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Isobaric Vapor−Liquid Equilibria for (Acetic Acid + Cyclohexane) and (Cyclohexane + Acetylacetone) at a Pressure of 101.3 kPa and for (Acetic Acid + Acetylacetone) at a Pressure of 60.0 kPa

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Isobaric vapor−liquid equilibrium (VLE) data for (acetic acid + cyclohexane) and (cyclohexane + acetylacetone) were determined at a pressure of 101.3 kPa and those for (acetic acid + acetylacetone) at a pressure of 60.0 kPa. A minimum boiling azeotrope was found for (acetic acid + cyclohexane). The nonideality of the vapor phase of (acetic acid + acetylacetone) and (acetic acid + cyclohexane) was investigated by using the Hayden−O'Connell equation. Thermodynamic consistency was tested for all of the VLE data. The experimental data were correlated satisfactorily by the Wilson, NRTL, and UNIQUAC models. Correlation results were in good agreement with experimental data.

Introduction

Acetylacetone (2,4-pentanedione) is an important reagent in analytical and coordination chemistry.[1] In the separation of acetylacetone using azeotrope distillation with water as entrainer,[2] there is a small quantity of acetylacetone and acetic acid left in the wastewater. Cyclohexane can be used to recycle acetylacetone from water by extraction, which is accompanied by coextraction of acetic acid, and then distillation is a feasible option for the separation of cyclohexane, acetylacetone, and acetic acid. Due to the large gap in volatility of cyclohexane in comparison to acetic acid and acetylacetone, normal pressure distillation is suitable for removal of cyclohexane from the extract phase, while reduced pressure distillation is preferably used for subsequent separation of acetylacetone and acetic acid considering the high boiling point of acetylacetone. Vapor−liquid equilibrium (VLE) data are essential to the design, operation, and optimization of distillation processes. However, the VLE data are not available in the literature. Lark et al.[3] reported the vapor pressures of the acetic acid + cyclohexane system at temperatures of 298.15 K and 318.15 K. Cui[4] investigated the VLE data of (acetic acid + acetylacetone) at a pressure of 101.3 KPa.

In this work, isobaric vapor−liquid equilibrium data for (acetic acid + cyclohexane) and (cyclohexane + acetylacetone) were investigated at a pressure of 101.3 kPa, and those for (acetic acid + acetylacetone), which have close boiling points, were determined at a pressure of 60.0 kPa. As the acetic acid molecules strongly associate with each other due to the hydrogen bond between two molecules, the association effect on vapor−liquid equilibrium should not be neglected. The nonideality of the vapor phase caused by the association of the acetic acid was considered by the chemical theory[5] and Hayden−O'Connell equation.[6] The thermodynamic consistency was tested with the Van Ness method,[7] which had been modified by Fredenslund et al.,[8] for these three systems. The Wilson,[9] NRTL,[10] and UNIQUAC[11] equations were used to correlate the experimental data.

Table 1. Densities (ρ), Refractive Index (n_D), and Boiling Points of Pure Compounds Compared with Literature Data[18]

	ρ/(g·cm^{-3}) (298.15 K)		n_D (293.15 K)		T_b (K) (1 atm)	
compound	exptl	lit.	exptl	lit.	exptl	lit.
acetylacetone	0.9717	0.9721	1.4489	1.4494	413.60	413.55
cyclohexane	0.7796	0.7792	1.4259	1.4264	353.90	353.87
acetic acid	1.0469	1.0446	1.3715	1.3720	391.44	391.50

Experimental Section

Chemicals. Acetylacetone was supplied by Huzhou Xinaote Pharmaceutical & Chemical Co., Ltd. with a minimum mass fraction purity of 0.998. Cyclohexane was provided by Shanghai Lingfeng Chemical Reagent Co., Ltd. and had a minimum mass fraction purity of 0.998. Acetic acid (glacial) was supplied by Shanghai Chemical Reagent No.1 Plant with a minimum mass fraction purity of 0.995. The purity of the chemicals was checked by a gas chromatograph (GC). All chemicals were used without further purification in this paper. The densities of the pure liquids were measured at a temperature of 298.15 K using an Anton Paar DMA 4100 densimeter. The temperature was controlled to ± 0.01 K with a thermostat bath. The accuracies in density and refractive index measurements are ± 0.0001 g·cm^{-3} and ± 0.0002, respectively. The experimental values of these properties and the boiling points are given in Table 1 together with those given in the literature.

