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Supporting Information

Liquid-Liquid Equilibria of Ionic Liquids-Water-Acetic Acid Mixtures

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Table S1. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + MTBE) at 293.15 K and 313.15 K and at 101 kPa. The mole fractions of water, acetic acid and MTBE are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			MTBE-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
$T = 293.15 \text{ K}$								
0.9890	0.0000	0.0110	0.0566	0.0000	0.9434	-	-	-
0.9739	0.0150	0.0111	0.1146	0.0643	0.8211	1.06	4.29	36.43
0.9397	0.0474	0.0129	0.2032	0.1532	0.6436	0.97	3.23	14.95
0.9246	0.0601	0.0153	0.3094	0.2041	0.4865	1.21	3.40	10.15
0.9077	0.0748	0.0175	0.3852	0.2151	0.3997	1.17	2.88	6.78
0.8943	0.0871	0.0186	0.4252	0.2181	0.3567	1.10	2.50	5.27
0.8864	0.0917	0.0219	0.4587	0.2180	0.3233	1.12	2.38	4.59
0.8798	0.0970	0.0232	0.4985	0.2177	0.2838	1.13	2.24	3.96
0.8398	0.1256	0.0346	0.5396	0.2195	0.2409	1.02	1.75	2.72
0.8280	0.1329	0.0391	0.5639	0.2200	0.2161	1.03	1.66	2.43
$T = 313.15 \text{ K}$								
0.9931	0.0000	0.0069	0.0466	0.0000	0.9534	-	-	-
0.9850	0.0075	0.0075	0.0674	0.0305	0.9021	0.93	4.07	59.43
0.9530	0.0394	0.0076	0.2098	0.1404	0.6498	1.04	3.56	16.19
0.9518	0.0397	0.0085	0.1794	0.1330	0.6876	0.95	3.35	17.77
0.9260	0.0582	0.0158	0.3071	0.1880	0.5049	1.14	3.23	9.74
0.8966	0.0845	0.0189	0.4786	0.2334	0.2880	1.32	2.76	5.17
0.8586	0.1121	0.0293	0.5652	0.2408	0.1940	1.28	2.15	3.26
0.8267	0.1331	0.0402	0.6127	0.2351	0.1522	1.21	1.77	2.38

$u(x_i) = 0.01$; $u(T) = 0.5 \text{ K}$; $u(p) = 2 \text{ kPa}$.

Table S2. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + MIBK) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and MIBK are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			MIBK-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
$T = 293.15$ K								
1.0000	0.0000	0.0000	0.0991	0.0000	0.9009	-	-	-
0.9697	0.0267	0.0036	0.1667	0.0758	0.7575	0.66	2.84	16.51
0.9630	0.0330	0.0040	0.2081	0.1208	0.6711	0.92	3.66	16.94
0.9361	0.0560	0.0079	0.2973	0.1622	0.5405	0.88	2.90	9.12
0.9138	0.0777	0.0085	0.3680	0.1991	0.4329	0.91	2.56	6.36
0.9072	0.0839	0.0089	0.4151	0.2075	0.3774	0.95	2.47	5.41
0.8921	0.0950	0.0129	0.4516	0.2258	0.3226	1.02	2.38	4.70
0.8877	0.0996	0.0127	0.4813	0.2305	0.2882	1.05	2.31	4.27
0.8618	0.1200	0.0182	0.5226	0.2261	0.2513	0.96	1.88	3.11
0.8560	0.1320	0.0120	0.5727	0.2238	0.2035	0.94	1.70	2.53
0.7800	0.1650	0.0550	0.6936	0.1908	0.1156	0.96	1.16	1.30

