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Densities of *m*-Xylene + Diphenylmethane and *m*-Cresol + Diphenylmethane from 333 K to 413 K and Pressures up to 30 MPa

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Densities were measured for liquid mixtures of *m*-xylene + diphenylmethane and *m*-cresol + diphenylmethane at temperatures from 333.15 K to 413.15 K and pressures up to 30 MPa. The Tait equation was used to correlate the results. Isothermal compressibilities of the fluids and their mixtures were calculated. The results showed that the excess volumes of *m*-xylene + diphenylmethane are negative and those of *m*-cresol + diphenylmethane are positive at the experimental conditions.

Introduction

Density of fluids and fluid mixtures is an important property in model development and engineering applications. As a continuation of our previous work (Chang and Lee, 1995, 1996; Chang et al., 1996), liquid densities of *m*-xylene + diphenylmethane and *m*-cresol + diphenylmethane were measured in the present study at temperatures from 333.15 K to 413.15 K and pressures up to 30 MPa. Most of the literature data for the constituents were available at atmospheric pressures and/or near ambient temperatures. Density data at high pressures are not so plentiful as those at ambient conditions. Among several others, Taxis et al. (1988) tabulated the densities of *m*-xylene at temperatures from 308 K to 360 K and pressures up to 40.4 MPa. Recently, Chang and Lee (1995, 1996) and Chang et al. (1996) reported the densities of binary mixtures containing *m*-xylene or *m*-cresol from 298 K to 413 K and pressures up to 30 MPa. No density data have been found in the literature at comparable conditions of this work for these diphenylmethane-containing mixtures.

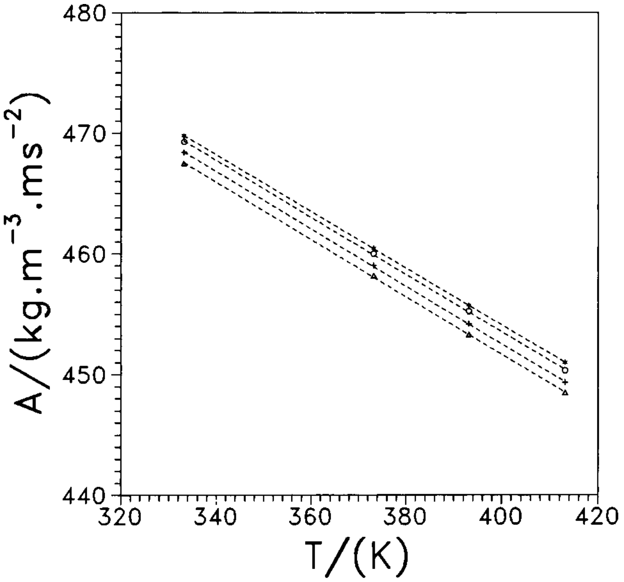

Figure 1. Temperature effects on the instrument parameter *A*: (*) 5.0 MPa, (○) 10.0 MPa, (+) 20.0 MPa, (△) 30.0 MPa, (- - -) calculated from a linear function.

Table 1. Densities of Pure Liquids at 0.1 MPa

substance	*T*/K	$\rho/(\mathrm{g\cdot cm^{-3}})$ this work	 lit.	ref
m-xylene	333.15	0.8302	0.8297	TRC, d-3290 (1977)
	373.15	0.7942	0.7936	TRC, d-3290 (1977)
	393.15	0.7752	0.7748	TRC, d-3290 (1977)
	413.15	0.7558[a]	0.7554[b]	TRC, d-3290 (1977)
m-cresol	333.15	1.0021	1.0018	TRC, d-6400 (1993)
	373.15	0.9682	0.9683	TRC, d-6400 (1993)
	393.15	0.9509	0.9509	TRC, d-6400 (1993)
	413.15	0.9326	0.9331	TRC, d-6400 (1993)
diphenylmethane	333.15	0.9755		
	373.15	0.9432		
	393.15	0.9268		
	413.15	0.9101		

[a] At 0.11 MPa. [b] At saturated pressure (0.104 MPa).

