The standard deviations, between the experimental data and those calculated using Redlich–Kister equation are also given in Table 4, show very small values at the investigated temperatures for all the systems.

4. Conclusion

In this work reports experimental values of densities, speeds of sound and refractive indices for (2PhEE +1-propanol or 2-propanol or 1-butanol or 2-butanol) binary systems were determined as a function of composition over the temperature range (293.15 to 323.15) K and at atmospheric pressure. The experimental values were used for the calculation of excess functions, which were then correlated using a Redlich-Kister-type polynomial equation. The excess molar volumes and deviation in isentropic compressibility are negative for all systems (2PhEE + 1-propanol, or 2-propanol, 2PhEE + 1-butanol, or 2-butanol) whereas deviation in refractive indices are positive. The results are analyzed in the light of molecular interactions between the 2PhEE and 1-propanol, or 2-propanol, 2PhEE + 1-butanol, or 2-butanol.

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Table 1: Molar mass, CAS #, suppliers and purities of chemicals used in this study

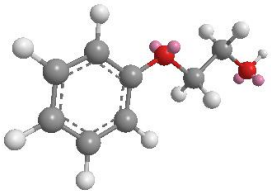
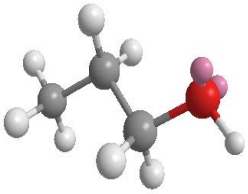
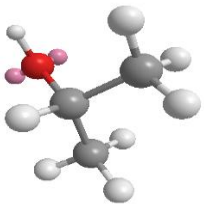
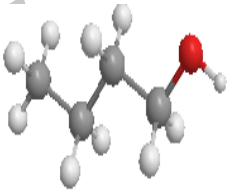
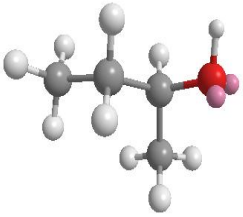
Chemical name	Structure	CAS #	Supplier	Lot #	Molar mass/(g.mole^{-1})	Mass fraction purity (as stated by the supplier)
2-PhEE		122-99-6	Sigma-Aldrich	BCBT1069	138.16	≥99%
1-propanol		71-23-8	Sigma-Aldrich	SZBF2320V	60.10	≥ 99%
2-propanol		67-63-0	Sigma-Aldrich	STBF8249V	60.10	≥99 .8%
1-butanol		71-36-3	Sigma-Aldrich	SZBB1160V	74.12	≥99.5%
2-butanol		78-92-2	Sigma-Aldrich	STBG2236V	74.12	≥99%

Table 2: Comparison of experimental density,ρ, and sound velocity, u, refractive indices n_D of the pure component with the corresponding literature values at (293.15, 298.15, 303.15, 313.15and 323.15) K and at pressure p = 0.1 MPa.

Component	T/(K)	ρ /(10^3×Kg m^{-3})		u/ (m·s^{-1})		n_D	
		Exp.	Lit.	Exp.	Lit.	Exp.	Lit.
2-PhEE	293.15	1.107	1.104[11]	1591.8	-	1.539	-
	298.15	1.103	1.10341[12]	1574.6	-	1.536	1.54[11]
							1.538[13]
	303.15	1.099	1.0933[14]	1557.4	1540.72[14]	1.534	-
	313.15	1.090	1.0830[14]	1522.9	1501.28[14]	1.530	-
	323.15	1.081	1.0739[14]	1489.1	1466.24[14]	1.526	-
1-propanol	293.15	0.803	0.80410[15]	1224.3	-	1.385	1.3852[15]
			0.8036[16]				1.3850[17]
			0.80428[18]				1.385[19]
			0.8032[19]				
	298.15	0.800	0.79993[15]	1207.3	1207.2[20]	1.383	1.3832[15]
			0.79960[16]		1208.1[21]		1.3832[17]
			0.80021[18]		1205.69 [22]		1.38304[22]
			0.79958[20]				1.3834[23]
			0.7995[21]				1.3834[24]
			0.79975[22]				1.3838[25]
			0.8000[23]				1.38307 [26]
			0.79966[24]				1.3830[27]

			0.79961[25]				1.3840[28]
			0.79950[26]				1.38307[29]
			0.79962[27]				
			0.7995[29]				
			0.7990[30]				
			0.79960[31]				
			0.7996[32]				
	303.15	0.796	0.79586[15]	1189.9	1192.6[21]	1.381	1.3811[15]
			0.79560[16]				1.3814[17]
			0.79642[18]				
			0.7955[21]				
			0.79560[33]				
			0.79550 [34]				
			0.79561[35]				
	313.15	0.788	0.78740[16]	1156.0	1160.2[21]	1.377	1.3774[17]
			0.78851[18]				
			0.7874[21]				
			0.78730[33]				
			0.78730 [34]				
	323.15	0.780	0.7791 [16]	1122.5	-	1.373	1.3732 [17]
			0.78102[18]				
			0.77860[33]				
			0.77900[34]				
2-propanol	293.15	0.785	0.78535 [18]	1157.8	-	1.377	1.378[19]
			0.7872[19]		-		1.377[36]

	298.15	0.781	0.7809[29] 0.78090 [31] 0.7807[32] 0.7810[37] 0.78105[38] 0.78116[39] 0.78098[40] 0.7810[41] 0.7810[42]	1140.2	1145.5[21] 1144[28]	1.375	1.3753[23] 1.3751[25] 1.3765[28] 1.37521[29] 1.3752[37] 1.37520[38] 1.37515[39] 1.3745[40] 1.37496[41] 1.37496[42]
	303.15	0.777	0.77712 [18] 0.7765[21] 0.77659[35] 0.77680 [43]	1122.6	1126.3[21]	1.373	-
	313.15	0.768	0.76879[18] 0.7682[21] 0.76800 [43]	1087.4	1091.3[21]	1.369	-
	323.15	0.759	0.75968 [18] 0.75930 [43]	1051.8	-	1.364	-
1-butanol	293.15	0.810	0.81034[15] 0.8098[16] 0.80943[44] 0.80965[45] 0.80953[46] 0.80960[49]	1258.4	1255.94[44] 1257.5[45] 1256.8[46] 1257.66[48]	1.399	1.3994[15] 1.3988[17] 1.3992[47]

