Electronic Supplementary Material (ESI) for RSC Advances.

Efficiency of Hydrophobic phosphonium ionic liquids and DMSO as recyclable cellulose dissolution and regeneration media

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Supporting Information

S1. NMR Spectra of Ionic Liquids

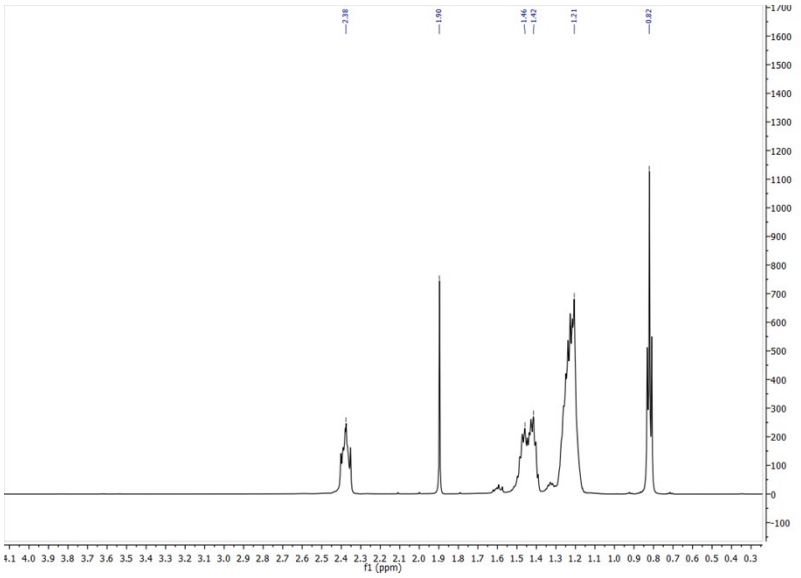

Figure 1: ^{1}H NMR spectra, [P_{8888}][OAc]

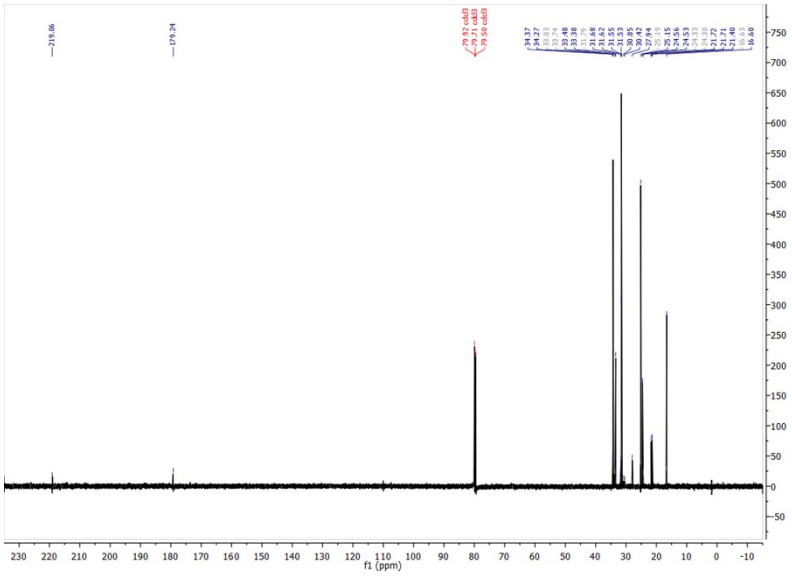

Figure 2: ^{13}C NMR spectra, [P_{8888}][OAc]

