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Liquid−Liquid Equilibria for Benzene + Cyclohexane + 1-Methyl-3-methylimidazolium Dimethylphosphate or + 1-Ethyl-3-methylimidazolium Diethylphosphate

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To screen suitable ionic liquids (ILs) for the extraction separation of benzene and cyclohexane, a close-boiling mixture, measurement of the corresponding liquid−liquid equilibria (LLE) data is necessary. Toward this aim, LLE data for ternary systems of ILs + benzene + cyclohexane were measured at atmospheric pressure and (298.2 and 313.2) K, and the experimental data were correlated using the nonelectrolyte NRTL equation. The ILs used in this work are 1-methyl-3-methylimidazolium dimethylphosphate ([C_1mim][DMP]) and 1-ethyl-3-methylimidazolium diethylphosphate ([C_2mim][DEP]). It was found that the selectivity of [C_1mim][DMP] and [C_2mim][DEP] for benzene is in the range of (4.4 to 2.9) and (4.3 to 2.5), respectively, and the selectivity is virtually independent of temperature in the temperature and concentration range studied. Considering the high extraction capacity and selectivity for benzene as well negligible solubility in benzene + cyclohexane mixtures, [C_2mim][DEP] may be used as a potential extracting solvent for the separation of benzene and cyclohexane.

Introduction

Separation of benzene and cyclohexane is one of the most important and difficult processes in the petrochemical industry. As an important commodity chemical, cyclohexane is produced via catalytic hydrogenation of benzene, and thus separation of the unreacted benzene from the product stream is inevitable. However, it is not practical to separate such a binary mixture by using a conventional distillation process considering their extremely close boiling points and low relative volatility in the whole composition range.[1] Presently, azeotropic distillation and extraction are commercially used for this separation, and the typical entrainers are molecular solvents such as sulfolane,[2] *N*-methyl-2-pyrrolidone (NMP),[3] and cyclodextrin,[4] which suffer from process complexity and high energy consumption due to their low extractive selectivity for benzene and high mutual solubility in a benzene + cyclohexane mixture. Vega et al.[5] evaluated the applicability of five molecular solvents, viz., DMF, NMP, *N*,*N*-dimethylacetamide, phenyl acetate, and dimethyl malonate, for the separation of the cyclohexane + benzene mixture by extractive distillation according to the limit selectivity derived from experimental infinite activity coefficients, and *N*,*N*-dimethylacetamide was recommended for such separation with its limit selectivity being 6.0 at 313 K. To reduce the energy cost, pervaporation separation processes based on membrane and/or liquid-supported membranes have been studied extensively. Although the membranes tailored to such separation showed high selectivity, their permeation rate is relatively low for practical use.

Liquid−liquid extraction is another widely used industrial separation process for a homogeneous liquid mixture in addition to distillation, and the key is to find a suitable extractant which is highly selective to benzene and sparsely soluble in a benzene + cyclohexane mixtures. In this regard, ionic liquids (ILs) as a class of neoteric solvents seem superior to the traditional molecular solvents for their unique attributes, e.g., good selectivity for aromatics versus alkanes, negligible solubility in a benzene + cyclohexane mixture, nonvolatility, and thermal stability up to about 200 °C.[6] In recent years, ILs have attracted much attention in chemical reaction and separation process development toward replacement of traditional volatile organic solvents with greener solvents, and some comprehensive reviews are available.[7–9] However, the liquid−liquid equilibria (LLE) data reported by now on the aromatic + aliphatic mixtures containing ILs is quite limited.[10–14] Letcher et al.[10–12] studied the performance of three different ILs, viz., 1-octyl-3-methylimidazolium chloride ([C_8mim]Cl), 1-hexyl-3-methylimidazolum tetrafluoroborate, or hexafluorophosphate ([C_6mim]BF_4 or PF_6), on the extraction of benzene from heptane, dodecane, and hexadecane, respectively, at 298.2 K.

