Densities, Viscosities, Refractive Indexes, and Surface Tensions for Binary and Ternary Mixtures of Tetrahydofuran, 2-Propanol, and 2,2,4-Trimethylpentane

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Densities, viscosities, refractive indexes, and surface tensions of a ternary system (tetrahydofuran + 2-propanol + 2,2,4-trimethylpentane) at $T = 298.15$ K and three constituent binary systems at $T =$ (288.15, 298.15, and 308.15) K were measured at atmospheric pressure. Densities were determined using a vibrating-tube densimeter. Viscosities were measured with an automatic microviscometer based on the rolling ball principle. Refractive indexes were measured using a digital Abbe-type refractometer. Surface tensions were determined by the Wilhelmy-plate method. These results were used to calculate excess molar volumes V^E, deviations in the viscosity $\Delta\eta$, deviations in the refractive index Δn_D, and deviations in the surface tension $\Delta\sigma$. The calculated quantities of V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ were fitted to variable-degree polynomials. The ternary results were compared with the values estimated by different empirical equations of prediction.

Introduction

Certain oxygenated compounds are usually added to gasoline to improve the octane number and reduce pollution. The present paper is concerned with the oxygenated compounds of the type {cyclic ether or aliphatic alcohol} and the alkane liquid that generally appears in gasoline. From the viewpoint of association, cyclic ethers can be regarded as an intermediate case between alkanes (inert compounds) and alkanols (highly self-associated compounds). For these reasons, we measured densities, viscosities, refractive indexes, and surface tensions for binary and ternary mixtures of tetrahydrofuran, 2-propanol, and 2,2,4-trimethylpentane at atmospheric pressure. As far as we know, no literature data are available for the systems investigated.

Experimental Section

The chemicals used were of analytical grade and were used without further purification. The mass purities and source of the chemicals employed were as follows: tetrahydrofuran (Merck, > 99.5 %); 2-propanol (Tedia, > 99.5 %); 2,2,4-trimethylpentane (Merck, > 99.7 %). The densities, viscosities, refractive indexes, and surface tensions at $T = 298.15$ K of these components agreed closely with the accepted literature values (Table 1).

Densities ρ were measured with an Anton Paar DMA-5000 vibrating-tube densimeter (Anton-Paar, Graz, Austria). Viscosities η were determined with an automatic microviscometer (Anton Paar type AMVn), which uses the rolling-ball principle. Refractive indices, n_D, were measured with an automatic Anton Paar RXA-156 refractometer, which runs with the wavelength of 589 nm corresponding to the D-ray of sodium. Surface tensions σ were measured with an automatic surface tension meter model CBVP-A3 (Kyowa, Japan), which works by the Wilhelmy-plate method. The detailed measuring procedures for these measurements have been described in previous studies.[1,2]

All samples were prepared by mass in a 50 cm^3 Erlenmeyer flask provided with a ground glass joint stopper, using a Precisa 262SMA balance with a precision of 10^{-5} g. The uncertainty in the composition is estimated to within $\pm 1 \cdot 10^{-4}$ mole fraction. All liquids were thermostatically controlled to within $\pm$ 0.01 K, $\pm$ 0.05 K, $\pm$ 0.03 K, and $\pm$ 0.05 K for the ρ, η, n_D, and σ measurements, respectively. All measurements were performed at least four times under atmospheric pressure (100.8 $\pm$ 0.4) kPa, and the results were averaged to give the final values. The uncertainty in the ρ, η, n_D, and σ measurements was estimated to be $\pm 1 \cdot 10^{-5}$ g·cm^{-3}, $\pm$ 0.006 mPa·s, $\pm$ 0.00002, and $\pm$ 0.05 mN·m^{-1}, respectively.

Results and Discussion

The experimental data of ρ, η, n_D, and σ for binary mixtures at $T =$ (288.15, 298.15, and 308.15) K and ternary mixtures at $T = 298.15$ K of tetrahydrofuran, 2-propanol, and 2,2,4-trimethylpentane are presented in Tables 2 to 5. Increasing the temperature from $T = 288.15$ K to $T = 3018.15$ K decreases the values of ρ, η, n_D, and σ for all these binary systems. Tables 6 and 7 list the values of molar excess volumes (V^E), viscosity deviations ($\Delta\eta$), deviations in the refractive index (Δn_D), and deviations in the surface tension ($\Delta\sigma$) for these binary and ternary mixtures at $T = 298.15$ K.

The molar excess volumes, V^E, were calculated from density data according to the following equation

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

where x_i, M_i, and ρ_i are the mole fraction, molar mass, and density of the pure component i, respectively. ρ is the density of the mixture, and N is the number of components. As can be seen from

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Table 1. Comparison of Measured Densities ρ, Viscosities η, Refractive Indexes, and Surface Tensions σ of Pure Components with Literature Values at $T = 298.15$ K

	ρ / g·cm^{-3}		η / mPa·s		n_D		σ / mN·m^{-1}	
component	exptl	lit.	exptl	lit.	exptl	lit.	exptl	lit.
tetrahydrofuran	0.88237	0.8829[a] 0.88209[b]	0.470	0.530[a] 0.4637[b]	1.40487	1.4049[a] 1.40496[c]	26.98	26.4[c]
2-propanol	0.78116	0.78126[c]	2.043	2.0436[c]	1.37515	1.3752[c]	20.90	20.95[f] 20.93[g]
2,2,4-trimethyl pentane	0.68795	0.68781[c] 0.68885[d]	0.481	0.4802[e]	1.38916	1.38898[c] 1.3892[d]	18.33	18.32[h]

[a] Nayak et al., 2003.[3] [b] Rodriguez et al., 1997.[4] [c] Riddick et al., 1986.[5] [d] Aralaguppi et al., 1999.[6] [e] Bouzas et al., 2000.[7] [f] Azizian and Bashavard, 2005.[8] [g] Ouyang et al., 2003.[9] [h] Vargaftik, 1975.[10]

