Vapor−Liquid Equilibria of Binary and Ternary Mixtures of Cyclohexane, 3-Methyl-2-Butanone, and Octane at 101.3 kPa

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Vapor−liquid equilibria were measured at 101.3 kPa for the three binary and one ternary mixtures of cyclohexane, 3-methyl-2-butanone, and octane. The isobaric $T-x-y$ data were reported, including an azeotropic point for the binary mixture cyclohexane + 3-methyl-2-butanone. The virial equation of state truncated after the second coefficient was used to calculate the vapor-phase fugacity coefficients. The Tsonopoulos correlation equation was applied to determine the second virial coefficients. Various activity coefficient models of the Wilson, the NRTL, and the UNIQUAC equations were used to correlate the binary experimental vapor−liquid equilibrium results. Optimally-fitted binary parameters of the activity coefficient models were obtained and those paramters of the NRTL model were employed to predict the ternary vapor−liquid equilibria. Satisfactory results were presented for the correlation and prediction of the vapor−liquid equilibrium data on binary and ternary mixtures.

Introduction

Vapor−liquid equilibria (VLE) are important to the design and improvement of chemical processes. To our knowledge, the experimental data for the VLE of the binary and ternary mixtures of cyclohexane, 3-methyl-2-butanone, and octane at a fixed pressure of 101.3 kPa were not all available in the literature. The VLE on these mixtures were measured in this work. All-glass recirculating equipment was used to measure the equilibrium temperatures and compositions of the coexisting phases. The results were examined for thermodynamic consistency and were correlated by various activity coefficient models. These models with their optimally-fitted binary parametes were then used to predict the VLE of binary and ternary mixtures.

Experimental Section

Chemicals. All the chemicals were high-purity grade purchased from the Merck Co. No detectable impurities of cyclohexane and octane were found on the gas chromatography (GC) analyses, and these two chemicals were used without further purification. 3-Methyl-2-butanone (MIPK) was purified in a distillation column at a reduced pressure. The purity of cyclohexane was better than 99.9%, and those of octane and 3-methyl-2-butanone were better than 99.6% on the GC analyses. The pure compound properties were measured in this work, and the comparisons with literature data are shown in Table 1. The refractive indices of pure chemicals were measured at (293.15 ± 0.1) K by an Abbe refractometer, Atago 3T, with an accuracy of ±0.0001. The densities of pure compounds were measured at (293.15 ± 0.01) K using the Anton Paar DMA 60/601 density meter with an accuracy of $\pm 1.0 \times 10^{-5}$ g/cm^3.

Apparatus and Procedures. The apparatus used was an all-glass recirculating still described by Paul (1976). This equipment has a side-heating unit which ensures complete mixing of the liquid mixture. The design also prevented liquid drop entrainment and partial condensation in the vapor phase. The equilibrium temperatures were measured by a digital quartz thermometer (DMT-610, Tokyo Electrical, Japan) with an accuracy of ±0.01 K. The pressure was maintained at 101.3 kPa through a dibutyl phthalate manometer. The accuracy of the pressure control was within ±0.05%.

Table 1. Comparison of the Measured Normal Boiling Temperatures, Refractive Indices, and Densities of Pure Fluids in This Work with Literature Data[a]

	T_b/K		n_D (293.15 K)		ρ (293.15 K)/g cm^{-3}	
component	exp	lit.	exp	lit.	exp	lit.
cyclohexane	353.87	353.93	1.4266	1.4262	0.7784	0.7785
3-methyl-2-butanone	367.44	367.50	1.3879	1.3882	0.8046	0.8032
octane	398.76	398.83	1.3974	1.3974	0.7024	0.7026

[a] Literature values were taken from TRC Data Bases (1995).

In each experiment, the liquid mixture was heated in a recirculating still at a fixed pressure of 101.3 kPa. Equilibrium was reached after 1 h where the temperatures of the liquid and vapor phases were constant and their difference was within 0.02 K. Samples of the equilibrium phases were taken at small volumes and were analyzed in a gas chromatograph.