The aim of the present work is to investigate the applicability of two novel ionic liquids, viz., 1-methyl-3-methylimidazolium dimethylphosphate ([C_1mim][DMP]) and 1-ethyl-3-methylimidazolium diethylphosphate ([C_2mim][DEP]), on the extractive separation of benzene + cyclohexane mixtures in terms of the experimental LLE data for the corresponding ternary systems at (298.2 and 313.2) K. Besides, the influence of temperature on extraction ability and selectivity is also investigated.

Experimental

Materials. The chemicals used in this study were benzene, cyclohexane, toluene, [C_1mim][DMP], and [C_2mim][DEP]. Benzene and cyclohexane both with a nominal minimum mass fraction of 0.990 and toluene with a nominal minimum mass fraction of 0.997 were used as received from Beijing Chemical Reagent Factory. [C_1mim][DMP] and [C_2mim][DEP] were synthe-

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Table 1. Liquid−Liquid Equilibrium Data in Mole Fraction for Ternary Systems [C_1mim][DMP] (1) + Benzene (2) + Cyclohexane (3) at (298.2 and 313.2) K and the Selectivity (*S*) of Benzene versus Cyclohexane

	cyclohexane-rich		IL-rich		
T/K	x'_2	x'_3	x''_2	x''_3	S
298.2	0.1663	0.8258	0.03958	0.05394	3.6
	0.2538	0.7413	0.06683	0.06215	3.1
	0.3174	0.6826	0.08792	0.05766	3.3
	0.3463	0.6536	0.1057	0.06028	3.3
	0.3841	0.6028	0.1218	0.05875	3.3
	0.4597	0.5294	0.1299	0.05157	2.9
313.2	0.1563	0.8348	0.03812	0.04644	4.4
	0.2222	0.7778	0.05974	0.04750	4.4
	0.2932	0.7024	0.08011	0.04494	4.3
	0.3449	0.6551	0.09497	0.04324	4.2
	0.4073	0.5927	0.1176	0.04197	4.1
	0.4592	0.5246	0.1280	0.04688	3.1
	0.5078	0.4922	0.1381	0.04441	3.0
	0.5555	0.4445	0.1548	0.04000	3.1

Table 2. Liquid−Liquid Equilibrium Data in Mole Fraction for Ternary Systems [C_2mim][DEP] (1) + Benzene (2) + Cyclohexane (3) at (298.2 and 313.2) K and the Selectivity (*S*) of Benzene versus Cyclohexane

	cyclohexane-rich		IL-rich		
T/K	x'_2	x'_3	x''_2	x''_3	S
298.2	0.2034	0.7965	0.1617	0.1469	4.3
	0.2666	0.7334	0.1943	0.1427	3.7
	0.2771	0.7229	0.2104	0.1477	3.7
	0.3321	0.6664	0.2230	0.1378	3.2
	0.4027	0.5973	0.2906	0.1397	3.1
	0.4540	0.5460	0.3222	0.1329	2.9
	0.5234	0.4766	0.3437	0.1174	2.7
	0.5626	0.4374	0.3759	0.1177	2.5
313.2	0.2472	0.7514	0.1749	0.1438	3.7
	0.2951	0.6998	0.2036	0.1370	3.5
	0.3581	0.6419	0.2556	0.1349	3.4
	0.4141	0.5859	0.2807	0.1270	3.1
	0.4704	0.5119	0.3197	0.1188	2.9
	0.5224	0.4776	0.3417	0.1188	2.6

sized according to the method in the literature.[15] The purities of ILs were above 0.980 in mass fraction in terms of NMR and elementary analysis. The ILs were treated at least 36 h by vacuum evaporation before use to remove the residual volatile impurities. The water mass fraction was less than $3 \cdot 10^{-4}$ as measured by the Karl−Fischer method (CBS-1A). All chemicals were free of halide as indicated by the absence of precipitate when mixed with silver nitrate aqueous solution, and the nominal mass fractions of water for benzene, cyclohexane, and toluene used were $2 \cdot 10^{-4}$, $2 \cdot 10^{-4}$, and $3 \cdot 10^{-4}$, respectively.

