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Liquid−Liquid Equilibria for Mixtures of (Furfuryl Alcohol + an Aromatic Hydrocarbon + an Alkane) at $T = 298.15$ K

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Liquid−liquid equilibrium results for mixtures of furfury alcohol + an aromatic hydrocarbon + an alkane at $T = 298.15$ K are reported, where an aromatic hydrocarbon refers to benzene or methyl benzene or 1,2-dimethylbenzene and an alkane refers to hexane or dodecane or hexadecane. The data presented indicate the utility of furfuryl alcohol as a solvent for the separation of aromatic and aliphatic hydrocarbons using solvent extraction. The compositions of the conjugated phases were correlated with the UNIQUAC and NRTL equations.

Introduction

Furfuryl alcohol is an inexpensive solvent that is formed as a byproduct in the manufacture of sugar.[1] In this work we investigate the usefulness of furfuryl alcohol as a solvent for the separation of aromatic and aliphatic hydrocarbons using solvent extraction. This is an area of active research.[2−5] The suitability of a new solvent for liquid−liquid extraction can be determined from its phase equilibrium properties, and in this work we report the liquid−liquid equilibrium results for the mixtures (furfuryl alcohol + an aromatic hydrocarbon + an alkane) at $T = 298.15$ K, where an aromatic hydrocarbon is benzene or methyl benzene or 1,2-dimethylbenzene and an alkane refers to hexane or dodecane or hexadecane. A search of the literature has indicated that data for mixtures presented here have not been reported previously.

The NRTL[6] model and the UNIQUAC[7] model were used to correlate the tie line data.

Experimental Section

Procedure. The binodal curves were determined at 298.15 K using the cloud point method, described in detail by Letcher et al.[8,9] The tie lines were determined using the refractive index method, described in detail by Chueh and Briggs.[10] The accuracy of this technique was established in a previous paper[5] by comparing results obtained in our laboratory with literature values for a test system and was found to be within 0.005 mole fraction. At least two tie lines for each of the systems discussed here were determined by GLC, confirming the results which were obtained by the refractive index method. The temperature was controlled to within 0.01 K using a Tronac temperature controller used in conjunction with a calibrated Hewlett-Packard quartz thermometer.

Chemicals. The chemicals used in this work were supplied by ACROS. The purities of the chemicals were determined by gas chromatography, and the results are recorded in Table 1. Furfuryl alcohol was distilled under vacuum and kept in a sealed bottle until use. Furfuryl alcohol was tested for moisture using the Karl Fischer method. The moisture was found to be less than 0.1% mole fraction. All other chemicals were not treated further.

Table 1. Details of the Chemicals: Percentage Mole Fraction Purities, UNIQUAC Structural Parameters, and Refractive Indices

	purity	UNIQUAC structural parameters[15]		n_D^{25}	
compd	percentage mole fraction	r	q^a	exp	lit.[14]
$C_5H_6O_2$	>99.0	3.84	3.27	1.4841	
C_6H_6	99.9	3.19	2.40	1.4990	1.4979
$C_6H_5CH_3$	99.8	3.92	2.98	1.4940	1.4940
1,2-$C_6H_4(CH_3)_2$	>99.0	4.66	3.54	1.5018	1.5029
$CH_3(CH_2)_4CH_3$	>99.0	4.50	3.86	1.3728	1.3723
$CH_3(CH_2)_{10}CH_3$	>99.0	8.55	7.10	1.4275	1.4269
$CH_3(CH_2)_{12}CH_3$	>99.0	11.24	8.26	1.4325	1.4325

[a] $q' = q$ for the compounds used in this work.