298.15	0.806	0.80585[9]	1241.8	1240.6[20]	1.397	1.3972[15]
		0.80567[15]		1238.99[44]		1.3967 [17]
		0.8060[16]		1239.8[46]		1.3971 [23]
		0.80589[20]		1240.2[50]		1.3973 [24]
		0.8059[23]		1241.0[51]		1.3975[25]
		0.80581[24]		1239.2[52]		1.3973[27]
		0.80577[25]		1240.5[53]		1.3983[28]
		0.80576[27]		1240.37[54]		1.39702[29]
		0.8053[30]		1240.25[55]		1.3978[49]
		0.8058[28]				1.3973[56]
		0.8059[29]				1.3973 [57]
		0.8060[37]				1.39716 [58]
		0.80556[51]				1.3973[59]
		0.80564[52]				
		0.80590[53]				
		0.80587[56]				
		0.80548[60]				
		0.80589[61]				
		0.8070[62]				
		0.8071[58]				
303.15	0.802	0.80201[9]	1225.0	1224[29]	1.395	1.3953[15]
		0.80195[15]		1222.08[44]		1.3947[17]
		0.8021 [16]		1223.6[45]		1.3946[63]
		0.80191[35]		1222.9[46]		
		0.80179[44]		1226.5[53]		
		0.80200[45]				

			0.8019[46]				
			0.80315[53]				
			0.80206[58]				
			0.8037[62]				
			0.8019[63]				
	313.15	0.794	0.79423 [9]	1191.8	1190[29]	1.391	1.3908[17]
			0.7943 [16]		1190.2[45]		1.3920[47]
			0.79421[45]		1189.9[50]		
			0.79420 [51]		1189.5[51]		
			0.79416[52]		1188.6[52]		
			0.7967[62]				
	323.15	0.787	0.78629[9]	1158.7	1156.5[46]	1.387	1.3867[17]
			0.7864[16]		1157.19 [48]		
			0.7861[46]				
2-butanol	293.15	0.806	0.8067[29]	1230.1	1230[29]	1.397	1.3971[47]
			0.80648[44]		1228.38[44]		
			0.80734[45]		1232.4[45]		
			0.8063[46]		1230.1[46]		
	298.15	0.802	0.80244[9]	1212.1	1210.43[44]	1.395	1.3954[25]
			0.80249[25]		1212.1[46]		1.39523[29]
			0.8024[29]		1212.2[50]		1.3948[40]
			0.80256[40]		1212.4[51]		1.3954[47]
			0.80241[50]		1211.5[52]		1.39503[64]
			0.80225[51]		1230.18[64]		1.3951[65]
			0.80220[52]				1.3952[66]

		0.80206[60]				1.39530[67]
		0.80241[64]				
		0.80250[68]				
303.15	0.798	0.7984[29]	1194.1	1192.47[44]	1.393	1.3928[47]
		0.79899[45]		1196.1[45]		
		0.7980[46]		1194[46]		
313.15	0.789	0.79028[45]	1157.7	1159.5[45]	1.389	1.3890[47]
		0.78963[50]		1157.5[50]		
		0.78941[51]		1157.3[51]		
		0.78959[52]		1157.1[52]		
323.15	0.780	0.7802[46]	1120.7	1120.6[46]	1.384	-
		0.78055[66]				

Standard uncertainties u are $u(T) = \pm 0.02$ K, $u(p) = \pm 0.04$ MPa and the combined expanded uncertainty Uc in mole fraction, density, sound velocity and refractive index were $Uc(x) = \pm 0.0005$, $Uc(\rho) = \pm 0.003$ g.cm^{-3}, $Uc(u) = \pm 1.2$ m.s^{-1} and $Uc(n) = \pm 0.005$ respectively, (0.95 level of confidence).

Table 3. Densities, ρ, sound velocity, u, isentropic compressibility,κs and refractive indices, $n_{D,}$ for the binary systems {2PhEE (1) + 1-propanol (2), or 2-propanol (2), or 1-butanol (2), or 2-butanol (2)}at (293.15, 303.15,313.15 and 323.15)K and at pressure p = 0.1 MPa.

x_1	ρ /($10^3 \times Kg\ m^{-3}$)	u / (ms^{-1})	κ_s/($10^{12} \times Pa^{-1}$)	n_D
		{2-PhEE (1) +1-propanol (2)}		
		T = 293.15 K		
0.0000	0.803	1224.3	830	1.385
0.1045	0.856	1281.0	712	1.411
0.2026	0.898	1328.3	631	1.433
0.3043	0.936	1372.9	567	1.453
0.3974	0.967	1410.5	520	1.469
0.5027	0.998	1449.7	477	1.484
0.5992	1.024	1482.4	444	1.497
0.6951	1.047	1512.1	418	1.508
0.8044	1.071	1543.0	392	1.520
0.8590	1.082	1557.4	381	1.526
0.9018	1.090	1568.2	373	1.530
1.0000	1.107	1591.8	356	1.539
		T = 303.15 K		
0.0000	0.796	1189.9	888	1.381
0.1045	0.847	1247.5	758	1.408
0.2026	0.890	1294.5	671	1.430
0.3043	0.928	1339.5	601	1.450
0.3974	0.959	1376.9	550	1.465
0.5027	0.990	1415.8	504	1.480
0.5992	1.016	1448.3	469	1.493
0.6951	1.039	1478.5	440	1.504
0.8044	1.062	1508.7	414	1.516

