

Densities and Viscosities for Binary and Ternary Mixtures of 1, 4-Dioxane + 1-Hexanol + *N,N*-Dimethylaniline from $T = (283.15$ to $343.15)$ K

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Viscosities and densities of the ternary solvent systems of 1,4-dioxane + 1-hexanol and *N,N*-dimethylaniline were measured at several temperatures between $T = (283.15$ and $343.15)$ K at atmospheric pressure over the whole composition range. The experimental results are used to calculate viscosity deviations, $\Delta\eta$, of the ternary system. The calculated binary data have been fitted to the Redlich-Kister equation to determine the appropriate coefficients. To determine the coefficients of ternary data, Cibulka, Singh, and Nagata equations were used. This work also provides a test of the Grunberg and Nissan equation for correlating the dynamic viscosities of binary and ternary mixtures with mole fractions.

Introduction

Multicomponent liquid mixtures have attracted the attention of researchers in the past decades. Physical properties are very important factors in chemical and engineering processes because of their influence upon the effectiveness of the operations. Mass and heat transfer processes and flow operations are evident examples of the importance of the knowledge of these properties.^{1,2} It is well-known that the knowledge of the dependence of dynamic viscosity on both temperature and composition of the system is needed for many engineering processes and the study of fluid phenomena. There are several predictive equations³ for estimating thermodynamic properties of multicomponent systems. Geometrical solution models are considered to predict excess molar volumes and deviations of the viscosity for the ternary mixture from binary contribution because of dependence of interactions in ternary systems on the interaction in binary systems.^{4–7} Recently, new models have been developed for the prediction of viscosities of mixtures. Some of them are based on the group contribution concept,^{8,9} and others are based on the molecular approach that requires binary interaction parameters for each binary system present in the multicomponent mixture.^{10,11} Such methods are rarely used for viscosity because some of them cannot be immediately extensible to multicomponent mixtures or they may require more parameters (such as three- and four-body interaction terms) for mixtures containing more than two components or require binary interaction parameters for each binary system present in the multicomponent mixture.

In this investigation, viscosity deviations are derived from experimental data and fitted to three empirical equations.^{12–14} A single-parameter semiempirical relation¹⁵ has been proposed to estimate the viscosities of binary mixtures in terms of pure component data.

There are a number of papers that discussed the thermodynamic behavior of liquid mixtures of the oxygenated compounds.^{16–19} The main objective of the present paper is to determine the densities and viscosities for the binary and ternary systems formed by two oxygenated compounds 1-hexanol + 1,4-dioxane and an aromatic compound *N,N*-dimethylaniline.

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Table 1. Densities and Viscosities of Pure Components at Several Temperatures

compound	<i>T/K</i>	$\rho/\text{kg}\cdot\text{m}^{-3}$		$\eta/\text{mPa}\cdot\text{s}$	
		exptl	lit.	exptl	lit.
1-hexanol	283.15	828.23		7.459	
	293.15	821.01		5.335	
	303.15	813.92	0.81353 ²⁷	3.763	3.765 ²⁷
	313.15	810.91	0.81050 ²⁷	2.937	2.934 ²⁷
	323.15	806.84	0.80650 ²⁷	2.172	2.169 ²⁷
	333.15	802.91	0.80340 ²⁷	1.654	1.655 ²⁷
	343.15	784.23		1.411	
	283.15	1.046.91		1.590	
1,4-dioxane	293.15	1.035.03	1.033642 ²⁸	1.312	1.3152 ²⁹
	303.15	1.022.71	1.022554 ²⁸	1.102	1.108 ²⁹
	313.15	1.011.32	1.011298 ²⁸	0.946	0.9458 ²⁹
	323.15	999.12	0.999838 ²⁸	0.825	0.8232 ²⁹
	333.15	987.92	0.988249 ²⁸	0.721	0.7212 ²⁹
	343.15	976.61	0.976726 ²⁸	0.640	0.6402 ²⁹
	283.15	969.97		1.696	
	293.15	963.01		1.439	
<i>N,N</i> -dimethylaniline	303.15	948.33	0.94815 ³⁰	1.170	1.173 ³⁰
	313.15	939.72	0.93975 ³⁰	0.981	0.985 ³⁰
	323.15	940.24		0.928	
	333.15	932.71		0.911	
	343.15	924.08		0.841	

The lack of these type of data motivated us to make this study which may be used in some industrial processes in the future. Viscosities of the ternary mixtures of 1,4-dioxane + 1-hexanol + *N,N*-dimethylaniline have been measured as well as binary mixtures 1-hexanol + *N,N*-dimethylaniline, 1,4-dioxane + *N,N*-dimethylaniline, and 1,4-dioxane + 1-hexanol, at several temperatures from (283.15 to 343.15) K. Viscosity deviations ($\Delta\eta$) have been calculated from experimental data.

Experimental Section

Materials. Extra pure *N,N*-dimethylaniline (CAS 121-69-7) (mole fraction > 99.0 %), 1-hexanol (CAS 111-27-3) (mole fraction > 99.0 %), and 1,4-dioxane (CAS 123-91-1) (mole fraction > 99.0 %) were provided by the Aldrich company. The purities of all the chemicals were checked by gas chromatography using a semicapillary methylsilicon column (o.d. 530 μm). The solvents were degassed by ultrasound and dried over molecular sieves (Sigma Union Carbide, 0.4 nm).

