Analysis of Surface Tension, Density, and Speed of Sound for the Ternary Mixture Dimethyl Carbonate + *p*-Xylene + *n*-Octane

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Surface tension at $T = 298.15$ K and atmospheric pressure has been measured for the ternary mixture dimethyl carbonate + *p*-xylene + *n*-octane. In addition, density and speed of sound at $T = (288.15$ to $308.15)$ K have also been measured for the same mixture. Excess molar volumes, excess isentropic compressibilities, and surface tension deviations were computed from experimental data and correlated with the Cibulka equation. The excess molar volumes were compared with predictions from the Nitta et al. model.

Introduction

In the last several years, investigations with the objective of finding new lubricants that are compatible with the alternative refrigerating agents, CFCs (chlorofluorocarbons) and HCFCs (hydrochlorofluorocarbons), have been carried out.[1−3]

The objective of this work deals with the necessity of having thermophysical data of mixtures that contain alternative refrigerants and lubricants that are required for the industries of refrigeration and of air conditioning and the manufacturers of lubricants. Among the three proposed groups of alternative lubricants, PAGs, POEs, and carbonates,[4] the last ones, carbonates, have been studied the least. Because of that, our group has realized a theoretical and experimental study about the thermophysical properties of mixtures containing carbonate molecules and alkyl benzene that confer good lubricant properties to the mixture and where the alkylic chain contributes to the thermal stability.

Thermophysical properties of binary mixtures containing dimethyl carbonate, *p*-xylene, and *n*-octane have been previously studied,[5−8] but the bibliography does not report ternary data for this kind of mixtures. In particular, this work reports experimental measurements of density and speed of sound for the ternary mixture dimethyl carbonate + *p*-xylene + *n*-octane at (288.15, 293.15, 298.15, 303.15, and 308.15) K and atmospheric pressure and at surface tension at 298.15 K. From experimental data, excess molar volumes, excess isentropic compressibilities, and surface tension deviation were computed. The Nagata and Tamura[9] equation was used to correlate the ternary contribution to the experimental excess molar volume and excess isentropic compressibility results. The Cibulka[10] equation was used to correlate the experimental surface tension deviation. Also, the group contribution model proposed by Nitta et al.[11] has been applied to estimate excess molar volumes.

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Experimental Section

The substances employed were supplied by Fluka and were kept under an argon (N-55) atmosphere. Analysis by gas−liquid chromatography using a Hewlett-Packard HP-6890 Series GC System chromatograph showed that the solvents had purities that conformed to supplier specifications. Their purities were > 99.0 % for dimethyl carbonate, > 99.0 % for *p*-xylene, and > 99.5 % for *n*-octane. Chromatograph operation conditions and chromatograms of pure compounds are gathered in Tables S1 and S2 in the Supporting Information, respectively. The substances were degassed and dried over molecular sieves (Sigma, 0.4 nm). Densities, speeds of sound, and surface tensions of the pure liquids show good agreement with values found in literature, as shown in Table 1, where most of the listed literature values agree with the those measured in this work within the experimental uncertainty.

Mixtures were prepared by mass using a Mettler AE-240 balance with an accuracy of $\pm\ 5 \cdot 10^{-5}$ g, which lead to an estimated uncertainty in mole fraction of $\pm\ 10^{-4}$. Samples were prepared in small stoppered bottles, and liquids were weighed in increasing order of volatility with the objective of avoiding losses by evaporation during manipulation and possible errors in mole fractions calculations.

Density (ρ) and speed of sound (u) of the pure liquids and mixtures were measured with an Anton-Paar DSA-48 densimeter and sound analyzer, respectively. The apparatus was automatically thermostatted at $\pm$ 0.02 K with an estimated uncertainty of $\pm\ 5 \cdot 10^{-5}$ g·m^{-3} and $\pm$ 0.5 m·s^{-1} for density and speed of sound measurements, respectively. The calibration was periodically performed using air and double-distilled Millipore-quality water. Further information about the experimental technique for density and speed of sound measurements has been provided in a previous work.[12]

Surface tension (σ) was measured using a Lauda TVT2 automated tensiometer with a precision of 10^{-2} mN·m^{-1} on the basis of the principle of the drop volume. This technique consists of measuring the volume of a drop detaching from a capillar with a circular cross section. The surface tension can be determined as follows