Experimental Section

m-Xylene (99 mass %), *m*-cresol (99 mass %), and diphenylmethane (99 mass %) were supplied by Aldrich Chemicals (Milwaukee, WI). The impurities in the chemicals were 0.3%, 0.1%, and 0.4% for *m*-xylene, *m*-cresol, and diphenylmethane, respectively, according to gas chromatography analysis. All substances were used without further purification. Mixture samples (about 30 g) were prepared by mass with an accuracy of 0.0002 in mole fraction. The sample was introduced into a high-pressure densimeter (DMA-512; Anton Paar) via a hand pump (Model 2426-801; Ruska). High pressure was generated by this hand pump. A pressure transducer (Model PDCR 330, 0−40 MPa; Druck) with a digital indicator (Model DPI 261; Druck) monitored the pressure in the measuring cell. The accuracy of pressure measurements was better than 0.75%. The temperature in the measuring cell was controlled by circulating thermostated silicon oil to within 0.03 K. A precision digital thermometer (Model 1506; Hart Scientific) incorporated with a platinum RTD probe measured the temperature to an accuracy of 0.02 K. The oscillation period of sample i in the vibrating U tube (t_i) was displayed by a DMA-60 processing unit (Anton Paar) which can be converted into density (ρ_i) via

$$\rho_i = A(t_i^2 - B) \times 10^{-3} \qquad (1)$$

where *A* and *B* are instrument constants determined by

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Table 2. Experimental Density and Calculated Isothermal Compressibility for Pure *m*-Cresol and Diphenylmethane

	T = 333.15 K		T = 373.15 K		T = 413.15K	
P/MPa	ρ/(g·cm^{-3})	$10^4\kappa_T$/MPa^{-1}	ρ/(g·cm^{-3})	$10^4\kappa_T$/MPa^{-1}	ρ/(g·cm^{-3})	$10^4\kappa_T$/MPa^{-1}
			Diphenylmethane			
0.1	0.9755	6.459	0.9432	8.246	0.9101	11.27
5.0	0.9786	6.242	0.9470	7.876	0.9149	10.32
10.0	0.9816	6.036	0.9506	7.532	0.9194	9.504
15.0	0.9845	5.844	0.9542	7.219	0.9237	8.813
20.0	0.9873	5.664	0.9575	6.931	0.9275	8.216
25.0	0.9901	5.495	0.9607	6.667	0.9313	7.698
30.0	0.9927	5.336	0.9639	6.423	0.9348	7.244
			m-Cresol			
0.1	1.0021	6.313	0.9682	7.840	0.9326	10.96
5.0	1.0052	6.057	0.9719	7.497	0.9375	10.02
10.0	1.0082	5.818	0.9755	7.177	0.9419	9.223
15.0	1.0110	5.597	0.9789	6.885	0.9461	8.545
20.0	1.0138	5.392	0.9822	6.616	0.9502	7.964
25.0	1.0164	5.203	0.9854	6.369	0.9536	7.455
30.0	1.0191	5.027	0.9885	6.140	0.9572	7.012

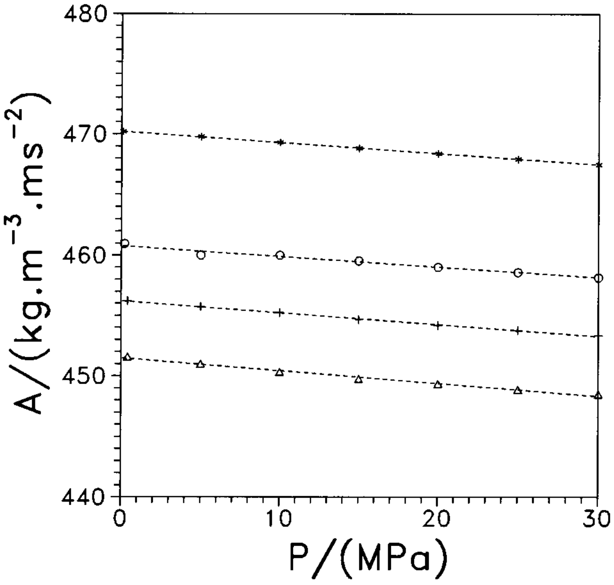

Figure 2. Pressure effects on the instrument parameter A: (*) 333.15 K, (○) 373.15 K, (+) 393.15 K, (△) 413.15 K, (- - -) calculated from eqs 2–5.