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S3. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [P_{666 14}]Cl) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [P_{666 14}]Cl are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
1.000	0.000	0.000	0.826	0.000	0.174	-	-	-
0.998	0.002	0.000	0.497	0.112	0.391	4.64	56.00	112.45
0.998	0.002	0.000	0.499	0.046	0.455	1.68	23.00	46.00
0.995	0.005	0.000	0.496	0.080	0.424	1.25	16.00	32.10
0.992	0.008	0.000	0.499	0.073	0.428	0.71	9.13	18.14
0.984	0.016	0.000	0.471	0.277	0.252	2.07	17.31	36.17
0.980	0.020	0.000	0.490	0.235	0.275	1.34	11.75	23.50
0.920	0.080	0.000	0.498	0.377	0.125	1.04	4.71	8.71
0.883	0.117	0.000	0.470	0.345	0.185	0.54	2.95	5.54
0.833	0.167	0.000	0.481	0.384	0.135	0.57	2.30	3.98
0.833	0.167	0.000	0.530	0.360	0.110	0.61	2.16	3.39
0.824	0.176	0.000	0.521	0.385	0.094	0.68	2.19	3.46
0.820	0.180	0.000	0.510	0.394	0.096	0.68	2.19	3.52
0.811	0.189	0.000	0.527	0.390	0.083	0.70	2.06	3.18
0.806	0.194	0.000	0.519	0.391	0.090	0.66	2.02	3.13
0.789	0.211	0.000	0.494	0.395	0.111	0.56	1.87	2.99
0.773	0.227	0.000	0.509	0.411	0.080	0.66	1.81	2.75
0.758	0.241	0.001	0.502	0.410	0.088	0.61	1.70	2.57
0.749	0.250	0.001	0.540	0.388	0.072	0.64	1.55	2.15
0.728	0.272	0.000	0.520	0.413	0.067	0.65	1.52	2.13
0.714	0.286	0.000	0.525	0.420	0.055	0.70	1.47	2.00
0.698	0.302	0.000	0.544	0.399	0.057	0.64	1.32	1.70

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

In the case of the (water + [P_{666,14}]Cl) binary system, a formation of an emulsion within the addition of water to this phosphonium-based ionic liquid was observed. This observation is in agreement with that already reported into the literature.^{1,2}

Table S4. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [P_{666,14}][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [P_{666,14}][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
1.000	0.000	0.000	0.127	0.000	0.873	-	-	-
0.958	0.042	0.000	0.298	0.070	0.632	0.07	1.67	5.36
0.943	0.057	0.000	0.309	0.081	0.610	0.06	1.42	4.34
0.902	0.098	0.000	0.354	0.118	0.528	0.06	1.20	3.07
0.892	0.108	0.000	0.355	0.121	0.524	0.06	1.12	2.82
0.867	0.133	0.000	0.420	0.147	0.433	0.08	1.11	2.28

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

In the case of the (water + [P_{666,14}][NTf₂]) binary system, a formation of an emulsion within the addition of water to this phosphonium-based ionic liquid was observed. This observation is in agreement with that already reported into the literature in the case of the [P_{666 14}][Cl].^{1,2}

Table S5. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [C₂mim][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [C₂mim][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
0.9995	0.0000	0.0005	0.2954	0.0000	0.7046	-	-	-
0.9836	0.0139	0.0025	0.2342	0.0285	0.7373	0.14	2.05	8.61
0.9758	0.0217	0.0025	0.2164	0.0478	0.7358	0.15	2.20	9.93
0.9439	0.0538	0.0023	0.2952	0.1253	0.5795	0.21	2.33	7.45
0.9400	0.0577	0.0023	0.2965	0.1358	0.5677	0.21	2.35	7.46
0.9368	0.0606	0.0026	0.3072	0.1407	0.5521	0.22	2.32	7.08
0.9251	0.0720	0.0029	0.3685	0.1545	0.4770	0.23	2.15	5.39
0.9075	0.0892	0.0033	0.3957	0.1920	0.4123	0.28	2.15	4.94
0.8697	0.1249	0.0054	0.4827	0.2282	0.2891	0.34	1.83	3.29
0.8569	0.1363	0.0068	0.5133	0.2355	0.2512	0.37	1.73	2.88

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S6. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [C₄mim][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [C₄mim][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
0.9995	0.0000	0.0005	0.2400	0.0000	0.7600	-	-	-
0.9945	0.0049	0.0006	0.2478	0.0178	0.7344	0.21	3.63	14.58
0.9835	0.0160	0.0005	0.2614	0.0414	0.6972	0.16	2.59	9.74
0.9690	0.0303	0.0007	0.3001	0.0700	0.6299	0.17	2.31	7.46
0.9301	0.0685	0.0014	0.3499	0.1200	0.5301	0.16	1.75	4.66
0.9086	0.0909	0.0005	0.4131	0.1697	0.4172	0.21	1.87	4.11
0.9014	0.0964	0.0022	0.4223	0.1756	0.4021	0.22	1.82	3.89
0.9013	0.0961	0.0026	0.4144	0.1713	0.4143	0.22	1.78	3.88
0.9009	0.0961	0.0030	0.4091	0.1777	0.4132	0.22	1.85	4.07
0.8793	0.1172	0.0035	0.4337	0.2048	0.3615	0.25	1.75	3.54
0.8694	0.1275	0.0031	0.4627	0.2267	0.3106	0.29	1.78	3.34
0.8582	0.1373	0.0045	0.4688	0.2247	0.3065	0.28	1.64	3.00
0.8090	0.1840	0.0070	0.5090	0.2370	0.2540	0.28	1.29	2.05

