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Liquid−Liquid Equilibria of the Ternary Systems of Alkane + Aromatic + 1-Ethylpyridinium Ethylsulfate Ionic Liquid at $T = (283.15 \text{ and } 298.15)$ K

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In this work, the ionic liquid [EPy][$EtSO_4$] was tested as a solvent for the separation of benzene from alkanes. The liquid−liquid equilibrium (LLE) data for the ternary mixtures of octane (1) or nonane (1) + benzene (2) + 1-ethylpyridinium ethylsulfate ([EPy][$EtSO_4$]) (3) at $T = (283.15 \text{ and } 298.15)$ K and atmospheric pressure were experimentally determined. The cloud-point method was used to determine the solubility curve, and the tie-line compositions were obtained by density measurements. The effectiveness of the extraction of benzene from an alkane was evaluated by means of the calculation of the solute distribution ratio and selectivity values. The consistency of tie-line data was ascertained by applying the Othmer−Tobias and Hand equations. A correlation of the experimental tie lines was conducted through the use of the nonrandom two-liquid (NRTL) equation, which provides a good correlation of the experimental data. The results show that [EPy][$EtSO_4$] can be used as an alternative solvent in liquid extraction processes for the removal of benzene from its mixtures with alkanes.

1. Introduction

In the petrochemical industry, the separation of aromatic hydrocarbon from aliphatic hydrocarbon mixtures is challenging because of the proximity of the boiling points of the hydrocarbons. This separation is made industrially by liquid extraction. However, nowadays improvements regarding environmental regulations and economic considerations have to be made to obtain a safe and environmentally benign process.

The ionic liquids (ILs) can be considered as environmentally friendly solvents due of their low vapor pressure. Compared to conventional organic solvents, the use of ILs for many applications has a number of advantages determined by the unique combination of their properties. The application of ILs on the extraction of aromatics from their mixtures with aliphatic hydrocarbons has previously been explored by experimental measurement of ternary liquid−liquid equilibrium (LLE), and these results can be found elsewhere.[1−23]

The purpose of this work was to investigate the possibility of using [EPy][$EtSO_4$] as a solvent in the separation of benzene from aliphatic compounds. With this aim, in this work, solubility curve data and tie-line data for the ternary mixtures of alkane (1) + benzene (2) + [EPy][$EtSO_4$] (3) were determined at $T = (283.15 \text{ and } 298.15)$ K and at atmospheric pressure. From the experimental data, the selectivity, S, and solute distribution ratio, β, were calculated to determine the feasibility of the IL for solvent extraction processes. The reliability of the experimentally measured LLE data was tested by the Othmer−Tobias[24] and Hand[25] equations. The experimental data were correlated through the nonrandom two-liquid (NRTL)[26] model, and the results were analyzed in terms of deviations between experimental and calculated compositions in both equilibrium phases and between experimental and calculated distribution coefficients.

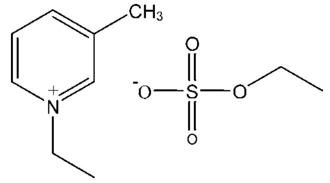

Figure 1. Structure of the IL [EPy][$EtSO_4$].

2. Experimental Section

2.1. Chemicals. Nonane and benzene were supplied by Sigma-Aldrich with mass fraction purities of > 99 % and 99.8 %, respectively. Octane was purchased from Fluka with a purity higher than 99.5 % by mass. They were degassed ultrasonically, dried over molecular sieves of type 4 nm supplied by Aldrich, and kept in an inert argon atmosphere.

The IL was synthesized and purified in our laboratory using a standard procedure previously published.[27] The IL was dried under high to vacuum ($P/\text{Pa} = 2 \cdot 10^{-1}$) and moderate temperature ($T/\text{K} = 323.15$) for several days to remove possible traces of volatile components including water, always prior to its use. Analysis using the 787 Karl Fischer Titrino techniques showed that the water mass fraction in the IL was $7 \cdot 10^{-4}$.

To ensure its purity, the structure of the final product was checked by nuclear magnetic resonance (NMR) spectroscopy. Its purity was found to be higher than 99 % in mass fraction. The IL was kept in bottles under inert atmosphere in a glovebox. The structure of this IL is presented in Figure 1.

The physical properties including the measured densities and refractive indices are listed in Table 1 together with literature[28−30] values where available (no literature data about the density and refractive index of [EPy][$EtSO_4$] have been found).

