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Densities of Binary Mixtures of Hexadecane with *m*-Xylene and Tetralin 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 + hexadecane and tetralin + hexadecane at temperatures from 333 K to 413 K and pressures up to 30 MPa. The Tait equation correlated accurately the density data. Isothermal compressibilities of hexadecane and the mixtures were then calculated with the aid of the Tait equation. The excess volumes of *m*-xylene + hexadecane are positive over the entire experimental conditions. The isothermal excess volumes of tetralin + hexadecane are negative at 333 K and 373 K but were found to vary from positive to negative with increasing tetralin mole fraction at 413 K.

Introduction

Liquid densities of the mixtures containing model compounds of coal liquids such as *m*-cresol, *m*-xylene, tetralin, quinoline, hexadecane, and 1-methylnaphthalene are useful for developing coal liquefaction processes. As a continuation of our previous work (Chang and Lee, 1995, 1996; Chang et al., 1996, 1997), liquid densities of *m*-xylene + hexadecane and tetralin + hexadecane were measured in the present study at temperatures from 333 K to 413 K and pressures up to 30 MPa. Density data are available in the literature for pure *m*-xylene, tetralin, and hexadecane (Heric and Brewer, 1967; Dymond et al., 1979; Oshmyansky et al., 1986; Goncalves et al., 1989; Serrano et al., 1990; Banipal et al., 1991; TRC Tables, 1993; Yu and Tsai, 1994), but most of the data were measured at near ambient conditions. Recently, Chang et al. (1996) reported the liquid densities of *m*-xylene + quinoline and *m*-xylene + tetralin in a temperature range of 333 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 two hexadecane-containing mixtures.

Table 1. Densities of Hexadecane

T/K	P/MPa	ρ/g·cm^{-3} this work	ρ/g·cm^{-3} lit.	ref
333.15	0.1	0.7462	0.746 1	TRC, d-1014 (1973)
			0.745 92	Banipal et al. (1991)
	5.0	0.7502	0.749 51	Banipal et al. (1991)
	10.0	0.7541	0.753 12	Banipal et al. (1991)
373.15	0.1	0.7183	0.718 0	TRC, d-1014 (1973)
			0.717 83	Banipal et al. (1991)
			0.718 6	Dymond et al. (1979)
	5.0	0.7233	0.722 46	Banipal et al. (1991)
	10.0	0.7279	0.726 69	Banipal et al. (1991)
413.15	0.1	0.6901		

Table 2. Experimental Density and Calculated Isothermal Compressibility for Hexadecane

	333.15 K		373.15 K		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}
0.1	0.7462	11.21	0.7183	14.55	0.6901	20.01
5.0	0.7502	10.58	0.7233	13.47	0.6964	17.75
10.0	0.7541	10.00	0.7279	12.53	0.7024	15.94
15.0	0.7577	9.491	0.7323	11.71	0.7077	14.47
20.0	0.7612	9.032	0.7365	11.00	0.7127	13.26
25.0	0.7647	8.619	0.7405	10.38	0.7172	12.25
30.0	0.7679	8.242	0.7443	9.819	0.7215	11.38

Experimental Section

m-Xylene (99 mass %), tetralin (99 mass %), and hexadecane (99 mass %) were purchased from Aldrich Chemicals. The impurities in the chemicals, analyzed with gas chromatography, were found to be 0.3%, 0.8%, and 0.4% for *m*-xylene, tetralin, and hexadecane, respectively. All the substances were used without further purification. Mixture samples (about 30 g) were prepared by mass with an accuracy of ±0.0002 in mole fraction. A hand pump (model 2426-801, Ruska) was employed to charge the sample into the oscillating U-tube of a DMA-512 densimeter (Anton Paar) and to adjust the pressure in the system. The pressure in the measuring cell was monitored by a pressure transducer (model-PDCR 330, 0-40 MPa, Druck) with a digital indicator (model-DPI 261, Druck). The accuracy of pressure measurements was better than ±0.75%. A circulating thermostated silicon oil bath was used to control the temperature of the measuring cell 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 U-tube (t_i) was displayed by a DMA-60 processing unit (Anton Paar), and t_i was then converted into density (ρ_i) via

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

where A and B are apparatus constants determined by using pure water (Haar et al., 1984) and dry nitrogen (Vargaftik, 1975) as calibrated fluids. The calibration was made at each temperature of interest over (0.1−30) MPa. It was found that the values of A decrease with increase in both pressure and temperature. The correlations of A