Table 2. Experimental Densities ρ, Viscosities η, Refractive Indexes n_D, and Surface Tensions σ for the Tetrahydrofuran (1) + 2-Propanol (2) System

x_1	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}	x_1	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}
				$T = 288.15$ K					
0.0000	0.78953	2.849	1.37933	21.75	0.5500	0.84640	0.713	1.39534	25.15
0.0500	0.79484	2.238	1.38085	22.18	0.6000	0.85153	0.678	1.39684	25.48
0.1000	0.80009	1.849	1.38233	22.53	0.6500	0.85668	0.643	1.39838	25.82
0.1500	0.80528	1.570	1.38377	22.85	0.7000	0.86184	0.613	1.39997	26.16
0.2001	0.81047	1.356	1.38520	23.13	0.7500	0.86701	0.589	1.40150	26.51
0.2500	0.81562	1.196	1.38662	23.38	0.8000	0.87219	0.569	1.40301	26.87
0.3000	0.82077	1.068	1.38802	23.65	0.8500	0.87741	0.554	1.40447	27.23
0.3500	0.82590	0.965	1.38945	23.93	0.9000	0.88264	0.540	1.40592	27.60
0.4000	0.83103	0.883	1.39088	24.22	0.9500	0.88778	0.530	1.40734	27.98
0.4500	0.83615	0.812	1.39235	24.52	1.0000	0.89302	0.520	1.40875	28.37
0.5000	0.84126	0.757	1.39384	24.83					
				$T = 298.15$ K					
0.0000	0.78116	2.043	1.37515	20.90	0.5500	0.83632	0.623	1.39118	24.04
0.0500	0.78631	1.706	1.37661	21.32	0.6000	0.84135	0.594	1.39269	24.34
0.1000	0.79135	1.445	1.37805	21.65	0.6500	0.84639	0.567	1.39421	24.65
0.1500	0.79635	1.248	1.37946	21.95	0.7000	0.85145	0.545	1.39578	24.97
0.2001	0.80135	1.113	1.38088	22.22	0.7500	0.85652	0.526	1.39735	25.30
0.2500	0.80634	0.988	1.38230	22.47	0.8000	0.86166	0.511	1.39889	25.63
0.3000	0.81133	0.896	1.38374	22.70	0.8500	0.86681	0.497	1.40041	25.97
0.3500	0.81633	0.812	1.38519	22.95	0.9000	0.87202	0.488	1.40191	26.30
0.4000	0.82131	0.752	1.38667	23.20	0.9500	0.87721	0.480	1.40339	26.64
0.4500	0.82630	0.703	1.38816	23.47	1.0000	0.88237	0.470	1.40487	26.98
0.5000	0.83129	0.659	1.38967	23.75					
				$T = 308.15$ K					
0.0000	0.77252	1.541	1.37061	20.17	0.5500	0.82606	0.549	1.38601	23.19
0.0500	0.77745	1.313	1.37192	20.60	0.6000	0.83096	0.526	1.38748	23.47
0.1000	0.78229	1.142	1.37328	20.93	0.6500	0.83586	0.507	1.38896	23.76
0.1500	0.78713	1.009	1.37462	21.23	0.7000	0.84081	0.489	1.39046	24.06
0.2001	0.79197	0.909	1.37596	21.50	0.7500	0.84580	0.474	1.39197	24.37
0.2500	0.79683	0.824	1.37735	21.75	0.8000	0.85082	0.461	1.39348	24.68
0.3000	0.80167	0.755	1.37875	21.98	0.8500	0.85587	0.452	1.39499	25.00
0.3500	0.80653	0.697	1.38017	22.22	0.9000	0.86097	0.444	1.39651	25.32
0.4000	0.81139	0.646	1.38161	22.45	0.9500	0.86617	0.440	1.39801	25.64
0.4500	0.81628	0.606	1.38307	22.68	1.0000	0.87133	0.433	1.39953	25.95
0.5000	0.82117	0.576	1.38454	22.93					

Tables 6 and 7, the V^E values are positive at all compositions. The uncertainty of excess molar volumes was estimated to be less than $\pm 1 \cdot 10^{-3}$ cm^3·mol^{-1}. The values of V^E at $T = 298.15$ K vary from 0.011 cm^3·mol^{-1} to 0.562 cm^3·mol^{-1}. The excess molar volume V^E ($x = 0.5$) increases in the order: 0 < tetrahydrofuran + 2,2,4-trimethylpentane < tetrahydrofuran + 2-propanol < 2-propanol + 2,2,4-trimethylpentane. Increasing the temperature from $T = 288.15$ K to $T = 308.15$ K increases the values of V^E for all these binary systems.

The dependence of V^E on both composition and temperature for the present mixtures may be explained as a balance between positive contributions (hydrogen bond rupture or dispersive interactions between unlike molecules) and negative contributions (intermolecular dipolar interactions or geometrical fitting between components). In the present investigation, tetrahydrofuran is associated through the dipole–dipole interaction and 2-propanol is associated through the hydrogen bonding of its hydroxyl group. In our systems, the observed V^E are positive, and the predominant contribution to the positive V^E is most likely from the breaking of these two kinds of interactions upon mixing. Larger V^E values in the mixtures of 2,2,4-trimethylpentane with 2-propanol than those with tetrahydrofuran lead us to believe that the contribution to the V^E values from the cleavage of the H-bond between 2-propanol molecules is greater than that of the O−O interaction between tetrahydrofuran molecules.

The values of the viscosity deviations, $\Delta\eta$, for the mixtures are calculated from the viscosity values of the pure liquids, η_i, and their mixtures, η, from eq 2

$$\Delta\eta = \eta - \sum_{i=1}^{N} x_i \eta_i \qquad (2)$$

It is observed that the binary $\Delta\eta$ values are negative over the whole mole fractions. The values of $\Delta\eta$ are negligibly small

Table 3. Experimental Densities ρ, Viscosities η, Refractive Indexes n_D, and Surface Tensions σ for the Tetrahydrofuran (1) + 2,2,4-Trimethylpentane (3) System

x_1	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}	x_1	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}
				$T = 288.15$ K					
0.0000	0.69610	0.537	1.39408	19.18	0.5500	0.76953		1.39975	21.33
0.0500	0.70095		1.39443	19.32	0.6000	0.77927	0.524	1.40053	21.68
0.1001	0.70607	0.534	1.39482	19.45	0.6500	0.78974		1.40138	22.05
0.1500	0.71148		1.39523	19.60	0.7000	0.80102	0.523	1.40229	22.47
0.2000	0.71720	0.531	1.39566	19.73	0.7500	0.81322		1.40324	22.97
0.2500	0.72326		1.39612	19.88	0.8000	0.82646	0.522	1.40425	23.57
0.3000	0.72972	0.528	1.39661	20.07	0.8500	0.84087		1.40530	24.35
0.3500	0.73664		1.39715	20.27	0.9000	0.85663	0.521	1.40640	25.32
0.4000	0.74066	0.527	1.39773	20.50	0.9500	0.87394		1.40775	26.50
0.4500	0.75199		1.39835	20.75	1.0000	0.89302	0.520	1.40875	28.37
0.5000	0.76046	0.525	1.39902	21.02					
				$T = 298.15$ K					
0.0000	0.68795	0.481	1.38916	18.33	0.5500	0.76031		1.39501	20.35
0.0500	0.69268		1.38949	18.47	0.6000	0.76992	0.472	1.39585	20.68
0.1001	0.69770	0.479	1.38987	18.63	0.6500	0.78026		1.39676	21.05
0.1500	0.70302		1.39028	18.77	0.7000	0.79141	0.472	1.39775	21.48
0.2000	0.70866	0.477	1.39071	18.92	0.7500	0.80347		1.39880	22.00
0.2500	0.71465		1.39116	19.10	0.8000	0.81655	0.471	1.39991	22.60
0.3000	0.72104	0.475	1.39166	19.27	0.8500	0.83080		1.40105	23.30
0.3500	0.72787		1.39222	19.43	0.9000	0.84638	0.471	1.40225	24.15
0.4000	0.73518	0.474	1.39284	19.63	0.9500	0.86349		1.40352	25.28
0.4500	0.74300		1.39351	19.83	1.0000	0.88237	0.470	1.40487	26.98
0.5000	0.75136	0.473	1.39423	20.05					
				$T = 308.15$ K					
0.0000	0.67962	0.434	1.38407	17.35	0.5500	0.75080		1.38950	19.60
0.0500	0.68420		1.38428	17.55	0.6000	0.76026	0.432	1.39031	19.90
0.1001	0.68910	0.433	1.38461	17.73	0.6500	0.77045		1.39120	20.25
0.1500	0.69433		1.38495	17.90	0.7000	0.78146	0.432	1.39220	20.67
0.2000	0.69991	0.432	1.38535	18.10	0.7500	0.79337		1.39326	21.20
0.2500	0.70584		1.38580	18.27	0.8000	0.80629	0.432	1.39438	21.82
0.3000	0.71216	0.432	1.38630	18.48	0.8500	0.82036		1.39557	22.55
0.3500	0.71889		1.38684	18.70	0.9000	0.83575	0.432	1.39682	23.45
0.4000	0.72608	0.431	1.38743	18.90	0.9500	0.85265		1.39814	24.55
0.4500	0.73377		1.38807	19.12	1.0000	0.87133	0.433	1.39953	25.95
0.5000	0.74199	0.431	1.38876	19.37					

