

Supplementary Information

Molecular interactions in aqueous biphasic systems composed of polyethylene glycol and crystalline vs. liquid cholinium-based salts

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Experimental Section

Materials

The following cholinium-based compounds were acquired from Sigma-Aldrich: cholinium chloride, [Ch]Cl, cholinium bicarbonate, [Ch][Bic], cholinium bitartrate, [Ch][Bit], and cholinium dihydrogen citrate, [Ch][DHcit]. The cholinium acetate, [Ch][Ac], cholinium dihydrogen phosphate, [Ch][DHph], and cholinium glycolate, [Ch][Gly], were obtained from Iolitec. The cholinium-based compounds that are ILs, namely cholinium propanoate, [Ch][Pro], cholinium butanoate, [Ch][But], and cholinium lactate, [Ch][Lac], were synthesized by our group according to standard protocols.¹⁻³ All the ILs were dried under constant agitation and vacuum, at a moderate temperature (50 °C), for a minimum of 48 h, to reduce the volatile compounds and water contents to negligible values. ¹H and ¹³C NMR was employed to evaluate the purity of each sample. All ILs showed a purity level higher than 98 wt%.

PEGs of average molecular weights 400 g.mol⁻¹, 600 g.mol⁻¹ and 1000 g.mol⁻¹ (abbreviated as PEG-400, PEG-600 and PEG-1000, respectively) were supplied by Fluka, and used as received.

The water used was double distilled, passed across a reverse osmosis system and further treated with a Milli-Q plus 185 water purification apparatus.

[Ch]-based salts and PEG 600/water mutual solubilities

The mutual solubilities measurements between [Ch]-based compounds and PEG or water were carried out at 25 °C and atmospheric pressure. For that purpose small amounts of each IL were added to small glass vials with pre-weighted PEG-600 or water and *vice-versa*. Then, each binary mixture was vigorously agitated during 12 h at constant temperature. After this period the vials were visually analysed. If a second phase was not detected, more IL, PEG or water (approximately 30 mg) were added and the procedure was repeated. The saturation values were taken at the first solid or second liquid phase appearance. At this stage, the vials were finally weighed and the solubilities were determined gravimetrically within $\pm 10^{-7}$ kg.

Determination of phase diagrams

Aqueous solution of each [Ch]-based compound (from 40 wt% to 80 wt%) and aqueous solutions of each PEG (80 wt% to 100 wt%) were prepared and used for the

determination of the binodal curves. The phase diagrams were determined by the cloud point titration method at 25 °C and 50 °C (± 1 °C) and atmospheric pressure, according to literature procedures.⁴⁻⁵ The composition of each system was calculated by the weight quantification of all components added within $\pm 10^{-7}$ kg.

pH and conductivity measurements

After phase separation, the pH values (± 0.02) and conductivity (± 0.01 mS.cm⁻¹) of both the salt-rich and PEG-rich phases were measured at 25 °C (± 1 °C) using a SevenMultiTM (Mettler Toledo Instruments). The calibration of the pH meter was carried out with two buffers (pH values of 4.00 and 7.00).

COSMO-RS predictions

The standard procedure for COSMO-RS modelling consists of two major steps. First, the continuum solvation COSMO calculations of electronic density and molecular geometry of PEG-600, [Ch]-based compounds and water were performed with the TURBOMOLE 6.1 program package on the density functional theory, utilizing the BP functional B88-P86 with a triple- ζ valence polarized basis set (TZVP) and the resolution of identity standard (RI) approximation.⁶ In a second step, the thermodynamic properties, such as activity coefficient, excess enthalpy and excess Gibbs free energy calculations were performed with the COSMOthermX_2.1 program using the parameter file BP_TZVP_C21_0111 (COSMOlogic GmbH & Co KG, Leverkusen, Germany). In all calculations, the salts or ILs were treated as isolated ions.

Results

Tables S1 to S12 present the experimental weight fraction data corresponding to the solubility curves of each ABS.

Table S1. Experimental binodal weight fraction data for the systems composed of PEG-600 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch]Cl		[Ch][Ac]		[Ch][Gly]	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
34.0819	39.1428	7.7463	57.7669	56.4588	20.7596
37.2452	36.5489	10.2532	52.8845	55.4419	21.4341
39.2156	34.6475	16.6263	47.2618	53.9444	22.5325
41.8640	32.5914	20.1027	44.4450	53.3623	22.9262
43.1425	31.8462	25.9081	40.3469	51.0288	24.4749
44.6782	30.7604	29.1567	37.9697	49.1718	25.8242
46.2828	29.6031	33.5656	35.0386	48.4817	26.3869
50.3988	26.4885	37.8865	32.2912	45.7609	28.4222
50.6779	26.2078	41.1845	30.0483	42.5650	30.8665
52.0774	25.4721	44.2316	27.9741	39.4323	33.3652
54.5077	23.6280	47.4464	25.8656	34.8857	36.8404
54.6391	23.1984	49.5218	24.4078	30.8054	40.1912
54.9489	23.5726	51.9556	22.8546	25.6866	44.1907
57.4056	21.5651	53.9060	21.5639	20.4765	48.4258
58.1009	20.8599	56.0332	20.2684	15.8067	52.5080
60.6128	19.5148	57.1339	19.5986		
61.8785	18.3621	58.3577	18.9164		
63.0859	17.4472	59.5557	18.1474		
66.3457	15.4835	61.2758	17.1357		
66.8194	15.0065	62.8528	16.2783		
67.3466	14.7846	63.6795	15.8088		
68.2108	14.0296	64.8256	15.1910		
69.1924	13.3523	66.0323	14.4888		
70.3181	12.7876	67.6526	13.6384		
70.5079	12.5991	68.8174	13.0049		
70.8827	12.2647	69.4803	12.6887		
70.8867	12.3326	70.7682	12.0323		
71.5790	12.0019				
72.5925	11.2409				
72.6452	11.2668				
74.1751	10.5506				