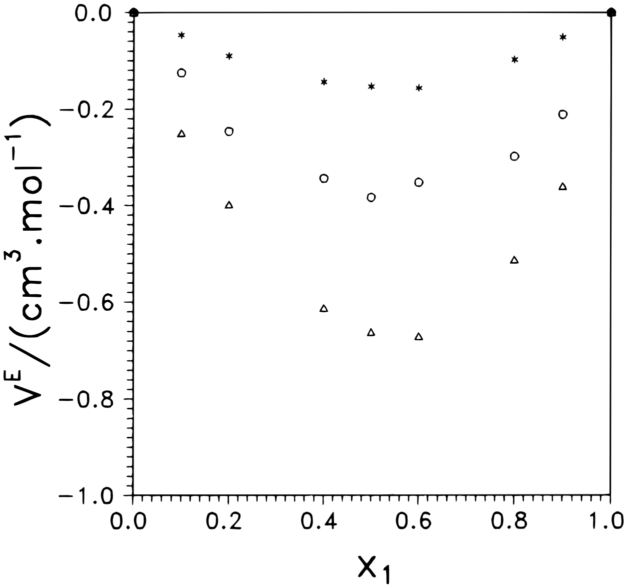

Figure 3. Temperature effects on the excess molar volumes at 0.1 MPa for *m*-xylene (1) + diphenylmethane (2): (*) 333.15 K, (○) 373.15 K, (△) 413.15 K.

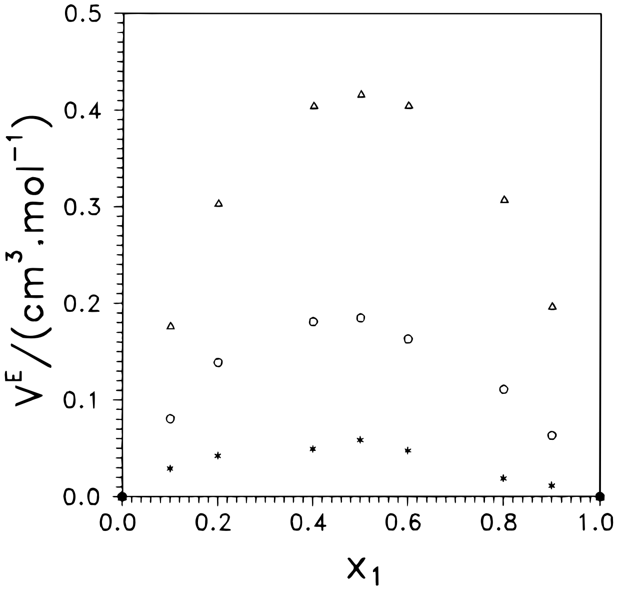

Figure 4. Temperature effects on the excess molar volumes at 0.1 MPa for *m*-cresol (1) + diphenylmethane (2): (*) 333.15 K, (○) 373.15 K, (△) 413.15 K.

