Liquid-liquid equilibria for methyl isobutyl ketone + cresols + water at 333.15K, 343.15K and 353.15K: Experimental results and data correlation

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ABSTRACT

In this work, the liquid-liquid equilibrium (LLE) data for ternary systems, methyl isobutyl ketone + *o*, *m* or *p*-cresol + water were measured at 333.15K, 343.15K and 353.15K under 101.3kPa. The nonrandom (NRTL) and universal quasichemical (UNIQUAC) models were used to correlate the experimental data, and the results indicated that, both models predicted LLE data quite accurately, with root mean square deviations (RMSD) less than 2.5%. The binary interaction parameters calculated from these two models were also reported. Distribution coefficient and selectivity were calculated to assess the extraction performance of methyl isobutyl ketone.

Keywords: Liquid-liquid equilibria; cresol; methyl isobutyl ketone; NRTL model; UNIQUAC model

1 Introduction

Coal gasification or distillation produces wastewater with highly concentrated phenols, which contains volatile phenols such as phenol and cresols, nonvolatile phenols such as hydroquinone and polyphenols, ammonia, organic acids and other substances. Among these pollutants, cresols are harmful to organism at concentration higher than $250 \text{ mg}\cdot\text{L}^{-1}$ [1], and may bring long-term adverse effects to the aquatic environment. Cresols are extremely toxic, even more toxic than phenol: e.g. the LD50 (rats oral) of *o*-, *m*-, *p*-cresol and phenol are 121, 242, 207 and 317 mg/kg respectively. They also have higher bio-accumulation potential than phenol as indicated by the octanol-water partition coefficient: e.g. log Kow of *o*-, *m*-, *p*-cresol and phenol are 1.95, 1.96, 1.95 and 1.46 respectively [2]. Thus it is necessary to remove cresols from waste waters before discharging them [3].

Solvent extraction is a frequently used method to treat phenols containing waste water with a range of advantages such as ease of implement, high throughput, versatility and economical efficiency [4]. This method has being used in China [5], South Africa [1], United states [1,6], etc., for quite a few decades, and the process simulation, operation cost and industrial implementation has been studied thoroughly [7,8]. Liquid-liquid equilibria (LLE) data are essential for designing or optimizing an extraction process [9-11]. Some LLE data of the ternary solvent-cresol-water systems have been published in recent years. The experimental data for (toluene + *o*-, *m*-, *p*-cresol + water), (ethylbenzene + *o*-, *m*-, *p*-cresol + water), (heptane + *o*-, *m*-, *p*-cresol + water) and (octane + *o*-, *m*-, *p*-cresol + water) systems were measured by Martin et al. [12,13]. Kupatkin et al. [14] studied the ternary systems, (trimethylcarbinol + *o*-cresol + water) and (trimethylcarbinol + *m*-cresol + water) at 298.2 and 323.2K. The system (methyl butyl ketone + *o*-, *m*-, *p*-cresol + water) at 298.2 and 313.2K was investigated by Lv et al. [15]. The LLE data of the systems, (2-methoxy-2-methylpropane + *o*-, *m*-, *p*-cresol + water) at 298.15 and 313.15 K were reported by Luo et al. [16-18].

Methyl isobutyl ketone (MIBK) is considered to be an excellent extraction solvent to searate cresols from water with high distribution coefficients, and has been used to treat phenolic waste water in industry [5,7]. It also has attracted the interest of researchers, with tie line data for the systems, (methyl isobutyl ketone + *o*- or *p*-cresol + water), measured at 303.2K by Telkikar et al. [19]. However, recovering phenols from waste water in industry are usually performed at temperatures above 333 K to avoid clogging the extraction

installation by paraffin wax (melting point between 328.15 and 335.15 K) in the industrial efflux [20], while corresponding LLE data in such temperature range remain unknown. Hence it is critical to study solvent extraction of cresols with MIBK above 333 K for designing or optimizing wastewater treatment process in industry.

The LLE data of ternary systems, (methyl isobutyl ketone + *o*-, *m*-, *p*-cresol + water) at (333.15, 343.15 and 353.15) K under 101.3kPa were measured in this work. The experimental data were correlated by NRTL [21] and UNIQUAC [22] activity coefficient to yield binary interaction parameters .

