2170 *J. Chem. Eng. Data* **2008,** *53,* 2170–2174

Ternary Liquid−Liquid Equilibria Measurement for Benzene + Cyclohexane + *N*-Methylimidazole, or *N*-Ethylimidazole, or *N*-Methylimidazolium Dibutylphosphate at 298.2 K and Atmospheric Pressure

Ruijie Wang,[†,‡] Chunxi Li,*[,†,‡] Hong Meng,[‡] Junfeng Wang,[†,‡] and Zihao Wang[‡]

State Key Laboratory of Chemical Resource Engineering, and College of Chemical Engineering, Beijing University of Chemical Technology, Beijing 10002, PR China

---

Liquid−liquid equilibrium (LLE) data for ternary systems of (benzene + cyclohexane + *N*-methylimidazole (MIM), or *N*-ethylimidazole (EIM), or *N*-methylimidazolium dibutylphosphate [HMIM][DBP]) were measured at 298.2 K and atmospheric pressure, and the experimental data were correlated using the nonelectrolyte NRTL equation. It was found that the selectivity of MIM, EIM, and [HMIM][DBP] for benzene is in the range of (413.6 to 10.7), (5.4 to 1.5), and (2.3 to 1.3), respectively. The variation of extractive performance of these solvents for the benzene component from its cyclohexane mixture is interpreted in terms of the molecular structure and corresponding variation of intermolecular interaction involved, e.g., polar-induced polar interaction, $\pi-\pi$ complexation, and dispersive interaction among different components.

Introduction

In addition to being used as solvent for paints and for the extraction of essential oils, cyclohexane is widely used as a feedstock for the production of cyclohexanone and hexane diacid, a monomer of nylon.[1] As a base chemical, cyclohexane is generally produced by catalytic hydrogenation of benzene, and residue of benzene in the product stream is inevitable due to the incompleteness of the reaction. For the separation of benzene and cyclohexane, traditional distillation is not viable because of their close boiling points (benzene, 80.10 °C; cyclohexane, 80.74 °C), and other approaches have to be resorted to, e.g., by using membrane pervaporation,[2−4] extraction, or extractive distillation. For the extractive distillation process, the key is to find an effective entrainer, which can be achieved by a quick screening according to their infinite activity coefficients in the entrainer.[5] For the extraction separation of aromatics from their aliphatic mixtures, some liquid−liquid equilibrium (LLE) data have been reported and some solvent candidates recommended, for example, sulfolane,[6,7] *N*-methyl-2-pyrrolidone (NMP),[7] glycols,[8−10] furfuryl alcohol,[11] and *N*-formyl morpholine (NFM).[12] In contrast, the LLE data with respect to the benzene + cyclohexane mixture are very limited to our knowledge.[13−15]

In our previous paper,[16] LLE measurements have been done for the ternary systems of benzene + cyclohexane + an ionic liquid (IL), viz., 1-methyl-3-methylimidazolium dimethylphosphate ([MMIM][DMP]) or 1-ethyl-3-methylimidazolium diethylphosphate ([EMIM][DEP]). It was found that the ionic liquid is insoluble in the benzene + cyclohexane mixture, and the selectivity of [MMIM][DMP] and [EMIM][DEP] for benzene is in the range of (4.7 to 2.9) and (4.3 to 2.5), respectively. The extractive selectivity for benzene is not very high, and thus more effective extracting solvents are expected. Inspired by the findings that the *N*-alkyl-substituted imidazoles, e.g., *N*-methylimidazole (MIM) and *N*-ethylimidazole (EIM), have excellent extractive ability for the thiophene series of sulfur compounds from fuel oils due to the $\pi-\pi$ electronic interaction between aromatic rings of imidazole and thiophene and that the extractive desulfurization ability of *N*-alkyl-substituted imidazoles is much higher than their corresponding ionic liquids,[17,18] the LLE data for the ternary systems of benzene + cyclohexane + MIM, or EIM, or dibutyl phosphate of MIM ([HMIM][DBP]) at 298.2 K are measured. On this basis, the selectivity (*S*) is calculated to determine the possibility of separating benzene from its cyclohexane mixtures using a solvent extraction process, and the structure−performance relationship for different extractants is discussed. The LLE data for the ternary systems studied are correlated using the NRTL equation with satisfaction.

