Supporting Information

Liquid-liquid equilibrium and extraction performance of aqueous biphasic systems composed of water, cholinium carboxylate ionic liquids and K_2CO_3

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NMR spectra of cholinium-based ILs

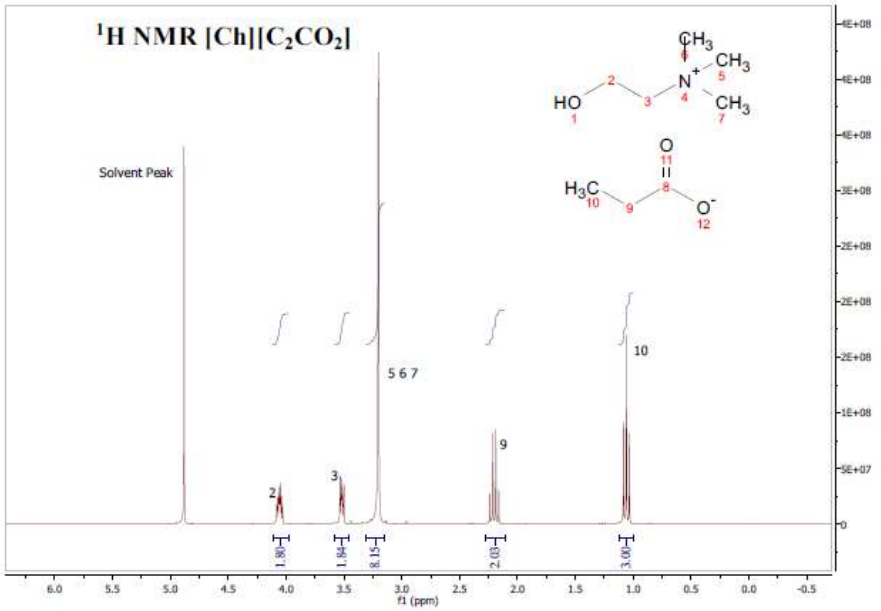

Figure S1. Cholinium propanoate, [Ch][C_2CO_2], ^{1}H NMR (D_2O, 300 MHz, [ppm]): 4.06 (m,); 3.52 (m, 2H); 3.20 (s, 9H); 2.20 (q, 2H, J_{HH}=7.7 Hz); 1.06 (t, 3H, J_{HH}=7.7 Hz).

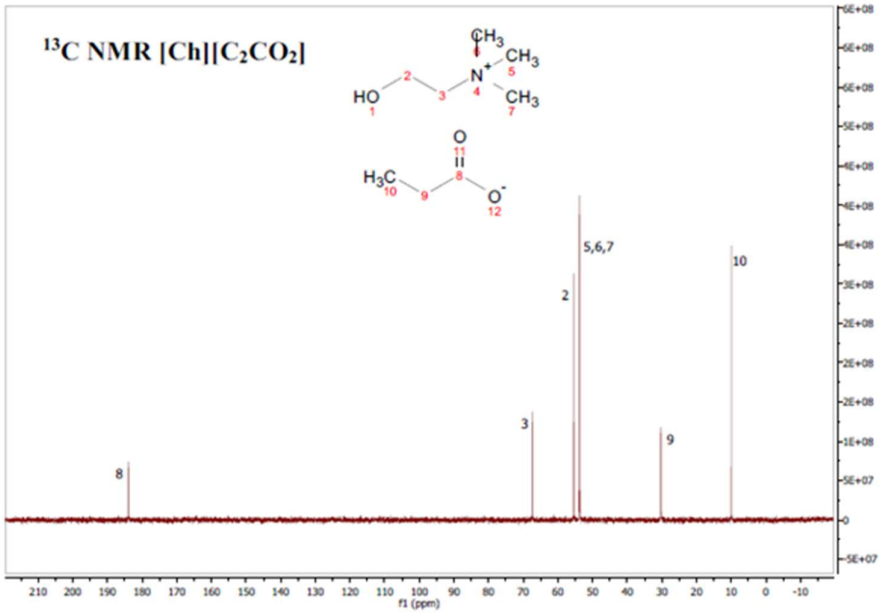

Figure S2. Cholinium propanoate, [Ch][C_2CO_2], ^{13}C NMR (D_2O, 75.47 MHz, [ppm]): 184.04; 67.40; 55.69; 53.75; 30.25; 9.60.