0.8590	1.073	1522.9	402	1.522
0.9018	1.081	1534.1	393	1.526
1.0000	1.099	1557.4	375	1.534
		T = 313.15 K		
0.0000	0.788	1156.0	950	1.377
0.1045	0.839	1214.0	809	1.405
0.2026	0.881	1261.1	714	1.426
0.3043	0.919	1306.4	637	1.446
0.3974	0.950	1343.5	583	1.461
0.5027	0.981	1382.3	533	1.476
0.5992	1.007	1414.7	496	1.490
0.6951	1.030	1444.8	465	1.500
0.8044	1.054	1474.8	436	1.512
0.8590	1.064	1488.9	424	1.518
0.9018	1.073	1500.2	414	1.521
1.0000	1.090	1522.9	396	1.530
		T = 323.15 K		
0.0000	0.780	1122.5	102	1.373
0.1045	0.831	1180.7	864	1.401
0.2026	0.872	1228.0	760	1.423
0.3043	0.911	1273.3	677	1.442
0.3974	0.942	1310.4	619	1.457
0.5027	0.973	1349.1	565	1.473
0.5992	0.998	1381.4	525	1.485
0.6951	1.021	1411.3	492	1.497
0.8044	1.045	1441.2	461	1.508
0.8590	1.056	1455.3	447	1.513
0.9018	1.064	1466.5	437	1.517
1.0000	1.081	1489.1	417	1.526

{2-PhEE (1) +2-propanol (2)}

T = 293.15 K

0.0000	0.785	1157.8	950	1.377
0.0980	0.837	1223.8	798	1.403
0.1981	0.882	1282.5	689	1.427
0.3023	0.924	1337.7	605	1.448
0.3974	0.958	1383.4	546	1.465
0.4981	0.990	1427.3	496	1.481
0.6071	1.020	1470.3	453	1.496
0.7009	1.044	1503.6	424	1.508
0.7974	1.066	1534.7	398	1.518
0.8826	1.085	1559.8	379	1.527
1.0000	1.107	1591.8	356	1.539

T = 303.15 K

0.0000	0.777	1122.6	1020	1.373
0.0980	0.828	1189.5	853	1.400
0.1981	0.874	1248.0	735	1.423
0.3023	0.915	1303.7	643	1.445
0.3974	0.949	1348.8	579	1.462
0.4981	0.981	1392.9	525	1.478
0.6071	1.012	1435.6	480	1.493
0.7009	1.036	1468.9	448	1.505
0.7974	1.058	1499.9	420	1.515
0.8826	1.076	1525.1	400	1.524
1.0000	1.099	1557.4	375	1.534

T = 313.15 K

0.0000	0.768	1087.4	1100	1.369

0.0980	0.819	1154.2	916	1.396
0.1981	0.865	1213.4	785	1.420
0.3023	0.907	1268.9	685	1.442
0.3974	0.940	1314.5	616	1.459
0.4981	0.972	1358.6	557	1.475
0.6071	1.003	1401.6	508	1.491
0.7009	1.027	1434.68	473	1.502
0.7974	1.049	1465.7	444	1.512
0.8826	1.067	1490.9	421	1.520
1.0000	1.090	1522.9	396	1.530

T = 323.15 K

0.0000	0.759	1051.8	1190	1.364
0.0980	0.810	1119.0	986	1.393
0.1981	0.856	1178.7	841	1.417
0.3023	0.897	1234.5	731	1.438
0.3974	0.931	1280.3	655	1.456
0.4981	0.963	1324.4	592	1.472
0.6071	0.994	1367.2	538	1.487
0.7009	1.018	1400.6	501	1.498
0.7974	1.040	1431.9	469	1.508
0.8826	1.059	1457.0	445	1.516
1.0000	1.081	1489.1	417	1.526

{2-PhEE (1) +1-butanol (2)}

T = 293.15 K

0.0000	0.810	1258.4	780	1.399
0.1033	0.851	1298.3	697	1.419
0.1974	0.887	1333.3	635	1.435
0.2967	0.921	1368.9	580	1.451

0.3958	0.953	1403.7	533	1.466
0.4913	0.981	1436.4	494	1.480
0.6029	1.013	1473.2	455	1.494
0.6971	1.037	1503.2	427	1.506
0.7989	1.062	1534.3	400	1.518
0.9011	1.086	1563.7	377	1.528
1.0000	1.107	1591.8	356	1.539
		T = 303.15 K		
0.0000	0.802	1225.0	831	1.395
0.1033	0.844	1265.3	740	1.415
0.1974	0.879	1299.9	674	1.431
0.2967	0.913	1335.6	614	1.447
0.3958	0.945	1370.3	564	1.462
0.4913	0.973	1402.9	522	1.476
0.6029	1.004	1439.9	480	1.491
0.6971	1.029	1469.3	450	1.502
0.7989	1.054	1500.0	422	1.514
0.9011	1.077	1530.1	396	1.524
1.0000	1.099	1557.4	375	1.534
		T = 313.15 K		
0.0000	0.794	1191.8	886	1.391
0.1033	0.836	1232.3	788	1.411
0.1974	0.870	1266.9	716	1.428
0.2967	0.904	1302.7	651	1.443
0.3958	0.936	1337.4	597	1.458
0.4913	0.965	1369.9	552	1.472
0.6029	0.996	1406.3	508	1.486
0.6971	1.020	1435.9	475	1.498
0.7989	1.045	1466.4	445	1.509