for tetrahydrofuran + 2,2,4-trimethylpentane mixtures. The values of $\Delta\eta$ at $T = 298.15$ K vary from –0.680 mPa·s to –0.001 mPa·s. The viscosity deviation $\Delta\eta$ ($x = 0.5$) increases in the order: tetrahydrofuran + 2-propanol ≈ 2-propanol + 2,2,4-trimethylpentane < tetrahydrofuran + 2,2,4-trimethylpentane < 0. The values of $\Delta\eta$ increase with a rise in temperature except for those of the tetrahydrofuran + 2,2,4-trimethylpentane system, which show no clear temperature dependence.

The deviations in the refractive index, Δn_D, were calculated from a mole fraction basis as:

$$\Delta n_D = n_D - \sum_{i=1}^{N} x_i n_D \tag{3}$$

where n_D and n_{Di} stand for the refractive index of the mixture and pure liquid i, respectively. The Δn_D values are negative at most of the compositions. For binary mixtures of tetrahydrofuran + 2-propanol, the Δn_D values are negative, while some positive values were found at high tetrahydrofuran mole fractions. On the other hand, the values of Δn_D are positive for the 2-propanol + 2,2,4-trimethylpentane mixture except for some negative values oberved at low 2-propanol mole fractions. The values of Δn_D at $T = 298.15$ K vary from −0.0034 to 0.0010. The Δn_D ($x = 0.5$) increases in the order: tetrahydrofuran + 2,2,4-trimethylpentane < tetrahydrofuran + 2-propanol < 2-propanol + 2,2,4-trimethylpentane. The Δn_D values decrease as the temperature increases from $T = 288.15$ K to $T = 308.15$ K for all these binary systems.

The deviations in the surface tension, $\Delta\sigma$, were calculated from the following equation:

$$\Delta\sigma = \sigma - \sum_{i=1}^{N} x_i \sigma_i \tag{4}$$

where σ and σ_i are the surface tension of the mixture and pure liquid i, respectively. The $\Delta\sigma$ values are negative values except for some positive values that were found for binary mixtures of tetrahydofuran + 2-propanol. The surface tension deviation $\Delta\sigma$ ($x = 0.5$) increases in the sequence: tetrahydrofuran + 2,2,4-trimethylpentane < 2-propanol + 2,2,4-trimethylpentane < tetrahydrofuran + 2-propanol. The values of $\Delta\sigma$ at $T = 298.15$ K vary from −2.90 mN·m^{-1} to 0.14 mN·m^{-1}. Increasing the temperature from $T = 288.15$ K to $T = 308.15$ K increases the values of $\Delta\sigma$ for mixtures of tetrahydrofuran + 2,2,4-trimethylpentane and tetrahydrofuran + 2-propanol. However, the system 2-propanol + 2,2,4-trimethylpentane shows a different temperature dependence.

The calculated quantities, V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$, at $T = 298.15$ K for the binary systems of tetrahydrofuran (1) + 2-propanol (2), tetrahydrofuran (1) + 2,2,4-trimethylpentane (3), and 2-propanol (2) + 2,2,4-trimethylpentane (3) have been fitted to the Redlich–Kister equation relation[11]

$$\Delta Q(x_i, x_j) = x_i x_j \sum_{k=0}^{m} a_k (x_i - x_j)^k \tag{5}$$

where $\Delta Q(x_i,x_j)$ refers to binary V^E/cm^3·mol^{-1}, $\Delta\eta$/mPa·s, Δn_D, or $\Delta\sigma$/mN·m^{-1} as a function of pure-component mole fractions

Table 4. Experimental Densities ρ, Viscosities η, Refractive Indexes n_D, and Surface Tensions σ for the 2-Propanol (2) + 2,2,4-Trimethylpentane (3) System