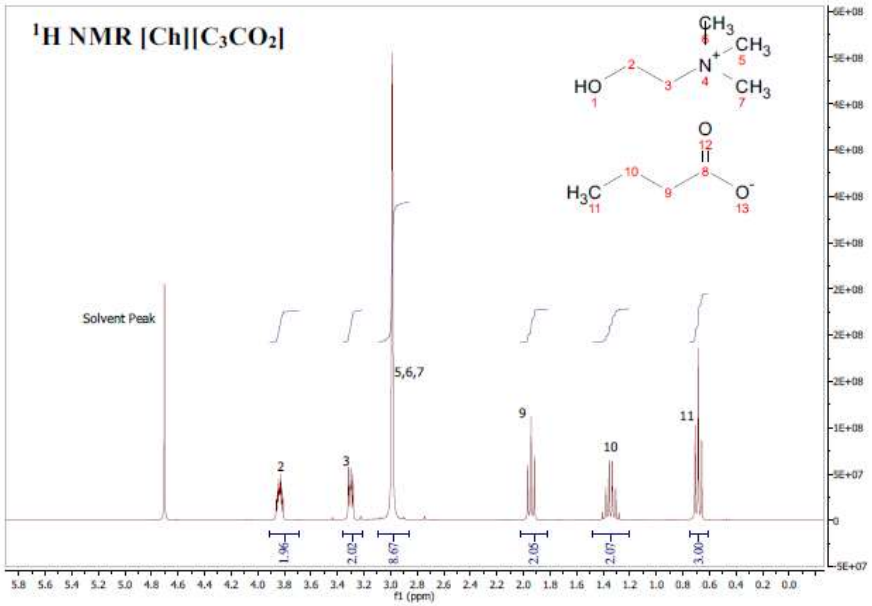

Figure S3. Cholinium Butanoate, [Ch][C_3CO_2], ^{1}H NMR (D_2O, 300 MHz, [ppm]): 3.66 (m, 2H); 3.32 (m, 2H); 3.01 (s, 9H); 1.98 (t, 2H, J_{HH}=7.7 Hz); 1.37 (m, 2H,); 0.71 (t, 3H, J_{HH}=7.7 Hz).

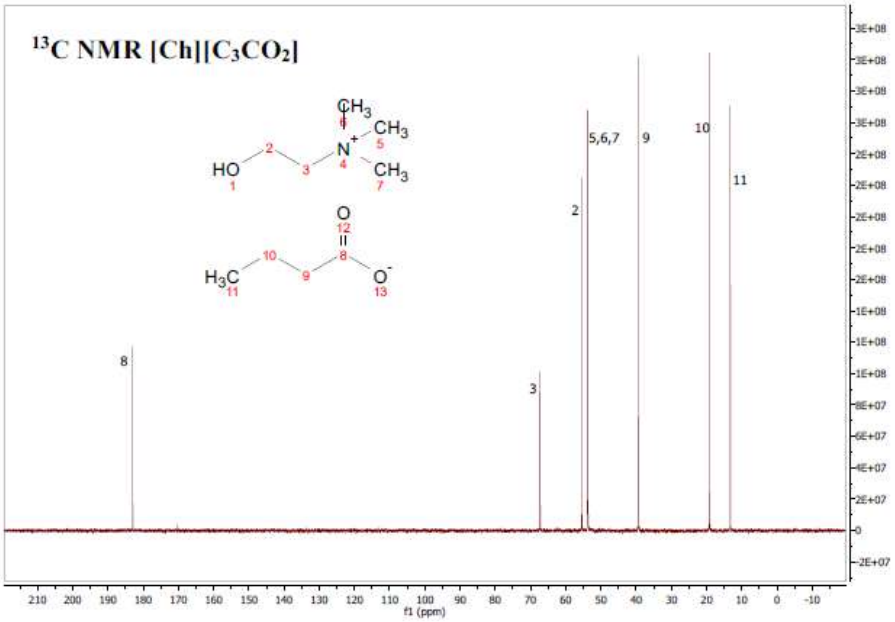

Figure S4. Cholinium Butanoate, [Ch][C_3CO_2], ^{13}C NMR (D_2O, 75.47 MHz, [ppm]): 183.07; 67.28; 55.43; 53.68.15; 39.30; 19.12; 13.27.

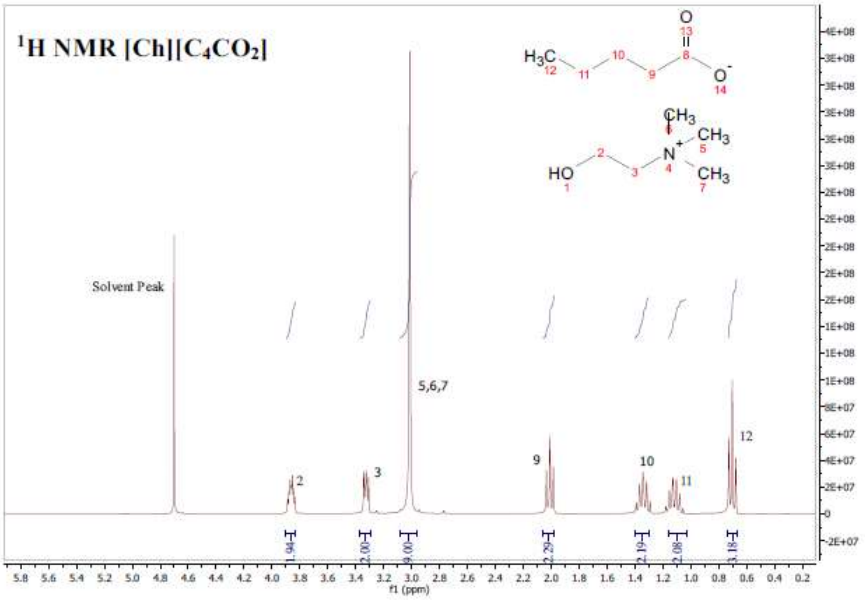

Figure S5. Cholinium Pentanoate, [Ch][C_4CO_2], ^{1}H NMR (D_2O, 300 MHz, [ppm]): 3.83 (m, 2H); 3.30 (m, 2H); 2.99 (s, 9H); 1.98 (t, 2H, J_{HH}=7.7 Hz); 1.31 (m, 2H,); 1.09 (m, 2H,); 0.68 (t, 3H, J_{HH}=7.7 Hz).