Table S2. Experimental binodal weight fraction data for the systems composed of PEG-600 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch][Bic]		[Ch][Bit]			
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
10.1364	53.3850	60.7244	13.5311	4.9682	67.0270
12.9063	50.8924	61.6429	12.8892	6.4409	65.0652
13.9666	50.0743	62.2029	12.5376	7.8021	62.0634
18.5083	46.4142	63.3127	11.8550	8.7913	60.9777
19.9134	44.9231	64.0030	11.4631	11.5956	57.5905
20.6432	44.3980	64.6590	11.0242	11.9558	56.1310
22.4662	42.7154	65.1924	10.7060	15.8215	52.5486
22.5157	42.7053	66.0494	10.1860	19.8116	48.7314
27.4700	39.1902	66.8701	9.7214	24.9897	43.6349
30.2757	36.8186	67.7031	9.2430	31.1285	38.9774
32.9258	34.7102	68.9080	8.7100	33.0364	37.4011
34.4811	33.3278	70.7096	7.6266		
37.4937	31.1626	72.1638	6.9511		
39.3993	29.6410	73.8744	6.2192		
43.3040	26.7841				
45.3727	24.9545				
47.5074	23.5082				
48.4397	22.7086				
49.4359	21.8419				
50.4330	21.0461				
51.6035	20.1329				
53.0482	19.1654				
53.5550	18.6675				
54.0985	18.1978				
55.5111	17.2987				
56.3702	16.5589				
57.2965	16.0009				
57.6738	15.6652				
58.4009	15.1774				
58.9815	14.7285				
60.1266	13.9539				

Table S3. Experimental binodal weight fraction data for the systems composed of PEG-600 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch][DHph]				[Ch][Lac]	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
3.5450	46.7961	30.4605	24.1434	5.0578	62.7497
5.5537	45.0241	31.4426	23.4425	8.5589	57.2474
6.5756	43.8340	32.0136	22.9432	12.7997	53.1147
7.5547	42.4903	32.6111	22.4686	21.5169	46.5027
10.4529	40.2952	33.4295	21.8383	23.8424	44.3971
11.4670	39.4321	34.2968	21.2053	31.2122	39.6178
12.2377	38.4571	35.1423	20.6526	31.5324	39.1553
13.6488	37.1970	35.6390	20.2979	36.4478	35.7286
14.9396	36.0185	36.0008	19.9463	39.4145	33.4585
16.3723	34.8275	36.6860	19.4659	40.1764	33.4619
18.2424	33.4277	37.6290	18.9087	44.3685	30.4271
19.4753	32.3956	38.0519	18.6007	46.3179	28.6724
20.5612	31.5413	38.5663	18.2132	48.1836	27.8172
22.2142	30.4096	39.1323	17.8482	50.2577	26.1887
23.6806	29.2131	39.7196	17.4718	53.0493	24.5721
24.5360	28.4287	40.0553	17.2073	57.5475	21.6293
25.9339	27.5070	40.7565	16.8094	61.4925	19.2269
27.1792	26.6414	41.0672	16.5481	65.4363	16.8539
28.0101	25.9146	41.4692	16.3546	69.4542	14.6192
29.0850	25.1764	41.8852	16.0180	5.0578	62.7497
30.1346	24.3811	42.4350	15.6749		

Table S4. Experimental binodal weight fraction data for the systems composed of PEG-600 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch][Dhct]					
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
15.4533	66.7641	52.1214	29.4278	70.5148	14.2540
23.8645	57.9325	52.5602	28.7738	70.8166	13.9656
24.5619	57.4332	54.2304	27.1186	72.5303	12.8493
30.4862	50.8230	55.5925	26.0604	73.7325	12.0379
34.0505	46.8840	57.4200	24.4744	74.8951	11.3147
37.7544	43.2658	58.6260	23.7582	76.4397	10.1839
38.7983	42.4853	59.7610	22.3311	79.8048	8.0702
41.1756	39.9710	61.1544	21.5643		
42.6086	38.1728	62.3750	20.2959		
43.8792	37.2230	63.5001	19.6611		
44.7644	35.7307	65.1885	18.1395		
46.6736	34.5025	66.1107	17.5926		
49.1516	32.0903	68.2303	15.8617		
49.4078	31.7846	68.3316	15.6764		

Table S5. Experimental binodal weight fraction data for the systems composed of PEG-400 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch]Cl		[Ch][Ac]		[Ch][Gly]	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
7.1213	76.8869	3.2068	76.0150	8.9800	73.0960
17.2346	62.9069	5.1602	71.1452	14.4505	64.3829
21.2144	59.4234	7.8633	65.7876	19.5541	57.2611
25.4565	55.8806	11.7567	61.4120	38.9308	42.4057
33.0541	49.3497	24.3122	51.7457		
41.2205	42.7683	46.8571	34.7135		
50.8729	34.9210				
55.7855	31.3935				
66.2262	23.4290				
79.4484	14.2674				

Table S6. Experimental binodal weight fraction data for the system composed of PEG-400 (1) + cholinium-based compounds (2) + H₂O (3) at 25 °C.

