

Densities and Viscosities for Binary Mixtures of Anisole with Pentyl Alcohol Isomers

Wen-Lu Weng,* Yule-Chen Chang, and Chu-Ping Huang

Department of Chemical Engineering, Ming-Hsin Institute of Technology, Hsin-Chu, Hsin-Feng 304, Taiwan, Republic of China

Densities and viscosities were measured for the binary mixtures of anisole with 2-pentanol, 3-pentanol, 2-methyl-1-butanol, 2-methyl-2-butanol, 3-methyl-1-butanol, and 3-methyl-2-butanol at 303.15 K, 313.15 K, and 323.15 K over the entire composition range. The excess volumes and viscosity deviations were calculated from the experimental data and are correlated by a Redlich–Kister type equation. McAllister's three-body and four-body interaction models were also used to correlate the kinematic viscosities.

Introduction

New density and viscosity data are reported in this article for six binary mixtures of anisole with isomers of pentyl alcohols at temperatures from 303.15 K to 323.15 K. These alcohol isomers include 2-pentanol, 3-pentanol, 2-methyl-2-butanol, 2-methyl-1-butanol, 3-methyl-1-butanol, and 3-methyl-2-butanol. The measurements are a continuation of studies on densities and viscosities for binary solutions containing alcohol isomers and polar constituents (Weng, 1999a,b). Although several similar studies have been reported (Aucejo et al., 1996; Artigas et al., 1996; Lafuente et al., 1993; Riggo et al., 1986), no available data were found in the literature for the binary mixtures of this study. The results not only show the effects of the self-association of the pentyl alcohols and the steric hindrance of methyl groups on both densities and viscosities but also add the availability of the physical property data, which are useful for model developments and engineering applications.

Experimental Section

Anisole (99%), 2-pentanol (98%), 3-pentanol (98%), and 2-methyl-2-butanol (99%) were R.D.H. products, and 2-methyl-1-butanol (98%), 3-methyl-1-butanol (99%), and 3-methyl-2-butanol (99%) were supplied by Fluka Chemie AG. The purities of these substances were checked with gas chromatography. All reagents were used without further purification. The measured densities and viscosities for these pure substances at 303.15 K were compared with literature values in Table 1.

An Anton Paar densimeter (DMA 60/602H) was employed to measure the density ρ . Each sample mixture was prepared by mass with an accuracy of ± 0.0001 in mole fraction. The temperature of the measuring cell in the densimeter was controlled within ± 0.03 K by circulating thermostatic water. A precision digital thermometer (model 1560, Hart Scientific) with a thermistor probe was used to read the cell temperature to an accuracy of ± 0.015 K. The oscillation period τ in the vibrating U-tube of the densimeter was converted into

Table 1. Densities ρ and Viscosities η for Pure Components at 303.15 K

component	$\rho/\text{g}\cdot\text{cm}^{-3}$		$\eta/\text{mPa}\cdot\text{s}$	
	exptl	lit.	exptl	lit.
anisole	0.9843	0.9846 ^a	0.908	0.9315 ^a 0.9070 ^b
2-pentanol	0.8013	0.8013 ^c 0.8010 ^d	2.888	2.884 ^c 2.77 ^d
3-pentanol	0.8115	0.8116 ^c	3.852	3.852 ^c
2-methyl-1-butanol	0.8110	0.8109 ^c	3.594	3.5956 ^c
2-methyl-2-butanol	0.8001	0.8000 ^c 0.8006 ^d	2.854	2.856 ^c 2.87 ^d
3-methyl-1-butanol	0.8017	0.8037 ^c 0.80178 ^e 0.80174 ^f 0.8027 ^d	3.191	3.195 ^c 2.961 ^f 2.95 ^d
3-methyl-2-butanol	0.8094	0.8093 ^c	3.163	3.163 ^c

^a Joshi et al. (1990a). ^b Joshi et al. (1990b). ^c TRC data (1994). ^d Riggo et al. (1986). ^e Kumar et al. (1992). ^f Venkatesu et al. (1996).

density by the following equation:

$$\rho = A(\tau^2 - B) \quad (1)$$

where A and B are apparatus constants determined by the literature density data of pure water (Harr et al., 1984) and dry air (Vargaftik, 1975) at temperatures of interest. The uncertainty of the density measurements is estimated to be less than $\pm 1 \times 10^{-4}$ g/cm³. While the composition of the mixture sample was checked frequently by gas chromatography after the measurement, the variation was found to be minimal.

