Supporting Information

Aqueous biphasic systems comprising analogues of glycine-betaine ionic liquids: toward greener separation platforms

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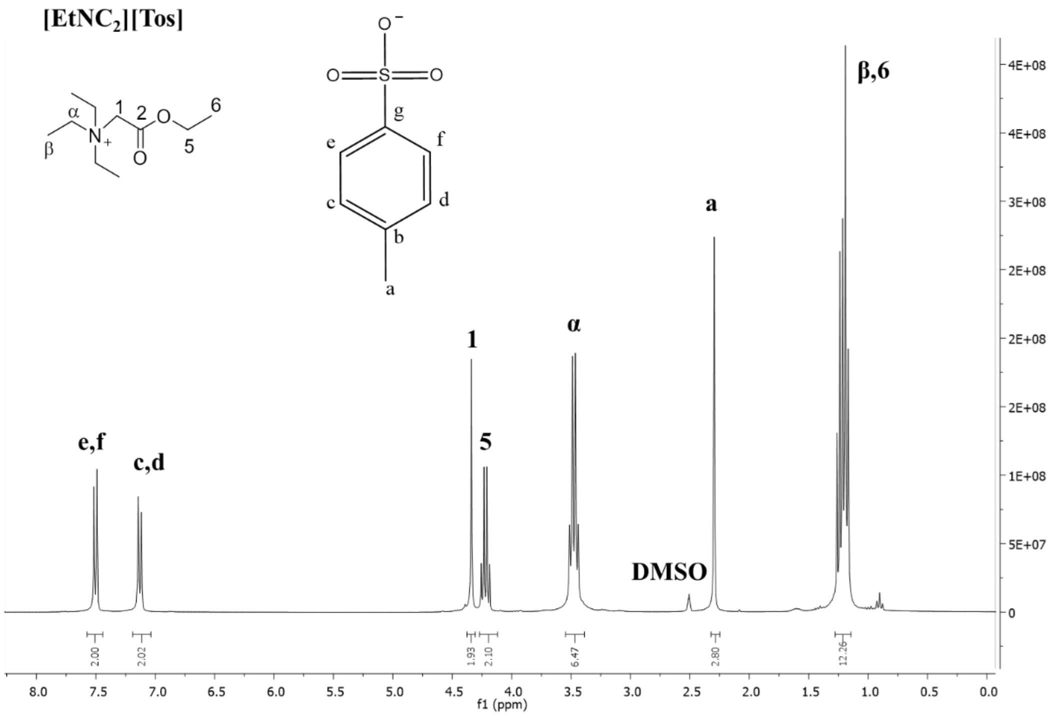

Figure S1. ^{1}H NMR spectrum of [EtNC$_2$][Tos].

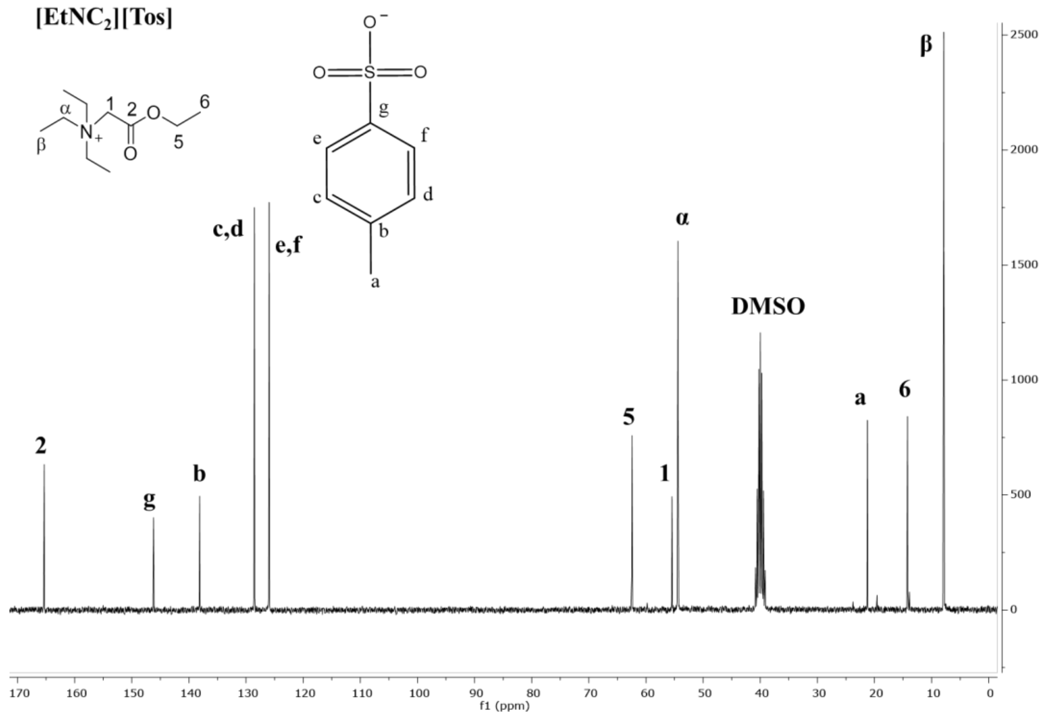

Figure S2. ^{13}C NMR spectrum of [EtNC$_2$][Tos].

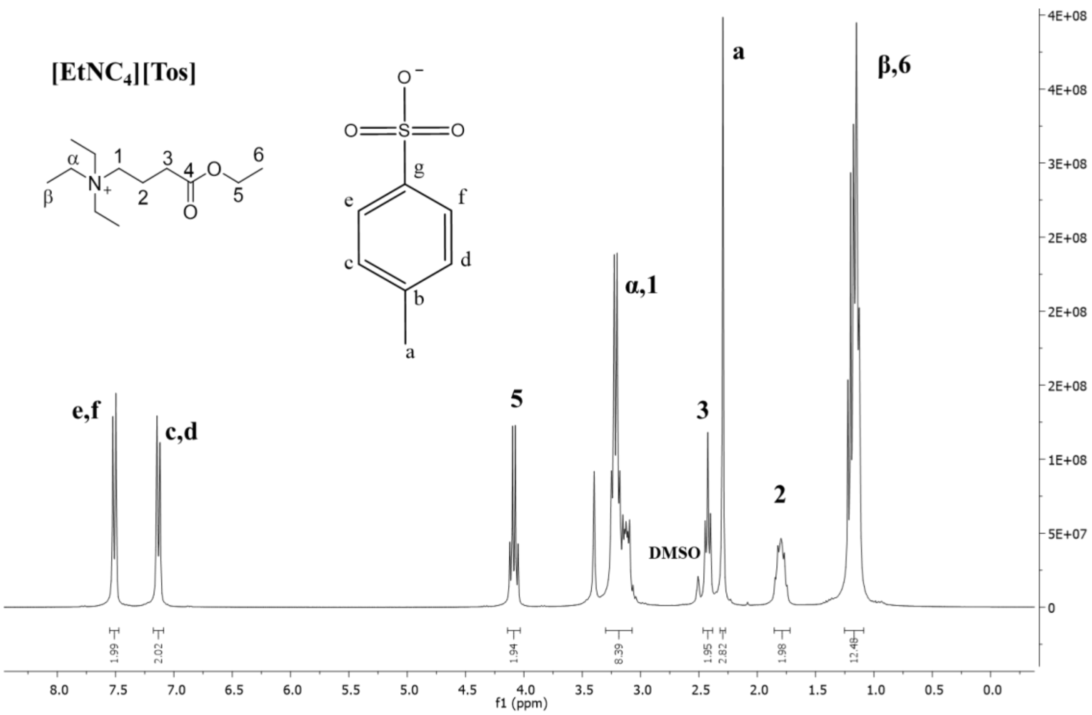

Figure S3. ^{1}H NMR spectrum of [EtNC$_4$][Tos].