x_2	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}	x_2	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}
				$T = 288.15$ K					
0.0000	0.69610	0.537	1.39408	19.18	0.5500	0.72729	0.836	1.38750	19.65
0.0500	0.69768	0.541	1.39346	19.21	0.6000	0.73185	0.916	1.38679	19.75
0.1000	0.69961	0.547	1.39285	19.23	0.6500	0.73684	1.009	1.38604	19.86
0.1501	0.70174	0.556	1.39227	19.27	0.7000	0.74233	1.126	1.38525	20.00
0.2000	0.70406	0.569	1.39170	19.30	0.7500	0.74832	1.264	1.38441	20.17
0.2500	0.70659	0.586	1.39114	19.33	0.8000	0.75493	1.437	1.38352	20.37
0.3000	0.70933	0.608	1.39058	19.37	0.8500	0.76225	1.652	1.38257	20.60
0.3500	0.71232	0.636	1.39001	19.40	0.9000	0.77037	1.933	1.38156	20.88
0.4000	0.71561	0.671	1.38942	19.45	0.9500	0.77942	2.314	1.38048	21.27
0.4500	0.71918	0.715	1.38881	19.50	1.0000	0.78953	2.849	1.37933	21.75
0.5000	0.72307	0.768	1.38817	19.57					
				$T = 298.15$ K					
0.0000	0.68795	0.480	1.38916	18.33	0.5500	0.71851	0.694	1.38241	18.72
0.0500	0.68936	0.482	1.38845	18.35	0.6000	0.72309	0.751	1.38175	18.80
0.1000	0.69113	0.486	1.38779	18.37	0.6500	0.72812	0.819	1.38105	18.90
0.1501	0.69320	0.493	1.38715	18.38	0.7000	0.73362	0.901	1.38031	19.02
0.2000	0.69548	0.503	1.38656	18.41	0.7500	0.73968	1.003	1.37954	19.18
0.2500	0.69796	0.515	1.38598	18.43	0.8000	0.74632	1.122	1.37875	19.38
0.3000	0.70066	0.530	1.38541	18.45	0.8500	0.75369	1.277	1.37791	19.62
0.3500	0.70364	0.550	1.38484	18.50	0.9000	0.76183	1.407	1.37705	19.95
0.4000	0.70690	0.576	1.38426	18.55	0.9500	0.77098	1.707	1.37613	20.37
0.4500	0.71045	0.608	1.38367	18.60	1.0000	0.78116	2.043	1.37515	20.90
0.5000	0.71431	0.646	1.38305	18.65					
				$T = 308.15$ K					
0.0000	0.67962	0.434	1.38407	17.35	0.5500	0.70950	0.586	1.37706	17.80
0.0500	0.68082	0.432	1.38317	17.37	0.6000	0.71409	0.628	1.37643	17.90
0.1000	0.68254	0.434	1.38246	17.38	0.6500	0.71911	0.677	1.37579	18.00
0.1501	0.68454	0.440	1.38181	17.40	0.7000	0.72465	0.736	1.37512	18.13
0.2000	0.68676	0.447	1.38117	17.42	0.7500	0.73074	0.806	1.37442	18.29
0.2500	0.68918	0.457	1.38056	17.43	0.8000	0.73740	0.898	1.37370	18.50
0.3000	0.69184	0.468	1.37998	17.47	0.8500	0.74487	1.006	1.37294	18.77
0.3500	0.69480	0.483	1.37941	17.52	0.9000	0.75306	1.145	1.37214	19.10
0.4000	0.69800	0.501	1.37884	17.58	0.9500	0.76226	1.310	1.37139	19.52
0.4500	0.70151	0.524	1.37826	17.65	1.0000	0.77252	1.541	1.37061	20.17
0.5000	0.70532	0.552	1.37767	17.72					

Table 5. Experimental Densities ρ, Viscosities η, Refractive Indexes n_D, and Surface Tensions σ for the Tetrahydrofuran (1) + 2-Propanol (2) + 2,2,4-Trimethylpentane (3) System at $T = 298.15$ K

x_1	x_2	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}	x_1	x_2	ρ / g·cm^{-3}	η / mPa·s	n_D	σ / mN·m^{-1}
0.0500	0.9000	0.77580	1.467	1.37645	20.75	0.3000	0.5500	0.78019	0.699	1.38424	21.35
0.0501	0.7999	0.75809	1.122	1.37804	20.15	0.3000	0.4500	0.76452	0.621	1.38542	20.50
0.0500	0.7000	0.74360	1.905	1.37951	19.67	0.3000	0.3500	0.75166	0.565	1.38650	19.90
0.0500	0.6000	0.73181	0.759	1.38085	19.33	0.3001	0.2500	0.74092	0.526	1.38765	19.45
0.0500	0.5001	0.72207	0.655	1.38208	19.05	0.3000	0.1500	0.73201	0.508	1.38871	19.25
0.0500	0.4000	0.71382	0.586	1.38324	18.89	0.3000	0.0500	0.72432	0.488	1.38983	19.15
0.0500	0.3000	0.70695	0.541	1.38436	18.75	0.4000	0.5500	0.80914	0.704	1.38572	22.75
0.0500	0.2000	0.70117	0.509	1.38551	18.67	0.4000	0.4500	0.78916	0.621	1.38686	21.63
0.0500	0.1000	0.69650	0.491	1.38666	18.60	0.4000	0.3500	0.77296	0.565	1.38795	20.70
0.0500	0.0500	0.69440	0.484	1.38727	18.55	0.3999	0.2501	0.75965	0.533	1.38901	20.15
0.1000	0.8500	0.78061	1.256	1.37445	21.30	0.4000	0.1500	0.74847	0.499	1.39001	19.85
0.1000	0.7500	0.76230	0.998	1.37907	20.20	0.4000	0.0500	0.73930	0.482	1.39109	19.75
0.1000	0.6500	0.74778	0.821	1.38054	19.60	0.5000	0.4500	0.81873	0.623	1.38857	23.55
0.1000	0.5500	0.73581	0.701	1.38187	19.33	0.5000	0.3500	0.79810	0.566	1.38955	22.20
0.1000	0.4500	0.72581	0.622	1.38308	19.12	0.5000	0.2500	0.78148	0.531	1.39052	21.20
0.1000	0.3499	0.71743	0.561	1.38423	18.97	0.5000	0.1501	0.76772	0.501	1.39148	20.45
0.1000	0.2500	0.71036	0.523	1.38534	18.85	0.5000	0.0500	0.75642	0.482	1.39254	20.10
0.1000	0.1501	0.70452	0.499	1.38649	18.75	0.6000	0.3500	0.82848	0.570	1.39168	24.40
0.1000	0.0500	0.69973	0.483	1.38770	18.65	0.6000	0.2500	0.80773	0.527	1.39255	22.65
0.2000	0.7500	0.79010	0.991	1.38028	21.75	0.6000	0.1500	0.79016	0.498	1.39343	21.25
0.2000	0.6500	0.77123	0.814	1.38173	20.75	0.6000	0.0500	0.77613	0.479	1.39439	20.70
0.2000	0.5500	0.75614	0.698	1.38302	20.05	0.7000	0.2500	0.83850	0.528	1.39462	25.35
0.2000	0.4500	0.74373	0.617	1.38422	19.70	0.7000	0.1500	0.81652	0.499	1.39537	22.85
0.2000	0.3500	0.73340	0.562	1.38535	19.45	0.6999	0.0500	0.79901	0.481	1.39621	21.45
0.2000	0.2500	0.72462	0.523	1.38646	19.25	0.8000	0.1500	0.84840	0.503	1.39760	26.65
0.2000	0.1501	0.71740	0.498	1.38756	19.05	0.8000	0.0500	0.82604	0.482	1.39915	23.25
0.2000	0.0500	0.71128	0.482	1.38872	18.87	0.8999	0.0501	0.85850	0.481	1.40186	27.85
0.3000	0.6500	0.79953	0.814	1.38296	22.25						