[Ch][Bic]		[Ch][Bit]			
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
4.6064	76.3149	7.8011	75.9681	43.0647	31.8304
8.3320	64.1211	9.4832	72.907	45.7267	28.9362
15.6190	55.3361	10.2361	72.6113	49.3708	24.8828
26.7269	44.5598	11.7189	70.1362	56.2237	18.692
32.0014	40.2773	13.8823	66.6712	60.6272	15.634
36.4901	36.9830	14.4581	66.0368		
40.6318	33.9896	17.13	62.1231		
48.0264	28.4390	18.0662	60.9821		
50.5827	26.7808	19.8168	58.6358		
52.9307	25.0938	21.0511	57.0553		
54.9675	23.6026	22.1392	55.4117		
56.6044	22.5111	24.0787	52.9587		
58.5185	21.1420	24.3736	53.2156		
61.2443	19.3907	26.3125	50.2153		
62.8251	18.1892	29.2908	47.42		
65.7587	16.3881	30.5618	46.0316		
67.9449	15.0253	33.564	42.823		
69.7628	13.8585	36.8994	38.8954		
71.5184	12.8512	37.6943	37.6425		
73.3357	11.7854	40.357	34.6342		

Table S7. Experimental binodal weight fraction data for the systems composed of PEG-400 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

		[Ch][DHph]		[Ch][DHcit]	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
3.6716	53.4546	42.0553	19.4554	13.1806	78.3618
4.8135	51.0734	42.7934	18.8797	15.3116	75.1863
6.4026	49.3956	43.7738	18.2112	17.7630	71.8563
7.2801	48.1931	44.4963	17.7162	19.7794	69.0637
8.9093	46.5262	45.1416	17.2364	21.4908	66.9473
9.0103	46.0556	45.8533	16.7336	22.9814	65.2655
9.8893	44.7814	46.6915	16.1961	26.9756	60.6960
11.6115	44.0309	47.4843	15.6883	31.5365	55.5813
11.6574	43.2697	47.7704	15.3936	33.5173	53.5943
13.3458	41.8102	48.4656	14.9302	55.9746	29.6529
14.0071	40.9596	49.1764	14.5247	63.7696	21.8183
14.1663	41.5895	49.6188	14.2025	78.0665	11.8720
15.3617	39.7276	50.0597	13.9099		
16.4821	39.4016	50.7538	13.5254		
19.7998	36.8986	51.2901	13.1531		
22.2638	34.8480	51.6791	12.8483		
25.2335	32.3340	52.3539	12.4772		
27.2864	30.8652	52.8065	12.1794		
29.0060	29.4020	53.2681	11.9716		
30.6375	28.1283	53.4129	11.7976		
32.3328	26.9291	53.8357	11.6034		
33.2111	26.0991	54.3215	11.3416		
34.6032	25.0208	54.8049	11.0756		
36.3226	23.8656				
37.1569	23.0901				
38.2859	22.2759				
39.4851	21.4441				
40.3493	20.7602				
41.1913	20.1146				

Table S8. Experimental binodal weight fraction data for the systems composed of PEG-1000 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch]Cl		[Ch][Ac]		[Ch][Gly]	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
10.3159	55.9164	14.1413	44.7570	3.7730	75.8240
15.4787	50.9733	11.7461	48.1524	3.9794	74.8555
23.9346	42.9799	8.2332	50.7311	10.1126	51.8951
26.8315	40.6761	4.9105	57.1192		
28.9920	38.7739				
30.9398	37.2033				
33.2309	35.6205				
36.1134	33.4080				
40.1175	30.0426				

Table S9. Experimental binodal weight fraction data for the systems composed of PEG-1000 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch][Bic]		[Ch][Bit]		[Ch][DHcit]	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
8.9373	50.2410	47.5877	18.7319	11.5142	65.9190
17.2464	43.1968	52.1811	15.6541	20.2953	55.4792
28.0776	34.5213	58.9611	11.3544	24.9578	50.4162
38.6946	26.5859			30.0832	44.9733
				34.3694	40.6179
				39.6771	35.4297
				65.9777	12.1468

Table S10. Experimental binodal weight fraction data for the systems composed of PEG-1000 (1) + cholinium-based compound (2) + H₂O (3) at 25 °C.

[Ch][DHph]		[Ch][Lac]	
100 w_1	100 w_2	100 w_1	100 w_2
1.7746	42.8039	15.7561	44.8122
5.1530	39.5994	16.1806	44.6486
5.9118	38.6642	16.5706	44.1932
8.3372	36.8751	17.1913	43.7647
9.5465	35.7104	17.5894	43.4275
11.9288	33.9082	18.0597	43.2344
14.1008	32.2892	19.1489	42.4859
15.6007	31.0811	19.8343	42.0052
16.1853	30.6909	23.6057	39.6832
18.0564	29.3371	24.1040	39.4349
20.0701	27.8683	25.2010	38.7108
20.8086	27.3407	25.8965	38.3027
22.3232	26.1851	27.9114	37.1174
23.7616	25.1932	28.5289	36.7135
24.9950	24.2966	31.4981	35.0675
26.1277	23.4752	33.0462	34.0997
27.7318	22.4400	34.7185	33.1887
28.4685	21.8366	37.6671	31.4616
29.6530	21.0477	43.7098	28.1400
30.1286	20.7187	45.0858	27.3435
30.5535	20.4044		
30.7845	20.2242		
31.2736	19.9092		
32.0671	19.3429		
32.4456	19.0838		

Table S11. Experimental binodal weight fraction data for the systems composed of PEG-600 (1) + cholinium-based compound (2) + H₂O (3) at 50 °C.