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

	333.15 K		373.15 K		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}
			$x_1 = 0.1000$			
0.1	0.7498	11.23	0.7212	14.54	0.6921	20.12
5.0	0.7538	10.55	0.7261	13.45	0.6986	17.77
10.0	0.7577	9.939	0.7309	12.51	0.7043	15.88
15.0	0.7614	9.399	0.7353	11.70	0.7098	14.38
20.0	0.7649	8.917	0.7395	10.99	0.7146	13.14
25.0	0.7682	8.485	0.7434	10.36	0.7192	12.10
30.0	0.7713	8.092	0.7472	9.807	0.7233	11.22
			$x_1 = 0.2000$			
0.1	0.7539	11.13	0.7248	14.73	0.6951	19.90
5.0	0.7580	10.52	0.7298	13.58	0.7015	17.71
10.0	0.7619	9.970	0.7346	12.58	0.7075	15.94
15.0	0.7655	9.474	0.7391	11.73	0.7130	14.51
20.0	0.7690	9.027	0.7433	10.98	0.7178	13.31
25.0	0.7725	8.624	0.7473	10.33	0.7223	12.31
30.0	0.7758	8.256	0.7511	9.760	0.7267	11.45
			$x_1 = 0.4000$			
0.1	0.7642	11.30	0.7339	14.67	0.7029	20.60
5.0	0.7683	10.61	0.7390	13.60	0.7096	18.25
10.0	0.7722	9.992	0.7440	12.67	0.7158	16.36
15.0	0.7760	9.446	0.7485	11.86	0.7213	14.84
20.0	0.7796	8.958	0.7528	11.16	0.7265	13.59
25.0	0.7830	8.520	0.7568	10.53	0.7310	12.53
30.0	0.7862	8.125	0.7608	9.977	0.7356	11.64
			$x_1 = 0.5000$			
0.1	0.7705	11.41	0.7397	14.89	0.7078	20.67
5.0	0.7746	10.72	0.7448	13.73	0.7145	18.29
10.0	0.7787	10.10	0.7498	12.72	0.7208	16.40
15.0	0.7825	9.546	0.7544	11.85	0.7265	14.86
20.0	0.7862	9.055	0.7588	11.10	0.7315	13.60
25.0	0.7897	8.615	0.7628	10.45	0.7363	12.55
30.0	0.7930	8.217	0.7667	9.865	0.7409	11.65
			$x_1 = 0.5999$			
0.1	0.7781	11.32	0.7464	15.23	0.7136	20.95
5.0	0.7823	10.65	0.7518	14.01	0.7206	18.56
10.0	0.7864	10.04	0.7569	12.95	0.7269	16.64
15.0	0.7902	9.506	0.7616	12.05	0.7327	15.10
20.0	0.7939	9.026	0.7660	11.27	0.7380	13.83
25.0	0.7974	8.595	0.7703	10.59	0.7428	12.76
30.0	0.8007	8.204	0.7742	9.990	0.7475	11.85
			$x_1 = 0.8000$			
0.1	0.7985	11.39	0.7649	15.14	0.7295	21.83
5.0	0.8028	10.74	0.7703	13.96	0.7368	19.16
10.0	0.8070	10.14	0.7755	12.93	0.7436	17.06
15.0	0.8110	9.613	0.7805	12.05	0.7495	15.38
20.0	0.8148	9.139	0.7851	11.29	0.7550	14.01
25.0	0.8185	8.712	0.7893	10.62	0.7601	12.88
30.0	0.8219	8.325	0.7934	10.03	0.7649	11.92
			$x_1 = 0.9000$			
0.1	0.8123	11.24	0.7775	15.18	0.7408	22.41
5.0	0.8166	10.60	0.7831	14.03	0.7485	19.55
10.0	0.8209	10.02	0.7884	13.03	0.7553	17.31
15.0	0.8249	9.507	0.7933	12.17	0.7614	15.55
20.0	0.8287	9.043	0.7981	11.42	0.7670	14.12
25.0	0.8324	8.625	0.8025	10.76	0.7724	12.95
30.0	0.8359	8.245	0.8067	10.18	0.7772	11.96

Table 4. Experimental Density and Calculated Isothermal Compressibility for Tetralin (1) + Hexadecane (2)