Results

The compositions of points on the binodal curve for the mixtures ($C_5H_6O_2$ + $C_6H_{6-m}(CH_3)_m$ + $CH_3(CH_2)_nCH_3$) at $T = 298.15$ K are reported in Table 2, where m is the number of methyl groups on the benzene ring and n is number of CH_2 units in the alkane compound. The compositions of conjugate phases for these mixtures (tie lines) are given in Table 3. The compositions of the plait points or critical points, which were determined following the method of Treybal,[11] are given in Table 4. The ternary phase diagrams showing the binodal curve together with tie lines and plait points are given in Figure 1. The ability of furfuryl alcohol to separate aromatic and aliphatic hydrocarbon mixtures is indicated by the selectivity, S, defined as[12]

$$S = (x_2'/x_3')/(x_2''/x_3'')$$

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Table 2. Compositions of Points on the Binodal Curve for the Mixtures $\{(x_1)C_5H_6O_2 + (x_2)C_6H_{6-m}(CH_3)_m + (1 - x_1 - x_2)CH_3(CH_2)_nCH_3\}$ at $T = 298.15$ K

x_1	x_2	x_1	x_2	x_1	x_2
$C_5H_6O_2 + CH_3(CH_2)_4CH_3$					
$+ C_6H_6$		$+ C_6H_5CH_3$		$+ 1,2\text{-}C_6H_4(CH_3)_2$	
0.006	0.000	0.006	0.000	0.006	0.000
0.018	0.130	0.029	0.252	0.033	0.219
0.036	0.246	0.047	0.296	0.071	0.295
0.080	0.330	0.084	0.320	0.095	0.322
0.157	0.368	0.161	0.355	0.150	0.352
0.244	0.368	0.217	0.351	0.233	0.358
0.322	0.349	0.333	0.336	0.330	0.338
0.398	0.340	0.416	0.313	0.422	0.303
0.478	0.309	0.494	0.286	0.504	0.274
0.597	0.255	0.556	0.261	0.623	0.222
0.694	0.201	0.614	0.232	0.738	0.156
0.780	0.149	0.719	0.171	0.812	0.113
0.866	0.072	0.831	0.094	0.889	0.052
0.943	0.000	0.943	0.000	0.943	0.000
$C_5H_6O_2 + CH_3(CH_2)_{10}CH_3$					
$+ C_6H_6$		$+ C_6H_5CH_3$		$+ 1,2\text{-}C_6H_4(CH_3)_2$	
0.011	0.000	0.011	0.000	0.011	0.000
0.015	0.263	0.022	0.342	0.020	0.263
0.019	0.405	0.030	0.479	0.037	0.457
0.031	0.449	0.045	0.562	0.052	0.525
0.041	0.491	0.091	0.582	0.082	0.564
0.073	0.544	0.133	0.581	0.143	0.583
0.126	0.571	0.207	0.572	0.231	0.559
0.193	0.573	0.294	0.535	0.291	0.535
0.281	0.547	0.361	0.498	0.367	0.493
0.356	0.505	0.436	0.450	0.445	0.443
0.419	0.473	0.518	0.400	0.543	0.381
0.506	0.422	0.649	0.308	0.641	0.309
0.623	0.338	0.796	0.187	0.721	0.244
0.804	0.184	0.994	0.000	0.803	0.178
0.994	0.000			0.994	0.000
$C_5H_6O_2 + CH_3(CH_2)_{14}CH_3$					
$+ C_6H$		$+ C_6H_5CH_3$		$+ 1,2\text{-}C_6H_4(CH_3)_2$	
0.014	0.000	0.014	0.000	0.014	0.000
0.020	0.210	0.020	0.263	0.020	0.364
0.031	0.370	0.031	0.482	0.028	0.505
0.050	0.583	0.046	0.555	0.040	0.609
0.086	0.648	0.058	0.609	0.060	0.653
0.162	0.647	0.084	0.659	0.094	0.674
0.222	0.627	0.162	0.649	0.143	0.668
0.279	0.598	0.217	0.633	0.212	0.633
0.327	0.573	0.268	0.603	0.277	0.599
0.381	0.544	0.320	0.574	0.341	0.561
0.445	0.499	0.399	0.521	0.406	0.520
0.506	0.457	0.484	0.461	0.486	0.459
0.624	0.356	0.586	0.383	0.590	0.377
0.717	0.270	0.715	0.272	0.747	0.242
0.998	0.000	0.998	0.000	0.998	0.000

and presented in Table 3. The ′ refers to the furfuryl alcohol-rich phase, and the ″ refers to the aliphatic-rich phase. For a separation to be effective, S must be different from unity, and the greater the disparity with unity the more efficient the separation.

