

Supporting Information

Evaluation of Cation Influence on the Formation and Extraction Capability of Ionic Liquid-Based Aqueous Biphasic Systems

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1,3-dimethylimidazolium chloride synthesis. 1,3-dimethylimidazolium chloride ([C₁im]Cl) has been synthesized by means of Carbonate Based Ionic Liquid Synthesis (CBILS[®]) of proionic / Sigma Aldrich.¹ 1,3-dimethylimidazolium hydrogenocarbonate (the CBIL precursor as a 45.91 % solution in H₂O : Methanol (3:2)) has been treated with an exact stoichiometric amount of hydrochloric acid (FIXANAL / Riedel-de Haën). After the evolution of CO₂ ceased, the solvents have been removed in vacuum, leaving white crystals of [C₁im]Cl.

¹H NMR Chemical Shifts (in CDCl₃, δ / ppm relative to TMS): 10.56 (s, 1H), 7.47 (d, 2H), 4.08 (s, 6H).

References

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http://www.sigmaaldrich.com/Area_of_Interest/Chemistry/Chemical_Synthesis/Product_Highlights/CBILS.html

Table S1 Experimental binodal curve mass fraction data for the system IL (1) + K₃PO₄ (2) + H₂O (3) at 298 K

[im]Cl		[C ₁ mim]Cl		[C ₂ mim]Cl	
100 w ₁	100 w ₂	100 w ₁	100 w ₂	100 w ₁	100 w ₂
14.071	26.440	40.215	7.716	38.727	4.175
13.364	26.266	36.696	8.386	34.749	6.366
12.892	26.429	33.897	8.938	31.369	7.142
12.333	26.353	30.416	11.312	26.796	8.785
11.909	26.472	27.791	12.334	25.026	10.285
11.469	26.551	25.358	14.071	23.370	11.511
10.953	26.776	22.861	15.973	21.547	13.050
10.496	27.030	21.368	17.092	20.019	14.420
7.475	30.409	19.788	18.484	18.419	15.884
7.009	30.785	18.399	19.692	17.045	17.150
6.296	31.437	16.665	21.215	15.757	18.396
5.581	32.212	15.173	22.492	14.579	19.557
		13.805	23.771	13.550	20.571
		12.578	24.931	12.685	21.426
		11.891	25.617	11.823	22.341
		10.786	26.693	10.781	23.435
		9.207	28.404	10.061	24.238
		7.592	30.292	9.164	25.244
				8.230	26.413
				7.369	27.499
				6.541	28.651
				5.602	30.035

Table S2 Experimental binodal curve mass fraction data for the system IL (1) + K₃PO₄ (2) + H₂O (3) at 298 K

[C ₄ mim]Cl				[OHC ₂ mim]Cl	
100 w ₁	100 w ₂	100 w ₁	100 w ₂	100 w ₁	100 w ₂
39.321	3.478	13.932	18.714	67.860	2.316
37.151	4.566	13.531	19.054	64.168	2.772
33.876	5.683	13.021	19.561	54.223	3.718
32.269	6.533	12.675	19.829	49.934	4.554
30.179	7.539	12.304	20.154	45.322	6.918
27.447	8.731	11.083	22.019	38.311	10.589
25.291	10.051	10.426	22.560	34.707	12.735
24.369	10.655	9.792	23.113	30.190	15.750
23.517	11.175	9.113	23.803	28.258	17.120
22.512	11.946	8.530	24.407	21.472	22.289
21.686	12.518	8.024	24.887	67.860	2.316
20.954	13.008	7.648	25.267	64.168	2.772
20.128	13.628	7.152	25.841	54.223	3.718
19.298	14.297	6.735	26.319	49.934	4.554
18.632	14.786	6.329	26.814	45.322	6.918
17.904	15.373	5.986	27.218	38.311	10.589
17.261	15.895	5.635	27.668	34.707	12.735
16.646	16.394	5.313	28.106	30.190	15.750
16.057	16.865	4.977	28.610	28.258	17.120
15.409	17.485	4.507	29.347	21.472	22.289
14.940	17.860	3.804	30.521		
14.343	18.403	2.912	32.157		

Table S3 Experimental binodal curve mass fraction data for the system IL (1) + K₃PO₄ (2) + H₂O (3) at 298 K