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S7. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [C₄mmim][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [C₄mmim][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
0.9996	0.0000	0.0004	0.1735	0.0000	0.8265	-	-	-
0.9984	0.0012	0.0004	0.1764	0.0073	0.8163	0.31	6.08	34.43
0.9813	0.0183	0.0004	0.2096	0.0419	0.7485	0.13	2.29	10.72
0.9635	0.0361	0.0004	0.2209	0.0665	0.7126	0.11	1.84	8.03
0.9539	0.0455	0.0006	0.2476	0.0828	0.6696	0.12	1.82	7.02
0.9290	0.0705	0.0005	0.2802	0.1143	0.6055	0.13	1.62	5.38
0.9085	0.0909	0.0006	0.331	0.1517	0.5173	0.15	1.67	4.58
0.8970	0.1017	0.0013	0.354	0.1801	0.4659	0.18	1.77	4.49
0.8603	0.1376	0.0021	0.4129	0.2217	0.3654	0.22	1.61	3.36
0.8263	0.1707	0.0030	0.4584	0.2472	0.2944	0.25	1.45	2.61

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S8. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [C₆mim][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [C₆mim][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
0.9998	0.0000	0.0002	0.1968	0.0000	0.8032	-	-	-
0.9941	0.0057	0.0002	0.2129	0.0329	0.7542	0.31	5.77	26.95
0.9753	0.0244	0.0003	0.2410	0.0655	0.6935	0.16	2.68	10.86
0.9706	0.0290	0.0004	0.2513	0.0805	0.6682	0.17	2.78	10.72
0.9453	0.0538	0.0009	0.2607	0.1111	0.6282	0.15	2.07	7.49
0.9392	0.0600	0.0008	0.2743	0.1207	0.6050	0.15	2.01	6.89
0.9193	0.0799	0.0008	0.2978	0.1506	0.5516	0.16	1.88	5.82
0.9090	0.0901	0.0009	0.3350	0.1798	0.4852	0.19	2.00	5.41
0.8993	0.1001	0.0006	0.3538	0.1868	0.4594	0.19	1.87	4.74
0.8882	0.1109	0.0009	0.3629	0.1995	0.4376	0.19	1.80	4.40
0.8713	0.1279	0.0008	0.3855	0.2131	0.4014	0.20	1.67	3.77
0.8444	0.1547	0.0009	0.4200	0.2479	0.3321	0.23	1.60	3.22
0.8401	0.1589	0.0010	0.4401	0.2575	0.3024	0.26	1.62	3.09
0.8268	0.1716	0.0016	0.4460	0.2699	0.2841	0.27	1.57	2.92
0.8157	0.1824	0.0019	0.4579	0.2750	0.2671	0.28	1.51	2.69
0.7806	0.2173	0.0021	0.5102	0.2801	0.2097	0.30	1.29	1.97

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S9. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [C₈mim][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [C₈mim][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
0.9996	0.0000	0.0004	0.1759	0.0000	0.8241	-	-	-
0.9921	0.0075	0.0004	0.1859	0.0335	0.7806	0.22	4.47	23.84
0.9872	0.0124	0.0004	0.1913	0.0432	0.7655	0.18	3.48	17.98
0.9715	0.0281	0.0004	0.2247	0.0964	0.6789	0.20	3.43	14.83
0.9543	0.0453	0.0004	0.2587	0.1456	0.5957	0.22	3.21	11.86
0.9194	0.0797	0.0009	0.3341	0.2153	0.4506	0.25	2.70	7.43
0.8619	0.1375	0.0006	0.3914	0.2637	0.3449	0.25	1.92	4.22
0.8525	0.1470	0.0005	0.3940	0.2643	0.3417	0.24	1.80	3.89
0.8490	0.1501	0.0009	0.3973	0.2691	0.3336	0.24	1.79	3.83
0.8051	0.1932	0.0017	0.4573	0.2951	0.2476	0.29	1.53	2.69