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Table 1. Comparison of Measured Densities (ρ), Speeds of Sound (u), and Surface Tensions (σ) of Pure Components with Literature Values and Molar Heat Capacity (C_p) Literature Values

	ρ / kg·m^{-3}		u / m·s^{-1}		σ / mN·m^{-1}		α / kK^{-1}	C_p / J·mol^{-1}·K^{-1}
component	exptl	lit.	exptl	lit.	exptl	lit.	exptl	lit.
				288.15 K				
dimethyl carbonate	1076.64	1076.56[a] 1076.46[b]	1240.7	1240.5[d]			1.220	164.3[f]
p-xylene	865.20		1350.7				0.996	178.6[f]
n-octane	706.58	706.5[c] 706.6[e]	1213.6	1213[c] 1214[e]			1.142	250.8[f]
				293.15 K				
dimethyl carbonate	1070.01	1070.02[a]	1218.1				1.236	164.6[f]
p-xylene	860.90	860.98[g] 861.41[h]	1329.6				1.001	178.6[f]
n-octane	702.57	702.56[i] 702.5[c]	1192.9.	1193[c]			1.151	250.8[f]
				298.15 K				
dimethyl carbonate	1063.39	1063.42[a] 1063.38[b]	1195.1	1197.06[a]	28.08	28.54[m]	1.248	165.4[f]
p-xylene	856.58	856.61[g] 856.5[j]	1308.4		27.43	28.00[g] 27.76[g]	1.014	181.9[f]
n-octane	698.55	698.62[g] 698.5[k]	1171.9	1172[l]	20.99	21.14[m] 21.18[g]	1.148	255.1[f]
				303.15 K				
dimethyl carbonate	1056.78	1056.6[n]	1173.2				1.259	165.3[f]
p-xylene	852.21	852.25[g] 852.2[j]	1287.4				1.027	183.6[f]
n-octane	694.48	694.5[o] 694.45[p]	1150.9	1151.6[o] 1156[q]			1.160	257.3[f]
				308.15 K				
dimethyl carbonate	1050.15	1050.11[a] 1050.04[b]	1151.5				1.273	166.7[f]
p-xylene	847.83	847.9[j]	1266.4				1.029	185.4[f]
n-octane	690.42	690.2[q] 690.4[o]	1130.3	1137[q] 1132.9[o]			1.185	259.5[f]

[a] Ref 15. [b] Ref 16. [c] Ref 17. [d] Ref 18. [e] Ref 19. [f] Ref 20. [g] Ref 21. [h] Ref 6. [i] Ref 22. [j] Ref 23. [k] Ref 24. [l] Ref 25. [m] Ref 26. [n] Ref 27. [o] Ref 28. [p] Ref 29. [q] Ref 30.

$$\sigma = \Delta\rho g V/2\pi r_{cap} f(r_{cap}/a) \quad (1)$$

$$a = (2\sigma/\Delta\rho g)^{1/2} \quad (2)$$

Where $\Delta\rho$ is the density difference between liquid and vapor phases, g is the gravitational acceleration, V is the drop volume, $2r_{cap}$ is the outer diameter of the capillary, and f is a correction function.

Results and Discussion

The density and speed of sound for the ternary mixture dimethyl carbonate + *p*-xylene + *n*-octane are reported in Table 2at the previously cited temperatures. In Table 3, surface tensions at 298.15 K are listed.

Excess molar volume (V_m^E) was calculated with the following equation

$$V_m^E = V - \sum_{i=1}^{n} x_i M_i/\rho_i \quad (3)$$

where V/m^3·mol^{-1} is the molar volume, x_i, M_i, and ρ_i stand for the mole fraction, molar mass, and density of component i, respectively, and n is the number of components in the mixture.

Excess isentropic compressibility (κ_s^E) was evaluated as follows

$$\kappa_s^E = \kappa_s - \sum_{i=1}^{n} \phi_i(\kappa_{s,i} + TV_i\alpha_i^2/C_{p,i}) - T(\sum_{i=1}^{n} x_i V_i)(\sum_{i=1}^{n} \phi_i\alpha_i)^2/\sum_{i=1}^{n} x_i C_{p,i} \quad (4)$$

where κ_s/TPa^{-1} is the isentropic compressibility, n represents the number of components of the mixture, T is the temperature, and ϕ_i, x_i, $\kappa_{s,i}$, V_i, α_i, and $C_{p,i}$ are the volume fraction, mole fraction, isentropic compressibility, molar volume, cubic expansion coefficient, and molar heat capacity of component i, respectively. The values of α_i were calculated from the densities, and the literature $C_{p,i}$ values are reported in Table 1.