Experimental

Materials. Di-*n*-butyl phosphoric acid (DBPA) of analytical grade was used as received from Jonnson Matthey Company with a quoted purity above 0.97 mass fraction. Benzene, cyclohexane, and imidazole 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. MIM, EIM, and BIM (*N*-butyl imidazole) of CP grade were also purchased from Beijing Chemical Reagent Factory, which were rectified before use with their purity above 0.992 according to acid−base titration analysis.

[HMIM][DBP] is an ionic liquid, which was prepared by a simple acid−base neutralization reaction of MIM and DBPA aqueous solutions according to the method described elsewhere. Its purity is 0.98 mass fraction in terms of NMR and elementary analysis. The IL was purified by means of vacuum evaporation at 1.0 kPa to remove the residual volatile impurities and traces of moistures. The water mass fraction was less than $3\cdot10^{-4}$ as measured by the Karl−Fischer method (CBS-1A).

---

* To whom correspondence should be addressed. E-mail: licx@mail.buct.edu.cn. Tel. & Fax: +86-010-64410308.
[†] State Key Laboratory of Chemical Resource Engineering.
[‡] College of Chemical Engineering.

10.1021/je800376f CCC: $40.75

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

cyclohexane-rich phase		MIM-rich phase		
x'_1	x'_2	x_1''	x_2''	S
0.0701	0.894	0.0537	0.0017	414
0.100	0.866	0.0794	0.00340	204
0.132	0.847	0.102	0.00420	155
0.152	0.795	0.123	0.00550	117
0.173	0.757	0.139	0.00660	92.8
0.219	0.687	0.167	0.00880	60.0
0.232	0.679	0.187	0.00990	55.6
0.250	0.649	0.213	0.0127	43.3
0.290	0.617	0.214	0.0146	31.1
0.304	0.566	0.237	0.0144	30.7
0.317	0.499	0.272	0.0183	23.3
0.3317	0.501	0.280	0.0287	15.4
0.331	0.470	0.304	0.0401	10.7

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

cyclohexane-rich phase		EIM-rich phase		
x'_1	x'_2	x_1''	x_2''	S
0.0536	0.889	0.0547	0.167	5.40
0.0776	0.839	0.0812	0.181	4.80
0.109	0.829	0.106	0.191	4.20
0.138	0.794	0.135	0.208	3.70
0.163	0.746	0.157	0.224	3.20
0.206	0.631	0.195	0.266	2.30
0.228	0.519	0.228	0.354	1.50
0.234	0.557	0.234	0.360	1.50

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

cyclohexane-rich		IL-rich		
x'_1	x'_2	x_1''	x_2''	S
0.0839	0.912	0.0820	0.444	2.30
0.100	0.889	0.100	0.440	2.00
0.128	0.860	0.125	0.439	1.90
0.141	0.847	0.126	0.434	1.70
0.171	0.815	0.160	0.437	1.70
0.235	0.751	0.232	0.431	1.70
0.292	0.687	0.268	0.436	1.40
0.337	0.633	0.314	0.441	1.30
0.341	0.627	0.317	0.463	1.30

Apparatus and Procedures. The liquid−liquid equilibrium measurements for the ternary mixture {benzene + cyclohexane + MIM, or EIM, or [HMIM][DBP]} were conducted in a jacketed glass cell of about 150 mL. The glass cell sealed by a silicon rubber cap and the heterogeneous 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.

The liquid admixture was stirred with a magnetic stirrer for 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 water and 3 mL of toluene with their mass weighted 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 for settling. In this process, the benzene and cyclohexane components are transferred into the toluene phase, while the hydrophilic solvent 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). 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 solvent in both phases was calculated via mass balance for the raffinate and extract 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 ± 2 % in mass fraction.