A Shimadzu GC, type 8A, equipped with a thermal conductivity detector, was used to determine the equilibrium compositions. The GC column was made of a 3 m length stainless steel tube with 3 mm diameter and was packed with Porapak Q. The GC response peaks were integrated by using a Shimadzu C-R3A integrator. The temperature of the injection port of the GC was maintained at 553.15 K. The oven temperature of the GC was at 523.15 K. Helium gas with a purity of 99.9% was used as the carrier gas at a flow rate of 25 cm^3/min. The GC was calibrated using mixtures of known compositions which were prepared gravimetrically. More than two analyses were made for each vapor and liquid composition, respectively. With these repeated procedures, the accuracy of the equilibrium composition measurements was within ±0.001 mole fraction.

Results and Discussion

VLE had been measured at 101.3 kPa for three binary mixtures of cyclohexane + 3-methyl-2-butanone, cyclohex-

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Table 2. Experimental VLE Data for Cyclohexane (1) + 3-Methyl-2-butanone (2) at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_2
367.44	0.0000	0.0000		1.0000
364.46	0.0523	0.1350	1.9982	0.9946
361.87	0.1057	0.2423	1.8884	0.9968
360.95	0.1277	0.2798	1.8462	0.9988
359.37	0.1701	0.3432	1.7682	1.0050
358.70	0.1890	0.3682	1.7365	1.0100
357.84	0.2185	0.4040	1.6843	1.0159
356.79	0.2590	0.4475	1.6168	1.0269
355.56	0.3112	0.4958	1.5393	1.0488
354.88	0.3467	0.5248	1.4887	1.0656
354.12	0.3963	0.5609	1.4199	1.0928
353.71	0.4209	0.5773	1.3911	1.1117
353.20	0.4620	0.6028	1.3412	1.1440
352.48	0.5351	0.6442	1.2612	1.2158
352.25	0.5635	0.6592	1.2329	1.2504
351.89	0.6255	0.6912	1.1754	1.3382
351.62	0.6820	0.7202	1.1310	1.4428
351.51	0.7334	0.7478	1.0946	1.5593
351.48	0.7643	0.7655	1.0756	1.6434
351.51	0.8037	0.7901	1.0541	1.7675
351.56	0.8215	0.8021	1.0452	1.8312
351.59	0.8353	0.8119	1.0393	1.8858
351.69	0.8525	0.8248	1.0313	1.9568
351.78	0.8693	0.8385	1.0252	2.0318
351.86	0.8795	0.8472	1.0213	2.0811
352.01	0.8969	0.8632	1.0157	2.1697
352.16	0.9116	0.8778	1.0116	2.2521
352.33	0.9254	0.8926	1.0082	2.3354
352.42	0.9318	0.8999	1.0068	2.3754
352.85	0.9576	0.9325	1.0023	2.5480
353.87	1.0000	1.0000	1.0000	

Table 3. Experimental VLE Data for Cyclohexane (1) + Octane (3) at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_3
398.76	0.0000	0.0000		1.0000
396.25	0.0372	0.1010	0.9670	0.9973
393.84	0.0728	0.1910	0.9828	0.9931
391.95	0.1023	0.2561	0.9763	0.9922
391.80	0.1047	0.2616	0.9775	0.9915
389.05	0.1481	0.3492	0.9791	0.9899
386.79	0.1861	0.4182	0.9809	0.9863
385.41	0.2093	0.4568	0.9826	0.9853
383.20	0.2494	0.5180	0.9832	0.9809
381.08	0.2871	0.5720	0.9903	0.9751
379.19	0.3231	0.6154	0.9896	0.9754
377.41	0.3591	0.6562	0.9903	0.9709
375.82	0.3912	0.6895	0.9924	0.9683
374.31	0.4230	0.7198	0.9939	0.9653
373.09	0.4493	0.7432	0.9954	0.9623
372.11	0.4712	0.7615	0.9964	0.9594
370.67	0.5033	0.7862	0.9983	0.9577
369.72	0.5258	0.8027	0.9992	0.9538
368.71	0.5499	0.8194	1.0005	0.9497
367.09	0.5898	0.8445	1.0020	0.9449
365.60	0.6281	0.8666	1.0035	0.9382
364.20	0.6653	0.8856	1.0042	0.9358
363.10	0.6958	0.9002	1.0047	0.9314
362.09	0.7247	0.9128	1.0047	0.9298
359.72	0.7959	0.9405	1.0045	0.9266
359.02	0.8284	0.9483	1.0039	0.9267
357.85	0.8573	0.9610	1.0028	0.9259
357.03	0.8848	0.9692	1.0023	0.9316
355.24	0.9491	0.9870	1.0001	0.9470
353.87	1.0000	1.0000	1.0000	