Surface tension deviation ($\Delta\sigma$) for the ternary mixtures was calculated by

$$\Delta\sigma = \sigma - \sum_{i=1}^{n} x_i\sigma_i \quad (5)$$

where σ/mN·m^{-1} is the surface tension of the mixture, σ_i is the surface tension of the component i, x_i is the mole fraction of the component i, and n is the number of components.

The estimated uncertainties, calculated analytically through the usual error propagation procedures, are $\pm 6\cdot10^{-9}$ m^3·mol^{-1} for V_m^E, 3 TPa^{-1} for κ_s^E, and 10^{-3} mN·m^{-1} for $\Delta\sigma$.

The ternary mixture derived properties were correlated using the equation

Table 2. Experimental Densities (ρ) and Speeds of Sound (u) for the Ternary Mixture Dimethyl Carbonate (1) + *p*-Xylene (2) + *n*-Octane (3) at Several Temperatures

x_1	x_2	ρ / kg·m^{-3}	u / m·s^{-1}	κ_s / TPa^{-1}	x_1	x_2	ρ / kg·m^{-3}	u / m·s^{-1}	κ_s / TPa^{-1}
				288.15 K					
0.06081	0.05129	723.60	1211.0	942	0.29132	0.39932	838.48	1245.0	769
0.04973	0.89958	861.30	1334.6	652	0.29266	0.50988	862.60	1267.4	722
0.10216	0.10109	738.40	1211.3	923	0.30192	0.59676	886.06	1288.2	680
0.09786	0.19949	751.55	1222.0	891	0.39734	0.10070	812.24	1194.6	863
0.10026	0.29971	767.32	1233.7	856	0.39369	0.19889	830.80	1210.6	821
0.10026	0.41495	785.83	1248.8	816	0.39900	0.30273	854.71	1230.1	773
0.09971	0.50716	801.40	1262.5	783	0.39507	0.40680	877.07	1252.0	727
0.10087	0.59211	817.02	1276.2	752	0.39324	0.50640	900.75	1276.1	682
0.10239	0.69438	836.95	1294.9	713	0.50935	0.09941	848.79	1194.5	826
0.10091	0.79753	857.42	1316.1	673	0.49467	0.19701	865.68	1213.0	785
0.19282	0.10115	757.99	1203.4	911	0.49025	0.30598	890.24	1236.9	734
0.19442	0.20125	774.32	1215.5	874	0.49958	0.40132	919.19	1262.2	683
0.19531	0.29965	791.10	1229.1	837	0.60641	0.09811	885.76	1198.3	786
0.21669	0.34533	805.12	1235.5	814	0.59792	0.20059	908.86	1221.7	737
0.20371	0.48837	828.29	1259.3	761	0.60211	0.29997	938.82	1249.2	683
0.19708	0.60273	849.24	1281.2	717	0.69358	0.10267	925.72	1207.5	741
0.19310	0.70599	870.16	1303.4	676	0.70387	0.19624	959.15	1235.7	683
0.29518	0.09655	782.56	1197.0	892	0.79674	0.10144	979.38	1223.7	682
0.29742	0.19789	801.15	1211.2	851	0.89452	0.05327	1022.72	1230.7	642
0.29716	0.29797	820.06	1227.1	810					
				293.15 K					
0.06081	0.05129	719.42	1190.6	981	0.29132	0.39932	833.75	1224.3	800
0.04973	0.89958	856.89	1314.2	676	0.29266	0.50988	857.82	1246.7	750
0.10216	0.10109	734.14	1190.8	961	0.30192	0.59676	881.24	1267.5	706