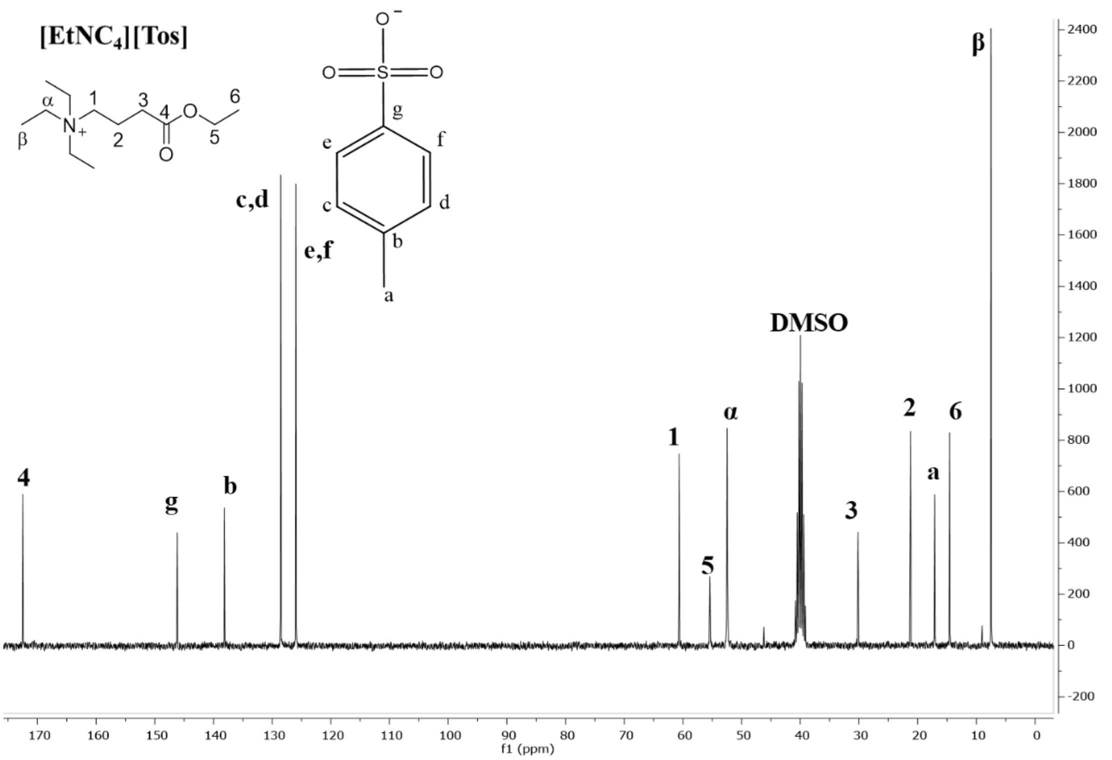

Figure S4. ^{13}C NMR spectrum of [EtNC$_4$][Tos].

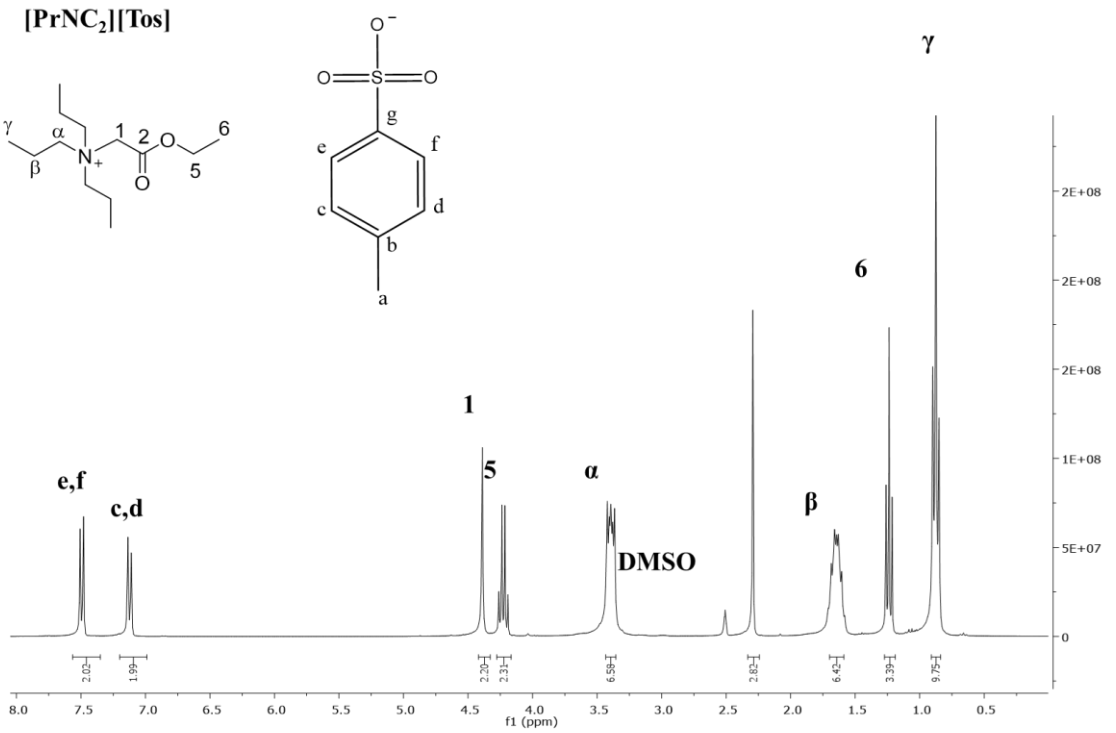

Figure S5. ^{1}H NMR spectrum of [PrNC$_2$][Tos].