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Table 1. Pure Component Properties Data at T/K = 298.15

	ρ/g·cm^{-3}		n_D	
component	exp.	lit.	exp.	lit.
octane	0.69860	0.6985[a] 0.69862[b]	1.39519	1.39510[a] 1.39505[b]
nonane	0.71399	0.7139[c] 0.71375[b]	1.40326	1.40322[c] 1.40311[b]
benzene	0.87357	0.87360[b]	1.49774	1.49792[b]
[EPy][EtSO$_4$]	1.2520	n.a.[d]	1.50525	n.a.[d]

[a] From ref 28. [b] From ref 29. [c] From ref 30. [d] n.a.: not available.

Table 2. Solubility Curves of Ternary Systems of Alkane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)

x_1	x_2	ρ / g·cm^{-3}
Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)		
T/K = 283.15		
0.004	0.000	1.26058
0.003	0.050	1.25265
0.003	0.099	1.24478
0.002	0.145	1.23708
0.001	0.210	1.22477
0.002	0.253	1.21597
0.001	0.312	1.20334
0.000	0.335	1.19857
T/K = 298.15		
0.005	0.000	1.25145
0.004	0.053	1.24263
0.003	0.094	1.23646
0.001	0.152	1.22696
0.001	0.213	1.21481
0.001	0.261	1.20523
0.001	0.300	1.19636
0.001	0.359	1.18428
0.000	0.406	1.17169
Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)		
T/K = 283.15		
0.004	0.000	1.26125
0.002	0.050	1.25363
0.002	0.099	1.24599
0.002	0.147	1.23711
0.002	0.210	1.22543
0.001	0.252	1.21582
0.000	0.335	1.19857
T/K = 298.15		
0.004	0.000	1.25084
0.003	0.052	1.24342
0.001	0.099	1.23568
0.001	0.150	1.22695
0.001	0.210	1.21582
0.001	0.262	1.20552
0.000	0.406	1.17169

2.2. Apparatus and Procedure. The density of the pure liquids and mixtures were measured using an Anton Paar DSA-5000 digital vibrating tube densimeter with an uncertainty of $\pm\ 3\cdot10^{-5}$ g·cm^{-3}. To measure refractive indices of pure components, an automatic refractometer (Abbemat-HP, Dr. Kernchen) with an uncertainty in the experimental measurements of $\pm\ 4\cdot10^{-5}$ was used. For the preparation of samples, a Mettler AX-205 Delta Range balance with an uncertainty of $\pm\ 3\cdot10^{-4}$ g was employed.

LLE data for the ternary systems of octane (1) or nonane (1) + benzene (2) + 1-ethylpyridinium ethylsulfate (3) were determined at T = (283.15 and 298.15) K. Two different temperatures, (283.15 and 298.15) K, were selected to study the ternary equilibrium system to observe the evaluation with the temperature of the solubility curve and tie lines. The points on the solubility curves were obtained using the "cloud point" method,[2] while the tie-line compositions were determined by density measurements.

Table 3. Validation Points of Ternary Systems of Alkane (1) + Aromatic (2) + [EPy][EtSO$_4$] (3)

x_1	x_2	ρ / g·cm^{-3}	x_1^{calc}	x_2^{calc}
Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)				
T/K = 283.15				
0.003	0.080	1.24836	0.003	0.078
0.001	0.193	1.22832	0.002	0.192
0.002	0.288	1.20891	0.001	0.288
T/K = 298.15				
0.003	0.081	1.23898	0.003	0.079
0.001	0.187	1.22013	0.002	0.186
0.000	0.290	1.19923	0.001	0.289
Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)				
T/K = 283.15				
0.004	0.082	1.24905	0.003	0.081
0.002	0.195	1.22792	0.002	0.195
0.001	0.288	1.20900	0.001	0.286
T/K = 298.15				
0.003	0.080	1.23920	0.002	0.078
0.000	0.183	1.22146	0.001	0.181
0.001	0.195	1.21873	0.001	0.193

The solubility curves of the studied systems were determined at T = (283.15 and 298.15) K, and at atmospheric pressure by titrating binary mixtures (3 mL) of known compositions with the third component, the end point was determined by observing the transition from a homogeneous to a heterogeneous solution. The density of each sample was measured, and a polynomial expression for the density as function of the three compositions was obtained. Note that the binary mixture of alkane (1) + benzene (2) is part of a solubility curve, since the miscibility of the IL in binary mixtures was not detected.