Table 6. Values of V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ for Binary Mixtures of Tetrahydrofuran, 2-Propanol, and 2,2,4-Trimethylpentane at T = 298.15 K

x	V^E / cm^3·mol^{-1}	$\Delta\eta$ / mPa·s	$\Delta n_D \cdot 10^3$	$\Delta\sigma$ / mN·m^{-1}	x	V^E / cm^3·mol^{-1}	$\Delta\eta$ / mPa·s	$\Delta n_D \cdot 10^3$	$\Delta\sigma$ / mN·m^{-1}
				x Tetrahydrofuran + (1−x) 2-Propanol					
0.0500	0.020	−0.258	−0.03	0.12	0.5500	0.191	−0.555	−0.32	−0.20
0.1000	0.048	−0.440	−0.07	0.14	0.6000	0.189	−0.506	−0.29	−0.21
0.1500	0.077	−0.559	−0.15	0.14	0.6500	0.183	−0.453	−0.26	−0.20
0.2001	0.103	−0.615	−0.22	0.10	0.7000	0.172	−0.397	−0.17	−0.19
0.2500	0.124	−0.662	−0.28	0.05	0.7500	0.157	−0.337	−0.09	−0.16
0.3000	0.144	−0.675	−0.33	−0.02	0.8000	0.134	−0.274	−0.04	−0.13
0.3500	0.159	−0.680	−0.36	−0.08	0.8500	0.107	−0.209	0.00	−0.10
0.4000	0.173	−0.662	−0.37	−0.13	0.9000	0.071	−0.139	0.01	−0.07
0.4500	0.184	−0.632	−0.36	−0.17	0.9500	0.035	−0.069	0.01	−0.04
0.5000	0.191	−0.598	−0.34	−0.19					
				x Tetrahydrofuran + (1−x) 2,2,4-Trimethylpentane					
0.0500	0.026		−0.46	−0.29	0.5500	0.104		−2.79	−2.74
0.1001	0.041	$-0.9\cdot10^{-3}$	−0.86	−0.57	0.6000	0.090	$-2.4\cdot10^{-3}$	−2.74	−2.84
0.1500	0.076		−1.24	−0.86	0.6500	0.075		−2.61	−2.90
0.2000	0.102	$-1.8\cdot10^{-3}$	−1.59	−1.14	0.7000	0.063	$-1.3\cdot10^{-3}$	−2.41	−2.90
0.2500	0.123		−1.93	−1.39	0.7500	0.051		−2.14	−2.82
0.3000	0.143	$-2.7\cdot10^{-3}$	−2.21	−1.65	0.8000	0.040	$-1.2\cdot10^{-3}$	−1.82	−2.65
0.3500	0.152		−2.44	−1.93	0.8500	0.029		−1.46	−2.38
0.4000	0.151	$-2.6\cdot10^{-3}$	−2.60	−2.16	0.9000	0.018	$-0.1\cdot10^{-3}$	−1.05	−1.96
0.4500	0.144		−2.72	−2.39	0.9500	0.011		−0.56	−1.27
0.5000	0.132	$-2.5\cdot10^{-3}$	−2.79	−2.60					
				x 2-Propanol + (1−x) 2,2,4-Trimethylpentane					
0.0500	0.190	−0.077	−0.01	−0.11	0.5500	0.511	−0.645	0.96	−1.02
0.1000	0.314	−0.150	0.03	−0.22	0.6000	0.479	−0.666	1.00	−1.07
0.1501	0.395	−0.221	0.09	−0.34	0.6500	0.436	−0.677	1.00	−1.10
0.2000	0.456	−0.290	0.20	−0.43	0.7000	0.388	−0.673	0.96	−1.11
0.2500	0.506	−0.356	0.32	−0.54	0.7500	0.332	−0.649	0.89	−1.08
0.3000	0.542	−0.419	0.45	−0.65	0.8000	0.276	−0.608	0.80	−1.01
0.3500	0.559	−0.477	0.58	−0.73	0.8500	0.211	−0.532	0.66	−0.89
0.4000	0.562	−0.529	0.70	−0.81	0.9000	0.147	−0.417	0.50	−0.69
0.4500	0.554	−0.576	0.81	−0.89	0.9500	0.071	−0.258	0.28	−0.40
0.5000	0.535	−0.615	0.89	−0.96					

Table 7. Values of V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ for Ternary Mixtures of Tetrahydrofuran (1) + 2-Propanol (2) + 2,2,4-Trimethylpentane (3) at T = 298.15 K

x_1	x_2	V^E / cm^3·mol^{-1}	$\Delta\eta$ / mPa·s	$\Delta n_D \cdot 10^3$	$\Delta\sigma$ / mN·m^{-1}	x_1	x_2	V^E / cm^3·mol^{-1}	$\Delta\eta$ / mPa·s	$\Delta n_D \cdot 10^3$	$\Delta\sigma$ / mN·m^{-1}
0.0500	0.9000	0.104	−0.419	−0.89	−0.02	0.3000	0.5500	0.324	−0.638	−1.93	−1.32
0.0501	0.7999	0.242	−0.608	−0.70	−0.62	0.3000	0.4500	0.381	−0.559	−2.15	−1.52
0.0500	0.7000	0.382	−0.669	−0.63	−0.91	0.3000	0.3500	0.400	−0.459	−2.47	−1.61
0.0500	0.6000	0.477	−0.658	−0.69	−1.15	0.3001	0.2500	0.390	−0.342	−2.72	−1.55
0.0500	0.5001	0.531	−0.606	−0.86	−1.20	0.3000	0.1500	0.322	−0.203	−3.06	−1.45
0.0500	0.4000	0.567	−0.519	−1.10	−1.09	0.3000	0.0500	0.241	−0.067	−3.34	−1.29
0.0500	0.3000	0.545	−0.407	−1.38	−0.93	0.4000	0.5500	0.256	−0.632	−2.02	−0.59
0.0500	0.2000	0.474	−0.283	−1.63	−0.78	0.4000	0.4500	0.320	−0.558	−2.28	−1.09
0.0500	0.1000	0.304	−0.144	−1.88	−0.57	0.4000	0.3500	0.353	−0.458	−2.59	−1.53
0.0500	0.0500	0.210	−0.073	−1.97	−0.49	0.3999	0.2501	0.346	−0.334	−2.93	−1.77
0.1000	0.8500	0.131	−0.552	−4.37	−0.23	0.4000	0.1500	0.317	−0.211	−3.33	−1.87
0.1000	0.7500	0.290	−0.653	−1.15	−0.87	0.4000	0.0500	0.208	−0.072	−3.65	−1.81
0.1000	0.6500	0.387	−0.674	−1.08	−1.17	0.5000	0.4500	0.265	−0.556	−2.14	−1.65
0.1000	0.5500	0.462	−0.638	−1.16	−1.31	0.5000	0.3500	0.309	−0.456	−2.56	−0.80
0.1000	0.4500	0.512	−0.560	−1.35	−1.25	0.5000	0.2500	0.304	−0.335	−2.99	−1.45
0.1000	0.3499	0.526	−0.465	−1.60	−1.14	0.5000	0.1501	0.271	−0.208	−3.43	−1.94
0.1000	0.2500	0.500	−0.347	−1.89	−1.09	0.5000	0.0500	0.173	−0.071	−3.77	−2.18
0.1000	0.1501	0.399	−0.214	−2.14	−0.93	0.6000	0.3500	0.247	−0.451	−2.00	−2.23
0.1000	0.0500	0.214	−0.074	−2.33	−0.77	0.6000	0.2500	0.255	−0.338	−2.53	−2.12
0.2000	0.7500	0.186	−0.659	−1.51	−0.39	0.6000	0.1500	0.225	−0.211	−3.05	−0.81
0.2000	0.6500	0.314	−0.680	−1.47	−0.98	0.6000	0.0500	0.140	−0.073	−3.50	−1.45
0.2000	0.5500	0.391	−0.640	−1.58	−0.02	0.7000	0.2500	0.190	−0.336	−2.03	−2.10
0.2000	0.4500	0.436	−0.564	−1.78	−0.62	0.7000	0.1500	0.196	−0.209	−2.69	−2.54
0.2000	0.3500	0.450	−0.463	−2.05	−0.91	0.6999	0.0500	0.118	−0.070	−3.24	−2.63
0.2000	0.2500	0.446	−0.346	−2.34	−1.15	0.8000	0.1500	0.136	−0.204	−2.03	−0.92
0.2000	0.1501	0.363	−0.214	−2.64	−1.20	0.8000	0.0500	0.090	−0.068	−1.88	−1.76
0.2000	0.0500	0.235	−0.074	−2.88	−1.09	0.8999	0.0501	0.052	−0.068	−0.74	−2.31
0.3000	0.6500	0.237	−0.679	−1.81	−0.93						