0.09786	0.19949	747.26	1201.5	927	0.39734	0.10070	807.36	1173.8	899
0.10026	0.29971	763.00	1213.3	890	0.39369	0.19889	825.89	1189.9	855
0.10026	0.41495	781.47	1228.4	848	0.39900	0.30273	849.76	1209.4	805
0.09971	0.50716	797.00	1242.1	813	0.39507	0.40680	872.10	1231.3	756
0.10087	0.59211	812.59	1255.8	780	0.39324	0.50640	895.75	1255.2	709
0.10239	0.69438	832.49	1274.5	739	0.50935	0.09941	843.63	1173.6	861
0.10091	0.79753	852.94	1295.7	698	0.49467	0.19701	860.54	1192.2	818
0.19282	0.10115	753.55	1182.8	949	0.49025	0.30598	885.08	1216.0	764
0.19442	0.20125	769.85	1195.0	910	0.49958	0.40132	913.98	1241.2	710
0.19531	0.29965	786.60	1208.6	870	0.60641	0.09811	880.37	1177.4	819
0.21669	0.34533	800.56	1214.9	846	0.59792	0.20059	903.46	1200.7	768
0.20371	0.48837	823.70	1238.8	791	0.60211	0.29997	933.39	1228.2	710
0.19708	0.60273	844.63	1260.7	745	0.69358	0.10267	920.09	1186.3	772
0.19310	0.70599	865.52	1282.8	702	0.70387	0.19624	953.48	1214.6	711
0.29518	0.09655	777.90	1176.3	929	0.79674	0.10144	973.49	1202.5	710
0.29742	0.19789	796.46	1190.5	886	0.89452	0.05327	1016.54	1209.3	673
0.29716	0.29797	815.34	1206.4	843					
				298.15 K					
0.06081	0.05129	715.25	1169.6	1022	0.29132	0.39932	829.00	1203.2	833
0.04973	0.89958	852.47	1293.2	701	0.29266	0.50988	853.03	1225.5	781
0.10216	0.10109	729.87	1169.7	1001	0.30192	0.59676	876.40	1246.2	735
0.09786	0.19949	742.97	1180.6	966	0.39734	0.10070	802.46	1152.5	938
0.10026	0.29971	758.67	1192.4	927	0.39369	0.19889	820.98	1168.6	892
0.10026	0.41495	777.10	1207.5	883	0.39900	0.30273	844.80	1188.1	839
0.09971	0.50716	792.61	1221.1	846	0.39507	0.40680	867.12	1210.0	788
0.10087	0.59211	808.17	1234.9	811	0.39324	0.50640	890.74	1233.8	738
0.10239	0.69438	828.04	1253.6	769	0.50935	0.09941	838.47	1152.2	898
0.10091	0.79753	848.45	1274.7	725	0.49467	0.19701	855.38	1170.8	853
0.19282	0.10115	749.10	1161.7	989	0.49025	0.30598	879.90	1194.6	796
0.19442	0.20125	765.36	1173.9	948	0.49958	0.40132	908.75	1219.7	740
0.19531	0.29965	782.09	1187.5	907	0.60641	0.09811	874.95	1155.9	855
0.21669	0.34533	795.99	1193.9	881	0.59792	0.20059	898.05	1179.3	801
0.20371	0.48837	819.10	1217.8	823	0.60211	0.29997	927.93	1206.5	740
0.19708	0.60273	840.02	1239.6	775	0.69358	0.10267	914.45	1164.8	806
0.19310	0.70599	860.88	1261.7	730	0.70387	0.19624	947.78	1192.9	741
0.29518	0.09655	773.24	1155.0	969	0.79674	0.10144	967.55	1180.8	741
0.29742	0.19789	791.77	1169.4	924	0.89452	0.05327	1010.31	1187.4	702
0.29716	0.29797	810.61	1185.3	878					