Apparatus and Procedure. The apparatus used for the VLE data measurements of the homogeneous binary system was a modified Ellis equilibrium still described by Walas.[12] In this still, both liquid and condensed vapor phases are continuously recirculated to provide intimate contact of the phases and ensure the equilibrium to be established rapidly.

Temperature was measured by using a calibrated precision mercury thermometer with an accuracy of ± 0.05 K. Pressure was controlled by using an automatic control system detailed

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Table 2. Experimental Vapor−Liquid Equilibrium Data: Temperature (T), Liquid-Phase and Vapor-Phase Mole Fractions (x_1, y_1), and Activity Coefficients (γ_i) for the Cyclohexane (1) + Acetyl Acetone (2) System at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_2
407.65	0.0088	0.1208	3.4051	1.0660
401.85	0.0244	0.2570	3.2829	1.0682
385.15	0.0871	0.5530	2.8553	1.0854
372.25	0.1851	0.7356	2.4355	1.0904
363.75	0.3131	0.8186	1.9954	1.1498
360.35	0.4716	0.8504	1.5074	1.3835
357.95	0.6477	0.8797	1.2128	1.8134
356.65	0.7452	0.9106	1.1313	1.9509
355.35	0.8714	0.9395	1.0353	2.7398
354.85	0.9382	0.9648	1.0015	3.3781

in the literature.[4,13] It consists of a vacuum pump, two $CaCl_2$ drying bottles, a mercury pressure gauge, a constant pressure tank (0.75 m^3), a magnetic valve, an electromagnetic delay, and a NaCl solution U tube. The pressure at the top part of the tank is maintained constant at preset pressure by adjusting the magnetic valve. If the pressure in the tank is higher than the setting pressure and the plug in the NaCl solution U-type tube touches the liquid surface, then the magnetic valve will open, and the pressure in the tank will decrease. The air is passed through a filter and a $CaCl_2$ drying bottle before entering the system. In this system, a TJ-800 Mercury U-type pressure gauge is used, whose precision is within ± 0.01 kPa. Atmospheric pressure was measured by a Fortin-type mercury barometer located adjacent to the experimental apparatus with an accuracy of ± 0.04 kPa. The uncertainty of the whole pressure measurement system was estimated to be less than ± 0.10 kPa.

The liquid and condensed phases were determined using a Varian CP-3800 gas chromatograph. A flame ionization detector was used together with a 30 m, 0.25 mm i.d. capillary column CP-Wax 52 CB. The GC response peaks were treated with Varian Star #1 for Windows. High-purity hydrogen was used as the carrier gas at a constant flow rate of 50 $mL\cdot min^{-1}$. The injector, detectors, and column temperature were kept at temperatures of (443.15, 453.15, and 433.15) K, respectively. The gas chromatograph was calibrated with mixtures of known compositions that were prepared gravimetrically by an electronic balance (uncertainty of ± 0.0001 g). The uncertainty of the measured mole fraction was ± 0.001.

Results and Discussion

The isobaric VLE data and the calculated activity coefficients are listed in Tables 2 to 4 for (cyclohexane + acetylacetone), (acetic acid + cyclohexane), and (acetic acid + acetylacetone), respectively.

The activity coefficients of the components in the liquid phase were calculated as follows

$$y_i\hat{\varphi}_i^{V}P = x_i\gamma_i P_i^{S}\varphi_i^{S}\exp\left\{\frac{V_i^{L}(P - P_i^{S})}{RT}\right\} \qquad (1)$$

where P is the total pressure; y_i is the mole fraction of component i in the vapor phase; x_i is the mole fraction of component i in the liquid phase; R is the gas constant; T is the temperature; and P_i^S is the vapor pressure of pure component i. P_i^S was correlated using the equation

$$\ln P_i^{S}\,(\mathrm{Pa}) = A + B/T + C\ln T + DT^{E} \qquad (2)$$

where A, B, C, D, and E are component specific coefficients for vapor pressure.