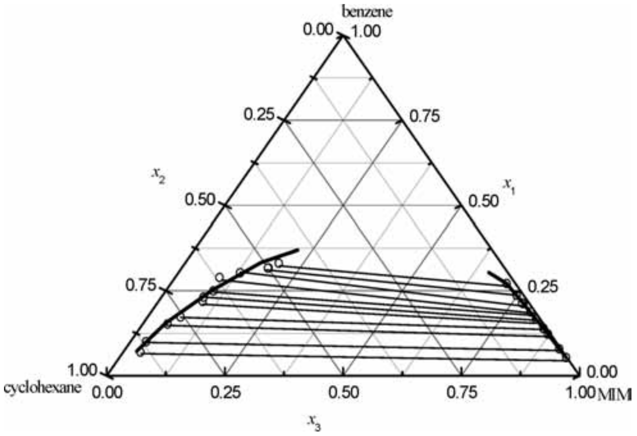

Figure 1. Binodal curves and tie-lines for the ternary mixture {benzene (1) + cyclohexane (2) + MIM (3)} at 298.2 K. −, Predicted solubility curves by the NRTL equation; ○, experimental data.

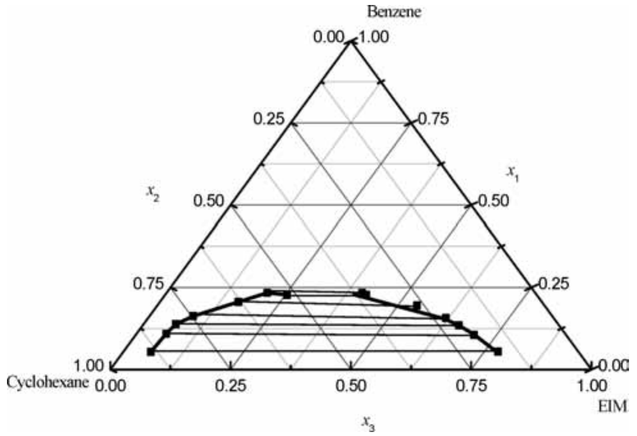

Figure 2. Binodal curves and tie-lines for the ternary mixture {benzene (1) + cyclohexane (2) + EIM (3)} at 298.2 K. −, Predicted solubility curves by the NRTL equation; ○, experimental data.

Results and Data Correlation

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

The selectivity (*S*) of a solvent with respect to benzene versus cyclohexane is calculated by eq 1[19]

$$S=\frac{(x'_1/x'_2)}{(x''_1/x''_2)} \tag{1}$$

where $x_1^{'}$ and $x_2^{'}$ refer to the mole fraction of benzene and cyclohexane in the extract phase and $x_1^{''}$ and $x_2^{''}$ refer to the mole fraction of benzene and cyclohexane in the raffinate phase, respectively. The selectivity values computed from the tie line data for MIM, EIM, and [HMIM][DBP] are presented in Tables 1 to 3, respectively. It is seen that the selectivity decreases regularly with the increase of benzene concentration in the raffinate phase as was observed in many published data,[16,19−21] and selectivity is always greater than unity, suggesting that extraction is possible.[22]

The NRTL equation[23] was used to correlate the experimental data for the ternary mixtures reported here. The algorithm employed by Walas[24] was used in the calculation of the tie line compositions. In the correlation process, the following objective function, F, was used, i.e., by minimizing the difference of activity in each of the phases

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

where n is the number of experimental data points; $\gamma_{1i}^{'}$, $\gamma_{2i}^{'}$ are the calculated activity coefficients in the extract phase; $\gamma_{1i}^{''}$, $\gamma_{2i}^{''}$ are the calculated activity coefficients in the raffinate phase; $x_{1i}^{'}$, $x_{2i}^{'}$ are the experimental mole fractions of the extract phase; and $x_{1i}^{''}$, $x_{2i}^{''}$ are the experimental mole fractions of the raffinate phase. The resulting NRTL parameters, viz., $g_{ij}-g_{jj}$, $g_{ji}-g_{ii}$, and α_{ij}, for the ternary system benzene (1) + cyclohexane (2) + solvent (3) are given in Table 4, along with the root mean square deviation (rmsd) as defined in eq 3

$$\mathrm{rmsd}=\left\{\sum_{i}\sum_{m}(\gamma'_{im}x'_{im}-\gamma''_{im}x''_{im})^2/2K\right\}^{1/2} \tag{3}$$

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 4 provide a measure of the fit of the correlation. As can be inferred from these values, a good correlation of the experimental values with the NRTL model was obtained.

