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Density, viscosity, excess molar volume and viscosity deviation for [chloroform (1)+methanol (3)] binary system and [chloroform (1)+di-isopropylether (2)+methanol (3)] ternary system at 298.15 K

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ABSTRACT

Densities ρ and viscosity η of the [chloroform (1)+methanol(3)] binary system and [chloroform (1)+di-isopropyaelther (DIPE) (2)+methanol (3)] ternary system have been measured at 298.15 K and a pressure of 960 hPa using an Anton Paar DMA 500 stavigmeter. Excess molar volumes V^E and viscosity deviation $\Delta\eta$ were calculated. The excess molar volume and viscosity deviation for binary system were fitted to a Redlich-Kister type equation and the ternary excess molar volumes $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ were correlated by a Redlich-Kister and Nagata and Tamura type equation. Also, the ternary excess molar volume and viscosity deviation Y^E_{123} were predicted using the Radojković equation. From the results we obtained conclusions about the molecular interactions in binary and ternary mixtures.

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Subject area	*Physical chemistry*
Compounds	Chloroform; di-isopropyaelther (DIPE); methanol
Data category	*Physicochemical*
Data acquisition format	*Physical properties*
Data type	*Raw and calculated.*
Procedure	*Determination: density with vibrating tube densimeter viscosity with concentric cylinder viscometer, Hall effect Excess Molar and viscosity deviation are calculated with the general expressions*
Data accessibility	*In this article*

1. Rationale

Properties such as density and viscosity of pure chemicals and of their binary and ternary liquid mixtures over the whole composition range are useful for a full understanding of their thermodynamic and transport properties as well as for practical chemical engineering purposes. On the other hand, excess thermodynamic functions and deviations of non-thermodynamic ones the liquid mixtures are fundamental for understanding of the interactions between molecules in these types of mixtures, particularly when polar components are involved. These functions have also been used as a qualitative and quantitative guide to predict the extent of complex formation in this kind of mixtures [1–3].

In this paper we report density and viscosity data at $T = 298.15$ K and 960 mHPa of three pure chemicals (chloroform, DIPE and methanol), as well as for the [chloroform (1)+methanol(3)] binary system and the ternary liquid mixture over the whole composition range, where these chemicals were included.

Empiric equations for the excess molar volumes $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ of the binary system as well as for the ternary system as a function of composition were developed, using OriginPro 8.5. These equations were fitted using least squares with all points equally weighed. The appropriate number of constants and significant digits are obtained by comparing with the experimental errors.

The excess molar volume and viscosity deviation for binary system were fitted to a Redlich-Kister [4] type equation and the ternary excess molar volumes $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ were correlated by a Redlich-Kister [4] type equation and Nagata and Tamura [5] type equation using least squares in order to obtain their respective dependency on concentration. Also, the ternary excess molar volume and viscosity deviation Y^E_{123}were predicted using the Radojković [6] equation. In all cases OriginPro 8.5 was used. Origin Pro 8.5 and SigmaPlot 10.0 were used for the figures.

We found three papers on density [7–9] and two on viscosity [8,9] of the binary system [chloroform (1)+methanol(3)]. To our knowledge no data density and viscosity, or excess molar volume values and viscosity deviation of [chloroform (1)+di-isopropyl ether (DIPE) (2)+methanol (3)] ternary system have been published.

Density and viscosity data for the other two binary systems at 298.15 KT have already been published by the group [10,11].

2. Procedure

2.1. Reagents

Chloroform (p.a.) and Methanol (p.a.) were supplied by Dorwill, while Dipe (p.a.) was supplied by MERK (Germany). The purity of the reagents determined by gas chromatography was 99.8%. Purity was checked periodically. In Table 1 we report the measured and literature values of density and viscosity of the reagents at 298.15 K.

Literature and experimental Dipe viscosities at 298.15 K exhibit a discrepancy. Literature data show a wide dispersion. When the data presented in this paper are used, the values fit well within the experimental error

Table 1
Densities and viscosities of the pure components at 298.15 K.

Reagent	ρ/kg.m^{-3}		η/mPa.s	
	Experimental	Literature	Experimental	Literature
Chloroform	1478.2	1478.82 [8]	0.5357	0.556 [8]
		1479.7 [21]		0.5357 [21]
		1478.8 [22]		0.556 [22]
Dipe	717.3	718.5 [21]	0.30424	0.379 [21]
Methanol	786.9	786.30 [8]	0.53741	0.551 [8]
		786.37 [21]		0.5513 [21]

2.2. Measurements

Liquid mixtures were prepared by mass in airtight-stoppered bottles. Were used for sample preparation the same techniques [12] and instruments [13] described in previous work. The uncertainty in the mole fractions for these mixtures is estimated to be around than $\pm 1 \times 10^{-4}$. The uncertainty in density and viscosity are ± 0.1 kg.m^{-3} and ± 0.0001 mPa.s, respectively.