Table 3. Experimental Vapor−Liquid Equilibrium Data: Temperature (T), Liquid-Phase and Vapor-Phase Mole Fractions (x_1, y_1), and Activity Coefficients (γ_i) for the Acetic Acid (1) + Cyclohexane (2) System at 101.3 kPa

T/K	x_1	y_1	γ_1	γ_2
353.15	0.0258	0.0650	10.2858	1.0393
352.65	0.0705	0.1165	6.5686	1.0690
352.15	0.1393	0.1689	4.3946	1.1071
351.95	0.2420	0.2149	3.1533	1.2391
352.15	0.3336	0.2460	2.3215	1.3634
352.55	0.4612	0.2757	1.7601	1.6324
352.95	0.5690	0.3017	1.4805	1.9789
353.95	0.7026	0.3320	1.2259	2.7320
354.35	0.7263	0.3402	1.1988	2.9070
354.95	0.7690	0.3544	1.1568	3.1256
357.45	0.8548	0.3816	1.0462	4.4724
361.05	0.9040	0.4548	1.0171	6.0832
364.15	0.9384	0.5057	1.0082	7.8756
380.45	0.9801	0.7897	0.9968	9.0320

Table 4. Experimental Vapor−Liquid Equilibrium Data: Temperature (T), Liquid-Phase and Vapor-Phase Mole Fractions (x_1, y_1), and Activity Coefficients (γ_i) for the Acetic Acid (1) + Acetylacetone (2) System at 60.0 kPa

T/K	x_1	y_1	γ_1	γ_2
393.75	0.0568	0.0846	2.0574	1.0611
391.45	0.1103	0.1637	1.8428	1.1330
389.75	0.1771	0.2418	1.5211	1.2117
388.95	0.2511	0.3570	1.4031	1.2346
387.85	0.3614	0.4887	1.2317	1.2743
386.45	0.4545	0.5955	1.1584	1.3241
384.75	0.5564	0.7017	1.1060	1.3276
383.75	0.6245	0.7572	1.0867	1.3310
382.65	0.6601	0.8037	1.0617	1.3386
381.75	0.7393	0.8580	1.0387	1.3422
380.15	0.8073	0.9043	1.0263	1.3552
378.85	0.8722	0.9464	1.0146	1.3681
378.25	0.9053	0.9615	1.0032	1.3725
377.25	0.9337	0.9725	1.0013	1.3748
376.95	0.9655	0.9903	0.9910	1.3886

The coefficients for vapor pressure and the properties of the pure components are given in Table 5.

In eq 1, V_i^L is the liquid molar volume of pure component i, calculated from the modified Rackett equation;[14] $\hat{\varphi}_i^V$ and φ_i^S are the fugacity coefficients of component i in the mixture vapor phase and in the pure state, respectively; and γ_i is the activity coefficient of component i.

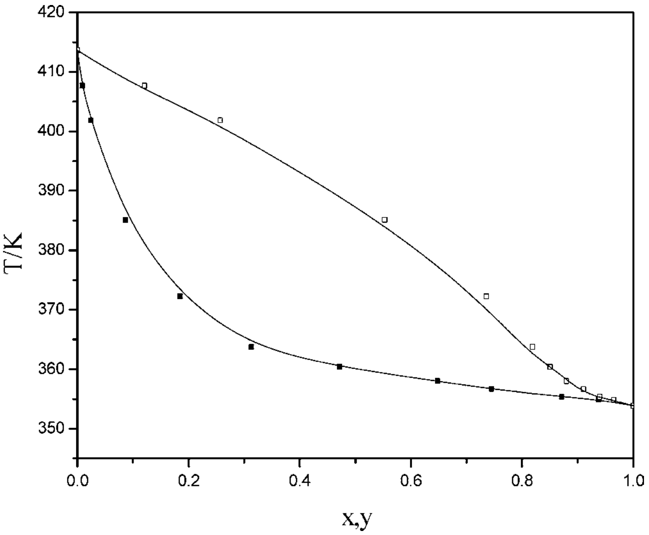

Figure 1. T−x−y diagram for cyclohexane (1) + acetylacetone (2) at a pressure of 101.3 kPa: ■, experimental liquid-phase mole fractions, x_1; □, experimental vapor-phase mole fractions, y_1; —, Wilson equation.

