Electronic Supplementary Material (ESI) for Physical Chemistry Chemical Physics.

Supplementary Information

Poly(ionic liquid)s as Phase Splitting Promoters in Aqueous Biphasic Systems

Karen João,[a‡] Liliana C. Tomé,[a‡] Mehmet Isik,[b] David Mecerreyes,[b,c] and Isabel M. Marrucho[a]*

[a] Instituto de Tecnologia Química e Biológica António Xavier, Universidade Nova de Lisboa, Av. da República, 2780-157 Oeiras, Portugal.

[b] POLYMAT, Institute for Polymer Materials, University of the Basque Country UPV/EHU, Joxe Mari Korta Center, Avda. Tolosa 72, 20018 Donostia-San Sebastian, Spain.

[c] IKERBASQUE, Basque Foundation for Science, E-48011 Bilbao, Spain.

‡ Equally contributing authors

* Corresponding author

Tel: +351 21 4469720

Fax: +351 21 4411277

E-mail: imarrucho@itqb.unl.pt

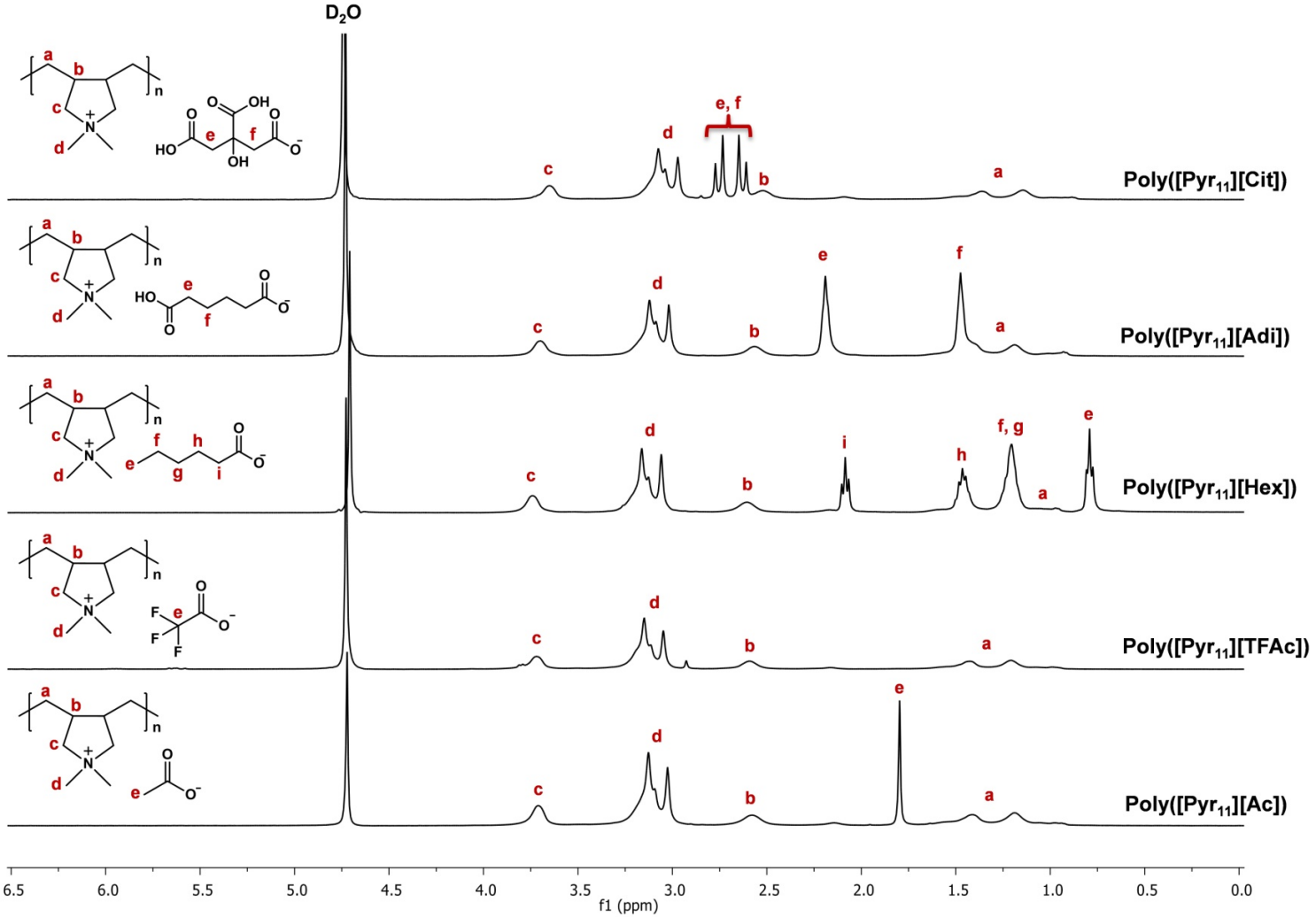

Fig. S1 ^{1}H – NMR spectra of the prepared pyrrolidinium-based PILs containing carboxylated counter-anions.