[Ch]Cl					
100 <i>w</i> ₁	100 <i>w</i> ₂	100 <i>w</i> ₁	100 <i>w</i> ₂	100 <i>w</i> ₁	100 <i>w</i> ₂
28.2913	40.1033	47.7682	25.7388	62.8462	16.1569
29.2787	39.0705	48.6565	24.8002	66.2151	13.6323
30.1001	38.2844	49.8244	23.8900	69.0106	11.8901
35.3568	32.9795	50.4489	23.5896	70.9403	10.9921
36.7088	32.2928	51.5359	22.6979	72.8610	9.9856
39.2230	30.3882	52.2768	22.5276	73.8627	9.3745
40.6534	29.4672	55.2205	20.4676		
41.8976	28.6241	57.1488	19.1507		
43.7878	28.0371	58.8008	18.2194		
45.0558	27.1202	60.4173	17.5116		
46.3820	26.5555	61.5336	16.8868		
46.7227	26.3233	62.6406	16.1757		

Table S12. Experimental binodal weight fraction data for the systems composed of PEG-600 (1) + cholinium-based salt (2) + H₂O (3) at 50 °C.

[Ch][DHph]					
100 <i>w</i> ₁	100 <i>w</i> ₂	100 <i>w</i> ₁	100 <i>w</i> ₂	100 <i>w</i> ₁	100 <i>w</i> ₂
31.3762	13.3265	22.2018	20.5149	17.6025	24.8837
30.2439	14.0226	21.7106	20.9190	17.3274	24.9135
29.3004	14.7128	21.2229	21.6157	17.1787	25.0806
28.4862	15.4347	20.8211	21.8461	17.0421	25.2753
27.5450	16.1061	20.2992	22.3654	16.8684	25.3990
26.8153	16.6050	20.0108	22.5466	16.6779	25.5152
26.1310	17.2072	19.4983	22.9400	16.5594	25.7225
25.4250	17.7209	19.0791	23.4066	16.3256	26.0864
24.9793	18.3478	18.7265	23.7561	16.0555	26.0677
24.2465	18.6779	18.5013	23.9286	15.9293	26.2669
23.8196	19.3007	18.3071	24.0724	15.7754	26.4472
23.2445	19.6310	18.1064	24.3007	15.5822	26.5295
22.6666	20.1209	17.9131	24.4555		

Table S13 presents the initial mixture compositions and the respective conductivity and pH values of each phase.

Table S13. Initial mixture compositions, pH, and conductivities of the coexisting phases at 25 °C.

Ternary System	Weight Fraction Composition / (wt %)		pH		Conductivity / (mS.cm ⁻¹)		Phase	
	PEG-600	[Ch] ⁺ salts	Top	Bottom	Top	Bottom	Top	Bottom
[Ch]Cl	57.93	29.93	7.19 ± 0.05	7.23 ± 0.09	30.50	0.601	IL	PEG
	57.85	26.84	7.44 ± 0.10	7.33 ± 0.06	20.70	3.330	IL	PEG
	54.69	27.73	-	-	10.98	0.507	IL	PEG
	57.73	22.88	7.14 ± 0.10	7.58 ± 0.37	9.810	1.691	IL	PEG
[Ch][Bic]	45.78	29.49	-	-	0.482	22.00	PEG	IL
	39.81	32.01	11.03 ± 0.19	10.33 ± 0.01	0.550	17.70	PEG	IL
[Ch][Bit]	35.97	39.93	-	-	0.313	4.96	PEG	IL
	35.17	38.73	4.92 ± 0.21	4.62 ± 0.06	0.517	4.88	PEG	IL
[Ch][Ac]	48.52	40.94	-	-	2.690	0.580	IL	PEG
	50.01	29.97	9.01 ± 0.01	9.00 ± 0.07	7.760	0.641	IL	PEG
[Ch][DHcit]	61.79	28.62	5.52 ± 0.12	5.33 ± 0.31	0.208	1.160	PEG	IL
	59.61	27.40	5.58 ± 0.02	5.33 ± 0.16	0.364	-	PEG	IL
[Ch][DHph]	40.19	30.07	6.86 ± 0.05	6.04 ± 0.08	0.092	2.640	PEG	IL
[Ch][Gly]	30.07	59.92	-	-	0.382	6.670	PEG	IL

Figures S1 to S6 show the comparison of different PEG molecular weights for the systems with [Ch][Bit], [Ch][Bic], [Ch][DHCit], [Ch][Lac], [Ch][Gly], and [Ch]Cl.

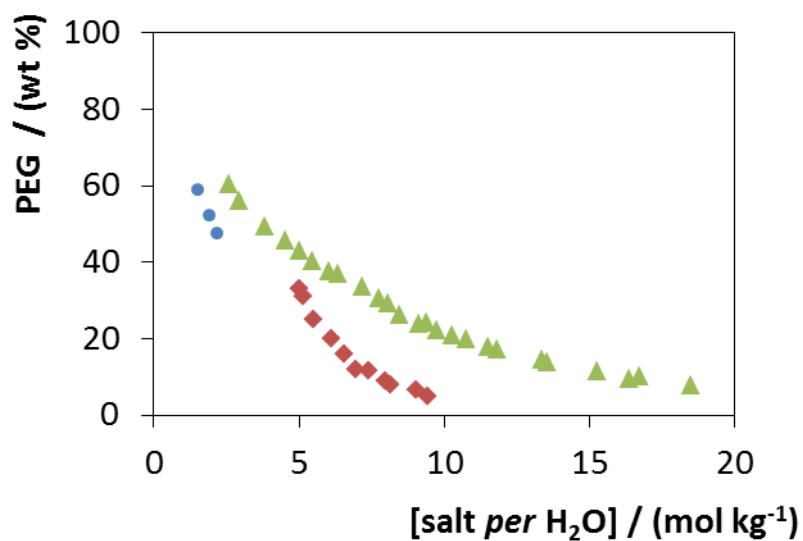


Figure S1. Experimental solubility data for PEG/[Ch][Bit] ABS at 25 °C (evaluation of the PEG molecular weight): (●) PEG-1000; (◆) PEG-600; (▲) PEG-400.