Table 2. Densities, Viscosities, and Deviations of the Viscosity for the Binary and Ternary Systems at Indicated Temperatures

x_1	x_2	$\rho/\text{kg}\cdot\text{m}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\Delta\eta/\text{mPa}\cdot\text{s}$	x_1	x_2	$\rho/\text{kg}\cdot\text{m}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\Delta\eta/\text{mPa}\cdot\text{s}$
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 283.15 K									
0.9538	0.0000	1043.01	1.588	-0.007	0.1400	0.6385	889.23	3.104	-2.257
0.9081	0.0000	1040.92	1.591	-0.008	0.1445	0.7576	871.21	3.872	-2.175
0.8551	0.0000	1034.31	1.602	-0.003	0.1143	0.8082	862.85	4.339	-2.003
0.7749	0.0000	1025.23	1.606	-0.007	0.2508	0.1372	962.43	1.823	-0.637
0.7182	0.0000	1019.31	1.607	-0.013	0.2506	0.2399	950.74	1.870	-1.182
0.6278	0.0000	1013.42	1.629	0.001	0.2503	0.3425	935.62	2.033	-1.610
0.5302	0.0000	1005.32	1.637	-0.002	0.2501	0.4448	920.66	2.282	-1.951
0.4246	0.0000	998.33	1.660	0.009	0.2499	0.5469	903.74	2.603	-2.218
0.3099	0.0000	990.33	1.680	0.017	0.2496	0.6488	891.55	2.941	-2.467
0.8795	0.1205	1013.54	1.601	-0.696	0.3094	0.1512	967.53	1.758	-0.777
0.7731	0.2269	981.11	1.691	-1.230	0.3092	0.2417	954.52	1.768	-1.288
0.6866	0.3134	957.86	1.815	-1.614	0.3090	0.3321	938.81	2.031	-1.546
0.5935	0.4065	938.47	2.007	-1.968	0.3087	0.4223	917.22	2.377	-1.720
0.4933	0.5067	916.23	2.324	-2.239	0.3094	0.5124	904.84	2.625	-1.991
0.3850	0.6150	896.72	2.785	-2.414	0.3081	0.6023	899.96	2.746	-2.388
0.2675	0.7325	873.31	3.520	-2.369	0.4380	0.1332	978.67	1.702	-0.715
0.1835	0.8165	860.24	4.488	-1.894	0.4525	0.2407	962.33	1.804	-1.231
0.0000	0.1009	958.16	1.749	-0.529	0.4521	0.3436	945.22	1.942	-1.686
0.0000	0.2017	944.54	1.867	-0.991	0.4517	0.4463	928.13	2.199	-2.021
0.0000	0.3022	928.83	2.079	-1.358	0.5761	0.0985	993.55	1.648	-0.555
0.0000	0.4025	915.52	2.306	-1.710	0.5756	0.1968	977.57	1.754	-1.015
0.0000	0.5026	904.21	2.676	-1.917	0.5400	0.2770	961.42	1.812	-1.423
0.0000	0.6025	890.94	3.092	-2.076	0.5395	0.3690	945.43	1.985	-1.780
0.0000	0.7022	876.26	3.708	-2.035	0.6674	0.0913	999.01	1.651	-0.500
0.0000	0.8016	861.23	4.614	-1.702	0.6669	0.1824	983.81	1.665	-1.011
0.0000	0.9009	848.23	5.687	-1.201	0.6663	0.2734	966.62	1.758	-1.443
0.1322	0.2109	957.74	1.797	-1.101	0.7575	0.0914	1007.62	1.648	-0.494
0.1282	0.3215	932.82	2.081	-1.454	0.7571	0.1523	981.23	1.704	-0.789
0.1270	0.4256	919.82	2.310	-1.826	0.8364	0.0880	970.05	1.434	-0.680
0.1338	0.5186	906.55	2.608	-2.063					
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 293.15 K									
0.9538	0.0000	1035.34	1.327	-0.008	0.1400	0.6385	881.11	2.406	-1.505
0.9081	0.0000	1031.25	1.330	-0.010	0.1445	0.7576	863.50	2.928	-1.446
0.8551	0.0000	1023.65	1.326	-0.020	0.1143	0.8082	855.45	3.249	-1.327