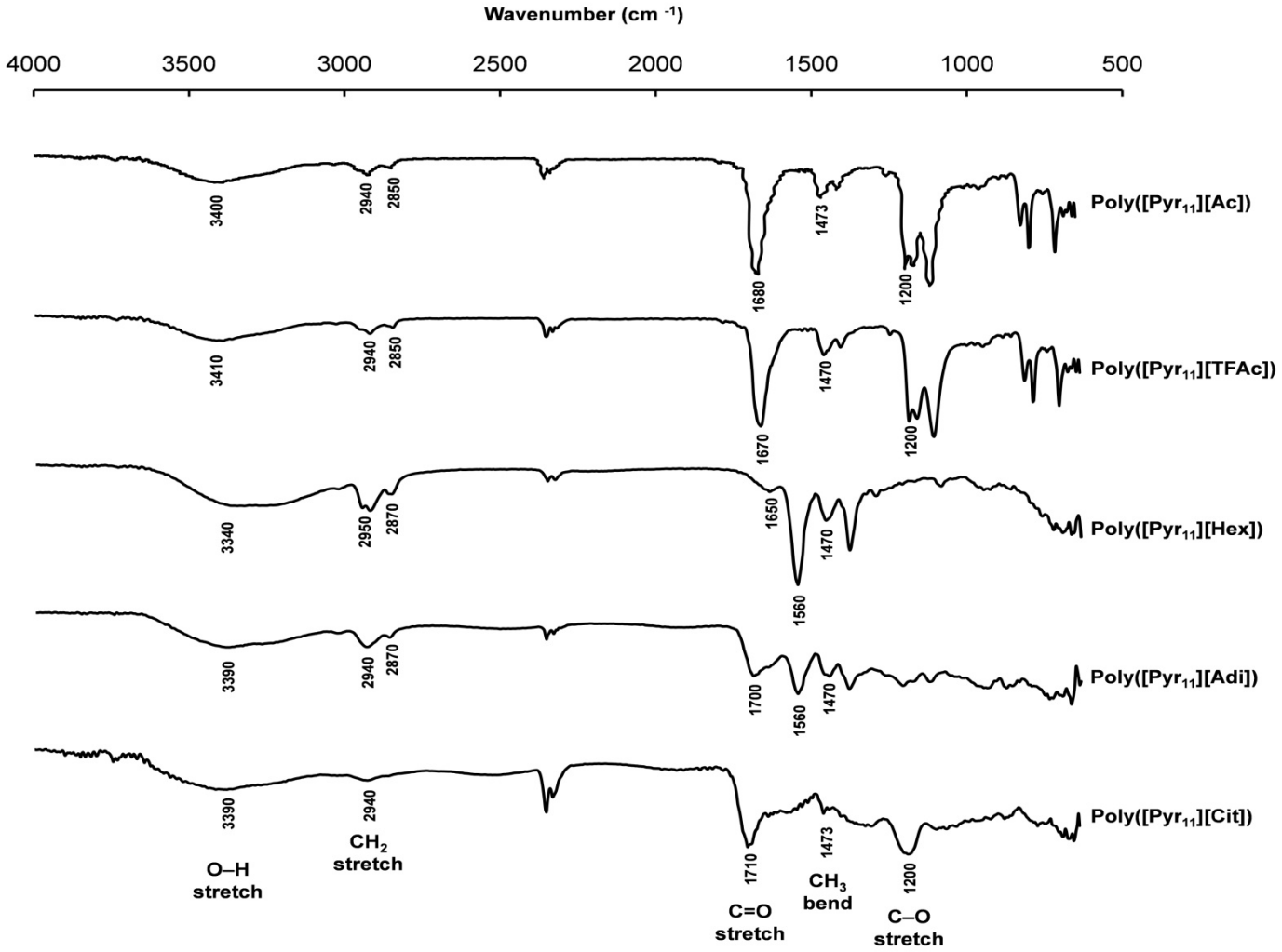

Fig. S2 FTIR transmission spectra of the prepared pyrrolidinium-based PILs containing carboxylate counter-anions.

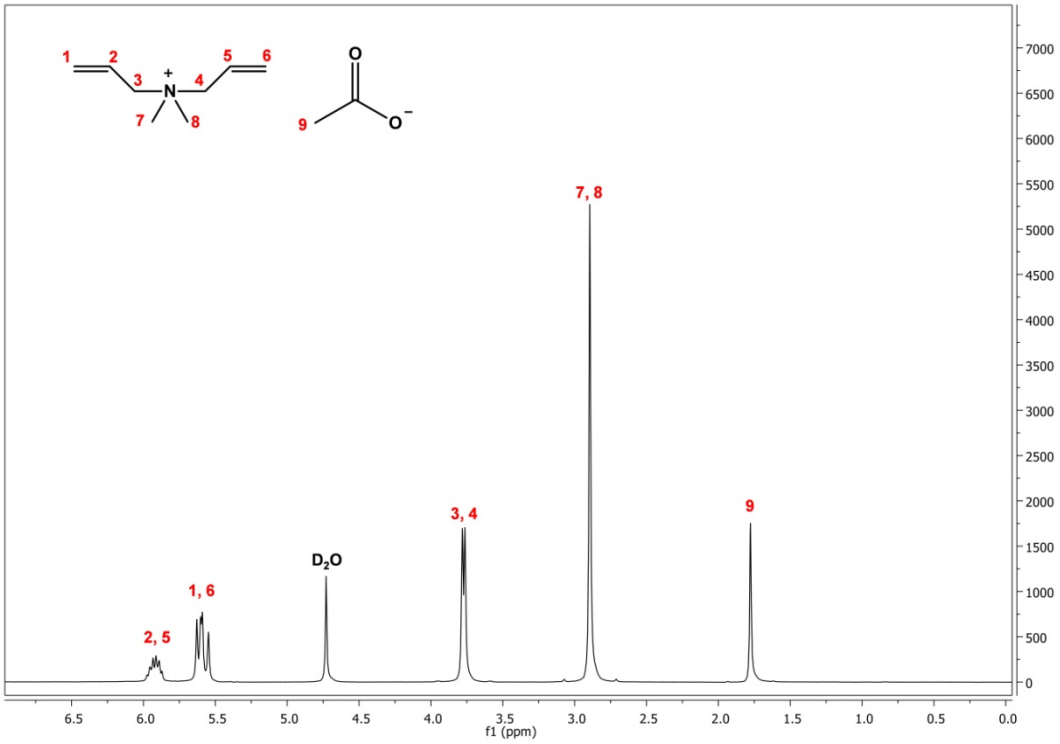

Fig. S3 ^{1}H-NMR spectrum of diallyldimethylammonium acetate monomer in D_2O.

Fig. S4 ^{13}C-NMR spectrum of diallyldimethylammonium acetate monomer in D_2O.