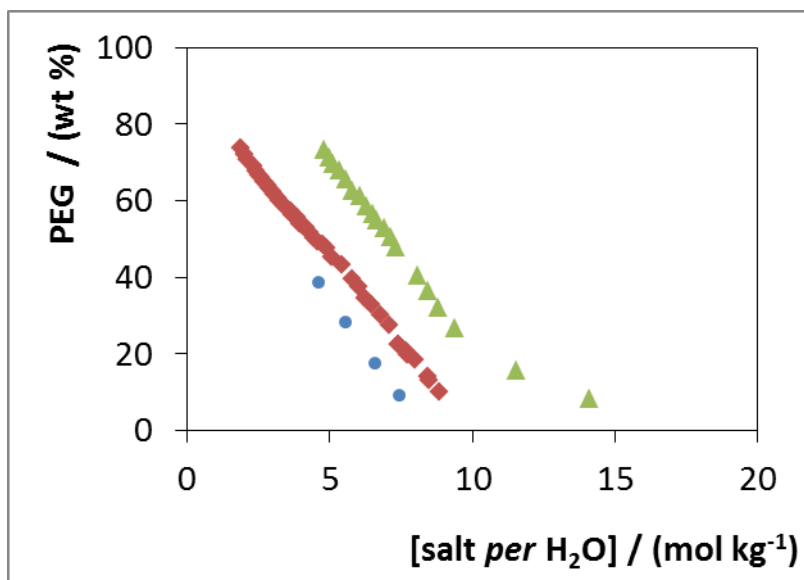


Figure S2. Experimental solubility data for PEG/[Ch][Bic] ABS at 25 °C (evaluation of the PEG molecular weight): (●) PEG-1000; (◆) PEG-600; (▲) PEG-400.

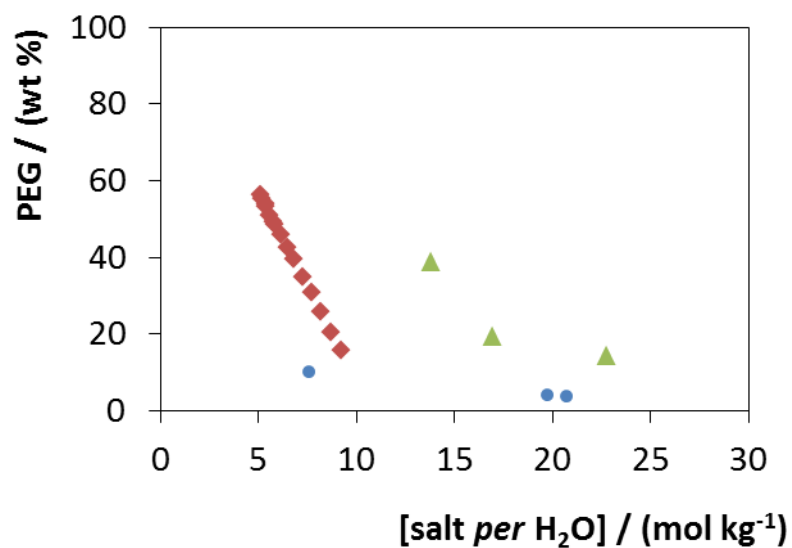


Figure S3. Experimental solubility data for PEG/[Ch][DHcit] ABS at 25 °C (evaluation of the PEG molecular weight): (●)-PEG 1000; (◆) PEG-600; (▲) PEG-400.

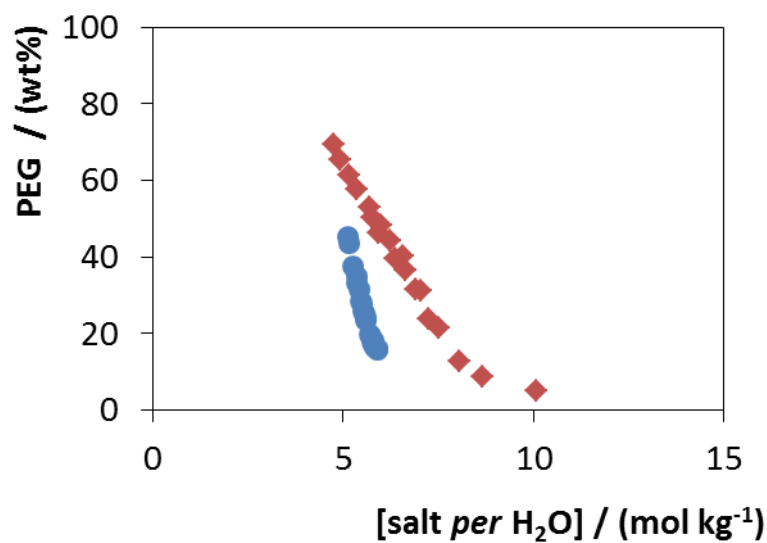


Figure S4. Experimental solubility data for PEG/[Ch][Lac] ABS at 25 °C (evaluation of the PEG molecular weight): (●) PEG-1000; (◆) PEG-600.