ane + octane, and 3-methyl-2-butanone + octane. The results are presented in Tables 2−4, respectively. The liquid-phase activity coefficients γ were calculated by the classical equation

$$\gamma_i = (\hat{\phi}_i y_i P)/\{x_i P_i^{\text{sat}} \phi_i^{\text{sat}} \exp[V_i^{\text{L}}(P - P_i^{\text{sat}})/RT]\} \quad (1)$$

where ϕ is the fugacity coefficient and x and y are the

Table 4. Experimental VLE Data for 3-Methyl-2-butanone (2) and Octane (3) at 101.3 kPa

T/K	x_2	y_2	γ_2	γ_3
398.76	0.0000	0.0000		1.0000
393.87	0.0310	0.1402	2.3494	1.0102
389.29	0.0681	0.2683	2.2676	1.0142
385.82	0.1057	0.3614	2.1333	1.0187
383.48	0.1380	0.4210	2.0131	1.0264
381.41	0.1672	0.4679	1.9428	1.0386
379.45	0.2110	0.5162	1.7831	1.0583
377.93	0.2377	0.5466	1.7421	1.0757
377.01	0.2736	0.5715	1.6199	1.0982
376.05	0.2991	0.5972	1.5869	1.1032
373.95	0.3857	0.6505	1.4158	1.1686
373.22	0.4206	0.6712	1.3656	1.1940
372.73	0.4465	0.6868	1.3334	1.2102
372.24	0.4793	0.7005	1.2835	1.2504
371.68	0.5101	0.7175	1.2539	1.2775
371.34	0.5379	0.7270	1.2158	1.3239
370.67	0.5799	0.7499	1.1844	1.3652
370.15	0.6222	0.7659	1.1434	1.4465
369.88	0.6596	0.7819	1.1091	1.5108
369.40	0.6903	0.7991	1.0973	1.5556
369.23	0.7207	0.8141	1.0756	1.6071
369.04	0.7471	0.8276	1.0602	1.6582
368.57	0.7776	0.8435	1.0517	1.7405
368.44	0.8037	0.8573	1.0379	1.8081
368.21	0.8280	0.8726	1.0319	1.8589
368.05	0.8616	0.8925	1.0187	1.9636
367.99	0.8757	0.9005	1.0129	2.0293
367.91	0.8994	0.9178	1.0074	2.0807
367.76	0.9235	0.9347	1.0033	2.1883
367.59	0.9536	0.9576	1.0002	2.3617
367.57	0.9565	0.9604	1.0007	2.3551
367.56	0.9655	0.9683	0.9998	2.3800
367.53	0.9756	0.9776	0.9998	2.3828
367.49	0.9808	0.9825	1.0007	2.3702
367.47	0.9824	0.9836	1.0007	2.4251
367.46	0.9880	0.9887	1.0005	2.4530
367.45	0.9912	0.9918	1.0007	2.4290
367.45	0.9927	0.9933	1.0007	2.3929
367.44	1.0000	1.0000	1.0000	