The kinematic viscosities ν were measured by using a Cannon–Fenske routine viscometer (size 75, supplied by Cannon Instrument Co.). The detailed procedure for viscosity measurements was described elsewhere (Weng, 1999a). The kinematic viscosities (cSt) were obtained from the following equation:

$$\nu = kt \quad (2)$$

where k is the capillary constant of the viscometer and t (s) is the flowing time. The absolute viscosities, η (mPa·s) were calculated from $\eta = \rho\nu$. The accuracy of the reported viscosities is to within $\pm 1.0\%$.

* To whom correspondence should be addressed. E-mail: wengwl@mh.it.edu.tw. Fax: 886-3-5595142.

Table 2. Densities ρ and Viscosities η for Anisole (1) + 2-Pentanol (2)

x_1	$T = 303.15$ K		$T = 313.15$ K		$T = 323.15$ K	
	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$
0.0	0.8013	2.888	0.7936	2.017	0.7843	1.466
0.1007	0.8192	2.097	0.8109	1.557	0.8012	1.202
0.2007	0.8372	1.590	0.8285	1.234	0.8186	1.014
0.3001	0.8550	1.279	0.8460	1.025	0.8360	0.887
0.4004	0.8732	1.095	0.8640	0.903	0.8538	0.803
0.5005	0.8916	0.998	0.8823	0.845	0.8718	0.753
0.5991	0.9097	0.951	0.9004	0.823	0.8898	0.725
0.6973	0.9277	0.931	0.9186	0.816	0.9077	0.711
0.7980	0.9468	0.924	0.9372	0.811	0.9261	0.704
0.8970	0.9651	0.919	0.9556	0.801	0.9443	0.697
1.0	0.9843	0.908	0.9749	0.786	0.9635	0.691

Table 3. Densities ρ and Viscosities η for Anisole (1) + 3-Pentanol (2)

x_1	$T = 303.15$ K		$T = 313.15$ K		$T = 323.15$ K	
	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$
0.0	0.8115	3.852	0.8023	2.272	0.7929	1.543
0.1007	0.8285	2.787	0.8190	1.745	0.8093	1.261
0.2006	0.8453	2.043	0.8359	1.355	0.8260	1.041
0.3001	0.8623	1.547	0.8527	1.093	0.8426	0.888
0.3996	0.8793	1.238	0.8697	0.938	0.8593	0.795
0.5000	0.8967	1.062	0.8870	0.863	0.8761	0.747
0.5999	0.9142	0.976	0.9046	0.835	0.8932	0.729
0.6973	0.9314	0.941	0.9217	0.824	0.9103	0.719
0.7998	0.9495	0.927	0.9397	0.811	0.9281	0.709
0.8971	0.9665	0.917	0.9569	0.793	0.9454	0.697
1.0	0.9843	0.908	0.9749	0.786	0.9635	0.691

Table 4. Densities ρ and Viscosities η for Anisole (1) + 2-Methyl-1-butanol (2)

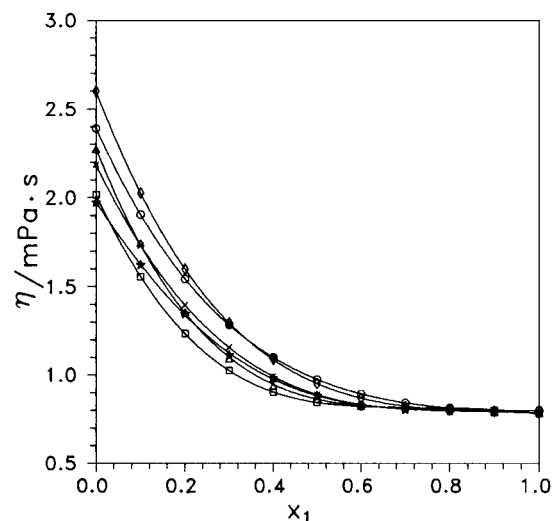
x_1	$T = 303.15$ K		$T = 313.15$ K		$T = 323.15$ K	
	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$
0.0	0.8110	3.594	0.8033	2.601	0.7951	1.936
0.1005	0.8283	2.761	0.8202	2.026	0.8116	1.552
0.2004	0.8454	2.126	0.8372	1.601	0.8282	1.246
0.3003	0.8626	1.665	0.8542	1.296	0.8449	1.022
0.4012	0.8798	1.347	0.8713	1.084	0.8617	0.872
0.5001	0.8971	1.149	0.8883	0.952	0.8786	0.784
0.6005	0.9146	1.032	0.9057	0.868	0.8956	0.739
0.6996	0.9320	0.968	0.9229	0.824	0.9124	0.718
0.8001	0.9494	0.932	0.9402	0.803	0.9293	0.707
0.9003	0.9669	0.912	0.9576	0.794	0.9463	0.698
1.0	0.9843	0.908	0.9749	0.786	0.9635	0.691