[amim]Cl			
100 w_1	100 w_2	100 w_1	100 w_2
44.178	2.719	14.929	19.269
39.549	4.183	14.461	19.632
37.573	5.123	13.862	20.170
34.552	5.983	13.113	20.911
33.073	6.908	12.533	21.427
31.568	7.611	12.038	21.819
30.238	8.287	11.606	22.222
29.013	9.001	11.107	22.723
27.213	10.187	10.645	23.184
26.089	10.706	10.281	23.525
24.566	11.889	9.964	23.818
23.027	12.958	9.571	24.199
21.720	13.898	9.198	24.594
20.633	14.586	8.864	24.927
19.420	15.559	8.555	25.229
18.306	16.492	8.264	25.519
17.579	16.961	7.804	26.106
16.624	17.803	7.467	26.468
15.716	18.584	6.944	27.055

Table S4 Experimental binodal curve mass fraction data for the system IL (1) + K₃PO₄ (2) + H₂O (3) at 298 K

[C ₆ mim]Cl					
100 w ₁	100 w ₂	100 w ₁	100 w ₂	100 w ₁	100 w ₂
42.378	3.902	9.074	21.725	4.327	27.228
35.976	5.403	8.959	21.877	4.247	27.354
33.612	6.214	8.818	21.977	4.192	27.421
31.267	7.301	8.596	22.238	4.121	27.553
29.172	8.245	8.362	22.460	4.050	27.675
27.419	9.054	8.238	22.535	3.955	27.817
25.951	9.812	8.038	22.786	3.908	27.878
24.565	10.488	7.927	22.863	3.859	27.913
23.574	11.200	7.743	23.090	3.796	28.012
22.427	11.794	7.635	23.136	3.734	28.097
21.477	12.342	7.449	23.368	3.674	28.210
20.717	12.886	7.371	23.469	3.575	28.355
20.085	13.472	7.199	23.620	3.504	28.481
19.238	13.869	7.048	23.810	3.390	28.685
18.584	14.336	6.906	24.006	3.341	28.766
17.971	14.732	6.824	24.041	3.199	29.032
17.371	15.141	6.684	24.221	3.112	29.191
16.849	15.528	6.553	24.381	3.033	29.345
16.369	15.888	6.427	24.538	2.948	29.515
15.909	16.229	6.302	24.688	2.852	29.649
15.494	16.575	6.187	24.826	2.798	29.760
14.758	17.246	6.073	24.959	2.746	29.861
14.375	17.489	6.009	24.994	2.685	29.992
14.018	17.743	5.901	25.132	2.626	30.120

13.656	17.960	5.700	25.391	2.542	30.301
13.337	18.195	5.552	25.543	2.482	30.434
12.832	18.758	5.463	25.675	2.406	30.565
12.513	18.911	5.373	25.794	2.359	30.676
12.045	19.408	5.288	25.908	2.316	30.791
11.773	19.573	5.205	26.016	2.237	30.968
11.542	19.758	5.124	26.127	2.174	31.107
11.317	19.938	5.047	26.227	2.105	31.285
11.066	20.011	4.971	26.334	2.047	31.428
10.843	20.136	4.893	26.415	1.959	31.647
10.626	20.273	4.861	26.472	1.907	31.789
10.279	20.651	4.787	26.553	1.800	32.069
10.094	20.781	4.693	26.710	1.713	32.330
9.769	21.111	4.596	26.845	1.606	32.629
9.526	21.284	4.530	26.920	1.489	32.982
9.439	21.405	4.441	27.067	1.385	33.326
9.215	21.661				

Table S5 Experimental binodal curve mass fraction data for the system IL (1) + K₃PO₄ (2) + H₂O (3) at 298 K

[C _{1im}]Cl					
100 w ₁	100 w ₂	100 w ₁	100 w ₂	100 w ₁	100 w ₂
19.992	22.214	8.537	21.342	3.830	24.046
18.153	22.151	8.316	21.507	3.751	24.172
17.569	22.179	7.928	21.785	3.672	24.266
16.842	22.019	7.613	21.839	3.593	24.365
16.310	22.004	7.383	21.842	3.515	24.442
15.702	21.837	7.188	21.898	3.449	24.545
15.232	21.804	7.037	22.060	3.383	24.658
14.665	21.604	6.856	22.103	3.253	24.868
14.250	21.584	6.693	22.173	3.175	24.927
13.788	21.456	6.518	22.169	3.105	25.045
13.421	21.454	6.317	22.300	3.045	25.104
12.974	21.294	6.128	22.401	2.980	25.199
12.578	21.171	5.984	22.391	2.909	25.347
12.244	21.150	5.860	22.431	2.849	25.440
11.886	21.051	5.747	22.520	2.792	25.540
11.618	21.061	5.525	22.622	2.732	25.594
11.303	20.966	5.356	22.867	2.678	25.668
11.049	20.970	5.124	22.812	2.609	25.801
10.773	20.918	4.957	23.181	2.544	25.913
10.536	20.915	4.737	23.174	2.484	26.047
10.312	20.934	4.579	23.412	2.389	26.273
10.089	20.915	4.384	23.396	2.287	26.428
9.925	20.982	4.261	23.702	2.221	26.626
9.694	20.895	4.083	23.733	2.124	26.824

