



(Liquid + liquid) equilibrium at $T = 298.15$ K for ternary mixtures of alkane + aromatic compounds + imidazolium-based ionic liquids



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ABSTRACT

Ionic liquids, with their unique and tunable properties, can be an advantageous alternative as extractive solvents in separation processes involving systems containing aliphatic and aromatic hydrocarbons. In this work, (liquid + liquid) equilibrium (LLE) data for the ternary systems {nonane (1) + benzene (2) + 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [BMim][NTf₂] (3)}, {octane (1) + benzene (2) + 1-methyl-3-propylimidazolium bis(trifluoromethylsulfonyl)imide, [PMim][NTf₂] (3)}, and {nonane (1) + aromatic compound (benzene or toluene or ethylbenzene) (2) + [PMim][NTf₂] (3)} were determined at $T = 298.15$ K and atmospheric pressure. Selectivity and solute distribution ratio, derived from the equilibrium data, were used to determine if this ionic liquid can be considered as a potential solvent for the separation of aromatic compounds (benzene, toluene, and ethylbenzene) from alkanes (octane and nonane). The experimental data were satisfactorily correlated with NRTL and UNIQUAC models.

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1. Introduction

Nowadays, the separation of aromatic and aliphatic compounds from hydrocarbon mixtures using ionic liquids (ILs) [1–14] is an increasingly attractive alternative to replace the conventional organic solvents in the petrochemical industry [15]. Generally, ILs have negligible vapor pressure, high thermal and chemical stability, good solvating ability for both organic and inorganic compounds [16] and cause less damage to the environment and human health than the conventional solvents. Furthermore, the ILs are known as “designer solvents” since it is possible to perform many different combinations of anion–cation, leading to almost an unlimited number of ionic liquids with different properties. This versatility of ILs presents multiple applications in different fields.

The number of publications concerning the extraction of aromatics from mixtures of aromatic/aliphatic hydrocarbons using ILs as solvents has increased considerably in recent years [6,7,17–19]. The present work is a continuation of the systematic study which carried out by our group in the determination of the (liquid + liquid) equilibria (LLE) for ternary systems containing ionic liquids as solvent [20–31]. The ILs selected for the current study are 1-methyl-3-propylimidazolium bis(trifluoromethylsulfonyl)imide, [PMim][NTf₂] and 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [BMim][NTf₂], since these ionic liquids

are known to be good solvents, to present relatively low viscosity, which facilitates handling, and to show an adequate performance in extractive applications. Taking into account these aspects, LLE data for the ternary systems {nonane (1) + benzene (2) + [BMim][NTf₂] (3)}, {octane (1) + benzene (2) + [PMim][NTf₂] (3)} and {nonane (1) + aromatic compound (benzene, toluene and ethylbenzene) (2) + [PMim][NTf₂] (3)} were determined at $T = 298.15$ K and atmospheric pressure. From the experimental data, the selectivity (S), and the solute distribution ratio (β) were calculated. These parameters were used to analyze the capability of the ILs [PMim][NTf₂] and [BMim][NTf₂] as solvents for the extraction of the studied aromatic hydrocarbons from their mixtures with alkanes.

As above mentioned, the number of possible combinations of anion–cation is very large; hence, the development of predictive and correlation models is indispensable for the optimal selection of a suitable IL for the aromatic/aliphatic extraction process. In this way, the Non-Random Two-Liquid (NRTL) [32] and Universal QUAsiChemical (UNIQUAC) [33] thermodynamic models were used to correlate the experimental data of the studied ternary systems.

2. Experimental section

2.1. Chemicals

All the organic compounds (octane, nonane, benzene, toluene and ethylbenzene) were purchased from Sigma–Aldrich with purities higher than 0.990 by mass and were ultrasonically degassed

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and dried over molecular sieves type $4 \cdot 10^{-10}$ m, supplied by Aldrich. Then, they were kept in bottles under inert argon atmosphere to avoid moisture.

