Thermochimica Acta, 232 (1994) 285–295
Elsevier Science B.V., Amsterdam
SSDI 0040-6031(93)01396-K

Liquid–liquid equilibria for one ternary and two quaternary systems containing acetonitrile at 25°C

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(Received 20 April 1993; accepted 10 June 1993)

Abstract

Experimental tie-lines are presented for (cyclohexane + 2-propanol + aceto-nitrile), (cyclohexane + benzene + acetonitrile + methanol) and (cyclohexane + 2-propanol + acetonitrile + methanol) at 25°C. The experimental results have been well reproduced by using the extended UNIQUAC and modified Wilson models with binary, ternary and quaternary parameters obtained in fitting the models to literature and the present experimental data.

LIST OF SYMBOLS

a_{ij}	binary energy parameter for i–j pair
F	objective function as defined by eqn. (9)
q_i	molecular geometric area parameter of pure component i
q_i'	interaction correction factor of pure component i
R	universal gas constant
r_i	molecular geometric volume parameter of pure component i
T	absolute temperature
V_i	liquid molar volume of pure component i
x_i	liquid mole fraction of component i
Z	lattice coordination number, here taken as 10

Greek letters

α_{ij}	binary parameter in modified Wilson model
γ_i	activity coefficient of component i
θ_i	surface fraction of component i
Λ_{ij}	Wilson-like parameter for i–j pair
Λ_{jki}, Λ_{jkli}	modified Wilson ternary and quaternary parameters
τ_{ij}	extended UNIQUAC parameter for i–j pair

τ_{jki}, τ_{jkli}	extended UNIQUAC ternary and quaternary parameters
Φ_i	segment fraction of component i

Subscripts

calc	calculated
exptl	experimental
i, j, k, l	components

INTRODUCTION

This work is concerned with the measurements of liquid–liquid equilibria (LLE) for cyclohexane + 2-propanol + acetonitrile, cyclohexane + benzene + acetonitrile + methanol, and cyclohexane + 2-propanol + acetonitrile + methanol at 25°C. The experimental LLE results are compared with those calculated from the extended UNIQUAC and modified Wilson models including binary, ternary, and quaternary parameters [1, 2]. Most of the binary and ternary parameters of the two models have been evaluated from published binary and ternary phase equilibrium data as follows: binary vapour–liquid equilibrium (VLE) data for acetonitrile + benzene at 20°C [3], acetonitrile + methanol at 55°C [4], acetonitrile + 2-propanol at 50°C [5], cyclohexane + benzene at 25°C [6], cyclohexane + 2-propanol at 50°C [7], methanol + benzene at 25°C [8], and methanol + 2-propanol at 55°C [9]; mutual solubilities at 25°C for acetonitrile + cyclohexane [10] and methanol + cyclohexane [5]; ternary tie-line data at 25°C for cyclohexane + benzene + acetonitrile [10], cyclohexane + methanol + acetonitrile [11], cyclohexane + benzene + methanol [12], and cyclohexane + 2-propanol + methanol [12].

EXPERIMENTAL

Acetonitrile, cyclohexane and 2-propanol (Wako Pure Chemical Industries Ltd., special grade) were used as received. Methanol (Wako Pure Chemical Industries Ltd., first grade) was fractionally distilled after shaking with calcium oxide. Benzene (Kanto Chemical Co., Inc., first grade) was subjected to repeated fractional recrystallization. The densities of the chemicals used, measured with an Anton Paar densimeter (DMA40) at 25°C, agreed well with literature values [13].

The experimental procedure of tie-line measurements was the same as described previously [14]. Compositions of two equilibrated liquids were determined using a Schimadzu gas chromatograph (GC-8C) and a Shimadzu Chromatopac (C-R3A). The experimental error of the observed mole fractions was 0.002 at most.