Table 5. Pure Component Properties Used in This Work[a]

compound	T_c/K	P_c/bar	ω	a	b	c
cyclohexane	553.5	41.23	0.212	6.032 45	1244.124	−44.911
3-methyl-2-butanone	553.4	39.01	0.331	6.088 47	1264.546	−57.754
n-octane	568.8	25.23	0.398	6.042 31	1351.497	−64.014

[a] The critical constants and acentric factors were taken from Reid et al. (1987). The parameters in the vapor pressure equation ($\log P_i^{\text{sat}}$ (kPa) $= a_i - b_i/(T\text{ (K)} + c_i)$) were taken from Richard and Stanislaw (1987).

equilibrium mole fractions in the liquid and vapor phases, respectively. P^{sat} is the saturated vapor pressure, and V^{L} is the saturated liquid molar volume.

The fugacity coefficient was calculated by using the virial equation of state truncated at the second virial coefficient. The second virial coefficients were calculated by the empirical correlations according to Tsonopoulos (1974). The critical constants and acentric factors of cyclohexane, 3-methyl-2-butanone, and octane were taken from the literature (Reid et al., 1987), and these values are listed in Table 5. The vapor pressures of the pure compounds were expressed by the Antoine equation:

$$\log P_i^{\text{sat}}/\text{kPa} = a_i - b_i/[T/\text{K} + c_i] \quad (2)$$

The constants a, b, and c in eq 2 were taken from the literature (Richard and Stanislaw, 1987), and their values are also listed in Table 5. The liquid molar volumes were calculated by the Rackett equation (Spenser and Danner,

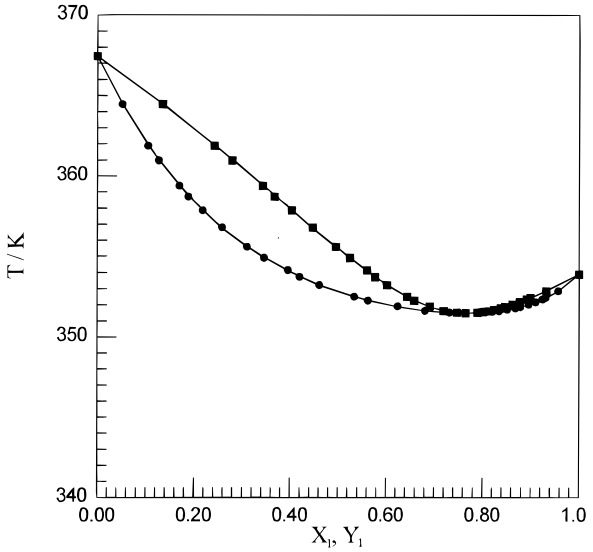

Figure 1. *Txy* curve for cyclohexane (1) + 3-methyl-2-butanone (2) at 101.3 kPa: (—) NRTL model. Experimental data: (●) liquid phase; (■) vapor phase.

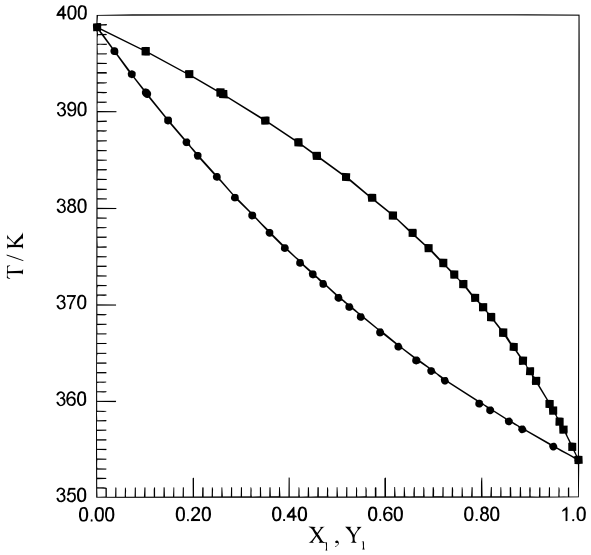

Figure 2. *Txy* curve for cyclohexane (1) + octane (3) at 101.3 kPa: (—) NTRL model. Experimental data: (●) liquid phase; (■) vapor phase.