The ionic liquids used in this work were supplied by IoLiTec GmbH (Germany) with a purity higher than 0.990 in mass fraction. The chemical structure of the studied ILs is shown in table 1. In order to reduce the moisture, they were dried with stirring at moderate temperature ($T = 343.15$ K) and under vacuum ($p = 0.2$ Pa) for at least 48 h prior to their use. The water contents were measured with a Mettler Toledo C20 Coulometric KF Titrator using Coulomat CG and Coulomat AG, supplied by Sigma–Aldrich, as cathodic and anodic titrants, respectively. The obtained mass fractions of water were less than $6 \cdot 10^{-4}$. The ionic liquids were kept in bottles under inert atmosphere.

The purities and experimental physical properties (density and refractive index) of the pure components at $T = 298.15$ K and literature data [34–38] are given in table 2.

2.2. Apparatus and procedure

All samples were prepared using a Mettler AX-205 Delta Range balance with an uncertainty of $\pm 3 \cdot 10^{-4}$ g. The density of the pure liquids and mixtures was measured using an Anton Paar DSA-5000 digital vibrating tube densimeter, with an uncertainty of $\pm 3 \cdot 10^{-5}$ g \cdot cm $^{-3}$. To measure refractive indices of pure components, an automatic refractometer (Abbat-HP, Dr. Kernchen) with an uncertainty in the experimental measurement of $\pm 4 \cdot 10^{-5}$ was used.

The LLE experiments were undertaken at $T = 298.15$ K and atmospheric pressure. The method used to study these systems includes the determination of the solubility curves and of the compositions of the tie-lines ends. The solubility curves were obtained using the “cloud point” method [39], by titrating binary mixtures (aromatic hydrocarbon + ionic liquid) of known composition with the third component (alkane) until a slight turbidity in samples was observed. Then, the samples were weighed to determine their composition, and the density of each sample was measured. From the density and composition values, a polynomial expression (density vs. mole fraction) was obtained. To estimate the error of the technique, several validation points were evaluated and comparing the experimental and calculated compositions, the maximum error was estimated to be ± 0.006 in mole fraction.

For the tie-lines determination, immiscible ternary mixtures of known composition were introduced into glass cells and sealed using a silicon cover. In order to ensure an intimate contact between phases, the mixtures were stirred using a magnetic stirrer for 6 h, and then they were left overnight in a thermostatic bath (PoliScience digital temperature controller, with a precision of ± 0.01 K) to ensure a complete phase separation. The temperature was controlled with a digital thermometer (ASL model F200) with an uncertainty of ± 0.01 K. Next, a sample from each phase was

TABLE 2

Mass fraction purity, density (ρ) and refractive index (n_D), of the pure components at $T = 298.15$ K.

Component	Purity	ρ /(g \cdot cm $^{-3}$)		n_D	
		Exp.	Lit.	Exp.	Lit.
[PMim][NTf $_2$]	>0.995	1.47444	1.47570 ^a	1.42526	n.a.
[BMim][NTf $_2$]	>0.999	1.43635	1.43658 ^b	1.42706	1.42692 ^b
Octane	>0.990	0.69860	0.69862 ^c	1.39519	1.39505 ^c
Nonane	>0.999	0.71390	0.71399 ^d	1.40326	1.40322 ^d
Benzene	>0.990	0.87357	0.87360 ^e	1.49774	1.49792 ^e
Toluene	>0.999	0.86217	0.86219 ^e	1.49399	1.49390 ^e
Ethylbenzene	>0.990	0.86251	0.86253 ^e	1.49304	1.49320 ^e

Standard uncertainties u are $u(\rho) = 3 \cdot 10^{-5}$ g \cdot cm $^{-3}$ and $u(n_D) = 4 \cdot 10^{-5}$.

n.a. = Not available.

^a From reference [34].

^b From reference [35].

^c From reference [36].

^d From reference [37].

^e From reference [38].

withdrawn using a syringe and the density of both phases was measured at $T = 298.15$ K.