Discussion

To compare the extraction performance of the solvents studied here with others reported in the literature, the selectivity value of benzene versus cyclohexane for different solvents is collected and showed in Table 5. As can be seen from the selectivity values listed in Table 5, MIM and EIM are two promising solvents for the extraction of benzene from its cyclohexane mixtures. The preferential extraction of these two solvents for benzene might be related to their higher polarity and aromaticity, which result in polar-induced polar and $\pi-\pi$ electron interaction or $\pi-\pi$ complexation, between two planar rings of benzene and imidazole molecules. In contrast, both attributes will not result in additional intermolecular attraction between the cyclohexane and imidazole ring, and only dispersive interaction is involved due to the negligible induced dipole moment and nonaromaticity of cyclohexane. In effect, many solvents with strong polarity and low miscibility with cyclohexane showed some extraction selectivity for benzene, for example, NMP, DMM, ISOP, NFM, and ethylene carbonate, as listed in Table 5, for which the polarity is originated from the carbonyl polar group. Also noted is that the selectivity of MIM is higher than any of the nonaromatic polar solvents reported in the literature, which contrast the importance of $\pi-\pi$ complexation interaction between aromatic rings.

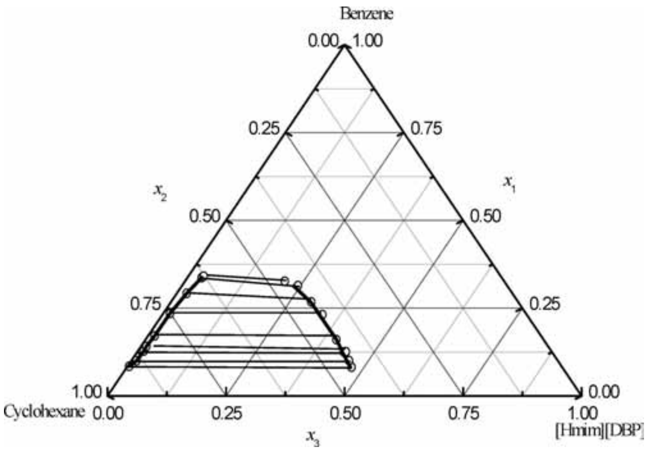

Figure 3. Binodal curves and tie-lines for the ternary mixture {benzene (1) + cyclohexane (2) + [HMIM] [DMP] (3)} at 298.2 K. —, Predicted solubility curves by the NRTL equation; ○, experimental data.

Table 4. Values of the NRTL Binary parameters Regressed from LLE Data of Ternary Mixtures Benzene (1) + Cyclohexane (2) + Solvent (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}
	Benzene (1) + Cyclohexane (2) + MIM(3)		
3−1	7043.28	262.350	0.52
3−2	14850.9	3393.47	0.18
1−2	178.050	5877.66	0.45
	rmsd = 0.044		
	Benzene (1) + Cyclohexane (2) + EIM (3)		
3−1	5962.22	10921.5	0.51
3−2	5399.20	13078.0	0.35
1−2	178.050	5877.66	0.45
	rmsd = 0.0064		
	Benzene (1) + Cyclohexane (2) + [HMIM][DMP] (3)		
3−1	5294.42	5405.89	0.68
3−2	−379.510	8617.54	0.24
1−2	178.050	5877.66	0.45
	rmsd = 0.0033		

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

Table 5. Selectivity Values of Benzene versus Cyclohexane for Different Molecule Solvents[a]

solvent	T/°C	S	remarks	ref
MIM	25	10.7 to 414	LLE data	this work
EIM	25	2.5 to 5.4	LLE data	this work
BIM	25	0.0	mutual soluble	this work
NMP	40	4.0	S^∞	26
DMM	40	14.7	S^∞	26
DMF	40	12.9	S^∞	26
ISOP	40	3.0	S^∞	26
NFM	25	1.3 to 5.2	LLE data	12
ethylene carbonate	30	3.9 to 9.3	LLE data	28
ethylene carbonate	40	4.0 to 8.5	LLE data	28
[MMIM][DMP]	25	2.9 to 3.6	LLE data	16
[EMIM][DEP]	25	2.5 to 4.3	LLE data	16

[a] S^∞ selectivity at infinite dilution estimated using the infinite activity coefficients of benzene (1) and cyclohexane (2) in a specified solvent by $S^\infty=\gamma_1^\infty/\gamma_2^\infty$.