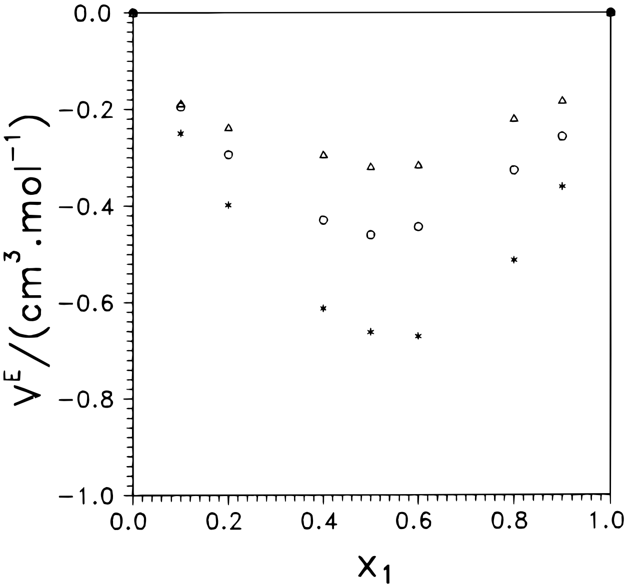

Figure 5. Pressure effects on the excess molar volumes at 413.15 K for *m*-xylene (1) + diphenylmethane (2): (*) 0.1 MPa, (○) 15.0 MPa, (△) 30.0 MPa.

Table 3. Experimental Density and Calculated Isothermal Compressibility for the *m*-Xylene (1) + Diphenylmethane (2)

	$T = 333.15$ K		$T = 373.15$ K		$T = 413.15$ K	
P/MPa	$\rho/(\mathrm{g \cdot cm^{-3}})$	$10^4\kappa_T/\mathrm{MPa^{-1}}$	$\rho/(\mathrm{g \cdot cm^{-3}})$	$10^4\kappa_T/\mathrm{MPa^{-1}}$	$\rho/(\mathrm{g \cdot cm^{-3}})$	$10^4\kappa_T/\mathrm{MPa^{-1}}$
			$x_1 = 0.1000$			
0.1	0.9647	6.817	0.9325	8.623	0.8993	11.67
5.0	0.9679	6.558	0.9364	8.216	0.9042	10.77
10.0	0.9710	6.314	0.9401	7.840	0.9090	9.984
15.0	0.9740	6.088	0.9437	7.498	0.9134	9.313
20.0	0.9769	5.879	0.9471	7.186	0.9174	8.727
25.0	0.9797	5.684	0.9505	6.900	0.9213	8.213
30.0	0.9825	5.502	0.9537	6.636	0.9250	7.760
			$x_1 = 0.2000$			
0.1	0.9533	7.040	0.9211	8.982	0.8874	12.53
5.0	0.9566	6.793	0.9250	8.560	0.8926	11.43
10.0	0.9598	6.559	0.9289	8.170	0.8976	10.49
15.0	0.9629	6.341	0.9327	7.817	0.9021	9.698
20.0	0.9658	6.138	0.9363	7.493	0.9064	9.023
25.0	0.9688	5.948	0.9396	7.196	0.9103	8.436
30.0	0.9716	5.770	0.9429	6.922	0.9140	7.923
			$x_1 = 0.4001$			
0.1	0.9283	7.899	0.8955	10.04	0.8613	14.07
5.0	0.9319	7.549	0.8998	9.507	0.8670	12.70
10.0	0.9353	7.223	0.9040	9.026	0.8723	11.56
15.0	0.9386	6.925	0.9080	8.592	0.8771	10.62
20.0	0.9418	6.652	0.9118	8.200	0.8815	9.815
25.0	0.9449	6.401	0.9154	7.843	0.8858	9.133
30.0	0.9479	6.169	0.9190	7.518	0.8897	8.541
			$x_1 = 0.5001$			
0.1	0.9146	8.189	0.8816	10.72	0.8469	15.04
5.0	0.9182	7.869	0.8860	10.07	0.8527	13.51
10.0	0.9218	7.569	0.8904	9.497	0.8584	12.26
15.0	0.9252	7.291	0.8946	8.985	0.8634	11.23
20.0	0.9284	7.034	0.8984	8.527	0.8679	10.35
25.0	0.9317	6.796	0.9022	8.116	0.8723	9.614
30.0	0.9348	6.574	0.9058	7.743	0.8765	8.976
			$x_1 = 0.6000$			
0.1	0.9000	8.826	0.8664	11.41	0.8314	15.81
5.0	0.9038	8.381	0.8711	10.72	0.8374	14.27
10.0	0.9075	7.972	0.8757	10.10	0.8432	12.99
15.0	0.9111	7.603	0.8799	9.550	0.8485	11.93
20.0	0.9144	7.268	0.8841	9.059	0.8533	11.03
25.0	0.9177	6.962	0.8879	8.617	0.8580	10.27
30.0	0.9208	6.682	0.8916	8.219	0.8622	9.605
			$x_1 = 0.7999$			
0.1	0.8675	9.886	0.8332	13.06	0.7967	18.43
5.0	0.8716	9.368	0.8384	12.16	0.8036	16.47
10.0	0.8756	8.895	0.8434	11.37	0.8099	14.88
15.0	0.8794	8.469	0.8480	10.67	0.8156	13.57
20.0	0.8830	8.084	0.8523	10.06	0.8210	12.48
25.0	0.8865	7.733	0.8566	9.524	0.8259	11.56
30.0	0.8899	7.414	0.8606	9.042	0.8305	10.77
			$x_1 = 0.9000$			
0.1	0.8495	10.33	0.8147	14.28	0.7774	20.24
5.0	0.8537	9.858	0.8202	13.23	0.7848	17.97
10.0	0.8579	9.421	0.8255	12.30	0.7914	16.14
15.0	0.8619	9.022	0.8304	11.51	0.7975	14.66
20.0	0.8656	8.657	0.8350	10.81	0.8030	13.44
25.0	0.8693	8.322	0.8394	10.19	0.8084	12.41
30.0	0.8728	8.013	0.8436	9.649	0.8132	11.54