Table 6. Consistency Test Results of the Binary VLE Experimental Data of This Work

binary systems	D	J	$D - J$
cyclohexane (1) + 3-methyl-2-butanone (2)	2.42	6.52	−4.10
cyclohexane (1) + octane (3)	0.0	10.03	−10.03
3-methyl-2-butanone (2) + octane (3)	0.13	12.79	−12.66

Table 7. Correlation Parameters and the Absolute Average Deviations in Boiling Temperatures (ΔT) and Vapor-Phase Mole Fractions (Δy) for the Binary and Ternary Mixtures

equations	A_{12}/J mol^{-1}	A_{21}/J mol^{-1}	α_{12}	Δy_1	ΔT/K
Cyclohexane (1) + 3-Methyl-2-butanone (2)					
Wilson	466.28	2693.32		0.0031	0.01
NRTL	4136.11	−1005.73	0.2	0.0033	0.02
UNIQUAC	1448.25	−537.07		0.0033	0.01
Cyclohexane (1) + Octane (3)					
Wilson	−822.88	1748.73		0.0053	0.02
NRTL	−237.23	122.96	0.2	0.0053	0.02
UNIQUAC	1191.78	−992.92		0.0061	0.02
3-Methyl-2-butanone (2) + Octane (3)					
Wilson	2969.61	212.98		0.0048	0.07
NRTL	1039.12	1896.50	0.2	0.0049	0.07
UNIQUAC	−666.42	1634.13		0.0051	0.07
Cyclohexane (1) + 3-Methyl-2-butanone (2) + Octane (3)					
NRTL				$\Delta y_1 = 0.0063$; $\Delta y_2 = 0.0026$; $\Delta T = 0.07$	

1972). The calculated activity coefficients for the binary systems were also presented in Tables 2−4. The binary mixture of cyclohexane and octane is a nearly ideal solution. The other two binary mixtures show positive deviations. These activity coefficients were used in the thermodynamic consistency test where the Herington method (Herington, 1951) was employed. In this method, the activity coefficient ratios of each binary system were plotted against the mole fraction and the following two terms were defined as

$$D = \frac{|K_1 - K_2|}{|K_1 + K_2|} \times 100 \qquad (3)$$

$$J = \frac{T_{max} - T_{min}}{T_{max}} \times 150 \qquad (4)$$

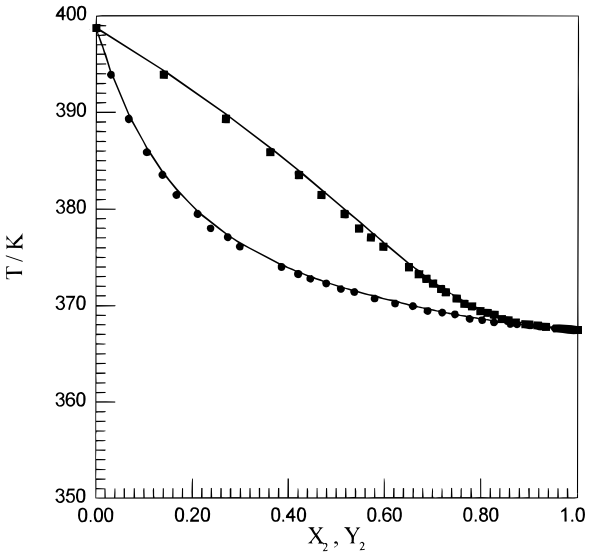

Figure 3. *Txy* curve for 3-methyl-2-butanone (2) + octane (3) at 101.3 kPa: (—) NRTL model. Experimental data: (●) liquid phase; (■) vapor phase.

where K_1 and K_2 are the areas lying above and below the axis where the logarithm of the activity ratio was zero, respectively. T_{max} and T_{min} were the maximum and minimum temperatures measured during the experiment. According to the Herington method, the experimental data were thermodynamically consistent if $(D - J)$ is less than 10. Table 6 lists the results of the thermodynamic consistency tests of this study. It is observed that the thermodynamic consistency requirement is satisfied for each of the binary systems. The experimental results also satisfied the thermodynamic consistency by using the Fredenslund method (Fredenslund et al., 1977), where the mean deviations in vapor-phase compositions were less than 0.006 for all three binary mixtures.