Tables 1 and 2 give the experimental tie-line results of the terniary cyclohexane + 2-propanol + methanol and quaternary cyclohexane + benzene + acetonitrile + methanol, and cyclohexane + 2-propanol + acetonitrile + methanol systems at 25°C.

ANALYSIS OF EXPERIMENTAL RESULTS

The experimental tie-line results have been correlated using the extended UNIQUAC and modified Wilson models with binary, ternary and quaternary parameters [1, 2]. The models give the activity coefficient of component 1 in a quaternary mixture as follows.

Extended UNIQUAC model

$$
\begin{aligned}
\ln \gamma_1 \\
= {} & \ln\frac{\Phi_1}{x_1} + 1 - \frac{\Phi_1}{x_1} - \frac{Z}{2} q_1\left(\ln\frac{\Phi_1}{\theta_1} + 1 - \frac{\Phi_1}{\theta_1}\right) \\
& - q_1' \ln\left(\sum_j^4 \theta_j\tau_{j1} + \theta_2\theta_3\tau_{231} + \theta_2\theta_4\tau_{241} + \theta_3\theta_4\tau_{341} + \theta_2\theta_3\theta_4\tau_{2341}\right) + q_1 \sum_j^4 \left(\frac{q_j'}{q_j}\right)\theta_j \\
& - q_1 \left\{ \frac{(q_1'/q_1)\theta_1(\tau_{11} - \theta_2\theta_3\tau_{231} - \theta_2\theta_4\tau_{241} - \theta_3\theta_4\tau_{341} - 2\theta_2\theta_3\theta_4\tau_{2341})}{\sum_j^4 \theta_j\tau_{j1} + \theta_2\theta_3\tau_{231} + \theta_2\theta_4\tau_{241} + \theta_3\theta_4\tau_{341} + \theta_2\theta_3\theta_4\tau_{2341}} \right. \\
& + \frac{(q_2'/q_2)\theta_2[\tau_{12} + (1-\theta_1)\theta_3\tau_{132} + (1-\theta_1)\theta_4\tau_{142} - \theta_3\theta_4\tau_{342} + (1-2\theta_1)\theta_3\theta_4\tau_{1342}]}{\sum_j^4 \theta_j\tau_{j2} + \theta_1\theta_3\tau_{132} + \theta_1\theta_4\tau_{142} + \theta_3\theta_4\tau_{342} + \theta_1\theta_3\theta_4\tau_{1342}} \\
& + \frac{(q_3'/q_3)\theta_3[\tau_{13} + (1-\theta_1)\theta_2\tau_{123} + (1-\theta_1)\theta_4\tau_{143} - \theta_2\theta_4\tau_{243} + (1-2\theta_1)\theta_2\theta_4\tau_{1243}]}{\sum_j^4 \theta_j\tau_{j3} + \theta_1\theta_2\tau_{123} + \theta_1\theta_3\tau_{143} + \theta_2\theta_4\tau_{243} + \theta_1\theta_2\theta_4\tau_{1243}} \\
& \left. + \frac{(q_4'/q_4)\theta_4[\tau_{14} + (1-\theta_1)\theta_2\tau_{124} + (1-\theta_1)\theta_3\tau_{134} - \theta_2\theta_3\tau_{234} + (1-2\theta_1)\theta_2\theta_3\tau_{1234}]}{\sum_j^4 \theta_j\tau_{j4} + \theta_1\theta_2\tau_{124} + \theta_1\theta_3\tau_{134} + \theta_2\theta_3\tau_{234} + \theta_1\theta_2\theta_3\tau_{1234}} \right\}
\end{aligned}
\tag{1}
$$

where Z is the lattice coordination number taken as 10, and the segment fraction Φ_i, the surface fraction θ_i, and the binary parameter τ_{ij} related to

TABLE 1

Experimental tie-line values for cyclohexane(1) + 2-propanol(2) + acetonitrile(3) at 25°C