2 Experimental

2.1 Materials

The purity and source of chemical reagents in this work are listed in Table 1. These chemicals were used without further purification since their purity had been verified with analysis methods listed in Table 1. Distilled water was used throughout all experiments.

2.2 Apparatus and procedure

The experimental LLE data for the ternary systems, MIBK + *o*, *m* or *p*-cresol + water were measured at 333.15K, 343.15K and 353.15K under 101.3kPa. Certain amounts of MIBK, *o*, *m* or *p*-cresol, and water were loaded into a 100 mL glass equilibrium cell to form a ternary mixture. The mixture was agitated vigorously for more than 2 hours and then was left to settle for over 20 hours for the system to reach the phase equilibrium. The temperature of the mixtures in the cell was kept constant by using a thermostatic bath with a fluctuation of 0.1 K.

When the phase equilibrium was reached and the mixture was split into two layers, the samples of both layers were collected with a syringe, and were analyzed by a gas chromatography (GC 6820, Agilent Technologies) equipped with a flame ionization detector (FID, with a sensitivity of 10-100 ppb) and a DB-5MS capillary column (30 m × 0.32 mm × 0.25 μm). The oven initial temperature was held at 313.15 K for 2 min and then increased 443.15 K at a rate of 30 K·min⁻¹. The detector and injector temperatures were held at 523.15 K and 533.15 K. The nitrogen was used as carrier gas with a rate of 30 ml·min⁻¹. The solvent was methanol.

The composition of the sample was determined by an internal standard method, where

n-butyl acetate was used as an internal standard for MIBK and 1, 3, 5-trimethylbenzene for cresols. The water' mole fraction was calculated from deducting those of the other two component (MIBK and cresols) from 1. The samples and internal standards were all weighed by an analytical balance (Shimadzu AUW220D) with an accuracy of $\pm 0.1\text{mg}$. Each sample was measured for at least 3 times, with a standard deviation of less than 0.02 %, thus the average value was reported in this work.

3 Results and discussion

3.1 Experimental LLE data.

Tables 2-4 show the LLE data of ternary systems, MIBK + cresols + water at (333.15, 343.15 and 353.15) K under 101.3kPa. All concentrations are expressed in mole fraction. The tie-lines data for the studied systems at were plotted in the triangular diagrams as shown in Figs. 1-3.

To estimate the capacity of MIBK to separate cresols from wastewater, the distribution coefficient (D) and separation factor (S) are calculated as follow

$$D = \frac{x_{21}}{x_{23}} \quad (1)$$

$$S = D \frac{x_{33}}{x_{31}} \quad (2)$$

where x_{21} and x_{23} are cresol mole fraction in organic and aqueous phases, respectively, x_{31} and x_{33} are water mole fraction in organic and aqueous phases, respectively. These distribution coefficient and selectivity at each temperature are listed in Tables 2-4. The results indicate that MIBK is an efficient solvent for extracting cresols. According to tables 2-4, the influence of temperature on LLE data is insignificant, in other words, temperature affect LLE data very slightly. The solubility of cresols in water is in the order of *o*-cresol > *m*-cresol > *p*-cresol, and the selectivity is in the order of *p*-cresol > *o*-cresol > *m*-cresol in the studied temperature range.

Distribution coefficient and selectivity of cresols as a function of the mole fraction in the aqueous phase at 333.15, 343.15 and 353.15K are shown in Figs. 4-9. According to these

figures, the distribution coefficient and selectivity decrease with increasing temperature. The reason may be attributed to that, elevated temperature breaks the hydrogen bonding network of water and thus increase the solubility of cresols in water significantly[23]. Nevertheless, D and S of cresols are still quite large even at 353K: $D > 400$ and $S > 1000$. In comparison, D and S of phenol in MIBK at 353K are 200 and 980 [18], both are smaller than cresol. This indicates cresols are very easy to extract, which further highlight the advantages of solvent extraction over other methods when treating phenolic wastewater. MIBK's solubility (1.7%) is less than methyl butyl ketone (2.0%) in water, and its boiling point is also lower, which indicates we can recover MIBK easier with less energy consumption after extraction. MIBK is also cheaper than MBK. All these data indicate MIBK can be used to treat phenolic wastewater as a very promising extractant.