The experimental results were then used to obtain the binary parameters of various activity coefficient models. The Wilson, NRTL, and UNIQUAC models were employed in our regressions. The expressions of the activity coefficients by these models were listed in the literature

Table 8. Experimental VLE Data for Cyclohexane (1) + 3-Methyl-2-butanone (2) + Octane (3) at 101.3 kPa

T/K	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3	T/K	x_1	x_2	y_1	y_2	γ_1	γ_2	γ_3
367.01	0.0259	0.8214	0.0592	0.8323	1.6044	1.0298	1.8301	370.95	0.0724	0.4004	0.1227	0.6057	1.0765	1.3678	1.1658
364.37	0.1102	0.7061	0.2095	0.6863	1.4291	1.0702	1.5959	369.01	0.1452	0.3614	0.2327	0.5378	1.0689	1.4248	1.1211
360.09	0.2255	0.6495	0.3764	0.5678	1.4062	1.0990	1.4548	367.71	0.2123	0.3136	0.3277	0.4715	1.0480	1.4965	1.0920
357.65	0.3321	0.5581	0.4837	0.4752	1.3114	1.1563	1.3291	366.21	0.2695	0.2840	0.3936	0.4236	1.0466	1.5530	1.0825
357.02	0.3735	0.5214	0.5208	0.4446	1.2774	1.1815	1.1954	365.37	0.3261	0.2485	0.4598	0.3756	1.0327	1.6143	1.0523
356.20	0.4087	0.4935	0.5471	0.4208	1.2545	1.2130	1.2273	364.37	0.3879	0.2066	0.5304	0.3232	1.0279	1.7225	1.0155
355.27	0.4728	0.4357	0.5931	0.3796	1.2065	1.2772	1.1535	363.56	0.4272	0.1919	0.5654	0.2983	1.0164	1.7546	1.0346
354.85	0.4980	0.4177	0.6105	0.3650	1.1930	1.2985	1.1408	362.91	0.4617	0.1752	0.6024	0.2720	1.0193	1.7878	1.0225
354.57	0.5242	0.3953	0.6276	0.3498	1.1743	1.3270	1.1133	361.99	0.5152	0.1481	0.6661	0.2302	1.0351	1.8416	0.9396
353.72	0.5764	0.3481	0.6603	0.3179	1.1508	1.4079	1.1809	361.06	0.5604	0.1317	0.6934	0.2050	1.0155	1.8984	1.0395
353.55	0.6108	0.3188	0.6814	0.2996	1.1261	1.4569	1.1107	359.88	0.6387	0.0967	0.7636	0.1573	1.0129	2.0586	0.9812
353.44	0.6326	0.3034	0.6947	0.2896	1.1120	1.4830	1.0395	358.98	0.6931	0.0769	0.8056	0.1271	1.0091	2.1518	0.9912
353.28	0.6590	0.2793	0.7105	0.2746	1.0967	1.5377	1.0037	358.38	0.7357	0.0618	0.8392	0.1059	1.0067	2.2738	0.9381
353.14	0.6686	0.2739	0.7166	0.2719	1.0945	1.5597	0.8355	357.72	0.7694	0.0533	0.8632	0.0923	1.0082	2.3465	0.8890
352.87	0.7229	0.2244	0.7507	0.2375	1.0687	1.6777	0.9447	357.37	0.8023	0.0415	0.8863	0.0719	1.0023	2.3740	0.9597
352.82	0.7559	0.1970	0.7712	0.2182	1.0514	1.7587	0.9513	356.89	0.8357	0.0321	0.9108	0.0553	1.0020	2.3971	0.9355
352.73	0.7895	0.1680	0.7951	0.1962	1.0405	1.8598	0.8682	355.29	0.8686	0.0436	0.9085	0.0724	1.0054	2.4327	0.8405