9.483	21.230	3.968	23.894	2.012	27.089
9.108	21.178	3.899	23.966	1.895	27.398
8.827	21.297				

Table S6 Experimental binodal curve mass fraction data for the system IL (1) + K₃PO₄ (2) + H₂O (3) at 298 K

[C _{2im}]Cl					
100 w ₁	100 w ₂	100 w ₁	100 w ₂	100 w ₁	100 w ₂
25.973	19.523	8.300	16.786	2.758	20.524
24.380	19.553	8.204	16.867	2.674	20.632
23.330	19.258	8.057	16.819	2.599	20.824
22.664	19.286	7.864	16.966	2.521	20.924
22.056	19.190	7.647	17.026	2.456	21.026
21.094	19.015	7.469	17.148	2.392	21.121
20.269	18.773	7.270	17.177	2.338	21.240
19.618	18.871	7.101	17.291	2.278	21.358
18.864	18.744	6.923	17.338	2.232	21.488
18.134	18.613	6.775	17.452	2.140	21.673
17.411	18.495	6.587	17.352	2.024	21.870
16.792	18.363	6.464	17.428	1.943	22.084
16.033	18.079	6.348	17.504	1.814	22.428
15.471	17.954	6.156	17.671	1.733	22.623
14.982	17.887	5.963	17.726	0.847	23.494
14.350	17.597	5.831	17.694	0.829	23.653
13.908	17.513	5.707	17.864	0.813	23.780
13.497	17.446	5.591	17.836	0.795	23.982
13.101	17.390	5.503	17.909	0.782	24.075
12.631	17.208	5.364	17.985	0.766	24.242
12.282	17.117	5.235	18.080	0.754	24.307
11.967	17.059	5.116	18.155	0.731	24.539
11.567	16.884	5.001	18.248	0.706	24.784
11.280	16.829	4.887	18.321	0.688	24.958

11.021	16.804	4.784	18.395	0.670	25.115
10.679	16.623	4.675	18.503	0.657	25.258
10.430	16.620	4.579	18.556	0.642	25.392
10.199	16.593	4.487	18.634	0.626	25.588
9.960	16.545	4.384	18.775	0.605	25.831
9.741	16.505	4.274	18.844	0.586	25.973
9.539	16.458	4.153	18.989	0.564	26.289
9.406	16.544	3.990	19.087	0.550	26.415
9.270	16.627	3.790	19.354	0.530	26.715
9.088	16.605	3.592	19.576	0.510	26.939
8.929	16.600	3.319	20.011	0.494	27.080
8.811	16.672	3.182	19.969	0.478	27.316
8.698	16.748	3.066	20.109	0.459	27.606
8.541	16.733	2.962	20.334	0.432	27.958
8.398	16.722	2.866	20.475		

Table S7 Experimental binodal curve mass fraction data for the system IL (1) + K₃PO₄ (2) + H₂O (3) at 298 K

[C ₇ H ₇ mim]Cl					
100 w ₁	100 w ₂	100 w ₁	100 w ₂	100 w ₁	100 w ₂
43.686	4.760	17.169	16.409	7.802	23.332
40.143	5.651	16.643	16.789	7.490	23.629
37.633	6.455	16.022	17.265	7.220	23.912
35.691	7.147	15.227	17.672	6.960	24.145
33.974	7.876	14.722	18.037	6.707	24.387
32.336	8.534	13.961	18.517	6.475	24.630
30.912	9.219	13.078	19.183	6.259	24.866
29.581	9.839	12.363	19.668	6.027	25.153
28.359	10.342	12.168	19.717	5.699	25.528
27.451	10.810	11.849	20.018	5.409	25.833
26.441	11.153	11.367	20.355	5.043	26.242
25.541	11.535	11.132	20.509	4.775	26.624
24.134	12.436	10.884	20.763	4.385	27.216
23.330	12.786	10.464	21.045	4.044	27.808
22.102	13.576	10.229	21.237	3.784	28.137
21.454	13.796	9.746	21.600	3.639	28.318
20.490	14.425	9.314	21.960	3.416	28.658
19.616	15.008	8.841	22.386	3.178	29.005
18.784	15.550	8.445	22.751	2.744	29.791
17.739	16.069	8.078	23.071	2.217	30.870