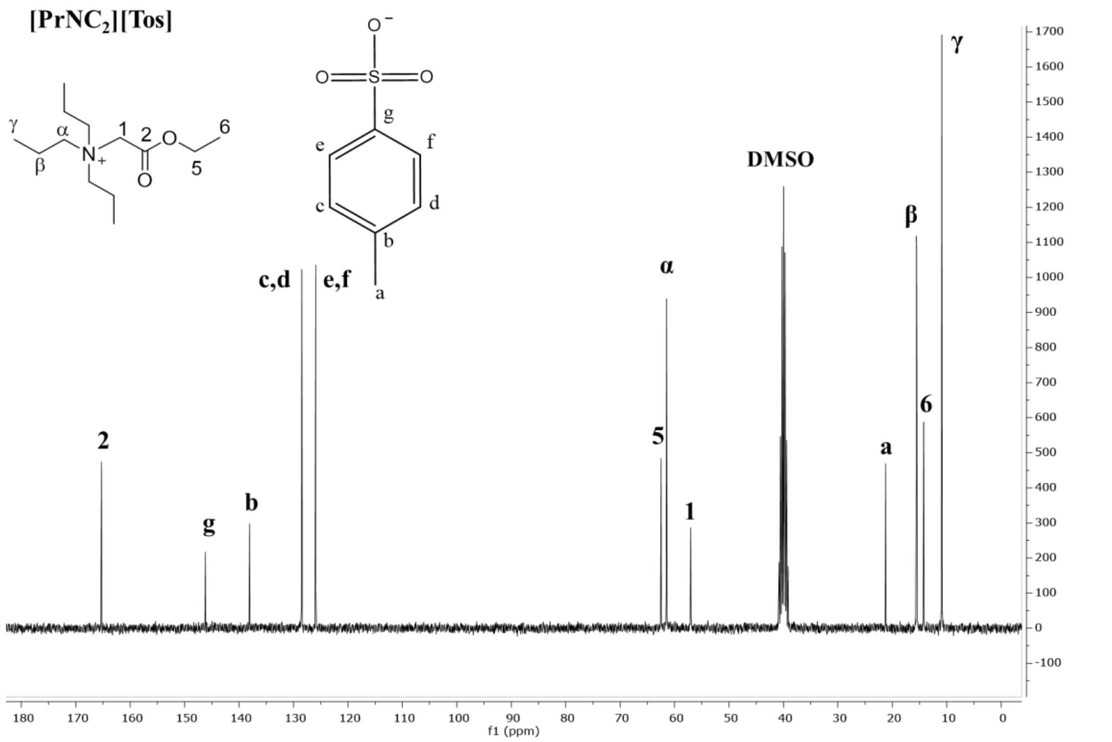

Figure S6. ^{13}C NMR spectrum of [PrNC$_2$][Tos].

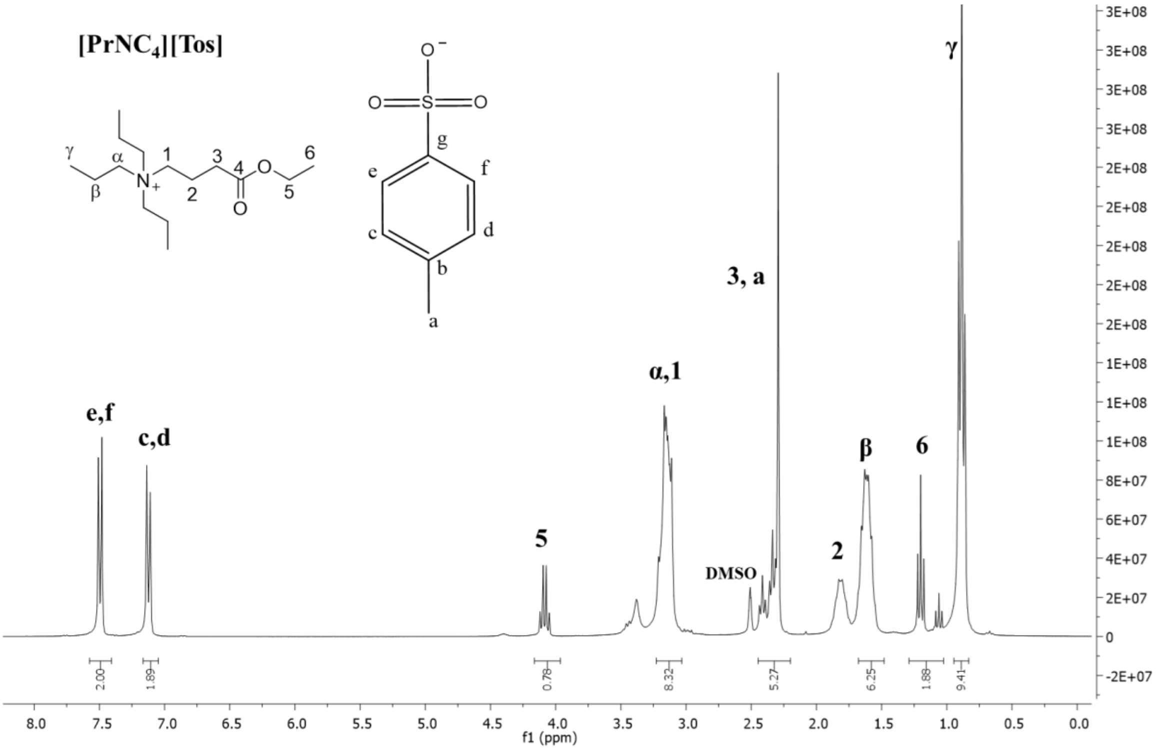

Figure S7. ^{1}H NMR spectrum of [PrNC$_4$][Tos].

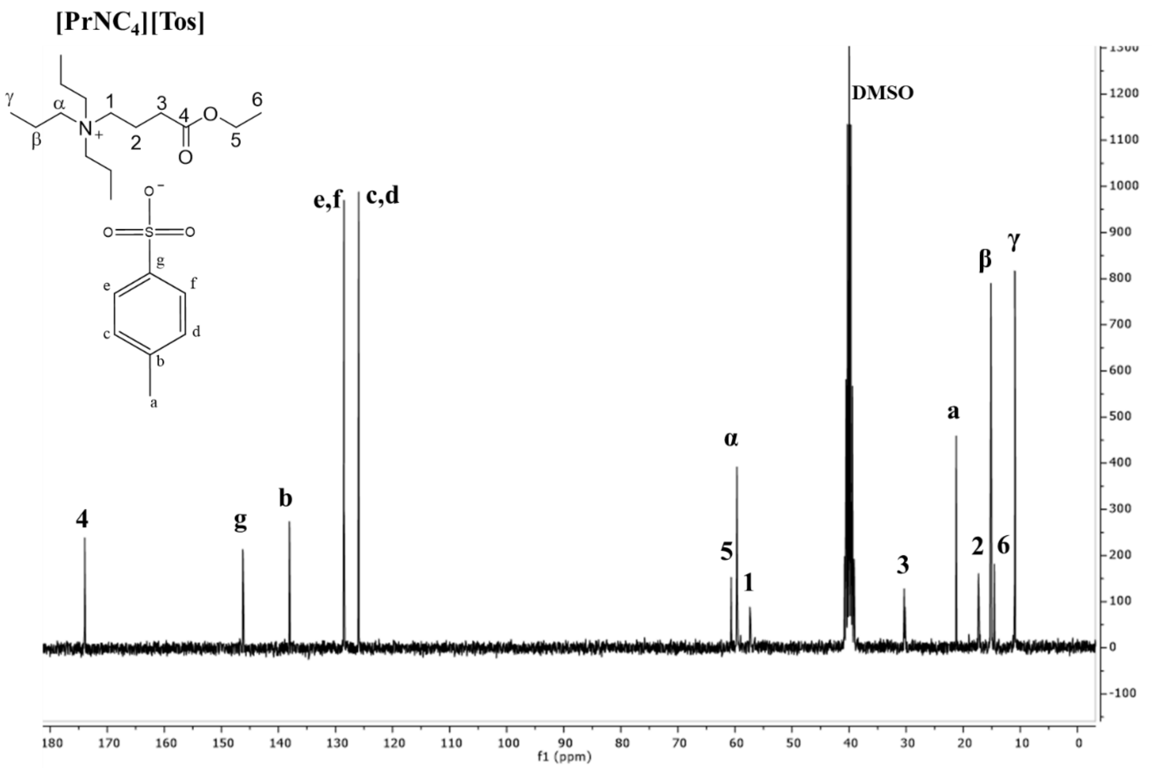

Figure S8. ^{13}C NMR spectrum of [PrNC$_4$][Tos].