The composition of the IL-rich phase was calculated using the above mentioned polynomial expression of density vs. composition. The composition of the hydrocarbon-rich phase was obtained using the literature data of density vs. mole fraction for the binary systems {octane (1) + benzene (2)} and {nonane (1) + benzene (2), or toluene (2), or ethylbenzene (2)} [40], since the ionic liquids are not miscible in the binary systems and their presence in the hydrocarbon-rich phase was assumed zero; this assumption was checked by 1 H NMR. This experimental procedure is described more in detail in our previous works [21,22].

3. Results and discussion

The (liquid + liquid) equilibrium data for the ternary mixtures {nonane (1) + benzene (2) + [BMim][NTf $_2$] (3)}, {octane (1) + benzene (2) + [PMim][NTf $_2$] (3)} and {nonane (1) + aromatic compound (benzene, or toluene, or ethylbenzene) (2) + [PMim][NTf $_2$] (3)} at $T = 298.15$ K and atmospheric pressure are reported in table 3, and the corresponding triangular diagrams are presented in figure 1. It can be observed that all the systems present one pair of components that shows total miscibility (alkane–aromatic) while the other two pairs show partial immiscibility (alkane–IL and aromatic–IL); therefore all the studied systems correspond to a Type 2 category, according to the classification proposed by Sørensen *et al.* [41].

By inspection of figure 1, it can be observed that the solubility of aromatic compounds in [PMim][NTf $_2$] decreases as the alkyl chain length at the benzene ring increases, that is, in the order: benzene > toluene > ethylbenzene. Table 4 This trend was also observed by other authors with different ionic liquids [16]. Besides, the solubility of benzene in [BMim][NTf $_2$] is slightly higher than

TABLE 1

Abbreviation, CAS number and chemical structure of the studied ILs.

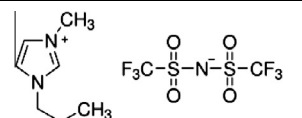
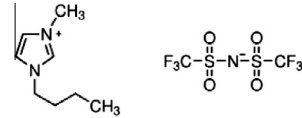
Name	Abbreviation	CAS number	Chemical structure
1-Methyl-3-propylimidazolium bis(trifluoromethylsulfonyl)imide	[PMim][NTf $_2$]	216299-72-8	
1-Butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide	[BMim][NTf $_2$]	174899-83-3	

TABLE 3

Experimental (liquid + liquid) equilibrium data, in mole fraction, for the ternary systems {aliphatic hydrocarbon (1) + aromatic hydrocarbon (2) + IL (3)} at $T = 298.15$ K and atmospheric pressure, together with solute distribution ratio (β), and selectivity (S) values.