352.67	0.8191	0.1447	0.8151	0.1769	1.0299	1.9507	0.9393	354.80	0.8531	0.0615	0.8817	0.0962	1.0072	2.3282	1.0177
352.68	0.8493	0.1197	0.8384	0.1547	1.0214	2.0615	0.9457	354.62	0.8696	0.0554	0.8907	0.0909	1.0032	2.4565	0.9711
352.74	0.8784	0.0961	0.8627	0.1316	1.0144	2.1801	0.9477	354.54	0.8870	0.0470	0.9096	0.0757	1.0066	2.4176	0.8842
352.87	0.9009	0.0774	0.8836	0.1118	1.0093	2.2897	0.8945	354.52	0.9018	0.0397	0.9212	0.0653	1.0033	2.4706	0.9168
352.97	0.9183	0.0633	0.9004	0.0956	1.0061	2.3862	0.9139	354.33	0.9144	0.0346	0.9332	0.0554	1.0077	2.4199	0.8942
353.08	0.9305	0.0535	0.9137	0.0817	1.0045	2.4041	1.2038	382.16	0.0804	0.1074	0.1644	0.3271	0.9916	2.0051	1.0006
365.51	0.1284	0.5607	0.2287	0.6244	1.2997	1.1843	1.2791	378.78	0.0876	0.1563	0.1640	0.4039	0.9827	1.8679	1.0114
362.31	0.2704	0.4553	0.4002	0.4923	1.1748	1.2684	1.1826	377.27	0.1972	0.0956	0.3551	0.2606	0.9797	2.0553	1.0074
361.81	0.2793	0.4598	0.4081	0.4885	1.1754	1.2658	1.2166	374.34	0.2686	0.0890	0.4546	0.2268	0.9885	2.0883	1.0074
359.76	0.3858	0.3739	0.5119	0.4060	1.1278	1.3793	1.1261	371.46	0.3513	0.0812	0.5538	0.1920	0.9886	2.1063	0.9973
358.81	0.4495	0.3245	0.5683	0.3602	1.1027	1.4530	1.0781	368.74	0.4273	0.0741	0.6335	0.1637	0.9956	2.1322	0.9892
358.22	0.4768	0.3092	0.5894	0.3432	1.0957	1.4803	1.0958	366.98	0.4792	0.0688	0.6800	0.1449	0.9968	2.1426	0.9985
357.34	0.5620	0.2435	0.6583	0.2846	1.0637	1.6031	1.0538	365.26	0.5324	0.0643	0.7237	0.1306	0.9984	2.1766	0.9862
356.82	0.6031	0.2143	0.6862	0.2603	1.0481	1.6939	1.0714	363.73	0.5779	0.0610	0.7604	0.1193	1.0059	2.1961	0.9577
356.43	0.6317	0.1977	0.7089	0.2434	1.0450	1.7386	1.0368	362.40	0.6195	0.0594	0.7843	0.1122	1.0025	2.2097	0.9697
356.23	0.6691	0.1718	0.7377	0.2226	1.0324	1.8415	0.9320	361.35	0.6632	0.0499	0.8173	0.0936	1.0036	2.2671	0.9687
356.14	0.7170	0.1408	0.7787	0.1863	1.0195	1.8860	0.9223	360.03	0.7180	0.0403	0.8544	0.0746	1.0041	2.3316	0.9592
355.88	0.7441	0.1274	0.7996	0.1699	1.0246	1.9355	0.9075	359.04	0.7661	0.0301	0.8871	0.0567	1.0037	2.4478	0.9323
355.22	0.7880	0.0998	0.8320	0.1327	1.0169	1.9523	1.2186	358.41	0.8001	0.0240	0.9079	0.0447	1.0006	2.4690	0.9314
354.90	0.8153	0.0873	0.8497	0.1292	1.0128	2.1957	0.8489	357.70	0.8296	0.0197	0.9227	0.0361	1.0001	2.4847	0.9690
354.62	0.8456	0.0717	0.8750	0.1062	1.0135	2.2175	0.8999	356.89	0.8606	0.0166	0.9387	0.0302	1.0028	2.5314	0.9239
354.41	0.8760	0.0580	0.8967	0.0885	1.0085	2.3001	0.8944								