Component-(1)-lean phase			Component-(1)-rich phase		
x_1	x_2	x_3	x_1	x_2	x_3
0.0824	0.0386	0.8790	0.9416	0.0075	0.0509
0.0889	0.0526	0.8585	0.9399	0.0102	0.0499
0.0971	0.0789	0.8240	0.9267	0.0178	0.0585
0.1081	0.0938	0.7981	0.9182	0.0230	0.0588
0.1109	0.1105	0.7786	0.9045	0.0306	0.0649
0.1264	0.1485	0.7251	0.8703	0.0507	0.0790

the energy parameter a_{ij} are defined by

$$\Phi_i = x_i r_i \Big/ \sum_j x_j r_j \qquad (2)$$

$$\theta_i = x_i q_i \Big/ \sum_j x_j q_j \qquad (3)$$

$$\tau_{ij} = \exp(-a_{ij}/T) \qquad (4)$$

The binary energy parameters a_{ij} are obtained from binary VLE or mutual solubility data, the ternary parameters $\tau_{jki(i\neq j\neq k)}$ are determined by fitting the model with the binary parameters to ternary tie-line data, and the quaternary parameters $\tau_{jkli(i\neq j\neq k\neq l)}$ are obtained similarly from quaternary tie-line data using the binary and ternary parameters derived. Binary VLE data reduction is performed using a computer program as given by Prausnitz et al. [15]. Computer calculations included vapour–phase non-ideality and the Poynting correction. The values of the energy parameters for partially miscible mixtures were obtained by solving the thermodynamic equation (eqn. (5)) for each component and eqn. (6) at two equilibrated liquid phases I and II.

$$(x_i\gamma_i)^{\mathrm{I}} = (x_i\gamma_i)^{\mathrm{II}} \qquad (5)$$

$$\sum_i x_i^{\mathrm{I}} = 1 \quad \text{and} \quad \sum_i x_i^{\mathrm{II}} = 1 \qquad (6)$$

The expressions of ln γ_2, ln γ_3 and ln γ_4 are obtained successively by cyclic advancement of the subscripts in eqn. (1), by changing 1 to 2, 2 to 3, 3 to 4, and 4 to 1.

Table 3 gives the pure-component molecular structural constants r and q of the extended UNIQUAC model and Table 4 presents the energy parameters and the root-mean-squared deviations between the experimental and calculated variables based on the extended UNIQUAC model.