Table 5. Physical Properties of the Pure Components[17,19,20]

	acetic acid	cyclohexane	acetylacetone
M.W./($g\cdot mol^{-1}$)	60.053	84.161	100.117
T_b/K	391.50	353.87	413.55
T_c/K	592.71	553.54	602.00
P_c/MPa	5.786	4.075	3.960
V_c/($m^3\cdot kmol^{-1}$)	0.171	0.308	0.323
Z_c	0.201	0.273	0.256
RD/Å	0.2610	0.3242	0.4017
DM/Debye	5.80	2.04	9.37
ω	0.4624	0.2118	0.4959
	Coefficients for Vapor Pressure		
A	70.23	116.69	129.02
B	−6846.5	−7109.1	−8624
C	−7.032	−15.521	−17.212
D	$5.021\cdot 10^{-6}$	0.017	0.01697
E	2	1	1

The vapor-phase fugacity coefficients were calculated from the virial equation of state truncated at the second virial term, which is given by

$$\ln \varphi_i = \left(2\sum_j y_j B_{ij} - B_{\mathrm{m}}\right)P/RT \tag{3}$$

where

$$B_{\mathrm{m}} = \sum_i \sum_j y_i y_j B_{ij} \tag{4}$$

B_{ii} and B_{ij} are the pure and cross second virial coefficients for the cyclohexane + acetylacetone system, and they are calculated with the Tsonopoulos[15,16] equation

$$\frac{B}{V} = \frac{BP_{\mathrm{c}}}{RT_{\mathrm{c}}} = f^{(0)} + \varpi f^{(1)} + af^{(2)} + bf^{(3)} \tag{5}$$

where

$$f^{(0)} = 0.1445 - 0.330/T_{\mathrm{r}} - 0.1385/T_{\mathrm{r}}^2 - 0.0121/T_{\mathrm{r}}^3 - 0.000607/T_{\mathrm{r}}^8 \tag{6}$$

$$f^{(1)} = 0.0637 + 0.331/T_{\mathrm{r}}^2 - 0.423/T_{\mathrm{r}}^3 - 0.008/T_{\mathrm{r}}^8 \tag{7}$$

$$f^{(2)} = 1/T_{\mathrm{r}}^6 \tag{8}$$

$$f^{(3)} = -1/T_{\mathrm{r}}^8 \tag{9}$$

$$T_{\mathrm{r}} = T/T_{\mathrm{c}} \tag{10}$$

$$\text{For this nonpolar system, } b = 0 \tag{11}$$

$$a = -2.14\cdot 10^{-4}\mu_{\mathrm{r}} - 4.308\cdot 10^{-21}(\mu_{\mathrm{r}})^8 \tag{12}$$

$$\mu_{\mathrm{r}} = 10^5\mu^2 p_{\mathrm{c}}/T_{\mathrm{c}}^2 \tag{13}$$

Because the association effect of acetic acid can not be neglected, B_{ii} and B_{ij} in (acetic acid + cyclohexane) and (acetic acid + acetylacetone) were estimated by the Hayden and O'Connell equation.[6] The fugacity coefficients of acetic acid were calculated by using the chemical theory[5]

$$\varphi_i = \frac{z_i}{y_i}\exp\left(\frac{B_i^{\mathrm{Free}}\cdot P}{RT}\right) \tag{14}$$

where z_i is the true vapor-phase mole fraction of monomers, for the associating component A

$$z_A = \frac{\sqrt{1 + 4k_{\mathrm{t}}y_A(2 - y_A)} - 1}{2k_{\mathrm{t}}(2 - y_A)} \tag{15}$$

and for nonassociating component N

$$z_{\mathrm{N}} = y_{\mathrm{N}}\frac{1 + 4k_{\mathrm{t}}(2 - y_A) - \sqrt{1 + 4k_{\mathrm{t}}y_A(2 - y_A)}}{2k_{\mathrm{t}}(2 - y_A)^2} \tag{16}$$