3.2 Data Correlation.

The NRTL and UNIQUAC models were used to correlate the experimental LLE data. The UNIQUAC structural parameters (r and q) taken from literatures [24, 25] are shown in Table 5. The binary interaction parameters (g_{ij} - g_{jj} and g_{ji} - g_{ii} , u_{ij} - u_{jj} and u_{ji} - u_{ii}) in the NRTL or UNIQUAC model for ternary systems, MIBK + cresols + water, were obtained by minimizing the objective function (OF) [26] given in the following equation:

$$OF = \sum_{i=1}^3 \sum_{j=1}^2 \sum_{k=1}^n \left[\frac{(T_k^{\text{exp}} - T_k^{\text{cal}})^2}{\sigma_T^2} + \frac{(x_{ijk}^{\text{exp}} - x_{ijk}^{\text{cal}})^2}{\sigma_x^2} \right] \quad (3)$$

where n is the number of the tie-lines, x^{exp} and T^{exp} are the experimental mole fraction and temperature, and x^{cal} and T^{cal} are the calculated mole fraction and temperature, respectively. The subscripts i , j and k refer to the component, the phase and the tie-line, respectively. σ_T and σ_x denote the standard deviation of the temperature and the mole fraction.

The root-mean-square-deviation (RMSD) was used to assess the agreement between the experimental data and calculated results from the NRTL or UNIQUAC model. The RMSD value is defined as:

$$\text{RMSD} = \left[\frac{\sum_{i=1}^3 \sum_{j=1}^2 \sum_{k=1}^n (x_{ijk}^{\text{exp}} - x_{ijk}^{\text{cal}})^2}{6n} \right]^{1/2} \quad (4)$$

The RMSD values (< 0.8%) of the two models are shown in Table 6. It can be seen that both NRTL and UNIQUAC models show good representation of the tie-line data for the studied systems. The binary interaction parameters calculated from the NRTL and UNIQUAC models at (333.15, 343.15 and 353.15) K are listed in Table 6 (the non-randomness parameter (α_{ij}) for the NRTL model are also shown). These binary interaction parameters can be used to design or simulate the extraction process of cresols.

The LLE tie lines, calculated from the NRTL or UNIQUAC model are shown in Figs. 1-3, with comparison to experimental data, which indicate the calculated results are in good agreement with the experimental data. Thus, both NRTL and UNIQUAC models are suitable for simulating the extraction process of cresols with MIBK.

4 Conclusions

The LLE data for the ternary systems, MIBK + *o*-, *m*-, *p*-cresol + water, were measured at 333.15K, 343.15K and 353.15K under 101.3kPa. These LLE data indicates MIBK extracts cresols from water with rather high distribution coefficients and selectivities. In addition, MIBK shows better physical properties than other extractants such as MBK (e.g. lower solubility and lower boiling point). All the results indicate MIBK is a very promising extractant to recovery cresols from water above 333 K. The experimental LLE data were correlated by the NRTL and UNIQUAC models, which both described the phase behavior of studied systems very accurately and yielded relevant binary interaction parameters among MIBK, water, and *o*-, *m*-, *p*-cresol. The experimental LLE data and calculated binary interaction parameters in this work should be useful for designing or optimizing the extraction process of phenolic compounds in industry, especially in the field of wastewater treatment.

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Captions of Tables and Figures

Table Captions

Table 1

Source and purity of the materials studied.

Table 2

Experimental LLE Data (mole fraction) for ternary system MIBK(1) + *o*-cresol(2) + water(3) at 333.15 K, 343.15K and 353.15K and 101.3kPa.^a

Table 3

Experimental LLE Data (mole fraction) for ternary system MIBK(1) + *m*-cresol(2) + water(3) at 333.15 K, 343.15K and 353.15K and 101.3kPa.^a

Table 4

Experimental LLE Data (mole fraction) for ternary system MIBK(1) + *p*-cresol(2) + water(3) at 333.15 K, 343.15K and 353.15K and 101.3kPa.^a

Table 5

UNIQUAC Structural (Area and Volume) Parameters.