Apparatus and Procedures. The liquid−liquid equilibrium measurements for the ternary mixture IL + benzene + cyclohexane were conducted in a jacketed glass cell of about 150 mL. The glass cell sealed by a silicon rubber cap and the liquid admixture inside mixed vigorously with a magnetic stirrer. The equilibrium liquid temperature was maintained by circulating water coming from a superthermostat (CNSHP) with temperature fluctuation within ± 0.3 °C.

First, known masses of ILs and liquid mixtures with known composition were in turn added into the glass cell. The mixture was stirred with a magnetic stirrer for at least 1.5 h at specified temperature and then left to stand for 2 h to achieve a clear phase separation. The time used here for equilibrium and phase splitting was fixed according to results from our preliminary tests. Two samples (approximately 0.5 mL for each) of known mass were taken out from both phases and immediately added into two 10 mL flasks. Each flask was filled with about 5 mL of toluene and approximately 3 mL of water of known mass in advance for the sake of mass balance. The flasks were sealed with PTFE/silicone sheet, shaken about 10 min by hand, and then put aside for 10 h or overnight for settling. In this process, the benzene and cyclohexane components are transferred into the toluene phase, while the ILs component into the water phase completely. As a result, the relative composition of benzene and cyclohexane in both phases can be analyzed using gas chromatography (SHIMADZU GC2010 equipped with a FID detector and FFAP capillary column, 30 m × 0.25 mm i.d. × 5 μm; carrier gas N_2; temperature program: (70 to 170) °C at $10\ \mathrm{K \cdot min^{-1}}$ and then maintained at 170 °C for 30 min without interference of ILs). The sample concentration was given by the GC Solution workstation according to the area of each chromatograph peak and the calibration curve made prior for the ternary mixture of toluene + benzene + cyclohexane. Once the amount of benzene and cyclohexane components had been determined, the mass fraction of ILs in both phases was calculated via mass balance for the upper and bottom phase samples, respectively. At least duplicate samples were made for each phase, and triplicate injections were made for each sample in the GC analysis. The reproducibility of the compositions was within ± 3 %. The uncertainty in temperature was 0.3 K, and the uncertainty of mole fraction for ILs was within 0.004 estimated from the water content of the ILs used.

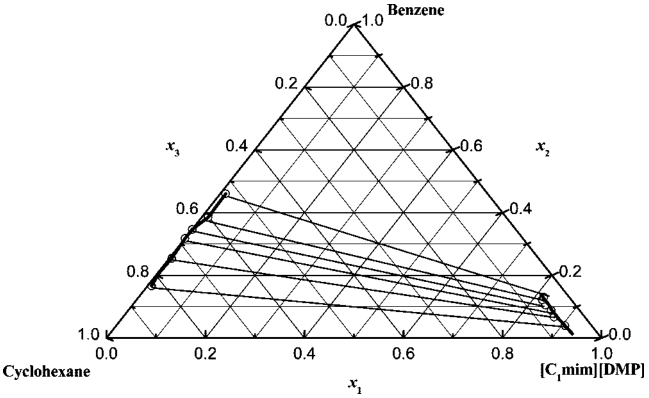

Figure 1. Binodal curves and tie-lines for the ternary mixture {[C_1mim][DMP] (1) + benzene (2) + cyclohexane (3)} at 298.2 K. —, Predicted line by the NRTL equation; ○, experimental data.

Results and Data Correlation

LLE data for ternary system, IL(1) + benzene(2) + cyclohexane(3), at (298.2 and 313.2) K were obtained experimentally in the mass fraction range of (0 to 0.5) for benzene. The results are listed in Tables 1 and 2, and the corresponding triangular diagrams shown in Figures 1 to 4.