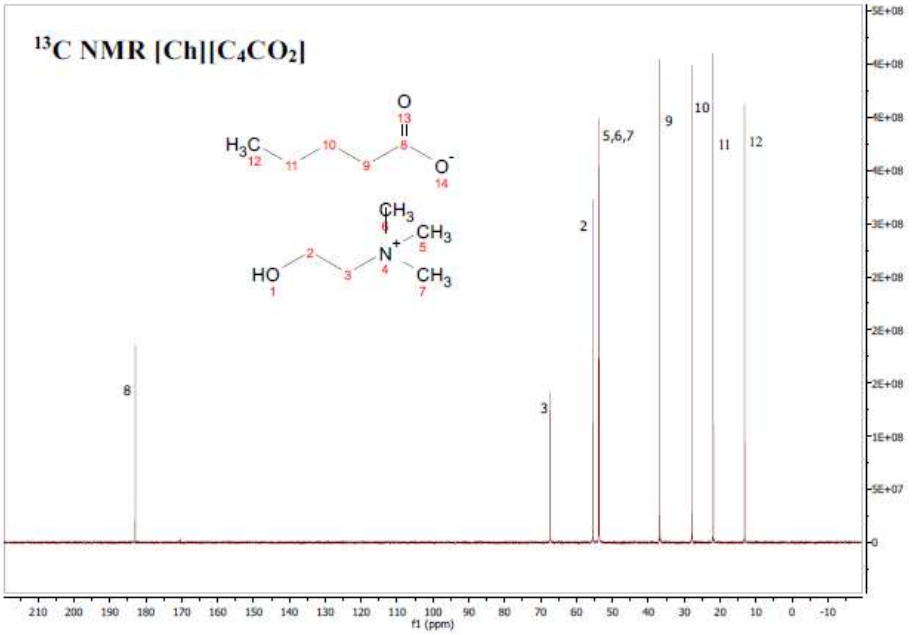

Figure S6. Cholinium Pentanoate, [Ch][C_4CO_2], ^{13}C NMR (D_2O, 75.47 MHz, [ppm]): 183.04; 67.35; 55.46; 53.71; 37.03; 27.96; 21.93; 13.57.

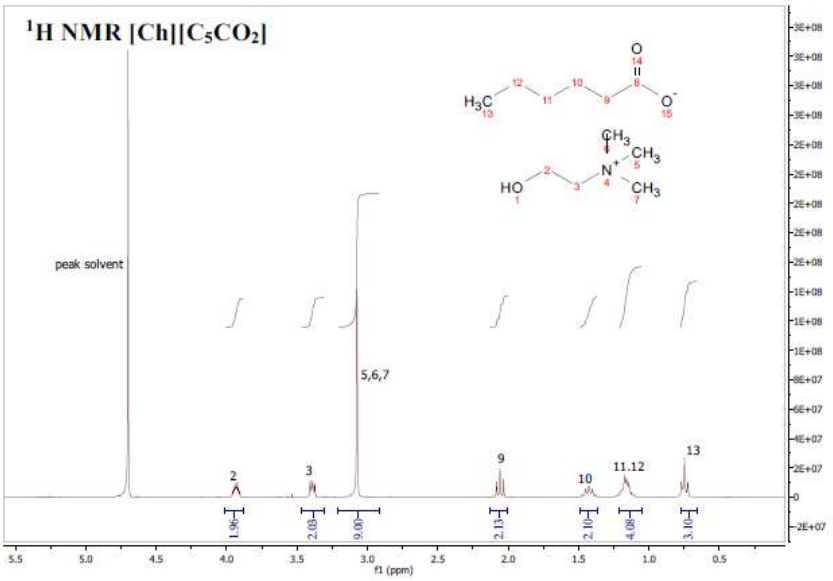

Figure S7. Cholinium Hexanoate, [Ch][C_5CO_2], ^{1}H NMR (D_2O, 300 MHz, [ppm]): 3.93 (m, 2H); 3.39 (m, 2H); 3.07 (s, 9H); 2.06 (t, 2H, J_{HH}=7.7 Hz); 1.41 (m, 2H,); 1.16 (m, 2H,); 0.75 (t, 3H, J_{HH}=7.7 Hz).

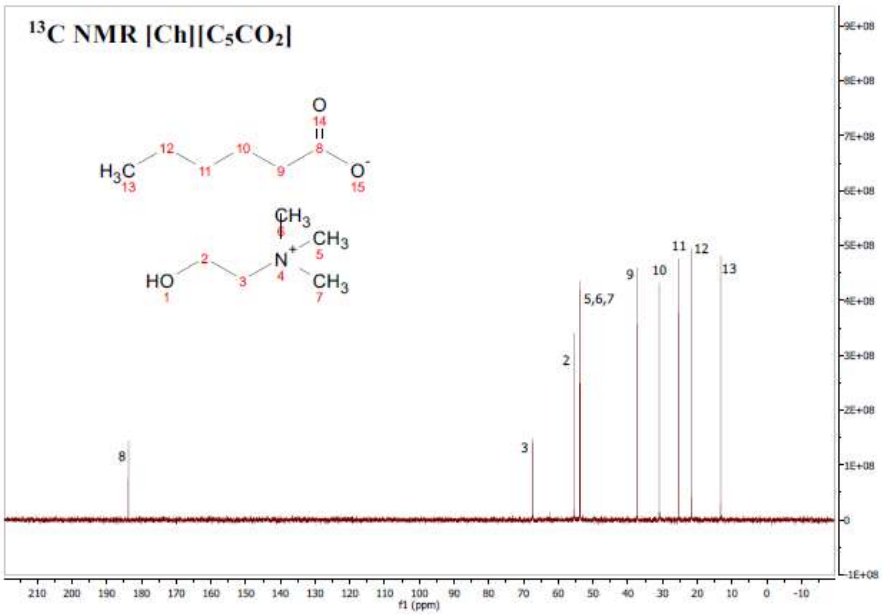

Figure S8. Cholinium Hexanoate, [Ch][C_5CO_2], ^{13}C NMR (D_2O, 75.47 MHz, [ppm]): 184.04; 67.38; 55.38; 53.74; 37.25; 30.92; 25.64; 21.55; 13.23.