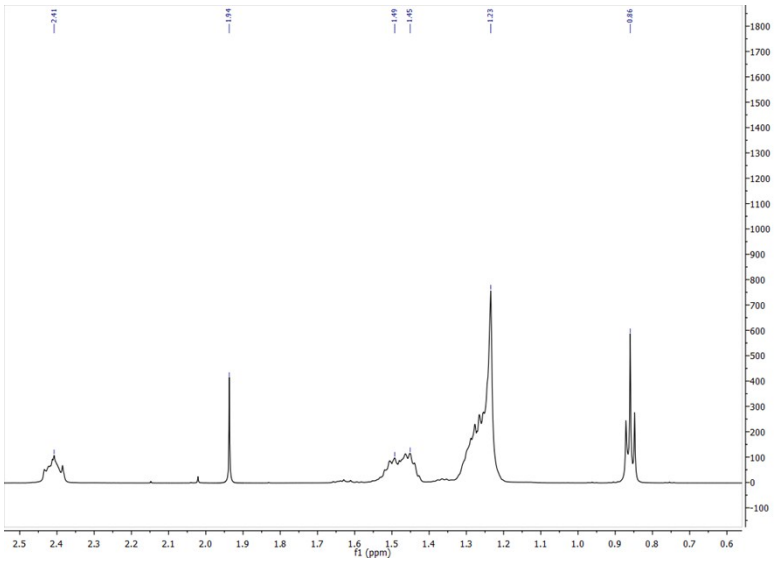

Figure 3: ^{1}H NMR spectra, [P_{14888}][OAc]

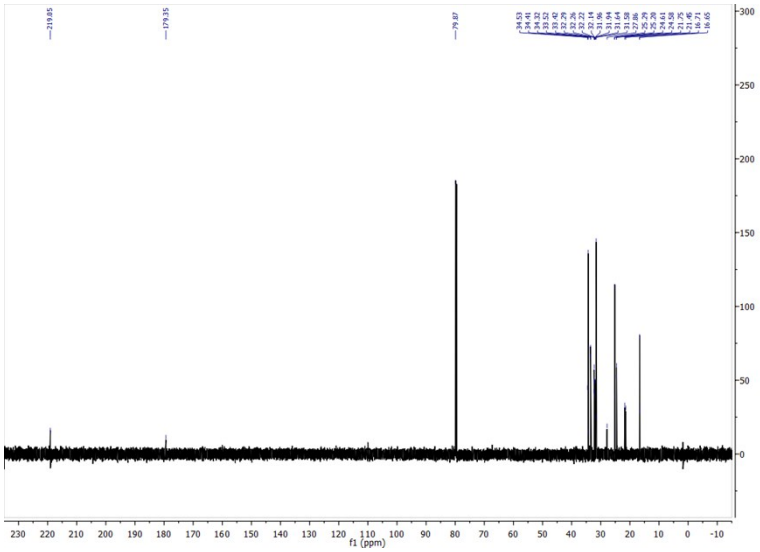

Figure 4: ^{13}C NMR spectra, $[P_{14888}][OAc]$

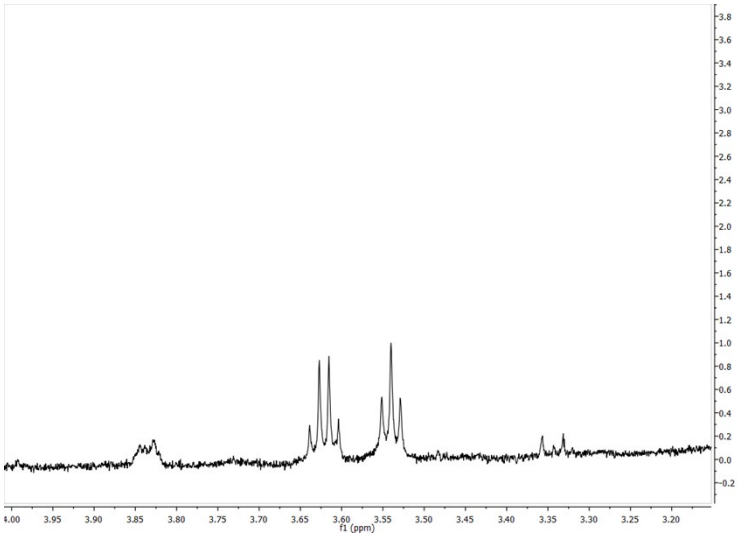

Figure 5: ^{1}H spectral impurties with $[P_{8888}][OAc]$ in cellulsoe backbone region, typically arising from residual alcohols

S2. Phase-Equilibria Data

Table 1: Liquid-liquid equilibrium data, DMSO distribution ratio (βDMSO), and selectivity (S) for the ternary system [P_{8888}][OAc] + DMSO + water at 2998.2 K and atmospheric pressure. The concentrations are expressed as mass fractions (w). Subscripts 1, 2 and 3 represent the ionic liquid, DMSO, and water, respectively.