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S10. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [C₁₀mim][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [C₁₀mim][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
0.9998	0.0000	0.0002	0.1526	0.0000	0.8474	-	-	-
0.9934	0.0064	0.0002	0.1592	0.0353	0.8055	0.25	5.52	34.42
0.9823	0.0175	0.0002	0.1976	0.0872	0.7152	0.25	4.98	24.77
0.9622	0.0375	0.0003	0.2115	0.1017	0.6868	0.15	2.71	12.34
0.9004	0.0993	0.0003	0.2367	0.1825	0.5808	0.13	1.84	6.99
0.8567	0.1430	0.0003	0.3001	0.2414	0.4585	0.16	1.69	4.82
0.8177	0.1820	0.0003	0.3718	0.2917	0.3365	0.21	1.60	3.52
0.7979	0.2018	0.0003	0.3953	0.3063	0.2984	0.23	1.52	3.06
0.7345	0.2652	0.0003	0.4502	0.3209	0.2289	0.25	1.21	1.97

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S11. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [C₄mpyrr][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [C₄mpyrr][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
1.0000	0.0000	0.0000	0.2194	0.0000	0.7806	-	-	-
0.9767	0.0233	0.0000	0.1681	0.0609	0.7710	0.15	2.61	15.19
0.9638	0.0362	0.0000	0.1760	0.0810	0.7430	0.14	2.24	12.25
0.9396	0.0604	0.0000	0.2028	0.1248	0.6724	0.14	2.07	9.57
0.9226	0.0771	0.0003	0.2685	0.1500	0.5815	0.16	1.95	6.69
0.9081	0.0916	0.0003	0.2996	0.1650	0.5354	0.16	1.80	5.46
0.8927	0.1066	0.0007	0.3011	0.1948	0.5041	0.18	1.83	5.42
0.8542	0.1444	0.0014	0.3584	0.2350	0.4066	0.21	1.63	3.88
0.8193	0.1777	0.0030	0.3724	0.2769	0.3507	0.24	1.56	3.43

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S12. Composition of the experimental tie-line ends, and values of the solute distribution ratios (β_x and β_w calculated from the mole and mass fractions, respectively) and selectivity (S) for the ternary system (water + acetic acid + [N₁₁₁₄][NTf₂]) at 293.15 K and at 101 kPa. The mole fractions of water, acetic acid and [N₁₁₁₄][NTf₂] are represented by x_1 , x_2 and x_3 , respectively.

Water-rich phase			Ionic Liquid-rich phase			β_w	β_x	S
x_1	x_2	x_3	x_1	x_2	x_3			
1.000	0.000	0.000	0.230	0.000	0.770	-	-	-
0.989	0.011	0.000	0.283	0.042	0.675	0.26	3.82	13.34
0.978	0.022	0.000	0.296	0.046	0.658	0.15	2.09	6.91
0.969	0.031	0.000	0.296	0.061	0.643	0.14	1.97	6.44
0.957	0.043	0.000	0.319	0.078	0.603	0.14	1.81	5.44
0.954	0.046	0.000	0.317	0.085	0.598	0.15	1.85	5.56
0.951	0.049	0.000	0.344	0.092	0.564	0.16	1.88	5.19
0.911	0.089	0.000	0.403	0.145	0.452	0.18	1.63	3.68
0.875	0.125	0.000	0.451	0.199	0.350	0.23	1.59	3.09
0.824	0.176	0.000	0.526	0.245	0.229	0.31	1.39	2.18

$u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa.

Table S13. Relative deviation between experimental water solubility in IL data reported herein with published data expressed in water mole fraction in IL, x_1 at 101 kPa.

IL	This work ^a	x_1 Literature data	Relative Deviation (%)
[P ₆₆₆₁₄][Cl]	0.8261	0.814 ^b [3]	1.49
		0.818 ^c [4]	0.99
		0.829 ^c [5]	-0.35
		0.824 ^c [6]	0.25
[P ₆₆₆₁₄][NTf ₂]	0.1206	0.081 ^b [3]	48.9
		0.088 ^c [4]	37.1
		0.230 ^c [6]	-47.6
[C ₂ mim][NTf ₂]	0.2954	0.2357 ^b [7]	25.3
		0.2869 ^b [8]	2.96
		0.31 ^d [9]	-4.71
		0.2970 ^e [10]	-0.54
		0.3050 ^d [11]	-3.15
[C ₄ mim][NTf ₂]	0.2400	0.2484 ^b [7]	-3.38
		0.2443 ^b [8]	-1.76
		0.27 ^d [9]	-11.1
		0.2431 ^f [10]	-1.28
		0.3210 ^d [11]	-25.2
		0.2931 ^b [12]	-18.1
[C ₄ mmim][NTf ₂]	0.1735	-	
[C ₆ mim][NTf ₂]	0.1968	0.1978 ^b [8]	-0.51
		0.2703 ^b [12]	-27.2
		0.2117 ^g [13]	-7.04
[C ₈ mim][NTf ₂]	0.1759	0.1781 ^b [8]	-1.24
		0.2411 ^b [12]	-27.0
		0.1951 ^g [13]	-9.84
[C ₁₀ mim][NTf ₂]	0.1526	-	
[C ₄ mpyrr][NTf ₂]	0.2194	0.2260 ^h [10]	-2.92
		0.199 ^b [14]	10.3
[N ₁₁₁₄][NTf ₂]	0.2300	0.2043 ⁱ [10]	12.6
		0.2420 ^d [11]	-4.96

^a This work at 293.15 K: $u(x_i) = 0.01$; $u(T) = 0.5$ K; $u(p) = 2$ kPa. ^b at 293.15 K. ^c at 298.15 K.