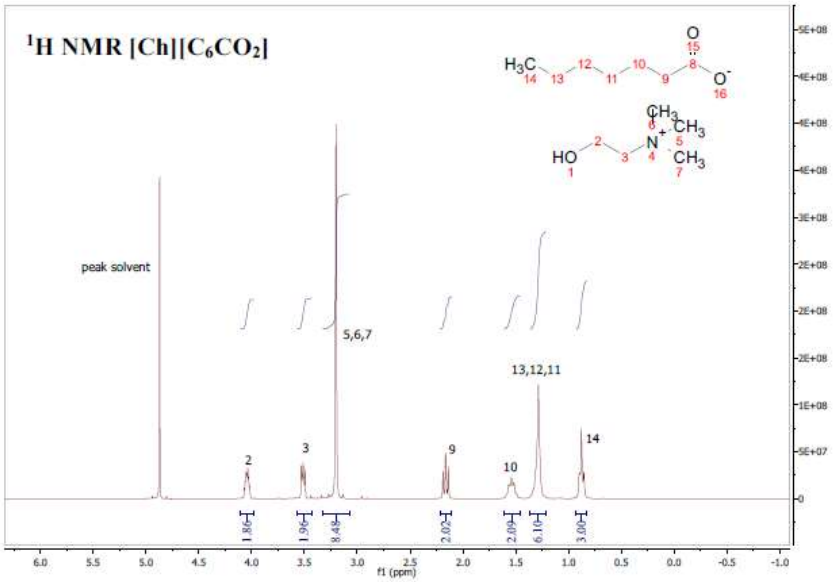

Figure S9. Cholinium Heptanoate, [Ch][C_6CO_2], ^{1}H NMR (D_2O, 300 MHz, [ppm]): 4.04 (m, 2H); 3.52 (m, 2H); 3.20 (s, 9H); 2.16 (t, 2H, J_{HH}=7.7 Hz); 1.54 (m, 2H,); 1.29 (s, 6H,); 0.88 (t, 3H, J_{HH}=7.7 Hz).

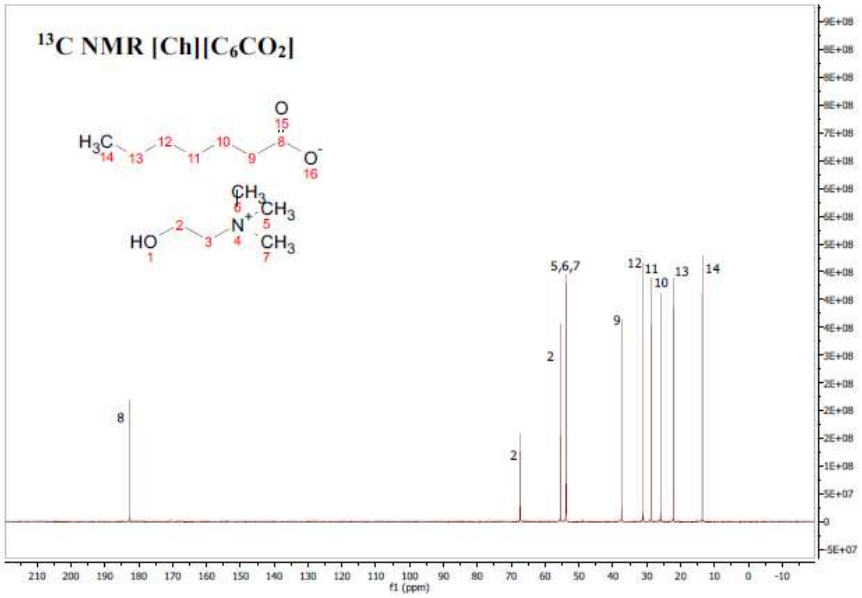

Figure S10. Cholinium Heptanoate, [Ch][C_6CO_2], ^{13}C NMR (D_2O, 75.47 MHz, [ppm]): 182.59; 68.38; 56.06; 52.32; 37.61; 30.60; 28.28; 25.63; 21.89; 13.90.

Dissociation curves of nitrogenous bases

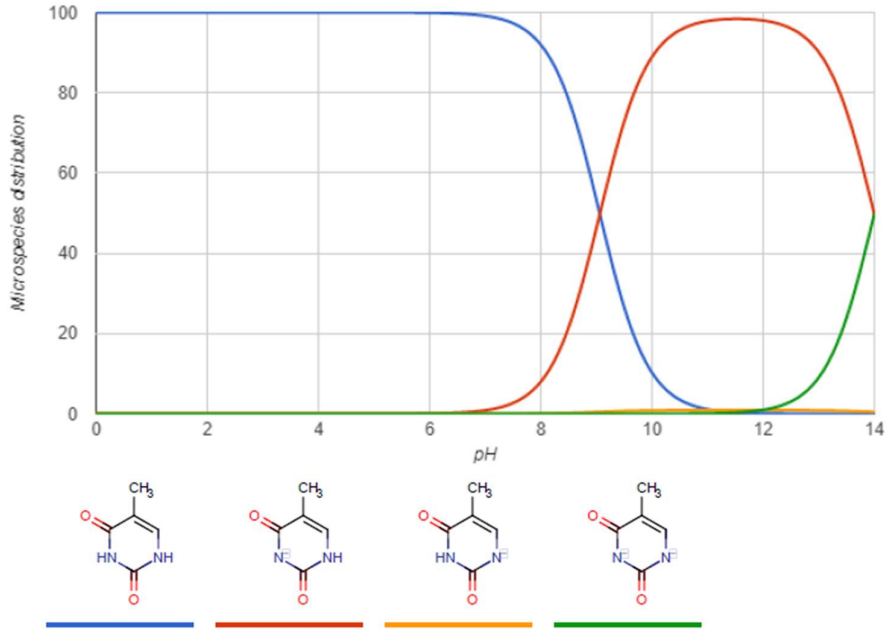

Figure S11. Dissociation curve of thymine.