0.7749	0.0000	1016.79	1.339	-0.015	0.2508	0.1372	954.23	1.499	-0.446
0.7182	0.0000	1011.33	1.345	-0.015	0.2506	0.2399	941.92	1.540	-0.806
0.6278	0.0000	1003.54	1.362	-0.008	0.2503	0.3425	927.63	1.637	-1.109
0.5302	0.0000	995.81	1.370	-0.011	0.2501	0.4448	912.94	1.828	-1.316
0.4246	0.0000	989.12	1.428	0.0354	0.2499	0.5469	895.62	2.051	-1.492
0.3099	0.0000	980.73	1.424	0.0195	0.2496	0.6488	883.44	2.297	-1.642
0.8795	0.1205	1002.74	1.311	-0.502	0.3094	0.1512	960.15	1.457	-0.537
0.7731	0.2269	973.80	1.395	-0.843	0.3092	0.2417	945.03	1.671	-0.676
0.6866	0.3134	951.11	1.554	-1.031	0.3090	0.3321	930.53	1.639	-1.060
0.5935	0.4065	929.82	1.626	-1.332	0.3087	0.4223	908.80	1.890	-1.161
0.4933	0.5067	903.63	1.845	-1.515	0.3094	0.5124	896.80	2.081	-1.320
0.3850	0.6150	889.20	2.184	-1.609	0.3081	0.6023	891.22	2.150	-1.602
0.2675	0.7325	865.64	2.707	-1.557	0.4380	0.1332	970.01	1.429	-0.481
0.1835	0.8165	853.33	3.221	-1.379	0.4525	0.2407	953.61	1.468	-0.859
0.0000	0.1009	950.00	1.448	-0.384	0.4521	0.3436	936.51	1.585	-1.143
0.0000	0.2017	936.43	1.527	-0.697	0.4517	0.4463	919.30	1.752	-1.377
0.0000	0.3022	920.62	1.667	-0.949	0.5761	0.0985	984.00	1.384	-0.376
0.0000	0.4025	909.23	1.837	-1.170	0.5756	0.1968	968.54	1.427	-0.716
0.0000	0.5026	896.74	2.086	-1.311	0.5400	0.2770	951.73	1.494	-0.965
0.0000	0.6025	882.60	2.359	-1.427	0.5395	0.3690	936.22	1.634	-1.184
0.0000	0.7022	868.60	2.821	-1.354	0.6674	0.0913	989.12	1.364	-0.358
0.0000	0.8016	852.26	3.401	-1.161	0.6669	0.1824	976.51	1.384	-0.692
0.0000	0.9009	841.25	4.138	-0.811	0.6663	0.2734	961.45	1.477	-0.954
0.1322	0.2109	949.43	1.483	-0.763	0.7575	0.0914	997.91	1.368	-0.345
0.1282	0.3215	924.62	1.669	-1.008	0.7571	0.1523	970.00	1.434	-0.515
0.1270	0.4256	910.94	1.836	-1.247	0.8364	0.0880	1002.74	1.348	-0.342
0.1338	0.5186	898.23	2.044	-1.400					
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 303.15 K									
0.9538	0.0000	1024.82	1.122	0.002	0.5935	0.4065	920.31	1.339	-0.915
0.9081	0.0000	1019.01	1.124	0.004	0.4933	0.5067	898.36	1.506	-1.028
0.8551	0.0000	1014.07	1.131	0.008	0.3852	0.615	879.87	1.748	-1.090
0.7749	0.0000	1005.98	1.136	-0.004	0.2675	0.7325	857.53	2.121	-1.047
0.7182	0.0000	1001.04	1.142	-0.005	0.1835	0.8165	845.02	2.632	-0.771
0.6278	0.0000	993.63	1.157	-0.006	0.0000	0.1009	942.24	1.221	-0.277
0.5302	0.0000	986.56	1.166	-0.001	0.0000	0.2017	928.31	1.276	-0.493
0.4246	0.0000	980.12	1.182	0.003	0.0000	0.3022	912.67	1.380	-0.659
0.3099	0.0000	973.40	1.199	0.007	0.0000	0.4025	901.18	1.496	-0.814
0.8795	0.1205	909.21	1.027	-0.425	0.0000	0.5026	888.09	1.668	-0.911
0.7731	0.2269	963.84	1.173	-0.578	0.0000	0.6025	875.63	1.891	-0.956
0.6866	0.3134	941.43	1.238	-0.755	0.0000	0.7022	860.74	2.160	-0.956