Alkane-rich phase		Ionic liquid-rich phase		β	S
x_1^I	x_2^I	x_1^{II}	x_2^{II}		
<i>{Nonane (1) + benzene (2) + [BMim][NTf₂] (3)}</i>					
0.958	0.042	0.025	0.068	1.62	62.04
0.904	0.096	0.024	0.141	1.47	55.32
0.861	0.139	0.024	0.199	1.43	51.36
0.820	0.180	0.025	0.254	1.41	46.28
0.775	0.225	0.026	0.301	1.34	39.88
0.741	0.259	0.030	0.349	1.35	33.28
0.633	0.367	0.031	0.437	1.19	24.31
0.527	0.473	0.031	0.516	1.09	18.55
0.41	0.590	0.028	0.594	1.01	14.74
0.272	0.728	0.026	0.667	0.92	9.58
0.204	0.796	0.023	0.702	0.88	7.82
<i>{Octane (1) + benzene (2) + [PMim][NTf₂] (3)}</i>					
0.959	0.041	0.028	0.061	1.49	50.96
0.911	0.089	0.027	0.125	1.40	47.39
0.864	0.136	0.028	0.182	1.34	41.29
0.765	0.235	0.031	0.288	1.23	30.24
0.718	0.282	0.033	0.335	1.19	25.85
0.672	0.328	0.034	0.377	1.15	22.72
0.569	0.431	0.035	0.459	1.06	17.31
0.452	0.548	0.032	0.544	0.99	14.02
0.322	0.678	0.026	0.617	0.91	11.27
0.182	0.818	0.021	0.669	0.82	7.090
<i>{Nonane (1) + benzene (2) + [PMim][NTf₂] (3)}</i>					
0.961	0.039	0.042	0.058	1.49	34.03
0.919	0.081	0.042	0.117	1.44	31.61
0.876	0.124	0.042	0.167	1.35	28.09
0.817	0.183	0.043	0.232	1.27	24.09
0.765	0.235	0.040	0.283	1.20	23.03
0.675	0.325	0.034	0.379	1.17	23.15
0.607	0.393	0.029	0.435	1.11	23.17
0.513	0.487	0.022	0.504	1.03	24.13
0.386	0.614	0.015	0.587	0.96	24.60
0.242	0.758	0.010	0.663	0.87	21.17
<i>{Nonane (1) + toluene (2) + [PMim][NTf₂] (3)}</i>					
0.950	0.050	0.029	0.048	0.96	31.45
0.887	0.113	0.028	0.105	0.93	29.44
0.839	0.161	0.028	0.146	0.91	27.17
0.787	0.213	0.030	0.198	0.93	24.39
0.733	0.267	0.031	0.232	0.87	20.55
0.664	0.336	0.032	0.284	0.85	17.54
0.571	0.429	0.032	0.366	0.85	15.22
0.455	0.545	0.030	0.421	0.77	11.72
0.329	0.671	0.024	0.497	0.74	10.15
0.197	0.803	0.017	0.574	0.71	8.28
0.133	0.867	0.013	0.613	0.71	7.23
<i>{Nonane (1) + ethylbenzene (2) + [PMim][NTf₂] (3)}</i>					
0.879	0.121	0.027	0.072	0.60	19.37
0.822	0.178	0.027	0.106	0.60	18.13
0.768	0.232	0.027	0.138	0.59	16.92
0.711	0.289	0.026	0.171	0.59	16.18
0.657	0.343	0.025	0.202	0.59	15.48
0.535	0.465	0.023	0.264	0.57	13.21
0.412	0.588	0.021	0.328	0.56	10.94
0.289	0.711	0.018	0.393	0.55	8.87
0.151	0.849	0.014	0.469	0.55	5.96
0.081	0.919	0.008	0.517	0.56	5.70

in [PMim][NTf₂], i.e., an increase of the alkyl chain length of the IL cation increases the solubility of this aromatic compound. Regarding the behavior of alkanes, no significant changes are found on the replacement of nonane by octane in the ternary systems {alkane (1) + benzene (2) + [PMim][NTf₂]}. Finally, the solubility of nonane is higher in [PMim][NTf₂] than in [BMim][NTf₂], since the increase of the alkyl chain length of the IL cation leads to an increase in the mixture solubility alkane–IL [42].

Together with the LLE experimental data, table 3 includes the corresponding values for the selectivity (S) and the solute distribution ratio (β), defined below:

$$\beta = x_2^{II}/x_2^I, \quad (1)$$

$$S = x_2^{II}x_1^I/x_2^Ix_1^{II}, \quad (2)$$

where x_2^I and x_2^{II} are the mole fractions of alkane and aromatic compound, respectively, in the alkane-rich phase (upper phase); and x_2^{II} and x_2^I are the mole fractions of alkane and aromatic compound, respectively, in the IL-rich phase (lower phase). These parameters allow to evaluate the feasibility of the studied ILs to perform the liquid–liquid extraction of aromatic compounds from the (alkane + aromatic) mixture.