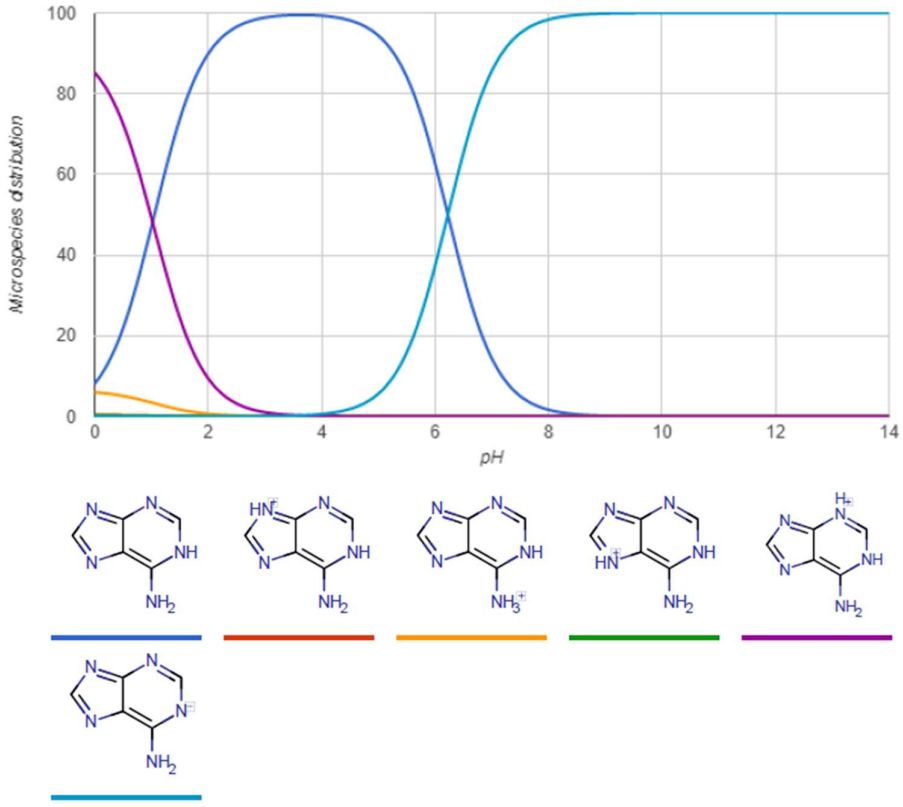

Figure S12. Dissociation curve of adenine.

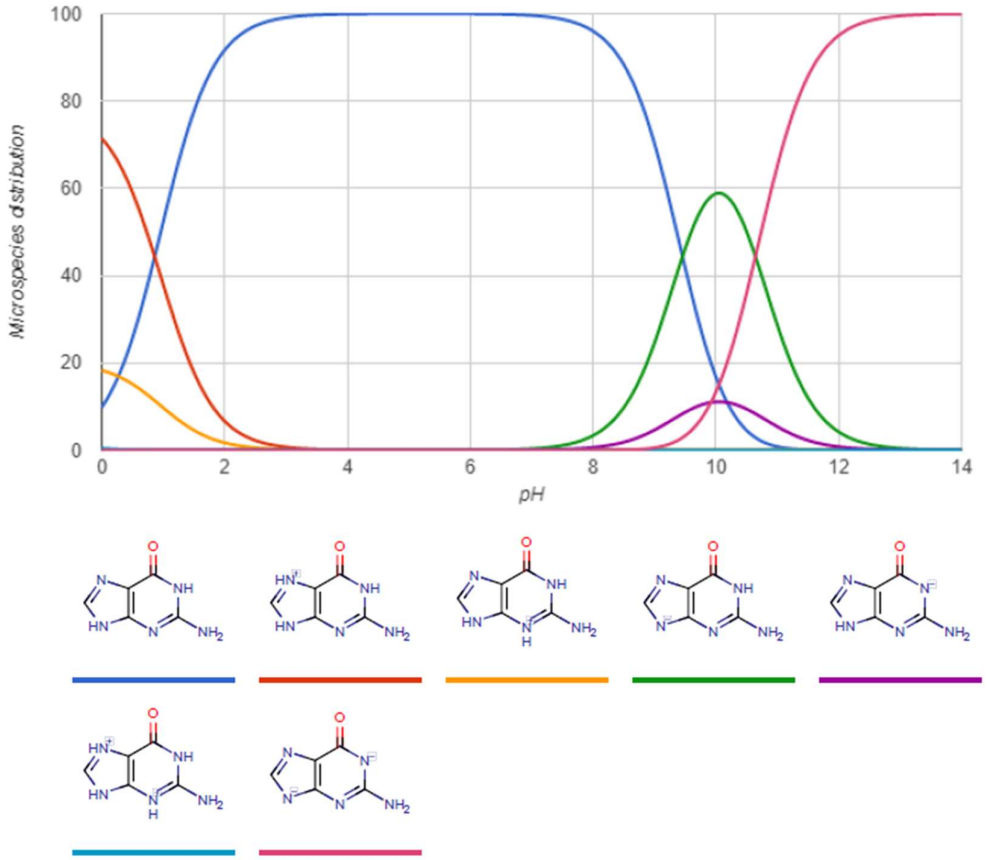

Figure S13. Dissociation curve of guanine.