With respect to the selectivity of EIM and MIM for benzene, the former is much lower than MIM. This may be attributed to the higher mutual solubility between EIM and the alkane/aromatic mixture due to the stronger dispersive interaction between them as the alkyl substitute of the imidazole ring changed from methyl to ethyl. The immiscible region in the triangle phase diagram of the benzene + cyclohexane + EIM system is narrower than that of benzene + cyclohexane + MIM, as shown in Figure 2 and Figure 1, due to the higher mutual solubility between EIM and the benzene component. Furthermore, as the alkyl substitute becomes larger to butyl, forming *N*-butylimidazole (BIM), BIM becomes totally miscible with cyclohexane and benzene, implying the nonapplicability of BIM as an extractant for the present system studied. As an opposite extreme, imidazole without any alkyl substitute on the ring is sparsely soluble with both benzene and cyclohexane and thus not applicable as an extractant for the present system. This observation of a higher selectivity with shorter R-groups is in accordance with the findings of Hanke et al.[25]

As a simple ionic liquid (IL), [HMIM][DBP] is composed of protonated MIM ([HMIM]$^+$) and dibutylphosphate anion [DBP]$^-$; however, the IL is believed to be presented as a highly polarized neutral entity in the nonpolar binary mixture of benzene and cyclohexane. By comparing Figure 1 and Figure 3, it is seen that the immiscible region for the ternary system of (benzene + cyclohexane + [HMIM][DBP]) is much narrower than that of (benzene + cyclohexane + MIM), and consequently, the selectivity of [HMIM][DBP] for benzene is lower than that of MIM. This is mainly originated from the two opposite variation trends; that is, when MIM is protonated forming [HMIM][DBP], IL solubility in the benzene + cyclohexane mixture is drastically decreased especially in the benzene-rich region, while the solubility of the benzene + cyclohexane mixture in the IL increased greatly. In effect, the size of the anion has a substantial influence on the IL solubility in the benzene + cyclohexane mixture and accordingly on the extraction selectivity; for example, the IL [MMIM][DMP] with a much smaller anion is insoluble in the benzene + cyclohexane mixture, and its extraction selectivity for benzene at 298.2 K is in the range of (3.6 to 2.9).[16] [HMIM][DBP] with a larger anion is partially soluble in the benzene + cyclohexane mixture with its selectivity lowered to the range of (2.3 to 1.3).

It should be pointed out that although molecular solvents NMP (4.0), DMM (14.7), DMF (12.9), and ISOP (3.0) have greater selectivity values than 3.0,[26] these values should be used with caution since the selectivity estimated from the infinite activity coefficients of benzene and cyclohexane in a specified solvent by $S^\infty = \gamma_1^\infty/\gamma_2^\infty$ can be different from the actual values up to a factor of 4.[27] The selectivity of ethylene carbonate is above 4.0 at room temperature.[28] These comparisons indicated the feasibility of using molecular solvents (MIM and EIM) for the extraction separation of the benzene + cyclohexane mixture.

Conclusions

The LLE data for the ternary systems of {benzene (1) + cyclohexane (2) + MIM, or EIM, or [HMIM][DBP] (3)} at 298.2 K and atmospheric pressure were measured and correlated using the nonelectrolyte NRTL equation. It is found that MIM and EIM are two promising solvents for the extraction of benzene from its cyclohexane mixtures in terms of their higher selectivity over traditional solely polar solvents, e.g., NMP, DMSO, etc. The preferential extraction of these two solvents for benzene might be related to their higher polarity and aromaticity, which imposed polar-induced polar and $\pi-\pi$ electron interaction between two planar rings of benzene and imidazole or the imidazolium cation. Ionic liquid [HMIM][DBP] has a much lower selectivity than MIM due to its much enhanced solubility for the mixture of benzene and cyclohexane and narrower immiscible region in the triangle-phase diagram.