Table 6

Binary Interaction Parameters of NRTL and UNIQUAC Model for the studied systems at different temperatures.^a

Figure Captions

Fig. 1.

Ternary diagram for LLE data of {MIBK(1) + *o*-cresol (2) + water (3)} at 333.15 K and 101.3kPa: □-□, experimental data; ▲, calculated data from NRTL model; ○, calculated data from UNIQUAC model.

Fig. 2.

Ternary diagram for LLE data of {MIBK(1) + *m*-cresol (2) + water (3)} at 333.15 K and 101.3kPa: □-□, experimental data; ▲, calculated data from NRTL model; ○, calculated data from UNIQUAC model.

Fig.3.

Ternary diagram for LLE data of {MIBK(1) + *p*-cresol (2) + water (3)} at 333.15 K and 101.3kPa: □-□, experimental data; ▲, calculated data from NRTL model; ○, calculated data from UNIQUAC model.

Fig. 4.

Distribution coefficient of *o*-cresol, *D*, plotted against the mole fraction of *o*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 5.

Distribution coefficient of *m*-cresol, *D*, plotted against the mole fraction of *m*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 6.

Distribution coefficient of *p*-cresol, *D*, plotted against the mole fraction of *p*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 7.

Selectivity of *o*-cresol, *S*, plotted against the mole fraction of *o*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 8.

Selectivity of *m*-cresol, *S*, plotted against the mole fraction of *m*-cresol in the aqueous phase at different

temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 9.

Selectivity of *p*-cresol, *S*, plotted against the mole fraction of *p*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Table 1

Source and purity of the chemical reagents.

Component	Source	Stated Mass fraction purity	Purification method	Analysis method
methanol	Xiya Reagent	≥0.99	None	GC ^a
2-cresol	Xiya Reagent	≥0.99	None	GC ^a
3-cresol	Xiya Reagent	≥0.99	None	GC ^a
4-cresol	Xiya Reagent	≥0.99	None	GC ^a
1,3,5-trimethylbenzene	Xiya Reagent	≥0.99	None	GC ^a
1-octanol	Xiya Reagent	≥0.99	None	GC ^a
4-Methyl-2-pentanone	Xiya Reagent	≥0.99	None	GC ^a

^a Gas chromatography

Table 2

Experimental LLE Data (mole fraction) for ternary system MIBK(1) + *o*-cresol(2) +water(3) at 333.15 K, 343.15K and 353.15K and 101.3kPa.^a

T/K	Organic Phase			Aqueous phase			D	S
	x_1	x_2	x_3	x_1	x_2	x_3		
333.15	0.2521	0.3588	0.3891	0.0007	0.0008	0.9985	449	1152
	0.2869	0.3363	0.3769	0.0009	0.0007	0.9984	480	1272
	0.3197	0.3148	0.3655	0.0010	0.0006	0.9984	525	1434
	0.3682	0.2828	0.3490	0.0011	0.0005	0.9984	566	1619
	0.4135	0.2459	0.3406	0.0013	0.0004	0.9983	615	1803
	0.4750	0.2017	0.3233	0.0014	0.0003	0.9983	672	2075
	0.5230	0.1615	0.3155	0.0015	0.0002	0.9983	808	2557
	0.5599	0.1357	0.3045	0.0016	0.0001	0.9983	1357	4449
	0.6330	0.0967	0.2703	0.0017	0.0001	0.9982	967	3571
	0.8112	0.0000	0.1888	0.0023	0.0000	0.9977		
343.15	0.2341	0.3650	0.4008	0.0006	0.0009	0.9985	406	1011
	0.2653	0.3446	0.3900	0.0008	0.0008	0.9984	431	1103
	0.3008	0.3212	0.3781	0.0009	0.0007	0.9984	459	1212
	0.3566	0.2905	0.3529	0.0011	0.0006	0.9984	484	1369
	0.4054	0.2512	0.3434	0.0012	0.0004	0.9984	628	1826
	0.4677	0.2084	0.3238	0.0014	0.0003	0.9983	695	2143
	0.5233	0.1698	0.3069	0.0015	0.0002	0.9983	849	2762
	0.5667	0.1393	0.2939	0.0016	0.0001	0.9983	697	2368
	0.6145	0.1053	0.2803	0.0017	0.0001	0.9983	1053	3750
	0.7413	0.0000	0.2587	0.0022	0.0000	0.9978		
353.15	0.2175	0.3710	0.4115	0.0006	0.0010	0.9985	371	900
	0.2375	0.3519	0.4106	0.0007	0.0009	0.9985	391	951
	0.2787	0.3251	0.3962	0.0008	0.0008	0.9984	406	1023
	0.3169	0.2998	0.3832	0.0009	0.0006	0.9984	500	1303
	0.3745	0.2509	0.3746	0.0011	0.0005	0.9984	502	1338
	0.4190	0.2229	0.3581	0.0013	0.0004	0.9984	557	1553
	0.4752	0.1844	0.3404	0.0014	0.0003	0.9983	615	1804
	0.5347	0.1437	0.3215	0.0015	0.0002	0.9983	719	2233
	0.5794	0.1104	0.3102	0.0016	0.0001	0.9983	1104	3553
	0.6928	0.0000	0.3072	0.0019	0.0000	0.9981		