Tie Line Correlation. The nonrandom two liquid[6] (NRTL) model and the universal quasichemical[7] (UNIQUAC) model are used to correlate the tie line data. The data were correlated using a computer program that minimized the following objective function using a simplex optimization routine.[13]

$$\mathrm{OF} = \sum_{k=1}^{n} \sum_{l=1}^{2} \sum_{i=1}^{3} (x_{kli} - \bar{x}_{kli})^2$$

where x_{kli} is the experimental composition of component i in phase l for the kth tie line and $\bar{x}_{kli}$ is the calculated composition of component i in phase l for the kth tie line.

Table 3. Compositions of Conjugate Phases for the Mixtures $\{(x_1)C_5H_4O_2 + x_2C_6H_{6-m}(CH_3)_m + (1 - x_1 - x_2)CH_3(CH_2)_nCH_3\}$ at $T = 298.15$ K and the Selectivity, S

x_{11}	x_{21}	x_{13}	x_{23}	S
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_4CH_3$				
0.852	0.086	0.021	0.161	7.0
0.768	0.158	0.046	0.282	5.1
0.618	0.243	0.111	0.351	2.7
0.532	0.286	0.207	0.371	1.8
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_4CH_3$				
0.838	0.084	0.012	0.159	5.6
0.756	0.144	0.032	0.263	3.9
0.686	0.193	0.092	0.323	2.9
0.601	0.237	0.176	0.354	1.9
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_4CH_3$				
0.888	0.050	0.021	0.130	5.3
0.839	0.091	0.043	0.249	3.7
0.783	0.129	0.105	0.333	2.5
0.697	0.180	0.229	0.358	1.7
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{10}CH_3$				
0.875	0.114	0.018	0.260	28.8
0.818	0.170	0.032	0.462	15.5
0.723	0.256	0.077	0.543	8.5
0.582	0.368	0.211	0.570	2.8
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_{10}CH_3$				
0.853	0.135	0.021	0.388	17.1
0.818	0.167	0.034	0.517	9.7
0.791	0.191	0.081	0.578	6.3
0.733	0.242	0.244	0.555	3.5
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_{10}CH_3$				
0.866	0.122	0.022	0.358	17.6
0.831	0.153	0.034	0.477	9.8
0.776	0.202	0.108	0.576	5.0
0.678	0.28	0.301	0.529	2.1
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{14}CH_3$				
0.802	0.189	0.024	0.285	50.9
0.722	0.267	0.034	0.425	30.9
0.611	0.368	0.046	0.559	12.4
0.499	0.464	0.096	0.649	4.9
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_{14}CH_3$				
0.860	0.132	0.022	0.344	30.4
0.763	0.228	0.040	0.529	20.6
0.635	0.343	0.065	0.632	7.5
0.469	0.471	0.162	0.652	2.2
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_{14}CH_3$				
0.705	0.276	0.020	0.398	21.2
0.627	0.347	0.028	0.522	11.5
0.551	0.410	0.040	0.593	6.5
0.446	0.488	0.066	0.658	3.1