^d at room temperature. ^e at 292.62 K. ^f at 290.13 K. ^g at 296.65 K. ^h at 290.35 K. ⁱ at 289.15 K.

Figure S1. ^1H -NMR of $[\text{C}_2\text{mim}][\text{NTf}_2]$ in d_6 -DMSO.

Figure S2. ^1H -NMR of $[\text{C}_4\text{mim}][\text{NTf}_2]$ in d_6 -DMSO.

Figure S3. ^1H -NMR of $[\text{C}_4\text{mmim}][\text{NTf}_2]$ in d_6 -DMSO.

Figure S4. ^1H -NMR of $[\text{C}_6\text{mim}][\text{NTf}_2]$ in d_6 -DMSO.

Figure S5. ^1H -NMR of $[\text{C}_8\text{mim}][\text{NTf}_2]$ in CDCl_3 .

Figure S6. ^1H -NMR of $[\text{C}_{10}\text{mim}][\text{NTf}_2]$ in CDCl_3 .

Figure S7. ^1H -NMR of $[\text{C}_4\text{mpyrr}][\text{NTf}_2]$ in d_6 -DMSO.

Figure S8. ^1H -NMR of $[\text{N}_{1114}][\text{NTf}_2]$ in d_6 -DMSO.

Figure S9. ^1H -NMR of $[\text{P}_{66614}][\text{NTf}_2]$ in CDCl_3 .

Figure S10. Equilibrium diagram of the ternary system (water + acetic acid + IL) at 293.15 K and at 101 kPa: ●, [P_{666,14}]Cl; □, [P_{666,14}][NTf₂].

Figure S11. Equilibrium diagram of the ternary system (water + acetic acid + $[C_n\text{mim}][\text{NTf}_2]$) at 293.15 K and at 101 kPa: $\diamond$, $n = 2$; $\bullet$, $n = 4$; $\triangle$, $n = 6$; $\blacksquare$, $n = 8$; ∇ , $n = 10$.

Figure S12. Equilibrium diagram of the ternary system (water + acetic acid + MTBE) at 101 kPa and at: a, 293.15 K; b, 313.15 K; (● and solid lines), experimental data; (○ and dashed lines), predicted using UNIQUAC model with parameters from Miao *et al.*¹⁵

Figure S13. Equilibrium diagram of the ternary system (water + acetic acid + MIBK) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S14. Equilibrium diagram of the ternary system (water + acetic acid + $[P_{666,14}]\text{Cl}$) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S15. Equilibrium diagram of the ternary system (water + acetic acid + $[P_{666,14}][NTf_2]$) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S16. Equilibrium diagram of the ternary system (water + acetic acid + [C₂mim][NTf₂]) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S17. Equilibrium diagram of the ternary system (water + acetic acid + [C₄mim][NTf₂]) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S18. Equilibrium diagram of the ternary system (water + acetic acid + [C₄mim][NTf₂]) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S19. Equilibrium diagram of the ternary system (water + acetic acid + [C₆mim][NTf₂]) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S20. Equilibrium diagram of the ternary system (water + acetic acid + [C₈mim][NTf₂]) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S21. Equilibrium diagram of the ternary system (water + acetic acid + [C₁₀mim][NTf₂]) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S22. Equilibrium diagram of the ternary system (water + acetic acid + [C₄mpyrr][NTf₂]) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S23. Equilibrium diagram of the ternary system (water + acetic acid + $[\text{N}_{1114}][\text{NTf}_2]$) at 293.15 K and at 101 kPa: (● and solid lines), experimental data; (○ and dashed lines), correlated using UNIQUAC model.

Figure S24. Equilibrium diagram of the ternary system (water + acetic acid + [C₄mim][NTf₂]) at 298.15 K and at 101 kPa: (● and solid lines), experimental data from Bharti and Banerjee;¹⁶ (○ and dashed lines), predicted using UNIQUAC model with parameters reported during this work.

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