0.9011	1.069	1495.7	418	1.520
1.0000	1.090	1522.9	396	1.530

T = 323.15 K

0.0000	0.787	1158.7	947	1.387
0.1033	0.828	1199.4	840	1.407
0.1974	0.862	1234.3	761	1.424
0.2967	0.896	1270.1	692	1.440
0.3958	0.928	1304.8	633	1.454
0.4913	0.956	1337.2	585	1.467
0.6029	0.987	1373.4	537	1.482
0.6971	1.012	1402.8	502	1.494
0.7989	1.037	1433.1	470	1.505
0.9011	1.060	1462.5	441	1.516
1.0000	1.081	1489.1	417	1.526

{2-PhEE (1) +2-butanol (2)}

T = 293.15 K

0.0000	0.806	1230.1	819	1.397
0.1062	0.849	1276.8	722	1.418
0.2025	0.885	1316.8	652	1.434
0.3030	0.920	1357.0	590	1.451
0.3989	0.951	1394.1	541	1.466
0.5066	0.984	1433.9	494	1.481
0.6032	1.011	1468.3	459	1.494
0.7042	1.038	1502.6	427	1.506
0.8005	1.062	1533.2	401	1.518
0.9011	1.085	1563.2	377	1.529
1.0000	1.107	1591.8	356	1.539

T = 303.15 K

0.0000	0.798	1194.1	879	1.393
0.1062	0.841	1241.8	771	1.413
0.2025	0.877	1281.8	694	1.430
0.3030	0.911	1322.3	627	1.447
0.3989	0.943	1359.5	574	1.462
0.5066	0.975	1399.7	523	1.477
0.6032	1.003	1433.8	485	1.490
0.7042	1.030	1468.4	451	1.501
0.8005	1.053	1498.6	423	1.514
0.9011	1.077	1529.2	397	1.524
1.0000	1.099	1557.4	375	1.534
T = 313.15 K				
0.0000	0.789	1157.7	945	1.389
0.1062	0.832	1205.8	827	1.409
0.2025	0.868	1246.8	741	1.427
0.3030	0.903	1287.7	668	1.443
0.3989	0.934	1325.1	610	1.458
0.5066	0.967	1365.5	555	1.473
0.6032	0.994	1399.6	514	1.486
0.7042	1.021	1433.8	477	1.499
0.8005	1.045	1464.4	446	1.510
0.9011	1.069	1494.6	419	1.520
1.0000	1.090	1522.9	396	1.530
T = 323.15 K				
0.0000	0.780	1120.7	1020	1.384
0.1062	0.823	1169.8	888	1.405
0.2025	0.859	1211.5	793	1.423
0.3030	0.894	1252.9	713	1.440
0.3989	0.925	1290.7	649	1.454

0.5066	0.958	1331.3	589	1.469
0.6032	0.985	1365.6	544	1.482
0.7042	1.012	1399.8	504	1.494
0.8005	1.036	1430.5	472	1.506
0.9011	1.060	1460.8	442	1.516
1.0000	1.081	1489.1	417	1.526

Standard uncertainties u are $u(T) = \pm 0.02$ K, $u(p) = \pm 0.04$ MPa and the combined expanded uncertainty Uc in mole fraction, density, sound velocity and refractive index were $U\text{c}(x) = \pm 0.0005$, $U\text{c}(\rho) = \pm 0.003$ g.cm^{-3}, $U\text{c}(u) = \pm 1.2$ m.s^{-1} and $U\text{c}(n) = \pm 0.005$ respectively, (0.95 level of confidence).

Table 4. Coefficients A_i, and standard deviations, obtained for the binary systems studied in this work at different temperatures and at pressure p = 0.1 MPa for the Redlich–Kister.

	T (K)	A_1	A_2	A_3	A_4	A_5	σ
			{2-PhEE (1) + 1-propanol (2)}				
V_m^E /(10^3×m^3.mol^{-1})	293.15	-1.644	0.533	-0.200	0.195	-0.137	0.003
	303.15	-1.691	0.563	-0.225	0.195	-0.137	0.003
	313.15	-1.741	0.592	-0.240	0.192	-0.139	0.003
	323.15	-1.794	0.620	-0.258	0.208	-0.151	0.003
$\Delta\kappa_S$ / (10^{-12}×Pa^{-1})	293.15	-462.6	207.9	-90.4	62.8	-38.4	0.1
	303.15	-505.9	230.0	-100.8	76.1	-49.4	0.3
	313.15	-554.1	255.8	-115.9	82.1	-52.6	0.4
	323.15	-607.5	284.3	-129.9	91.8	-59.1	0.4
Δn_D	293.15	0.087	-0.027	0.005	0.006	-	0.000
	303.15	0.088	-0.028	0.009	0.003	-	0.000
	313.15	0.089	-0.026	0.014	-0.008	-	0.000
	323.15	0.091	-0.024	0.018	-0.017	-	0.000
			{2-PhEE (1) + 2-propanol (2)}				
V_m^E /(10^3×m^3.mol^{-1})	293.15	-2.209	0.734	-0.211	0.396	-0.260	0.004
	303.15	-2.273	0.764	-0.188	0.380	-0.305	0.004
	313.15	-2.369	0.796	-0.232	0.390	-0.250	0.004
	323.15	-2.504	0.857	-0.250	0.389	-0.262	0.004
$\Delta\kappa_S$ / (10^{-12}×Pa^{-1})	293.15	-632.5	309.0	-144.0	106.8	-68.4	0.3
	303.15	-695.6	345.5	-160.7	126.5	-88.5	0.5
	313.15	-768.4	385.7	-184.0	137.6	-89.4	0.3
	323.15	-853.2	435.6	-211.1	154.3	-100.5	0.3