Table 4. Compositions of Plait Points for the Mixtures $\{(x_1)C_5H_6O_2 + (x_2)C_6H_{6-m}(CH_3)_m + (1 - x_1 - x_2)CH_3(CH_2)_nCH_3\}$ at $T = 298.15$ K

	x_1	x_2
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_4CH_3$	0.409	0.332
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_4CH_3$	0.468	0.295
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_4CH_3$	0.591	0.237
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{10}CH_3$	0.432	0.467
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_{10}CH_3$	0.596	0.346
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_{10}CH_3$	0.568	0.363
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{14}CH_3$	0.303	0.588
$C_5H_6O_2 + C_6H_5 + CH_3(CH_2)_{14}CH_3$	0.340	0.560
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_{14}CH_3$	0.283	0.593

In fitting the NRTL equation, the nonrandomness parameter α of 0.45 was found to yield the best results. The pure component structural parameters (r, q, and q') from the UNIQUAC model were defined in the original paper[7] and are given in Table 1. The resulting binary interaction parameters and the root-mean-square (rms) deviations are reported in Tables 5 and 6. The symbols and notation used

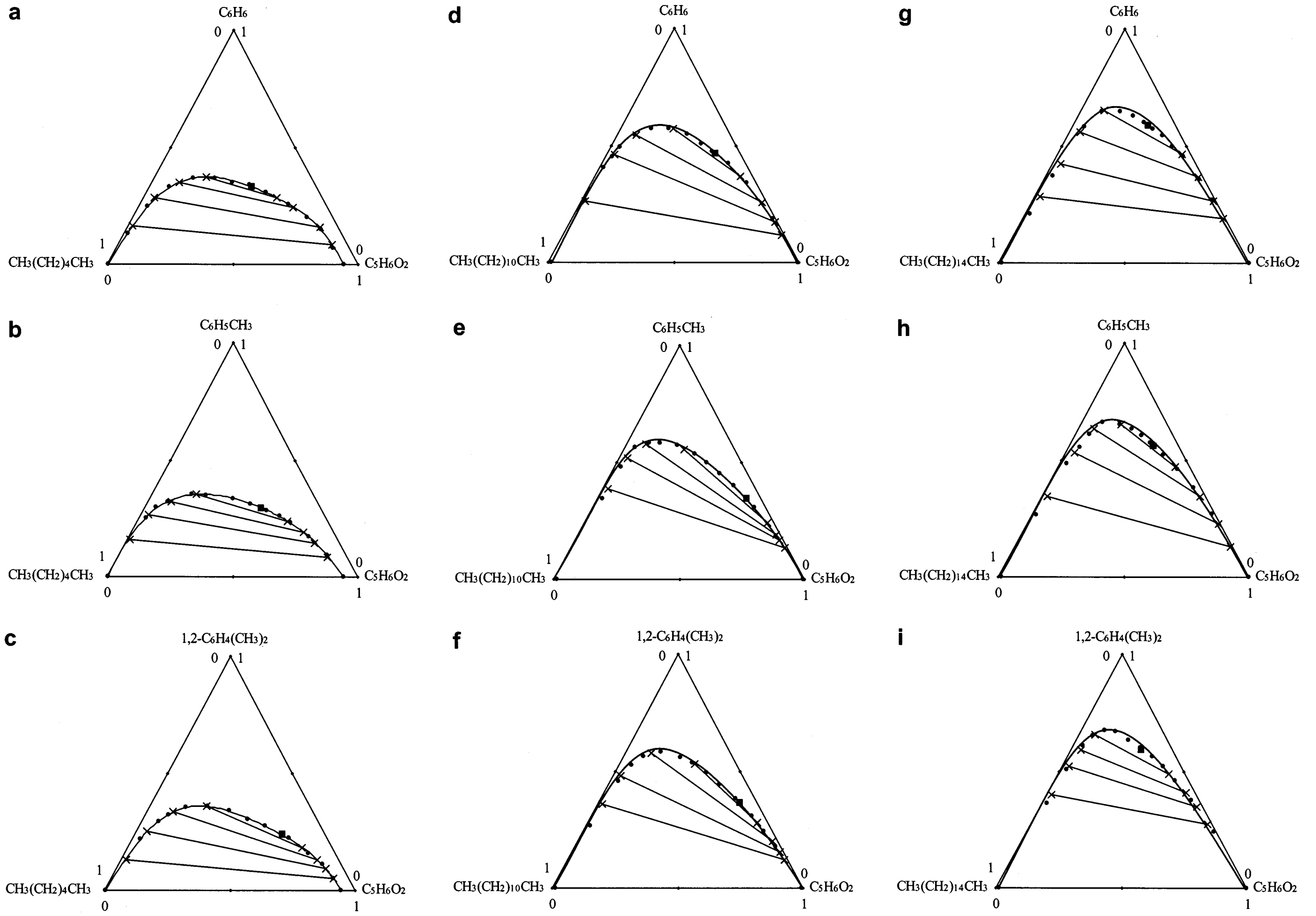

Figure 1. Liquid−liquid equilibrium results for the mixtures (a) $\{(x_1)C_5H_6O_2 + (x_2)C_6H_6 + (1 - x_1 - x_2)CH_3(CH_2)_4CH_3\}$; (b) $\{(x_1)C_5H_6O_2 + (x_2)C_6H_5CH_3 + (1 - x_1 - x_2)CH_3(CH_2)_4CH_3\}$; (c) $\{(x_1)C_5H_6O_2 + (x_2)1,2\text{-}C_6H_4(CH_3)_m + (1 - x_1 - x_2)CH_3(CH_2)_4CH_3\}$; (d) $\{(x_1)C_5H_6O_2 + (x_2)C_6H_6 + (1 - x_1 - x_2)CH_3(CH_2)_{10}CH_3\}$; (e) $\{(x_1)C_5H_6O_2 + (x_2)C_6H_5CH_3 + (1 - x_1 - x_2)CH_3(CH_2)_{10}CH_3\}$; (f) $\{(x_1)C_5H_6O_2 + (x_2)1,2\text{-}C_6H_4(CH_3)_2 + (1 - x_1 - x_2)CH_3(CH_2)_{10}CH_3\}$; (g) $\{(x_1)C_5H_6O_2 + (x_2)C_6H_6 + (1 - x_1 - x_2)CH_3(CH_2)_{14}CH_3\}$; (h) $\{(x_1)C_5H_6O_2 + (x_2)C_6H_5CH_3 + (1 - x_1 - x_2)CH_3(CH_2)_{14}CH_3\}$; and (i) $\{(x_1)C_5H_6O_2 + (x_2)1,2\text{-}C_6H_4(CH_3)_2 + (1 - x_1 - x_2)CH_3(CH_2)_{14}CH_3\}$ at $T = 298.15$ K: ●, points on the binodal curve; ×, points connecting conjugate phases; ■, critical or plait point.

Table 5. NRTL Binary Interaction Parameters and the Root-Mean-Square Deviations (rms) for the Mixtures[a] $\{(x_1)C_5H_6O_2 + (x_2)C_6H_{6-m}(CH_3)_m + (1 - x_1 - x_2)CH_3(CH_2)_nCH_3\}$

	$\frac{g_{12} - g_{22}}{J \cdot mol^{-1}}$	$\frac{g_{21} - g_{11}}{J \cdot mol^{-1}}$	$\frac{g_{13} - g_{33}}{J \cdot mol^{-1}}$	$\frac{g_{31} - g_{11}}{J \cdot mol^{-1}}$	$\frac{g_{23} - g_{33}}{J \cdot mol^{-1}}$	$\frac{g_{32} - g_{22}}{J \cdot mol^{-1}}$	rms
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_4CH_3$	−41.34	−3050	−5345	−1597	−2548	166.4	0.005
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_4CH_3$	−46.41	−2902	−4890	−1813	−2144	311.5	0.003
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_4CH_3$	−56.42	−3014	−4933	−1788	−2252	594.5	0.004
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{10}CH_3$	−23.90	−2907	−5957	−3617	−1638	115.4	0.004
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_{10}CH_3$	−53.83	−2909	−6170	−3335	−1263	180.0	0.004
$C_5H_6O_2 +1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_{10}CH_3$	−95.60	−2910	−6126	−3169	−1265	230.5	0.004
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{14}CH_3$	−233.8	−2054	−6043	−3759	−1000	395.2	0.006
$C_5H_6O_2 + C_6H_5 + CH_3(CH_2)_{14}CH_3$	−257.7	−2650	−5989	−3758	−856	418.0	0.005
$C_5H_6O_2 + 1,2\text{-}C_6H_4(CH_3)_2 + CH_3(CH_2)_{14}CH_3$	−263.2	−2663	−6629	−3613	−1903	319.4	0.005