Density and viscosity were simultaneously measured with an Anton Paar Stabinger viscometer (SVM 3000/G2) calibrated by the manufacturer. This is equipped with its own Peltier effect control system, which maintains the temperature at ± 0.01 K. The repeatability of the results, as provided by the manufacturer, is $\pm 0.1\%$ of the measured viscosity value, ± 0.1 kg m^{-3} for density, and ± 0.005 K for temperature. Total uncertainties in this work are ± 0.0001 mPa.s of for viscosity value, ± 0.1 kg m^{-3} for density, and ± 0.01 K for temperature. The calibration of the apparatus was checked using standard oils provided by the manufacturer. At least three measurements were made at each temperature and for each solution or pure component.

2.3. Results and discussion

The experimental values of the density ρ and viscosity η for the [chloroform (1)+methanol(3)] binary system are shown in Table 2.

To study ternary mixtures, binary mixtures of constant molar fraction relation $\gamma = x_1 / x_2$ are prepared. A known volume of the binary mixture was added the third component, in this case methanol (3). Each set of ternary mixture with constant relation $\gamma = x_1 / x_2$, it is called serie.

The experimental values of the density ρ and viscosity η for the [chloroform (1)+di-isopropyl ether (DIPE) (2)+methanol (3)] ternary system are shown in Table 3.

Table 2
Experimental density ρ and viscosity η for the [chloroform (1)+methanol(3)] binary system at (298.15 ± 0.01) K.

x_1	ρ/kg.m^{-3}	η/mPa.s
Chloroform (1)+Methanol (3)		
0.0000	786.4	0.5327
0.1020	914.1	0.6114
0.2062	1023.0	0.6617
0.3020	1108.0	0.6732
0.4013	1183.7	0.6654
0.5050	1251.9	0.6413
0.5995	1306.1	0.6178
0.7041	1358.8	0.5877
0.7873	1396.2	0.5659
0.8909	1438.3	0.5451
1.0000	1478.2	0.5357

Table 3
Experimental density ρ and viscosity η ,excess molar volume V^E and viscosity deviation $\Delta\eta$ for the [chloroform (1)+di-isopropyl ether (DIPE) (2)+methanol (3)] ternary system at (298.15 ± 0.01) K.