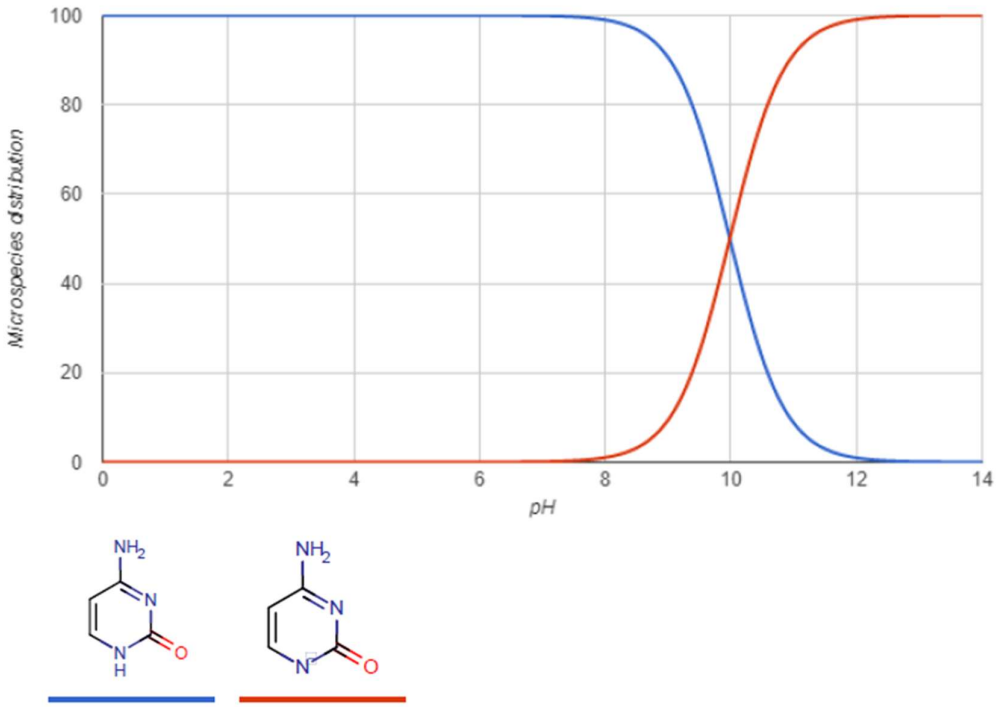

Figure S14. Dissociation curve of cytosine.

Table S1. Experimental data for the binodal weight fraction percentage of the ABS formed by [Ch][C_2CO_2], [Ch][C_3CO_2] or [Ch][C_4CO_2] (1) + K_2CO_3 (2) + water (3) at (298 ± 1) K and atmospheric pressure (0.10 MPa).[a]

[Ch][C_2CO_2]			[Ch][C_3CO_2]			[Ch][C_4CO_2]		
$100w_1$	$100w_2$	$100w_3$	$100w_1$	$100w_2$	$100w_3$	$100w_1$	$100w_2$	$100w_3$
39.932	18.391	41.677	44.358	12.930	42.713	39.979	14.822	45.199
38.885	17.909	43.206	43.459	12.668	43.873	39.137	14.509	46.354
36.276	20.080	43.644	41.420	14.438	44.143	37.318	16.167	46.515
35.646	19.731	44.623	40.555	14.136	45.308	36.594	15.854	47.553
31.951	22.895	45.153	38.916	15.602	45.483	34.503	17.815	47.682
31.634	22.668	45.698	38.161	15.299	46.540	33.863	17.485	48.653
28.007	25.832	46.162	36.334	16.979	46.687	32.365	18.931	48.704
27.683	25.533	46.784	35.655	16.661	47.684	31.827	18.616	49.557
24.295	28.560	47.146	33.357	18.835	47.809	29.808	20.619	49.573
24.011	28.226	47.764	32.848	18.547	48.605	29.372	20.317	50.311
20.027	31.882	48.092	31.022	20.317	48.661	28.064	21.647	50.288
19.836	31.579	48.585	30.487	19.966	49.548	27.626	21.309	51.066
17.144	34.115	48.742	28.617	21.831	49.552	25.958	23.052	50.990
16.976	33.782	49.242	28.216	21.525	50.259	25.550	22.689	51.761
13.761	36.903	49.336	25.925	23.868	50.207	23.860	24.508	51.632
13.693	36.720	49.587	25.604	23.572	50.824	23.540	24.179	52.280
12.016	38.378	49.606	24.416	24.816	50.768	22.089	25.783	52.128
11.938	38.128	49.934	24.115	24.510	51.375	21.792	25.437	52.771
			22.376	26.376	51.249	20.326	27.102	52.572
			22.126	26.081	51.793	20.098	26.798	53.104
			20.641	27.711	51.647	19.002	28.074	52.924
			20.440	27.441	52.119	18.807	27.786	53.408
			19.076	28.972	51.952	17.782	29.006	53.212
			18.935	28.758	52.307	17.595	28.699	53.706
			18.406	29.362	52.232	16.762	29.717	53.522
			18.287	29.173	52.540	16.606	29.440	53.953
			17.287	30.333	52.380	15.904	30.318	53.778
			17.163	30.115	52.723	15.776	30.073	54.151
			16.596	30.783	52.621	15.025	31.031	53.944
			16.494	30.592	52.914	14.888	30.748	54.365
			15.622	31.638	52.740	13.999	31.909	54.093
			15.520	31.431	53.050	13.890	31.661	54.448
			14.859	32.237	52.904	13.304	32.443	54.253
			14.778	32.060	53.162	13.194	32.174	54.632
			14.272	32.688	53.040	12.533	33.076	54.391
			14.187	32.494	53.319	12.445	32.843	54.711
			13.488	33.374	53.137	11.944	33.543	54.514
			13.400	33.155	53.445	11.862	33.312	54.826
			12.934	33.754	53.312	11.225	34.218	54.557
			12.858	33.558	53.584	11.151	33.993	54.856