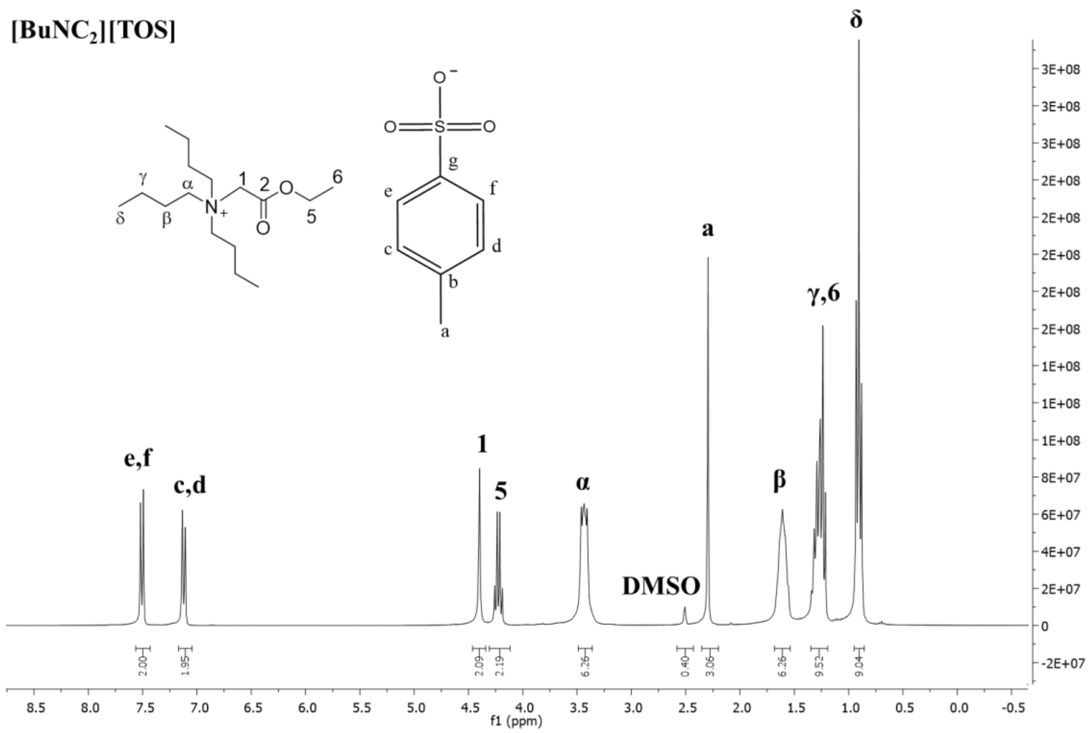

Figure S9. ^{1}H NMR spectrum of [BuNC$_2$][Tos].

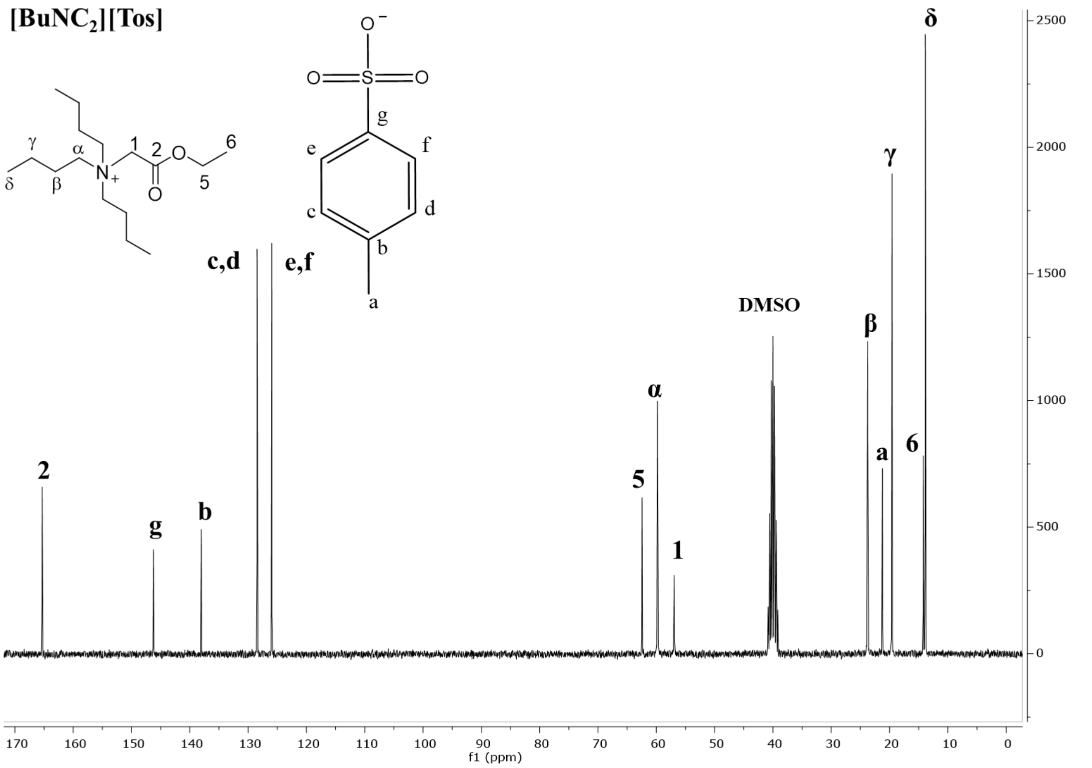

Figure S10. ^{13}C NMR spectrum of [BuNC$_2$][Tos].

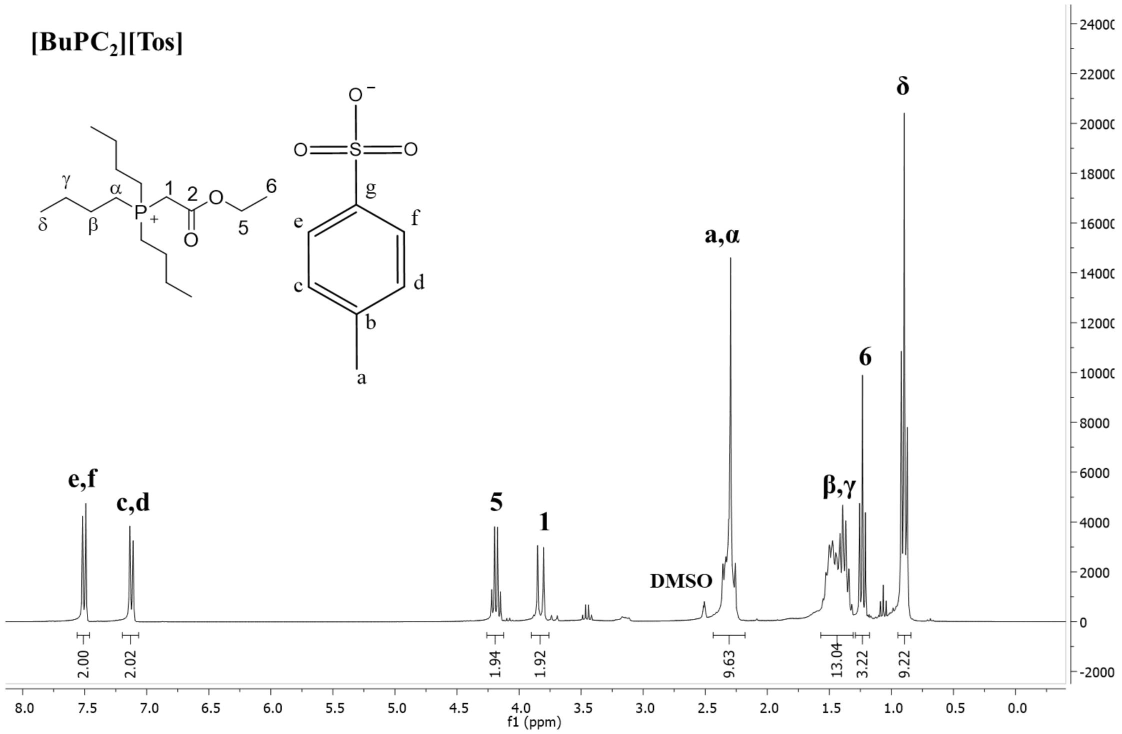

Figure S11. ^{1}H NMR spectrum of $[BuPC_2][Tos]$.