X_1	X_3	ρ/kg.m^{-3}	η/mPa.s	V^E/m^3.mol^{-1}	$\Delta\eta$/mPa.s
δ = 0.1286					
0.0991	0.0000	818.2	0.3595	$-9.206.10^{-6}$	$2.677.10^{-2}$
0.0821	0.1714	817.9	0.3769	$-7.859.10^{-6}$	$6.474.10^{-3}$
0.0819	0.1739	817.9	0.3775	$-7.840.10^{-6}$	$6.510.10^{-3}$
0.0656	0.3378	817.4	0.4239	$-6.537.10^{-6}$	$1.687.10^{-2}$
0.0612	0.3825	817.1	0.4393	$-6.165.10^{-6}$	$2.244.10^{-2}$
0.0392	0.6046	813.9	0.5170	$-4.207.10^{-6}$	$5.126.10^{-2}$
0.0305	0.6923	811.2	0.5419	$-3.358.10^{-6}$	$5.688.10^{-2}$
0.0239	0.7586	808.2	0.5560	$-2.677.10^{-6}$	$5.640.10^{-2}$
0.0148	0.8509	802.4	0.5665	$-1.691.10^{-6}$	$4.660.10^{-2}$
0.0061	0.9388	794.1	0.5637	$-6.988.10^{-7}$	$2.447.10^{-2}$
0.0034	0.9655	791.0	0.5600	$-3.956.10^{-7}$	$1.488.10^{-2}$
0.0027	0.9732	789.9	0.5586	$-3.006.10^{-7}$	$1.180.10^{-2}$
0.0019	0.9808	788.9	0.5572	$-2.128.10^{-7}$	$8.721.10^{-3}$
0.0018	0.9819	788.7	0.5569	$-1.974.10^{-7}$	$8.183.10^{-3}$
0.0000	1.0000	786.4	0.5527	0.000	0.000
δ = 0.5174					
0.3069	0.0000	881.8	0.4610	$-1.531.10^{-6}$	$7.684.10^{-2}$
0.2933	0.0443	880.9	0.4607	$-1.538.10^{-6}$	$6.908.10^{-2}$
0.2335	0.2392	875.3	0.4776	$-1.466.10^{-6}$	$5.312.10^{-2}$
0.2221	0.2763	873.9	0.4832	$-1.438.10^{-6}$	$5.247.10^{-2}$
0.2018	0.3425	871.2	0.4945	$-1.385.10^{-6}$	$5.261.10^{-2}$
0.1427	0.5349	859.8	0.5305	$-1.123.10^{-6}$	$5.618.10^{-2}$
0.1026	0.6656	848.2	0.5515	$-8.739.10^{-7}$	$5.515.10^{-2}$
0.0952	0.6897	845.6	0.5546	$-8.234.10^{-7}$	$5.421.10^{-2}$
0.0485	0.8420	823.9	0.5649	$-4.499.10^{-7}$	$3.884.10^{-2}$
0.0294	0.9043	811.6	0.5634	$-2.820.10^{-7}$	$2.683.10^{-2}$
0.0218	0.9291	805.8	0.5617	$-2.054.10^{-7}$	$2.094.10^{-2}$
0.0104	0.9660	796.3	0.5577	$-9.697.10^{-8}$	$1.072.10^{-2}$
0.0000	1.0000	786.4	0.5527	0.000	0.000
δ = 0.9404					
0.4459	0.0000	968.7	0.5248	$-1.442.10^{-6}$	$1.062.10^{-1}$
0.3510	0.2129	949.5	0.5395	$-8.204.10^{-7}$	$9.237.10^{-2}$
0.3458	0.2246	948.7	0.5410	$-8.295.10^{-7}$	$9.231.10^{-2}$
0.2806	0.3707	937.0	0.5622	$-9.207.10^{-7}$	$9.391.10^{-2}$
0.2289	0.4868	925.2	0.5792	$-9.790.10^{-7}$	$9.534.10^{-2}$
0.1821	0.5916	910.5	0.5910	$-9.144.10^{-7}$	$9.307.10^{-2}$
0.1468	0.6707	896.0	0.5960	$-7.878.10^{-7}$	$8.747.10^{-2}$
0.1223	0.7257	883.7	0.5968	$-6.596.10^{-7}$	$8.089.10^{-2}$
0.1020	0.7712	872.0	0.5955	$-5.378.10^{-7}$	$7.348.10^{-2}$
0.0776	0.8260	855.8	0.5911	$-3.775.10^{-7}$	$6.174.10^{-2}$
0.0394	0.9117	825.3	0.5773	$-1.386.10^{-7}$	$3.644.10^{-2}$
0.0174	0.9609	804.5	0.5651	$-3.296.10^{-8}$	$1.764.10^{-2}$
0.0000	1.0000	786.4	0.5527	0.000	0.000
δ = 1.2482					
0.5165	0.0000	1019.8	0.5479	$-1.594.10^{-6}$	$1.119.10^{-1}$
0.3952	0.2348	991.3	0.5727	$-8.008.10^{-7}$	$1.093.10^{-1}$
0.3197	0.3811	975.0	0.5954	$-8.930.10^{-7}$	$1.149.10^{-1}$
0.2611	0.4945	959.1	0.6107	$-9.495.10^{-7}$	$1.170.10^{-1}$
0.2143	0.5852	942.5	0.6188	$-9.050.10^{-7}$	$1.145.10^{-1}$
0.1730	0.6650	923.9	0.6211	$-7.796.10^{-7}$	$1.075.10^{-1}$
0.1345	0.7395	902.5	0.6181	$-6.045.10^{-7}$	$9.579.10^{-2}$
0.0897	0.8264	871.7	0.6068	$-3.586.10^{-7}$	$7.436.10^{-2}$
0.0367	0.9290	825.6	0.5804	$-9.101.10^{-8}$	$3.599.10^{-2}$
0.0173	0.9666	805.7	0.5667	$-2.953.10^{-8}$	$1.790.10^{-2}$
0.0000	1.0000	786.4	0.5527	0.000	0.000

(*continued on next page*)

Table 3 (*continued*)