Selectivity (*S*) is an important parameter in assessing the feasibility of utilizing a solvent in liquid−liquid extraction. With regards to the pseudobinary mixture of benzene (2) + cyclohexane (3) studied, the feasibility of extracting aromatics from aliphatic is given by eq 1[11]

$$S = \frac{(x'_2/x'_3)}{(x''_2/x''_3)} \tag{1}$$

where x_2 and x_3 refer to the mole fraction of benzene and cyclohexane, respectively, and ′ is the IL-rich phase and ″ is the alkane-rich phase. The selectivity values computed from the tie line data for [C_1mim][DMP] (1) + benzene (2) + cyclohexane (3) and [C_2mim][DEP] (1) + benzene (2) + cyclohexane (3) are presented in Table 1 and Table 2, respectively. It is noted

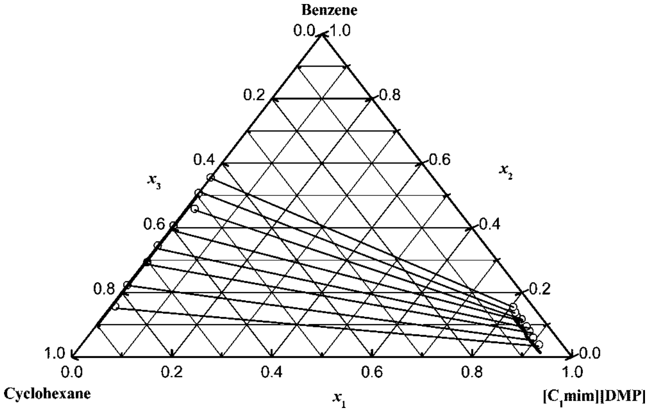

Figure 2. Binodal curves and tie-lines for the ternary mixture {[C$_1$mim][DMP] (1) + benzene (2) + cyclohexane (3)} at 313.2 K. —, Predicted line by the NRTL equation; ○, experimental data.

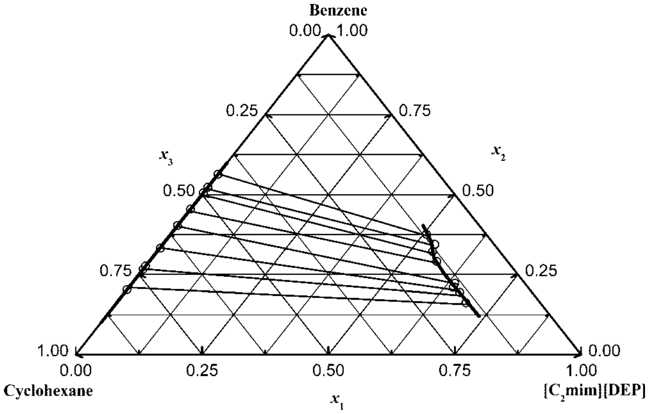

Figure 3. Binodal curves and tie-lines for the ternary mixture {[C$_2$mim][DEP] (1) + benzene (2) + cyclohexane (3)} at 298.2 K. —, Predicted line by the NRTL equation; ○, experimental data.

that the selectivity is always greater than unity, suggesting that extraction is possible.[16]

The nonrandom two-liquid equation (NRTL)[17] was used to correlate the experimental data for the ternary mixtures reported here. The algorithm employed by Walas[18] was used in the calculation of the tie line compositions. For the correlation of the experimental data, the following objective function, F, was used, i.e., by minimizing the difference of activity in each of the phases

$$F=\sum_{i=1}^{n}[\gamma'_{1i}x'_{1i}-\gamma''_{1i}x''_{1i}]^2+[\gamma'_{2i}x'_{2i}-\gamma''_{2i}x''_{2i}]^2 \qquad (2)$$

where n is the number of experimental data points; $\gamma'_{1i},\gamma'_{2i}$ are the calculated activity coefficients of the IL-rich phase; $\gamma''_{1i},\gamma''_{2i}$ are the calculated activity coefficients of the alkane-rich phase; x'_{1i},x'_{2i} are the experimental mole fractions of the IL-rich phase; and x''_{1i},x''_{2i} are the experimental mole fractions of the alkane-rich phase. The resulting NRTL parameters, viz., $g_{ij}-g_{jj}$, $g_{ji}-g_{ii}$, and α_{ij}, for the ternary systems IL (1) + benzene (2) + cyclohexane (3) are given in Table 3, along with the root mean square deviation (rmsd) as defined in eq 3:

$$\mathrm{rmsd}=\left\{\sum_i\sum_m(\gamma'_{im}x'_{im}-\gamma''_{im}x''_{im})^2/2K\right\}^{1/2} \qquad (3)$$

where the subscripts of i and m provide a designation for the component and the tie line, respectively. The value of K is the number of interaction components. The values of rmsd in Table 3 provide a measure of the fit of the correlation. As can be inferred from these values, a fairly good correlation of the experimental values with the NRTL model was obtained.

