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ORIGINAL PAPER

Thermodynamic and transport properties for binary and ternary mixtures of 2-methyltetrahydrofuran + chlorobenzene + cyclopentanone at $T = 298.15$ K

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Abstract Experimental densities ρ, viscosities η, and refractive indices n_D of the ternary mixtures consisting of 2-methyltetrahydrofuran + chlorobenzene + cyclopentanone and constituted binary mixtures were measured at $T = 298.15$ K for the liquid region and at ambient pressure for the whole composition range. Excess molar volumes V_m^E, deviations in the viscosity $\Delta\eta$, and deviations in the refractive index Δn_D from the mole fraction average for the mixtures were derived from the experimental data. The excess partial molar volumes $V_{m,i}^E$ were also calculated. The binary and ternary data of V_m^E, $\Delta\eta$, and Δn_D were correlated as a function of the mole fraction by using the Redlich–Kister and the Cibulka equations, respectively. McAllister's three-body interaction model is used for correlating the kinematic viscosity of binary mixtures with the mole fraction.

Keywords Excess molar volume · Viscosity deviation · Refractive index deviation · 2-Methyltetrahydrofuran · Cyclopentanone · Chlorobenzene

Introduction

This paper is a continuation of our earlier work related to the study of thermodynamic and transport properties of binary and ternary mixtures [1–3]. Excess and deviation properties of mixtures provide information about the molecular interactions between the various components and can be used for the development of molecular models describing the thermodynamic behavior of mixtures [4–7].

The thermodynamic properties of mixtures containing ketones, cyclic ethers, and aromatic compounds are of great industrial interest. The excess and deviation properties of such mixtures have proved to be meaningful from a thermodynamic point of view, as they provide direct information about the energetic effects arising between the molecules present in the mixture; this knowledge can help to explain the rearranging of the bondings that occurs during the mixing process, which is essential when studying new theoretical approaches to the liquid state matter and its mixtures. Here, we present experimental densities ρ, viscosities η, and refractive indices n_D for the binary and ternary mixtures formed by 2-methyltetrahydrofuran, chlorobenzene, and cyclopentanone at $T = 298.15$ K for the liquid region and at ambient pressure for the whole composition range.

The derived properties (excess molar volumes V_m^E, deviations in the viscosity $\Delta\eta$, and deviations in the refractive index Δn_D) in combination with other mixing properties provide valuable information for qualitatively analyzing the molecular interactions between molecules. Excess partial molar volumes $V_{m,i}^E$ were also calculated from experimental data for these mixtures. The excess and deviation values for the binary mixtures were fitted by the least-squares method of the Redlich–Kister equation. For correlating the ternary data, the Cibulka equation was used. As far as we know, no ternary data are available for the mixtures investigated in the open literature. This work will also provide a test of the semiempirical McAllister three-body model to correlate the kinematic viscosity of the aforementioned binary mixtures with the mole fraction.

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Results and discussion

The experimental densities ρ, viscosities η, and refractive indices n_D for three binary mixtures 2-methyltetrahydrofuran + cyclopentanone, chlorobenzene + 2-methyltetrahydrofuran, and chlorobenzene + cyclopentanone at $T = 298.15$ K are reported in Table 1. Excess molar volumes V_m^E, deviations in the viscosity $\Delta\eta$, and deviations in the refractive index Δn_D from the mole fraction average for three binary mixtures at $T = 298.15$ K were calculated and are tabulated in Table 1.

Excess molar volumes V_m^E were calculated from density data according to

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

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 mixture, and N is the number of components. In the mixtures studied, excess molar volumes are negative for the three binary mixtures over the whole composition range. The excess molar volume V_m^E ($x = 0.5$) decreases in the sequence: 2-methyltetrahydrofuran + cyclopentanone > chlorobenzene + cyclopentanone > chlorobenzene + 2-methyltetrahydrofuran. Figure 1 shows the excess molar volumes for the three binary mixtures at $T = 298.15$ K. For the mixture 2-methyltetrahydrofuran + cyclopentanone the negative value for V_m^E is due to dipole–dipole interactions between the carbonyl group of cyclopentanone and the oxygen atom of 2-methyltetrahydrofuran. The interactions between chlorobenzene + cyclopentanone give a negative contribution to V_m^E. The negative value of V_m^E for this mixture suggests a specific interaction between the components owing to the existence of London and dipolar forces between the ketone and chlorobenzene. For the mixture chlorobenzene + 2-methyltetrahydrofuran the negative value of V_m^E may be due to dipolar forces between the chlorine atom of chlorobenzene and the oxygen atom of 2-methyltetrahydrofuran.