Table 5. Densities ρ and Viscosities η for Anisole (1) + 2-Methyl-2-butanol (2)

x_1	$T = 303.15$ K		$T = 313.15$ K		$T = 323.15$ K	
	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$
0.0	0.8001	2.854	0.7911	1.976	0.7807	1.416
0.1000	0.8183	2.246	0.8089	1.623	0.7983	1.206
0.2000	0.8364	1.792	0.8269	1.339	0.8161	1.023
0.2997	0.8543	1.463	0.8448	1.125	0.8340	0.885
0.4001	0.8727	1.232	0.8629	0.976	0.8518	0.798
0.5007	0.8910	1.079	0.8814	0.885	0.8701	0.751
0.5997	0.9093	0.988	0.8997	0.831	0.8885	0.730
0.7012	0.9284	0.941	0.9189	0.808	0.9074	0.719
0.8005	0.9472	0.922	0.9374	0.799	0.9261	0.709
0.9000	0.9657	0.917	0.9561	0.792	0.9447	0.697
1.0	0.9843	0.908	0.9749	0.786	0.9635	0.691

Results and Discussion

Experimental results for the six binary systems of anisole with the isomers of pentyl alcohol are listed in Tables 2–7, respectively. Figure 1 shows the variations of the absolute viscosities with the mole fraction of anisole x_1 for these six systems at 313.15 K. The viscosities decrease monotonically with an increase of x_1 for each system.

**Figure 1.** Viscosity η at 313.15 K: (□) anisole (1) + 2-pentanol (2); (△) anisole (1) + 3-pentanol (2); (◇) anisole (1) + 2-methyl-1-butanol (2); (☆) anisole (1) + 2-methyl-2-butanol (2); (O) anisole (1) + 3-methyl-1-butanol (2); (x) anisole (1) + 3-methyl-2-butanol (2).**Table 6. Densities ρ and Viscosities η for Anisole (1) + 3-Methyl-1-butanol (2)**

x_1	$T = 303.15$ K		$T = 313.15$ K		$T = 323.15$ K	
	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$
0.0	0.8017	3.191	0.7952	2.391	0.7889	1.827
0.1002	0.8198	2.520	0.8128	1.905	0.8058	1.484
0.2000	0.8378	2.023	0.8304	1.545	0.8231	1.224
0.3005	0.8557	1.657	0.8482	1.283	0.8403	1.036
0.3997	0.8736	1.401	0.8660	1.101	0.8574	0.908
0.5004	0.8922	1.216	0.8841	0.974	0.8751	0.823
0.6014	0.9108	1.087	0.9023	0.893	0.8930	0.769
0.7004	0.9290	0.999	0.9203	0.843	0.9104	0.735
0.8003	0.9473	0.944	0.9385	0.816	0.9279	0.715
0.9008	0.9659	0.916	0.9567	0.801	0.9456	0.701
1.0	0.9843	0.908	0.9749	0.786	0.9635	0.691

Table 7. Densities ρ and Viscosities η for Anisole (1) + 3-Methyl-2-butanol (2)

x_1	$T = 303.15$ K		$T = 313.15$ K		$T = 323.15$ K	
	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\rho/\text{g}\cdot\text{cm}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$
0.0	0.8094	3.163	0.8013	2.185	0.7916	1.573
0.1006	0.8265	2.405	0.8182	1.731	0.8081	1.273
0.2007	0.8439	1.858	0.8354	1.397	0.8251	1.066
0.3004	0.8609	1.476	0.8522	1.157	0.8417	0.925
0.4000	0.8781	1.223	0.8694	0.991	0.8587	0.830
0.5008	0.8962	1.067	0.8869	0.889	0.8760	0.771
0.6009	0.9139	0.981	0.9044	0.832	0.8935	0.736
0.6997	0.9314	0.937	0.9219	0.808	0.9109	0.718
0.8003	0.9491	0.919	0.9398	0.799	0.9287	0.707
0.8998	0.9666	0.913	0.9572	0.794	0.9458	0.699
1.0	0.9843	0.905	0.9749	0.786	0.9635	0.691