[a] $\alpha = 0.45$.

in these tables are consistent with the original work by Renon and Prausnitz[6] and Abrams and Prausnitz.[7]

Discussion

All the data reported here contribute new information to the literature. The mixtures (furfuryl alcohol + an aromatic hydrocarbon + an alkane) were studied in order to determine the suitability of furfuryl alcohol for separating aromatic−aliphatic hydrocarbon mixtures. Aromatic hydrocarbons with increasing numbers of methyl groups (0 and 1 and 2) on the benzene ring were investigated to establish the effect of substitution of the benzene ring on the phase equilibrium. Alkanes of three different chain lengths (6 and 10 and 16) were investigated to establish the effect of chain length on the phase equilibrium.

The area of the two-phase region for the mixtures (furfuryl alcohol + an aromatic hydrocarbon + an alkane) is significantly large, indicating the mutual immiscibility of the components of the mixture. As the number of carbon atoms in the alkane increases from 6 to 16, there is an increase in the area of the two-phase region. This indicates a decrease in the mutual solubility of the components as the alkane chain length increases. The number of methyl groups on the benzene ring has a marginal effect on the ternary liquid−liquid equilibria for the mixtures looked at

Table 6. UNIQUAC Binary Interaction Parameters and the Root-Mean-Square Deviations (rms) for the Mixtures $\{(x_1)C_5H_4O_2 + (x_2)C_6H_{6-m}(CH_3)_m + (1 - x_1 - x_2)CH_3(CH_2)_nCH_3\}$

	$\frac{u_{12} - u_{22}}{J \cdot mol^{-1}}$	$\frac{u_{21} - u_{11}}{J \cdot mol^{-1}}$	$\frac{u_{13} - u_{33}}{J \cdot mol^{-1}}$	$\frac{u_{31} - u_{11}}{J \cdot mol^{-1}}$	$\frac{u_{23} - u_{33}}{J \cdot mol^{-1}}$	$\frac{u_{32} - u_{22}}{J \cdot mol^{-1}}$	rms
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_4CH_3$	268.7	−263.6	−280.7	70.88	−340.0	977.3	0.02
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_4CH_3$	272.0	−243.5	−293.6	98.29	−303.7	1193	0.02
$C_5H_6O_2$ + 1,2-$C_6H_4(CH_3)_2 + CH_3(CH_2)_4CH_3$	410.2	−274.6	−185.0	−72.3	−133.8	341.9	0.02
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{10}CH_3$	948.4	−344.4	−329.1	286.5	−243.0	789.0	0.03
$C_5H_6O_2 + C_6H_5CH_3 + CH_3(CH_2)_{10}CH_3$	134.9	−207.6	−325.6	286.3	−249.3	981.3	0.02
$C_5H_6O_2$ +1,2-$C_6H_4(CH_3)_2 + CH_3(CH_2)_{10}CH_3$	165.4	−199.1	−334.9	310.8	−234.1	949.1	0.03
$C_5H_6O_2 + C_6H_6 + CH_3(CH_2)_{14}CH_3$	1903	−390.6	−307.5	267.9	−271.3	945.8	0.03
$C_5H_6O_2 + C_6H_5 + CH_3(CH_2)_{14}CH_3$	794.4	−382.5	−320.6	299.4	−253.3	789.8	0.03
$C_5H_6O_2$ + 1,2-$C_6H_4(CH_3)_2 + CH_3(CH_2)_{14}CH_3$	824.5	−362.5	−332.0	300.1	−241.6	778.1	0.03