The excess partial molar volumes $V_{m,i}^E$ can be determined from excess molar volume data using

$$V_{m,i}^E = V_m^E + (1 - x_i)\left(\partial V_m^E / \partial x_i\right)_{T,P} \qquad (2)$$

The values of excess partial molar volumes $V_{m,1}^E$ and $V_{m,2}^E$ for the three binary mixtures at $T = 298.15$ K are listed in Table 1 and graphically represented in Figs. 2 and 3. The results are in good agreement with the Gibbs–Duhem equation.

The deviation in the viscosity from the mole fraction average $\Delta\eta$ is given by

$$\Delta\eta = \eta - \sum_{i=1}^{N} x_i \eta_i \qquad (3)$$

where η is the absolute viscosity of the mixtures and η_i is the absolute viscosity of pure component i. The $\Delta\eta$ values are also graphically represented as a function of mole fraction at $T = 298.15$ K in Fig. 4. The $\Delta\eta$ values are negative for 2-methyltetrahydrofuran + cyclopentanone over the whole composition range. This reveals that the strength of specific interaction is not the only factor influencing the viscosity deviation of liquid mixtures. The molecular size and shape of the components also play an equally important role. Deviations in the viscosity for the mixture chlorobenzene + 2-methyltetrahydrofuran are positive and may be due to interactions between branched groups of unlike molecules. For the mixture chlorobenzene + cyclopentanone an inversion of the sign of $\Delta\eta$ is observed over part of the concentration range as expected as a result of steric effects. In this mixture $\Delta\eta$ values are positive at lower concentrations of chlorobenzene and negative at higher concentrations of chlorobenzene.

The deviation in the refractive index Δn_D was calculated from the mole fraction average as suggested by Brocos et al. [8] and is given by

$$\Delta n_D = n_D - \sum_{i=1}^{N} x_i n_{D_i} \qquad (4)$$

where n_D, n_{D_i}, and x_i are the refractive index of the mixture, the refractive index of pure component i, and the mole fraction of pure component i, respectively. Figure 5 shows the results of Δn_D for the three binary mixtures at $T = 298.15$ K. For the whole composition range, the Δn_D values are positive for the three binary mixtures. The values of Δn_D ($x = 0.5$) follow the order chlorobenzene + cyclopentanone > chlorobenzene + 2-methyltetrahydrofuran > 2-methyltetrahydrofuran + cyclopentanone. The mixing functions V_m^E, $\Delta\eta$, and Δn_D were represented mathematically by the Redlich–Kister equation for correlating the experimental data [9]:

$$\Delta Q_{ij} = x_1(1 - x_1)\sum_{i=0}^{k} A_i (2x_1 - 1)^i \qquad (5)$$

where ΔQ_{ij} refers to V_m^E (cm^3 mol^{-1}), $\Delta\eta$ (mPa s), or Δn_D, x_i is the mole fraction of component i, and A_i are adjustable parameters. The values of coefficients A_i were determined by a multiple regression analysis based on the least-squares method and are summarized along with the standard deviations between the experimental and the fitted values of the respective functions in Table 2. The standard deviation is defined by

$$\sigma = \left[\frac{\sum_{i=1}^{n}\left(\Delta Q_i^{\text{exptl}} - \Delta Q_i^{\text{calcd}}\right)^2}{n - p}\right]^{1/2} \qquad (6)$$