Excess volumes $V^E/\text{cm}^3\cdot\text{mol}^{-1}$ and viscosity deviations $\delta\eta/\text{mPa}\cdot\text{s}$ were calculated from the experimental results by the following equations, respectively.

$$V^E = V_m - (x_1 V_1 + x_2 V_2) \quad (3)$$

$$\delta\eta = \eta_m - (x_1 \eta_1 + x_2 \eta_2) \quad (4)$$

where x_i , V_i , and η_i are the mole fraction, molar volume, and viscosity of the pure component i , respectively. The subscript m represents mixture properties. The uncertainty of the excess molar volumes is estimated to be less than

Table 8. Correlated Results for Excess Molar Volume V^E

system	T/K	a_0	a_1	a_2	a_3	$10^3\sigma/\text{cm}^3\cdot\text{mol}^{-1}$
anisole + 2-pentanol	303.15	0.6475	-0.0909	-0.1306	-0.1940	0.20
	313.15	0.9922	-0.5163	0.1063	0.1950	0.15
	323.15	1.0440	-0.4885	0.3980	-0.0072	0.18
anisole + 3-pentanol	303.15	0.8106	-0.4857	-0.4285	0.1550	0.10
	313.15	0.9473	-0.3452	-0.1667	-0.1579	0.18
	323.15	1.2094	0.1824	-0.1304	-0.7739	0.25
anisole + 2-methyl-1-butanol	303.15	0.5049	-0.2462	-0.1846	0.3516	0.18
	313.15	0.5962	-0.1588	-0.0068	-0.0224	0.18
	323.15	0.6347	-0.3230	0.3236	0.3879	0.17
anisole + 2-methyl-2-butanol	303.15	0.5662	-0.1416	-0.5992	0.1080	0.23
	313.15	0.7403	-0.2284	-0.2580	0.0583	0.23
	323.15	0.8807	-0.1723	-0.3001	-0.0845	0.28
anisole + 3-methyl-1-butanol	303.15	0.4403	-0.2693	-0.2135	0.5414	0.22
	313.15	0.5296	-0.2719	0.0332	0.2820	0.10
	323.15	0.6370	-0.2855	0.3861	0.3335	0.31
anisole + 3-methyl-2-butanol	303.15	0.6056	-0.5362	0.0157	0.3807	0.35
	313.15	0.8184	-0.2984	-0.1366	0.0124	0.27
	323.15	0.9402	-0.5106	0.0685	0.2043	0.42

Table 9. Correlated Results for Viscosity Deviation ($\delta\eta$)

system	T/K	a_0	a_1	a_2	a_3	$10\sigma/\text{mPa}\cdot\text{s}$
anisole + 2-pentanol	303.15	-3.5995	2.5952	-1.1089	0.3004	0.10
	313.15	-2.2298	1.7255	-0.3627	-0.2487	0.18
	323.15	-1.3016	0.8011	-0.1939	-0.0217	0.07
anisole + 3-pentanol	303.15	-5.2701	3.4216	-0.8771	-0.1516	0.11
	313.15	-2.6645	2.0406	-0.3269	-0.6607	0.10
	323.15	-1.4795	1.0954	-0.0747	-0.4599	0.16
anisole + 2-methyl-1-butanol	303.15	-4.4045	2.3005	-0.2813	-0.3806	0.09
	313.15	-2.9726	1.5067	-0.2579	0.0060	0.20
	323.15	-2.1176	1.2104	0.0487	-0.3688	0.11
anisole + 2-methyl-2-butanol	303.15	-3.2045	1.5120	-0.1930	0.1091	0.08
	313.15	-1.9890	0.9863	0.0981	-0.2271	0.26
	323.15	-1.2133	0.8179	0.1215	-0.5092	0.21
anisole + 3-methyl-1-butanol	303.15	-3.3383	1.4983	-0.5355	0.0595	0.34
	313.15	-2.4575	1.1836	-0.2449	0.0962	0.18
	323.15	-1.7476	0.9285	-0.1590	-0.0901	0.22
anisole + 3-methyl-2-butanol	303.15	-3.8707	2.1573	-0.4548	-0.0305	0.21
	313.15	-2.3794	1.2500	-0.1242	-0.0027	0.38
	323.15	-1.4391	0.8527	-0.2677	0.0788	0.24