Table 2 Continued

x_1	x_2	ρ / kg·m^{-3}	u / m·s^{-1}	κ_s / TPa^{-1}	x_1	x_2	ρ / kg·m^{-3}	u / m·s^{-1}	κ_s / TPa^{-1}
				303.15 K					
0.06081	0.05129	711.00	1148.7	1066	0.29132	0.39932	824.20	1182.2	868
0.04973	0.89958	848.02	1272.3	728	0.29266	0.50988	848.18	1204.3	813
0.10216	0.10109	725.53	1148.9	1044	0.30192	0.59676	871.52	1225.0	765
0.09786	0.19949	738.61	1159.7	1007	0.39734	0.10070	797.52	1131.2	980
0.10026	0.29971	754.28	1171.5	966	0.39369	0.19889	816.01	1147.4	931
0.10026	0.41495	772.67	1186.7	919	0.39900	0.30273	839.79	1166.9	875
0.09971	0.50716	788.16	1200.4	880	0.39507	0.40680	862.09	1188.8	821
0.10087	0.59211	803.70	1214.1	844	0.39324	0.50640	885.69	1212.5	768
0.10239	0.69438	823.54	1232.7	799	0.50935	0.09941	833.26	1130.9	938
0.10091	0.79753	843.92	1253.8	754	0.49467	0.19701	850.19	1149.5	890
0.19282	0.10115	744.59	1140.7	1032	0.49025	0.30598	874.69	1173.3	831
0.19442	0.20125	760.82	1153.0	989	0.49958	0.40132	903.48	1198.4	771
0.19531	0.29965	777.51	1166.6	945	0.60641	0.09811	869.50	1134.5	894
0.21669	0.34533	791.34	1172.9	919	0.59792	0.20059	892.60	1157.8	836
0.20371	0.48837	814.46	1196.9	857	0.60211	0.29997	922.44	1185.1	772
0.19708	0.60273	835.36	1218.6	806	0.69358	0.10267	908.77	1143.4	842
0.19310	0.70599	856.21	1240.7	759	0.70387	0.19624	942.05	1171.4	774
0.29518	0.09655	768.52	1133.9	1012	0.79674	0.10144	961.58	1159.2	774
0.29742	0.19789	787.01	1148.2	964	0.89452	0.05327	1004.05	1165.7	733
0.29716	0.29797	805.82	1164.2	916					
				308.15 K					
0.06081	0.05129	706.91	1127.9	1112	0.29132	0.39932	819.50	1161.1	905
0.04973	0.89958	843.67	1251.5	757	0.29266	0.50988	843.46	1183.4	847
0.10216	0.10109	721.34	1128.0	1090	0.30192	0.59676	866.74	1204.0	796
0.09786	0.19949	734.39	1138.9	1050	0.39734	0.10070	792.69	1110.0	1024
0.10026	0.29971	750.02	1150.7	1007	0.39369	0.19889	811.15	1126.3	972
0.10026	0.41495	768.37	1165.9	957	0.39900	0.30273	834.88	1145.7	912
0.09971	0.50716	783.84	1179.6	917	0.39507	0.40680	857.15	1167.7	856
0.10087	0.59211	799.34	1193.4	878	0.39324	0.50640	880.71	1191.3	800
0.10239	0.69438	819.14	1212.0	831	0.50935	0.09941	828.13	1109.6	981
0.10091	0.79753	839.49	1232.9	784	0.49467	0.19701	845.07	1128.2	930
0.19282	0.10115	740.21	1119.7	1077	0.49025	0.30598	869.54	1152.1	866
0.19442	0.20125	756.40	1132.0	1032	0.49958	0.40132	898.28	1177.1	803
0.19531	0.29965	773.06	1145.7	986	0.60641	0.09811	864.13	1113.2	934
0.21669	0.34533	786.83	1152.0	958	0.59792	0.20059	887.21	1136.5	873
0.20371	0.48837	809.91	1175.9	893	0.60211	0.29997	917.00	1163.7	805
0.19708	0.60273	830.81	1197.7	839	0.69358	0.10267	903.16	1122.0	880
0.19310	0.70599	851.62	1219.7	789	0.70387	0.19624	936.37	1149.9	808
0.29518	0.09655	763.92	1112.8	1057	0.79674	0.10144	955.64	1137.6	809
0.29742	0.19789	782.38	1127.2	1006	0.89452	0.05327	997.79	1144.0	766
0.29716	0.29797	801.16	1143.1	955					

Table 3. Experimental Surface Tensions (σ) for the Ternary Mixture Dimethyl Carbonate (1) + *p*-Xylene (2) + *n*-Octane (3) at 298.15 K

x_1	x_2	σ / mN·m^{-1}	x_1	x_2	σ / mN·m^{-1}	x_1	x_2	σ / mN·m^{-1}
0.04868	0.04947	21.07	0.19108	0.41338	23.04	0.39936	0.39406	23.99
0.05586	0.88962	26.52	0.19619	0.49536	23.64	0.43295	0.47381	25.39
0.09269	0.10329	21.31	0.19663	0.60143	24.56	0.49699	0.09846	21.97
0.09518	0.19771	21.71	0.19354	0.7067	25.67	0.49401	0.19785	22.63
0.10059	0.28393	22.11	0.29371	0.09794	21.62	0.49797	0.29962	23.67
0.09549	0.40025	22.73	0.28901	0.20129	22.11	0.49624	0.40272	25.06
0.09803	0.49404	23.31	0.29914	0.29199	22.66	0.58898	0.10018	22.22
0.10041	0.60555	24.08	0.30965	0.39328	23.44	0.60089	0.19465	23.23
0.09932	0.69979	24.84	0.29583	0.49630	24.25	0.60114	0.29883	24.85
0.09602	0.80411	25.92	0.30129	0.59781	25.52	0.69914	0.09767	22.85
0.19314	0.09851	21.44	0.40899	0.10150	21.75	0.70245	0.19802	24.63
0.19473	0.19843	21.92	0.40699	0.19651	22.28	0.79526	0.10160	24.28
0.19320	0.29939	22.44	0.37245	0.29515	22.93	0.89859	0.05069	25.56