	293.15	0.095	-0.029	0.000	0.004	-	0.000
Δn_D	303.15	0.099	-0.023	0.004	-0.014	-	0.000
	313.15	0.105	-0.024	0.004	-0.011	-	0.000
	323.15	0.111	-0.024	0.003	-0.018	-	0.000
	{2-PhEE (1) +1-butanol (2)}						
V_m^E	293.15	-1.098	0.203	-0.080	0.144	-	0.006
/(10^3×m^3.mol^{-1})	303.15	-1.122	0.219	-0.094	0.129	-	0.005
	313.15	-1.149	0.231	-0.091	0.121	-	0.006
	323.15	-1.184	0.247	-0.094	0.110	-	0.006
$\Delta\kappa_S$ /	293.15	-309.5	99.1	-37.6	21.7	-0.4	0.1
(10^{-12}×Pa^{-1})	303.15	-337.6	108.3	-30.1	26.7	-24.7	0.1
	313.15	-369.1	120.7	-36.9	28.5	-21.4	0.1
	323.15	-405.0	136.5	-41.4	26.5	-25.7	0.1
	293.15	0.048	-0.007	0.000	-0.002	-	0.000
Δn_D	303.15	0.049	-0.008	0.000	0.000	-	0.000
	313.15	0.049	-0.009	0.002	-0.001	-	0.000
	323.15	0.050	-0.009	0.004	-0.004	-	0.000
	{2-PhEE (1) +2-butanol (2)}						
V_m^E	293.15	-0.982	0.024	0.117	0.105	-	0.006
/(10^3×m^3.mol^{-1})	303.15	-1.036	0.033	0.110	0.105	-	0.006
	313.15	-1.133	0.068	0.108	0.094	-	0.006
	323.15	-1.282	0.122	0.090	0.105	-	0.006
$\Delta\kappa_S$ /	293.15	-364.1	121.8	-43.2	27.6	-7.9	0.1
(10^{-12}×Pa^{-1})	303.15	-403.3	137.5	-43.0	36.6	-28.9	0.2
	313.15	-449.4	160.2	-54.6	33.3	-18.9	0.1
	323.15	-504.7	186.5	-65.6	38.4	-21.5	0.1

	293.15	0.048	-0.006	0.001	0.001	-	0.000
Δn_D	303.15	0.050	-0.005	0.001	-0.006	-	0.000
	313.15	0.051	-0.007	0.004	-0.003	-	0.000
	323.15	0.054	-0.010	0.007	0.002	-	0.000

Standard uncertainties u are $u(T) = \pm 0.02$ K, $u(p) = \pm 0.04$ MPa and the combined expanded uncertainty Uc in mole fraction, density, sound velocity and refractive index were $U\text{c}(x) = \pm 0.0005$, $U\text{c}(\rho) = \pm 0.003$ g.cm^{-3}, $U\text{c}(u) = \pm 1.2$ m.s^{-1} and $U\text{c}(n) = \pm 0.005$ respectively, (0.95 level of confidence).

Figure captions

Figure 1. Plot of excess molar volumes, V_m^E ,for the binary mixtures:(a){2PhEE (1) + 1-propanol (2)},(b){2PhEE (1) + 2-propanol (2)},(c) **{**2PhEE (1) + 1-butanol (2)} and (d){2PhEE (1) + 2-butanol (2)} as function of the composition expressed in the mole fraction of 2PhEE at 293.15 K (♦), 303.15 K (■), 313.15 K (▲) and 323.15 K (●). The dotted lines were generated using Redlich-Kister polynomial curve-fitting.

Figure 2. Plot of deviation in isentropic compressibility, $\Delta\kappa_s$,of the binary mixtures:(a){2PhEE (1) + 1-propanol (2)},(b){2PhEE (1) + 2-propanol (2)},(c) {2PhEE (1) + 1-butanol (2)} and (d){2PhEE (1) + 2-butanol (2)} as function of the composition expressed in the mole fraction of 2PhEE at 293.15 K (♦), 303.15 K (■), 313.15 K (▲) and 323.15 K (●). The dotted lines were generated using Redlich-Kister polynomial curve-fitting.

Figure 3. Plot of deviation in refractive index, Δn_D, of the binary mixtures: (a){2PhEE (1) + 1-propanol (2)}, (b){2PhEE (1) + 2-propanol (2)}, (c) **{**2PhEE (1) + 1-butanol (2)} and (d){2PhEE (1) + 2-butanol (2)} as function of the composition expressed in the mole fraction of 2PhEE at 293.15 K (♦), 303.15 K (■), 313.15 K (▲)and 323.15 K (●). The dotted lines were generated using Redlich-Kister polynomial curve-fitting.

Figure 1 (a)

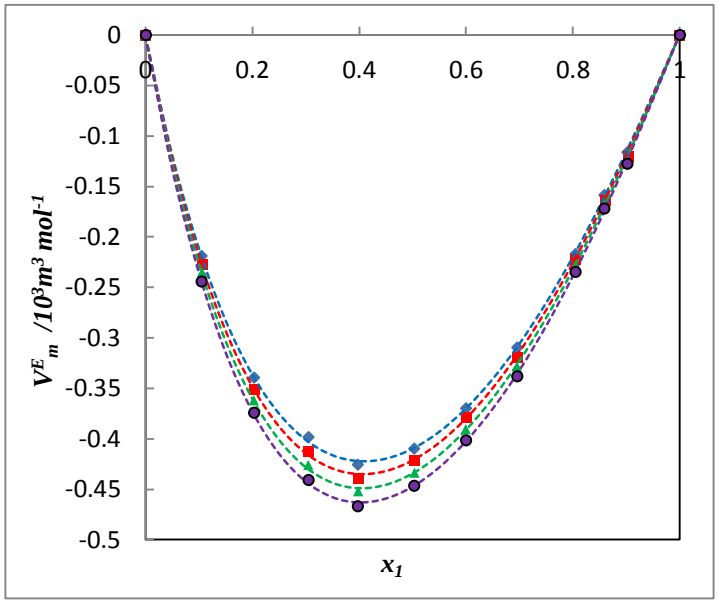


Figure 1 (b)