Table 2. Continued

x_1	x_2	$\rho/\text{kg}\cdot\text{m}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\Delta\eta/\text{mPa}\cdot\text{s}$	x_1	x_2	$\rho/\text{kg}\cdot\text{m}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\Delta\eta/\text{mPa}\cdot\text{s}$
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 303.15 K (Continued)									
0.0000	0.8016	846.02	2.585	-0.798	0.3090	0.3321	921.83	1.361	-0.724
0.0000	0.9009	832.65	3.101	-0.550	0.3087	0.4223	900.22	1.545	-0.783
0.0000	1.0000	813.96	3.917	0.000	0.3094	0.5124	889.69	1.661	-0.909
0.1322	0.2109	940.87	1.251	-0.529	0.3081	0.6023	882.77	1.729	-1.083
0.1282	0.3215	916.52	1.318	-0.759	0.4380	0.1332	961.04	1.197	-0.339
0.1270	0.4256	902.93	1.508	-0.85	0.4525	0.2407	944.06	1.228	-0.595
0.1338	0.5186	890.34	1.659	-0.948	0.4521	0.3436	927.71	1.308	-0.792
0.1400	0.6385	874.15	1.907	-1.022	0.4517	0.4463	910.30	1.445	-0.932
0.1445	0.7576	855.86	2.266	-0.983	0.5761	0.0985	974.52	1.185	-0.242
0.1143	0.8082	847.78	2.497	-0.891	0.5756	0.1968	959.35	1.195	-0.497
0.2508	0.1372	945.73	1.257	-0.311	0.5400	0.2770	942.41	1.240	-0.672
0.2506	0.2399	934.55	1.276	-0.568	0.5395	0.3690	926.90	1.335	-0.824
0.2503	0.3425	919.61	1.361	-0.759	0.6674	0.0913	979.77	1.156	-0.242
0.2501	0.4448	903.86	1.502	-0.893	0.6669	0.1824	966.24	1.181	-0.462
0.2499	0.5469	887.65	1.649	-1.021	0.6663	0.2734	950.86	1.212	-0.675
0.2496	0.6488	875.23	1.826	-1.118	0.7575	0.0914	988.03	1.141	-0.247
0.3094	0.1512	949.71	1.250	-0.348	0.7571	0.1523	961.02	1.211	-0.341
0.3092	0.2417	937.00	1.211	-0.631	0.8364	0.0880	993.57	1.156	-0.214
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 313.15 K									
0.9538	0.0000	1014.66	0.968	0.005	0.1400	0.6385	865.35	1.541	-0.709
0.9081	0.0000	1008.93	0.965	-0.003	0.1445	0.7576	848.02	1.792	-0.682
0.8551	0.0000	1003.65	0.976	0.003	0.1143	0.8082	839.81	1.958	-0.615
0.7749	0.0000	995.85	0.984	0.002	0.2508	0.1372	937.01	1.072	-0.221
0.7182	0.0000	991.21	0.987	0.004	0.2506	0.2399	926.13	1.086	-0.401
0.6278	0.0000	984.40	1.002	0.006	0.2503	0.3425	910.72	1.142	-0.538
0.5302	0.0000	977.93	1.010	0.004	0.2501	0.4448	894.86	1.243	-0.631
0.4246	0.0000	970.47	1.025	0.008	0.2499	0.5469	879.67	1.359	-0.707
0.3099	0.0000	963.88	1.029	0.009	0.2496	0.6488	867.89	1.489	-0.769
0.8795	0.1205	980.82	0.965	-0.232	0.3094	0.1512	941.13	1.043	-0.271
0.7731	0.2269	953.63	1.002	-0.407	0.3092	0.2417	928.05	1.080	-0.405
0.6866	0.3134	931.85	1.053	-0.528	0.309	0.3321	912.82	1.143	-0.512
0.5935	0.4065	909.94	1.127	-0.639	0.3087	0.4223	892.16	1.286	-0.539
0.4933	0.5067	889.72	1.254	-0.712	0.3094	0.5124	879.68	1.371	-0.624
0.3850	0.6150	871.16	1.431	-0.749	0.3081	0.6023	874.43	1.416	-0.748
0.2675	0.7325	849.44	1.705	-0.709	0.4380	0.1332	950.35	1.022	-0.245
0.1835	0.8165	836.88	2.285	-0.296	0.4525	0.2407	935.32	1.084	-0.384
0.0000	0.1009	933.77	1.051	-0.200	0.4521	0.3436	918.58	1.105	-0.557
0.0000	0.2017	920.41	1.086	-0.355	0.4517	0.4463	902.05	1.202	-0.654
0.0000	0.3022	904.59	1.160	-0.470	0.5761	0.0985	963.19	1.003	-0.184
0.0000	0.4025	892.85	1.246	-0.574	0.5756	0.1968	949.56	1.050	-0.322
0.0000	0.5026	879.80	1.369	-0.639	0.5400	0.2770	935.34	1.055	-0.472
0.0000	0.6025	867.83	1.524	-0.673	0.5395	0.3690	918.17	1.136	-0.565
0.0000	0.7022	852.77	1.732	-0.652	0.6674	0.0913	970.32	1.002	-0.162
0.0000	0.8016	839.15	2.023	-0.549	0.6669	0.1824	957.08	1.000	-0.336
0.0000	0.9009	824.98	2.370	-0.389	0.6663	0.2734	940.85	1.031	-0.477
0.1322	0.2109	932.43	1.065	-0.38	0.7575	0.0914	977.53	0.981	-0.174
0.1282	0.3215	907.95	1.157	-0.497	0.7571	0.1523	951.24	1.008	-0.262
0.1270	0.4256	895.54	1.264	-0.586	0.8364	0.0880	982.61	0.972	-0.169
0.1338	0.5186	881.74	1.363	-0.661					
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 323.15 K									
0.9538	0.0000	1002.40	0.845	0.002	0.0000	0.8016	831.15	1.610	-0.398
0.9081	0.0000	997.95	0.848	0.002	0.0000	0.9009	818.33	1.869	-0.273
0.8551	0.0000	993.17	0.857	0.005	0.0000	1.0000	804.22	2.276	0.000
0.7749	0.0000	985.13	0.861	0.003	0.1322	0.2109	924.05	0.922	-0.278
0.7182	0.0000	981.34	0.872	0.008	0.1282	0.3215	899.56	0.989	-0.361
0.6278	0.0000	974.24	0.879	0.007	0.1270	0.4256	886.83	1.071	-0.419
0.5302	0.0000	968.52	0.886	0.006	0.1338	0.5186	873.54	1.150	-0.465
0.4246	0.0000	961.76	0.901	0.011	0.1400	0.6385	857.33	1.290	-0.486
0.3099	0.0000	955.01	0.912	0.012	0.1445	0.7576	839.84	1.468	-0.468
0.8795	0.1205	971.57	0.843	-0.169	0.1143	0.8082	832.15	1.584	-0.422
0.7731	0.2269	943.38	0.869	-0.295	0.2508	0.1372	928.06	0.932	-0.159
0.6866	0.3134	921.84	0.907	-0.381	0.2506	0.2399	916.68	0.938	-0.29
0.5935	0.4065	900.90	0.964	-0.459	0.2503	0.3425	902.13	0.985	-0.382
0.4933	0.5067	880.42	1.056	-0.510	0.2501	0.4448	886.75	1.048	-0.457
0.3850	0.6150	864.56	1.196	-0.526	0.2499	0.5469	871.06	1.135	-0.508
0.2675	0.7325	841.13	1.403	-0.488	0.2496	0.6488	860.02	1.240	-0.54
0.1835	0.8165	829.74	1.699	-0.313	0.3094	0.1512	932.08	0.857	-0.247
0.0000	0.1009	925.31	0.917	-0.147	0.3092	0.2417	918.84	0.933	-0.293
0.0000	0.2017	912.27	0.939	-0.261	0.309	0.3321	904.39	0.986	-0.361
0.0000	0.3022	896.34	0.992	-0.344	0.3087	0.4223	883.40	1.081	-0.388
0.0000	0.4025	885.58	1.056	-0.414	0.3094	0.5124	872.23	1.170	-0.421
0.0000	0.5026	872.20	1.138	-0.467	0.3081	0.6023	865.84	1.178	-0.534
0.0000	0.6025	859.03	1.269	-0.471	0.4380	0.1332	942.45	0.896	-0.173
0.0000	0.7022	843.94	1.404	-0.470	0.4525	0.2407	926.25	0.941	-0.270

