Densities of *m*-Xylene + Quinoline and *m*-Xylene + Tetralin from (333 to 413) K and up to 30 MPa

Ji-Sheng Chang, Ming-Jer Lee,* and Ho-mu Lin

Department of Chemical Engineering, National Taiwan Institute of Technology, Taipei, 106 Taiwan, ROC

Densities were measured for liquid mixtures of *m*-xylene + quinoline and *m*-xylene + tetralin (1,2,3,4-tetrahydronaphthalene) at temperatures from 333.15 K to 413.15 K and pressures up to 30 MPa. The Tait equation correlated accurately the results. Isothermal compressibilities of the fluids and their mixtures were calculated with the aid of the Tait equation. The excess volumes of *m*-xylene + quinoline and *m*-xylene + tetralin were found to be negative at the experimental conditions.

Introduction

Densities of fluids and fluid mixtures are of importance for model development and engineering applications. The liquid densities of *m*-xylene + quinoline and *m*-xylene + tetralin are measured in the present study at temperatures from 333 K to 413 K and pressures up to 30 MPa. Density measurements for the constituent compounds at the atmospheric pressures have been made by several investigators (e.g., Oshmyansky et al., 1986; Goncalves et al., 1989; Yu and Tsai, 1994; Et-Tahir et al., 1995). Chang and Lee (1995, 1996) reported the densities of *m*-cresol + *m*-xylene, +tetralin, +quinoline, and +1-methylnaphthalene at temperatures from 298 K to 348 K and pressures up to 30 MPa. No density data have been found under similar conditions of the present study for these two binary systems.

Experimental Section

m-Xylene (99 mass %) and tetralin (99 mass %) were purchased from Aldrich Chemicals (USA), and quinoline (99 mass %) was purchased from Janssen Chimica (Belgium). The impurities in the chemicals were detected by gas chromatography analysis to be less than 1% (0.3% for m-xylene, 0.5% for quinoline, and 0.8% for tetralin). All the substances were used without further purification. Mixture samples (about 30 g) were prepared by mass with an accuracy of better than ± 0.5 mg. 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. Pressure in the sample tube was measured by a pressure transducer (model PDCR 330, 0-40 MPa, Druck) with a digital indicator (model DPI 261, Druck). The pressure readings were accurate to $\pm 0.75\%$. A circulating thermostated bath was used to control the temperature of the measuring cell within ± 0.03 K. A precision digital thermometer (model 1506, Hart Scientific) incorporated with a thermistor probe read the temperature to an accuracy of ± 0.015 K. The oscillation period of the sample *i* in the vibrating U tube (t_i) was displayed by a DMA-60 processing unit (Anton Paar) which was converted into density (ρ_i) by

$$\rho_i = A(t_i^2 - B) \tag{1}$$

where A and B are apparatus constants determined by using pure water (Haar et al., 1984) and dry nitrogen (Vargaftik, 1975) as standard fluids. The calibration was

Table 1.	Densities	of Pure	Liquids	at 0).1 M	Pa
----------	-----------	---------	---------	------	-------	----

		ρ/ g·c	m^{-3}	
substance	<i>T</i> /K	this work	lit.	ref
<i>m</i> -xylene	333.15	0.8302	0.8297	TRC, d-3290 (1996)
	373.15	0.7942	0.7936	TRC, d-3290 (1996)
	393.15	0.7752	0.7748	TRC, d-3290 (1996)
	413.15	0.7558	0.7554	TRC, d-3290 (1996)
quinoline	333.15	1.0612	1.062	TRC, d-9435 (1996)
-	373.15	1.0292	1.030	TRC, d-9435 (1996)
	393.15	1.0126	1.014	TRC, d-9435 (1996)
	413.15	0.9960	0.997	TRC, d-9435 (1996)
tetralin	333.15	0.9387	(0.9379) ^a	Goncalves et al. (1989)
	373.15	0.9063		
	393.15	0.8896		
	413.15	0.8732		

 $^a\,\rm Extrapolated$ value from density data in the temperature range of 298.1 K to 328.1 K.