k_{t} is the dimerization equilibrium constant of associating component A, calculated by the following equation

$$k_{\mathrm{t}} = -\frac{-B_A^D}{RT}\cdot P\cdot \exp\frac{B_A^{\mathrm{Free}}P}{RT} \tag{17}$$

$$B^D = B_{\mathrm{bound}} + B_{\mathrm{metastable}} + B_{\mathrm{chem}} \tag{18}$$

where $B_{\mathrm{bound}} + B_{\mathrm{metastable}}$, B_{chem}, and B_i^{Free} were obtained by the Hayden and O'Connell equation.

The experimental data and calculated values of $T-x-y$ relationship and activity coefficients for (cyclohexane + acetylacetone), (acetic acid + cyclohexane), and (acetic acid + acetylacetone) are shown in Figures 1 to 6.

The results reported in these tables indicated that all the systems exhibit a positive deviation from ideal behavior. The

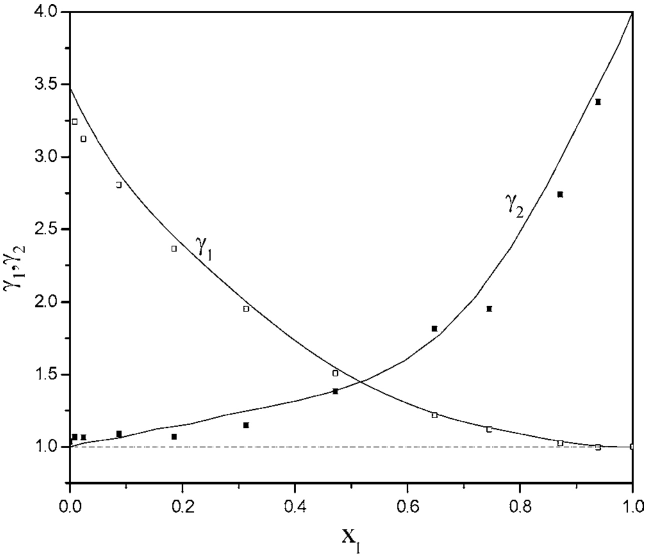

Figure 2. Activity coefficient diagram for cyclohexane (1) + acetylacetone (2) at a pressure of 101.3 kPa: ■, experimental data, γ_1; □, experimental data, γ_2; —, calculated data using the Wilson equation.

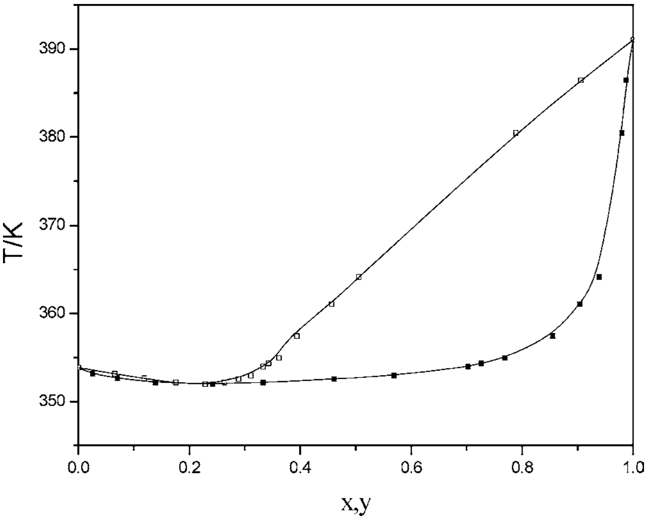

Figure 3. $T-x-y$ diagram for acetic acid (1) + cyclohexane (2) at a pressure of 101.3 kPa: ■, experimental liquid-phase mole fractions, x_1; □, experimental vapor-phase mole fractions, y_1; —, NRTL equation.