The plots of the variation of the solute distribution ratio and the selectivity with the composition of the aromatic compound in the raffinate phase for the studied ternary systems are presented in figure 2a and b, respectively. As it can be observed in figure 2a, in general the solute distribution ratio decreases with increasing concentration of the aromatic compound in the alkane-rich phase, except for the system {nonane (1) + ethylbenzene (2) + [PMim][NTf₂] (3)} whose values stand almost constant. Similar values of β are observed in the ternary systems {alkane (1) + benzene (2) + [PMim][NTf₂] (3)} when replacing the alkane, whereas the values of this parameter are slightly higher when [BMim][NTf₂] is used as solvent and nonane as alkane. With a last comparison between the systems involving different aromatic compounds it is possible to conclude that the presence of substituents on the benzene ring leads to a decrease of the β values.

Regarding the selectivity, all the values of S for the benzene ternary systems are higher than one and decrease with the increase of aromatic content in the alkane-rich phase. The systems with benzene show higher selectivities than those containing the other aromatic compounds. Comparing the systems {alkane (1) + benzene (2) + [PMim][NTf₂] (3)}, higher S are observed when the alkane is octane at x_2^I lower than 0.30. Moreover, the systems {nonane (1) + benzene (2) + IL (3)} show higher values of S when the IL is [BMim][NTf₂] at x_2^I lower than 0.40. Finally, similar values of S are found for the systems containing the different studied aromatic compounds, with the exception of the system with benzene at x_2^I higher than 0.30.

The obtained values of selectivity and solute distribution ratio show that both ionic liquids, [BMim][NTf₂] and [PMim][NTf₂], could be successfully used in the separation of (alkane + aromatic compound) mixtures, being octane or nonane the alkanes and benzene, or toluene, or ethylbenzene the aromatic compounds.

4. Thermodynamic correlation

The experimental LLE for the ternary systems investigated were correlated using the NRTL (NonRandom Two-Liquid) model [32]. The UNIQUAC (UNIversal QUAsi-Chemical) model [33] was only used to correlate the LLE data for the system containing [BMim][NTf₂], since the required van der Waals parameters for the other IL are not available in the literature. These models have provided adequate correlating capability for ternary systems containing ILs as shown in literature [28–30].

For the NRTL model, the non-randomness parameter in the NRTL equation, α_{ij} , was set to different values between 0.05 and 0.3 during calculations. The best results achieved are presented in table 5. The typical values of α_{ij} are found in the range (0.2 to 0.47), but in this work the best results, for some systems, were achieved using values outside this range. Some studies were found in literature where α_{ij} values outside the typical range provide the