x_i and x_j. The binary interaction coefficients, a_k, have been determined from a least-squares procedure, and the results are presented in Table 8. The parameters a_k were then used to calculate the curves of V^E for these binary systems as shown in Figure 1.

Table 8. Binary Coefficients a_k of the Redlich–Kister Equation and Standard Deviations δ of V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ for the Binary Systems at T = (288.15, 298.15, and 308.15) K

ΔQ_{ij}	T/K	a_0	a_1	a_2	a_3	a_4	$\delta \cdot 10^3$
			Tetrahydrofuran (1) + 2-Propanol (2)				
V^E / cm^3·mol^{-1}	288.15	0.5638	0.1368	−0.0254	−0.0027	−0.1496	2.3
	298.15	0.7547	0.1712	0.0644	−0.0072	−0.3167	1.2
	308.15	0.8939	0.1672	0.1750	0.0500	−0.2654	2.1
$\Delta\eta$ / mPa·s	288.15	−3.7128	2.6990	−1.5144	0.5500	−1.9308	3.8
	298.15	−2.3927	1.5854	−0.9562	0.4833	−0.5101	3.4
	308.15	−1.6463	1.0358	−0.5160	0.0844	−0.4356	1.2
Δn_D	288.15	−0.00086	0.00114	0.00427	−0.00113	−0.00227	0.014
	298.15	−0.00143	0.00100	0.00166	−0.00046		0.013
	308.15	−0.00218	0.00092	0.00009	−0.00031		0.011
$\Delta\sigma$ / mN·m^{-1}	288.15	−0.9260	−0.5818	1.1945	−1.6191	0.6266	4.6
	298.15	−0.7771	−0.8017	1.8818	−1.1263		4.1
	308.15	−0.5069	−1.3267	1.9717	−0.5006		5.4
			Tetrahydrofuran (1) + 2,2,4-Trimethylpentane (3)				
V^E / cm^3·mol^{-1}	288.15	0.3793	−0.5651	0.1511	0.4676	−0.3115	2.6
	298.15	0.4766	−0.5690	0.1754	0.3050	−0.1720	1.8
	308.15	0.5954	−0.4757	0.1481	−0.0782	0.1854	0.7
$\Delta\eta$ / mPa·s	288.15	−0.0135	0.0091	−0.0027	−0.0018		0.04
	298.15	−0.0104	0.0097	−0.0001	−0.0215	0.0028	0.03
	308.15	−0.0079	0.0058	0.0019	−0.0066		0.02
Δn_D	288.15	−0.00959	−0.00153	0.00143	0.00139		0.040
	298.15	−0.01119	−0.00122	0.00164	-3.18×10^{-6}	−0.00108	0.011
	308.15	−0.01219	−0.00201	0.00019	0.00176		0.014
$\Delta\sigma$ / mN·m^{-1}	288.15	−11.0210	−6.4838	−4.8004	−6.3588	−3.8660	27.0
	298.15	−10.3780	−6.4989	−1.7021	−4.7612	−6.5641	26.8
	308.15	−9.1965	−7.2081	−4.0309	−1.1641		15.9
			2-Propanol (2) + 2,2,4-Trimethylpentane (3)				
V^E / cm^3·mol^{-1}	288.15	1.7639	−0.7583	0.2085	0.6411	0.2645	3.2
	298.15	2.1563	−0.9141	0.1610	0.2627	0.6696	2.9
	308.15	2.5797	−1.0039	0.0456	0.0690	1.0753	4.2
$\Delta\eta$ / mPa·s	288.15	−3.6903	−2.2474	−1.2547	−1.0125	−1.2662	0.9
	298.15	−2.4618	−1.3794	−0.7282	−0.7792	−0.5956	2.4
	308.15	−1.7357	−0.9740	−0.5055	−0.4382	−0.3545	2.0
Δn_D	288.15	0.00585	0.00336	−0.00051	0.00027		0.005
	298.15	0.00357	0.00299	−0.00118	0.00041		0.008
	308.15	0.00129	0.00300	−0.00136	0.00041	−0.00197	0.015
$\Delta\sigma$ / mN·m^{-1}	288.15	−3.5883	−2.1691	−0.6106	−0.9420	−1.1769	5.3
	298.15	−3.8499	−2.6157	−1.9065	−1.0292		4.9
	308.15	−4.1566	−2.4301	−2.5014	−2.1210		11.5
			Tetrahydrofuran (1) + 2-Propanol (2) + 2,2,4-Trimethylpentane (3)				
ΔQ_{123}	C_{00}	C_{10}	C_{01}	C_{11}	C_{20}	C_{02}	$\delta \cdot 10^3$
V^E/cm^3·mol^{-1}	2.123	−14.050	−6.596	16.332	18.265	10.260	10.5
$\Delta\eta$/mPa·s	9.649	−57.105	20.372	3.974	−4.599		6.5
Δn_D	−0.401	1.105	1.173	−1.293	−1.036	−1.162	0.61
$\Delta\sigma$/mN·m^{-1}	167.020	−157.361	−419.990	−281.812	375.711	528.591	40.7

Table 9. Standard Deviations of Equations 7 to 12 in Estimating V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ for the Tetrahydrofuran + 2-Propanol + 2,2,4-Trimethylpentane Ternary System at T = 298.15 K

ΔQ_{123}	Scatchard et al.	Tsao and Smith	Toop	Kohler	Colinet	Jacob and Fitzner
V^E/cm^3·mol^{-1}	0.022	0.074	0.024	0.027	0.046	0.023
$\Delta\eta$/mPa·s	0.108	0.199	0.117	0.086	0.021	0.062
Δn_D	0.0016	0.0020	0.0018	0.0018	0.0017	0.0018
$\Delta\sigma$/mN·m^{-1}	0.30	0.18	0.29	0.16	0.21	0.16