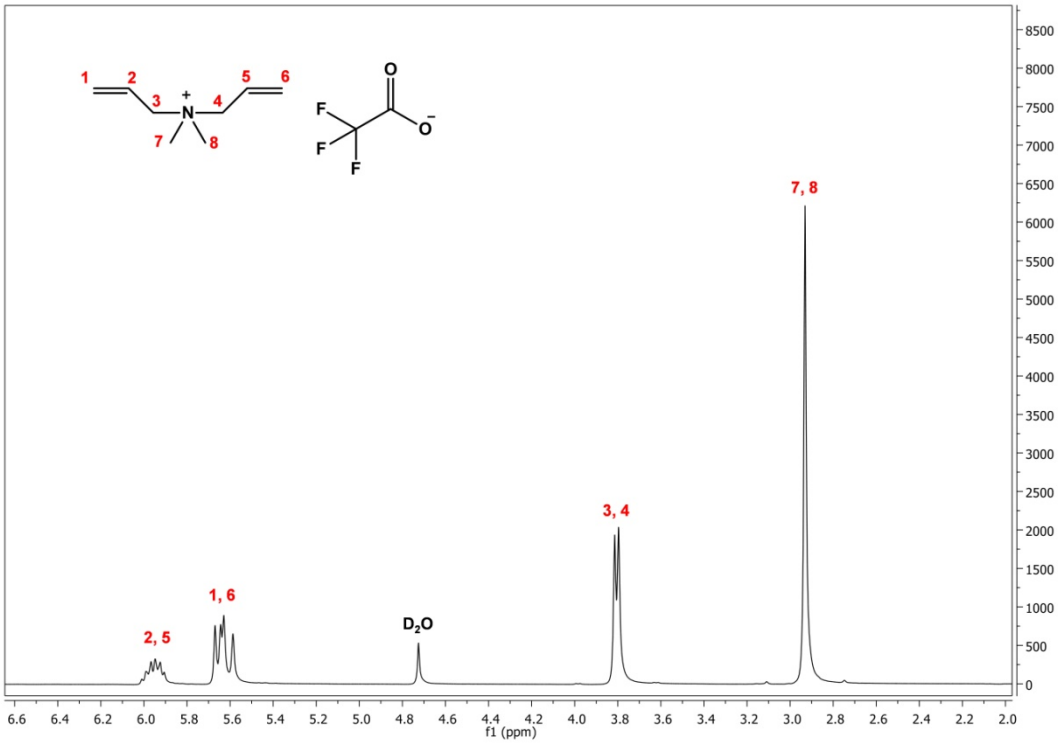

Fig. S5 ^{1}H-NMR spectrum of diallyldimethylammonium trifluoroacetate monomer in D_2O.

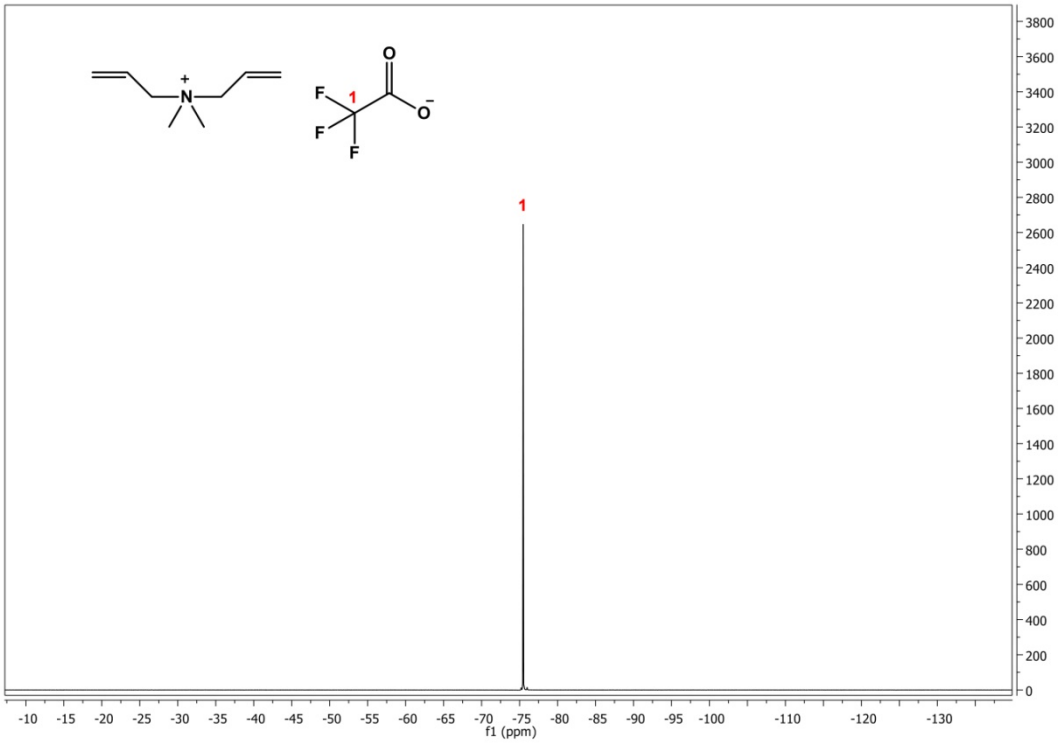

Fig. S6 ^{19}F-NMR spectrum of diallyldimethylammonium trifluoroacetate monomer in D_2O.