X_1	X_3	ρ/kg.m^{-3}	η/mPa.s	V^E/m^3.mol^{-1}	$\Delta\eta$/mPa.s
δ = 1.8328					
0.6107	0.0000	1085.8	0.5772	$-9.293.10^{-7}$	$1.179.10^{-1}$
0.4648	0.2388	1055.6	0.6036	$-9.291.10^{-7}$	$1.220.10^{-1}$
0.4421	0.2760	1050.2	0.6096	$-9.509.10^{-7}$	$1.244.10^{-1}$
0.3943	0.3543	1037.5	0.6219	$-9.743.10^{-7}$	$1.295.10^{-1}$
0.3154	0.4835	1011.4	0.6392	$-9.199.10^{-7}$	$1.347.10^{-1}$
0.2718	0.5549	993.4	0.6452	$-8.277.10^{-7}$	$1.341.10^{-1}$
0.2053	0.6638	959.8	0.6463	$-6.185.10^{-7}$	$1.250.10^{-1}$
0.1737	0.7156	940.7	0.6426	$-4.937.10^{-7}$	$1.165.10^{-1}$
0.1442	0.7639	920.8	0.6361	$-3.728.10^{-7}$	$1.054.10^{-1}$
0.1075	0.8239	893.1	0.6237	$-2.313.10^{-7}$	$8.744.10^{-2}$
0.0781	0.8722	868.0	0.6096	$-1.305.10^{-7}$	$6.884.10^{-2}$
0.0501	0.9180	841.5	0.5927	$-5.514.10^{-8}$	$4.765.10^{-2}$
0.0000	1.0000	786.4	0.5527	0.000	0.000
δ = 2.6855					
0.6968	0.0000	1161.7	0.5949	$-1.135.10^{-6}$	$1.142.10^{-1}$
0.6021	0.1360	1129.8	0.6021	$-2.671.10^{-7}$	$1.116.10^{-1}$
0.5649	0.1893	1119.1	0.6094	$-1.809.10^{-7}$	$1.151.10^{-1}$
0.4667	0.3302	1091.4	0.6344	$-2.802.10^{-7}$	$1.300.10^{-1}$
0.4498	0.3545	1086.4	0.6390	$-3.248.10^{-7}$	$1.328.10^{-1}$
0.3129	0.5509	1036.5	0.6685	$-5.951.10^{-7}$	$1.482.10^{-1}$
0.2551	0.6339	1007.8	0.6721	$-5.967.10^{-7}$	$1.458.10^{-1}$
0.2436	0.6504	1001.3	0.6719	$-5.818.10^{-7}$	$1.444.10^{-1}$
0.2040	0.7072	977.1	0.6682	$-5.201.10^{-7}$	$1.366.10^{-1}$
0.1207	0.8268	914.1	0.6431	$-2.928.10^{-7}$	$1.029.10^{-1}$
0.0456	0.9345	840.8	0.5957	$-8.152.10^{-8}$	$4.772.10^{-2}$
0.0222	0.9682	814.0	0.5751	$-3.826.10^{-8}$	$2.469.10^{-2}$
0.0168	0.9759	807.5	0.5699	$-2.923.10^{-8}$	$1.893.10^{-2}$
0.0000	1.0000	786.4	0.5527	0.000	0.000
δ = 4.7481					
0.8025	0.0000	1260.3	0.6003	$-8.801.10^{-7}$	$9.348.10^{-2}$
0.7058	0.1205	1227.0	0.6078	$-3.412.10^{-7}$	$9.545.10^{-2}$
0.6526	0.1869	1210.1	0.6170	$-2.771.10^{-7}$	$1.016.10^{-1}$
0.5422	0.3244	1174.1	0.6417	$-3.948.10^{-7}$	$1.200.10^{-1}$
0.3780	0.5289	1106.6	0.6734	$-6.264.10^{-7}$	$1.423.10^{-1}$
0.3081	0.6161	1068.5	0.6780	$-6.228.10^{-7}$	$1.429.10^{-1}$
0.2365	0.7053	1021.3	0.6732	$-5.236.10^{-7}$	$1.340.10^{-1}$
0.1544	0.8077	955.1	0.6521	$-3.256.10^{-7}$	$1.082.10^{-1}$
0.1033	0.8713	906.3	0.6288	$-1.842.10^{-7}$	$8.200.10^{-2}$
0.0694	0.9135	870.4	0.6084	$-1.011.10^{-7}$	$5.967.10^{-2}$
0.0342	0.9574	829.5	0.5826	$-3.056.10^{-8}$	$3.185.10^{-2}$
0.0000	1.0000	786.4	0.5527	0.000	0.000
δ = 10.3307					
0.8984	0.0000	1359.4	0.6034	$-4.782.10^{-7}$	$7.285.10^{-2}$
0.7761	0.1361	1316.0	0.6017	$-1.800.10^{-7}$	$6.813.10^{-2}$
0.7568	0.1576	1309.0	0.6042	$-1.605.10^{-7}$	$7.016.10^{-2}$
0.6164	0.3139	1254.3	0.6372	$-1.251.10^{-7}$	$9.970.10^{-2}$
0.5133	0.4287	1208.1	0.6684	$-1.781.10^{-7}$	$1.284.10^{-1}$
0.4326	0.5185	1166.5	0.6900	$-2.248.10^{-7}$	$1.480.10^{-1}$
0.4297	0.5216	1165.0	0.6906	$-2.290.10^{-7}$	$1.485.10^{-1}$
0.3570	0.6026	1122.0	0.7033	$-2.584.10^{-7}$	$1.594.10^{-1}$
0.2944	0.6723	1080.0	0.7064	$-2.668.10^{-7}$	$1.610.10^{-1}$
0.1704	0.8103	979.2	0.6821	$-2.198.10^{-7}$	$1.336.10^{-1}$
0.0800	0.9110	886.6	0.6300	$-1.306.10^{-7}$	$7.927.10^{-2}$
0.0296	0.9671	825.8	0.5853	$-5.486.10^{-8}$	$3.333.10^{-2}$
0.0293	0.9674	825.4	0.5851	$-5.257.10^{-8}$	$3.312.10^{-2}$
0.0164	0.9817	808.7	0.5716	$-3.635.10^{-8}$	$1.930.10^{-2}$
0.0000	1.0000	786.4	0.5527	0.000	0.000