Validation points for the solubility curve were obtained in the same way; the compositions of these points were calculated through the above-mentioned polynomial expression, and the obtained values were compared with the known compositions. If the mean deviation is low, the equation is validated and can be used for the tie-line determination. The maximum error was estimated to be 0.003 in mole fraction.

Tie-line data were obtained preparing ternary mixtures (12 mL) of known composition within the immiscible region; they were thermostatted at T = (283.15 and 298.15) K in a thermostatic bath (PoliScience digital temperature controller) with a precision of ± 0.01 K. Special care was taken in covering the whole immiscibility region and getting well-distributed tie-lines throughout it. To guarantee the thermodynamic equilibrium, all mixtures were vigorously stirred using a magnetic stirrer for 6 h to get a good contact between both phases and kept overnight to settle down. Then, a suitable amount of each layer was withdrawn to carry out the compositional analysis. Analysis of the composition of the two-phase equilibrium mixtures was carried by measuring densities, using the polynomial expression for the density as a function of the three components, obtained for solubility curves. No presence of IL was observed with the NMR technique in the upper equilibrium phase of the tie-lines of the studied systems. The composition of the upper phase was determined using the density curves of the binary systems of alkane (1) + aromatic (2), taken from literature.[31]

3. Results and Discussion

The compositions of the ternary mixtures (mole fraction) on the solubility curves at T = (283.15 and 298.15) K for both systems at studied temperatures are given in Table 2, and the validation points are summarized in Table 3.

Table 4. Fitting Parameters for Equation 1

a	*b*	*c*	*d*	*e*	*f*	*g*
Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3) at *T*/K = 283.15						
1.26149	−0.24538	−0.00155	−0.00001	−0.15326	−0.07750	−0.07720
Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3) at *T*/K = 298.15						
1.25363	−0.47107	0.01918	0.00011	−0.16755	−0.01527	−0.16498
Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3) at *T*/K = 283.15						
1.25768	0.99272	0.50070	0.00011	−0.11540	−0.31368	0.39426
Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3) at *T*/K = 298.15						
1.24952	0.33723	0.02352	0.00012	−0.13088	−0.13352	−0.0.04809

Table 5. Experimental LLE Data in Mole Fraction for the Ternary System of Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3) at Several Temperatures, Solute Distribution Ratio, *β*, and Selectivity, *S*, Values

alkane-rich layer		IL-rich layer			
x_1^{I}	x_2^{I}	x_1^{II}	x_2^{II}	β	S
		T/K = 283.15			
0.938	0.062	0.005	0.029	0.47	87.75
0.874	0.126	0.004	0.057	0.45	98.85
0.800	0.200	0.004	0.090	0.45	90.00
0.744	0.256	0.004	0.114	0.45	82.83
0.680	0.320	0.004	0.140	0.44	74.38
0.618	0.382	0.004	0.163	0.43	65.93
0.549	0.451	0.004	0.190	0.42	57.82
0.467	0.533	0.004	0.218	0.41	47.75
0.400	0.600	0.004	0.242	0.40	40.33
0.340	0.660	0.004	0.261	0.40	33.61
		T/K = 298.15			
0.873	0.127	0.005	0.057	0.45	78.36
0.816	0.184	0.004	0.081	0.44	89.80
0.753	0.247	0.004	0.107	0.43	81.55
0.697	0.303	0.004	0.129	0.43	74.19
0.637	0.363	0.004	0.152	0.42	66.68
0.510	0.490	0.004	0.198	0.40	51.52
0.372	0.628	0.004	0.247	0.39	36.58
0.250	0.750	0.004	0.288	0.38	24.00

The polynomial expression used for the fitting the density as function of composition for each solubility curve is the following:

$$\rho/(\mathrm{g\cdot cm^{-3}}) = a + b\cdot x_1 + c\cdot {x_1}^2 + d\cdot {x_1}^3 + e\cdot x_2 + f\cdot {x_2}^2 + g\cdot {x_2}^3 \quad (1)$$

where *a*, *b*, *c*, *d*, *e*, *f*, and *g* are the adjustable parameters; these parameters are presented in Table 4.