Table 2.	Experimental	l Density	and (Calcul	ated
Isotherm	nal Ĉompressi	bility for	Pure	<i>m</i> -Xyl	ene,
Quinolin	e, and Tetrali	n		•	

	333.15 K		373.	15 K	413.15 K		
	ρ/	$10^4 \kappa_{\rm T}$	ρ/	$10^4 \kappa_{\rm T}$	ρ/	$10^4 \kappa_{\rm T}$	
P∕ MPa	g•cm ^{−3}	MPa^{-1}	g•cm ^{−3}	MPa^{-1}	g•cm ^{−3}	MPa^{-1}	
			<i>m</i> -Xylene				
0.1	0.8302	11.24	0.7942	15.36	0.7558	22.03	
5.0	0.8347	10.61	0.8000	14.16	0.7636	19.57	
10.0	0.8390	10.04	0.8055	13.12	0.7706	17.58	
15.0	0.8432	9.528	0.8106	12.23	0.7772	15.98	
20.0	0.8470	9.069	0.8153	11.46	0.7831	14.65	
25.0	0.8508	8.655	0.8199	10.78	0.7885	13.53	
30.0	0.8544	8.279	0.8242	10.19	0.7938	12.59	
		(Quinoline				
0.1	1.0612	5.584	1.0292	6.912	0.9960	9.268	
5.0	1.0641	5.392	1.0325	6.619	1.0004	8.537	
10.0	1.0669	5.210	1.0359	6.347	1.0045	7.904	
15.0	1.0696	5.040	1.0392	6.096	1.0082	7.359	
20.0	1.0723	4.881	1.0423	5.865	1.0119	6.888	
25.0	1.0749	4.733	1.0453	5.652	1.0153	6.474	
30.0	1.0774	4.593	1.0482	5.454	1.0185	6.108	
			Tetralin				
0.1	0.9387	7.464	0.9063	9.645	0.8732	12.67	
5.0	0.9422	7.151	0.9105	9.074	0.8784	11.66	
10.0	0.9454	6.855	0.9145	8.560	0.8834	10.78	
15.0	0.9485	6.586	0.9184	8.103	0.8880	10.03	
20.0	0.9516	6.337	0.9220	7.694	0.8923	9.386	
25.0	0.9546	6.108	0.9254	7.326	0.8965	8.820	
30.0	0.9574	5.895	0.9288	6.993	0.9002	8.319	

made at each temperature of interest over 0.1 MPa to 30 MPa. The values of A were correlated with a linear function of pressure at a given temperature. Equation 1

© 1996 American Chemical Society

^{*} To whom correspondence should be addressed. Fax: 886-2-737-6644. E-mail: mjl@ch.ntit.edu.tw.

Table 3. Experimental Density and CalculatedIsothermal Compressibility for m-Xylene (1) + Quinoline(2)

Table 4.	Experimental Density	and Calculated	l
Isotherm	al Compressibility for	<i>m</i> -Xylene (1) +	Tetralin
(2)	- 0	-	