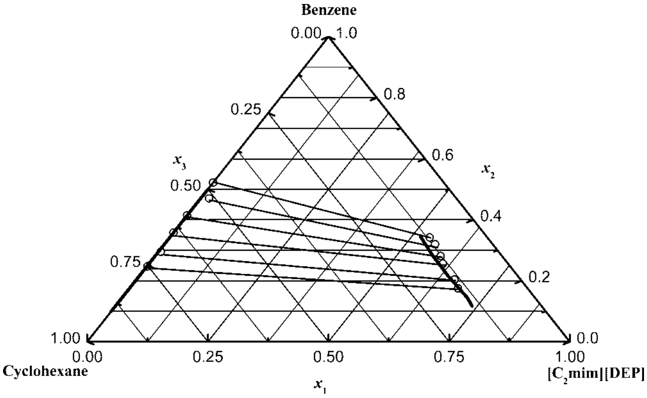

Figure 4. Binodal curves and tie-lines for the ternary mixture {[C$_2$mim][DEP] (1) + benzene (2) + cyclohexane (3)} at 313.2 K. —, Predicted line by the NRTL equation; ○, experimental data.

Table 3. Values of the NRTL Binary Parameters Regressed from LLE Data of Ternary Mixtures {IL (1) + Benzene (2) + Cyclohexane (3)} and the Fitting Deviation in rmsd[a]

component	NRTL parameters		
$(i)+(j)$	$(g_{ij}-g_{jj})$/ (J·mol^{-1})	$(g_{ji}-g_{ii})$/ (J·mol^{-1})	α_{ij}
[MMIM][DMP]			
IL (1) + benzene (2)	9105.0	5746.5	0.55
IL (1) + cyclohexane (3)	1659.2	12268	0.14
benzene (2) + cyclohexane (3)	178.05	5877.7	0.45
	rmsd = 0.022		
[EMIM][DEP]			
IL (1) + benzene (2)	10990	9532.5	0.48
IL (1) + cyclohexane (3)	5414.8	12249	0.33
benzene (2) + cyclohexane (3)	178.05	5877.7	0.45
	rmsd = 0.007		

[a] Note: rmsd is root mean square deviation of activity as defined in eq 3.

Discussion

Solubilities of pure solutes (benzene and cyclohexane) in ILs ([C$_1$mim][DMP] and [C$_2$mim][DEP]) at 298.2 K are measured, respectively, via a gravimetric method by weighing the mass difference of the solute-saturated IL samples before and after vacuum vaporization. The mole fraction solubility of (benzene and cyclohexane) in [C$_1$mim][DMP] and [C$_2$mim][DEP] are (0.215 and 0.00876) and (0.712 and 0.0345), respectively. The results suggest that the extraction capacity of [C$_2$mim][DEP] for benzene is much higher than that of [C$_1$mim][DMP], and accordingly, the immiscibility region of [C$_2$mim][DEP] is smaller than that of [C$_1$mim][DMP] for the ternary systems of IL + benzene + cyclohexane, as shown in Figures 1 through 4. The solubility ratio of benzene to cyclohexane in [C$_1$mim][DMP] and [C$_2$mim][DEP] is calculated as 24.5 and 20.7, respectively, implying that the extraction selectivity of [C$_1$mim][DMP] for benzene is slightly higher than that of [C$_2$mim][DEP], which is consistent with the order observed in the finite concentration range, i.e., [C$_1$mim][DMP] > [C$_2$mim][DEP], as shown in Tables 1 and 2. This difference might be attributed to the large difference of solubility of cyclohexane in two different ILs.