TABLE 2

Experimental tie-line values for two quaternary systems at 25°C

Component-(1)-lean phase				Component-(1)-rich phase			
x_1	x_2	x_3	x_4	x_1	x_2	x_3	x_4
Cyclohexane(1) + benzene(2) + acetonitrile(3) + methanol(4) [a]							
$x_3' = 0.75$							
0.0992	0.0429	0.6459	0.2120	0.8555	0.0693	0.0584	0.0168
0.1365	0.0936	0.5778	0.1921	0.7262	0.1371	0.1064	0.0303
0.1827	0.1117	0.5289	0.1767	0.6417	0.1658	0.1483	0.0442
$x_3' = 0.50$							
0.0929	0.0212	0.4456	0.4403	0.8934	0.0332	0.0405	0.0329
0.1101	0.0392	0.4238	0.4269	0.8325	0.0688	0.0540	0.0447
0.1329	0.0626	0.4012	0.4033	0.7763	0.1037	0.0658	0.0542
0.1564	0.0870	0.3768	0.3798	0.7101	0.1360	0.0857	0.0682
$x_3' = 0.25$							
0.1238	0.0176	0.2128	0.6458	0.8690	0.0356	0.0280	0.0674
0.1230	0.0262	0.2099	0.6409	0.8459	0.0519	0.0310	0.0712
0.1550	0.0183	0.0614	0.7653	0.8442	0.0390	0.0141	0.1027
0.1595	0.0231	0.0740	0.7434	0.9063	0.0473	0.0155	0.1309
0.1578	0.0326	0.0993	0.7103	0.7921	0.0637	0.0219	0.1223
0.1387	0.0373	0.2038	0.6202	0.8119	0.0712	0.0352	0.0817
Cyclohexane(1) + 2-propanol(2) + acetonitrile(3) + methanol(4) [b]							
$x_3' = 0.75$							
0.0833	0.0340	0.6687	0.2140	0.9380	0.0051	0.0415	0.0154
0.1030	0.0749	0.6178	0.2043	0.9129	0.0149	0.0517	0.0205
0.1150	0.0982	0.5936	0.1932	0.9006	0.0233	0.0532	0.0229
0.1481	0.1362	0.5384	0.1773	0.8560	0.0415	0.0702	0.0323
0.1653	0.1681	0.5035	0.1631	0.8211	0.0609	0.0798	0.0382
$x_3' = 0.50$							
0.1013	0.0395	0.4322	0.4270	0.9116	0.0070	0.0413	0.0401
0.1229	0.0684	0.4035	0.4052	0.8983	0.0135	0.0437	0.0445
0.1372	0.0919	0.3856	0.3853	0.8915	0.0203	0.0416	0.0466
0.1474	0.1047	0.3763	0.3716	0.8727	0.0261	0.0482	0.0530
0.1759	0.1279	0.3498	0.3464	0.8366	0.0389	0.0579	0.0666
$x_3' = 0.2$							
0.1317	0.0358	0.2075	0.6250	0.8892	0.0070	0.0292	0.0746
0.1554	0.0630	0.1947	0.5869	0.8716	0.0145	0.0317	0.0822
0.1735	0.0783	0.1879	0.5603	0.8585	0.0200	0.0314	0.0901
0.1796	0.0860	0.1830	0.5514	0.8320	0.0243	0.0369	0.1068

[a] Tie-lines were obtained by mixing pure cyclohexane and benzene with x_3' acetonitrile + $(1 - x_3')$ methanol. [b] Tie-lines were obtained by mixing pure cyclohexane and 2-propanol with x_3' acetonitrile + $(1 - x_3')$methanol.

TABLE 3

Molecular structural constants for pure components

Component	r	q	q'
Acetonitrile	1.87	1.72	$q^{0.2}$
Benzene	3.19	2.40	$q^{0.2}$
Cyclohexane	3.97	3.01	$q^{0.2}$
Methanol	1.43	1.43	1.00
2-Propanol	2.78	2.51	0.89

TABLE 4

Binary results of phase equilibrium data reduction obtained by using the extended UNIQUAC model

System (1 + 2)	Temp./ °C	Number of data points	Energy parameters		Root-mean-squared deviations			
			a_{12}/ K	a_{21}/ K	δP/ Torr	δT/ K	δx ($\times 10^3$)	δy ($\times 10^3$)
Acetonitrile +benzene	20	45	37.28	251.01	0.76	0.01	0.6	4.3
Acetonitrile +methanol	55	13	205.45	134.51	1.79	0.00	1.1	4.7
Acetonitrile +2-propanol	50	15	70.27	356.68	0.82	0.02	0.5	3.3
Benzene +cyclohexane	25	11	37.77	85.90	0.23	0.00	0.1	0.9
Cyclohexane +2-propanol	50	9	869.11	123.13	1.27	0.04	0.6	5.6
Methanol +benzene	25	9	80.75	826.56	0.69	0.02	1.0	4.1
Methanol +2-propanol	55	20	80.25	18.06	1.73	0.07	0.9	4.0
Acetonitrile +cyclohexane	25	MS[a]	432.82	948.65				
Methanol +cyclohexane	25	MS[a]	280.74	1122.7				

[a] MS means mutual solubilities.