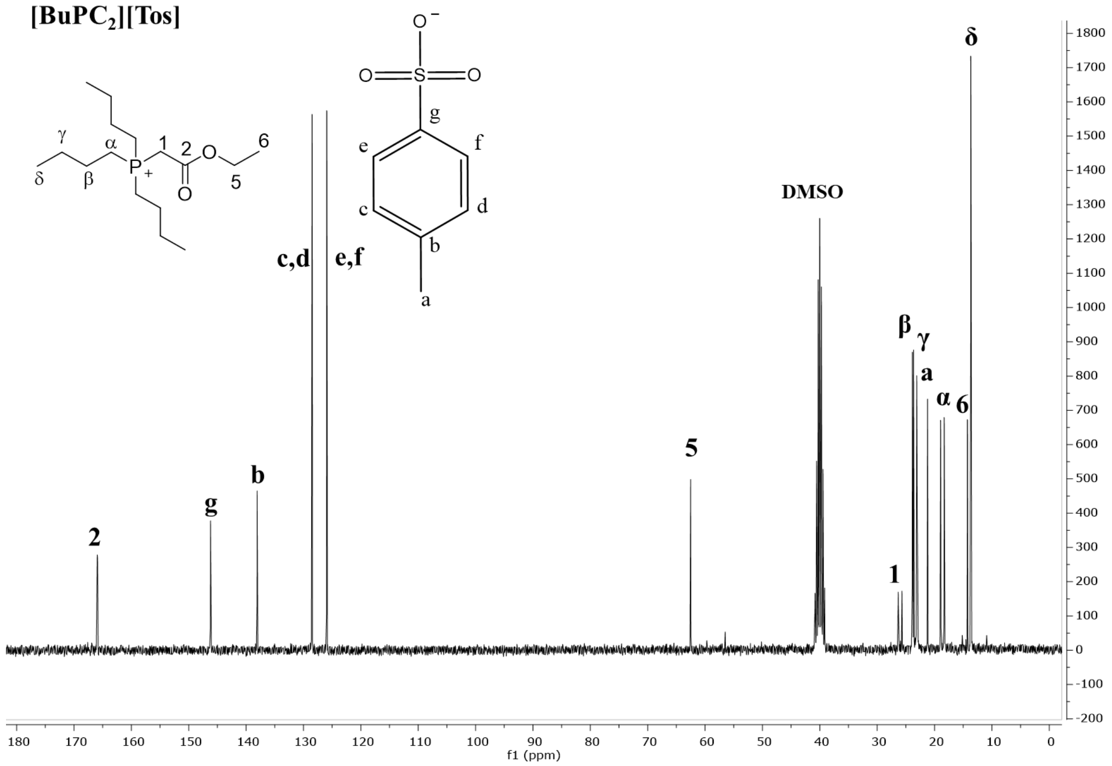

Figure S12. ^{13}C NMR spectrum of $[BuPC_2][Tos]$.

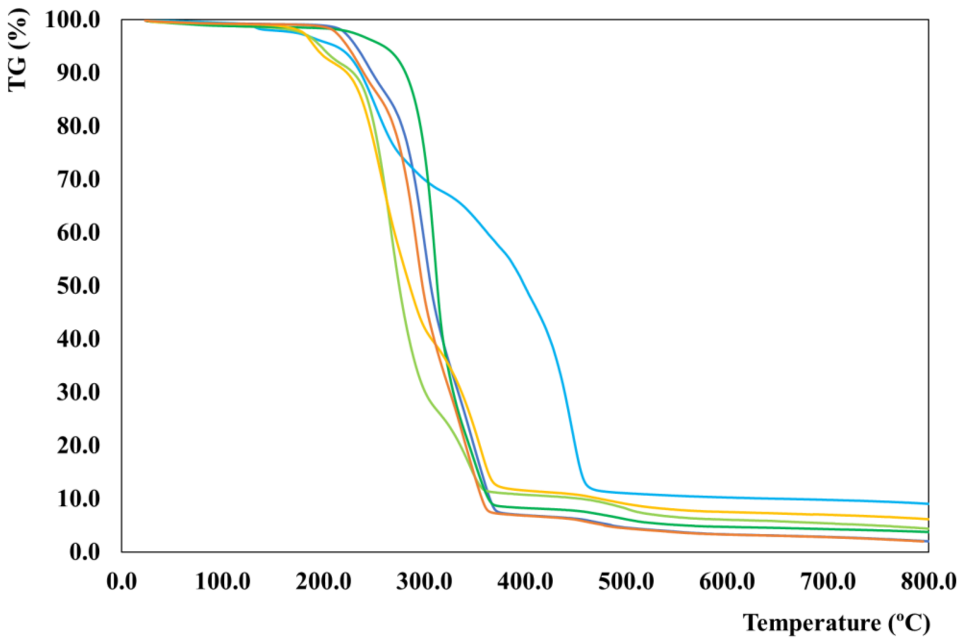

Figure S13. TGA profiles of AGB-ILs: (—) $[EtNC_2][Tos]$; (—) $[EtNC_4][Tos]$; (—) $[PrNC_2][Tos]$; (—) $[PrNC_4][Tos]$; (—) $[BuNC_2][Tos]$; (—) $[BuPC_2][Tos]$.

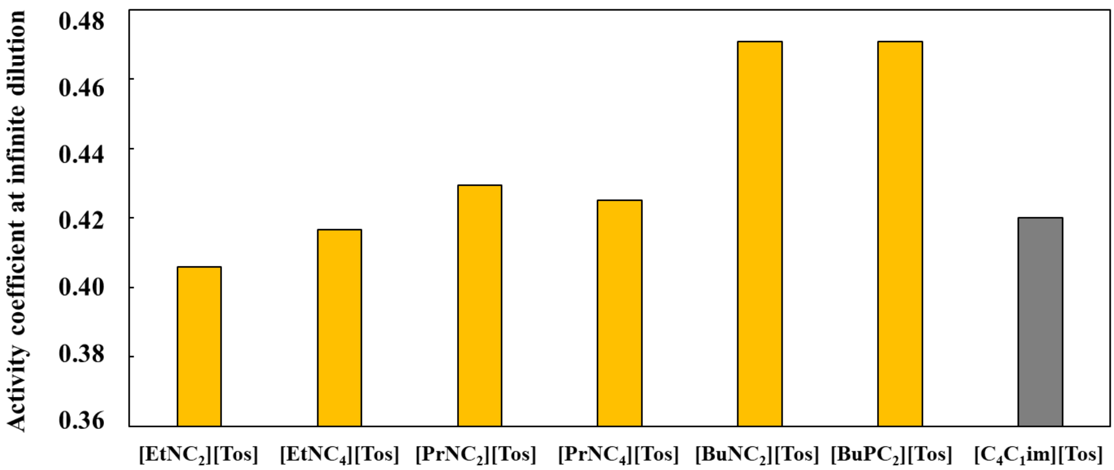

Figure S14. Activity coefficients at infinite dilution (γ^{∞}) of water at 25 °C.