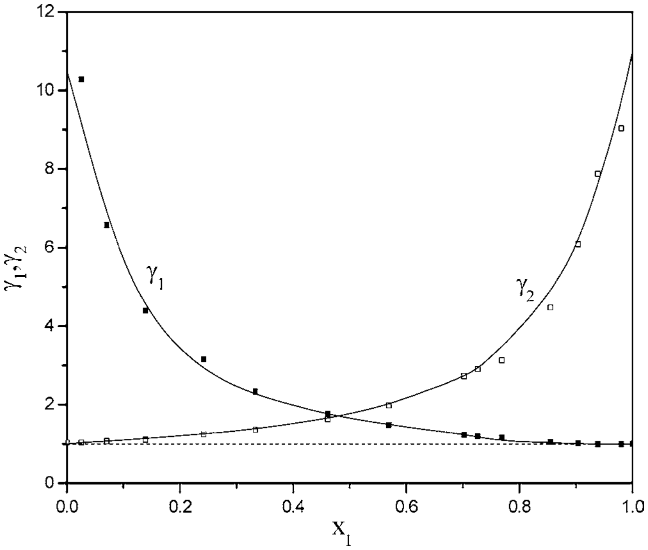

Figure 4. Activity coefficient diagram for acetic acid (1) + cyclohexane (2) at a pressure of 101.3 kPa: ■, experimental data, γ_1; □, experimental data, γ_2; —, calculated data using the NRTL equation.

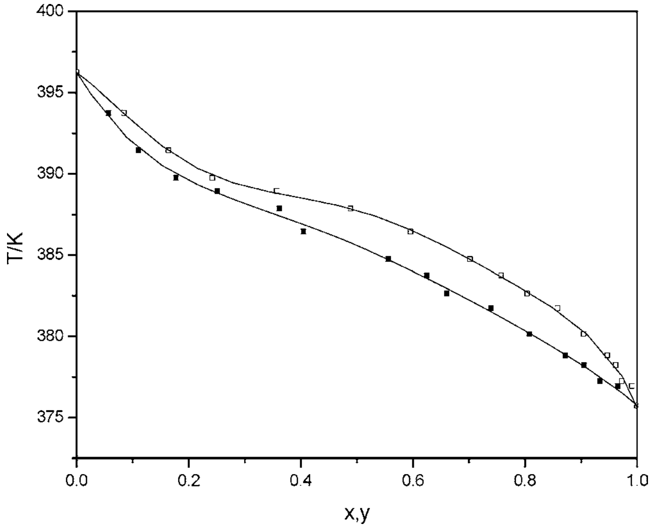

Figure 5. *T*−*x*−*y* diagram for acetic acid (1) + acetylacetone (2) at a pressure of 60.0 kPa: ■, experimental liquid-phase mole fractions, x_1; □, experimental vapor-phase mole fractions, y_1; —, NRTL equation.

acetic acid (1) + cyclohexane (2) system shows a minimum boiling azeotrope illustrated in Figure 3. Azeotropic compositions were obtained by determining the x_1 values that make the function $(x_1 - y_1) = f(x_1)$ equal to zero. The corresponding azeotropic temperatures were computed from a polynomial equation $T = f(x_1)$, whose coefficients were obtained by fitting the experimental results around the azeotropic point, using the x_1 values previously determined. The liquid composition of acetic acid and boiling temperature of the azeotrope for acetic acid (1) + cyclohexane (2) are 0.206 at a temperature of 352.03 K and pressure of 101.3 kPa.

The experimental results of the binary systems were tested for thermodynamic consistency by means of the point-to-point test of Van Ness,[9] modified by Fredenslund et al.[10] According to this test, the experimental data are consistent if the mean absolute deviation between calculated and measured vapor phase compositions, Δy, is less than 0.01. The results of this test for the mixtures were 0.0043, 0.0038, and 0.0057 for (acetic acid + cyclohexane), (cyclohexane + acetylacetone), and (acetic acid + acetylacetone), respectively, indicating that the VLE results for all three systems are thermodynamically consistent.