Modified Wilson model

$$\begin{aligned}
\ln \gamma_1 &= -\ln\left[\left(\sum_j^4 \alpha_{1j}\Lambda_{1j}x_j + \Lambda_{231}x_2x_3 + \Lambda_{241}x_2x_4 + \Lambda_{341}x_3x_4 + \Lambda_{2341}x_2x_3x_4\right) \Big/ \sum_j^4 \alpha_{1j}x_j\right] \\
&\quad - x_1\left[\frac{1 - \Lambda_{231}x_2x_3 - \Lambda_{241}x_2x_4 - \Lambda_{341}x_3x_4 - 2\Lambda_{2341}x_2x_3x_4}{\sum_j^4 \alpha_{1j}\Lambda_{1j}x_j + \Lambda_{231}x_2x_3 + \Lambda_{241}x_2x_4 + \Lambda_{341}x_3x_4 + \Lambda_{2341}x_2x_3x_4}\right. \\
&\qquad \left. - \frac{\alpha_{11}}{\sum_j^4 \alpha_{1j}x_j}\right] \\
&\quad - x_2\left[\frac{\alpha_{21}\Lambda_{21} + \Lambda_{132}x_3(1-x_1) + \Lambda_{142}x_4(1-x_1) - \Lambda_{342}x_3x_4 + \Lambda_{1342}x_3x_4(1-2x_1)}{\sum_j^4 \alpha_{2j}\Lambda_{2j}x_j + \Lambda_{132}x_1x_3 + \Lambda_{142}x_1x_4 + \Lambda_{342}x_3x_4 + \Lambda_{1342}x_1x_3x_4}\right. \\
&\qquad \left. - \frac{\alpha_{21}}{\sum_j^4 \alpha_{2j}x_j}\right] \\
&\quad - x_3\left[\frac{\alpha_{31}\Lambda_{31} + \Lambda_{123}x_2(1-x_1) + \Lambda_{143}x_4(1-x_1) - \Lambda_{243}x_2x_4 + \Lambda_{1243}x_2x_4(1-2x_1)}{\sum_j^4 \alpha_{3j}\Lambda_{3j}x_j + \Lambda_{123}x_1x_2 + \Lambda_{143}x_1x_4 + \Lambda_{243}x_2x_4 + \Lambda_{1243}x_1x_2x_4}\right. \\
&\qquad \left. - \frac{\alpha_{31}}{\sum_j^4 \alpha_{3j}x_j}\right] \\
&\quad - x_4\left[\frac{\alpha_{41}\Lambda_{41} + \Lambda_{124}x_2(1-x_1) + \Lambda_{134}x_3(1-x_1) - \Lambda_{234}x_2x_3 + \Lambda_{1234}x_2x_3(1-2x_1)}{\sum_j^4 \alpha_{4j}\Lambda_{4j}x_j + \Lambda_{124}x_1x_2 + \Lambda_{134}x_1x_3 + \Lambda_{234}x_2x_3 + \Lambda_{1234}x_1x_2x_3}\right. \\
&\qquad \left. - \frac{\alpha_{41}}{\sum_j^4 \alpha_{4j}x_j}\right] \qquad (7)
\end{aligned}$$

where α_{ij} and Λ_{ij} are the binary parameters. The values of α_{ij} are unity for completely miscible mixtures and are empirically assigned values which are slightly larger than unity for partially miscible mixtures. Λ_{ij} is defined by

$$\Lambda_{ij} = (V_j/V_i)\exp(-a_{ij}/T) \qquad (8)$$

$\Lambda_{jki(i \neq j \neq k)}$ and $\Lambda_{jkli(i \neq j \neq k \neq l)}$ are also the ternary and quaternary parameters to