^a Standard uncertainties u are $u(T) = 0.1$ K, $u(p)=1$ kPa, $u(x)=0.0002$

Table 3

Experimental LLE Data (mole fraction) for ternary system MIBK(1) + *m*-cresol(2) + water(3) at 333.15K, 343.15K and 353.15K and 101.3kPa.^a

T/K	Organic Phase			Aqueous phase			D	S
	x_1	x_2	x_3	x_1	x_2	x_3		
333.15	0.2413	0.3989	0.3598	0.0007	0.0009	0.9984	443	1229
	0.3010	0.3563	0.3426	0.0009	0.0008	0.9983	445	1297
	0.3391	0.3318	0.3291	0.0010	0.0007	0.9983	474	1438
	0.3971	0.2865	0.3164	0.0011	0.0006	0.9983	478	1508
	0.4566	0.2365	0.3069	0.0013	0.0005	0.9983	473	1539
	0.4929	0.2102	0.2969	0.0014	0.0004	0.9982	526	1768
	0.5293	0.1886	0.2821	0.0015	0.0003	0.9982	629	2226
	0.5864	0.1433	0.2703	0.0016	0.0002	0.9982	717	2648
	0.6361	0.1007	0.2632	0.0018	0.0001	0.9981	1007	3819
	0.8112	0.0000	0.1888	0.0023	0.0000	0.9977		
343.15	0.2263	0.4042	0.3695	0.0007	0.0010	0.9984	404	1092
	0.2805	0.3529	0.3666	0.0008	0.0008	0.9983	441	1201
	0.3178	0.3267	0.3555	0.0009	0.0007	0.9983	467	1311
	0.3702	0.2846	0.3452	0.0011	0.0006	0.9983	474	1371
	0.4277	0.2397	0.3326	0.0013	0.0005	0.9982	479	1438
	0.4628	0.2126	0.3245	0.0013	0.0004	0.9982	532	1636
	0.5030	0.1859	0.3111	0.0014	0.0003	0.9982	620	1989
	0.5577	0.1492	0.2932	0.0015	0.0002	0.9982	746	2540
	0.6188	0.1063	0.2749	0.0017	0.0002	0.9982	532	1932
	0.7413	0.0000	0.2587	0.0022	0.0000	0.9978		
353.15	0.2210	0.4011	0.3779	0.0006	0.0010	0.9984	401	1059
	0.2786	0.3500	0.3714	0.0008	0.0009	0.9984	389	1046
	0.3073	0.3277	0.3650	0.0009	0.0008	0.9983	410	1121
	0.3573	0.2931	0.3496	0.0010	0.0007	0.9983	419	1196
	0.4181	0.2420	0.3399	0.0012	0.0005	0.9983	484	1422
	0.4575	0.2157	0.3268	0.0013	0.0005	0.9983	431	1317
	0.4950	0.1851	0.3198	0.0014	0.0004	0.9982	463	1445
	0.5379	0.1470	0.3151	0.0015	0.0003	0.9982	490	1552
	0.5865	0.1029	0.3106	0.0016	0.0002	0.9982	515	1655
	0.6928	0.0000	0.3072	0.0019	0.0000	0.9981		