To study the ability of the IL [EPy][EtSO$_4$] to separate aliphatic + benzene mixtures, LLE for the ternary systems of octane (1) + benzene (2) + 1-ethylpyridinium ethylsulfate (3) and nonane (1) + benzene (2) + 1-ethypyridinium ethylsulfate (3) were experimentally determined at T = (283.15 and 298.15) K and at atmospheric pressure. Tables 5 and 6 list the compositions of the experimental tie-lines for the two investigated ternary systems at T = (283.15 and 298.15) K, together with the LLE data. Tables 5 and 6 include the corresponding values for the solute distribution ratio (β) and the selectivity (S), which are widely used parameters to characterize the suitability of a solvent in liquid extraction. These parameters, β and S, were calculated according to the following expressions:

$$\beta = \frac{x_2^{\mathrm{II}}}{x_2^{\mathrm{I}}} \quad (2)$$

$$S = \frac{x_2^{\mathrm{II}} x_1^{\mathrm{I}}}{x_2^{\mathrm{I}} x_1^{\mathrm{II}}} \quad (3)$$

where x_1^{I} and x_2^{I} are the mole fractions of alkane and benzene, respectively, in the alkane rich-phase, and x_1^{II} and x_2^{II} are the mole fractions of alkane and benzene, respectively, in the IL-rich phase. Figure 2 shows graphical representations of the tie-lines of both ternary systems at the studied temperatures. The evolution of the β and S for each system as a function of the mole fraction of the solute in the organic phase at the studied temperatures is plotted in Figures 3 and 4, respectively. In these figures it can be observed that the selectivity and solute distribution ratio decreases with an increase of benzene in alkane-rich phase, as was observed in several published data.[2,5,9,10,12,19−21,23] The S values increase in the order nonane > octane, and the solute distribution ratio increases in the order octane > nonane. These results are in agreement with the works presented by Letcher et al.[2,3] and Deenadayalu and co-workers.[14] Considering the type of ternary diagrams and that a small variation in the compositions has a great effect on selectivity, this parameter should be interpreted as a range. As can be seen, the effect of the temperature is rather small, with the characterizing parameters of the extraction (S and β) being slightly higher than β for the lower temperatures. However, the selectivity values in the systems in the study are higher than unity. As a result of the above equations, the IL [EPy][EtSO$_4$] can be confirmed as a potential alternative solvent for the separation of benzene from alkanes.

The equations provided by Othmer−Tobias[24] and Hand[25] were used to ascertain the reliability of the experimental tie-line compositions:

$$\ln\left(\frac{1 - w_1^{\mathrm{I}}}{w_1^{\mathrm{I}}}\right) = a + b \ln\left(\frac{1 - w_3^{\mathrm{II}}}{w_3^{\mathrm{II}}}\right) \quad (4)$$

$$\ln\left(\frac{w_2^{\mathrm{I}}}{w_1^{\mathrm{I}}}\right) = c + d \ln(w_2^{\mathrm{II}}/w_3^{\mathrm{II}}) \quad (5)$$

where w_1^{I} and w_2^{I} are the mass fractions of alkane and benzene, respectively, in the alkane-rich phase; w_2^{II} and w_3^{II} are the mass

Table 6. Experimental LLE Data in Mole Fraction for the Ternary System of Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3) at Several Temperatures, Solute Distribution Ratio, *β*, and Selectivity, *S*, Values

alkane-rich layer		IL-rich layer			
x_1^{I}	x_2^{I}	x_1^{II}	x_2^{II}	β	S
		T/K = 283.15			
0.871	0.129	0.004	0.056	0.43	94.53
0.810	0.190	0.003	0.082	0.43	116.53
0.751	0.249	0.003	0.107	0.43	107.57
0.686	0.314	0.003	0.133	0.42	96.86
0.628	0.372	0.003	0.156	0.42	87.78
0.498	0.502	0.003	0.205	0.41	67.79
0.375	0.625	0.003	0.248	0.40	49.60
0.249	0.751	0.003	0.292	0.39	32.27
0.12	0.88	0.003	0.336	0.38	15.27
		T/K = 298.15			
0.935	0.065	0.004	0.028	0.43	100.69
0.874	0.126	0.003	0.054	0.43	124.86
0.812	0.188	0.003	0.079	0.42	113.74
0.698	0.302	0.003	0.125	0.41	96.30
0.636	0.364	0.003	0.147	0.40	85.62
0.500	0.500	0.003	0.198	0.40	66.00
0.379	0.621	0.003	0.241	0.39	49.03
0.252	0.748	0.003	0.281	0.38	31.56