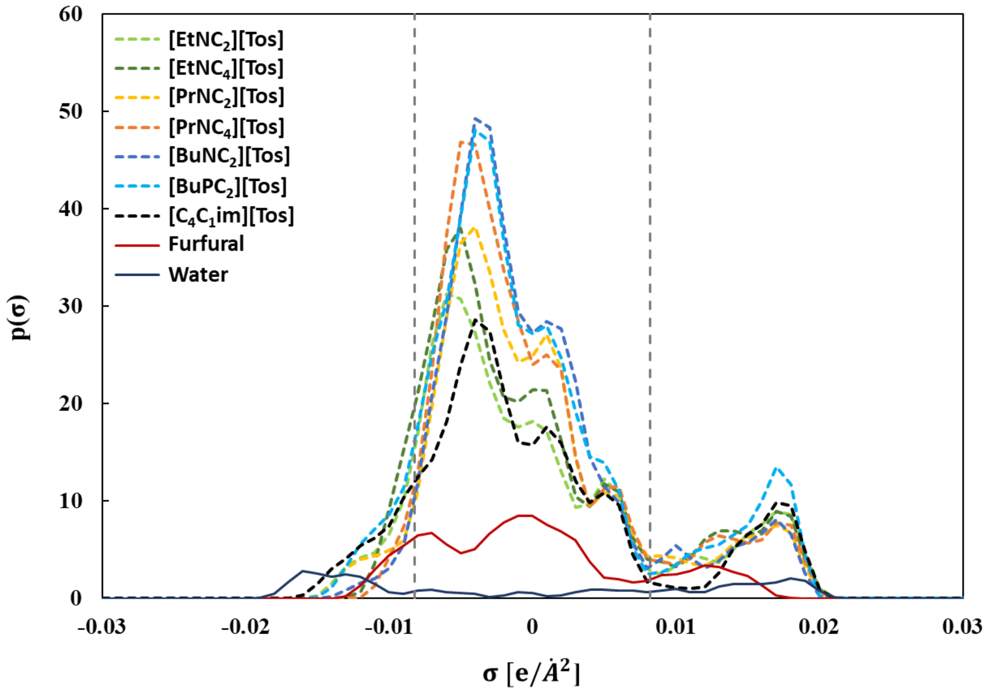

Figure S15. σ-profiles of water, furfural and the studied ILs.

The liquid-liquid phase diagrams were obtained by applying the cloud point titration method at atmospheric pressure and room temperature (25 °C). The quantification of all components added to the system (± 10^{-4} g) was carried out, allowing to obtain the corresponding system compositions and binodal curves. The experimental data corresponding to the binodal curves were correlated using Equation (ES1):

$$[IL] = A\,exp[(B\,[salt^{0.5}]) - (C\,[salt^{3}])] \qquad \text{(ES1)}$$

where [IL] and [salt] correspond to the IL and salt weight percentages, respectively, and the constants A, B and C are constants and are determined by the regression analysis of the experimental data.

Table S1. Experimental data for the binodal weight fraction for the system composed of $[EtNC_2][Tos]$ (1) + $C_6H_5K_3O_7.H_20$ (2) + H_20 (3) at 25ºC and atmospheric pressure (0.1 MPa)[a].

[EtNC2][Tos]								
100 w_1	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**
68.06	6.21	25.72	29.54	18.39	52.07	15.04	26.72	58.24
58.34	8.93	32.73	28.49	18.79	52.73	14.65	27.04	58.31
54.29	10.10	35.62	27.41	19.33	53.25	14.01	27.61	58.38
52.28	10.71	37.02	24.43	21.32	54.25	13.63	27.99	58.38
49.00	11.50	39.50	20.71	22.70	56.59	13.25	28.35	58.40
46.78	12.18	41.04	20.04	23.38	56.58	13.08	28.52	58.39
43.23	13.40	43.36	19.32	23.74	56.95	12.75	28.88	58.37
41.09	14.06	44.86	18.68	24.13	57.20	12.34	29.31	58.36
39.47	14.58	45.94	18.18	24.53	57.28	11.82	29.61	58.57
37.60	15.08	47.32	18.01	24.53	57.46	11.36	30.08	58.56
35.66	16.25	48.09	17.04	25.35	57.61	11.04	30.44	58.52
33.41	16.84	49.75	16.72	25.43	57.85	10.54	30.99	58.47
32.31	17.10	50.59	15.91	25.85	58.25			
30.46	18.13	51.41	15.34	26.39	58.27			

[a] The standard uncertainty for the weight fraction $u(100\ w)$ is 0.01, the standard uncertainty for the temperature $u(T)$ is 1 ºC, and the standard uncertainty for pressure $u(P)$ is 10 kPa.

Table S2. Experimental data for the binodal weight fraction for the system composed of [$EtNC_4$][Tos] (1) + $C_6H_5K_3O_7.H_20$ (2) + H_20 (3) at 25ºC and atmospheric pressure (0.1 MPa)[a].

[$EtNC_4$][Tos]								
100 w_1	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**
73.16	3.27	23.57	18.80	20.34	60.86	10.01	26.05	63.95
69.67	3.51	26.82	18.14	20.89	60.97	9.82	26.28	63.90
57.35	5.36	37.29	17.77	21.04	61.19	9.67	26.35	63.98
52.81	6.81	40.37	17.31	21.31	61.38	9.46	26.57	63.97
50.16	7.50	42.34	16.96	21.49	61.56	9.22	26.76	64.03
47.61	8.51	43.87	16.65	21.60	61.75	8.93	27.07	63.99
44.47	9.31	46.22	16.27	21.76	61.97	8.61	27.18	64.21
44.72	8.93	46.35	15.90	22.00	62.11	8.00	27.29	64.71
40.35	10.29	49.37	15.37	22.48	62.15	7.95	27.90	64.15
38.12	11.34	50.54	15.05	22.62	62.32	7.71	28.18	64.11
35.76	12.58	51.65	14.74	22.76	62.49	7.47	28.47	64.06
34.24	13.10	52.66	14.39	23.01	62.59	7.22	28.79	63.99
32.34	14.29	53.37	14.09	23.17	62.74	7.03	29.01	63.96
29.83	15.54	54.63	13.81	23.35	62.84	6.69	29.44	63.87
29.35	16.02	54.63	13.57	23.50	62.93	6.42	29.83	63.75
27.49	15.95	56.56	13.24	23.79	62.97	6.19	30.11	63.70
26.49	16.53	56.98	13.03	23.85	63.12	5.92	30.46	63.62
25.77	16.81	57.42	12.71	24.13	63.16	5.73	30.75	63.51
24.95	17.25	57.81	12.52	24.16	63.32	5.59	30.90	63.51
24.29	17.56	58.15	12.15	24.48	63.37	5.43	31.12	63.45
23.52	17.93	58.55	11.87	24.71	63.42	5.22	31.41	63.37
22.73	18.44	58.83	11.69	24.82	63.49	4.80	32.33	62.87
21.95	19.05	59.00	11.52	24.91	63.56	4.73	32.17	63.10
21.35	19.03	59.62	11.13	25.21	63.66	4.59	32.50	62.90
20.74	19.40	59.86	10.85	25.40	63.75	4.42	32.99	62.59
20.31	19.57	60.12	10.64	25.59	63.76	3.93	33.83	62.24
19.65	20.01	60.34	10.48	25.68	63.84			
19.15	20.32	60.53	10.33	25.81	63.85			

[a] The standard uncertainty for the weight fraction $u(100\ w)$ is 0.01, the standard uncertainty for the temperature $u(T)$ is 1 ºC, and the standard uncertainty for pressure $u(P)$ is 10 kPa.