TABLE 5

Binary Wilson-like parameters

System (1 + 2)	Temp./ °C	Parameters			
		a_{12}/ K	a_{21}/ K	α_{12}	α_{21}
Acetonitrile + benzene	45	392.49	−7.60	1.0	1.0
Acetonitrile + methanol	30	21.43	335.80	1.0	1.0
Acetonitrile + 2-propanol	50	945.69	−26.29	1.0	1.0
Benzene + cyclohexane	25	85.77	67.31	1.0	1.0
Cyclohexane + 2-propanol	60	142.66	797.96	1.0	1.0
Methanol + benzene	35	899.85	92.17	1.0	1.0
Methanol + 2-propanol	40	627.74	−451.28	1.0	1.0
Acetonitrile + cyclohexane	25	1217.8	679.03	1.1	1.1
Methanol + cyclohexane	25	1158.4	471.58	1.0	1.1

be determined from the experimental tie-line results. Table 5 shows the binary Wilson-like parameters; those for the completely miscible mixtures were mainly taken from Gmehling et al. [3, 6, 7, 9]. The ternary parameters of the two models were evaluated by minimizing the following objective

TABLE 6

The results of fitting the extended UNIQUAC and modified Wilson models to ternary tie-lines at 25°C

System (1 + 2 + 3)	Type	Number of data points	Ternary parameters		F/mol%	
			I[a]	II[b]	I	II
Cyclohexane	II	6	$\tau_{231} = 1460$	$\Lambda_{231} = -0.2427$	0.49	0.38
+benzene			$\tau_{132} = 0.1098$	$\Lambda_{132} = 0.4265$		
+acetonitrile			$\tau_{123} = -0.1517$	$\Lambda_{123} = -0.3536$		
Cyclohexane	I	7	$\tau_{231} = 0.4016$	$\Lambda_{231} = 0.4016$	0.43	0.49
+methanol			$\tau_{132} = -0.1534$	$\Lambda_{132} = -0.1534$		
+acetonitrile			$\tau_{123} = -0.1083$	$\Lambda_{123} = -0.1083$		
Cyclohexane	I	6	$\tau_{231} = -0.0364$	$\Lambda_{231} = -0.1286$	0.40	0.45
+2-propanol			$\tau_{132} = -0.1743$	$\Lambda_{132} = 0.2002$		
+acetonitrile			$\tau_{123} = 0.1502$	$\Lambda_{123} = 0.0150$		
Cyclohexane	I	6	$\tau_{231} = 0.5750$	$\Lambda_{231} = 0.5260$	0.30	0.30
+benzene			$\tau_{132} = -0.1749$	$\Lambda_{132} = 0.1309$		
+methanol			$\tau_{123} = 0.1325$	$\Lambda_{123} = -0.1653$		
Cyclohexane	I	7	$\tau_{231} = -0.4940$	$\Lambda_{231} = -0.1110$	0.52	0.50
+2-propanol			$\tau_{132} = 0.5619$	$\Lambda_{132} = 0.3723$		
+methanol			$\tau_{123} = -0.4545$	$\Lambda_{123} = -0.0350$		

[a] Extended UNIQUAC model. [b] Modified Wilson model.

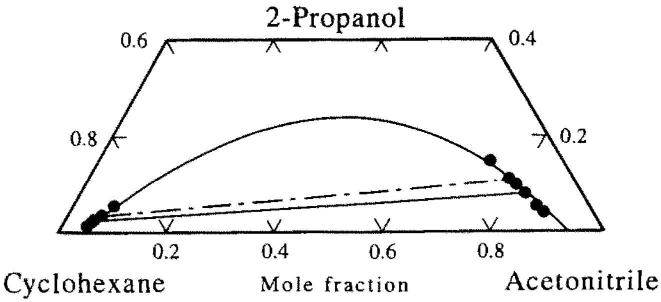

Fig. 1. Calculated liquid–liquid equilibria for cyclohexane + 2-propanol + acetonitrile at 25°C: ●— — —●, experimental tie line; ———, calculated from the extended UNIQUAC model with binary and ternary parameters.

function with a simplex method [16]

$$F=\left[\sum_{i}\sum_{j}\sum_{k}(x_{ijk,\mathrm{calc}}-x_{ijk,\mathrm{exptl}})^2/6M\right]^{0.5} \tag{9}$$

where $i=1$, 2, 3 (components), $j=1$, 2 (phases) and $k=1,2,\ldots M$ (tie-lines). Table 6 gives the ternary calculated results. The two models gave similar results. Figure 1 shows the experimental tie-lines and the calculated results for cyclohexane + 2-propanol + acetonitrile. Table 7 also gives the quaternary calculated results and Table 8 shows the detailed deviations between the experimental and calculated liquid mole fractions.