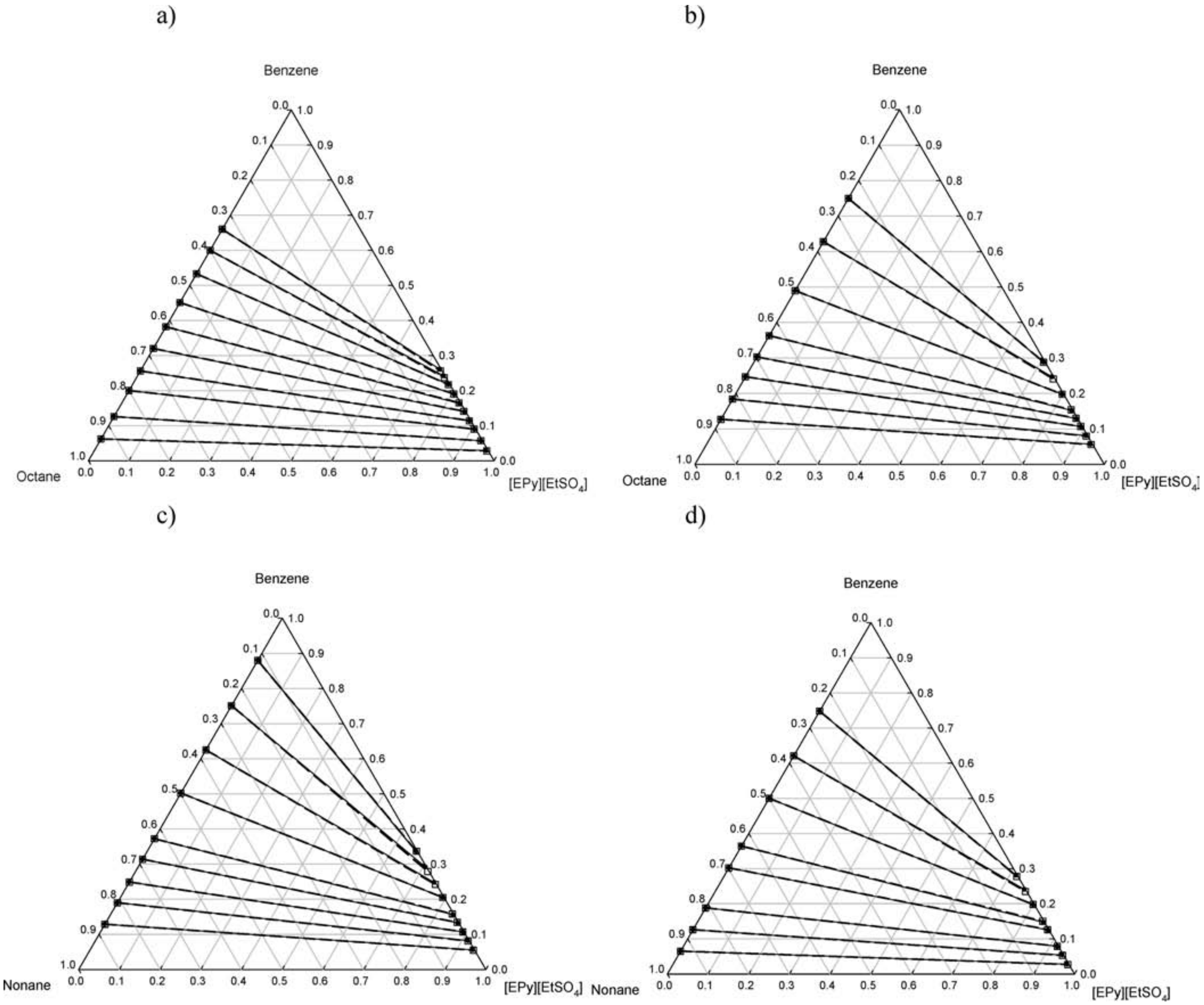

Figure 2. Experimental LLE of the ternary systems of octane (1) + benzene (2) + [EPy][EtSO$_4$] (3): (a) T/K = 283.15; (b), T/K = 298.15; and nonane (1) + benzene (2) + [EPy][EtSO$_4$] (3): (c) T/K = 283.15; (d) T/K = 298.15. Solid lines and full points indicate experimental tie-lines, and dashed lines and empty squares indicate calculated data from the NRTL model.