2.4. Excess molar volume and viscosity deviation

The excess molar volumes V^E and viscosity deviation $\Delta\eta$ for binary and ternary systems were calculated from the following equations:

$$V^E = \sum_{i=1}^{n} x_i M_i \left[\left(\frac{1}{\rho}\right) - \left(\frac{1}{\rho_i}\right)\right] \quad (1)$$

$$\Delta\eta = \eta - \left(\sum_{i=1}^{n} \eta_i x_i\right) \quad (2)$$

where n is the number of components, x_i the mole fraction of component i in the mixture, M_i its molecular weight, ρ, η, are the density and viscosity of the mixture and η_i, ρ_i the measured densities and viscosities of the pure component, respectively.

Excess molar Volume and viscosity deviation of binary systems were fitted using the Redlich-Kister [4] polynomial equation of the type:

$$Y_{ij} = x_i x_j \sum_{p=0}^{k} a_p (1 - 2x_i)^p \quad (3)$$

where Y_{ij} is the excess property of the *ij* binary system and a_p are adjustable parameters. These equations were fitted using least squares [14] with all points equally weighed. The appropriate number of constants and significant digits are obtained by comparison with the experimental errors mentioned above.

A series of equations that adjust properties of excess and deviations from ideality of ternary systems were proposed. Some of these equations predict the excess properties from those of binary systems [15–17]. There are several papers in the literature [17–20] in which these settings are tested. The results are varied and the best setting depends on the type of system.

In this paper the ternary excess molar volumes and viscosity deviation Y^E_{123} were predicted using the Radojković [6] equation:

$$Y^E_{123} = Y^E_{12} + Y^E_{13} + Y^E_{23} \quad (4)$$

where $Y^E_{12}; Y^E_{13}; Y^E_{23}$ are the properties for the three binary systems.

The ternary excess molar volumes V^E and viscosity deviation $\Delta\eta$ were correlated by Nagata and Tamura equation type [5]:

$$Y^E_{123} = Y^E_{12} + Y^E_{13} + Y^E_{23} + x_1x_2x_3\left(B_0 - B_1x_1 - B_2x_2 - B_3x_1^2 - B_4x_2^2 - B_5x_1x_2 - B_6x_1^3 - B_7x_2^3 - B_8x_1^2x_2\right) \quad (5)$$

and the Redlich-Kister equation type [4]:

$$Y^E_{123} = Y^E_{12} + Y^E_{13} + Y^E_{23} + x_1x_2x_3.[B_0 + B_1.(x_1 - x_2) + B_2.(x_2 - x_3) + B_3.(x_1 - x_3) + B_4.(x_1 - x_2)^2 + B_5.(x_2 - x_3)^2 + B_6.(x_1 - x_3)^2 + \cdots] \quad (6)$$

where B_n are the adjustable parameters obtained from fitting the V^E and $\Delta\eta$ data (calculated from experimental data).

In all cases the standard deviation is calculated with the equation

$$\sigma = \sqrt{\left(\frac{\sum_{i=1}^{N}\left(Y^E_{\exp} - Y^E_{calc}\right)^2}{N - p}\right)} \quad (7)$$

Numerical values of the coefficients a_p of Eq. 3 obtained from a least squares analysis of the data for the binary systems are listed in Table 4 with standard deviations.

Numerical values of the coefficients B_n of Eqs. (5) and (6), obtained from a least squares analysis of the data for ternary systems are listed in Table 5 with standard deviations. Table 5 also shows the standard deviation that is obtained by applying Eq. (4) corresponding to the Radojković equation.

Equations for adjustment and also for predicting, the OriginPro 8.5 software was used.

Figs. 1 and 2 show excess molar volume and viscosity deviation plotted against the mole fraction of chloroform for the systems: [chloroform (1)+dipe (2)] and [chloroform (1)+methanol (3)] and against the mole fraction of DIPE for the system [dipe (2)+methanol (3)] at 298.15 K.