Table 1 Densities ρ, excess molar volumes $V_{\mathrm{m}}^{\mathrm{E}}$, excess partial molar volume $V_{\mathrm{m},i}^{\mathrm{E}}$, viscosities η, deviations in the viscosity $\Delta\eta$, refractive indices n_{D}, and deviations in the refractive indices Δn_{D} of binaries at 298.15 K

x	ρ (g cm^{-3})	$V_{\mathrm{m}}^{\mathrm{E}}$ (cm^3 mol^{-1})	$V_{\mathrm{m},1}^{\mathrm{E}}$ (cm^3 mol^{-1})	$V_{\mathrm{m},2}^{\mathrm{E}}$ (cm^3 mol^{-1})	η	$\Delta\eta$ (mPa s)	n_{D}	Δn_{D}
(x) 2-Methyltetrahydrofuran + (1 − x) cyclopentanone								
0.0000	0.94407	0.000	0.00	0.00	1.125	0.000	1.4337	0.0000
0.0212	0.94195	−0.017	−0.78	0.00	1.103	−0.007	1.4332	0.0001
0.0637	0.93769	−0.047	−0.70	0.00	1.061	−0.021	1.4323	0.0004
0.1277	0.93133	−0.090	−0.59	−0.02	1.001	−0.039	1.4308	0.0008
0.1917	0.92498	−0.123	−0.50	−0.03	0.944	−0.054	1.4293	0.0011
0.2563	0.91860	−0.149	−0.41	−0.06	0.890	−0.065	1.4277	0.0014
0.3212	0.91224	−0.168	−0.33	−0.09	0.840	−0.073	1.4260	0.0016
0.3856	0.90595	−0.179	−0.26	−0.13	0.792	−0.078	1.4242	0.0016
0.4507	0.89965	−0.185	−0.20	−0.17	0.747	−0.079	1.4224	0.0017
0.5157	0.89341	−0.186	−0.15	−0.22	0.705	−0.078	1.4205	0.0017
0.5812	0.88714	−0.176	−0.11	−0.27	0.665	−0.075	1.4185	0.0016
0.6466	0.88095	−0.163	−0.07	−0.32	0.628	−0.069	1.4164	0.0014
0.7069	0.87529	−0.146	−0.05	−0.38	0.596	−0.061	1.4145	0.0012
0.7785	0.86863	−0.119	−0.03	−0.44	0.560	−0.050	1.4121	0.0009
0.8445	0.86255	−0.089	−0.01	−0.50	0.529	−0.037	1.4100	0.0007
0.9107	0.85652	−0.056	0.00	−0.57	0.500	−0.022	1.4078	0.0004
0.9775	0.85049	−0.014	0.00	−0.63	0.472	−0.006	1.4056	0.0001
1.0000	0.84848	0.000	0.00	0.00	0.463	0.000	1.4048	0.0000
(x) Chlorobenzene + (1 − x) 2-methyltetrahydrofuran								
0.0000	0.84848	0.000	0.00	0.00	0.463	0.000	1.4048	0.0000
0.0188	0.85358	−0.038	−2.12	0.00	0.470	0.002	1.4072	0.0002
0.0509	0.86232	−0.105	−1.97	0.00	0.482	0.005	1.4111	0.0004
0.1030	0.87641	−0.202	−1.74	−0.02	0.501	0.009	1.4177	0.0009
0.1570	0.89089	−0.287	−1.51	−0.06	0.520	0.013	1.4243	0.0013
0.2126	0.90570	−0.361	−1.30	−0.11	0.540	0.017	1.4312	0.0017
0.2712	0.92119	−0.425	−1.10	−0.17	0.560	0.021	1.4383	0.0020
0.3298	0.93651	−0.470	−0.91	−0.25	0.579	0.024	1.4454	0.0023
0.3913	0.95246	−0.503	−0.74	−0.35	0.598	0.026	1.4528	0.0025
0.4548	0.96874	−0.519	−0.58	−0.46	0.617	0.027	1.4603	0.0026
0.5206	0.98543	−0.517	−0.44	−0.60	0.635	0.027	1.4680	0.0027
0.5892	1.00246	−0.497	−0.32	−0.75	0.654	0.026	1.4759	0.0026
0.6601	1.02018	−0.455	−0.21	−0.93	0.671	0.024	1.4839	0.0024
0.7334	1.03809	−0.393	−0.13	−1.12	0.689	0.021	1.4921	0.0021
0.8094	1.05639	−0.307	−0.06	−1.34	0.705	0.016	1.5005	0.0016
0.8890	1.07527	−0.194	−0.02	−1.58	0.722	0.011	1.5091	0.0010
0.9713	1.09447	−0.054	0.00	−1.84	0.737	0.003	1.5179	0.0002
1.0000	1.10109	0.000	0.00	0.00	0.742	0.000	1.5210	0.0000
(x) Chlorobenzene + (1 − x) cyclopentanone								
0.0000	0.94407	0.000	0.00	0.00	1.125	0.000	1.4337	0.0000
0.0165	0.94731	−0.026	−1.56	0.00	1.122	0.004	1.4355	0.0004
0.0498	0.95372	−0.070	−1.41	0.00	1.117	0.011	1.4390	0.0009
0.1006	0.96348	−0.146	−1.23	−0.02	1.108	0.021	1.4443	0.0018
0.1542	0.97338	−0.201	−1.04	−0.05	1.097	0.031	1.4498	0.0026
0.2087	0.98326	−0.254	−0.88	−0.09	1.084	0.039	1.4551	0.0032
0.2660	0.99325	−0.286	−0.71	−0.13	1.068	0.045	1.4606	0.0037
0.3245	1.00329	−0.319	−0.58	−0.19	1.050	0.046	1.4662	0.0042
0.3841	1.01316	−0.335	−0.45	−0.26	1.023	0.045	1.4715	0.0043