Table 4. Coefficients D_i and C_i of Equations *8* and *9*, Standard Deviations for Excess Molar Volume (V_m^E), Excess Isentropic Compressibility (κ_s^E) and Surface Tension Deviation ($\Delta\sigma$)

T/K	D_0	D_1	D_2	D_3	D_4	D_5	D_6	D_7	D_8	s
					$V_m^E \cdot 10^6/m^3 \cdot mol^{-1}$					
288.15	0.0008	0.0103	0.0003	−0.0292	$3 \cdot 10^{-6}$	−0.0042	0.0197	−0.0003	0.008	0.006
293.15	0.0011	0.0102	0.0019	−0.0277	−0.0026	−0.0039	0.0182	0.0005	0.0054	0.006
298.15	0.0015	0.0121	0.0037	−0.0301	−0.0059	−0.0075	0.0191	0.0035	0.0091	0.006
303.15	0.0019	0.0131	0.0046	−0.0317	−0.0060	−0.0079	0.0202	0.0026	0.0083	0.007
308.15	0.0014	0.0125	0.0025	−0.0315	−0.0037	−0.0063	0.0207	0.0021	0.0081	0.006
					κ_s^E/TPa^{-1}					
288.15	0.07	0.63	0.08	−1.37	0.19	−0.50	1.15	−0.21	0.69	0.4
293.15	0.08	0.48	0.20	−0.89	−0.13	−0.30	0.81	0.04	0.36	0.4
298.15	0.12	0.51	0.39	−0.86	−0.46	−0.26	0.86	0.24	0.02	0.4
303.15	−0.06	0.46	−0.22	−1.66	0.41	−0.51	−1.25	−0.19	1.79	0.4
308.15	0.21	0.31	0.81	0.36	−1.10	−0.07	−0.07	0.59	−0.99	0.6
					$\Delta\sigma$/mN·m^{-1}					
		C_0			C_1			C_2		s
298.15		6.328			− 34.705			− 16.671		0.06

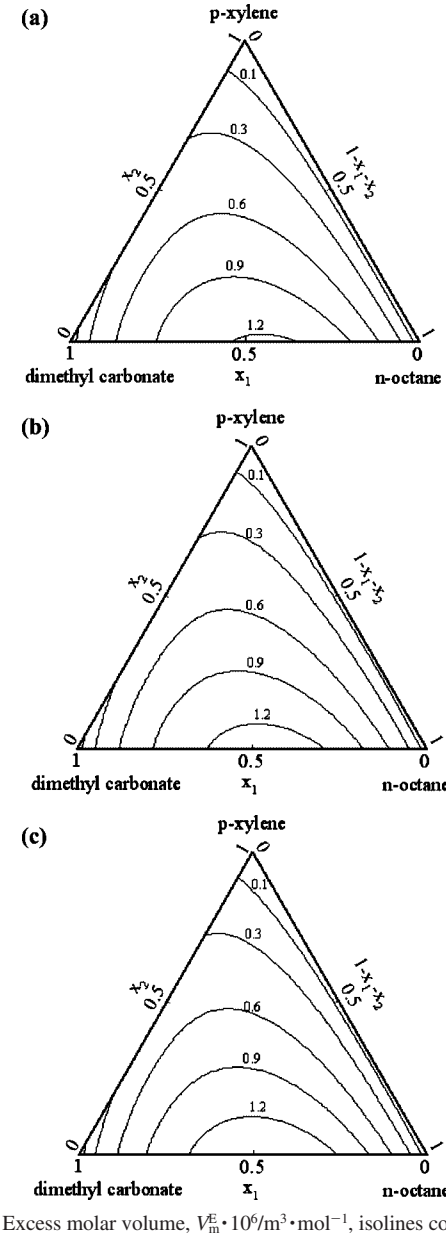

Figure 1. Excess molar volume, $V_m^E \cdot 10^6/m^3 \cdot mol^{-1}$, isolines correlated with eq 6 for the ternary system dimethyl carbonate (1) + *p*-xylene (2) + *n*-octane (3) at: (a) 288.15 K, (b) 298.15 K, and (c) 308.15 K.