	333.15 K		373.15 K		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}
			$x_1 = 0.1000$			
0.1	0.7566	10.73	0.7279	14.18	0.6988	19.57
5.0	0.7606	10.22	0.7327	13.14	0.7050	17.30
10.0	0.7644	9.748	0.7374	12.23	0.7110	15.48
15.0	0.7679	9.317	0.7418	11.44	0.7162	14.02
20.0	0.7713	8.924	0.7459	10.75	0.7210	12.82
25.0	0.7748	8.567	0.7498	10.15	0.7255	11.81
30.0	0.7781	8.238	0.7535	9.609	0.7296	10.96
			$x_1 = 0.2000$			
0.1	0.7676	10.99	0.7384	13.92	0.7086	18.97
5.0	0.7716	10.29	0.7433	12.92	0.7149	16.89
10.0	0.7755	9.666	0.7479	12.04	0.7205	15.20
15.0	0.7791	9.116	0.7523	11.28	0.7258	13.83
20.0	0.7825	8.628	0.7565	10.62	0.7307	12.69
25.0	0.7858	8.192	0.7603	10.03	0.7351	11.74
30.0	0.7890	7.800	0.7640	9.503	0.7392	10.92
			$x_1 = 0.4000$			
0.1	0.7937	10.06	0.7636	13.17	0.7325	18.34
5.0	0.7975	9.526	0.7684	12.23	0.7387	16.24
10.0	0.8012	9.043	0.7730	11.41	0.7444	14.56
15.0	0.8048	8.609	0.7772	10.69	0.7495	13.20
20.0	0.8082	8.216	0.7812	10.07	0.7543	12.08
25.0	0.8114	7.859	0.7851	9.512	0.7586	11.14
30.0	0.8145	7.533	0.7887	9.017	0.7628	10.34
			$x_1 = 0.5000$			
0.1	0.8095	9.721	0.7791	12.73	0.7477	17.52
5.0	0.8132	9.232	0.7838	11.85	0.7538	15.63
10.0	0.8170	8.786	0.7884	11.08	0.7595	14.09
15.0	0.8206	8.383	0.7926	10.40	0.7646	12.84
20.0	0.8239	8.015	0.7966	9.804	0.7692	11.80
25.0	0.8270	7.680	0.8004	9.275	0.7736	10.92
30.0	0.8302	7.374	0.8040	8.803	0.7777	10.16
			$x_1 = 0.6001$			
0.1	0.8279	9.361	0.7970	12.59	0.7654	17.00
5.0	0.8315	8.908	0.8017	11.60	0.7713	15.12
10.0	0.8351	8.491	0.8062	10.75	0.7769	13.60
15.0	0.8386	8.114	0.8104	10.02	0.7820	12.36
20.0	0.8420	7.771	0.8143	9.378	0.7866	11.34
25.0	0.8452	7.456	0.8180	8.821	0.7909	10.47
30.0	0.8483	7.167	0.8215	8.328	0.7949	9.735
			$x_1 = 0.8000$			
0.1	0.8745	8.775	0.8426	11.06	0.8103	15.32
5.0	0.8781	8.264	0.8471	10.38	0.8161	13.70
10.0	0.8817	7.803	0.8513	9.772	0.8213	12.37
15.0	0.8850	7.392	0.8554	9.234	0.8262	11.28
20.0	0.8881	7.023	0.8592	8.754	0.8307	10.38
25.0	0.8912	6.692	0.8629	8.324	0.8348	9.613
30.0	0.8942	6.391	0.8664	7.935	0.8388	8.955
			$x_1 = 0.9000$			
0.1	0.9040	7.987	0.8718	10.35	0.8389	14.21
5.0	0.9074	7.657	0.8761	9.712	0.8445	12.81
10.0	0.9109	7.350	0.8802	9.143	0.8496	11.65
15.0	0.9142	7.067	0.8841	8.640	0.8543	10.69
20.0	0.9174	6.806	0.8879	8.192	0.8588	9.876
25.0	0.9205	6.565	0.8915	7.789	0.8630	9.183
30.0	0.9232	6.339	0.8948	7.425	0.8667	8.583

with pressure have been reported by Chang et al. (1997). Densities of water were reproduced to an average absolute deviation of 0.01% over the entire range of the calibrated conditions. The uncertainty of the reported densities in Tables 1−4 was estimated to be $\pm 1.0 \times 10^{-4}$ g·cm^{-3}.