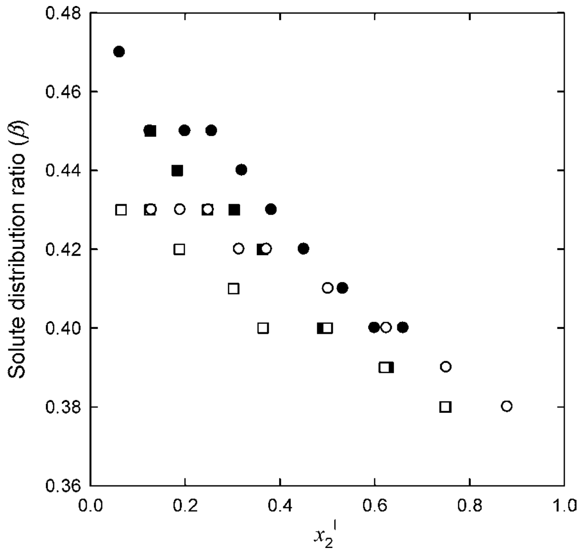

Figure 3. Solute distribution ratio for the ternary systems of octane (1) + benzene (2) + [EPy][EtSO$_4$] (3): ●, T/K = 283.15; ■, T/K = 298.15; and nonane (1) + benzene (2) + [EPy][EtSO$_4$]: (3) ○, T/K = 283.15; □, T/K = 298.15, as a function of the mole fraction of benzene in the alkane-rich phase.

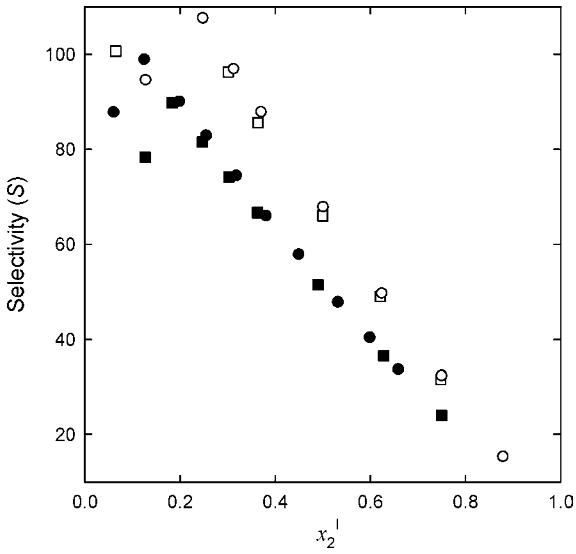

Figure 4. Selectivity for the ternary systems of octane (1) + benzene (2) + [EPy][EtSO$_4$]: (3) ●, T/K = 283.15; ■, T/K = 298.15; nonane (1) + benzene (2) + [EPy][EtSO$_4$]: (3) ○, T/K = 283.15; □, T/K = 298.15, as a function of the mole fraction of benzene in the alkane-rich phase.

Table 7. Othmer−Tobias and Hand Equation Parameters Together with the Correlation Factor at Every Studied Temperature for Both Ternary Systems

T/K	a	b	R^2
Othmer−Tobias Equation			
Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)			
283.15	2.9095	1.344	0.984
298.15	3.7165	1.6338	0.984
Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)			
283.15	4.108	1.1785	0.957
298.15	3.2961	1.4912	0.984
T/K	c	d	R^2
Hand Equation			
Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)			
283.15	3.1416	1.4514	0.990
298.15	3.5687	1.5545	0.980
Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)			
283.15	3.9801	1.1713	0.951
298.15	3.0765	1.3906	0.978

fractions of benzene and IL, respectively, in the IL-rich phase; and a, b, c, and d are adjustable parameters. The linearity of these fittings indicates the degree of consistency of the experimental data. The parameters obtained from the proposed equations are presented in Table 7, together with the correlation factor, R^2, for both systems at the studied temperatures. As can be inferred from R^2 values presented in this table, the experimental data show a satisfactory linearity.

In Figures 5 and 6, experimental and literature selectivities[16,17,32−34] for the ternary systems of octane (1) + benzene (2) + IL or sulfolane (3) and nonane (1) + benzene (2) + IL (3) are compared, respectively. As it can be observed in Figure 5 for the system of octane (1) + benzene (2) + IL or sulfolane (3), the selectivity values obtained for this system using ILs are higher than those obtained with sulfolane, and the selectivity of [EMPy][EtSO$_4$] for this system is the higher. Figure 6 shows that the selectivities obtained for the system studied in this work of nonane (1) + benzene (2) + [EPy][EtSO$_4$] (3) are similar to the literature selectivities obtained for the system containing [EMPy][EtSO$_4$].