12.239	34.368	53.393	10.699	34.649	54.652
12.178	34.195	53.627	10.632	34.432	54.935
11.740	34.777	53.483	10.224	35.038	54.739
11.683	34.609	53.708	10.166	34.838	54.996
10.954	35.593	53.453	9.571	35.737	54.693
10.913	35.459	53.628	9.520	35.547	54.933
10.558	35.944	53.498	9.075	36.231	54.693
10.512	35.785	53.703	9.025	36.031	54.943
10.126	36.321	53.553	8.631	36.650	54.719
10.083	36.170	53.747	8.587	36.464	54.949
9.653	36.777	53.571	8.180	37.115	54.705
9.604	36.590	53.806	8.101	36.755	55.144
9.032	37.412	53.556	7.341	38.015	54.644
8.994	37.256	53.750	7.307	37.838	54.855
8.734	37.635	53.630	6.684	38.890	54.426
8.702	37.494	53.805	6.632	38.586	54.782
8.306	38.079	53.615			
8.276	37.940	53.784			
7.834	38.604	53.562			
7.806	38.462	53.732			
7.312	39.215	53.472			
7.285	39.070	53.645			
6.778	39.857	53.365			
6.736	39.606	53.659			

[a]The combined standard uncertainty for the weight fraction $u_r(w)$ is 0.01, the standard uncertainty for the temperature $u(T)$ is 1 K, and the standard uncertainty for pressure $u(p)$ is 10 kPa.

Table S2. Experimental data for the binodal weight fraction percentage of the ABS formed by [Ch][C_5CO_2] or [Ch][C_6CO_2] (1) + K_2CO_3 (2) + water (3) at (298 ± 1) K and atmospheric pressure (0.1 MPa).[a]

[Ch][C_5CO_2]			[Ch][C_6CO_2]		
$100w_1$	$100w_2$	$100w_3$	$100w_1$	$100w_2$	$100w_3$
41.894	16.225	41.881	40.749	17.833	41.419
41.060	15.902	43.038	39.913	17.467	42.620
38.941	17.672	43.388	37.326	19.651	43.022
38.102	17.291	44.607	36.588	19.263	44.149
35.603	19.448	44.949	34.247	21.305	44.448
34.947	19.090	45.963	33.635	20.924	45.440
32.751	21.044	46.205	31.420	22.916	45.663
32.208	20.695	47.097	30.939	22.565	46.496
29.750	22.945	47.305	29.243	24.134	46.624
29.315	22.609	48.076	28.803	23.771	47.426
27.815	24.021	48.165	26.933	25.550	47.517
27.434	23.692	48.874	26.543	25.179	48.278
25.669	25.396	48.935	25.019	26.672	48.310
25.324	25.055	49.621	24.679	26.310	49.011
23.482	26.882	49.635	23.189	27.811	49.000
23.226	26.588	50.186	22.911	27.478	49.611
21.807	28.030	50.163	21.544	28.892	49.564
21.543	27.690	50.767	21.304	28.571	50.125
20.021	29.280	50.700	20.306	29.630	50.064
19.801	28.958	51.241	20.078	29.297	50.626
18.719	30.119	51.163	18.928	30.549	50.523
18.522	29.803	51.675	18.738	30.241	51.021
17.411	31.025	51.564	17.642	31.465	50.893
17.270	30.774	51.956	17.473	31.165	51.362
16.264	31.904	51.832	16.664	32.092	51.244
16.131	31.643	52.227	16.527	31.830	51.643
15.332	32.560	52.107	15.706	32.791	51.503
15.220	32.321	52.460	15.583	32.536	51.881
14.409	33.273	52.319	15.092	33.124	51.785
14.299	33.020	52.681	14.969	32.854	52.177
13.585	33.878	52.537	14.352	33.609	52.039
13.495	33.653	52.853	14.246	33.359	52.395
12.877	34.409	52.714	13.649	34.106	52.246
12.797	34.195	53.008	13.554	33.869	52.577
12.131	35.027	52.841	12.922	34.676	52.402
12.052	34.799	53.148	12.832	34.436	52.731
11.501	35.503	52.996	12.422	34.971	52.607
11.435	35.299	53.267	12.335	34.726	52.939
10.891	36.006	53.103	11.732	35.531	52.738
10.830	35.802	53.369	11.663	35.324	53.013