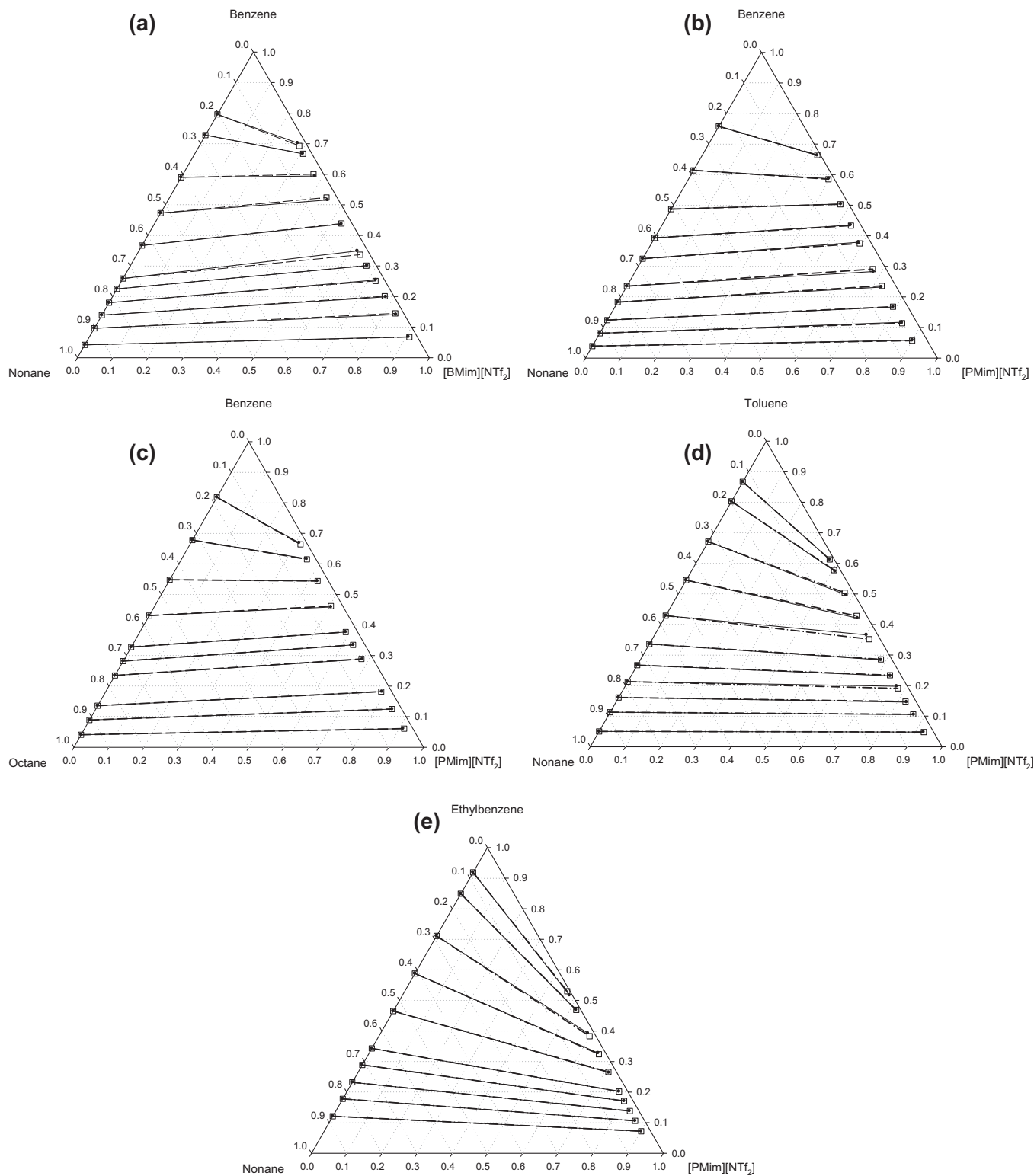


FIGURE 1. Tie-lines of the ternary systems (a) {nonane (1) + benzene (2) + [BMimNTf₂] (3)}; (b) {octane (1) + benzene (2) + [PMimNTf₂] (3)}; (c) {nonane (1) + benzene (2) + [PMimNTf₂] (3)}; (d) {nonane (1) + toluene (2) + [PMimNTf₂] (3)} and (e) {nonane (1) + ethylbenzene (2) + [PMimNTf₂] (3)} at $T = 298.15$ K. Solid lines and full points indicate experimental tie-lines and dashed lines and empty squares indicate those calculated from NRTL model.

lower deviations in the correlation of LLE of systems containing ionic liquids [3,9,12,43].

The volume, r_i , and surface area, q_i , van der Waals parameters for the UNIQUAC model were taken from literature [44,45]. The adjustable parameters of both models were determined minimizing the next objective function:

$$F.O = \sum_{i=1}^m \sum_{j=1}^n \left(\frac{(1/\beta_{ij})^{cal} - (1/\beta_{ij})^{exp}}{(1/\beta_{ij})^{exp}} \right)^2 \quad (3)$$

where M is the number of tie lines, N is the number of components in the mixture, and $(1/\beta)^{exp}$ and $(1/\beta)^{cal}$ are the experimental and

TABLE 4
Structural parameters for the UNIQUAC model.

Component	r_i	q_i
[PMim][NTf ₂]		
[BMim][NTf ₂] ^a	11.200	10.200
Octane ^b	5.845	4.936
Nonane ^b	6.523	5.476
Benzene ^b	3.188	2.400
Toluene ^b	3.923	2.968
Ethylbenzene ^b	4.597	3.508

^a From reference [44].

^b From reference [45].