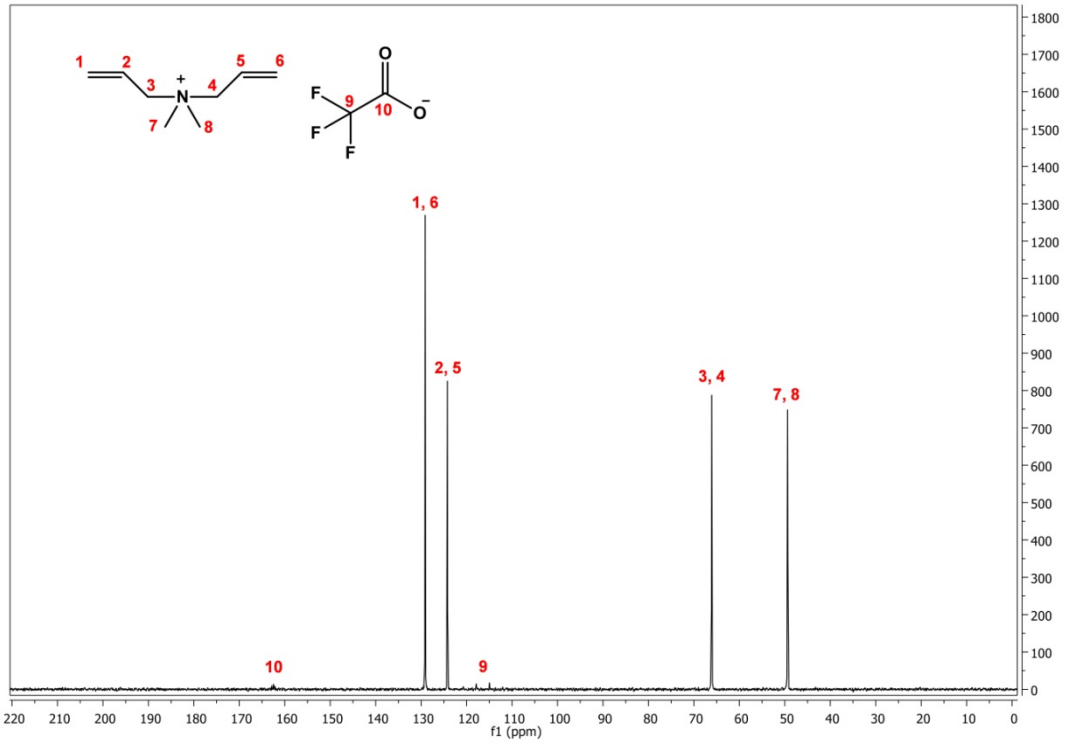

Fig. S7 ^{13}C-NMR spectrum of diallyldimethylammonium trifluoroacetate monomer in D_2O.

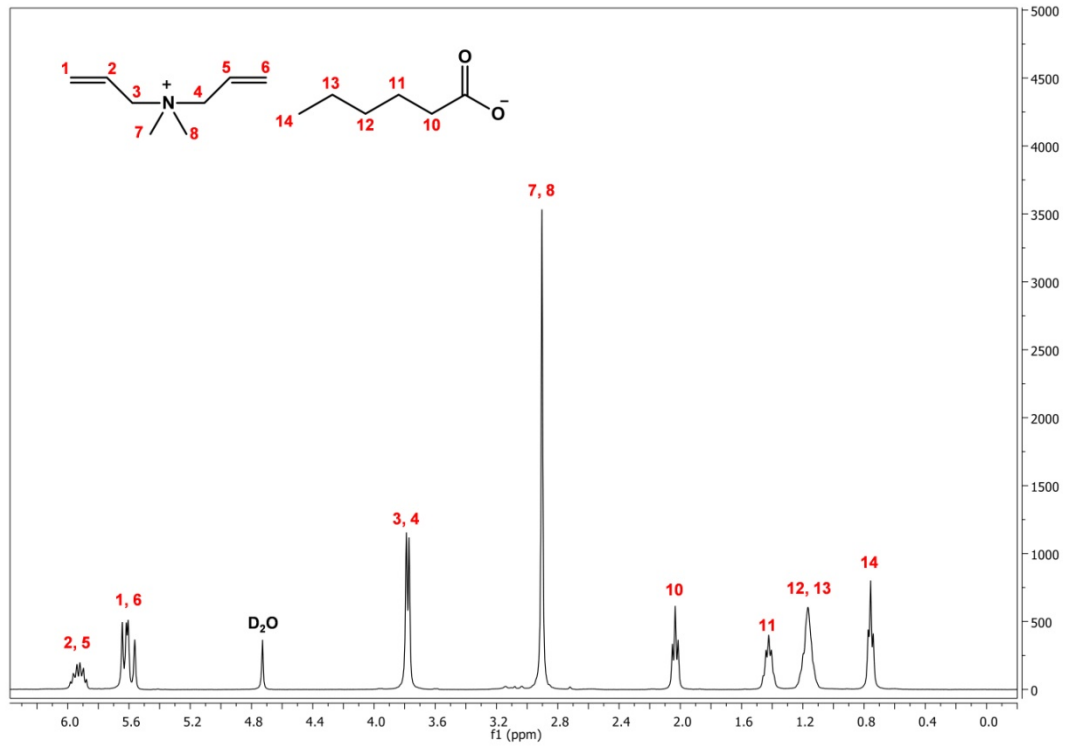

Fig. S8 ^{1}H-NMR spectrum of diallyldimethylammonium hexanoate monomer in D_2O.