^a Standard uncertainties u are $u(T) = 0.1$ K, $u(p) = 1$ kPa, $u(x) = 0.0002$

Table 4

Experimental LLE Data (mole fraction) for ternary system MIBK(1) + *p*-cresol(2) + water(3) at 333.15 K, 343.15K and 353.15K and 101.3kPa.^a

T/K	Organic Phase			Aqueous phase			D	S
	x_1	x_2	x_3	x_1	x_2	x_3		
333.15	0.2320	0.3882	0.3798	0.0006	0.0009	0.9984	431	1133
	0.2703	0.3600	0.3697	0.0008	0.0008	0.9984	450	1215
	0.3168	0.3173	0.3659	0.0009	0.0007	0.9984	453	1236
	0.3654	0.2844	0.3502	0.0011	0.0005	0.9984	569	1622
	0.4131	0.2516	0.3353	0.0013	0.0004	0.9983	629	1873
	0.4630	0.2170	0.3200	0.0014	0.0003	0.9983	723	2256
	0.5197	0.1645	0.3159	0.0015	0.0002	0.9983	823	2601
	0.5555	0.1519	0.2926	0.0016	0.0001	0.9983	1519	5183
	0.6123	0.1110	0.2767	0.0017	0.0001	0.9982	1110	4004
	0.8112	0.0000	0.1888	0.0023	0.0000	0.9977		
343.15	0.2241	0.3948	0.3811	0.0006	0.0009	0.9985	439	1150
	0.2617	0.3621	0.3762	0.0007	0.0009	0.9984	402	1067
	0.2937	0.3337	0.3726	0.0009	0.0007	0.9984	477	1278
	0.3544	0.2866	0.3590	0.0011	0.0005	0.9984	573	1594
	0.3943	0.2568	0.3489	0.0012	0.0004	0.9984	642	1837
	0.4418	0.2215	0.3366	0.0014	0.0003	0.9983	738	2189
	0.4837	0.1901	0.3261	0.0015	0.0002	0.9983	951	2911
	0.5329	0.1530	0.3140	0.0016	0.0002	0.9983	765	2432
	0.5874	0.1144	0.2982	0.0017	0.0001	0.9982	1144	3829
	0.7413	0.0000	0.2587	0.0022	0.0000	0.9978		
353.15	0.2090	0.3943	0.3967	0.0006	0.0010	0.9984	394	992
	0.2454	0.3698	0.3848	0.0007	0.0009	0.9984	411	1066
	0.2935	0.3274	0.3791	0.0009	0.0007	0.9984	468	1233
	0.3412	0.2916	0.3672	0.0010	0.0006	0.9984	486	1321
	0.3831	0.2601	0.3568	0.0012	0.0005	0.9984	520	1455
	0.4294	0.2252	0.3454	0.0013	0.0003	0.9984	751	2171
	0.4840	0.1743	0.3417	0.0014	0.0003	0.9983	581	1697
	0.5144	0.1606	0.3251	0.0015	0.0002	0.9983	803	2466
	0.5697	0.1196	0.3107	0.0016	0.0001	0.9983	1196	3843
	0.6928	0.0000	0.3072	0.0019	0.0000	0.9981		

^a Standard uncertainties u are $u(T) = 0.1$ K, $u(p) = 1$ kPa, $u(x) = 0.0002$

Table 5

UNIQUAC Structural (Area and Volume) Parameters

component	r	q
water	0.9200	1.4000
MIBK	4.5967	3.9560
<i>o</i> -cresol	4.8180	3.6480
<i>m</i> -cresol	4.8180	3.6480
<i>p</i> -cresol	4.8180	3.6480

Table 6

Binary Interaction Parameters of NRTL and UNIQUAC Model for the studied systems at different temperatures.^a