The derived data, V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$, for ternary mixtures of tetrahydrofuran (1) + 2-propanol (2) + 2,2,4-trimethylpentane (3) at T = 298.15 K were correlated, respectively, using the equation

$$\Delta Q_{123} = \Delta Q(x_1,x_2) + \Delta Q(x_1,x_3) + \Delta Q(x_2,x_3) + x_1x_2x_3\sum_{i=0}^{2}\sum_{j=0}^{2-i} C_{ij}x_1^i x_2^j \quad (6)$$

where ΔQ_{123} refers to ternary V^E/cm^3·mol^{-1}, $\Delta\eta$/mPa·s, Δn_D, or $\Delta\sigma$/mN·m^{-1} and $x_3 = 1 - x_1 - x_2$. ΔQ is the binary contribution functions for V^E, $\Delta\eta$, Δn_D, or $\Delta\sigma$ as defined in eq 5. The ternary parameters C_{ij} were determined with the optimization algorithm similar to that for the binary parameters. The parameters C_{ij} and the corresponding standard deviations are also given in Table 8.

The curves of constant V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ at T = 298.15 K for the ternary mixtures were calculated from eq 6 and plotted in Figures 2 to 5, respectively. As can be expected from the behavior of the binary mixtures, the experimental values of ternary V^E are positive at all compositions (Figure 2). A maximum V^E value is found near the 2-propanol + 2,2,4-trimethylpentane side with a composition at about x = 0.4 of 2-propanol. As shown in Figure 3, the values of ternary $\Delta\eta$ are

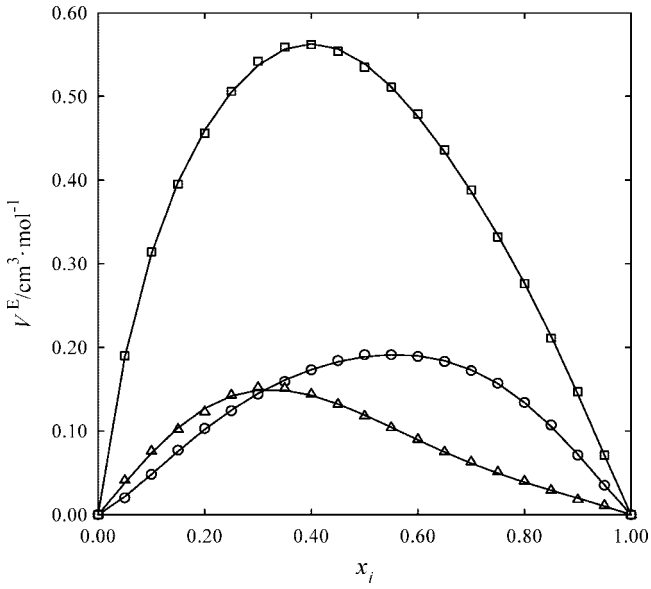

Figure 1. Variation of excess molar volume V^E with mole fraction x_i for the binary systems at $T = 298.15$ K: ○, tetrahydrofuran (1) + 2-propanol (2), $x_i = x_1$; Δ, tetrahydrofuran (1) + 2,2,4-trimethylpentane (3), $x_i = x_1$; , 2-propanol (2) + 2,2,4-trimethylpentane (3), $x_i = x_2$. Solid curves were calculated from the Redlich–Kister equation.

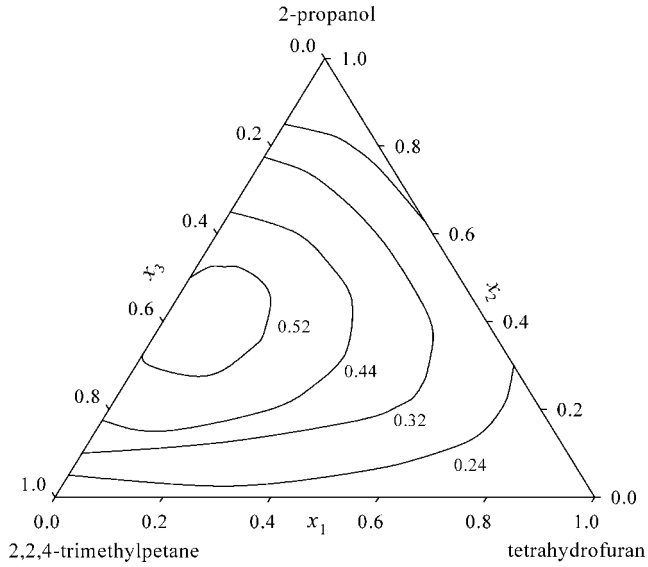

Figure 2. Iso-lines of V^E for the ternary system tetrahydrofuran (1) + 2-propanol (2) + 2,2,4-trimethylpentane (3) at $T = 298.15$ K.

negative at all compositions, with a minimum value near the tetrahydrofuran + 2-propanol side at the composition about $x = 0.7$ of 2-propanol. Curves of constant Δn_D and $\Delta\sigma$ in Figures 4 and 5 show negative values at almost all compositions, with a minimum value close to the side of tetrahydrofuran + 2,2,4-trimethylpentane.

The ternary V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ for the system tetrahydrofuran (1) + 2-propanol (2) + 2,2,4-trimethylpentane (3) at $T = 298.15$ K may be estimated, from binary functions ΔQ, using the following expressions:

Scatchard et al.[12]

$$\Delta Q_{123} = \frac{x_2}{1-x_1}\Delta Q(x_1, 1-x_1) + \frac{x_3}{1-x_1}\Delta Q(x_1, 1-x_1) + \Delta Q\left(\frac{x_2}{x_2+x_3}, \frac{x_3}{x_2+x_3}\right) \quad (7)$$

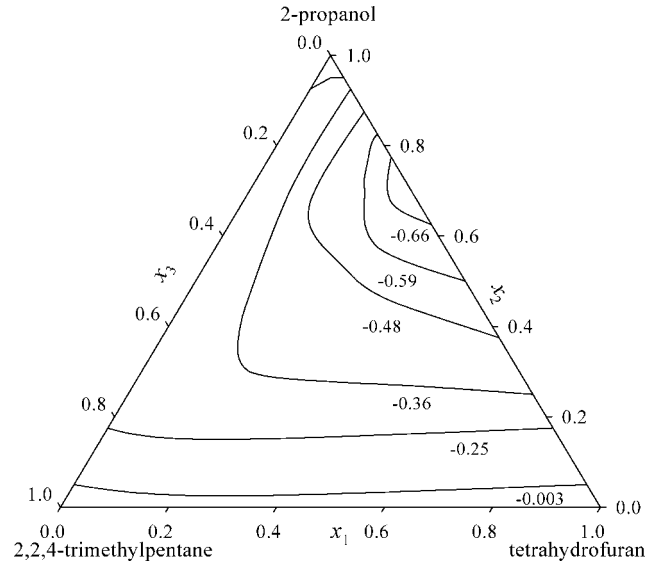

Figure 3. Iso-lines of $\Delta\eta$ for the ternary system tetrahydrofuran (1) + 2-propanol (2) + 2,2,4-trimethylpentane (3) at $T = 298.15$ K.