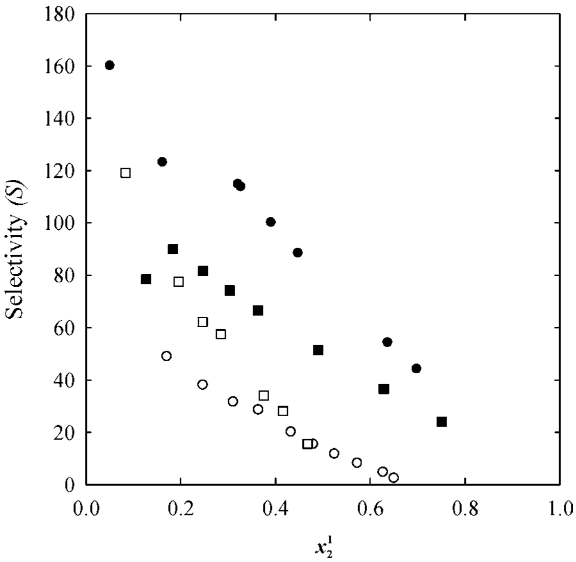

Figure 5. Selectivity of benzene for the ternary systems of octane (1) + benzene (2) + solvent (3) at T/K = 298.15: ■, [EPy][EtSO$_4$] (this work); ●, [EMPy][EtSO$_4$] (from ref 32); ○, sulfolane (from ref 33); □, sulfolane (from ref 34).

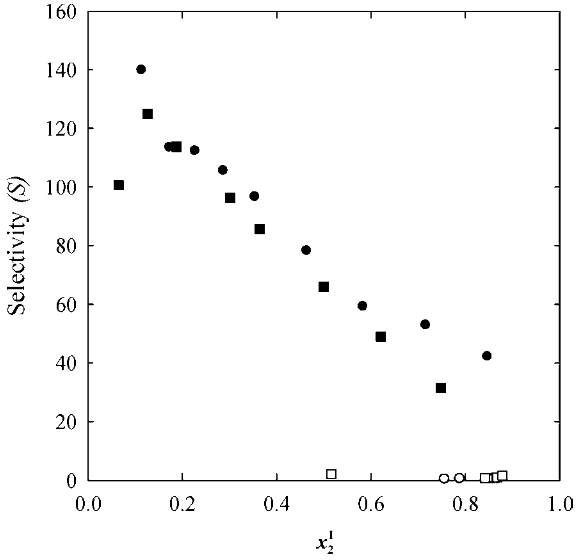

Figure 6. Selectivity of benzene for the ternary systems of nonane (1) + benzene (2) + solvent (3) at T/K = 298.15: ■, [EPy][EtSO$_4$] (this work); ●, [EMPy][EtSO$_4$] (from ref 30); ○, [BMim][PF$_6$] (from ref 16); □, [OMim][PF$_6$] (from ref 17).

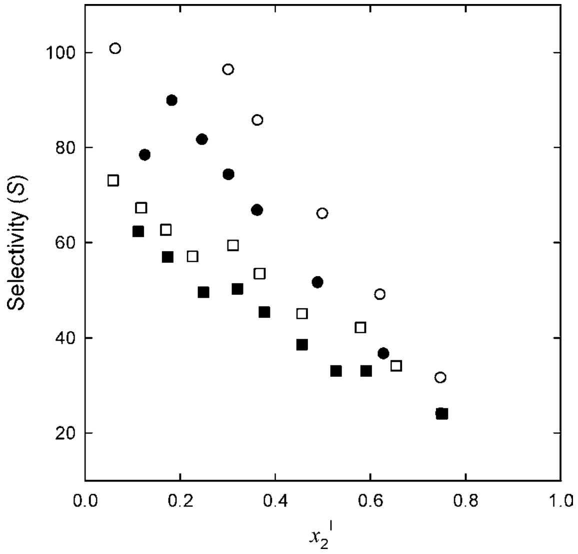

Figure 7. Selectivity for the ternary systems at T = 298.15 K: ■, hexane (1) + benzene (2) + [EPy][EtSO$_4$] (3); □, heptane (1) + benzene (2) + [EPy][EtSO$_4$] (3); ●, octane (1) + benzene (2) + [EPy][EtSO$_4$] (3); ○, nonane (1) + benzene (2) + [EPy][EtSO$_4$] (3), as a function of the mole fraction of benzene in the alkane-rich phase.