Table 2. Continued

x_1	x_2	$\rho/\text{kg}\cdot\text{m}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\Delta\eta/\text{mPa}\cdot\text{s}$	x_1	x_2	$\rho/\text{kg}\cdot\text{m}^{-3}$	$\eta/\text{mPa}\cdot\text{s}$	$\Delta\eta/\text{mPa}\cdot\text{s}$
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 323.15 K (Continued)									
0.4521	0.3436	910.16	0.949	-0.401	0.6674	0.0913	960.22	0.871	-0.121
0.4517	0.4463	892.79	1.018	-0.471	0.6669	0.1824	947.21	0.868	-0.246
0.5761	0.0985	955.30	0.891	-0.118	0.6663	0.2734	931.15	0.902	-0.335
0.5756	0.1968	940.48	0.895	-0.247	0.7575	0.0914	967.97	0.892	-0.091
0.5400	0.2770	923.90	0.914	-0.339	0.7571	0.1523	941.25	0.885	-0.181
0.5395	0.3690	908.15	0.957	-0.420	0.8364	0.0880	972.53	0.853	-0.119
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 333.15 K									
0.9538	0.0000	991.84	0.751	0.004	0.1400	0.6385	837.84	1.089	-0.330
0.9081	0.0000	986.57	0.750	0.000	0.1445	0.7576	831.93	1.213	-0.319
0.8551	0.0000	983.43	0.761	0.006	0.1143	0.8082	824.26	1.286	-0.296
0.7749	0.0000	974.75	0.763	0.002	0.2508	0.1372	919.59	0.817	-0.118
0.7182	0.0000	971.52	0.771	0.005	0.2506	0.2399	908.13	0.823	-0.210
0.6278	0.0000	964.37	0.779	0.005	0.2503	0.3425	892.97	0.854	-0.275
0.5302	0.0000	958.78	0.786	0.004	0.2501	0.4448	878.85	0.909	-0.318
0.4246	0.0000	953.15	0.798	0.008	0.2499	0.5469	863.21	0.964	-0.359
0.3099	0.0000	945.84	0.811	0.011	0.2496	0.6488	850.18	1.037	-0.383
0.8795	0.1205	958.09	0.742	-0.124	0.3094	0.1512	923.20	0.800	-0.143
0.7731	0.2269	933.31	0.763	-0.213	0.3092	0.2417	910.33	0.819	-0.210
0.6866	0.3134	911.92	0.792	-0.273	0.3090	0.3321	895.05	0.869	-0.246
0.5935	0.4065	890.93	0.839	-0.322	0.3087	0.4223	874.63	0.920	-0.28
0.4933	0.5067	869.91	0.903	-0.361	0.3094	0.5124	863.94	0.967	-0.318
0.3854	0.6150	856.26	1.012	-0.365	0.3081	0.6023	857.32	1.007	-0.364
0.2675	0.7325	833.54	1.160	-0.337	0.4380	0.1332	932.68	0.785	-0.131
0.1835	0.8165	821.17	1.289	-0.295	0.4525	0.2407	916.95	0.841	-0.175
0.0000	0.1009	916.93	0.812	-0.110	0.4521	0.3436	900.77	0.836	-0.278
0.0000	0.2017	905.29	0.826	-0.192	0.4517	0.4463	880.41	0.881	-0.330
0.0000	0.3022	887.96	0.861	-0.252	0.5761	0.0985	946.80	0.777	-0.094
0.0000	0.4025	876.93	0.908	-0.300	0.5756	0.1968	930.66	0.783	-0.182
0.0000	0.5026	864.04	0.971	-0.331	0.5400	0.2770	916.53	0.882	-0.162
0.0000	0.6025	849.87	1.044	-0.353	0.5395	0.3690	899.36	0.835	-0.295
0.0000	0.7022	837.74	1.157	-0.334	0.6674	0.0913	950.55	0.771	-0.086
0.0000	0.8016	823.68	1.310	-0.276	0.6669	0.1824	937.78	0.766	-0.177
0.0000	0.9009	810.66	1.423	-0.257	0.6663	0.2734	921.41	0.783	-0.247
0.1322	0.2109	915.63	0.812	-0.203	0.7575	0.0914	957.69	0.761	-0.088
0.1282	0.3215	891.12	0.856	-0.264	0.7571	0.1523	931.54	0.765	-0.142
0.1270	0.4256	879.69	0.909	-0.310	0.8364	0.0880	962.37	0.785	-0.054
0.1338	0.5186	865.10	0.962	-0.344					
1,4-Dioxane (1) + 1-Hexanol (2) + <i>N,N</i> -Dimethylaniline (3) at 343.15 K									
0.9538	0.0000	980.14	0.670	0.002	0.1400	0.6385	841.04	0.906	-0.252
0.9081	0.0000	977.83	0.674	0.004	0.1445	0.7576	823.85	1.004	-0.233
0.8551	0.0000	971.97	0.678	0.002	0.1143	0.8082	816.72	1.074	-0.200
0.7749	0.0000	964.44	0.683	0.004	0.2508	0.1372	910.66	0.722	-0.091
0.7182	0.0000	962.15	0.689	0.002	0.2506	0.2399	900.68	0.726	-0.157
0.6278	0.0000	954.22	0.711	0.017	0.2503	0.3425	884.77	0.745	-0.206
0.5302	0.0000	948.37	0.710	0.009	0.2501	0.4448	869.74	0.782	-0.238
0.4246	0.0000	944.04	0.716	0.007	0.2499	0.5469	854.62	0.830	-0.258
0.3099	0.0000	936.89	0.725	0.008	0.2496	0.6488	842.56	0.932	-0.225
0.8795	0.1205	947.05	0.662	-0.093	0.3094	0.1512	914.54	0.712	-0.107
0.7731	0.2269	923.91	0.678	-0.157	0.3092	0.2417	901.22	0.798	-0.081
0.6866	0.3134	965.08	0.748	-0.151	0.3090	0.3321	886.64	0.775	-0.165
0.5935	0.4065	881.04	0.732	-0.237	0.3087	0.4223	866.08	0.800	-0.201
0.4933	0.5067	862.93	0.786	-0.257	0.3094	0.5124	855.16	0.839	-0.222
0.3853	0.6152	843.77	0.863	-0.261	0.3081	0.6023	848.54	0.858	-0.264
0.2675	0.7325	824.52	0.975	-0.236	0.4380	0.1332	924.11	0.707	-0.090
0.1835	0.8165	815.14	1.074	-0.200	0.4525	0.2407	906.70	0.715	-0.153
0.0000	0.1009	969.05	0.774	-0.034	0.4521	0.3436	891.55	0.734	-0.203
0.0000	0.2017	895.76	0.731	-0.145	0.4517	0.4463	874.98	0.772	-0.234
0.0000	0.3022	880.00	0.737	-0.206	0.5761	0.0985	936.93	0.693	-0.071
0.0000	0.4025	867.83	0.790	-0.220	0.5756	0.1968	920.91	0.693	-0.136
0.0000	0.5026	854.24	0.830	-0.248	0.5400	0.2770	905.10	0.715	-0.171
0.0000	0.6025	842.51	0.902	-0.243	0.5395	0.3690	891.34	0.770	-0.178
0.0000	0.7022	829.06	0.973	-0.238	0.6674	0.0913	939.37	0.688	-0.064
0.0000	0.8016	813.99	1.080	-0.198	0.6669	0.1824	928.42	0.690	-0.123
0.0000	0.9009	803.44	1.218	-0.126	0.6663	0.2734	911.87	0.751	-0.123
0.1322	0.2109	906.96	0.723	-0.149	0.7575	0.0914	946.73	0.688	-0.057
0.1282	0.3215	882.53	0.752	-0.195	0.7571	0.1523	920.08	0.684	-0.102
0.1270	0.4256	870.61	0.790	-0.227	0.8364	0.0880	952.19	0.676	-0.061
0.1338	0.5186	856.87	0.837	-0.241					