Table S3. Experimental data for the binodal weight fraction for the system composed of [$PrNC_2$][Tos] (1) + $C_6H_5K_3O_7.H_20$ (2) + H_20 (3) at 25ºC and atmospheric pressure (0.1 MPa)[a].

[$PrNC_2$][Tos]								
100 w_1	100 w_2	100 w_3	100 w_1	100 w_2	100 w_3	100 w_1	100 w_2	100 w_3
78.75	0.58	20.67	25.60	15.26	59.14	12.23	24.49	63.28
71.36	1.01	27.63	24.88	15.40	59.72	11.82	24.81	63.37
57.17	2.72	40.11	23.60	16.42	59.98	11.65	24.90	63.45
54.59	3.30	42.11	21.41	17.62	60.97	11.40	25.16	63.44
52.39	4.03	43.58	21.02	17.66	61.32	11.01	25.87	63.13
50.41	4.35	45.24	20.58	17.87	61.56	10.89	25.98	63.13
48.66	4.86	46.48	20.21	17.98	61.81	10.74	26.07	63.19
47.08	5.20	47.72	19.40	18.77	61.83	10.53	26.18	63.29
45.32	5.74	48.94	18.68	19.42	61.90	10.39	26.22	63.39
43.90	6.27	49.83	18.27	19.64	62.09	10.24	26.30	63.46
42.20	7.04	50.76	17.97	19.72	62.32	9.98	26.59	63.43
40.86	7.38	51.76	17.69	19.78	62.53	9.82	26.70	63.48
39.69	7.74	52.56	17.27	20.06	62.68	9.60	26.74	63.66
38.15	8.61	53.23	16.36	21.23	62.41	9.42	26.87	63.71
36.94	9.01	54.05	16.12	21.22	62.66	9.22	27.08	63.70
35.71	9.58	54.70	15.75	21.45	62.80	9.10	27.32	63.58
34.49	10.17	55.34	15.53	21.46	63.01	8.94	27.38	63.69
33.36	10.70	55.94	15.18	21.71	63.11	8.78	27.45	63.77
32.44	11.10	56.46	14.99	21.70	63.31	8.65	27.48	63.87
31.63	11.31	57.05	14.64	21.99	63.36	7.56	29.58	62.86
30.50	12.00	57.49	14.21	22.45	63.34			
29.77	12.18	58.05	13.42	23.61	62.97			
28.89	12.61	58.50	12.90	24.18	62.92			
27.87	13.23	58.90	12.71	24.28	63.00			
26.18	14.67	59.15	12.48	24.44	63.08			

[a] The standard uncertainty for the weight fraction *u*(100 *w*) is 0.01, the standard uncertainty for the temperature *u*(*T*) is 1 ºC, and the standard uncertainty for pressure *u*(*P*) is 10 kPa.

Table S4. Experimental data for the binodal weight fraction for the system composed of [$PrNC_4$][Tos] (1) + $C_6H_5K_3O_7.H_20$ (2) + H_20 (3) at 25ºC and atmospheric pressure (0.1 MPa)[a].

[$PrNC_4$][Tos]								
100 w_1	100 w_2	100 w_3	100 w_1	100 w_2	100 w_3	100 w_1	100 w_2	100 w_3
78.17	0.05	21.77	25.12	18.64	56.25	10.22	30.28	59.50
71.28	0.87	27.85	23.27	19.88	56.86	9.98	30.29	59.74
60.11	3.46	36.43	21.41	20.99	57.60	9.51	30.61	59.88
53.11	5.75	41.13	20.53	21.22	58.25	9.07	31.01	59.91
48.85	7.11	44.04	20.01	21.53	58.46	8.84	31.46	59.70
46.09	8.25	45.67	19.62	21.78	58.60	8.49	31.95	59.56
44.04	9.50	46.45	18.85	22.45	58.70	8.22	32.06	59.73
41.86	10.73	47.42	16.75	24.76	58.48	7.82	32.48	59.70
40.04	11.47	48.49	16.35	24.95	58.70	7.41	32.96	59.63
36.81	12.86	50.33	15.97	25.28	58.75	6.70	34.26	59.04
34.54	13.61	51.85	15.48	25.68	58.85	6.54	34.25	59.20
33.29	14.30	52.41	14.90	25.78	59.31	6.37	34.31	59.32
32.29	14.83	52.88	14.25	26.27	59.48	6.25	34.44	59.31
29.77	16.21	54.02	13.71	26.82	59.47			
28.89	16.52	54.59	13.54	26.81	59.66			
27.75	17.34	54.90	13.29	26.85	59.86			
26.78	17.82	55.40	12.51	27.88	59.61			
26.09	18.00	55.92	10.40	29.97	59.63			

[a] The standard uncertainty for the weight fraction $u(100\ w)$ is 0.01, the standard uncertainty for the temperature $u(T)$ is 1 ºC, and the standard uncertainty for pressure $u(P)$ is 10 kPa.

Table S5. Experimental data for the binodal weight fraction for the system composed of $[BuPC_2][Tos]$ (1) + $C_6H_5K_3O_7.H_20$ (2) + H_20 (3) at 25ºC and atmospheric pressure (0.1 MPa)[a].

[BuPC2][Tos]								
100 w_1	100 w_2	100 w_3	100 w_1	100 w_2	100 w_3	100 w_1	100 w_2	100 w_3
79.73	0.33	19.95	13.94	11.75	74.31	6.81	20.67	72.52
54.13	1.38	44.49	13.43	12.12	74.44	6.69	21.14	72.18
51.56	1.64	46.80	12.82	12.98	74.20	6.60	21.42	71.98
47.23	1.99	50.79	12.27	13.38	74.36	6.50	21.62	71.88
44.08	2.59	53.32	11.73	14.21	74.06	6.35	21.87	71.77
39.03	3.22	57.75	11.47	14.40	74.12	6.25	21.98	71.76
36.08	3.84	60.09	11.16	14.86	73.98	6.19	22.00	71.82
33.48	4.54	61.97	10.93	14.96	74.11	6.05	22.21	71.73
31.10	5.16	63.74	10.80	15.16	74.03	5.59	24.20	70.22
28.73	5.43	65.84	10.48	15.78	73.74	5.51	24.09	70.40
27.55	5.74	66.71	10.24	16.03	73.73	5.43	24.11	70.47
26.12	6.22	67.66	9.89	16.56	73.55	5.34	24.19	70.47
24.18	6.89	68.93	9.74	16.47	73.78	5.26	24.47	70.28
22.73	7.48	69.79	9.65	17.00	73.34	5.20	24.55	70.26
21.62	7.66	70.73	9.27	16.91	73.82	5.13	24.58	70.30
20.49	8.11	71.40	9.06	17.21	73.73	4.99	25.20	69.81
19.36	8.72	71.91	8.85	17.21	73.94	4.88	25.61	69.50
18.51	9.30	72.19	8.52	17.53	73.95	4.81	25.73	69.46
17.85	9.43	72.72	8.29	18.36	73.35	4.73	25.80	69.47
17.20	9.60	73.21	8.15	18.50	73.35	4.64	26.14	69.22
16.66	9.97	73.37	7.93	18.85	73.22			
16.24	10.39	73.37	7.77	18.89	73.35			
15.64	10.76	73.60	7.56	19.09	73.35			
15.08	11.03	73.89	7.32	19.49	73.19			
14.51	11.54	73.95	7.07	20.21	72.71			