T/K	components	UNIQUAC			NRTL			RMSD
	$i-j$	$u_{ij}-u_{jj}$ /J·mol ⁻¹	$u_{ji}-u_{ii}$ /J·mol ⁻¹	RMSD	$g_{ij}-g_{jj}$ /J·mol ⁻¹	$g_{ji}-g_{ii}$ /J·mol ⁻¹	α_{ij}	
MIBK(1) + <i>o</i> -cresol(2) + water (3)								
333.15	1-2	-289.5	280.5	0.0078	594.7	-646.1	0.3	0.0079
	1-3	-251.9	-193.3		-35.2	2000.0	0.2	
	2-3	208.0	-603.5		-431.8	2497.7	0.2	
343.15	1-2	-293.5	280.9	0.0051	635.9	-661.1	0.3	0.0051
	1-3	-257.4	-202.8		-37.2	2070.8	0.2	
	2-3	216.1	-623.5		-453.4	2574.3	0.2	
353.15	1-2	-280.1	275.4	0.0054	565.6	-633.7	0.3	0.0066
	1-3	-215.3	-233.8		-90.0	2183.3	0.2	
	2-3	226.4	-648.7		-464.5	2643.1	0.2	
MIBK(1) + <i>m</i> -cresol(2) + water (3)								
333.15	1-2	-221.6	217.9	0.0061	470.6	-503.1	0.3	0.0054
	1-3	-250.7	-200.3		-22.4	2014.9	0.2	
	2-3	152.6	-512.8		-357.8	2399.9	0.2	
343.15	1-2	-122.0	144.3	0.0056	403.2	-439.8	0.3	0.0043
	1-3	-253.5	-210.6		-50.0	2113.3	0.2	
	2-3	175.8	-599.0		-390.1	2507.3	0.2	
353.15	1-2	-169.7	166.8	0.0031	350.4	-369.1	0.3	0.0026
	1-3	-180.7	-262.6		-111.5	2247.9	0.2	
	2-3	158.2	-545.2		-365.0	2543.2	0.2	
MIBK(1) + <i>p</i> -cresol(2) + water (3)								
333.15	1-2	-313.3	306.1	0.0083	637.1	-706.8	0.3	0.0082
	1-3	-258.3	-185.7		-34.1	1978.1	0.2	
	2-3	203.4	-590.1		-415.0	2464.7	0.2	
343.15	1-2	-316.7	306.5	0.0089	608.0	-679.8	0.3	0.0077
	1-3	-235.2	-207.5		-69.7	2076.1	0.2	
	2-3	226.9	-693.4		-406.4	2523.8	0.2	
353.15	1-2	-302.8	295.2	0.0073	591.9	-656.4	0.3	0.0062
	1-3	-207.9	-233.8		-100.7	2177.1	0.2	
	2-3	230.3	-711.4		-416.5	2599.8	0.2

Fig. 1. Ternary diagram for LLE data of {MIBK(1) + *o*-cresol (2) + water (3)} at 333.15 K and 101.3kPa: □-□, experimental data; ▲, calculated data from NRTL model; ○, calculated data from UNIQUAC model.

Fig. 2. Ternary diagram for LLE data of {MIBK(1) + *m*-cresol (2) + water (3)} at 333.15 K and 101.3kPa: □-□, experimental data; ▲, calculated data from NRTL model; ○, calculated data from UNIQUAC model.

Fig. 3. Ternary diagram for LLE data of {MIBK(1) + *p*-cresol (2) + water (3)} at 333.15 K and 101.3kPa: □-□, experimental data; ▲, calculated data from NRTL model; ○, calculated data from UNIQUAC model.

Fig. 4. Distribution coefficient of *o*-cresol, D , plotted against the mole fraction of *o*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 5. Distribution coefficient of *m*-cresol, D , plotted against the mole fraction of *m*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 6. Distribution coefficient of *p*-cresol, D , plotted against the mole fraction of *p*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 7. Selectivity of o -cresol, S , plotted against the mole fraction of o -cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 8. Selectivity of m -cresol, S , plotted against the mole fraction of m -cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.

Fig. 9. Selectivity of *p*-cresol, S , plotted against the mole fraction of *p*-cresol in the aqueous phase at different temperatures: ■, at 333.15K; ○, at 343.15K; ▲, at 353.15K.