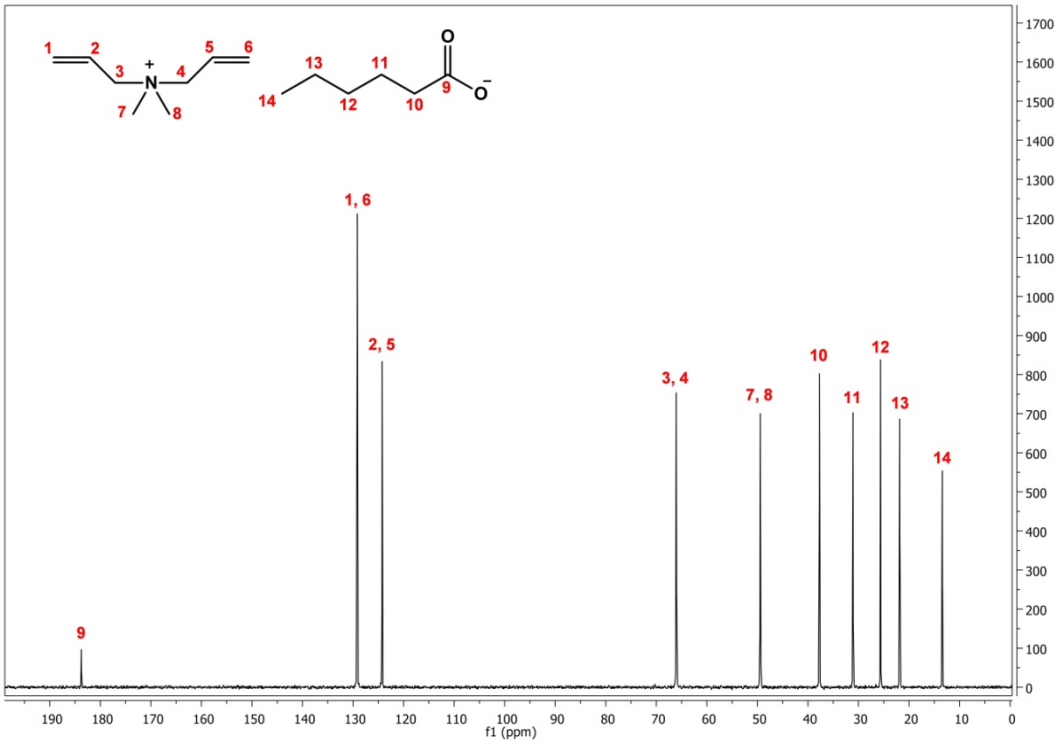

Fig. S9 ^{13}C-NMR spectrum of diallyldimethylammonium hexanoate monomer in D_2O.

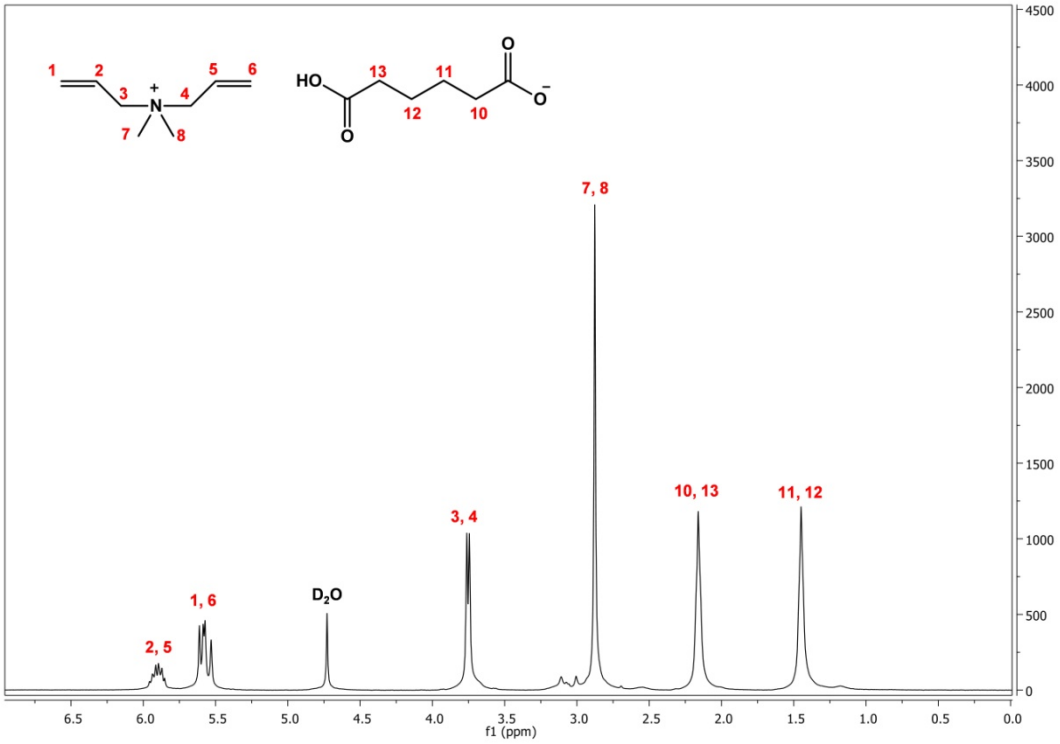

Fig. S10 ^{1}H-NMR spectrum of diallyldimethylammonium adipate monomer in D_2O.