It is noted that the selectivity values of the ILs, [C$_1$mim][DMP] and [C$_2$mim][DEP], for benzene are in the range of (4.4 to 2.9) and (4.3 to 2.5), respectively, which is much higher than unity, implying that these ILs are potentially applicable for the extraction of benzene from its binary mixture

Table 4. Selectivity Values of Benzene versus Alkanes for Different Ionic Liquids at 298.2 K

alkanes	[C$_1$mim] [DMP][a]	[C$_2$mim] [DEP][a]	[C$_2$mim] [OcSO$_4$][b]	[C$_6$mim] [PF$_6$][c]	[C$_4$mim] [PF$_6$][d]
cyclohexane	2.9 to 4.4	2.5 to 4.3			3.1
heptane			1.3 to 2.7	5.25 to 14.20	
dodecane				4.20 to 18.78	
hexadecane			7.3 to 19.0	14.11 to 39.94	

[a] Measured by this work. [b] Taken from ref 12. [c] Taken from ref 11. [d] Taken from ref 20 measured at 295.2 K.

of cyclohexane. Besides, the influence of temperature on the extraction selectivity of benzene is not obvious for the two ILs studied in the limited temperature range of (298.2 to 313.2) K. This behavior seems common for the extraction of aromatics from their alkane mixtures using other ILs, e.g., toluene + heptane + IL,[16] because the interaction of ionic liquid with the aromatic benzene is mainly π-ionic in nature and not very dependent on temperature.[19]

In comparison with other ILs reported, e.g., [C$_4$mim][PF$_6$], [C$_6$mim][PF$_6$], and [C$_2$mim][OcSO$_4$], the ILs used here show a higher extraction selectivity for benzene from its cyclohexane mixture. As shown in Table 4, the extraction selectivity of [C$_2$mim][OcSO$_4$] and [C$_6$mim][PF$_6$] for benzene from its heptane mixture is in the range of (1.3 to 2.7) and (5.25 to 14.2), respectively, from which it is inferred that their selectivity for benzene from its cyclohexane mixture should be lower, since cyclohexane is a shorter alkane than heptane and thus its solubility in a specific IL is higher, leading to a lower solubility ratio of benzene to alkane in the IL phase. The selectivity variation of different ILs for benzene with respect to alkanes can be well explained by the increasing lipophilicity of the ILs with the increase of the alkyl length of substitutes in both cations and anions.[7]

The advantage of using IL as an alternative solvent for the extractive separation of a alkane + aromatic mixtures is obvious. On one hand, the extractive selectivity of IL for benzene from its cyclohexane mixture is comparable to that of traditional molecular solvents; for example, the selectivity of ethylene carbonate[21] is 8.5 at 40 °C. On the other hand, the solubility of ILs in benzene + cyclohexane mixtures is negligible in the whole concentration range which makes the recycle of IL much easier. On the contrary, the mutual solubility of molecular solvent and the mixture especially in the benzene-rich region is usually so high that it introduces an extra separation cost for the recycle of extractant from both phases.

The equilibria composition of the IL-rich phase was predicted at varying compositions of the alkane-rich phase by using the binary parameters regressed, and the results were shown by solid lines in Figures 1 to 4, respectively. It is seen that the predicted lines virtually pass through the scattered experimental data points, which justified the applicability of the NRTL equation for the systems studied. This may be largely attributed to the molecular attributes of the ILs considering their negligible dissociation in such an aromatic/alkane mixture that has very low permittivity and polarity.

Conclusions

The LLE data for the ternary systems of IL ([C$_1$mim][DMP] or [C$_2$mim][DEP]) + benzene + cyclohexane at atmospheric pressure and (298.2 and 313.2) K were measured experimentally and correlated using the nonelectrolyte NRTL equation with satisfaction. The solubility of IL ([C$_1$mim][DMP] or [C$_2$mim][DEP]) in the benzene + cyclohexane mixture is negligible, and the selectivity of ILs for benzene with respect to cyclohexane is virtually independent of temperature in the limited temperature range of (298.2 to 313.2) K studied. The selectivity of the ILs for benzene vs cyclohexane decreases with the increase of benzene content in the mixture. The extraction selectivity of [C$_1$mim][DMP] for benzene is a little higher than that of [C$_2$mim][DEP], while the extraction capacity of [C$_2$mim][DEP] is much higher than that of [C$_1$mim][DMP].

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