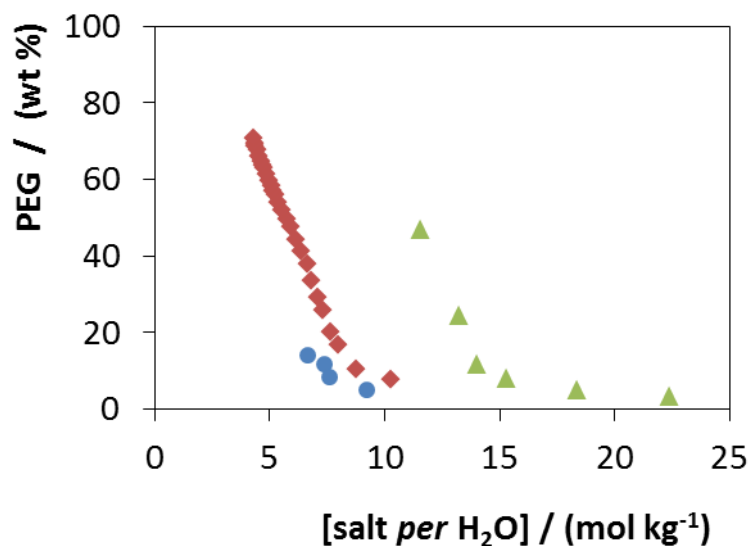


Figure S5. Experimental solubility data for PEG/[Ch][Gly] ABS at 25 °C (evaluation of the PEG molecular weight): (●) PEG-1000; (◆) PEG-600; (▲) PEG-400.

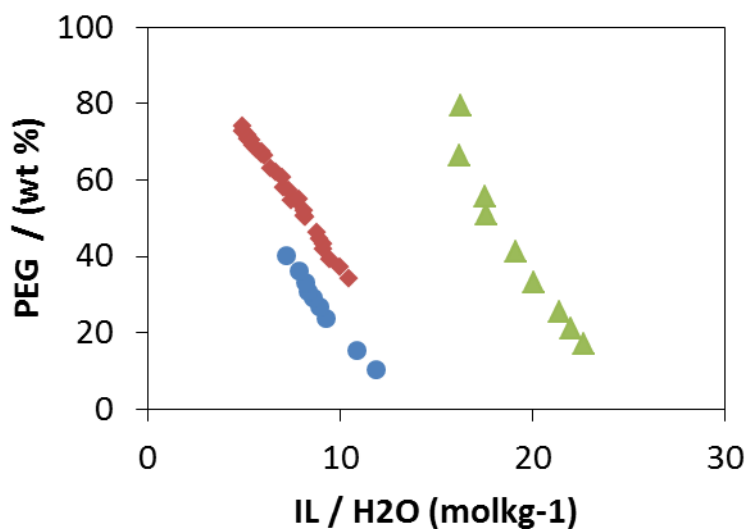


Figure S6. Experimental solubility data for PEG/[Ch]Cl ABS at 25 °C (evaluation of the PEG molecular weight): (●) PEG-1000; (◆) PEG-600; (▲) PEG-400.

Figures S7 to S12 show the COSMO-RS prediction results.

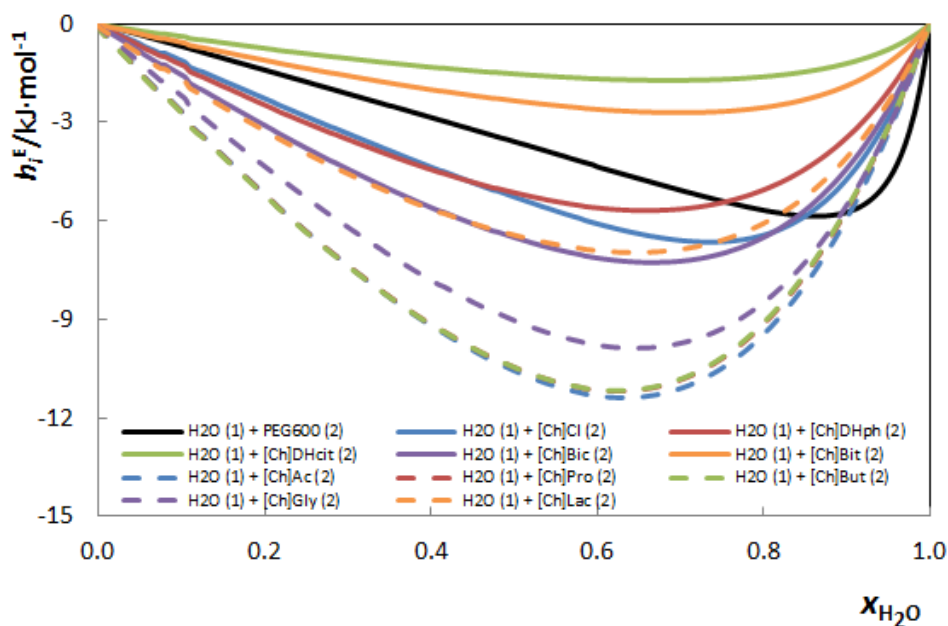


Figure S7. Excess enthalpies between water and the IL, salt or PEG-600 predicted by COSMO-RS as a function of the water mole fraction ($x_{\text{H}_2\text{O}}$).