979 15 V

419 15 V

999 15 V

	333.	15 K	373.	15 K	413.15 K		
		$10^4 \kappa_{\rm T}$	ρ/	$10^4 \kappa_{\rm T}$	ρ/	$10^{4}\kappa_{\rm T}/$	
P∕ MPa	g∙cm ⁻³	MPa ⁻¹	g•cm ^{−3}	MPa^{-1}	g∙cm ⁻³	MPa ⁻¹	
		X	$i_1 = 0.100$	l			
0.1	1.0397	5.825	1.0069	7.532	0.9731	9.870	
5.0	1.0427	5.642	1.0106	7.164	0.9776	9.119	
10.0	1.0456	5.466	1.0140	6.824	0.9818	8.465	
15.0	1.0484	5.302	1.0174	6.516	0.9859	7.902	
20.0	1.0511	5.148	1.0206	6.235	0.9897	7.411	
25.0	1.0538	5.003	1.0238	5.978	0.9933	6.979	
30.0	1.0564	4.866	1.0268	5.743	0.9967	6.595	
		X	$t_1 = 0.2001$	l			
0.1	1.0167	6.158	0.9833	8.044	0.9491	10.65	
5.0	1.0197	5.967	0.9871	7.633	0.9539	9.843	
10.0	1.0227	5.784	0.9908	7.258	0.9586	9.139	
15.0	1.0256	5.612	0.9943	6.918	0.9626	8.530	
20.0	1.0285	5.451	0.9977	6.610	0.9666	8.000	
25.0	1.0312	5.299	1.0010	6.330	0.9704	7.535	
30.0	1.0339	5.156	1.0040	6.073	0.9739	7.122	
		X	$i_1 = 0.400$	1			
0.1	0.9707	7.038	0.9368	9.396	0.9020	12.49	
5.0	0.9740	6.803	0.9410	8.828	0.9072	11.48	
10.0	0.9772	6.579	0.9450	8.317	0.9125	10.61	
15.0	0.9804	6.370	0.9488	7.863	0.9170	9.857	
20.0	0.9835	5.175	0.9525	7.459	0.9214	9.213	
20.0	0.9800	5.992	0.9500	7.090	0.9200	8.049 0.154	
30.0	0.9694	5.620	0.9595	0.707	0.9294	0.154	
			1 = 0.4999)			
0.1	0.9477	7.571	0.9133	10.10	0.8778	13.81	
5.0	0.9512	7.294	0.9176	9.498	0.8835	12.54	
10.0	0.9546	7.032 6.790	0.9219	8.950	0.8888	11.48	
20.0	0.9579	0.709	0.9200	0.475	0.0937	0.825	
25.0	0.9011	6 352	0.9298	0.04J 7.658	0.8982	9.825	
30.0	0.9672	6 155	0.9370	7 308	0.9066	8 601	
0010	010012	0.100))	0.0000	0.001	
0.1	0 0949	× 2002	1 = 0.6000	J 10.07	0.9540	15 91	
0.1 5.0	0.9243	0.203	0.0099	10.07	0.0040	12.31	
10.0	0.9280	7.671	0.8944	9 608	0.8001	12.79	
15.0	0.0010	7 974	0.0000	9.079	0.8711	11 49	
20.0	0.9384	7.009	0.9072	8.608	0.8759	10.61	
25.0	0.9416	6.764	0.9109	8.185	0.8803	9.860	
30.0	0.9447	6.537	0.9146	7.804	0.8845	9.213	
		v	y = 0.8000	า			
0.1	0 8780	9 609	1 - 0.0000 0 8425	, 12 79	0 8055	18 20	
5.0	0.8820	9.156	0.8477	11.96	0.8122	16.30	
10.0	0.8860	8.738	0.8526	11.22	0.8187	14.75	
15.0	0.8898	8.357	0.8572	10.57	0.8244	13.47	
20.0	0.8934	8.010	0.8616	9.993	0.8298	12.41	
25.0	0.8969	7.692	0.8658	9.479	0.8346	11.50	
30.0	0.9003	7.399	0.8699	9.019	0.8394	10.73	
		X	$t_1 = 0.9001$	1			
0.1	0.8546	10.55	0.8190	13.97	0.7814	20.00	
5.0	0.8589	9.955	0.8244	12.98	0.7886	17.84	
10.0	0.8630	9.417	0.8296	12.11	0.7953	16.09	
15.0	0.8670	8.938	0.8345	11.36	0.8015	14.66	
20.0	0.8708	8.507	0.8391	10.70	0.8072	13.47	
25.0	0.8744	8.117	0.8434	10.11	0.8123	12.47	
30.0	0.8779	7.763	0.8476	9.585	0.8173	11.61	

reproduced the water densities to an average absolute percent deviation of 0.01% over the entire range of the calibrated conditions. The uncertainty of the density measurements was estimated to be less than $\pm 1.0 \times 10^{-4}~g\text{-cm}^{-3}$.

Results and Discussion

Table 1 compares our measurements with the literature values for the constituent compounds at 0.1 MPa. The agreement is generally within $\pm 0.1\%$. Table 2 compiles the experimental densities and the calculated isothermal