using pure water (Haar et al., 1984) and dry nitrogen (Vargaftik, 1975) as standard fluids. The calibration was made at each temperature of interest over the pressure range (0.1 to 30) MPa. The values of A, determined from the calibration, decrease linearly with increasing both temperature and pressure as shown in Figures 1 and 2, respectively. To preserve the quality of the experimental results, each temperature-specific parameter A was treated as a function of pressure by the following correlations:

$$A = 470.213 - 0.0909P \quad (\text{at } T = 333.15\ \text{K}) \qquad (2)$$

$$A = 460.939 - 0.0937P \quad (\text{at } T = 373.15\ \text{K}) \qquad (3)$$

$$A = 456.202 - 0.0980P \quad (\text{at } T = 393.15\ \text{K}) \qquad (4)$$

$$A = 451.486 - 0.1052P \quad (\text{at } T = 413.15\ \text{K}) \qquad (5)$$

where A is in $\mathrm{kg \cdot m^{-3} \cdot ms^{-2}}$ and P is in MPa. Equation 1 reproduced the water densities to an average absolute deviation of 0.01% over the entire range of the calibrated conditions. The accuracy of the reported densities in Tables 1−4 was estimated to be $1.0 \times 10^{-4}\ \mathrm{g \cdot cm^{-3}}$.

Results and Discussion

Table 1 lists the experimental densities in comparison with the literature values for the pure liquids at 0.1 MPa. Only the result of pure *m*-xylene at 413.15 K was actually measured at 0.11 MPa, which is slightly higher than its vapor pressure (0.104 MPa). Its corresponding literature value was reported at the saturated pressure. The agreement between experimental results and literature values

Table 4. Experimental Density and Calculated Isothermal Compressibility for the *m*-Cresol (1) + Diphenylmethane (2)