Table 4
Parameters a_p of Eq. (3) and the corresponding standard deviation.

a_0	a_1	a_2	a_3	$\sigma\,\Sigma$
chloroform (1) +dipe(2)				
$-6.4955.10^{-6}$	$-6.31588.10^{-7}$	$1.54409.10^{-6}$		8.10^{-8} m^3.mol^{-1}
0.3308	−0.15135	−0.13991		3.10^{-3} mPa.s
dipe (2)+methanol (3)				
$-4.03108.10^{-6}$	$3.55177.10^{-7}$	$-5.22092.10^{-7}$		2.10^{-8} m^3.mol^{-1}
−0.16265	0.02473	0.14481	0.15987	2.10^{-3} mPa.s
chloroform (1)+ methanol (3)				
$-5.1004.10^{-7}$	$-1.151.10^{-7}$	$3.95839.10^{-7}$		2.10^{-9} m^3.mol^{-1}
0.44163	0.51485	0.10657		2.10^{-3} mPa.s

Table 5
Parameters B_n and standard deviations σ of Eqs. (5) and (6) and standard deviations σ_R of Eq. (4) for [chloroform(1)+dipe (2)+methanol (3)] ternary system at 298.15 K.

Parameter	V^E/m^3.mol^{-1}		$\Delta\eta$/mPa.s	
	R K	N&T	R K	N&T
B_0	$2.7409.10^{-5}$	$-5.38236.10^{-5}$	0.58384	1.79845
B_1	−9.33957	$-7.22634.10^{-4}$	−4786.10335	4.36207
B_2	−9.33953	0.00122	−4787.66615	4.93869
B_3	9.33964	0.0027	4787.50156	−20.59061
B_4	$-7.32305.10^{-4}$	−0.00211	2.71062	−27.26336
B_5	$2.83652.10^{-4}$	−0.00464	−0.60595	31.23574
B_6	$-2.46277.10^{-4}$	−0.00281	1.20912	20.44343
B_7	0.00156	0.00295	−2.78848	25.40283
B_8	$-2.2734.10^{-4}$	0.00604	1.02984	−45.06006
B_9	$2.07338.10^{-4}$		−1.15661	
σ	2.10^{-6}	2.10^{-6}	1.10^{-2}	1.10^{-2}
σ_R	2.10^{-6}		2.10^{-2}	

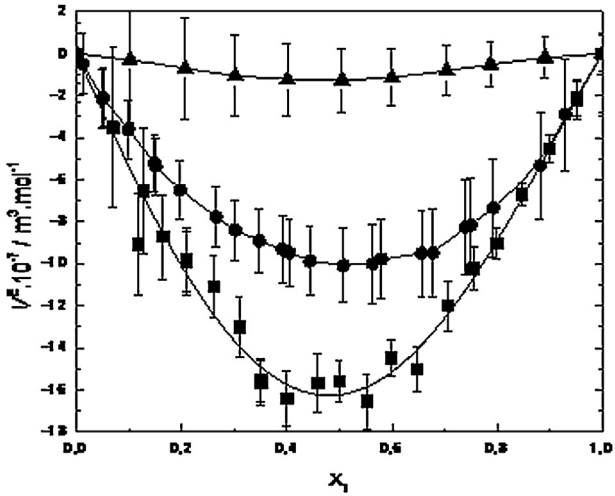

Fig. 1. Experimental values of V^E against x_i $(i=1,2)$ for the binary systems: (■): chloroform (1)+dipe (2); (●): dipe (2)+methanol (3) and (▲) : chloroform (1)+methanol (3) at 298.15 K.

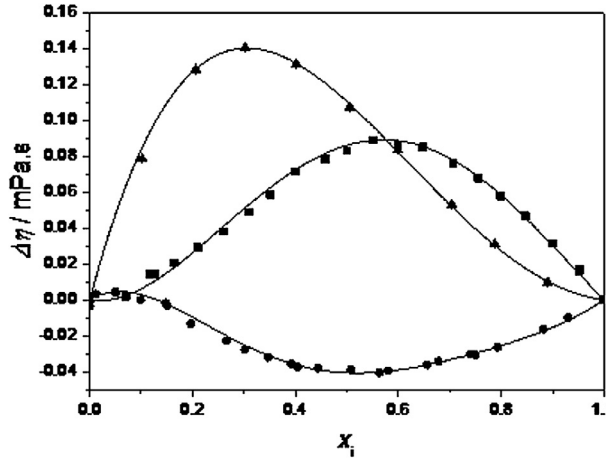

Fig. 2. Experimental values of $\Delta\eta$ against x_i $(i=1,2)$ for the binary systems: (■): chloroform (1)+dipe (2); (●): dipe (2)+methanol (3) and (▲) : chloroform (1)+methanol (3) at 298.15 K.

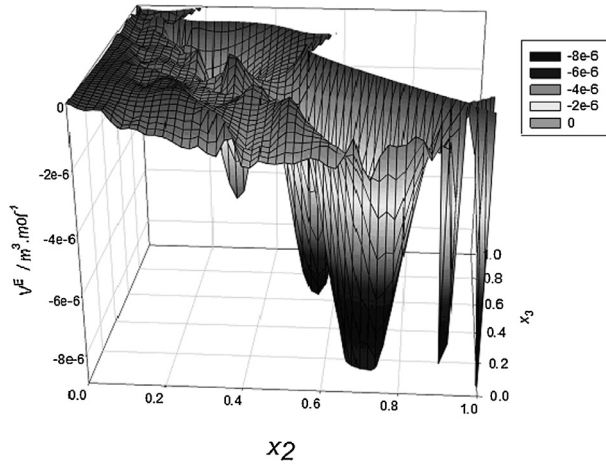

Fig. 3. 3D surface of V^E against molar fractions of dipe (x_2) and methanol (x_3) at 298.15 K.