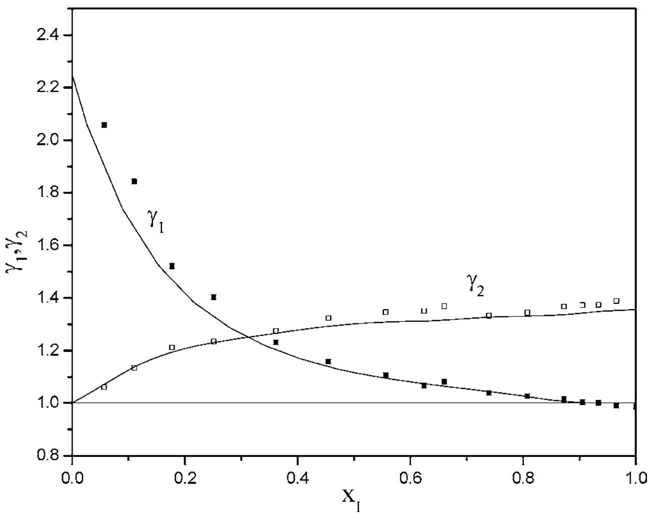

Figure 6. Activity coefficient diagram for acetic acid (1) + acetylacetone (2) at a pressure of 60.0 kPa: ■, experimental data, γ_1; □, experimental data, γ_2; —, calculated data using the NRTL equation.

Table 6. Interaction Parameters A_{ij}, Root Mean Squared Deviations between Calculated and Experimental Vapor-Phase Mole Fractions σy_1, and Temperature σT/K for the Binary Systems with Different Models

model	A_{12}[a] J·mol^{-1}	A_{21}[a] J·mol^{-1}	α	σT[b] K	σy_1[b]
	Cyclohexane (1) + Acetylacetone (2)				
Wilson	147.815	442.414		0.26	0.011
NRTL	430.976	96.601	0.3	0.32	0.013
UNIQUAC	143.449	−2.930		0.28	0.013
	Acetic Acid (1) + Cyclohexane (2)				
Wilson	273.913	1378.14		0.36	0.009
NRTL	1172.26	−114.184	0.3	0.31	0.008
UNIQUAC	412.623	−72.721		0.33	0.010
	Acetic Acid (1) + Acetylacetone (2)				
Wilson	−229.866	688.926		0.30	0.010
NRTL	−138.46	71.66	0.3	0.24	0.008
UNIQUAC	526.393	−315.943		0.26	0.010

[a] The interaction parameters for various models are as follows: Wilson, $A_{ij} = (\lambda_{ij} - \lambda_{ii})/R$; NRTL, $A_{ij} = (g_{ij} - g_{ii})/R$; UNIQUAC, $A_{ij} = (U_{ij} - U_{ii})/R$. [b] $\sigma T = [\sum_{i=1}^{n}(T_i^{\text{calc}} - T_i^{\text{expt}})^2/n]^{1/2}$; $\sigma y_1 = [\sum_{i=1}^{n}(y_{1,i}^{\text{calc}} - y_{1,i}^{\text{expt}})^2/n]^{1/2}$.

The VLE experimental data were correlated with Wilson, NRTL, and UNIQUAC equations by minimizing the objective function *F*

$$F = \sum_{k=1}^{n} \sum_{i=1}^{2} \left[\left(\frac{\gamma_i^{\text{expt}} - \gamma_i^{\text{calc}}}{\gamma_i^{\text{expt}}} \right)^2 \right]_k \tag{19}$$

where *n* is the number of experimental VLE data. As recommended by Renon and Prausnitz, the mixture nonrandomness parameter in the NRTL equation was set as 0.3, and the structural parameters *r* and *q* for the UNIQUAC equation were taken from ref 21.

The interaction parameters for the Wilson, NRTL, and UNIQUAC equations, A_{12} and A_{21}, and the root mean squared deviations (rmsd) between the experimental and calculated values are listed in Table 6.

Conclusions

The isobaric vapor−liquid equilibrium (VLE) data for (acetic acid + cyclohexane) and (cyclohexane + acetylacetone) were obtained at a pressure of 101.3 kPa, and those for (acetic acid

+ acetylacetone) were obtained at a pressure of 60.0 kPa. The thermodynamic consistency was tested for all the binary VLE data by Van Ness's method. Three activity coefficient models, namely, Wilson, NRTL, and UNIQUAC, were used for correlations. The correlated results are in good agreement with experimental data. The system (acetic acid + cyclohexane) shows a minimum boiling azeotrope, while there is no azeotropism in other two systems.

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