Table 1 continued

x	ρ (g cm^{-3})	V_m^E (cm^3 mol^{-1})	$V_{m,1}^E$ (cm^3 mol^{-1})	$V_{m,2}^E$ (cm^3 mol^{-1})	η	$\Delta\eta$ (mPa s)	n_D	Δn_D
0.4488	1.02358	−0.341	−0.34	−0.34	0.993	0.040	1.4772	0.0043
0.5148	1.03387	−0.333	−0.25	−0.42	0.959	0.031	1.4828	0.0042
0.5836	1.04429	−0.316	−0.17	−0.52	0.920	0.019	1.4887	0.0040
0.6542	1.05465	−0.286	−0.11	−0.62	0.882	0.007	1.4944	0.0036
0.7390	1.06665	−0.233	−0.05	−0.74	0.835	−0.007	1.5011	0.0029
0.8057	1.07580	−0.184	−0.03	−0.83	0.802	−0.014	1.5063	0.0023
0.8869	1.08665	−0.117	−0.01	−0.94	0.769	−0.016	1.5124	0.0013
0.9704	1.09745	−0.040	−0.01	−1.05	0.745	−0.008	1.5188	0.0004
1.0000	1.10109	0.000	0.00	0.00	0.742	0.000	1.5210	0.0000

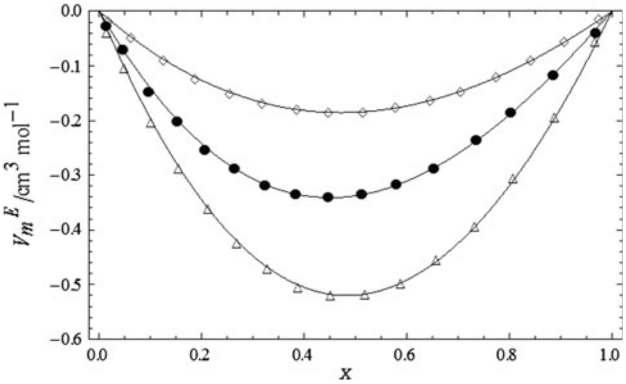

Fig. 1 Excess molar volumes V_m^E versus mole fraction x of binary mixtures at 298.15 K: *open diamonds* 2-methyltetrahydrofuran + cyclopentanone; *open triangles* chlorobenzene + 2-methyltetrahydrofuran; *filled circles* chlorobenzene + cyclopentanone; *solid line* calculated from the Redlich–Kister equation

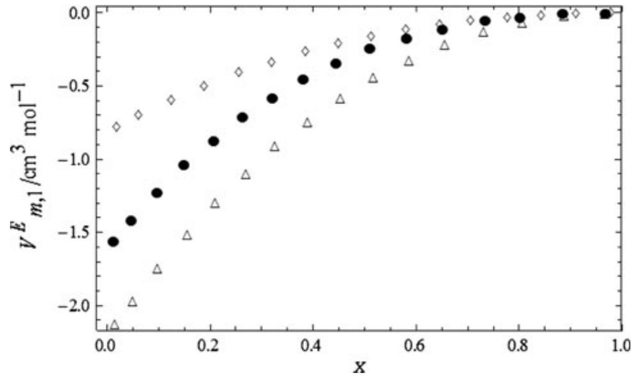

Fig. 2 Calculated excess partial molar volumes $V_{m,1}^E$ versus mole fraction x of binary mixtures at 298.15 K: *open diamonds* 2-methyltetrahydrofuran (1) + cyclopentanone (2); *open triangles* chlorobenzene (1) + 2-methyltetrahydrofuran (2); *filled circles* chlorobenzene (1) + cyclopentanone (2)