10.261	36.557	53.182	11.218	35.928	52.854
10.210	36.373	53.417	11.159	35.739	53.102
9.745	37.002	53.253	10.752	36.302	52.946
9.696	36.816	53.489	10.694	36.105	53.201
9.257	37.420	53.323	10.284	36.683	53.033
9.215	37.250	53.535	10.234	36.503	53.263
8.798	37.836	53.367	9.968	36.884	53.148
8.760	37.673	53.567	9.921	36.709	53.371
8.235	38.423	53.342	9.664	37.083	53.253
8.207	38.293	53.501	9.617	36.903	53.480
7.904	38.730	53.365	9.255	37.440	53.305
7.875	38.584	53.542	9.211	37.259	53.530
7.485	39.158	53.357	8.879	37.761	53.361
7.455	39.003	53.542	8.838	37.585	53.577
7.140	39.475	53.384	8.658	37.861	53.481
7.115	39.333	53.552	8.620	37.692	53.688
			8.286	38.215	53.500
			8.250	38.052	53.697
			7.996	38.456	53.548
			7.962	38.293	53.745
			7.690	38.734	53.576
			7.655	38.560	53.785
			7.434	38.924	53.642
			7.405	38.773	53.821
			7.207	39.106	53.687
			7.183	38.975	53.842
			7.012	39.264	53.723
			6.988	39.127	53.885
			6.758	39.523	53.719
			6.734	39.383	53.883
			6.569	39.673	53.759
			6.546	39.534	53.920
			6.338	39.903	53.759
			6.319	39.782	53.899
			6.177	40.037	53.785
			6.157	39.905	53.939
			5.946	40.290	53.764
			5.912	40.056	54.033

[a]The combined standard uncertainty for the weight fraction $u_r(w)$ is 0.01, the standard uncertainty for the temperature $u(T)$ is 1 K, and the standard uncertainty for pressure $u(p)$ is 10 kPa.

Table S3. Weight fraction compositions (wt%) of the initial mixture (M), moles of IL cation and cation *per* g of the IL-rich phase (determined by ^{1}H NMR), and cation:anion ratio in the IL-rich phase of the ABS composed of water + cholinium-based ILs + K_2CO_3 at (298 ± 1) K.

IL	$[IL]_M$/ wt%	$[salt]_M$/ wt%	mol IL Cation/g	mol IL Anion/g	cation:anion[a]
[Ch][C_2CO_2]	22.73	21.85	0.0015 ± 0.0002	0.0017 ± 0.0001	1:1
	26.30	30.92	0.0017 ± 0.0004	0.0019 ± 0.0005	1:1
[Ch][C_3CO_2]	25.62	23.82	0.0013 ± 0.0002	0.0014 ± 0.0003	1:1
	21.90	28.82	0.0017 ± 0.0002	0.0023 ± 0.0006	1:1
[Ch][C_4CO_2]	25.27	30.47	0.0014 ± 0.0005	0.0017 ± 0.0003	1:1
	27.38	27.71	0.0022 ± 0.0007	0.0027 ± 0.0009	1:1

[a]Determined through the excel ARRED function.

Table S4. Activity coefficients of each compound at each phase in the ABS formed by cholinium-based ionic liquid + K_2CO_3 and water.

Top phase			Bottom phase		
H_2O	**K_2CO_3**	**IL**	**H_2O**	**K_2CO_3**	**IL**
[Ch][C_2CO_2]					
1.4308	1.0826	1.4927	1.5477	1.8491	1.0164
1.5087	1.0501	1.6104	1.5362	1.8188	1.0193
1.5421	1.0384	1.6715	1.5288	1.7959	1.0217
IL Critical Concentration / wt% = 19.31					
[Ch][C_3CO_2]					
1.8197	1.0733	1.5233	2.7200	1.9140	1.0113
1.9032	1.0581	1.5739	2.6829	1.8857	1.0133
1.9163	1.0429	1.6454	2.6665	1.8601	1.0154
IL Critical Concentration / wt% = 25.93					
[Ch][C_4CO_2]					
1.9867	1.0884	1.4737	3.3643	1.8963	1.0126
2.0526	1.0524	1.5983	3.3685	1.8792	1.0138
1.8752	1.041	1.6709	3.3409	1.8650	1.0150
IL Critical Concentration / wt% = 11.72					
[Ch][C_5CO_2]					
2.2399	1.0898	1.4727	1.8549	1.8848	1.0134
2.4778	1.0615	1.5604	1.8522	1.8726	1.0144
2.5666	1.0417	1.6547	1.8532	1.8465	1.0166
IL Critical Concentration / wt% = 15.80					
[Ch][C_6CO_2]					
2.6861	1.1642	1.3126	3.6007	1.8796	1.0138
2.4753	1.1103	1.4185	3.6268	1.8714	1.0145
2.5870	1.0855	1.4783	3.5684	1.8450	1.0168
IL Critical Concentration / wt% = 11.17					

Table S5. Extraction efficiencies (*EE*%) of the studied ABS for thymine, adenine, guanine and cytosine, and respective standard deviation (σ), and pH of the ABS phases, at (298 ± 1) K.

Cholinium-based IL	$EE\%_{ADE} \pm \sigma$	$EE\%_{THY} \pm \sigma$	$EE\%_{CYT} \pm \sigma$	$EE\%_{GUA} \pm \sigma$	pH	
					IL-rich phase	K_2CO_3-rich phase
[Ch][C_2CO_2]	97.32 ± 0.82	94.22 ± 0.54	89.32 ± 0.74	90.25 ± 0.27	12.42 ± 0.07	12.22 ± 0.06
[Ch][C_3CO_2]	95.22 ± 0.02	93.91 ± 0.27	87.06 ± 0.09	88.03 ± 0.60	11.98 ± 0.11	11.79 ± 0.05
[Ch][C_4CO_2]	96.40 ± 0.07	92.59 ± 0.25	87.10 ± 0.45	84.12 ± 0.01	12.17 ± 0.14	12.00 ± 0.12
[Ch][C_5CO_2]	92.77 ± 0.01	92.32 ± 0.59	84.36 ± 0.75	81.41 ± 0.80	12.19 ± 0.10	12.04 ± 0.06
[Ch][C_6CO_2]	93.10 ± 0.51	92.68 ± 0.74	88.46 ± 0.62	82.97 ± 0.01	12.10 ± 0.28	11.94 ± 0.25