Fig. 3 show surface of V^E against molar fractions of DIPE (2) and methanol(3). Figs. 4 and 5 show contourn lines of excess molar volumen and viscosity deviation for the [chloroform (1)+Dipe(2)+methanol (3)] at 298.15 K, respectively.

Origin Pro 8.5 was used for the Figs. 1,2,4 and 5. For Fig. 3 SigmaPlot 10.0 was used

3. Data, value and validation

Binary systems presented in this paper are part of the studies conducted in the research group on the intermolecular hydrogen bonds, how they affect the thermophysical properties of the systems where they are present and the effect of adding a third component to them.

The information available in the open literature of thermophysical properties of binary systems studied is very scarce, particularly in systems where the DIPE is present. The ternary systems were

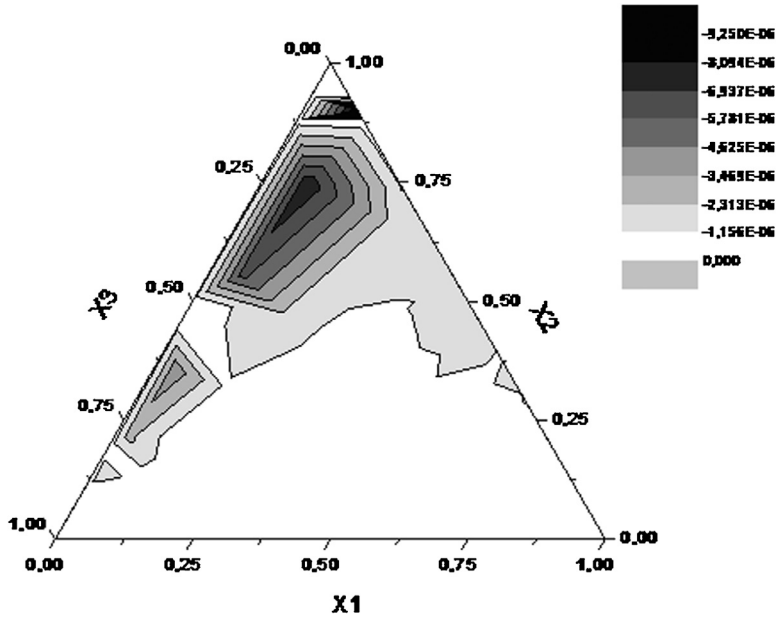

Fig. 4. Contourn lines of excess molar volumen for the [chloroform (1)+dipe(2)+methanol (3)] ternary system at 298.15 K.

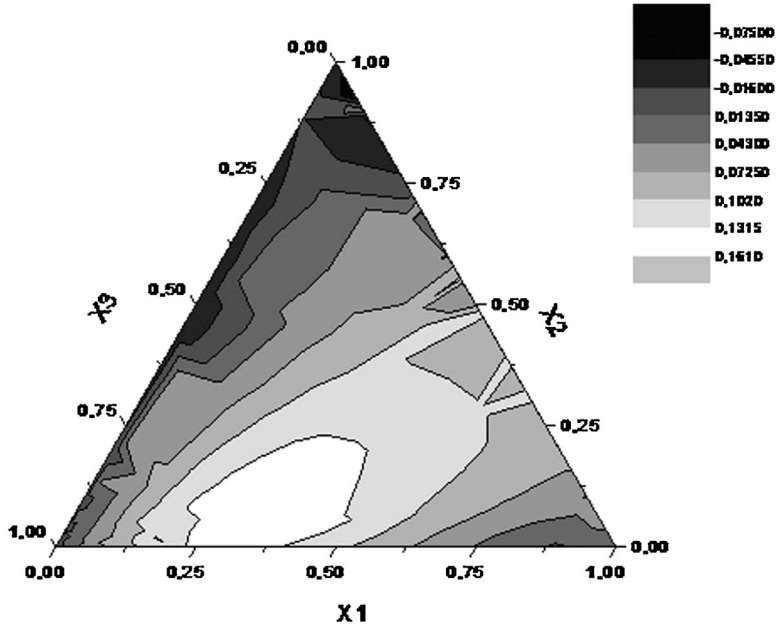

Fig. 5. Contourn lines of viscosity deviation for the [chloroform (1)+dipe(2)+methanol(3)] ternary system at 298.15 K.

not studied, as far as could be found. Thus these data are very useful for scientific and technological community. Both the alkanols and ethers are used as fuel additives.