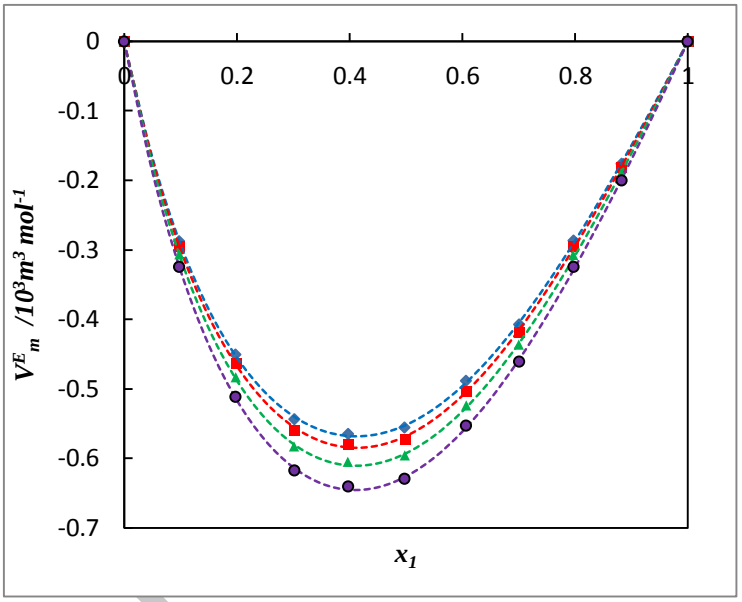


Figure 1 (c)

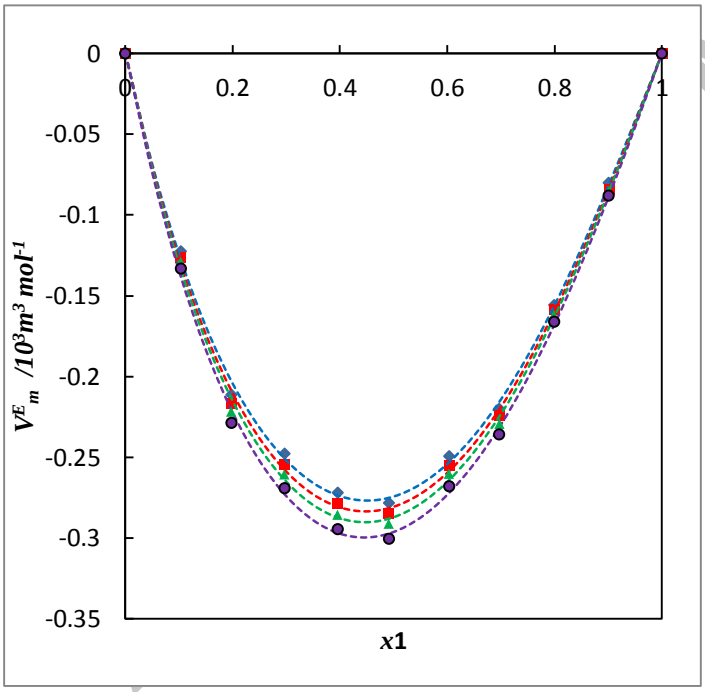


Figure 1 (d)

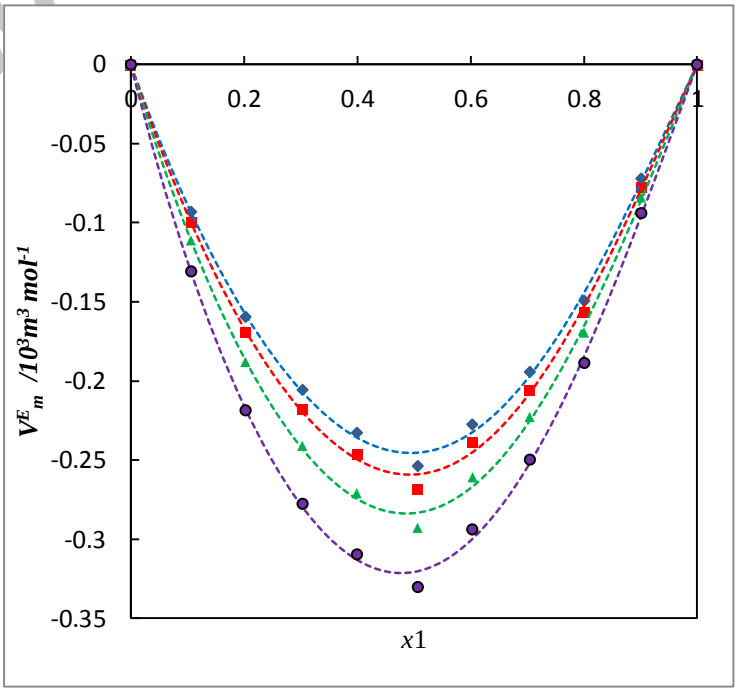
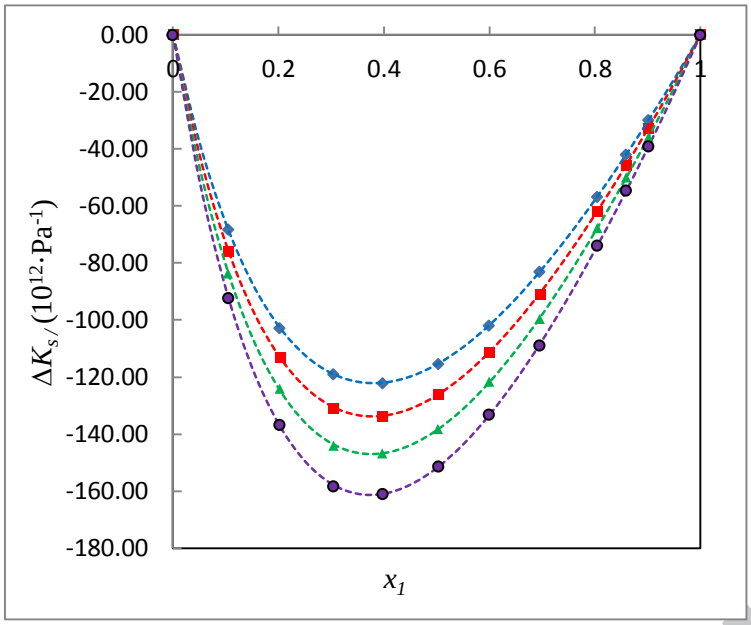