(Gmehling et al., 1979). The following objection function was minimized in our regression:

$$Q = \sum_N \sum_i \left(\frac{\gamma_i^{\text{exp}} - \gamma_i^{\text{cal}}}{\gamma_i^{\text{exp}}} \right)^2 \qquad (5)$$

Table 7 lists these regression results. The deviations of the regressions are reasonably small, and it is indicated that all activity coefficient models are suitable to represent the binary experimental data. The *Txy* diagrams for the three binary mixtures are shown in Figures 1−3, respectively. The binary mixture of cyclohexane (1) + 3-methyl-2-butanone (2) has an azeotrope. The azeotropic temperature at 101.3 kPa is 351.49 K with $x_1 = 0.7703$. No azeotrope was observed for the other two binary mixtures.

The VLE of the ternary system of cyclohexane (1) + 3-methyl-2-butanone (2) + octane (3) were also measured at 101.3 kPa, and the results are given in Table 8. The binary parameters of the NRTL model given in Table 7 were used to predict the VLE of the ternary system, and the calculated deviations are also listed in Table 7. It is again observed that the predictions are satisfactory. The equilibrium $x-y$ diagram of the ternary system is shown in Figure 4.

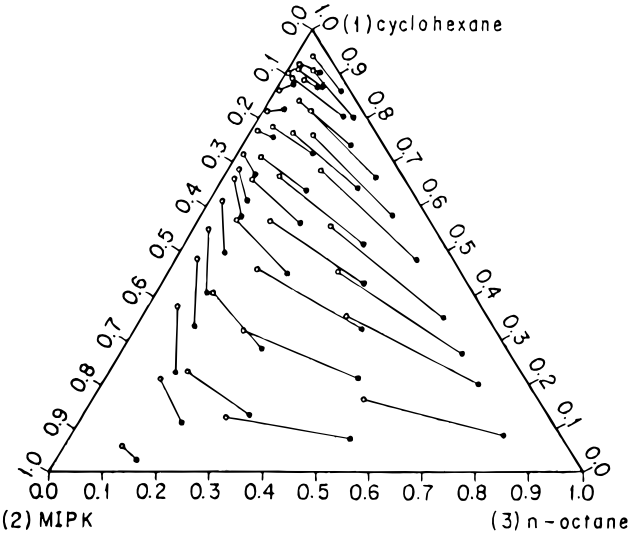

Figure 4. Experimental VLE data for cyclohexane (1) + 3-methyl-2-butanone (2) + octane (3) at 101.3 kPa: (●) liquid phase; (○) vapor phase.

Conclusion

Vapor−liquid equilibria of the binary and ternary mixtures of cyclohexane, 3-methyl-2-butanone, and octane were measured at 101.3 kPa. The results of the binary mixtures satisfied the thermodynamic consistency test and the calculated activity coefficients were fitted by various models. Predictions of the VLE of the ternary system also show satisfactory results by using directly the parameters obtained from the regression of the binary data.

Glossary

A	binary parameters in the activity coefficient models
a, b, c	constants in the vapor pressure equation

D, J	parameters in the Herington test method, defined in eqs 4 and 5
K	area parameter used in the Herington test method
n_D	refractive index
P	pressure
R	gas constant
T	temperature
T_b	normal boiling temperature
V	volume
x, y	mole fractions of the liquid and vapor phases, respectively

Greek Letters

ϕ	fugacity coefficient
γ	activity coefficient
ρ	density

Superscripts

cal	calculated results
exp	experimental data
L	liquid phase property
sat	saturated property

Subscripts

c	critical property
i	component i
N	index for all data points

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