Figure 7 shows the selectivity values obtained for the systems studied in this work at a temperature of 298.15 K and the selectivity of hexane or heptane (1) + benzene (2) + [EPy][EtSO$_4$] (3) systems presented by us in previous work,[35] observing that the selectivity increases in the order nonane > octane > heptane > hexane. The ternary system of hexane (1) + benzene (2) + [EPy][EtSO$_4$] (3) has the lowest S because hexane is the most soluble alkane in the IL-rich phase.

4. Thermodynamic Correlation

The NRTL equation proposed by Renon and Prausnitz was used to correlate the experimental tie-line data for mixtures investigated here. Previous works demonstrate that the original NRTL equation can successfully correlate LLE data of ternary systems involving an IL.[2−5,8−10,12,13,15−17,19−21] The α values were set to different values between 0.1 and 0.4, and the best

Table 8. NRTL Binary Interaction Parameters and Deviations for LLE Data of Ternary Systems with $\alpha = 0.1$

T / K	$i-j$	Δg_{ij} / $\mathrm{kJ \cdot mol^{-1}}$	Δg_{ji} / $\mathrm{kJ \cdot mol^{-1}}$	σx	$\Delta\beta$
		Octane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)			
283.15	1−2	−1.666	5.671	0.029	0.939
	1−3	24.389	4.498		
	2−3	120.657	3.999		
298.15	1−2	−1.692	5.948	0.096	1.270
	1−3	25.636	4.753		
	2−3	130.217	4.415		
		Nonane (1) + Benzene (2) + [EPy][EtSO$_4$] (3)			
283.15	1−2	−2.891	7.141	0.154	1.473
	1−3	24.709	5.205		
	2−3	112.234	3.542		
298.15	1−2	−2.444	6.361	0.110	1.882
	1−3	25.866	5.452		
	2−3	118.505	3.665		

results found for the correlation were with α equal to 0.1 for both systems at $T = (283.15$ and $298.15)$ K. The binary interaction parameters, Δg_{ij}, are estimated from experimental data. The objective function used minimizes the difference between the experimental and the calculated mole fractions of the components in both phases. In this work, among the multiple solutions obtained by minimizing the objective function, the solution which achieves the lower deviations in composition and solute distribution ratio has been chosen.

The NRTL binary interaction parameters of the ternary systems correlated are listed in Table 8, as well as the values of the corresponding deviations. The values of σx and $\Delta\beta$ in this table provide a measure of the accuracy of the correlation. These deviations were calculated as follows:

$$\sigma x = 100\sqrt{\frac{\sum_{i}^{M}\sum_{j}^{N-1}(x_{ij}^{\mathrm{I,exp}} - x_{ij}^{\mathrm{I,calc}})^2 + (x_{ij}^{\mathrm{II,exp}} - x_{ij}^{\mathrm{II,calc}})^2}{2MN}} \tag{6}$$

$$\Delta\beta = 100\sqrt{\frac{1}{M}\sum_{k}\left(\frac{\beta_k - \beta_k^{\mathrm{calc}}}{\beta_k}\right)^2} \tag{7}$$

where M is the number of tie lines and N the number of components of the mixture.

The correlated tie lines are plotted in Figure 1 along with the experimental ones. As can be seen from the results depicted in Figure 1, the experimental data are well-correlated with the NRTL equation. The tie-lines in the ternary diagrams coincide in all cases. The visual comparison of both sets of tie lines for each system supports the general validity of NRTL correlations carried out. As can be inferred from the deviation values, a fairly good correlation of the experimental values with the NRTL model was obtained.

5. Conclusions

In this work, the LLE for the ternary systems of octane (1) + benzene (2) + 1-ethylpyridinium ethylsulfate (3) and nonane (1) + benzene (2) + 1-ethylpyridinium ethylsulfate (3) were experimentally determined at $T = (283.15$ and $298.15)$ K and at atmospheric pressure, and the corresponding selectivity and distribution coefficient were calculated. The selectivity values are higher than unity for both studied systems at $T = (283.15$ and $298.15)$ K and higher for the systems containing alkanes with larger chain, following the relation nonane > octane. A small effect of temperature has been observed in the studied systems.

The consistency of the LLE data was proved by the linearity of the Othmer−Tobias and Hand equations, and the classical NRTL model was proven to acceptably correlate the experimental data of LLE. The results are very satisfactory, with deviations between calculated and experimental compositions in both equilibrium phases of about 0.1. The results obtained in this work indicating that the [EPy][EtSO$_4$] IL would be a good choice as a solvent in the separation of aromatic from aliphatic hydrocarbons.

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