Figure 2 (a)



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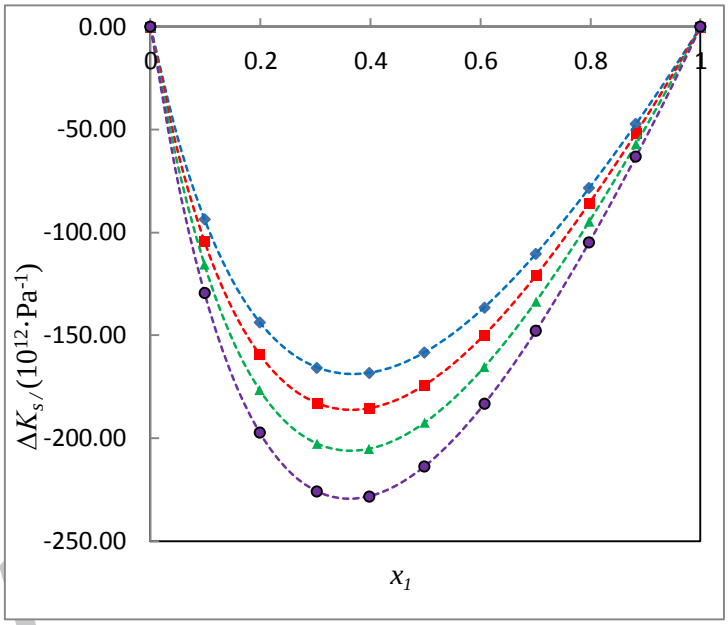


Figure 2 (c)

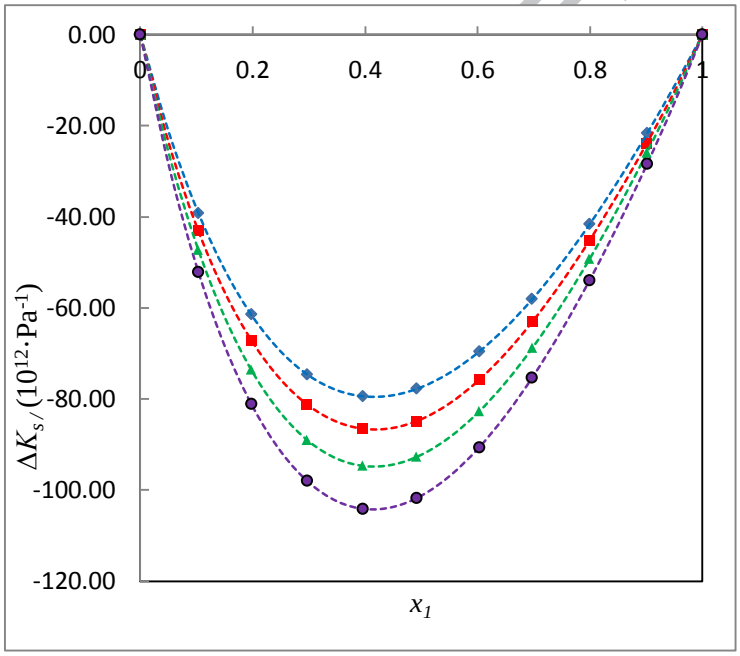


Figure 2 (d)

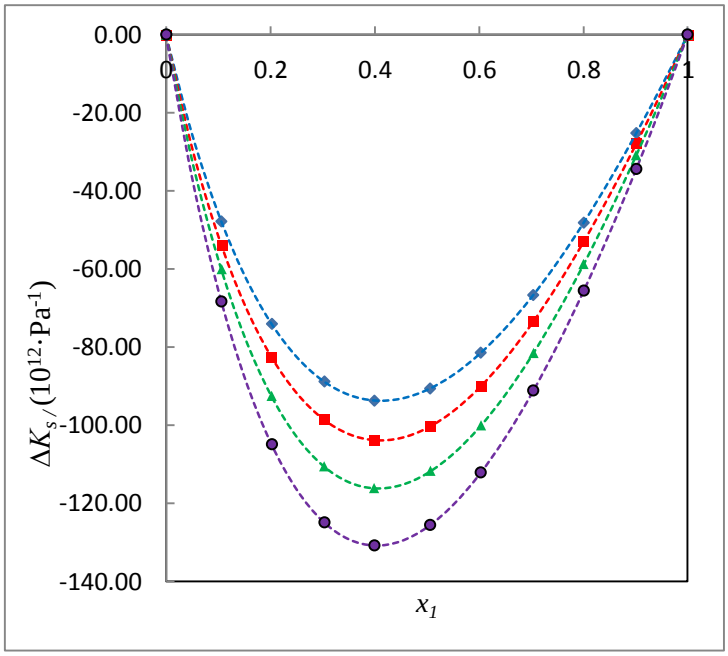


Figure 3 (a)