Literature Cited

(1) *Kirk-Othmer Encyclopedia of Chemical Technology*, 3rd ed.; Wiley: New York, 1978.

(2) Fang, Z. P.; Jiang, Z. Y. Progress and Prospect in Pervaporation Membrane for Separation of Benzene and Cyclohexane. *Petrochem. Technol.* **2005**, *34* (9), 885–890.

(3) Kuniaki, I.; Kenji, O.; Takashi, M.; Tadashi, U. Effect of mesogenic groups on characteristics of permeation and separation for benzene/cyclohexane mixtures of side-chain liquid-crystalline polymer membranes. *J. Membr. Sci.* **1998**, *143*, 93–104.

(4) Jeong, B. H.; Hasegaw, A. Y.; Kusakabe, K. Separation of Benzene and Cyclohexane Mixtures Using an NaY-Type Zeolite Membrane. *Sep. Sci. Technol.* **2002**, *37* (6), 12251 239.

(5) Aurelio, V.; Fernando, D.; Ricardo, E.; José, C. Activity Coefficients for Cyclohexane, Cyclohexene, and Benzene in Extractive Distillation Solvents Using Non-Steady-State Gas Chromatography. *J. Chem. Eng. Data* **2001**, *46*, 98–101.

(6) Choi, Y. J.; Cho, K. W.; Cho, B. W.; Yeo, Y.-K. Optimization of the Sulfolane Extraction Plant Based on Modeling and Simulation. *Ind. Eng. Chem. Res.* **2002**, *41*, 5504–5509.

(7) Krishna, R.; Goswami, A. N.; Nanoti, S. M.; Rawat, B. S.; Khana, M. K.; Dobhal, J. Extraction of Aromatics from 63- 69 °C Naphtha Fraction for Food Grade Hexane Production Using Sulpholane and NMP as Solvents. *Ind. J. Technol* **1987**, *25*, 602–606.

(8) Al-Sahhaf, T. A.; Kapetanovic, E. Measurement and Prediction of Phase Equilibria in the Extraction of Aromatics from Naphtha Reformate by Tetraethylene glycol. *Fluid Phase Equilib.* **1996**, *118*, 271–285.

(9) Wang, W.; Gou, Z. M.; Zhu, S. L. Liquid-Liquid Equilibria for Aromatics Extraction Systems with Tetraethylene glycol. *J. Chem. Eng. Data* **1998**, *43*, 81–83.

(10) Yorulmaz, Y.; Karpuzcu, F. Sulpholane versus Diethylene glycol in Recovery of Aromatics. *Chem. Eng. Res. Des.* **1985**, *63*, 184–190.

(11) Morawski, P.; Letcher, T. M.; Naicker, P. K.; Domanska, U. Liquid−Liquid Equilibria for Mixtures of (Furfuryl Alcohol + an Aromatic Hydrocarbon + an Alkane) at $T = 298.15$ K. *J. Chem. Eng. Data* **2002**, *47* (6), 1453–1456.

(12) Chen, D. C.; Ye, H. Q.; Wu, H. (Liquid + Liquid) Equilibria of Three Ternary Systems: (Heptane + Benzene + N-formylmorpholine), (Heptane + Toluene + N-formylmorpholine), (Heptane + Xylene + N-formylmorpholine) from $T = (298.15$ to $353.15)$ K. *J. Chem. Thermodyn.* **2007**, *39*, 1182–1188.

(13) Arlt, W.; Seiler, M.; Jork, C.; Schneider, T. (BASF), Ionic liquids as selective additives for the separation of close-boiling or azeotropic mixtures, PCT Int. Appl. WO 2002/074718 A2, 26-09-2002(2002).

(14) Chen, J.; Li, Z.; Duan, L. Liquid−liquid equilibria of ternary and quaternary systems including cyclohexane, 1-heptane, benzene, toluene, and sulfolane at 298.15 K. *J. Chem. Eng. Data* **2000**, *45*, 689–692.