Results and Discussion

While the comparison of experimental densities with literature has been made by Chang et al. (1996) for *m*-xylene and tetralin, Table 1 lists the measured densities of hexadecane in comparing with the literature values. The agreement is satisfactory at low pressures. However, our measurements are higher than those of Banipal et al. (1991) by about 0.001 g·cm^{-3} at 10.0 MPa. Table 2 presents the experimental densities and the calculated isothermal compressibilities (κ_T) of hexadecane. Those for *m*-xylene and tetralin have been reported by Chang et al. (1996). The results for *m*-xylene + hexadecane and tetralin + hexadecane mixtures are compiled in Tables 3 and 4, respectively. The pressure effects on liquid den-

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

		m-xylene (1) + hexadecane (2)				tetralin (1) + hexadecane (2)			
T/K	x_1	C	D/MPa	$10^4\pi_1{}^a$	$10^5\sigma^b$/g·cm^{-3}	C	D/MPa	$10^4\pi_1{}^a$	$10^5\sigma^b$/g·cm^{-3}
333.15	0.0	0.083 95	74.81	0.4	5.0	0.083 95	74.81	0.4	5.0
333.15	0.1	0.078 61	69.92	0.4	6.3	0.094 41	87.85	0.8	10.0
333.15	0.2	0.085 93	77.10	0.3	3.6	0.073 35	66.67	0.4	5.2
333.15	0.4	0.078 47	69.36	0.2	2.2	0.081 27	80.72	0.2	1.8
333.15	0.5	0.079 55	69.64	0.2	2.0	0.082 59	84.86	0.5	6.2
333.15	0.6	0.080 62	71.12	0.1	0.8	0.082 73	88.28	0.5	6.1
333.15	0.8	0.083 36	73.08	0.2	2.3	0.064 95	73.93	0.4	5.5
333.15	0.9	0.083 37	74.06	0.1	1.1	0.083 33	104.23	0.6	9.2
333.15	1.0^c	0.085 66	76.30	0.3	3.8	0.076 58	102.50	0.3	7.9
373.15	0.0	0.081 24	55.73	0.3	3.6	0.081 24	55.73	0.3	3.6
373.15	0.1	0.081 16	55.74	0.2	2.6	0.080 38	56.60	0.2	1.8
373.15	0.2	0.078 08	52.90	0.2	2.0	0.080 74	57.91	0.3	3.3
373.15	0.4	0.083 72	56.98	0.4	4.9	0.077 45	58.72	0.3	4.0
373.15	0.5	0.078 81	52.82	0.2	2.2	0.077 34	60.65	0.3	3.4
373.15	0.6	0.078 31	51.31	0.2	2.0	0.067 39	53.42	0.2	2.7
373.15	0.8	0.079 91	52.67	0.5	5.5	0.076 36	68.95	0.2	2.5
373.15	0.9	0.082 99	54.57	0.3	4.8	0.071 91	69.41	0.2	3.5
373.15	1.0^c	0.081 28	52.82	0.3	3.2	0.069 77	72.24	0.3	4.4
413.15	0.0	0.071 38	35.58	0.4	5.7	0.071 38	35.58	0.4	5.7
413.15	0.1	0.068 86	34.12	0.6	6.5	0.067 66	34.47	0.5	6.9
413.15	0.2	0.072 86	36.52	0.6	7.8	0.069 74	36.66	0.5	4.7
413.15	0.4	0.072 30	35.00	0.8	9.8	0.064 79	35.23	0.4	5.7
413.15	0.5	0.072 11	34.79	0.7	6.8	0.066 08	37.62	0.6	7.3
413.15	0.6	0.073 51	34.99	0.4	6.5	0.062 47	36.64	0.3	3.9
413.15	0.8	0.070 95	32.40	0.5	5.5	0.059 43	38.70	0.3	3.5
413.15	0.9	0.069 35	30.84	1.0	12.3	0.059 81	41.99	0.3	4.4
413.15	1.0^c	0.077 76	35.10	0.5	5.8	0.066 43	52.32	0.4	5.7

[a] π_1 as defined in eq 3. [b] σ(g·cm^{-3}) = $[(\sum_{k=1}^{n}(\rho_{k,\text{calc}} - \rho_k)^2)/(n - 2)]^{1/2}$, where n is number of data points. All the points at 0.1 MPa are not included. [c] Densities for pure *m*-xylene and tetralin have been reported by Chang et al. (1996).