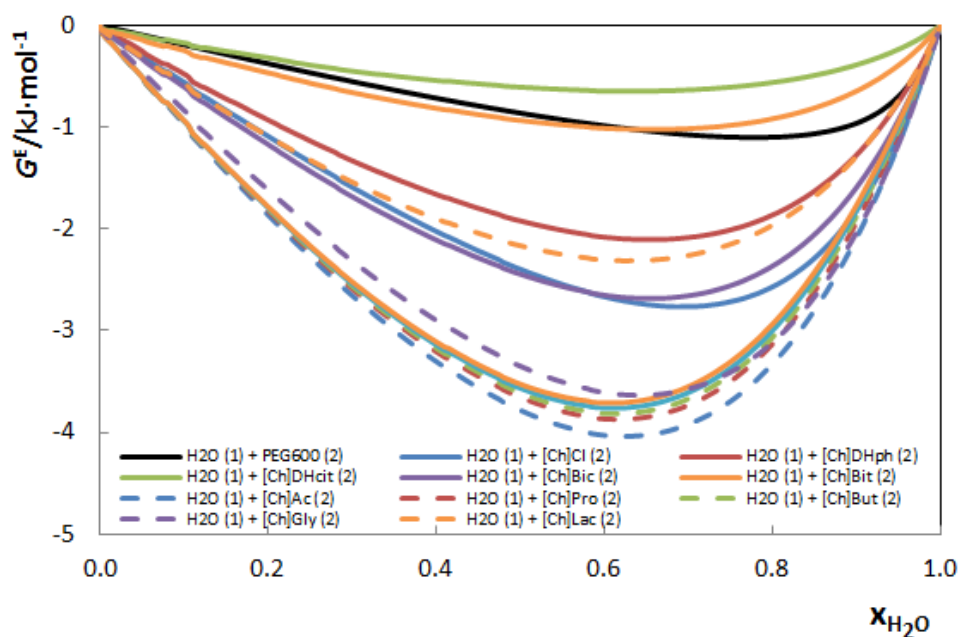


Figure S8. Excess Gibbs free energy of mixing, G^E , between water and the IL, salt or PEG-600 predicted by COSMO-RS as a function of the water mole fraction ($x_{\text{H}_2\text{O}}$).

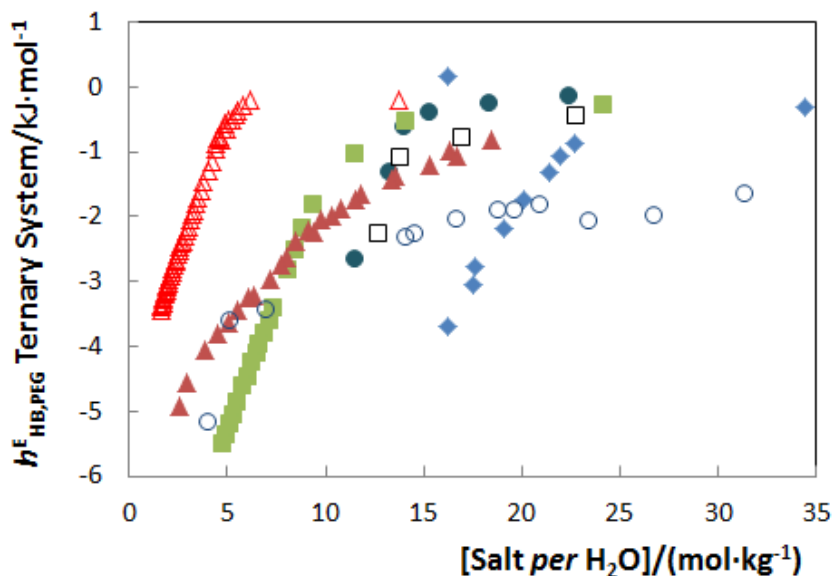


Figure S9. Partial molar excess enthalpies of PEG-400 in the ternary system at 25 °C as a function of the concentration of salt *per* H₂O predicted by COSMO-RS: (Δ) [Ch][DHph]; (\blacktriangle) [Ch][Bit]; (\circ) [Ch][DHcit]; (\blacksquare) [Ch][Bic]; (\square) [Ch][Gly]; (\bullet) [Ch][Ac]; (\blacklozenge) [Ch]Cl.