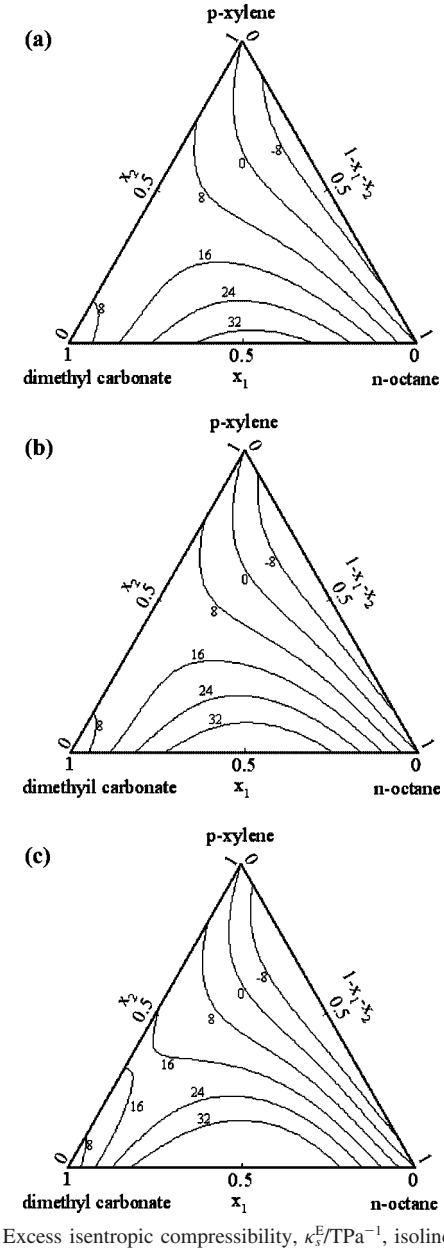

Figure 2. Excess isentropic compressibility, κ_s^E/TPa^{-1}, isolines correlated with eq 6 for the ternary system dimethyl carbonate (1) + *p*-xylene (2) + *n*-octane (3) at: (a) 288.15 K, (b) 298.15 K, and (c) 308.15 K.

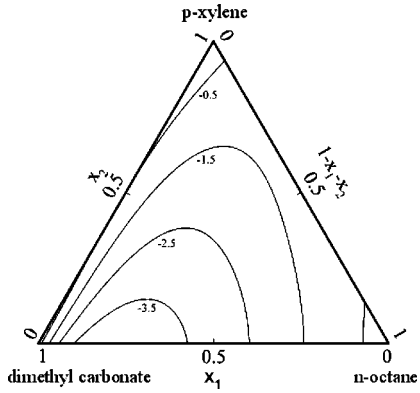

Figure 3. Surface tension deviation, $\Delta\sigma$/mN·m^{-1}, isolines correlated with eq 6 for the ternary system dimethyl carbonate (1) + *p*-xylene (2) + *n*-octane (3) at $T = 298.15$ K.

Table 5. Standard Deviations (*s*) of the Estimated Ternary Excess Molar Volume from Experimental Data

T/K	$s \cdot 10^{6a}$/m^3·mol^{-1}	$s \cdot 10^{6b}$/m^3·mol^{-1}
288.15	0.099	0.921
293.15	0.102	0.982
298.15	0.107	1.046
303.15	0.088	1.073
308.15	0.112	1.169

[a] Mosteiro[14] recalculated parameters. [b] Koukios et al. parameters.

$$Q^{E}_{123} = \sum_{i=1}^{3}\sum_{\substack{j=1 \\ j>i}}^{3} Q^{E}_{ij} + x_1x_2x_3\Delta_{123} \tag{6}$$

This expression includes three terms that correspond to the binary contributions, Q^{E}_{ij}, each of them correlated using the following equation

$$Q^{E}_{ij} = x_ix_j\sum_{p=1}^{m} A_p(x_i - x_j)^{p-1}/1 + B_0(x_i - x_j) \tag{7}$$

where A_p and B_0 are the adjustable fitting parameters. These parameters were computed using an unweighted least-squares method. The adjustable fitting parameters A_p and B_0 and the corresponding standard deviation are given in Table S3 in the Supporting Information.