	ა აა.	15 K	373.	15 K	413.13 K		
	0/	$104 \mu r$	0/	$104 \mu r$	0/	$10^{4} \kappa_{T}$	
<i>P</i> /MPa	$\sigma \cdot cm^{-3}$	MPa^{-1}	$\sigma \cdot cm^{-3}$	MPa^{-1}	$\sigma \cdot cm^{-3}$	MPa^{-1}	
171011 u	5 cm	MI u	g cm	MI u	5 cm	wir u	
		X	$x_1 = 0.100$	1			
0.1	0.9302	7.757	0.8973	9.991	0.8636	13.52	
5.0	0.9337	7.393	0.9016	9.382	0.8690	12.33	
10.0	0.9370	7.056	0.9057	8,835	0.8742	11.32	
15.0	0 9402	6 749	0 9096	8 350	0 8791	10.47	
20.0	0.0434	6 470	0.0000	7 0 1 8	0.8835	0 7/9	
25.0	0.9454	6 9 1 9	0.0169	7.510	0.0033	0.111	
20.0	0.9404	0.213	0.9100	7.550	0.0015	9.111	
30.0	0.9493	5.977	0.9203	7.180	0.8915	8.558	
		2	$x_1 = 0.200$	0			
0.1	0 9201	7 850	0 8868	10 50	0 8529	14 04	
5.0	0.9235	7 537	0.8913	9 848	0.8585	12 84	
10.0	0.0270	7 9 4 4	0.0015	0.262	0.0000	11 09	
15.0	0.3270	0.079	0.0333	9.202	0.0040	10.0%	
15.0	0.9303	0.973	0.8995	8.745	0.8088	10.95	
20.0	0.9334	6.723	0.9034	8.284	0.8733	10.20	
25.0	0.9365	6.491	0.9071	7.872	0.8776	9.554	
30.0	0.9395	6.275	0.9105	7.499	0.8818	8.988	
				n			
0.1	0 0000	0 6 2 0	0.400	11 44	0.0910	15 56	
0.1	0.9008	8.039	0.8009	11.44	0.8318	10.00	
5.0	0.9045	8.234	0.8715	10.69	0.8378	14.13	
10.0	0.9082	7.860	0.8761	10.02	0.8435	12.92	
15.0	0.9116	7.520	0.8804	9.434	0.8488	11.92	
20.0	0.9150	7.209	0.8844	8.915	0.8536	11.06	
25.0	0.9183	6.924	0.8883	8.451	0.8582	10.32	
30.0	0.9214	6.662	0.8920	8.036	0.8624	9.676	
				-			
		λ	$x_1 = 0.499$	9			
0.1	0.8900	8.967	0.8559	12.03	0.8208	16.33	
5.0	0.8938	8.542	0.8607	11.20	0.8271	14.77	
10.0	0.8976	8.150	0.8655	10.47	0.8330	13.46	
15.0	0.9011	7.793	0.8698	9.830	0.8383	12.38	
20.0	0.9045	7.467	0.8740	9.269	0.8433	11.46	
25.0	0 9079	7 1 7 0	0 8779	8 771	0 8480	10.67	
20.0	0.9111	6 896	0.8818	8 3 2 5	0.8524	9 990	
30.0	0.3111	0.830	0.0010	0.525	0.0524	3.330	
		λ	$x_1 = 0.600$	1			
0.1	0.8793	9.146	0.8444	12.47	0.8083	17.40	
5.0	0.8831	8.760	0.8493	11.65	0.8148	15.66	
10.0	0 8870	8 400	0 8542	10.93	0.8210	14 22	
15.0	0.8907	8 070	0.8588	10.00	0.8266	13.03	
20.0	0.8042	7 766	0.8630	0 794	0.0200	12.03	
25.0	0.0342	7.100	0.8030	0.999	0.0310	11.10	
20.0	0.6970	7.400	0.0071	9.222	0.8300	11.10	
30.0	0.9008	7.224	0.8710	8.770	0.8411	10.44	
		,	$x_1 = 0.800$	1			
0.1	0 8557	10.22	0 8204	13.82	0 7832	1977	
5.0	0.8500	0 708	0.8258	12.02	0.7002	17 51	
10.0	0.0000	0.228	0.0200	11.09	0.7000	15.60	
10.0	0.6040	9.230	0.8309	11.90	0.7970	13.09	
15.0	0.8679	8.812	0.8358	11.23	0.8030	14.23	
20.0	0.8716	8.427	0.8403	10.58	0.8084	13.02	
25.0	0.8752	8.075	0.8447	9.995	0.8133	12.01	
30.0	0.8787	7.752	0.8487	9.477	0.8182	11.15	
		-	~ — 0 000	n			
0.1	0.0400	10.01	1 - 0.300	14 50	0 7700	00.01	
0.1	0.8438	10.01	0.8084	14.33	0.7706	20.81	
5.0	0.8481	10.12	0.8140	13.49	0.7780	18.51	
10.0	0.8524	9.668	0.8193	12.57	0.7851	16.66	
15.0	0.8564	9.255	0.8243	11.77	0.7912	15.16	
20.0	0.8603	8.877	0.8291	11.08	0.7970	13.91	
25.0	0.8640	8.530	0.8335	10.46	0.8023	12.86	
30.0	0.8676	8.211	0.8377	9.916	0.8072	11.97	