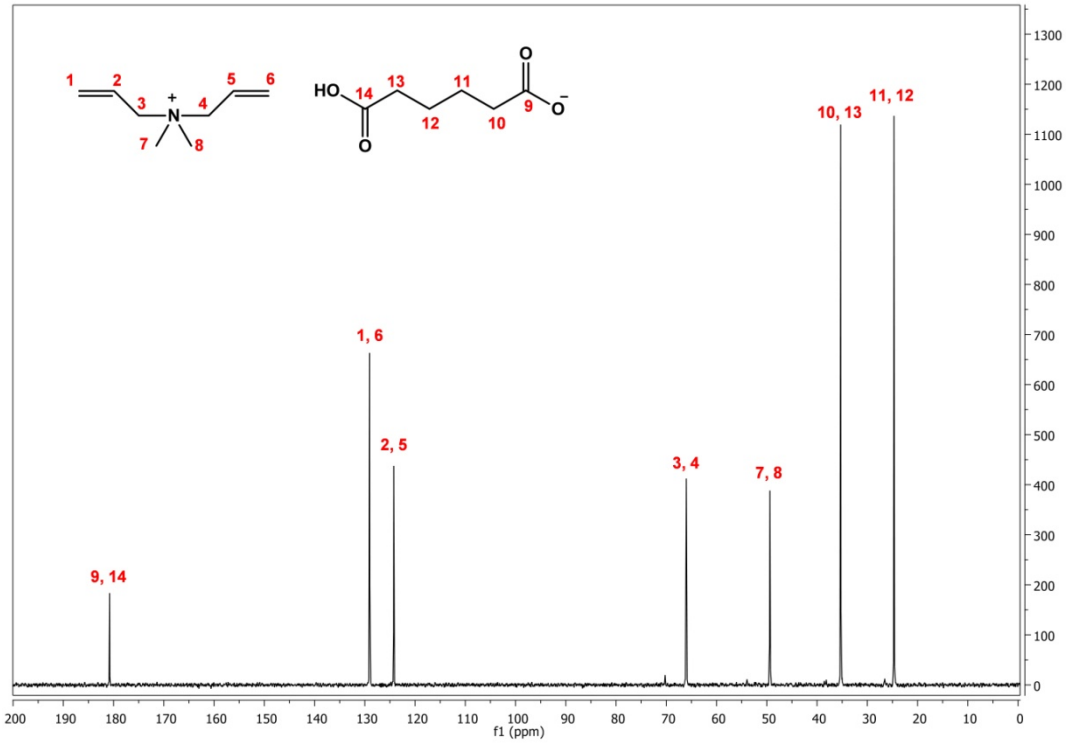

Fig. S11 ^{13}C-NMR spectrum of diallyldimethylammonium adipate monomer in D_2O.

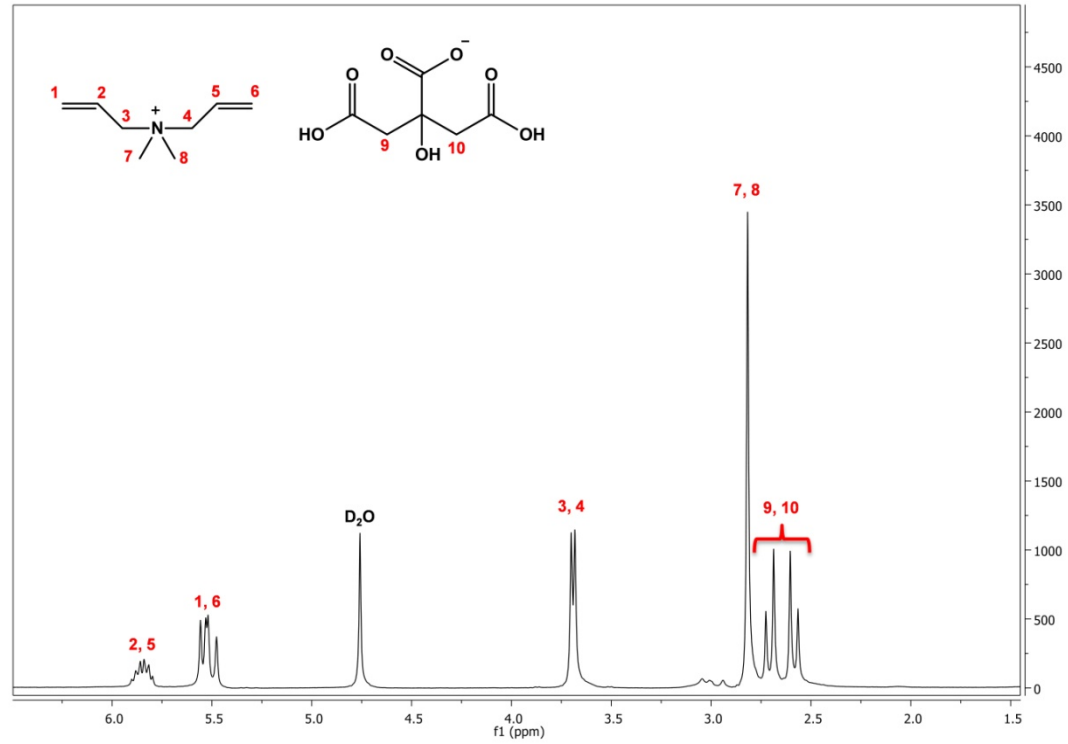

Fig. S12 ^{1}H-NMR spectrum of diallyldimethylammonium citrate monomer in D_2O.