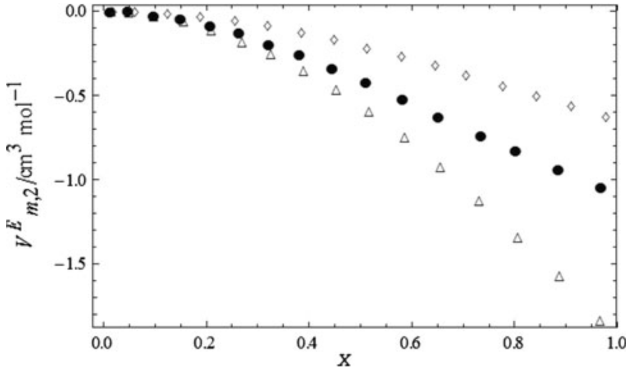

Fig. 3 Calculated excess partial molar volumes $V_{m,2}^E$ versus mole fraction x of binary mixtures at 298.15 K: *open diamonds* 2-methyltetrahydrofuran (1) + cyclopentanone (2); *open triangles* chlorobenzene (1) + 2-methyltetrahydrofuran (2); *filled circles* chlorobenzene (1) + cyclopentanone (2)

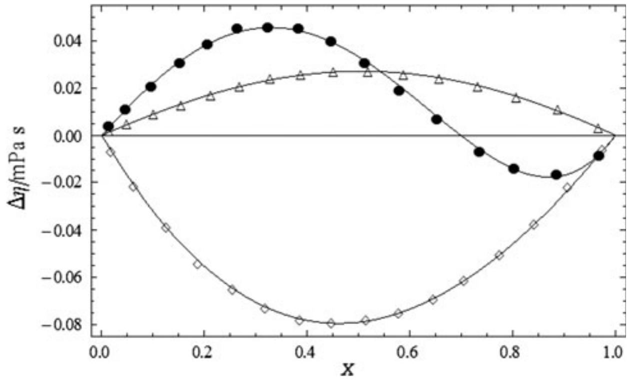

Fig. 4 Deviations in the viscosity $\Delta\eta$ versus mole fraction x of binary mixtures at 298.15 K: *open diamonds* 2-methyltetrahydrofuran + cyclopentanone; *open triangles* chlorobenzene + 2-methyltetrahydrofuran; *filled circles* chlorobenzene + cyclopentanone; *solid line* calculated from the Redlich–Kister equation

where n is the number of experimental points and p is the number of adjustable parameters. The standard deviations σ at $T = 298.15$ K lie between 0.00078 and 0.0035 cm^3 mol^{-1}, between 0.00035 and 0.00087 mPa s, and between 0.000033 and 0.000057 for V_m^E, $\Delta\eta$, and Δn_D, respectively.

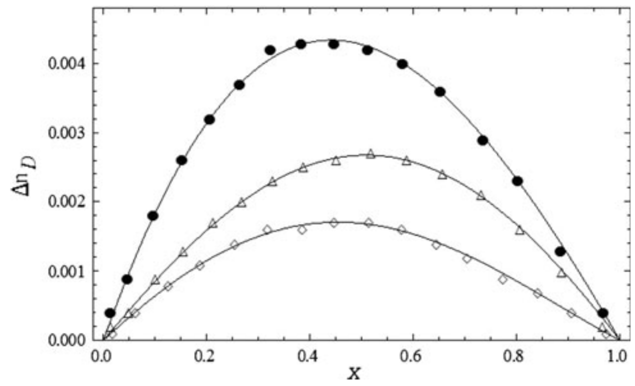

Fig. 5 Deviations in the refractive indices Δn_D versus mole fraction x of binary mixtures at 298.15 K: *open diamonds* 2-methyltetrahydrofuran + cyclopentanone; *open triangles* chlorobenzene + 2-methyltetrahydrofuran; *filled circles* chlorobenzene + cyclopentanone; *solid line* calculated from the Redlich–Kister equation