Table 6. Excess Volume for *m*-Xylene (1) + Hexadecane (2)

	V^E/cm^3·mol^{-1}						
x_1	0.1 MPa	5.0 MPa	10.0 MPa	15.0 MPa	20.0 MPa	25.0 MPa	30.0 MPa
			T = 333.15 K				
0.1	0.06	0.07	0.07	0.05	0.05	0.10	0.17
0.2	0.10	0.11	0.10	0.10	0.11	0.13	0.12
0.4	0.15	0.15	0.14	0.12	0.13	0.17	0.18
0.5	0.18	0.17	0.15	0.14	0.13	0.14	0.14
0.6	0.16	0.16	0.15	0.14	0.13	0.15	0.16
0.8	0.10	0.08	0.07	0.06	0.04	0.05	0.05
0.9	0.08	0.08	0.07	0.08	0.07	0.08	0.08
			T = 373.15 K				
0.1	0.22	0.24	0.22	0.21	0.23	0.26	0.26
0.2	0.30	0.30	0.28	0.28	0.29	0.30	0.31
0.4	0.36	0.38	0.34	0.35	0.32	0.35	0.34
0.5	0.38	0.39	0.37	0.36	0.35	0.36	0.37
0.6	0.38	0.35	0.32	0.30	0.28	0.27	0.28
0.8	0.25	0.27	0.26	0.22	0.21	0.23	0.24
0.9	0.19	0.19	0.19	0.19	0.17	0.17	0.16
			T = 413.15 K				
0.1	0.46	0.39	0.53	0.47	0.51	0.53	0.59
0.2	0.56	0.57	0.62	0.58	0.64	0.67	0.65
0.4	0.66	0.61	0.60	0.63	0.59	0.65	0.60
0.5	0.66	0.65	0.64	0.64	0.68	0.67	0.66
0.6	0.65	0.61	0.62	0.61	0.60	0.62	0.59
0.8	0.52	0.47	0.43	0.47	0.47	0.46	0.48
0.9	0.32	0.27	0.25	0.30	0.31	0.27	0.31

Table 7. Excess Volume for Tetralin (1) + Hexadecane (2)

	V^E/cm^3·mol^{-1}						
x_1	0.1 MPa	5.0 MPa	10.0 MPa	15.0 MPa	20.0 MPa	25.0 MPa	30.0 MPa
			T = 333.15 K				
0.1	−0.35	−0.36	−0.34	−0.31	−0.28	−0.27	−0.30
0.2	−0.48	−0.49	−0.50	−0.51	−0.47	−0.42	−0.43
0.4	−0.61	−0.56	−0.54	−0.53	−0.52	−0.47	−0.45
0.5	−0.63	−0.56	−0.57	−0.58	−0.55	−0.49	−0.49
0.6	−0.66	−0.60	−0.57	−0.58	−0.58	−0.54	−0.53
0.8	−0.63	−0.60	−0.62	−0.60	−0.56	−0.53	−0.52
0.9	−0.35	−0.32	−0.31	−0.29	−0.28	−0.29	−0.25
			T = 373.15 K				
0.1	−0.15	−0.11	−0.13	−0.12	−0.10	−0.07	−0.05
0.2	−0.23	−0.21	−0.20	−0.21	−0.21	−0.17	−0.15
0.4	−0.33	−0.30	−0.29	−0.26	−0.22	−0.22	−0.18
0.5	−0.39	−0.34	−0.35	−0.33	−0.31	−0.28	−0.25
0.6	−0.43	−0.42	−0.41	−0.40	−0.36	−0.34	−0.29
0.8	−0.47	−0.45	−0.43	−0.42	−0.39	−0.40	−0.37
0.9	−0.44	−0.39	−0.41	−0.40	−0.40	−0.39	−0.36
			T = 413.15 K				
0.1	0.09	0.12	0.15	0.15	0.21	0.24	0.29
0.2	0.20	0.17	0.30	0.29	0.29	0.34	0.37
0.4	0.25	0.21	0.28	0.30	0.31	0.38	0.38
0.5	0.06	0.06	0.10	0.13	0.18	0.22	0.21
0.6	−0.10	−0.09	−0.05	−0.04	−0.01	0.04	0.08
0.8	−0.32	−0.34	−0.27	−0.27	−0.24	−0.19	−0.17
0.9	−0.25	−0.26	−0.23	−0.22	−0.20	−0.18	−0.16