	$T = 333.15$ K		$T = 373.15$ K		$T = 413.15$ K	
P/MPa	ρ/(g·cm^{-3})	$10^4\kappa_T$/MPa^{-1}	ρ/(g·cm^{-3})	$10^4\kappa_T$/MPa^{-1}	ρ/(g·cm^{-3})	$10^4\kappa_T$/MPa^{-1}
			$x_1 = 0.1000$			
0.1	0.9771	6.590	0.9444	8.276	0.9106	11.44
5.0	0.9802	6.328	0.9483	7.896	0.9155	10.43
10.0	0.9832	6.082	0.9519	7.542	0.9201	9.571
15.0	0.9861	5.855	0.9554	7.221	0.9243	8.846
20.0	0.9890	5.646	0.9587	6.926	0.9283	8.226
25.0	0.9917	5.451	0.9620	6.656	0.9319	7.689
30.0	0.9943	5.270	0.9651	6.407	0.9355	7.220
			$x_1 = 0.2000$			
0.1	0.9788	6.565	0.9458	8.484	0.9115	11.37
5.0	0.9819	6.304	0.9497	8.031	0.9164	10.40
10.0	0.9850	6.059	0.9534	7.617	0.9209	9.572
15.0	0.9879	5.833	0.9569	7.245	0.9252	8.869
20.0	0.9907	5.624	0.9603	6.909	0.9292	8.264
25.0	0.9935	5.430	0.9636	6.604	0.9329	7.739
30.0	0.9961	5.250	0.9667	6.326	0.9365	7.279
			$x_1 = 0.4000$			
0.1	0.9830	6.505	0.9495	8.339	0.9144	11.58
5.0	0.9861	6.243	0.9533	7.927	0.9192	10.47
10.0	0.9891	5.996	0.9571	7.549	0.9238	9.537
15.0	0.9920	5.770	0.9606	7.206	0.9281	8.763
20.0	0.9948	5.560	0.9639	6.894	0.9320	8.108
25.0	0.9976	5.366	0.9671	6.608	0.9357	7.547
30.0	1.0002	5.185	0.9702	6.346	0.9392	7.060
			$x_1 = 0.5000$			
0.1	0.9853	6.494	0.9517	8.418	0.9162	11.28
5.0	0.9885	6.238	0.9554	7.957	0.9211	10.31
10.0	0.9915	5.998	0.9592	7.538	0.9257	9.480
15.0	0.9944	5.776	0.9627	7.162	0.9299	8.778
20.0	0.9972	5.571	0.9661	6.824	0.9337	8.176
25.0	0.9999	5.380	0.9693	6.517	0.9376	7.655
30.0	1.0026	5.203	0.9724	6.237	0.9410	7.196
			$x_1 = 0.6000$			
0.1	0.9880	6.518	0.9542	8.353	0.9184	11.43
5.0	0.9912	6.248	0.9580	7.901	0.9233	10.38
10.0	0.9942	5.995	0.9618	7.490	0.9279	9.492
15.0	0.9971	5.763	0.9652	7.120	0.9322	8.749
20.0	0.9999	5.549	0.9686	6.787	0.9361	8.117
25.0	1.0026	5.351	0.9718	6.484	0.9397	7.572
30.0	1.0053	5.167	0.9750	6.209	0.9432	7.098
			$x_1 = 0.8000$			
0.1	0.9944	6.416	0.9603	8.206	0.9240	11.41
5.0	0.9974	6.150	0.9640	7.765	0.9290	10.33
10.0	1.0005	5.902	0.9677	7.364	0.9336	9.424
15.0	1.0033	5.673	0.9711	7.003	0.9377	8.667
20.0	1.0061	5.462	0.9744	6.677	0.9416	8.026
25.0	1.0088	5.267	0.9777	6.381	0.9453	7.476
30.0	1.0115	5.086	0.9808	6.112	0.9488	6.998
			$x_1 = 0.9000$			
0.1	0.9980	6.327	0.9640	8.043	0.9278	11.11
5.0	1.0011	6.093	0.9678	7.646	0.9326	10.15
10.0	1.0040	5.872	0.9713	7.279	0.9371	9.322
15.0	1.0070	5.668	0.9748	6.947	0.9413	8.625
20.0	1.0098	5.477	0.9780	6.646	0.9452	8.028
25.0	1.0124	5.300	0.9812	6.370	0.9489	7.511
30.0	1.0151	5.134	0.9843	6.118	0.9525	7.059