[a] The standard uncertainty for the weight fraction *u*(100 *w*) is 0.01, the standard uncertainty for the temperature *u*(*T*) is 1 ºC, and the standard uncertainty for pressure *u*(*P*) is 10 kPa.

Table S6. Experimental data for the binodal weight fraction for the system composed of $[BuNC_2][Tos]$ (1) + $C_6H_5K_3O_7.H_20$ (2) + H_20 (3) at 25ºC and atmospheric pressure (0.1 MPa)[a].

[BuNC₂][Tos]								
100 w_1	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**
77.31	1.50	21.19	16.70	11.58	71.72	9.00	19.12	71.88
56.64	1.89	41.47	15.97	12.03	71.99	8.73	19.49	71.78
50.47	2.10	47.44	15.11	13.05	71.84	8.54	19.51	71.95
46.29	2.40	51.31	14.34	13.51	72.15	8.29	19.72	71.99
43.26	2.97	53.77	13.61	14.46	71.92	8.08	19.83	72.09
38.37	3.54	58.09	13.27	14.68	72.05	7.71	20.38	71.91
35.50	4.12	60.38	12.78	15.36	71.85	7.39	20.85	71.76
32.49	5.46	62.05	12.56	15.48	71.96	7.24	21.35	71.41
27.17	6.95	65.88	12.38	15.69	71.94	7.14	21.65	71.21
25.94	7.49	66.57	11.97	16.32	71.71	7.03	21.86	71.11
24.40	8.00	67.60	11.66	16.52	71.82	6.86	22.13	71.01
22.35	8.60	69.05	11.19	17.08	71.74	6.74	22.25	71.02
21.57	9.08	69.36	10.86	17.39	71.76	6.66	22.25	71.08
20.84	9.48	69.68	10.36	17.43	72.21	6.50	22.48	71.01
20.18	9.89	69.93	10.05	18.07	71.88	5.97	24.57	69.46
19.21	10.34	70.45	9.81	18.37	71.82			
18.37	10.69	70.94	9.46	18.78	71.76			
17.53	11.32	71.15	9.17	19.09	71.73			

[a] The standard uncertainty for the weight fraction $u(100\ w)$ is 0.01, the standard uncertainty for the temperature $u(T)$ is 1 ºC, and the standard uncertainty for pressure $u(P)$ is 10 kPa.

Table S7. Experimental data for the binodal weight fraction for the system composed of $[C_4C_1im][Tos]$ (1) + $C_6H_5K_3O_7.H_20$ (2) + H_20 (3) at 25ºC and atmospheric pressure (0.1 MPa)[a].

$[C_4C_1im][Tos]$								
100 w_1	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**	**100 w_1**	**100 w_2**	**100 w_3**
75.05	2.11	22.84	19.81	19.90	60.29	9.15	27.15	63.70
70.89	2.55	26.56	19.32	20.13	60.55	8.75	27.56	63.70
65.57	3.16	31.28	18.35	20.80	60.85	8.35	27.99	63.66
62.65	3.72	33.63	17.56	21.16	61.28	8.04	28.25	63.71
55.46	5.47	39.07	16.49	21.86	61.65	7.72	28.62	63.66
50.54	7.02	42.43	16.07	22.11	61.82	7.54	28.81	63.65
46.37	8.29	45.34	15.28	22.61	62.11	7.30	29.11	63.59
44.25	8.58	47.17	14.84	22.78	62.38	6.97	29.50	63.53
42.08	9.58	48.34	14.31	23.16	62.53	6.78	29.92	63.30
39.84	10.42	49.74	14.05	23.29	62.66	6.61	30.11	63.28
36.97	11.67	51.36	13.68	23.64	62.68	6.37	30.44	63.19
35.54	12.43	52.03	13.24	23.88	62.87	5.88	31.08	63.05
33.40	13.01	53.59	12.86	24.22	62.93	5.72	31.32	62.96
31.61	14.25	54.14	12.17	24.64	63.18	5.46	31.70	62.84
29.99	14.90	55.11	11.82	24.89	63.29	5.17	32.14	62.68
28.48	15.50	56.02	11.55	25.09	63.36	5.02	32.39	62.59
26.66	16.47	56.87	11.06	25.46	63.48	4.82	32.76	62.42
25.18	17.18	57.64	10.76	25.66	63.58	4.73	32.90	62.37
23.96	17.77	58.27	10.57	25.84	63.59	4.60	33.18	62.22
22.39	18.56	59.05	10.14	26.21	63.64	4.20	33.94	61.86
21.79	18.81	59.40	9.63	26.65	63.73	4.05	34.22	61.72
20.82	19.43	59.74	9.38	26.90	63.73	3.45	35.56	60.99

[a] The standard uncertainty for the weight fraction $u(100\ w)$ is 0.01, the standard uncertainty for the temperature $u(T)$ is 1 ºC, and the standard uncertainty for pressure $u(P)$ is 10 kPa.

Table S8. Correlation parameters of Equation (S1) used to describe the experimental binodal data at 25 °C and atmospheric pressure (0.1 MPa).[a]

AGB-ILs	***A*** **±** ***σ***	***B*** **±** ***σ***	$\mathbf{10^{-5}\,(\mathit{C} \pm \sigma)}$	$\boldsymbol{R^2}$
$[EtNC_2]$[Tos]	178.96 ± 13.23	-0.381 ± 0.023	2.697 ± 0.309	0.9938
$[EtNC_4]$[Tos]	112.25 ± 3.96	-0.302 ± 0.013	4.938 ± 0.261	0.9939
$[BuNC_2]$[Tos]	121.24 ± 7.92	-0.585 ± 0.034	1.427 ± 1.262	0.9657
$[BuPC_2]$[Tos]	108.81 ± 3.98	-0.590 ± 0.020	0.935 ± 0.882	0.9797
$[PrNC_2]$[Tos]	87.51 ± 2.05	-0.283 ± 0.009	4.027 ± 0.282	0.9925
$[PrNC_4]$[Tos]	79.81 ± 1.89	-0.201 ± 0.009	3.803 ± 0.233	0.9916
$[C_4C_1im]$[Tos]	52.13 ± 0.51	-0.214 ± 0.003	4.290 ± 0.250	0.9985

[a] The standard uncertainty for the temperature $u(T)$ is 1 ºC, and the standard uncertainty for pressure $u(P)$ is 10 kPa.