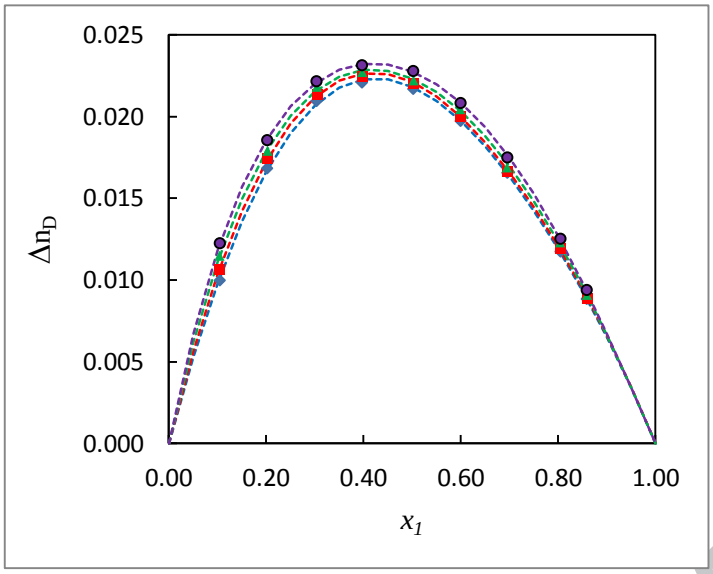


Figure 3 (b)

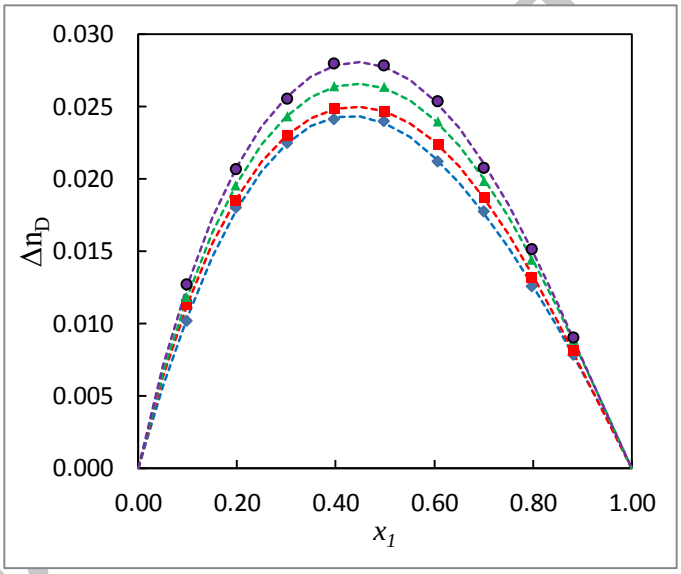


Figure 3 (c)

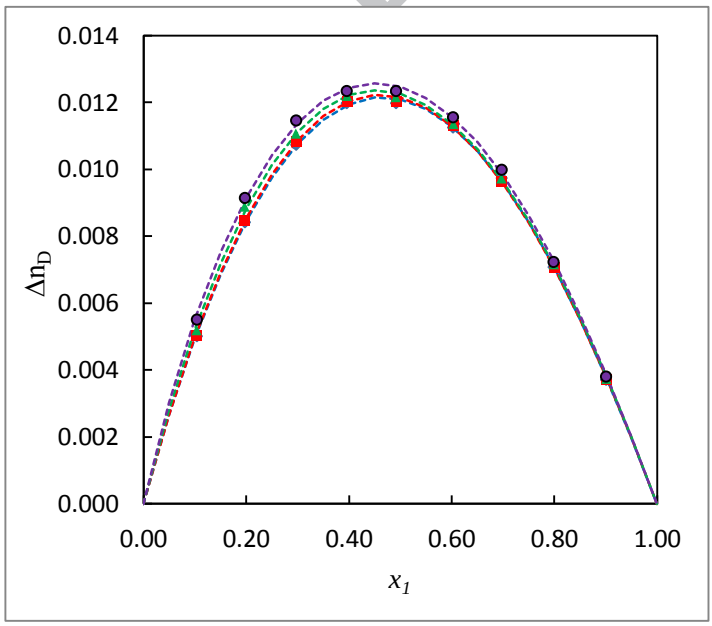
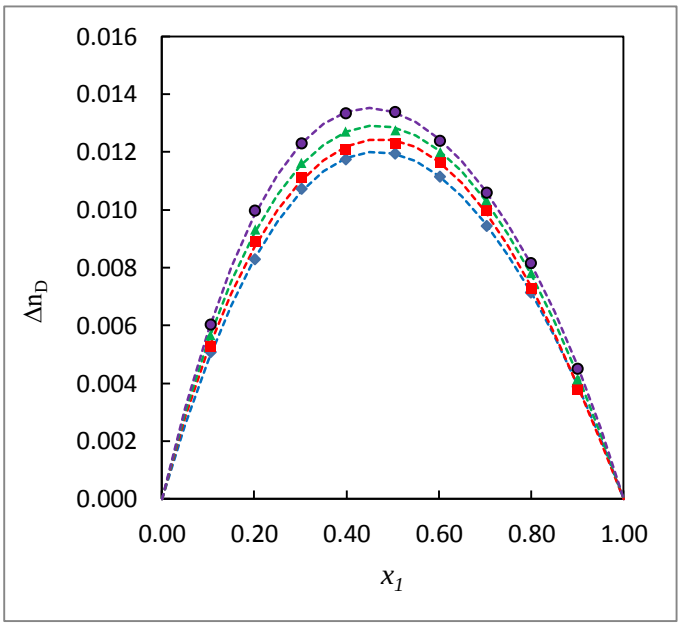


Figure 3 (d)



Highlights

- Densities, sound velocities and refractive indexes for binary systems containing 2-phenoxyethanol + alcohol were measured.
- Derived properties were calculated from measured ρ, u and n_D respectively.
- Redlich–Kister polynomial was used to fit the experimental results.