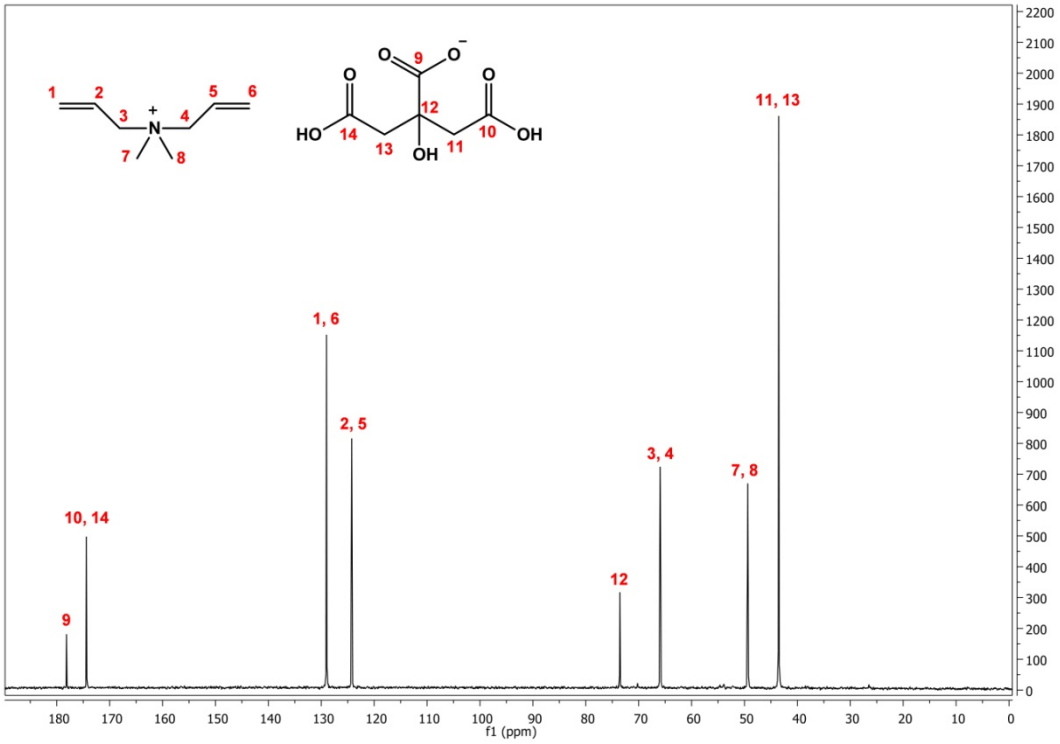

Fig. S13 ^{13}C-NMR spectrum of diallyldimethylammonium citrate monomer in D_2O

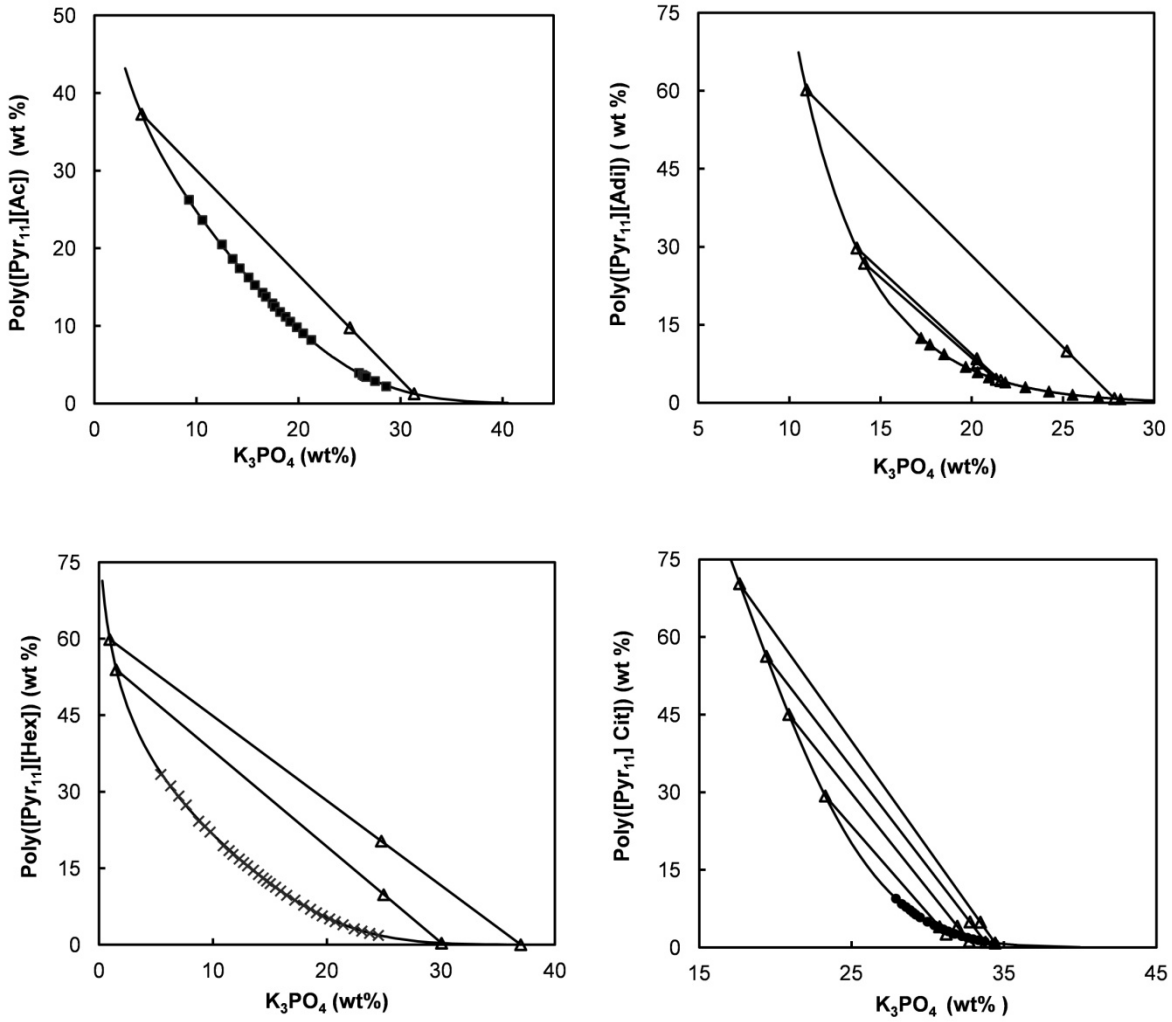

Fig. S14 Phase diagrams and experimental tie-lines of the PIL + K_3PO_4 + H_2O ternary systems at 25 ºC: TL data (Δ).

Table S1. Weight fraction data for the ternary systems composed of PIL (1) + K_3PO_4 (2) + H_2O (3) at 25 ºC.

Poly([Pyr_{11}][Ac]) M_w = 52 kDa		Poly([Pyr_{11}][TFAc]) M_w = 41 kDa		Poly([Pyr_{11}]Cl) High M_w (400–500 kDa)	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
26.2596	9.2460	20.1130	9.0706	25.8046	8.0396
23.6251	10.5594	18.3199	9.7905	23.6962	9.1665
20.4992	12.4717	17.1880	10.3080	21.4650	10.1486
18.6420	13.5263	16.2908	10.7877	20.1946	10.7919
17.4376	14.2218	15.6233	11.0443	18.9313	11.5523
16.2429	15.0783	14.8718	11.5248	17.5925	12.2591
15.2695	15.7040	13.9168	11.8824	16.6004	12.9244
14.2799	16.4490	13.1502	12.3178	15.8620	13.3244
13.7514	16.7815	12.4401	12.7331	15.1564	13.6620
12.9176	17.4303	11.6786	13.1785	13.9121	14.5306
12.4770	17.6629	10.8677	13.6576	12.5483	15.3530
11.8025	18.1863	10.1428	14.0940	11.3299	16.1939
11.1769	18.7167	9.2839	14.7144	10.2933	17.0193
10.5376	19.1782	8.3619	15.4104	9.3169	17.7953
9.8251	19.8267	7.6017	16.0023	8.4428	18.4450
9.0529	20.4304	6.9327	16.6163	7.7168	19.1538
8.1961	21.2268	6.2680	17.2076	6.9568	19.9035
3.9362	25.9181	5.5884	17.9142	6.4959	20.4209
3.6874	26.2579	4.9642	18.5869	6.0738	20.8780
3.5535	26.4338	4.4495	19.2114	5.6254	21.3720
3.4284	26.6076	3.9709	19.8345	4.9988	22.1552
2.8864	27.4917	3.5277	20.4825	4.3846	22.9050
2.2169	28.5805	3.0997	21.1735	3.6505	24.1190
-	-	2.6971	21.8946	1.9116	27.4357
-	-	2.2861	22.7370	-	-
-	-	1.8250	23.8209	-	-
-	-	1.3759	25.1175	-	-
-	-	1.0118	26.4352	-	-