sity at constant conditions of temperature and concentration are represented by the Tait equation

$$\frac{\rho - \rho_0}{\rho} = C \ln\left(\frac{D + P}{D + 0.1}\right) \tag{2}$$

where ρ_0 is the density at 0.1 MPa and P is the system pressure in MPa. The values of C and D were determined by fitting the Tait equation to the isothermal density data at a given composition. The objective function of the optimization is given by

$$\pi_1 = [\sum_{k=1}^{n} |\rho_{k,\text{calc}} - \rho_k|/\rho_k]/n \tag{3}$$

where n is the number of data points. $\rho_{k,\text{calc}}$ and ρ_k represent the calculated and experimental densities, respectively, for the kth point. Table 5 lists the calculated results of C, D, π_1, and the standard deviations of the fits

Table 8. Results of the Excess Volume Correlations with Eq 7

		m-xylene (1) + hexadecane (2)				tetralin (1) + hexadecane (2)			
T/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	0.6574	0.0810	0.0941	0.8	−2.506	−0.6610	−2.890	0.7
333.15	5.0	0.6163	−0.0080	0.2226	1.0	−2.292	−0.3457	−2.957	1.3
333.15	10.0	0.5513	−0.0232	0.2705	1.1	−2.260	−0.5180	−3.115	1.1
333.15	15.0	0.5040	0.0495	0.2492	1.3	−2.302	−0.5631	−2.721	1.9
333.15	20.0	0.4938	−0.0680	0.2253	1.4	−2.212	−0.7294	−2.531	1.3
333.15	25.0	0.5679	−0.2448	0.4594	1.7	−1.995	−0.7348	−2.681	0.8
333.15	30.0	0.5199	−0.5122	1.043	3.3	−1.955	−0.4345	−2.693	1.0
373.15	0.1	1.454	−0.2187	1.132	1.5	−1.520	−1.310	−1.948	0.7
373.15	5.0	1.458	−0.3112	1.287	1.3	−1.421	−1.373	−1.576	0.9
373.15	10.0	1.331	−0.1647	1.339	1.3	−1.392	−1.186	−1.632	0.3
373.15	15.0	1.292	−0.2286	1.337	2.2	−1.340	−1.166	−1.527	0.8
373.15	20.0	1.220	−0.4198	1.413	1.6	−1.221	−1.189	−1.496	1.4
373.15	25.0	1.264	−0.5313	1.561	2.0	−1.151	−1.355	−1.429	1.2
373.15	30.0	1.281	−0.5716	1.535	1.9	−1.014	−1.286	−1.165	1.9
413.15	0.1	2.575	−0.6900	2.620	2.9	0.3368	−2.527	−1.864	2.6
413.15	5.0	2.548	−0.7180	1.771	2.1	0.2364	−2.666	−1.660	1.7
413.15	10.0	2.431	−1.558	2.818	5.3	0.5002	−2.772	−1.400	2.2
413.15	15.0	2.469	−0.9422	2.647	2.9	0.5658	−2.708	−1.411	2.0
413.15	20.0	2.436	−1.176	3.209	4.0	0.6569	−2.835	−1.073	1.5
413.15	25.0	2.564	−1.488	2.886	3.7	0.8717	−2.915	−0.9082	1.6
413.15	30.0	2.367	−1.513	3.856	5.4	0.8891	−3.023	−0.4158	1.5

[a] $\pi_2 = [\sum_{k=1}^{n}|V^E_{k,\mathrm{calc}} - V^E_k|]/n$.