Apparatus and Procedures. Densities were measured by an Anton Paar DMA-58 vibrating tube density meter. The density meter was calibrated with deionized doubly distilled water and dry air. Ubbelohde viscosimeters (Scott) of relatively long flow

times [(60 to 600) s, with water] were used to minimize the kinetic energy corrections. For each specified composition, five readings were taken for the flow time with variations not exceeding ± 0.01 s. The viscosities of all mixtures were

Table 3. Coefficients of the Redlich–Kister Equation (2), (A_p), and σ (Standard Deviations) for Deviation Viscosity of Binary Systems at (283.15 to 343.15) K

T	A_0	A_1	A_2	A_3	σ
K	(mPa·s)	(mPa·s)	(mPa·s)	(mPa·s)	(mPa·s)
1,4-Dioxane + <i>N,N</i> -Dimethylaniline					
283.15	0.001	-0.132	0.114	-0.099	0.005
293.15	0.04	-0.3	-0.1	0.3	0.01
303.15	0.003	-0.1	0.05	0.2	0.003
313.15	0.024	0.03	-0.04	0	0.003
323.15	0.033	-0.03	0.07	-0.04	0.002
333.15	0.023	-0.04	0.09	-0.02	0.002
343.15	0.04	0.01	-0.1	-0.0	0.003
1,4-Dioxane + 1-Hexanol					
283.15	-8.99	5.09	-2.17	-0.73	0.04
293.15	-5.95	3.4	-2.4	0.3	0.03
303.15	-4.12	2.5	-0.7	-2.8	0.02
313.15	-3.0	1.8	1.2	-4	0.07
323.15	-2.08	0.9	0.4	-1.2	0.02
333.15	-1.42	0.47	-0.38	0.3	0.005
343.15	-0.99	0.5	-0.2	-0.4	0.02
1-Hexanol + <i>N,N</i> -Dimethylaniline					
283.15	-7.69	-3.68	-2.52	-1.23	0.04
293.15	-5.25	-2.3	-1.8	-0.8	0.03
303.15	-3.62	-1.6	-1.3	-0.4	0.01
313.15	-2.54	-1.0	-1.0	-0.4	0.01
323.15	-1.83	-0.7	-0.7	-0.3	0.008
333.15	-1.30	-0.3	-0.8	-0.9	0.02
343.15	-0.99	-0.1	-0.1	-0.8	0.02

calculated from the average flow time, whereas the viscosimeter constants were determined by using values from Marsh²⁰ for the water viscosity together with the corresponding flow times measured by the means of this viscosimeter. The uncertainty of the density and viscosity measurements was $3 \cdot 10^{-4}$ g·cm⁻³ and ± 0.003 mPa·s. The viscosimeter was held in a water bath Heidolph whose temperature was controlled to within ± 0.01 K. Finally, all binary and ternary mixtures were prepared in all cases by mass using a Mettler H20T balance. The mass measurements were accurate to ± 0.01 mg. The precision of all mole fractions is estimated to be better than $\pm 2 \cdot 10^{-4}$. The details of the methods and techniques of the measurements have been described earlier.^{31–35} Data processing and curve fitting were performed by DataFit ver. 8.1.69 (Oakdale Engineering).³⁶