Table 2 Parameters and standard deviations of Eqs. (5) and (6) for binary mixtures at 298.15 K

System	A_0	A_1	A_2	σ
(x) 2-Methyltetrahydrofuran + $(1 - x)$ cyclopentanone				
V_m^E (cm^3 mol^{-1})	−0.7394	0.0865		0.001
$\Delta\eta$ (mPa s)	−0.3159	0.0500		2×10^{-4}
Δn_D	0.0067	0.0015	−0.0013	6×10^{-5}
(x) Chlorobenzene + $(1 - x)$ 2-methyltetrahydrofuran				
V_m^E (cm^3 mol^{-1})	−2.0778	0.1423		0.001
$\Delta\eta$ (mPa s)	0.1086	0.0023	−0.0111	3×10^{-4}
Δn_D	0.0107	0.0004	−0.0014	4×10^{-5}
(x) Chlorobenzene + $(1 - x)$ cyclopentanone				
V_m^E (cm^3 mol^{-1})	−1.3500	0.2794		0.003
$\Delta\eta$ (mPa s)	0.1332	0.2711	−0.1626	0.001
Δn_D	0.0171	−0.0042		0.0001

The experimental densities, viscosities, refractive indices, and calculated excess molar volumes, deviations in the viscosity, and deviations in the refractive index from the mole fraction average of ternary mixtures 2-methyltetrahydrofuran + chlorobenzene + cyclopentanone at $T = 298.15$ K are listed in Table 3. The derived data V_m^E, $\Delta\eta$, and Δn_D as defined in Eqs. (1), (3), and (4) for the ternary mixture were correlated using the equations

$$\Delta Q_{123} = \Delta Q_{\text{bin}} + x_1 x_2 x_3 \Delta_{123} \tag{7}$$

and

$$\Delta Q_{\text{bin}} = \sum_{i=1}^{3} \sum_{j>i}^{3} \Delta Q_{ij} \tag{8}$$

where ΔQ_{123} refers to V_m^E, $\Delta\eta$, and Δn_D for the ternary mixture 2-methyltetrahydrofuran + chlorobenzene + cyclopentanone and $x_3 = 1 - x_1 - x_2$. ΔQ_{ij} in Eq. (8) is the binary contribution of each *i–j* pair to the V_m^E, $\Delta\eta$, or Δn_D given by Eq. (5) with the parameters shown in Table 2. The ternary contribution term Δ_{123} was correlated using the expression suggested by Cibulka [10]

$$\Delta_{123} = B_0 + B_1 x_1 + B_2 x_2 \tag{9}$$

The ternary parameters, B_0, B_1, and B_2, were determined with the optimization algorithm similar to that for the binary parameters. The fitting parameters and the corresponding standard deviations are given in Table 4. The standard deviations σ are 0.0098 cm^3 mol^{-1}, 0.00095 mPa s, and 0.000071 for V_m^E, $\Delta\eta$, and Δn_D, respectively. As can be expected, the ternary mixture shows negative values of V_m^E and positive values of Δn_D at all compositions. But $\Delta\eta$ values are negative at almost all compositions (Table 3) except those close to the binary system chlorobenzene + 2-methyltetrahydrofuran where a change in sign occurs.

McAllister's three-body interaction model [11] is widely used for correlating the kinematic viscosity of binary mixtures with mole fraction. The three-body model is defined as

$$\begin{aligned}\ln v = {} & x_1^3 \ln v_1 + 3x_1^2 x_2 \ln v_{12} + 3x_1 x_2^2 \ln v_{21} \\ & + x_2^3 \ln v s_2 - \ln\left(x_1 + \frac{x_2 M_2}{M_1}\right) + 3x_1^2 x_2 \ln\left(\frac{2 + M_2/M_1}{3}\right) \\ & + 3x_1 x_2^2 \ln\left(\frac{1 + 2M_2/M_1}{3}\right) + x_2^3 \ln\left(\frac{M_2}{M_1}\right)\end{aligned} \tag{10}$$

where v, v_1, and v_2 are the kinematic viscosities of the mixture and the viscosities of pure components 1 and 2, respectively. v_{12} and v_{21} are the model parameters. Table 5 records the calculated results with the standard deviation as defined by Eq. (6). The standard deviations σ (mm^2 s^{-1}) for this model lie between 0.00025 and 0.0072, and the largest value corresponds to chlorobenzene + cyclopentanone.