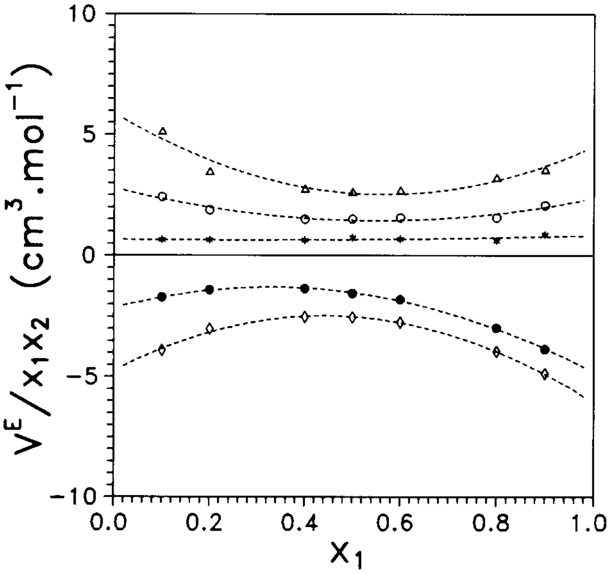

Figure 1. Temperature effects on the excess volumes at 0.1 MPa for *m*-xylene (1) + hexadecane (2), (*) 333.15 K, (○) 373.15 K, (△) 413.15 K and for tetralin (1) + hexadecane (2), (◇) 333.15 K, (●) 373.15 K; (- - -) calculated from eq 7.

(σ). It indicates that the Tait equation correlates accurately the densities over the entire pressure range. The isothermal compressibilities κ_T as tabulated in Tables 2−4 were obtained by differentiation of the Tait equation

$$\kappa_T = \frac{-1}{V}\left(\frac{\partial V}{\partial P}\right)_{T,x} = \frac{V_0}{V}\left(\frac{C}{D+P}\right) \tag{4}$$

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

Volume change of mixing or excess volume (V^E) is related to the intermolecular interactions in a mixture. The excess volume can be calculated from experimental density data via

$$V^E = V_m - x_1V_1{}^\circ - x_2V_2{}^\circ \tag{5}$$

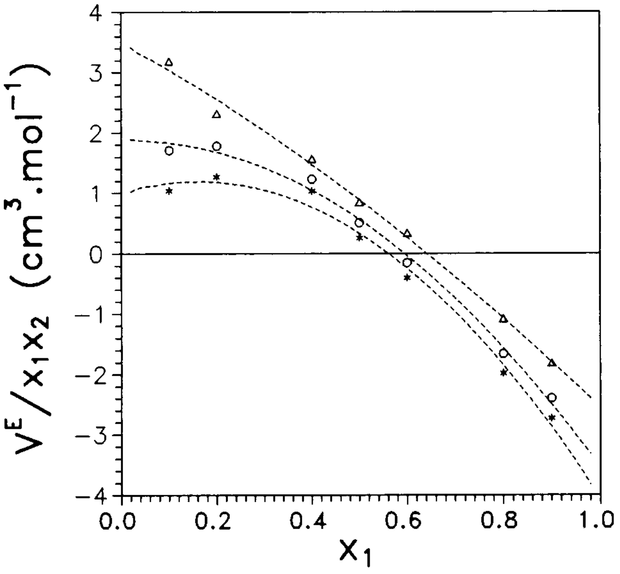

Figure 2. Pressure effects on the excess volumes at 413.15 K for tetralin (1) + hexadecane (2), (*) 0.1 MPa, (○) 15.0 MPa, (△) 30.0 MPa; (- - -) calculated from eq 7.

with

$$V_m = \frac{x_1M_1 + x_2M_2}{\rho} \tag{6}$$

where V_m is the molar volume of a mixture. x_i, $V_i{}^\circ$, and M_i are the mole fraction, molar volume, and molecular weight, respectively, for the component i. Tables 6 and 7 give the excess volumes for *m*-xylene + hexadecane and tetralin + hexadecane, respectively. The uncertainty of the calculated excess volumes is about ±0.05 cm^3·mol^{-1}. The isothermal excess volumes were correlated with a Redlich−Kister type equation:

$$V^E/x_1x_2 = \sum_{k=1}^{3} E_k(x_1 - x_2)^{k-1} \tag{7}$$

The optimized values of E_k were determined by a leastsquares algorithm. The correlated results are listed in Table 8 and represented by the dashed lines in Figures 1 and 2.

The excess volumes of *m*-xylene + hexadecane, as shown in Figure 1, are positive and increase with increasing temperature at a constant pressure. Figure 1 also illustrates that the excess volumes of tetralin + hexadecane are negative at lower temperatures (333 K and 373 K). V^E for tetralin + hexadecane at 413 K is shown as a function of pressure in Figure 2, in which the excess volumes vary from positive to negative with increase in the mole fraction of tetralin. Pressure may either enhance the volume expansion or reduce the volume contraction. At the transition points ($V^E = 0\ \mathrm{cm^3 \cdot mol^{-1}}$), the mixtures behave as a pseudo ideal solution. This particular behavior may be of interest in studying the intermolecular interactions.

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