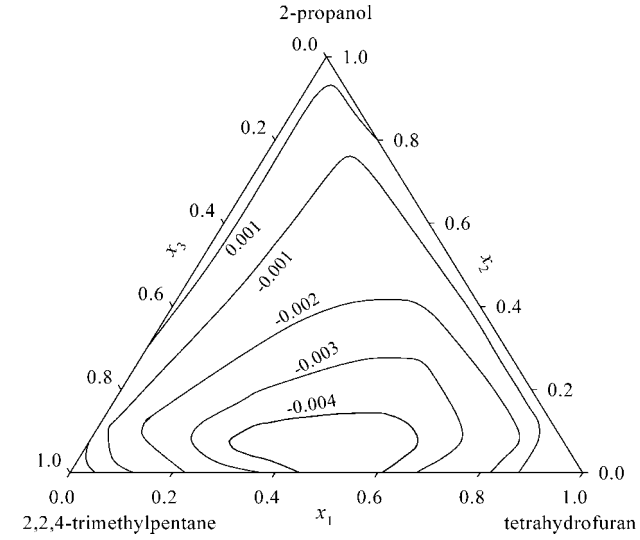

Figure 4. Iso-lines of Δn_D for the ternary system tetrahydrofuran (1) + 2-propanol (2) + 2,2,4-trimethylpentane (3) at $T = 298.15$ K.

Tsao and Smith[13]

$$\Delta Q_{123} = \frac{x_2}{1-x_1}\Delta Q(x_1, 1-x_1) + \frac{x_3}{1-x_1}\Delta Q(x_1, 1-x_1) + (1-x_1)\Delta Q\left(\frac{x_2}{x_2+x_3}, \frac{x_3}{x_2+x_3}\right) \quad (8)$$

Toop[14]

$$\Delta Q_{123} = \frac{x_2}{1-x_1}\Delta Q(x_1, 1-x_1) + \frac{x_3}{1-x_1}\Delta Q(x_1, 1-x_1) + (1-x_1)^2\Delta Q\left(\frac{x_2}{x_2+x_3}, \frac{x_3}{x_2+x_3}\right) \quad (9)$$

Kohler[15]

$$\Delta Q_{123} = (x_1+x_2)^2\Delta Q\left(\frac{x_1}{x_1+x_2}, \frac{x_2}{x_1+x_2}\right) + (x_1+x_3)^2\Delta Q\left(\frac{x_1}{x_1+x_3}, \frac{x_3}{x_1+x_3}\right) + (x_2+x_3)^2\Delta Q\left(\frac{x_2}{x_2+x_3}, \frac{x_3}{x_2+x_3}\right) \quad (10)$$

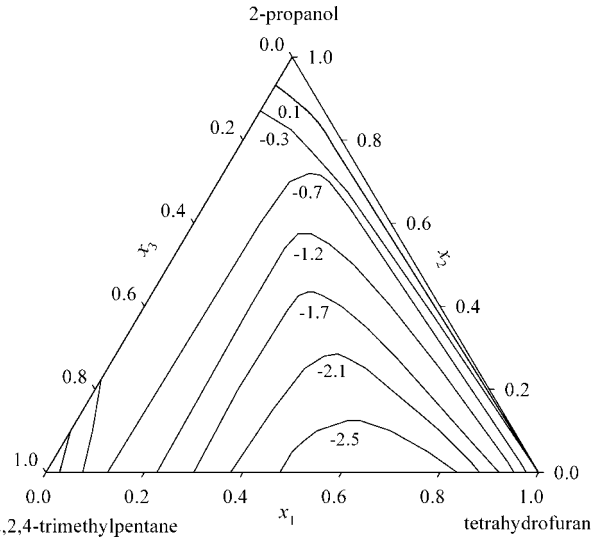

Figure 5. Iso-lines of $\Delta\sigma$ for the ternary system tetrahydrofuran (1) + 2-propanol (2) + 2,2,4-trimethylpentane (3) at $T = 298.15$ K.

Colinet[16]

$$\Delta Q_{123} = 0.5 \left[\begin{array}{l} \frac{x_2}{1-x_1}\Delta Q(x_1, 1-x_1) + \frac{x_1}{1-x_2}\Delta Q(1-x_2, x_2) + \\ \frac{x_3}{1-x_1}\Delta Q(x_1, 1-x_1) + \frac{x_1}{1-x_3}\Delta Q(1-x_3, x_3) + \\ \frac{x_3}{1-x_2}\Delta Q(x_2, 1-x_2) + \frac{x_2}{1-x_3}\Delta Q(1-x_3, x_3) \end{array} \right] \quad (11)$$

Jacob and Fitzner[17]

$$\Delta Q_{123} = \frac{4x_1x_2}{1-(x_1-x_2)^2}\Delta Q\left(\frac{1+x_1-x_2}{2}, \frac{1-x_1+x_2}{2}\right) + \frac{4x_1x_3}{1-(x_1-x_3)^2}\Delta Q\left(\frac{1+x_1-x_3}{2}, \frac{1-x_1+x_3}{2}\right) + \frac{4x_2x_3}{1-(x_2-x_3)^2}\Delta Q\left(\frac{1+x_2-x_3}{2}, \frac{1-x_2+x_3}{2}\right) \quad (12)$$

The standard deviations for these estimations are shown in Table 9. As can be seen from this result, the Scatchard equation gives lower deviations for estimating the ternary V^E, whereas the Colinet equation predicts better values for the ternary $\Delta\eta$. With respect to the ternary Δn_D, there are no significant differences between the various equations. On the other hand, the Kohler equation and the Jacob and Fitzner equation predict equally well for ternary $\Delta\sigma$.

Conclusion

This paper reports the experimental data of densities ρ, viscosities η, refractive indexes n_D, and surface tensions σ for the systems formed by tetrahydrofuran, 2-propanol, and 2,2,4-trimethylpentane at atmospheric pressure. The values of V^E are positive at all compositions, while the $\Delta\eta$, Δn_D, and $\Delta\sigma$ values are negative at most of the compositions. The calculated V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ data were fitted to variable-degree polynomials in terms of liquid mole fractions.

The ternary V^E, $\Delta\eta$, Δn_D, and $\Delta\sigma$ data were compared with those estimated from binary results using the empirical equations of Scatchard et al., Tsao and Smith, Toop, Kohler, Colinet, and Jacob and Fitzner. As we have pointed out above, the Toop equation leads to a good agreement with experimental values of V^E, whereas the same equation does not predict good values for $\Delta\sigma$. Alternately, the Scatchard at al. equation predicts good results for V^E, while the same equation does not give good values for $\Delta\sigma$.

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