Poly([Pyr_{11}]Cl) Medium M_w (200–350 kDa)		Poly([Pyr_{11}]Cl) Low M_w (< 100 kDa)		Poly([Pyr_{11}][Hex]) Mw = 53 kDa	
100 w_1	100 w_2	100 w_1	100 w_2	100 w_1	100 w_2
28.0804	6.3072	27.4065	7.1018	33.4319	5.4320
25.5056	7.5317	25.4169	7.8315	31.1727	6.3029
23.6835	8.4730	23.3960	8.8055	29.2123	7.0147
22.1401	9.2245	21.1792	10.0928	27.4774	7.6531
20.4171	9.9699	19.7409	10.8721	26.2518	7.8902
18.7790	10.8067	18.4385	11.6105	25.1050	8.5309
17.1123	11.9289	17.1289	12.5842	24.2942	8.7540
16.0596	12.4389	15.2265	13.6780	23.2578	9.2987
14.8766	13.2595	13.0583	15.0552	22.1119	9.7388
13.3804	14.3868	11.7321	16.0789	20.6702	10.6775
11.9669	15.2181	10.4187	17.1103	19.4208	10.9106
11.0020	15.9985	9.5497	17.8319	18.5079	11.4175
9.8745	16.9520	8.7117	18.6504	17.7499	11.7460
8.7849	17.8502	7.4660	19.7302	16.8723	12.3133
7.9404	18.6015	6.6567	20.5798	16.1797	12.6817
7.1880	19.3276	6.0333	21.2744	15.5120	13.0355
6.3646	20.2068	5.0364	22.4768	14.6703	13.5454
5.4585	21.2498	3.7428	24.2894	13.8179	13.9930
4.4784	22.5157	2.8569	25.8212	13.1396	14.4006
3.6918	23.6931	2.3227	26.9320	12.5304	14.7101
3.1105	24.6746	1.8704	27.9495	12.0027	15.0169
2.5726	25.6230	1.3977	29.4635	11.3467	15.4919
2.0376	26.7827	-	-	10.5947	15.9475
1.4612	28.3001	-	-	9.7573	16.4706
-	-	-	-	8.7911	17.1887
-	-	-	-	7.7706	17.9594
-	-	-	-	6.9835	18.5629
-	-	-	-	6.3134	19.0761
-	-	-	-	5.7100	19.5988

-	-	-	-	5.1167	20.2240
-	-	-	-	4.5542	20.7250
-	-	-	-	3.9381	21.4057
-	-	-	-	3.1403	22.4014
-	-	-	-	2.6903	23.0655
-	-	-	-	2.2803	23.7447
-	-	-	-	1.8873	24.5169

Poly([Pyr_{11}][Adi]) Mw = 50 kDa		Poly([Pyr_{11}][Cit]) Mw = 31 kDa	
100 w_1	100 w_2	100 w_1	100 w_2
16.2146	16.2602	9.4685	27.8959
15.1523	16.5998	8.4626	28.2809
14.1028	16.7876	7.8686	28.5673
13.2847	17.0620	7.2712	28.8307
12.4588	17.2050	6.7639	29.0353
11.1991	17.6956	6.3972	29.1983
9.3271	18.4763	5.8366	29.4870
7.9456	18.9798	5.0251	29.9689
6.8789	19.6499	4.3260	30.4141
5.8598	20.3072	3.8578	30.7657
4.9019	20.9270	3.5230	31.0061
3.9267	21.8240	3.1336	31.3298
2.9797	22.9269	2.6640	31.7649
2.1761	24.2171	2.2285	32.2239
1.5420	25.5190	1.9158	32.6041
1.0659	26.9295	1.6502	32.9566
0.7195	28.1532	1.4225	33.3210
-	-	1.1701	33.7333
-	-	0.8549	34.3658

Table S2. Weight fraction data for the ternary systems composed of poly([Pyr_{11}]Cl) high M_w (400–500 kDa) (1) + K_3PO_4 (2) + H_2O (3) at 40 ºC and 50 ºC.

Poly([Pyr_{11}]Cl) 40 ºC		Poly([Pyr_{11}]Cl) 50 ºC	
100 w_1	100 w_2	100 w_1	100 w_2
26.0203	8.7972	26.3240	9.2903
24.3447	9.4210	24.2191	10.3755
22.3937	10.5640	21.5039	11.3209
20.4943	11.2979	20.0747	12.0556
18.8006	12.3349	18.5554	13.0256
17.5516	12.9834	17.1118	13.7603
16.4738	13.7424	15.9488	14.5412
15.4574	14.3025	14.9763	15.1714
14.6820	14.7578	14.0864	15.7337
13.9325	15.2505	13.6405	15.9533
13.2139	15.7357	12.4914	16.6140
12.2814	16.3693	10.8497	18.0426
10.5734	17.6728	9.5972	19.0802
9.1872	18.8952	8.7112	19.8904
8.1092	19.9785	7.9455	20.6774
7.4815	20.5826	7.1256	21.5504
6.2985	21.6968	6.4991	22.2353
5.2284	22.9240	5.8385	23.0930
3.9837	24.7486	5.0986	24.0146
3.2152	26.1229	4.4151	24.9874
2.6891	27.0787	3.6926	26.1375
-	-	2.8772	27.5851