compressibilities (κ_T) of pure *m*-xylene, quinoline, and tetralin at temperatures of 333.15 K to 413.15 K and pressures up to 30 MPa. The results of *m*-xylene + quinoline and *m*-xylene + tetralin mixtures are presented in Tables 3 and 4, respectively. The isothermal compressibilities, as tabulated in Tables 2–4, were calculated from the following equation:

$$\kappa_{\rm T} = \frac{-1}{V} \left(\frac{\partial V}{\partial P} \right)_{T,x} = \frac{V_{\rm o}}{V} \left(\frac{C}{D+P} \right) \tag{2}$$

where V stands for the molar volume, V_0 for the molar

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

			m-xylene (1) + quinoline (2)			m-xylene (1) + tetralin (2)			
<i>T</i> /K	<i>X</i> 1	С	D/MPa	$10^{4}\pi_{1}{}^{a}$	$10^5 \sigma^{b/} \text{g} \cdot \text{cm}^{-3}$	С	D/MPa	$10^{4}\pi_{1}{}^{a}$	$10^5 \sigma^{b/} \text{g} \cdot \text{cm}^{-3}$
333.15	0.0	0.071 29	127.57	0.2	3.2	0.076 58	102.50	0.3	8.5
333.15	0.100	0.080 49	138.07	0.1	2.4	0.071 45	92.01	0.2	3.1
333.15	0.200	0.085 77	139.18	0.1	2.0	0.084 61	107.68	0.2	3.1
333.15	0.400	0.090 44	128.40	0.1	2.0	0.079 12	91.48	0.2	3.3
333.15	0.500	0.088 66	117.00	0.2	3.4	0.080 93	90.15	0.4	4.7
333.15	0.600	0.086 79	105.70	0.2	3.5	0.092 05	100.54	0.2	3.2
333.15	0.800	0.086 64	90.07	0.3	4.7	0.086 40	84.44	0.3	3.8
333.15	0.900	0.079 70	75.47	0.1	1.9	0.096 45	90.77	0.5	6.2
333.15	1.0	0.085 66	76.30	0.3	4.1	0.085 66	76.30	0.3	3.8
373.15	0.0	0.071 09	102.75	0.3	4.5	0.069 77	72.24	0.3	4.5
373.15	0.100	0.066 73	88.49	0.3	5.2	0.069 93	69.89	0.3	4.7
373.15	0.200	0.068 25	84.75	0.2	2.9	0.071 71	68.18	0.2	2.8
373.15	0.400	0.066 60	70.78	0.2	3.6	0.073 53	64.15	0.2	3.0
373.15	0.500	0.072 26	71.44	0.5	6.1	0.073 66	61.15	0.3	3.8
373.15	0.600	0.075 28	69.15	0.4	5.2	0.079 91	63.99	0.5	6.0
373.15	0.800	0.082 41	64.34	0.2	4.4	0.081 20	58.64	0.2	3.2
373.15	0.900	0.082 12	58.67	0.2	3.8	0.083 82	57.59	0.2	2.7
373.15	1.0	0.081 28	52.82	0.3	3.4	0.081 28	52.82	0.3	3.4
413.15	0.0	0.050 25	54.12	0.4	5.9	0.066 43	52.32	0.4	5.7
413.15	0.100	0.055 39	56.02	0.4	6.8	0.064 06	47.27	0.5	6.6
413.15	0.200	0.059 56	55.82	0.6	10.5	0.068 27	48.53	0.6	7.2
413.15	0.400	0.064 53	51.55	0.6	10.1	0.069 71	44.70	0.2	3.5
413.15	0.500	0.062 76	45.36	0.6	7.8	0.070 00	42.77	0.5	6.5
413.15	0.600	0.063 48	41.36	0.4	4.8	0.070 90	40.64	0.5	5.3
413.15	0.800	0.070 84	38.82	0.7	8.8	0.069 37	34.98	0.7	8.7
413.15	0.900	0.074 62	37.21	0.7	8.8	0.075 73	36.30	0.7	10.7
413.15	1.0	0.077 76	35.10	0.5	5.9	0.077 76	35.10	0.5	5.9

^{*a*} π_1 as defined in eq 4. ^{*b*} $\sigma/\text{g-cm}^{-3} = \{ [\sum_{k=1}^{n} (\rho_{\text{calc},k} - \rho_{\text{expt},k})^2]/[n-2] \}^{1/2}$, where *n* is the number of data points. The point at 0.1 MPa is not included.