is within 0.1% for both *m*-xylene and *m*-cresol. Table 2 compiles the experimental densities and the calculated isothermal compressibilities (κ_T) of pure *m*-cresol and diphenylmethane from 333.15 K to 413.15 K and at pressures up to 30 MPa. These values for *m*-xylene have been reported by Chang et al. (1996). The results of *m*-xylene + diphenylmethane and *m*-cresol + diphenylmethane mixtures are listed in Tables 3 and 4, respectively. The isothermal compressibilities as tabulated in Tables 2−4 were calculated according to the following definition with the aid of the Tait equation:

$$\kappa_T = \frac{-1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,x} = \frac{V_0}{V}\left(\frac{C}{D + P}\right) \qquad (6)$$

where V is the molar volume, V_0 is the molar volume at 0.1 MPa, T is the temperature, and x is the mole fraction. The constants C and D are parameters of the Tait equation:

$$\frac{\rho - \rho_0}{\rho} = C \ln\left(\frac{D + P}{D + 0.1}\right) \qquad (7)$$

where ρ_0 is the density at 0.1 MPa, except for pure *m*-xylene at 413.15 K at which the density at a pressure of 0.11 MPa was used in the calculation. The optimized values of C and D were obtained from fitting the Tait equation to the isothermal density data at a given composition by the

Table 5. Results of the Density Correlations with the Tait Equation

		m-xylene (1) + diphenylmethane (2)				*m*-cresol (1) + diphenylmethane (2)			
T/K	x_1	C	D/MPa	$10^4\pi_1{}^a$	$10^5\sigma^b/(\text{g}\cdot\text{cm}^{-3})$	C	D/MPa	$10^4\pi_1{}^a$	$10^5\sigma^b/(\text{g}\cdot\text{cm}^{-3})$
333.15	0.0	0.076 13	116.87	0.1	2.0	0.076 13	116.87	0.1	2.0
333.15	0.1	0.077 85	114.10	0.2	3.5	0.072 28	109.59	0.2	3.0
333.15	0.2	0.086 46	122.71	0.1	2.0	0.071 99	109.55	0.1	1.7
333.15	0.4	0.076 82	97.15	0.2	3.2	0.070 38	108.10	0.2	2.7
333.15	0.5	0.089 62	109.34	0.2	3.5	0.071 95	110.70	0.3	5.1
333.15	0.6	0.075 10	84.99	0.2	2.9	0.068 76	105.40	0.2	3.1
333.15	0.8	0.080 36	81.19	0.2	2.1	0.067 72	105.45	0.2	2.7
333.15	0.9	0.095 12	91.96	0.4	5.2	0.074 63	117.86	0.3	3.9
333.15	1.0	0.092 42	83.33	0.5	7.1	0.068 13	107.82	0.3	4.8
373.15	0.0	0.079 01	95.72	0.2	2.7	0.079 01	95.72	0.2	2.7
373.15	0.1	0.078 39	90.81	0.4	5.4	0.077 32	93.33	0.5	8.5
373.15	0.2	0.081 80	90.97	0.5	8.5	0.068 40	80.52	0.2	3.5
373.15	0.4	0.081 16	80.78	0.3	4.1	0.072 75	87.14	0.5	8.7
373.15	0.5	0.075 94	70.76	0.2	2.6	0.066 40	78.78	0.2	3.6
373.15	0.6	0.079 52	69.57	0.4	5.4	0.066 68	79.73	0.2	3.7
373.15	0.8	0.079 46	60.77	0.3	4.0	0.066 08	80.43	0.4	6.8
373.15	0.9	0.080 16	56.02	0.3	3.6	0.070 23	87.22	0.3	6.3
373.15	1.0	0.077 71	50.02	0.4	5.1	0.077 19	98.35	0.2	3.0
413.15	0.0	0.056 33	49.88	0.4	6.4	0.056 33	49.88	0.4	6.4
413.15	0.1	0.063 84	54.63	0.5	7.1	0.054 49	47.53	0.3	5.2
413.15	0.2	0.059 59	47.46	0.4	5.7	0.056 19	49.31	0.4	6.2
413.15	0.4	0.059 98	42.54	0.3	4.5	0.050 56	43.56	0.5	6.8
413.15	0.5	0.061 30	40.67	1.0	12.8	0.055 34	48.98	0.3	4.9
413.15	0.6	0.066 83	42.16	0.6	8.3	0.052 31	45.68	0.3	4.6
413.15	0.8	0.070 30	38.04	0.2	3.1	0.050 61	44.26	0.4	6.4
413.15	0.9	0.072 47	35.71	0.4	5.5	0.053 93	48.44	0.4	6.3
413.15	1.0	0.077 76	35.10	0.5	5.9	0.054 26	49.42	0.5	10.0