Ionic liquid-rich phase (*I*)			**Water-rich phase (*II*)**			β_{DMSO}	**S**
w_1	w_2	w_3	w_1	w_2	w_3		
0.840	0.000	0.160	0.001	0	0.999	-	-
0.839	0.007	0.155	0.006	0.095	0.898	13.5	1.90×10^3
0.820	0.027	0.153	0.005	0.248	0.747	9.19	1.51×10^3
0.761	0.050	0.189	0.009	0.373	0.618	7.46	631
0.761	0.124	0.115	0.014	0.600	0.386	4.84	263
0.717	0.200	0.083	0.104	0.705	0.191	3.52	24.3
0.564	0.357	0.080	0.213	0.695	0.092	1.95	5.15

Table 2: Liquid-liquid equilibrium data and DMSO distribution ratio (β_{DMSO}) for the ternary system [P_{14888}][OAc] + DMSO + water at 2998.2 K and atmospheric pressure. The concentrations are expressed as mass fractions (w). Subscripts 1, 2 and 3 represent the ionic liquid, DMSO, and water, respectively.

Ionic liquid-rich phase (*I*)			**Water-rich phase (*II*)**			β_{DMSO}
w_1	w_2	w_3	w_1	w_2	w_3	
0.887	0.000	0.113	0.000	0.000	1.000	-
0.880	0.002	0.118	0.000	0.180	0.820	90.0
0.879	0.010	0.111	0.000	0.399	0.601	39.9
0.853	0.052	0.095	0.000	0.608	0.392	11.7
0.765	0.169	0.066	0.000	0.742	0.258	4.39

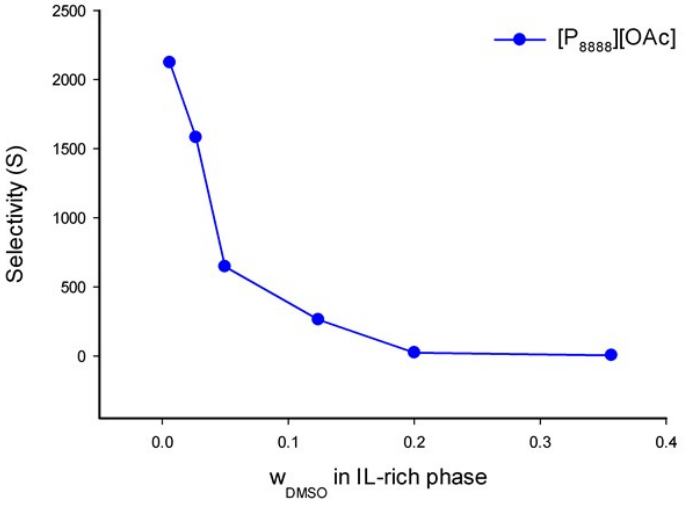

Figure 6: Selectivity (S) for the ternary system [P_{8888}][OAc] + DMSO + water, at 25 ^{O}C and atmospheric pressure, as a function of the mass fraction of DMSO in the ionic liquid-rich phase

S3. IR spectra of Regenerated and Treated Cellulose

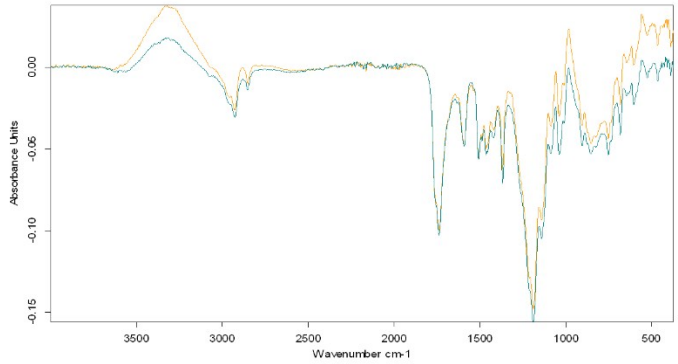

Figure 7: FTIR Spectra of Cellulose, 10wt% MCC treated with [P_{8888}][OAc] and 40wt% DMSO, IR spectra (Blue) versus unmodified cellulose (Yellow)