$\pm 0.005 \text{ cm}^3\cdot\text{mol}^{-1}$, and the viscosity deviations are accurate to $\pm 0.03 \text{ mPa}\cdot\text{s}$. The composition dependence of either the V^E or $\delta\eta$ isotherm was represented by a Redlich-Kister type equation:

$$Y = x_1 x_2 \sum_{i=0}^P a_i (x_1 - x_2)^i \quad (5)$$

where Y refers to V^E or $\delta\eta$, and x_1 and x_2 are the mole fractions of anisole and the alcohol component, respectively. The coefficients a_i were obtained by fitting the experimental results to eq 5 with a least-squares method. The correlated results for excess volumes and viscosity deviations are given respectively in Tables 8 and 9, in which the tabulated standard deviation (σ) was defined as

$$\sigma = \left[\frac{\sum (Y_{\text{exp}} - Y_{\text{cal}})^2}{n - p} \right]^{1/2} \quad (6)$$

where n is the number of data points and p is the number of coefficients. The subscript cal denotes the calculated value.

The variations of V^E and $\delta\eta$ with the mole fraction of anisole at 313.15 K are presented in Figures 2 and 3, respectively. Figure 2 shows that the excess molar volumes are positive for all these investigated systems. It implies that volume expansion takes place when anisole mixes with the pentyl alcohol isomers. The magnitude of the volume expansion follows the sequence 2-pentanol > 3-pentanol

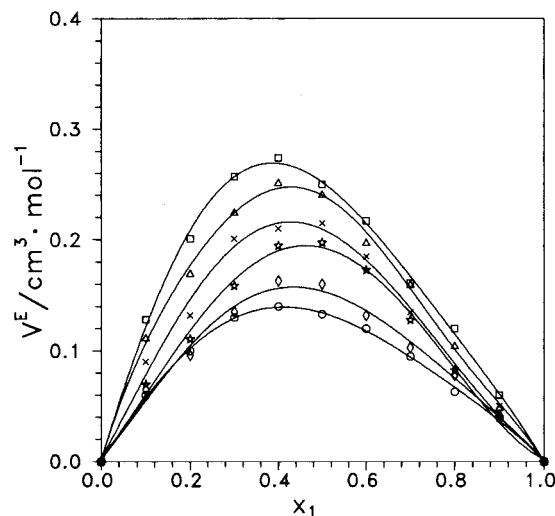


Figure 2. Excess volumes V^E at 313.15 K: (\square) anisole (1) + 2-pentanol (2); (\triangle) anisole (1) + 3-pentanol (2); (\diamond) anisole (1) + 2-methyl-1-butanol (2); (\star) anisole (1) + 2-methyl-2-butanol (2); (\circ) anisole (1) + 3-methyl-1-butanol (2); (\times) anisole (1) + 3-methyl-2-butanol (2); (—) calculated from eq 5.

> 3-methyl-2-butanol > 2-methyl-2-butanol > 2-methyl-1-butanol > 3-methyl-1-butanol. Moreover, the excess volumes were found to increase with increasing temperature. Figure 3 illustrates that the viscosity deviations are negative for each binary system. As evidenced from the