We may conclude that the experimental tie-line results for the ternary and quaternary systems studied here have been well correlated with the two models using binary, ternary and quaternary parameters.

TABLE 7

The results of fitting the extended UNIQUAC and modified Wilson models to the quaternary tie-lines of the two systems at 25°C

System (1 + 2 + 3 + 4)	No. of data points	Quaternary parameters				Deviations/mol%			
		I[a]		II[b]		AAM[c]		RMS[d]	
						I[a]	II[b]	I	II
Cyclohexane	13	$\tau_{2341}=$	0.2141	$\Lambda_{2341}=$	−0.7108	0.56	0.59	0.62	0.66
+benzene		$\tau_{1342}=$	1.6823	$\Lambda_{1342}=$	1.5830	0.70[e]	0.78	0.90	0.98
+acetonitrile		$\tau_{1243}=$	−2.8095	$\Lambda_{1243}=$	−2.5885				
+methanol		$\tau_{1234}=$	2.4411	$\Lambda_{1234}=$	2.2347				
Cyclohexane	14	$\tau_{2341}=$	−1.9557	$\Lambda_{2341}=$	−0.8886	0.40	0.51	0.49	0.58
+2-propanol		$\tau_{1342}=$	0.1171	$\Lambda_{1342}=$	−9.6756	0.48[e]	0.67	0.56	0.79
+acetonitrile		$\tau_{1243}=$	−0.3581	$\Lambda_{1243}=$	−1.5987				
+methanol		$\tau_{1234}=$	0.6832	$\Lambda_{1234}=$	8.5811				

[a] Extended UNIQUAC model. [b] Modified Wilson model. [c] AAM means absolute arithmetic mean deviation. [d] RMS means root-mean-squared deviation. [e] Predicted value based on the binary and ternary parameters.

TABLE 8

Detailed calculated results for the two quaternary systems at 25°C

	Component-(1)-lean phase				Component-(1)-rich phase			
	AAM[a]		RMS[b]		AAM		RMS	
	I[c]	II[d]	I	II	I	II	I	II
Cyclohexane(1) + benzene(2) + acetonitrile(3) + methanol(4)								
δx_1	0.0048	0.0035	0.0059	0.0047	0.0099	0.0068	0.0112	0.0085
δx_2	0.0016	0.0028	0.0022	0.0030	0.0012	0.0027	0.0017	0.0028
δx_3	0.0051	0.0076	0.0057	0.0084	0.0051	0.0072	0.0074	0.0080
δx_4	0.0069	0.0071	0.0078	0.0078	0.0099	0.0093	0.0106	0.0098
Cyclohexane(1) + 2-propanol(2) + acetonitrile(3) + methanol(4)								
δx_1	0.0031	0.0063	0.0053	0.0080	0.0058	0.0080	0.0077	0.0109
δx_2	0.0030	0.0018	0.0033	0.0021	0.0029	0.0019	0.0032	0.0022
δx_3	0.0060	0.0073	0.0062	0.0079	0.0053	0.0049	0.0058	0.0057
δx_4	0.0023	0.0018	0.0027	0.0023	0.0037	0.0049	0.0049	0.0066

[a] AAM means absolute arithmetic mean deviation between the experimental and calculated liquid mole fractions. [b] RMS means root-mean-squared deviation between the experimental and calculated liquid mole fractions. [c] Extended UNIQUAC model. [d] Modified Wilson model.

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