The purity of the reagents used was controlled by chromatography and IR spectroscopy which guarantees its purity.

The instruments used are certified by the manufacturer and monitored regularly, each time a series of measurements starts.

Experimental determinations were repeated at least three times. Mixtures of any composition are also prepared and their properties are determined experimentally to obtain the total uncertainty of the proposed relationship. Additionally, residual analysis is performed in each case.

The knowledge of the properties of excess and deviations from ideality is vital both to model behavior at the molecular level, as forecast in the construction of equipment which amply justifies available data and correlations. Residual analysis was also performed on these.

Excess thermodynamic functions and deviations of nonthermodynamic ones of binary and ternary liquid mixtures are very important for the design of industrial equipment and for the interpretation of the liquid state, particularly when polar components are involved because there exists a possibility of drawing conclusions about the interactions between the components of the mixture.

4. Discussion and conclusions

Experimental data of density and viscosity are provided for the [chloroform (1)+methanol (3)] binary system and [chloroform (1) DIPE (2)+methanol (3)] ternary system at 298.15 K.

Adjustment equations for binary and ternary system are provided across the range of composition.

The excess molar volume $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ for binary systems correlate well within the order of magnitude of the experimental error by a Redlich-Kister [4] type equation. The ternary excess molar volumes $\boldsymbol{V^E}$ and viscosity deviation $\boldsymbol{\Delta\eta}$ correlate well within the order of magnitude of the experimental error by a Redlich-Kister [4] type equation and Nagata and Tamura [5] type equation. Also, the ternary excess molar volumes and viscosity deviation Y^E_{123}were predicted using the Radojković [6] equation.

The prediction using the Radojković equation fits well with the data within the experimental error with a deviation of the same order as the correlation equations.

We know that chloroform and DIPE are not associated at pure state while methanol is strongly associated with chains linked by hydrogen bondings.

In the mixture of chloroform (1)+DIPE (2) intermolecular bonds appear and therefore the excess molar volume is negative over the full range of composition and with a minimum near to $x_1 \approx 0.5$. The viscosity deviation is positive over the range of composition with a maximum nearest 0.5. For [chloroform (1)+methanol (3)] and [DIPE (2)+methanol (3)] systems, solvent effect appears which is responsible to break the self-association of methanol. In both cases it is possible that the monomers of methanol can be accommodated in the most complex structure of the n-mers and / or form bonds with the other component i.e. a hetero-association. Most likely, these systems have a negative excess molar volume of the entire range of composition. The viscosity deviation corroborates this assertion.

Fig. 2 shows that the formation of hetero-association is dominant in the chloroform+DIPE system, as previously reported [6]. For DIPE+methanol system, at low concentrations of DIPE, the formation of hetero-association is the predominant effect. For concentrations greater than $X_2 = 0.15$, the bond-breaking is the predominant process, as had previously been reported [7]. For chloroform+methanol system the formation of hetero-association is the predominant effect.

Figs. 3 and 4 show that the molar excess volume is negative, showing remarkable minimum at low concentrations of chloroform and methanol and high of DIPE, which could be interpreted as a hetero-association and / or interstitial accommodation of methanol in a more complex structure.

Figs. 5 and 6 corroborates the proposal of hetero-linked and interstitial accommodation due to small negative values in the zone. In the zone near the binary [chloroform (1)+methanol (3)] the positive values would show that the presence of DIPE favors the formation of chloroform methanol links

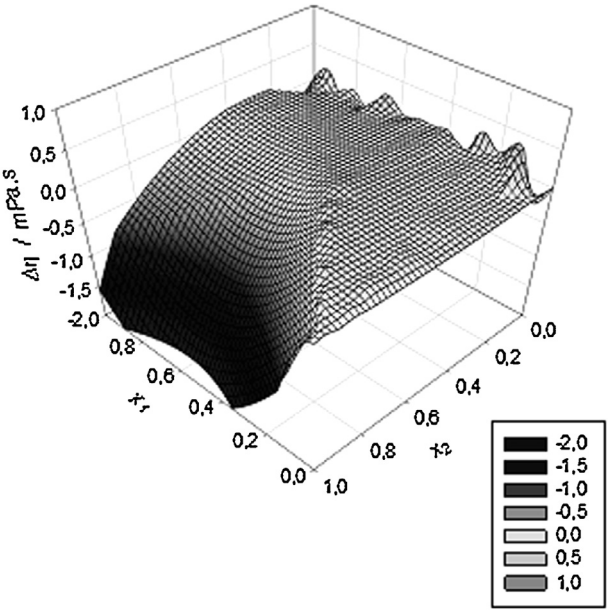

Fig. 6. 3D surface of Viscosity deviation against molar fractions of dipe (x_2) and chloroform (x_1) at 298.15 K.

Acknowledgments

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