(15) Shyu, L.-J.; Zhang, Z.; Zhang, Q. (Akzo Nobel), Process for the extraction of an aromatic compound from an aliphatic phase using a non-neutral ionic liquid, PCT Int. Appl. WO, 2001. 40150 A1, 07-06-2001 (2001).

(16) Wang, R. J.; Wang, J. F.; Meng, H.; Li, C. X.; Wang, Z. H. Liquid-Liquid Equilibria for Benzene + Cyclohexane + 1-Methyl-3-methylimidazolium Dimethylphosphate or + 1-Ethyl-3-methylimidazolium Diethylphosphate. *J. Chem. Eng. Data* **2008**, *53* (5), 1159–1162.

(17) Nie, Y.; Li, C. X.; Wang, Z. H. Extractive Desulfurization of Fuel Oil Using Alkylimidazole nd Its Mixture with Dialkylphosphate Ionic Liquids. *Ind. Eng. Chem. Res.* **2007**, *46*, 5108–5112.

(18) Jiang, X. C.; Nie, Y.; Chunxi Li, C. L.; Wang, Z. H. Imdazolium-based phosphate ionic liquids- apotential solvent for extractive desulfurization of fuel. *Fuel* **2008**, *87* (1), 79–84.

(19) Letcher, T. M.; Deenadayalu, N. Liquid−liquid Equilibria for Mixtures of an 1-methyl-3-octyl-imidazolium Chloride + Benzene + an Alkane at 298.15 K and 1 atm. *J. Chem. Thermodyn.* **2003**, *35*, 67–76.

(20) Letcher, T. M.; Reddy, P. S. Ternary (liquid +liquid) Equilibria for Mixtures of 1-hexyl-3-methylimdazolium (terafluoroborate or hexafluorophosphate) + Benzene + an Alkane at $T = 298.2$ K and $P = 0.1$ MPa. *J. Chem. Thermodyn.* **2005**, *37*, 415–421.

(21) Chen, J.; Li, Z. C.; Duan, L. P. Liquid−Liquid Equilibria of Ternary and Quaternary Systems Including Cyclohexane, 1-Heptene, Benzene, Toluene, and Sulfolane at 298.15 K. *J. Chem. Eng. Data* **2000**, *45*, 689–692.

(22) Meindersma, G. W.; Podt, A. Selection of Ionic Liquids for the Extraction of Aromatic Hydrocarbons from Aromatic/aliphatic Mixtures. *Fuel Proces Technol.* **2005**, *87*, 59–70.

(23) Renon, H.; Prausnitz, J. M. Local Compositions in Thermodynamic Excess Functions for Liquid Mixtures. *AIChE J.* **1968**, *14*, 135–144.

(24) Walas, S. W. *Phase Equilibria in Chemical Engineering*; Butterworth: Boston, 1985.

(25) Hanke, C. G.; Johansson, A.; Harper, J. B.; Lynden-Bell, R. M. Why are Aromatic Compounds more Soluble than Aliphatic Hydrocarbons in Dimethylimidazolium Ionic Liquids? A Simulation Study. *Chem. Phys. Lett.* **2003**, *374*, 85–90.

(26) Vega, A.; Diez, F.; Esteban, R.; Coca, J. Solvent Selection for Cyclohexane -Cyclohexene- Benzene Separation by Extractive Distillation Using Non -Steady-State Gas Chromatography. *Ind. Eng. Chem. Res.* **1997**, *36*, 803–807.

(27) Letcher, T. M.; Reddy, P. Ternary Liquid-Liquid Equilibria for Mixtures of 1-Hexyl-3-Methylimidozolium (Tetrafluoroborate or Hexafluorophosphate) + Ethanol + an Alkene at $T = 298.2$ K. *Fluid Phase Equilib.* **2004**, *219*, 107–112.

(28) Mohsen-Nia, M.; Mohammad Doulabi, F. S. Liquid-Liquid Eequilibria for Mixtures of (Ethylene Carbonate + Aromatic Hydrocarbon + Cyclohexane). *Thermochim. Acta* **2006**, *44*, 82–85.

Received for review May 25, 2008. Accepted June 23, 2008.

JE800376F