Experimental

The purity of the components from Merck was as follows: 2-methyltetrahydrofuran ≥99%, chlorobenzene ≥99.5%, cyclopentanone ≥99.5%. Densities and refractive indices were measured without further purification, and their values were in good agreement with those found in the literature [12, 13] and reported in Table 6.

Apparatus and procedure

The density of the pure compounds and mixtures was measured by means of an Anton Parr DMA 4500 oscillating U-tube densimeter, provided with automatic

Table 3 Densities ρ, excess molar volumes $V_{\mathrm{m}}^{\mathrm{E}}$, viscosities η, deviations in the viscosity $\Delta\eta$, refractive indices n_{D}, and deviations in the refractive indices of ternary mixtures at 298.15 K

x_1	x_2	ρ (g cm^{-3})	$V_{\mathrm{m}}^{\mathrm{E}}$ (cm^{-3} mol^{-1})	η (mPa s)	$\Delta\eta$ (mPa s)	n_{D}	Δn_{D}
0.0500	0.0503	0.94873	−0.111	1.068	−0.005	1.4378	0.0012
0.0500	0.2501	0.92867	−0.209	0.891	−0.049	1.4331	0.0022
0.0500	0.4499	0.90906	−0.247	0.743	−0.065	1.4274	0.0024
0.0501	0.6500	0.88986	−0.224	0.622	−0.053	1.4212	0.0019
0.0499	0.8495	0.87107	−0.138	0.524	−0.019	1.4146	0.0011
0.0501	0.8996	0.86642	−0.102	0.501	−0.009	1.4128	0.0007
0.0501	0.6994	0.88521	−0.213	0.598	−0.044	1.4197	0.0018
0.0501	0.4998	0.90428	−0.252	0.711	−0.064	1.4257	0.0021
0.0502	0.3000	0.92383	−0.230	0.852	−0.055	1.4317	0.0022
0.0986	0.2467	0.93800	−0.260	0.888	−0.036	1.4379	0.0027
0.0999	0.4492	0.91834	−0.311	0.740	−0.049	1.4323	0.0029
0.1002	0.6498	0.89903	−0.291	0.620	−0.036	1.4259	0.0022
0.0998	0.8498	0.87999	−0.198	0.522	−0.002	1.4190	0.0012
0.2000	0.0501	0.97643	−0.270	1.042	0.027	1.4530	0.0033
0.2000	0.2499	0.95614	−0.375	0.871	−0.012	1.4475	0.0036
0.1996	0.4506	0.93604	−0.412	0.725	−0.025	1.4415	0.0034
0.2000	0.6498	0.91670	−0.397	0.609	−0.009	1.4348	0.0024
0.2002	0.7499	0.90711	−0.363	0.558	0.006	1.4314	0.0019
0.2001	0.5498	0.92648	−0.421	0.663	−0.021	1.4384	0.0031
0.2000	0.3501	0.94613	−0.407	0.793	–0.023	1.4447	0.0036
0.2001	0.1498	0.96634	−0.337	0.951	0.002	1.4503	0.0035
0.2999	0.4498	0.95331	−0.484	0.706	−0.006	1.4505	0.0036
0.3003	0.6500	0.93364	−0.464	0.594	0.014	1.4436	0.0025
0.4000	0.0498	1.01056	−0.373	0.972	0.033	1.4716	0.0044
0.3999	0.2497	0.98994	−0.479	0.813	0.007	1.4656	0.0042
0.3999	0.4516	0.96947	−0.517	0.682	0.009	1.4590	0.0035
0.3999	0.5498	0.95968	−0.516	0.627	0.019	1.4556	0.0029
0.3990	0.3498	0.97953	−0.500	0.744	0.004	1.4622	0.0038
0.5000	0.0498	1.02640	−0.374	0.928	0.027	1.4801	0.0042
0.5000	0.2499	1.00561	−0.474	0.777	0.009	1.4740	0.0039
0.5000	0.4499	0.98531	−0.522	0.655	0.019	1.4673	0.0030
0.6000	0.0499	1.04148	−0.346	0.876	0.014	1.4884	0.0037
0.5994	0.2499	1.02054	−0.447	0.740	0.010	1.4821	0.0033
0.6004	0.3500	1.01040	−0.474	0.682	0.019	1.4787	0.0027
0.6912	0.0618	1.05336	−0.303	0.820	0.001	1.4954	0.0032
0.7003	0.2498	1.03508	−0.397	0.706	0.014	1.4902	0.0025
0.8500	0.0501	1.07638	−0.176	0.757	−0.009	1.5081	0.0017
0.8497	0.0999	1.07115	−0.213	0.735	0.001	1.5065	0.0015
0.8996	0.0500	1.08293	−0.133	0.742	−0.005	1.5119	0.0011