Results and Discussion

Table 1 presents density, ρ , and dynamic viscosity, η , data of pure components 1,4-dioxane, 1-hexanol, and *N,N*-dimethylaniline, which are compared with values found in the literature. Table 2 presents densities, viscosities, and viscosity deviations, $\Delta\eta$, for the binary and ternary mixtures of 1,4-dioxane + 1-hexanol + *N,N*-dimethylaniline at seven temperatures between (283.15 and 343.15) K over the full range of mole fractions. The viscosity deviations, $\Delta\eta$, for binary and ternary mixtures were calculated according to the following equations

$$\Delta\eta/(mPa\cdot s) = \eta - \sum_{i=1}^n x_i \eta_i \quad (1)$$

where η is the absolute viscosity of the mixture; η_i is the absolute and dynamic viscosity of pure component i ; x_i is the mole fraction in component i ; and n is the number of

Table 4. Adjustable Parameters (G_{12}) of Equation 3 and σ (Standard Deviations) for Binary Mixtures of 1,4-Dioxane + 1-Hexanol, 1-Hexanol + *N,N*-Dimethylaniline, and 1,4-Dioxane + *N,N*-Dimethylaniline

T	G_{12}	σ
K	(mPa·s)	(mPa·s)
1,4-Dioxane + 1-Hexanol		
283.15	1.63	0.04
293.15	1.54	0.04
303.15	1.20	0.06
313.15	1.04	0.09
323.15	0.88	0.04
333.15	0.73	0.01
343.15	0.75	0.02
1-Hexanol + <i>N,N</i> -Dimethylaniline		
283.15	1.22	0.04
293.15	1.21	0.07
303.15	0.93	0.01
313.15	1.01	0.08
323.15	0.87	0.01
333.15	0.97	0.04
343.15	1.13	0.02
1,4-Dioxane + <i>N,N</i> -Dimethylaniline		
283.15	0.01	0.01
293.15	0.04	0.02
303.15	-0.13	0.003
313.15	-0.21	0.008
323.15	-0.09	0.007
333.15	0.07	0.01
343.15	0.09	0.02

components in the mixture. The viscosity deviations for binary mixtures were fitted to a Redlich–Kister equation²¹

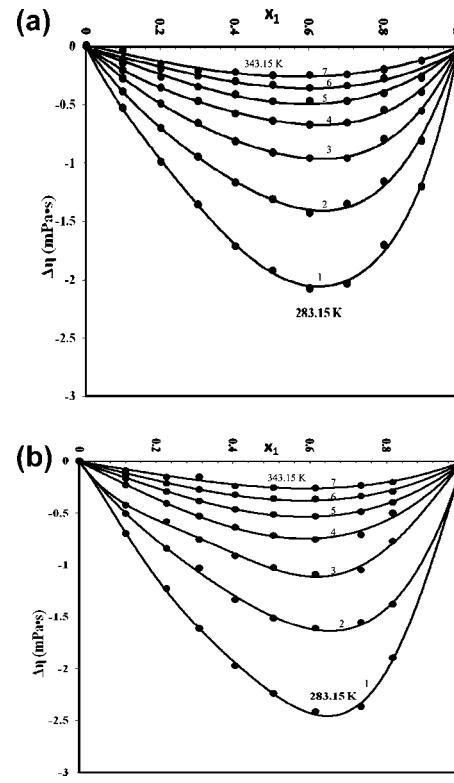
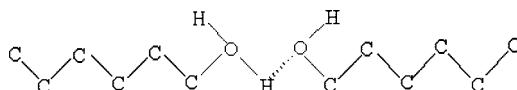
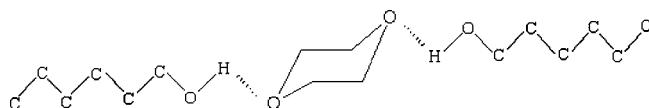


Figure 1. (a) Viscosity deviations $\Delta\eta$ (mPa·s) for the binary mixtures 1-hexanol (x_1) + *N,N*-dimethylaniline (x_1) at: 1, 283.15 K; 2, 293.15 K; 3, 303.15 K; 4, 313.15 K; 5, 323.15 K; 6, 333.15 K; 7, 343.15 K. (b) Viscosity deviations $\Delta\eta$ (mPa·s) for the binary mixtures 1,4-dioxane (x_1) + 1-hexanol (x_1) at: 1, 283.15 K; 2, 293.15 K; 3, 303.15 K; 4, 313.15 K; 5, 323.15 K; 6, 333.15 K; 7, 343.15 K.