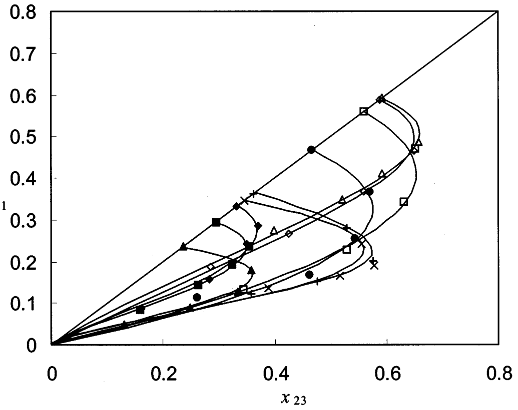

Figure 2. Distribution of the aromatic hydrocarbon between the furfuryl alcohol-rich phase and the alkane compound-rich phase at T = 298.15 K. x_{21} and x_{23} are the concentration of the aromatic hydrocarbon in the furfuryl alcohol-rich phase and the concentration of the alkanol in the alkane-rich phase, respectively. ▲, $\{(x_1)C_5H_6O_2 + (x_2)C_6H_6 + (1 - x_1 - x_2)CH_3(CH_2)_4CH_3\}$; ■, $\{(x_1)C_5H_6O_2 + (x_2)C_6H_5CH_3 + (1 - x_1 - x_2)CH_3(CH_2)_4CH_3\}$; ◆, $\{(x_1)C_5H_6O_2 + (x_2)$1,2-$C_6H_4(CH_3)_m + (1 - x_1 - x_2)CH_3(CH_2)_4CH_3\}$; ×, $\{(x_1)C_5H_6O_2 + (x_2)C_6H_6 + (1 - x_1 - x_2)CH_3(CH_2)_{10}CH_3\}$; +, $\{(x_1)C_5H_6O_2 + (x_2)C_6H_5CH_3 + (1 - x_1 - x_2)CH_3(CH_2)_{10}CH_3\}$; ●, $\{(x_1)C_5H_6O_2 + (x_2)$1,2-$C_6H_4(CH_3)_2 + (1 - x_1 - x_2)CH_3(CH_2)_{10}CH_3\}$; ◇, $\{(x_1)C_5H_6O_2 + (x_2)C_6H_6 + (1 - x_1 - x_2)CH_3(CH_2)_{14}CH_3\}$; □, $\{(x_1)C_5H_6O_2 + (x_2)C_6H_5CH_3 + (1 - x_1 - x_2)CH_3(CH_2)_{14}CH_3\}$; △, $\{(x_1)C_5H_6O_2 + (x_2)$1,2-$C_6H_4(CH_3)_2 + (1 - x_1 - x_2)CH_3(CH_2)_{14}CH_3\}$.

in this work. There is a very slight increase in the area of the two-phase region as the number of methyl groups on the benzene rings increases.

The solubility of the aromatic hydrocarbon in the aliphatic-rich phase is greater than the solubility of the aromatic hydrocarbon in the furfuryl alcohol-rich phase, as can be seen in Figure 2.

The significant two-phase region as well as the S values (ranging from 1.7 to 50) indicate that furfuryl alcohol is a viable solvent in the liquid−liquid extraction processes for separating aromatic hydrocarbons from alkanes.

Both the NRTL and UNIQUAC models are able to model the tie line data. The rms deviation for the NRTL model is an order of magnitude better than that of the UNIQUAC model. This is not entirely unexpected, as the NRTL model is a three parameter model while the UNIQUAC model is a two parameter model.

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