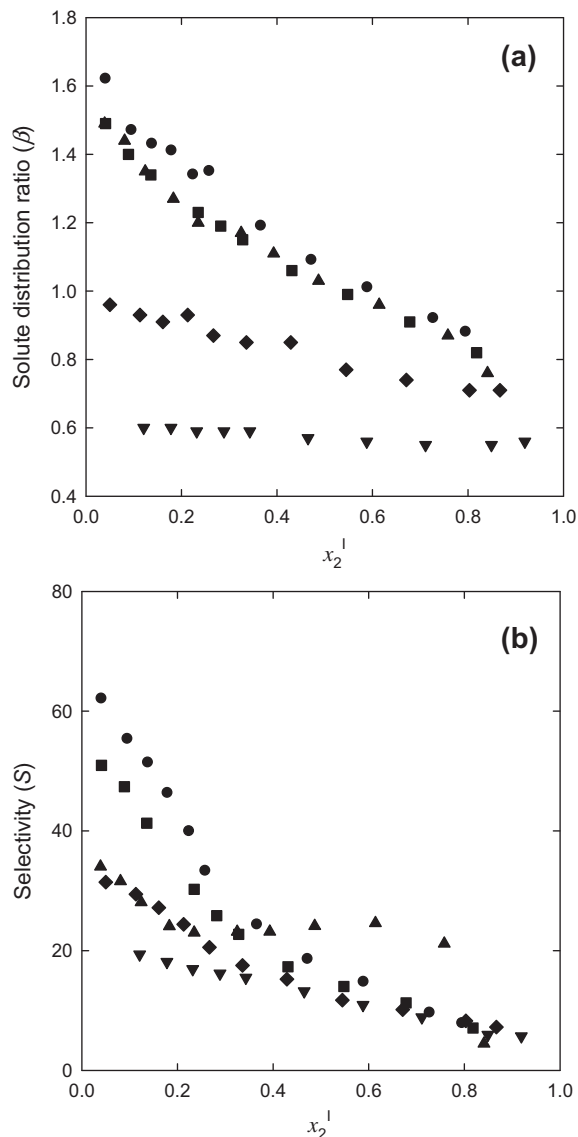


FIGURE 2. (a) Solute distribution ratio and (b) selectivity for the ternary systems {aliphatic hydrocarbon (1) + aromatic hydrocarbon (2) + IL (3)} at $T = 298.15$ K as a function of the mole fraction of aromatic hydrocarbon in the alkane-rich phase: (●) {nonane (1) + benzene (2) + [BMim][NTf₂] (3)}; (■) {octane (1) + benzene (2) + [PMim][NTf₂] (3)}; (▲) {nonane (1) + benzene (2) + [PMim][NTf₂] (3)}; (◆) {nonane (1) + toluene (2) + [PMim][NTf₂] (3)} and (▼) {nonane (1) + ethylbenzene (2) + [PMim][NTf₂] (3)}.

calculated solute distribution ratio, respectively. The validity of these models was verified by means of the of the root-mean-square deviation of the composition, σ_x , and the mean error of the solute distribution ratio, $\Delta\beta$, which were calculated as follows:

TABLE 5
NRTL binary interaction parameters and deviations for LLE data of the ternary systems at $T = 298.15$ K and atmospheric pressure.