The so-called ternary contribution ($x_1x_2x_3\Delta_{123}$) for excess molar volume and excess isentropic compressibility was correlated using the equation proposed by Nagata and Tamura[9]

$$\frac{\Delta_{123}}{RT} = \frac{D_0 - D_1x_1 - D_2x_2 - D_3x_1^2 - D_4x_2^2 - D_5x_1x_2 - D_6x_1^3 - D_7x_2^3 - D_8x_2x_1^2}{(1 + (x_2 - x_3))} \tag{8}$$

Surface tension deviation was correlated using the expression suggested by Cibulka[10]

$$\Delta_{123} = C_0 + C_1x_1 + C_2x_2 \tag{9}$$

The adjustable fitting parameters D_i and C_i of eqs 8 and 9 and the corresponding standard deviations are given in Table 4.

Figures 1 and 2 show the isolines of V^{E}_m and κ^{E}_s, respectively, at (288.15, 298.15, and 308.15) K. The excess molar volume values are positive over the whole composition range, and the maximum V^{E}_m value is found near $x_1 = 0.5$ of the binary system dimethyl carbonate + *n*-octane for all studied temperatures. V^{E}_m positive values slightly increase with temperature. The positive excess molar volumes indicate that there are no strong specific interactions between the components of the mixture, and this behavior can be explained by considering the disruption of the dipolar order in the carbonate group and packing effects. κ^{E}_s ternary plots present, at all temperatures studied, an ideal behavior isoline (zero value isoline). A temperature increment produces a negligible effect on the negative values, and the positive ones become more positive.

The surface tension deviations at 298.15 K are negative over the whole composition range. The correlated values are plotted in Figure 3, and the minimum $\Delta\sigma$ value is found near $x_1 = 0.75$ of the binary system dimethyl carbonate (1) + *n*-octane (2).

Theoretical Model

The group contribution model proposed by Nitta et al.[11] was applied to predict the excess molar volumes for the ternary mixture dimethyl carbonate (1) + *p*-xylene (2) + *n*-octane (3) using the original parameters calculated by Koukios et al.[13] and those recalculated by García et al.[7] and Mosteiro.[14] The standard deviations (*s*) of the estimated ternary V^{E}_m from experimental data at different temperatures are reported in Table 5. Predictions

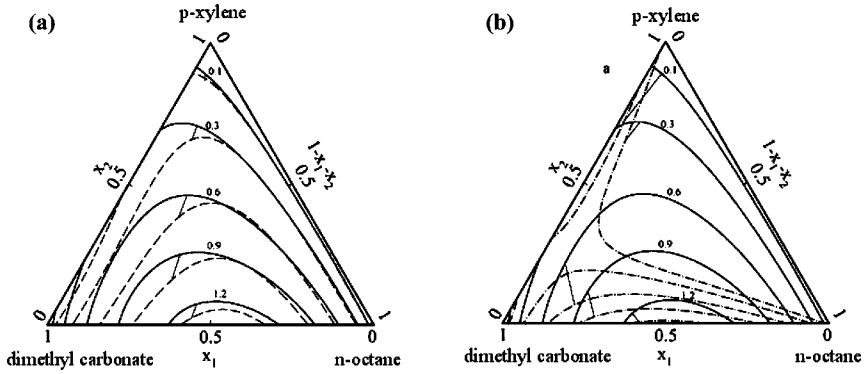

Figure 4. Excess molar volume, $V^{E}_m \cdot 10^6$/m^3·mol^{-1}, isolines correlated with eq 6 for the ternary system dimethyl carbonate (1) + *p*-xylene (2) + *n*-octane (3) at $T = 298.15$ K (—) and estimated values with Nitta et al.[11] (---): (a) Mosteiro[14] recalculated parameters, (b) Koukios et al.[13] original parameters.

with the recalculated parameters by Mosteiro[14] lead to better results, as shown in Figure 4.

Supporting Information Available:

Chromatograph operation conditions and chromatograms of pure compounds, coefficients of eq 7, and standard deviations for excess molar volume, excess isentropic compressibility, and surface tension deviation of binary mixtures. This material is available free of charge via the Internet at http://pubs.acs.org.

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