[a] π_1 as defined in eq 8. [b] $\sigma/(\text{g}\cdot\text{cm}^{-3}) = \{[\sum_{k=1}^{n}(\rho_{k,\text{calc}} - \rho_{k,\text{expt}})^2]/[n-2]\}^{1/2}$ where n is the number of data points. All the points at 0.1 MPa are not included.

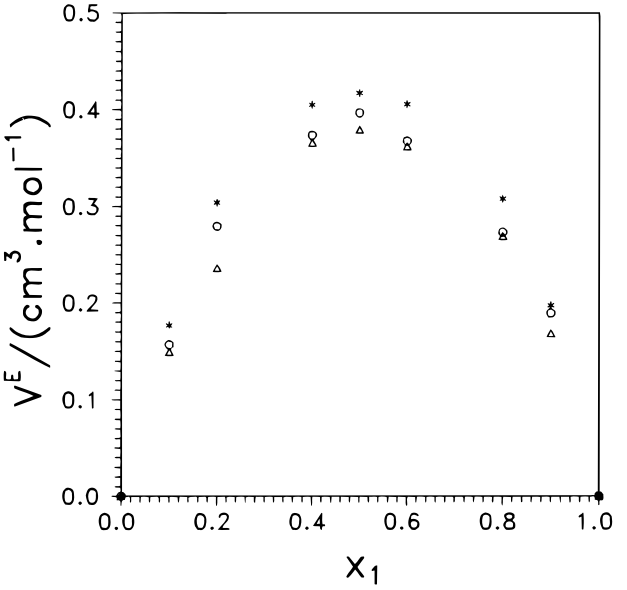

Figure 6. Pressure effects on the excess molar volumes at 413.15 K for *m*-cresol (1) + diphenylmethane (2): (*) 0.1 MPa, (○) 15.0 MPa, (△) 30.0 MPa.

modified Levenberg–Marquardt algorithm with the objective function π_1:

$$\pi_1 = [\sum_{k=1}^{n} |\rho_{k,\text{calc}} - \rho_{k,\text{expt}}|/\rho_{k,\text{expt}}]/n \tag{8}$$

where n is the number of data points. $\rho_{k,\text{calc}}$ and $\rho_{k,\text{expt}}$ represent the calculated and experimental densities, respectively, for the kth point. Table 5 reports the calculated results, including the optimized values of C and D, π_1, and the standard deviations of the fits (σ), which show the accuracy of the Tait equation in correlating the densities over the entire pressure range.

By definition, molar excess volume (V^E) can be computed from the experimental density via

$$V^E = V_m - x_1 V_1{}^0 - x_2 V_2{}^0 \tag{9}$$

with

$$V_m = \frac{x_1 M_1 + x_2 M_2}{\rho} \tag{10}$$

where V_m is the molar volume of a mixture. x_i, $V_i{}^0$, and M_i are the molar fraction, molar volume, and molecular weight, respectively, for the component i. Note that the molar volume of pure *m*-xylene at 413.15 K and 0.11 MPa was used in the excess volume calculations for *m*-xylene + diphenylmethane at 413.15 K and 0.1 MPa. The excess volumes are negative for *m*-xylene + diphenylmethane and positive for *m*-cresol + diphenylmethane over the investigated conditions. Figures 3 and 4 illustrate the temperature effects on the excess volumes, while Figures 5 and 6 show the pressure effects. Obviously, the absolute values of the excess volumes increase with temperature and decrease with pressure for both binary systems.

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