Table 10. Correlated Results of McAllister's Models

system	T/K	three-body model			four-body model			
		ν_{12}	ν_{21}	AAD% ^a	ν_{1112}	ν_{1122}	ν_{2221}	AAD% ^a
anisole + 2-pentanol	303.15	1.0299	0.9158	1.01	1.0627	0.8444	1.4189	0.48
	313.15	0.9424	0.7803	1.22	0.9716	0.7229	1.1854	0.74
	323.15	0.7899	0.7965	0.55	0.7987	0.7290	1.0365	0.23
anisole + 3-pentanol	303.15	0.9253	1.1685	2.49	1.1058	0.7124	2.0560	0.49
	313.15	0.9003	0.8313	1.75	0.9817	0.6772	1.3394	1.15
	323.15	0.8209	0.7484	1.56	0.8441	0.6631	1.0719	1.20
anisole + 2-methyl-1-butanol	303.15	0.8986	1.4752	1.79	1.0297	0.8791	2.2537	0.30
	313.15	0.7834	1.1662	1.41	0.8878	0.7960	1.6552	0.07
	323.15	0.7489	0.8940	1.80	0.8432	0.6172	1.3558	0.47
anisole + 2-methyl-2-butanol	303.15	0.9049	1.3239	1.45	1.0162	0.8918	1.8838	0.13
	313.15	0.8263	1.0352	1.50	0.9161	0.7443	1.4608	0.21
	323.15	0.7931	0.8133	1.21	0.8364	0.6766	1.1239	0.77
anisole + 3-methyl-1-butanol	303.15	0.9520	1.5772	0.32	0.9523	1.1878	2.0370	0.08
	313.15	0.8438	1.1890	0.89	0.8933	0.8869	1.5997	0.05
	323.15	0.7735	0.9580	0.75	0.7998	0.7738	1.2737	0.20
anisole + 3-methyl-2-butanol	303.15	0.9055	1.2395	1.66	1.0277	0.8332	1.8845	0.23
	313.15	0.8206	1.0148	1.50	0.9079	0.7403	1.4562	0.17
	323.15	0.7895	0.8213	0.49	0.7934	0.7526	1.0682	0.12

$$^a \text{AAD\%} = (100/n) \sum_{k=1}^n |\nu_k^{\text{cal}} - \nu_k^{\text{exp}}| / \nu_k^{\text{exp}}$$

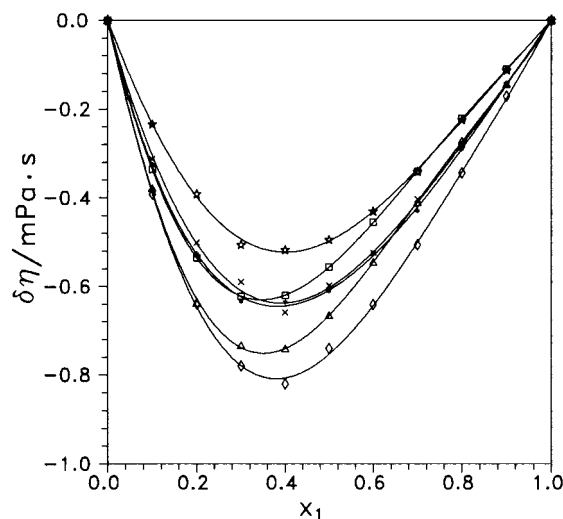


Figure 3. Viscosity deviations $\delta\eta$ at 303.15 K: (\square) anisole (1) + 2-pentanol (2); (\triangle) anisole (1) + 3-pentanol (2); (\diamond) anisole (1) + 2-methyl-1-butanol (2); (\star) anisole (1) + 2-methyl-2-butanol (2); (\circ) anisole (1) + 3-methyl-1-butanol (2); (\times) anisole (1) + 3-methyl-2-butanol (2); (—) calculated from eq 5.

calculations, the viscosity deviations decrease with an increase of temperature.

McAllister's multibody interaction model (McAllister, 1960) was widely used to correlate kinematic viscosity ν data. The three-body McAllister model was defined as

$$\ln \nu = x_1^3 \ln \nu_1 + 3x_1^2 x_2 \ln \nu_{12} + x_2^3 \ln \nu_{21} - \ln[x_1 + x_2(M_2/M_1)] + 3x_1^2 x_2 \ln[(2 + M_2/M_1)/3] + 3x_1 x_2^2 \ln[(1 + 2M_2/M_1)/3] + x_2^3 \ln(M_2/M_1) \quad (7)$$

and the four-body model was given by

$$\ln \nu = x_1^4 \ln \nu_1 + 4x_1^3 x_2 \ln \nu_{1112} + 6x_1^2 x_2^2 \ln \nu_{1122} + 4x_1 x_2^3 \ln \nu_{2221} + x_2^4 \ln \nu_2 - \ln[x_1 + x_2(M_2/M_1)] + 4x_1^3 x_2 \ln[(3 + M_2/M_1)/4] + 6x_1^2 x_2^2 \ln[(1 + M_2/M_1)/2] + 4x_1 x_2^3 \ln[(1 + 3M_2/M_1)/4] + x_2^4 \ln(M_2/M_1) \quad (8)$$

where ν_{12} , ν_{21} , ν_{1112} , ν_{1122} , and ν_{2221} are model parameters. The calculated results are presented in Table 10. The

average deviations are approximately within the experimental uncertainty, regardless of whether the three-body or the four-body model was used.

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