$i-j$	$\Delta g_{ij}/(\text{kJ} \cdot \text{mol}^{-1})$	$\Delta g_{ji}/(\text{kJ} \cdot \text{mol}^{-1})$	α_{ij}	σ_x	$\Delta\beta$
{Nonane (1) + benzene (2) + [BMim][NTf ₂] (3)}					
1 to 2	-2.4772	6.5488	0.30	0.241	1.64
1 to 3	18.990	8.6374			
2 to 3	28.064	-1.7195			
{Octane (1) + benzene (2) + [PMim][NTf ₂] (3)}					
1 to 2	-2.8782	4.0392	0.30	0.102	1.23
1 to 3	22.278	7.7924			
2 to 3	17.862	-4.3665			
{Nonane (1) + benzene (2) + [PMim][NTf ₂] (3)}					
1 to 2	-0.7836	-5.9394	0.10	0.154	1.50
1 to 3	45.822	0.7779			
2 to 3	43.082	-16.846			
{Nonane (1) + toluene (2) + [PMim][NTf ₂] (3)}					
1 to 2	-5.0292	6.3530	0.10	0.253	1.91
1 to 3	79.843	6.2461			
2 to 3	115.26	-1.0951			
{Nonane (1) + ethylbenzene (2) + [PMim][NTf ₂] (3)}					
1 to 2	-1.9008	5.4949	0.10	0.220	1.22
1 to 3	49.889	2.3640			
2 to 3	124.78	3.1195			

TABLE 6
UNIQUAC binary interaction parameters and deviations for LLE data of the ternary system {nonane (1) + benzene (2) + [BMim][NTf₂] (3)} at $T = 298.15$ K and atmospheric pressure.

$i-j$	$\Delta u_{ij}/(\text{kJ} \cdot \text{mol}^{-1})$	$\Delta u_{ji}/(\text{kJ} \cdot \text{mol}^{-1})$	σ_x	$\Delta\beta$
{Nonane (1) + benzene (2) + [BMim][NTf ₂] (3)}				
1 to 2	1.8884	-1.2431	0.320	1.99
1 to 3	3.4420	-0.1306		
2 to 3	13.616	-2.5455		

$$\sigma_x = 100 \left(\frac{\sum_i^M \sum_j^{N-1} \left[\left(x_{ij}^{I,\text{exp}} - x_{ij}^{I,\text{calc}} \right)^2 + \left(x_{ij}^{II,\text{exp}} - x_{ij}^{II,\text{calc}} \right)^2 \right]}{2MN} \right)^{1/2}, \quad (4)$$

$$\Delta\beta = 100 \left(\frac{1}{M} \sum_{k=1}^M \left(\frac{\beta_k - \beta_k^{\text{calc}}}{\beta_k} \right)^2 \right)^{1/2}, \quad (5)$$

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

The values of the adjustable parameters, together with the values of the root-mean-square deviation and the mean error of the solute distribution ratio using the NRTL model are given in table 5 and those for the UNIQUAC model in table 6. From the deviation values, it can be inferred that the experimental data were satisfactorily correlated by the NRTL and UNIQUAC models. For a visual confirmation the experimental tie-lines and those calculated with the NRTL model are plotted together in figure 1, where the goodness of the correlation can be confirmed.

5. Conclusions

(Liquid + liquid) equilibrium data for the ternary systems {nonane (1) + benzene (2) + 1-butyl-3-methylimidazolium bis(trifluoromethylsulfonyl)imide, [BMim][NTf₂] (3)}, {octane (1) + benzene (2) + 1-methyl-3-propyl imidazolium bis(trifluoromethylsulfonyl)imide, [PMim][NTf₂] (3)} and {nonane (1) + aromatic compound (benzene or toluene or ethylbenzene) (2) + [PMim][NTf₂] (3)} were

determined at $T = 298.15$ K and atmospheric pressure. The corresponding values of the solute distribution ratio and selectivity were calculated. The highest values of β was found for the system {nonane (1) + benzene (2) + [BMim][NTf₂] (3)}. In general, the value of β decreases with increasing concentration of the aromatic compound in the alkane-rich phase, except for the system {nonane (1) + ethylbenzene (2) + [PMim][NTf₂] (3)}, whose values stand almost constant.

The values of S for all the ternary systems are higher than the unity, which confirms that the aromatic extraction for these systems is possible with both studied ionic liquids. Moreover, the high values of β and S indicate that [BMim][NTf₂] is a good solvent for the extraction of benzene from nonane. Finally, the LLE data reported were satisfactorily correlated by the NRTL model for all the studied systems. UNIQUAC model also adequately correlated the data for the system containing [BMim][NTf₂].

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