 Table 6. Results of the Excess Volume Correlations with Eq 7

			<i>m</i> -xylene (1) + quinoline (2)			m-xylene (1) + tetralin (2)			
<i>T</i> /K	P/MPa	E_1	E_2	E_3	$10^2 \pi_2^{a}$ /cm ³ ·mol ⁻¹	E_1	E_2	E_3	$10^2 \pi_2^a$ /cm ³ ·mol ⁻¹
333.15	0.1	-2.406	-0.1159	-1.856	1.7	-1.741	-0.5142	-1.339	3.8
333.15	5.0	-2.192	-0.1081	-1.878	1.8	-1.633	-0.6015	-1.134	3.5
333.15	10.0	-2.011	-0.1550	-1.904	1.6	-1.629	-0.4004	-1.232	3.5
333.15	15.0	-1.889	-0.1882	-1.958	1.7	-1.523	-0.6248	-1.187	3.8
333.15	20.0	-1.776	-0.1063	-1.833	1.9	-1.475	-0.8548	-0.2496	4.2
333.15	25.0	-1.648	-0.1178	-1.733	1.8	-1.438	-0.7828	0.0224	4.3
333.15	30.0	-1.552	-0.1095	-1.750	1.6	-1.403	0.6428	-0.1130	4.2
373.15	0.1	-3.024	-0.5308	-1.581	1.8	-1.969	-0.0239	-0.7324	4.3
373.15	5.0	-2.689	-0.3407	-1.755	1.8	-1.765	-0.1047	-0.7978	4.4
373.15	10.0	-2.438	-0.3929	-1.734	2.0	-1.776	-0.0350	-0.5537	4.2
373.15	15.0	-2.209	-0.3458	-1.648	2.0	-1.694	-0.1006	-0.5886	4.0
373.15	20.0	-2.052	-0.4012	-1.650	1.8	-1.588	-0.1563	-0.7222	4.4
373.15	25.0	-1.858	-0.1682	-1.542	1.8	-1.567	-0.1712	-0.6940	3.9
373.15	30.0	-1.697	-0.3331	-1.782	2.0	-1.447	-0.1830	-0.6609	4.6
413.15	0.1	-4.106	-1.366	-1.971	3.1	-2.455	-0.3040	-0.5901	5.1
413.15	5.0	-3.618	-1.166	-1.525	2.4	-2.197	-0.2099	-0.6506	5.4
413.15	10.0	-3.232	-1.284	-1.473	2.5	-2.140	-0.2533	-0.6637	5.2
413.15	15.0	-2.792	-1.054	-1.846	3.3	-1.953	-0.00614	-0.8775	4.9
413.15	20.0	-2.415	-1.066	-1.935	3.5	-1.859	0.08577	-0.6011	4.8
413.15	25.0	-2.218	-0.8258	-1.808	3.1	-1.755	0.1457	-0.2214	5.2
413.15	30.0	-1.983	-0.8191	-1.795	3.1	-1.634	0.1874	-0.2959	4.7

^{*a*} π_2 as defined in eq 8.

volume at 0.1 MPa, T for temperature, and x for the mole fraction. The constants C and D are the parameters in the Tait equation:

$$\frac{\rho - \rho_0}{\rho} = C \ln \left(\frac{D + P}{D + 0.1} \right) \tag{3}$$

where ρ_0 is the density at 0.1 MPa. The optimized values of *C* and *D* were obtained from fitting the Tait equation to the isothermal density data at a given composition by means of the modified Levenberg–Marquardt algorithm to minimize the following objective function π_1 .

$$\pi_1 = \left[\sum_{k=1}^n |\rho_{k,\text{calc}} - \rho_{k,\text{expt}}| / \rho_{k,\text{expt}}\right] / n \tag{4}$$

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

Molar excess volumes (V^{E}) can be readily computed from density data via

$$V^{\rm E} = V_{\rm m} - x_1 V_1^{\,\rm o} - x_2 V_2^{\,\rm o} \tag{5}$$



Figure 1. Temperature effects on the molar excess volumes at 0.1 MPa for *m*-xylene (1) + quinoline (2): (*) 333.15 K; (\bigcirc) 373.15 K; (\triangle) 413.15 K; (- - -) calculated from eq 7.