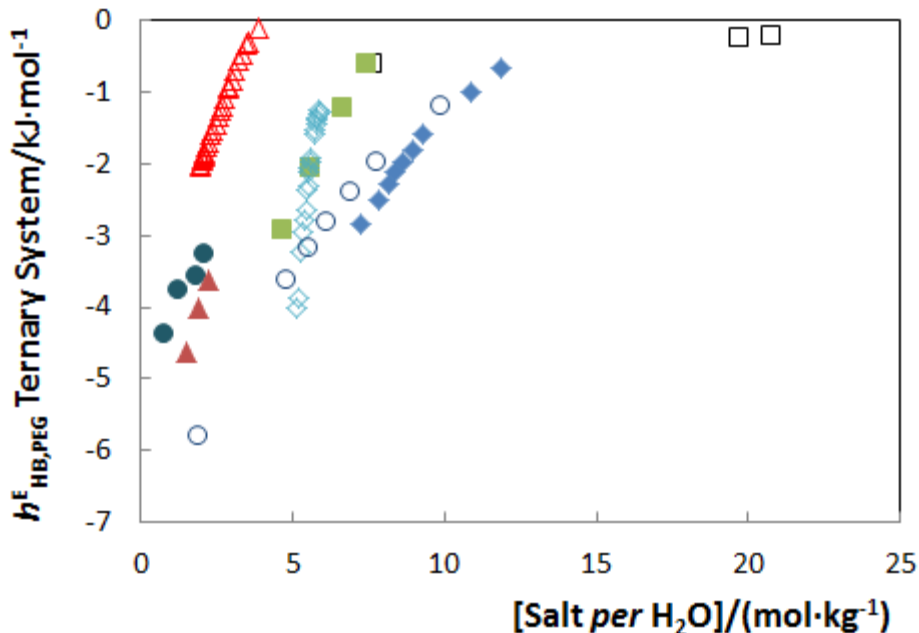


Figure S10. Partial molar excess enthalpies of PEG-1000 in the ternary system at 25 °C as a function of the concentration of salt *per* H₂O predicted by COSMO-RS: (Δ) [Ch][DHph]; (\blacktriangle) [Ch][Bit]; (\circ) [Ch][DHcit]; (\blacksquare) [Ch][Bic]; (\diamond) [Ch][Lac]; (\square) [Ch][Gly]; (\bullet) [Ch][Ac]; (\blacklozenge) [Ch]Cl.

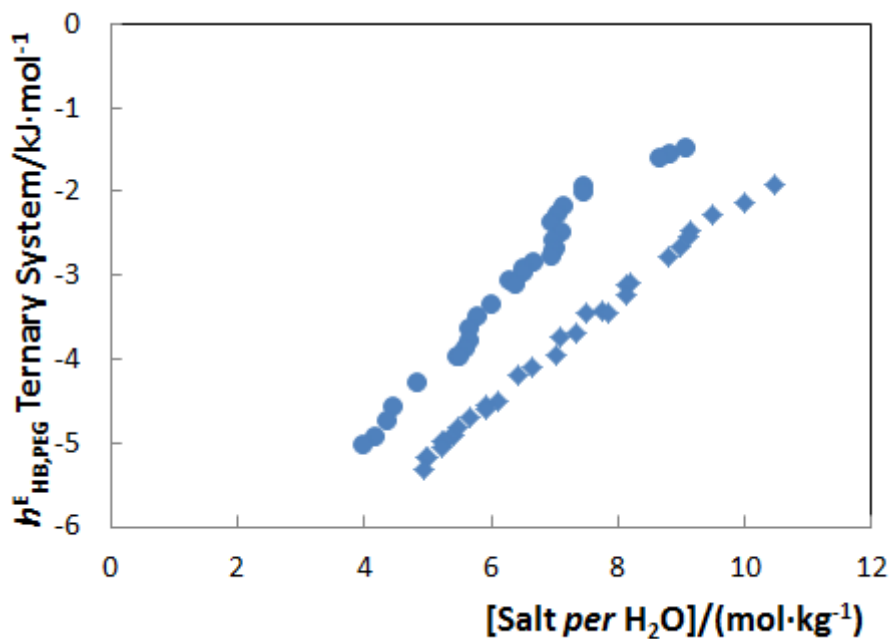


Figure S11. Partial molar excess enthalpies of PEG-600 in the ternary system at 25 °C as a function of the concentration of salt *per* H₂O predicted by COSMO-RS at 25 and 50 °C: (◆) PEG 600 + [Ch]Cl at 25 °C; (●) PEG-600 + [Ch]Cl at 50 °C.

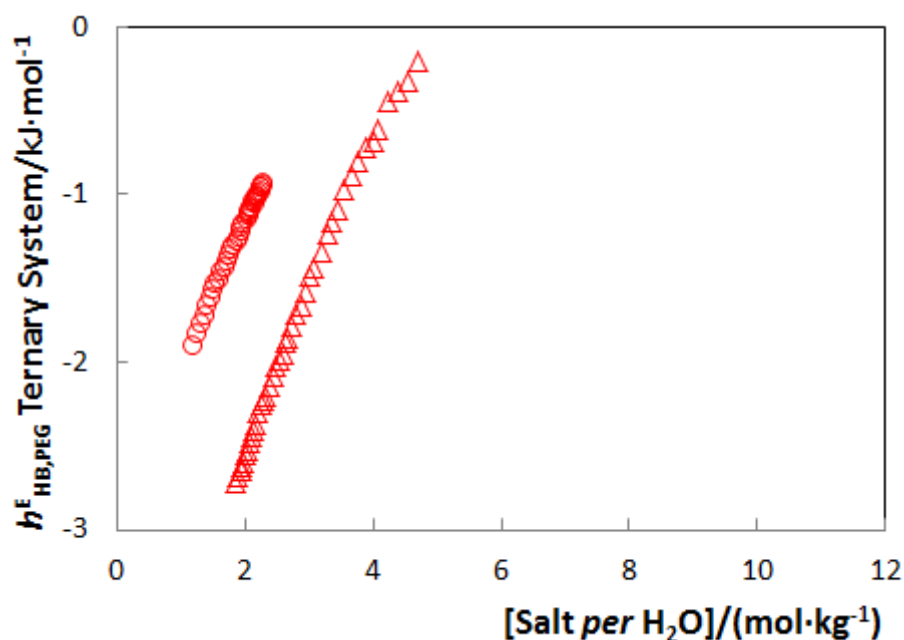


Figure S12. Partial molar excess enthalpies of PEG-600 in the ternary system at 25 °C as a function of the concentration of salt *per* H₂O predicted by COSMO-RS at 25 and 50 °C: (Δ) PEG-600 + [Ch][DHph] at 25 °C; (○) PEG-600 + [Ch][DHph] at 50 °C.

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