Table 5. Coefficients of the Cibulka Equation (4), Singh Equation (5), and Nagata Equation (6), B_P , and σ (Standard Deviations) for Deviation Viscosity of the Ternary System 1,4-Dioxane (1) + 1-Hexanol (2) + *N,N*-Dimethylaniline (3) at (283.15 to 343.15) K

	B_1 (mPa·s)	B_2 (mPa·s)	B_3 (mPa·s)	σ (mPa·s)
<i>T</i> = 283.15 K				
Cibulka	2.3	55	-39	0.09
Singh	7.8	-0.18	0.24	0.19
Nagata	7.8	-	-	0.19
<i>T</i> = 293.15 K				
Cibulka	1.31	38	-26	0.08
Singh	5.5	-0.1	0.2	0.11
Nagata	5.5	-	-	0.11
<i>T</i> = 303.15 K				
Cibulka	0.2	23	-13.9	0.03
Singh	3.4	-0.06	0.1	0.13
Nagata	3.4	-	-	0.13
<i>T</i> = 313.15 K				
Cibulka	2.7	8.9	-10.5	0.06
Singh	2.2	-0.06	0.01	0.09
Nagata	2.2	-	-	0.09
<i>T</i> = 323.15 K				
Cibulka	-0.15	9	-4.5	0.07
Singh	1.5	0.0	0.1	0.1
Nagata	1.6	-	-	0.1
<i>T</i> = 333.15 K				
Cibulka	-0.75	8.52	-2.5	0.08
Singh	1.28	0.0	0.06	0.12
Nagata	1.30	-	-	0.12
<i>T</i> = 343.15 K				
Cibulka	0.50	4.68	-3.5	0.09
Singh	0.9	0.0	0.07	0.14
Nagata	0.9	-	-	0.14

Scheme 1**Scheme 2**

$$Y_{ij}^E = x_i x_j \sum_{P=0}^P A_P (x_i - x_j)^P \quad (2)$$

where Y_{ij}^E is $\Delta\eta$ and A_P are adjustable parameters. Table 3 lists the A_P coefficients and the standard deviations of $\Delta\eta$ for the binary mixtures 1,4-dioxane + 1-hexanol, 1-hexanol + *N,N*-dimethylaniline, and 1,4-dioxane + *N,N*-dimethylaniline at seven temperatures from (298.15 to 343.15) K. The viscosity deviations for 1,4-dioxane + 1-hexanol and 1-hexanol + *N,N*-dimethylaniline mixtures are plotted in Figure 1a and b, respectively. The Grunberg and Nissan interaction model¹⁵ that has been used to correlate the dynamic viscosity of binary mixtures with mole fractions used is

$$\eta = \exp(x_1 \ln \eta_1 + x_2 \ln \eta_2 + x_1 x_2 G_{12}) \quad (3)$$

where G_{12} is a parameter proportional to the interchange energy. The standard deviation and adjustable parameter of this equation for 1-hexanol + 1,4-dioxane, 1-hexanol + *N,N*-dimethylaniline, and 1,4-dioxane + *N,N*-dimethylaniline are given in Table 4.

The viscosity deviations for the ternary mixtures have been fitted to the Cibulka,⁴ Singh,⁵ and Nagata and Sakura⁶ equations.

The Cibulka,⁴ Singh,⁵ and Nagata and Sakura⁶ equations are shown in equations 4, 5, and 6, respectively.

Cibulka equation:⁴

$$Y^E = Y_{12}^E + Y_{13}^E + Y_{23}^E = x_1 x_2 x_3 (B_1 + B_2 x_1 + B_3 x_2) \quad (4)$$

Singh equation:⁵

$$Y^E = Y_{12}^E + Y_{13}^E + Y_{23}^E + B_1 x_1 x_2 x_3 + B_2 x_1 (x_2 - x_3) + B_3 x_1^2 (x_2 - x_3)^2 \quad (5)$$

Nagata and Sakura equation:⁶

$$Y^E = Y_{12}^E + Y_{13}^E + Y_{23}^E + B_1 x_1 x_2 x_3 \quad (6)$$

where in all equations B_1 , B_2 , and B_3 are fitting parameters.

The fitted parameters and standard deviations obtained by the least-squares method are given in Table 5. The standard deviations for the Cibulka equation were better than the Nagata and Singh equations. The viscosity of a mixture according to Kauzman and Eyring²² strongly depends on the entropy of the mixture, which is related to the liquid's structure and bond enthalpy and consequently with molecular interactions between the components of the mixture. So, the viscosity deviations are a function of molecular interactions and the size and shape of molecules. Hence, it has been pointed out in the literature that the value of viscosity deviations of multicomponent systems can constitute a reliable criterion for assessing or for excluding the presence of interactions of any kind between dissimilar molecules.^{23–30} Therefore, the magnitude of these deviations from ideality of the system that can be negative, positive, or zero may be explained as a balance between positive contributions (hydrogen bond rupture and dispersive interactions between unlike molecules) and negative contributions (intermolecular dipolar interactions and geometrical fitting between components).

The magnitude of $\Delta\eta$ for binary systems in this investigation follows the order 1-hexanol + 1,4-dioxane > 1-hexanol + *N,N*-dimethylaniline > 1,4-dioxane + *N,N*-dimethylaniline. In the 1-hexanol + 1,4-dioxane binary system, because of the presence of two donor sites in 1,4-dioxane, there must be a hydrogen bond formation between dioxane and hexanol which results in positive deviations of viscosity (Scheme 1). Negative deviations for viscosity show the geometry effects of molecules.

Two molecules, at least, are attached by a hydrogen bond in pure 1-hexanol. This makes the solute more viscous, and sharing of two parallel plates of molecules gets harder (Scheme 1).

However, in the binary mixtures of 1,4-dioxane and 1-hexanol in spite of a longer chain and strong solute–solvent interaction, we have a negative deviation for viscosity, and this must be caused by the geometry of the chains (Scheme 2).

In the two systems containing the 1-hexanol maximum deviation from lineal behavior of viscosity is the coordinate at $x_{1\text{-hexanol}} = 0.65$, so the mole fraction of 1-hexanol is higher than the other compound. For all systems, by increasing the temperature, the magnitude of $\Delta\eta$ decreases. The negative values observed for $\Delta\eta$ of those two binary mixtures correspond to a system containing an associated component.²⁶

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