viscosity correction. The uncertainty of the density measurement was estimated to be 1×10^{-5} g cm^{-3}. The apparatus was calibrated once a day with dry air and doubly distilled fresh water. The temperature in the cell was regulated to ±0.01 K with a solid-state thermostat.

The mixtures were prepared by weighing known masses of pure liquids in air-tight, narrow-mouth, ground-glass stoppered bottles taking due precautions to minimize evaporation losses. All the mass measurements were performed on an electronic balance (Mettler AE 163, Switzerland) accurate to 0.01 mg. The possible error in the mole fraction is estimated to be less than $\pm 1 \times 10^{-4}$.

Viscosities were measured with an Ubbelohde viscometer. The equation for viscosity, according to Poiseuille's law, is

Table 4 Parameters and standard deviations of Eqs. (9) and (6) for ternary mixtures at 298.15 K

ΔQ_{123}	B_0	B_1	B_2	σ
V_m^E (cm^3 mol^{-1})	0.61093	−0.85117	−0.47422	0.010
$\Delta\eta$ (mPa s)	0.20044	−0.17923	−0.35130	0.001
Δn_D	0.00425	−0.00944	−0.00271	0.0001

Table 5 Binary coefficients of McAllister's three-body interaction equations and standard deviations σ for kinematic viscosities at 298.15 K

ν_{12} (mm^2 s^{-1})	ν_{21} (mm^2 s^{-1})	σ (mm^2 s^{-1})
(x) 2-Methyltetrahydrofuran + (1 − x) cyclopentanone		
0.6987	0.9089	2.6 × 10^{-4}
(x) Chlorobenzene + (1 − x) 2-methyltetrahydrofuran		
0.6696	0.6455	2.5 × 10^{-4}
(x) Chlorobenzene + (1 − x) cyclopentanone		
0.7922	1.1279	0.0072

Table 6 Experimental and literature values of densities ρ and refractive indices n_D of pure components at 298.15 K

Component	ρ (g cm^{-3})		n_D	
	Expt.	Lit.	Expt.	Lit.
Chlorobenzene	1.10109	1.10099 [12]	1.5210	1.52185 [12]
2-Methyltetrahydrofuran	0.84848	0.84882 [12]	1.4048	1.40508 [12]
Cyclopentanone	0.94407	0.94400 [13]	1.4337	1.4347 [13]

$$\eta = \rho\nu = \rho(kt - c/t) \tag{11}$$

where k and c are the viscometer constants and t, η, and ν are the efflux time, dynamic viscosity, and kinematic viscosity, respectively. The viscometer was suspended in a thermostated water bath maintained to ±0.01 K. An electronic digital stopwatch with uncertainty to ±0.01 s was used for flow time measurements. At least three repetitions of each data point obtained were reproducible to ±0.05 s, and results were averaged. The uncertainty of the viscosity measurement was estimated to be less than ±2 × 10^{-3} mPa s.

Refractive indices were measured using a digital Abbe-type refractometer. The uncertainty of refractive index measurement was estimated to be ±2 × 10^{-4}.

Airtight stoppered bottles were used for the preparation of the mixtures. The mass of the dry bottle was first determined. The less volatile component of the mixture was introduced into the bottle, and the total mass was recorded. Subsequently, the other component was introduced, and the mass of the bottle along with the two components was determined. Ternary mixtures were prepared by mixing of the three components. A total of 39 compositions were measured at $T = 298.15$ K for the ternary mixture of 2-methyltetrahydrofuran + chlorobenzene + cyclopentanone. Each mixture was immediately used after it was well mixed by shaking. All the weighings were performed on an electronic balance (AB 204-N Mettler) accurate to 0.1 mg. The uncertainty in the mole fraction is estimated to be lower than ±2 × 10^{-4}.

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