with

$$V_{\rm m} = \frac{x_1 M_1 + x_2 M_2}{\rho} \tag{6}$$

where $V_{\rm m}$ is the molar volume of a mixture. x_i , $V_i^{\rm o}$, and M_i are the mole fraction, molar volume, and the molecular weight for the component *i*, respectively. The uncertainty of the calculated excess volumes is about ± 0.05 cm³·mol⁻¹. For these two investigated binary systems, the excess volumes are negative. The isothermal excess volumes are correlated with a Redlich–Kister type equation:

$$V^{E}/x_{1}x_{2} = \sum_{k=1}^{3} E_{k}(x_{1} - x_{2})^{k-1}$$
(7)

The optimized values of E_k are determined from fitting eq 7 to the experimental excess volumes by minimization of the objective function π_2 :

$$\pi_2 = \left[\sum_{k=1}^{n} |V_{k,\text{calc}}^E - V_{k,\text{expt}}^E\right] / n$$
(8)

where *n* is the number of data points of the mixtures. Table 6 lists the calculated results. Figures 1 and 2 illustrate the effects of temperature and pressure, respectively, on the molar excess volumes for *m*-xylene + quinoline. The dashed curves on the graphs represent the calculated values from eq 7. Over the entire investigated conditions, the absolute values of excess volumes increase with temperature and decrease with pressure for both binary systems.



Figure 2. Pressure effects on the molar excess volumes at 333.15 K for *m*-xylene (1) + quinoline (2): (*) 0.1 MPa; (\bigcirc) 15.0 MPa; (\triangle) 30.0 MPa; (- -) calculated from eq 7.

Literature Cited

- Chang, J. S.; Lee, M. J. Densities of m-Cresol + m-Xylene and m-Cresol + Tetralin Mixtures at 298–348 K and up to 30 MPa. *J. Chem. Eng. Data* **1995**, *40*, 1115–1118.
- Chang, J. S.; Lee, M. J. Densities of m-Cresol + Quinoline and m-Cresol + 1-Methylnaphthalene Mixtures at (298–348) K and up to 30 MPa. *J. Chem. Eng. Data* 1996, *41*, 275–278.
 Goncalves, F. A.; Hamano, K.; Sengers, J. V. Density and Viscosity of
- Goncalves, F. A.; Hamano, K.; Sengers, J. V. Density and Viscosity of Tetralin and trans-Decalin. *Int. J. Thermophys.* **1989**, *10*, 845–856.
- Et-Tahir, A.; Boned, C.; Lagourette, B.; Xans, P. Determinations of the Viscosity of Various Hydrocarbons and Mixtures of Hydrocarbons Versus Temperature and Pressure. *Int. J. Thermophys.* 1995, *16*, 1309–1334.
- Haar, L.; Gallagher, J. S.; Kell, G. S. NBS/NRC Steam Tables: Thermodynamic and Transport Properties and Computer Programs for Vapor and Liquid States of Water in SI Units; Hemisphere: New York, 1984.
- Oshmyansky, Y.; Hanley, H. J. M.; Ely, J. F.; Kidnay, A. J. The Viscosities and Densities of Selected Organic Compounds and Mixtures of Interest in Coal Liquefaction Studies. *Int. J. Thermo*phys. **1986**, 7, 99–608.
- TRC Data Bases for Chemistry and Engineering-TRC Thermodynamic Tables, Version 1996-1S; Thermodynamics Research Center, The Texas A&M University System: College Station, TX, 1996, bf 1977; d-3290; d-9435.
- Vargaftik, N. B. Tables on the Thermodynamical Properties of Liquids and Gases, 2nd ed.; Hemisphere: Washington, DC, 1975.
- Yu, C. H.; Tsai, F. N. Excess Volumes of (Tetralin + an n-Alkan-1-ol). J. Chem. Thermodyn. 1994, 26, 191–195.

Received for review April 1, 1996. Accepted June 19, 1996. $^{\circ}$ The financial support from the National Science Council, ROC, through Grant No. NSC83-0402-E011-07 is gratefully acknowledged.

JE960120F

[®] Abstract published in Advance ACS Abstracts, August 1, 1996.