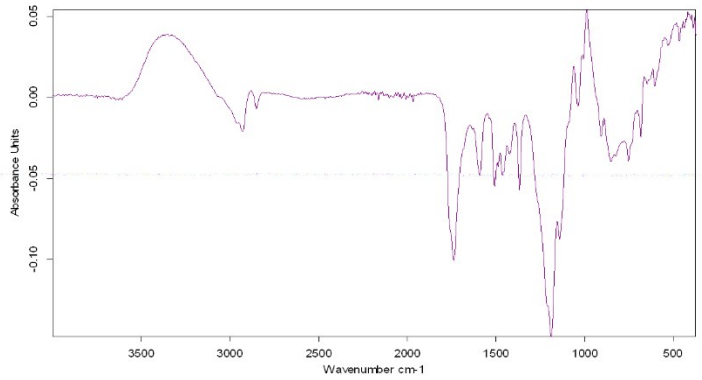

Figure 8: FTIR Spectra of Regenerated Cellullose from Large Scale Dissolution-Regeneration

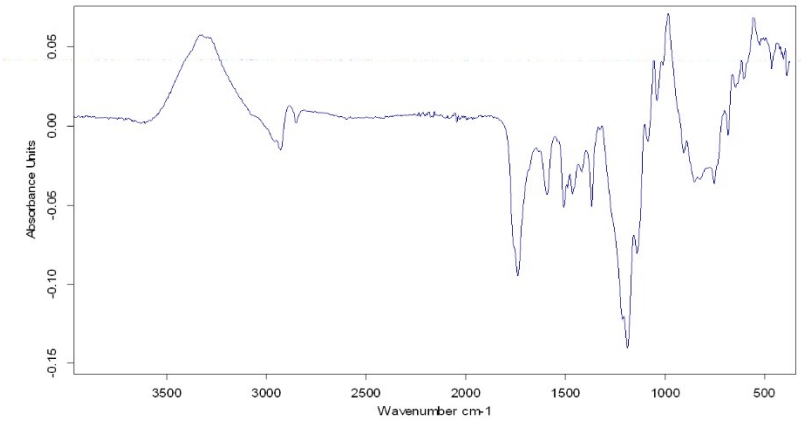

Figure 9: FTIR Spectra of Cellulose 10 wt% (Enocell Pulp) treated with pure [P_{8888}][OAc]

S4. Microscopy of Regenerated and Treated Cellulose

Figure 10: Dissolved and Regenerated cellulose (MCC) from large-scale dissolution experiment (x5 zoom)

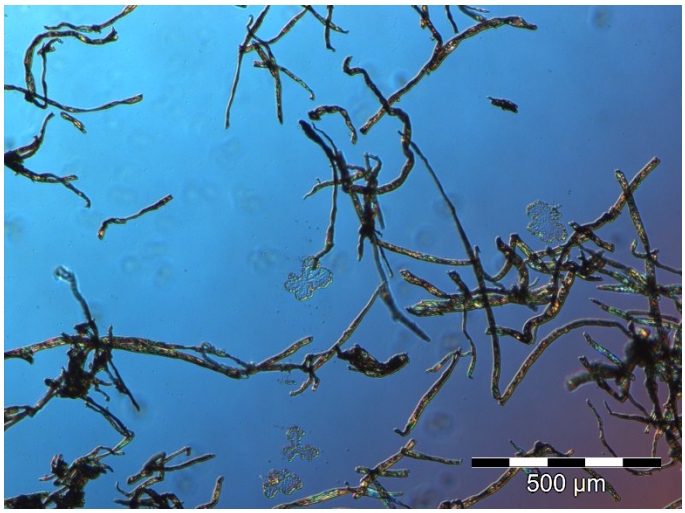

Figure 11: Cellulose (Enocell Pulp) treated with pure [P_{8888}][OAc] (x5 zoom)

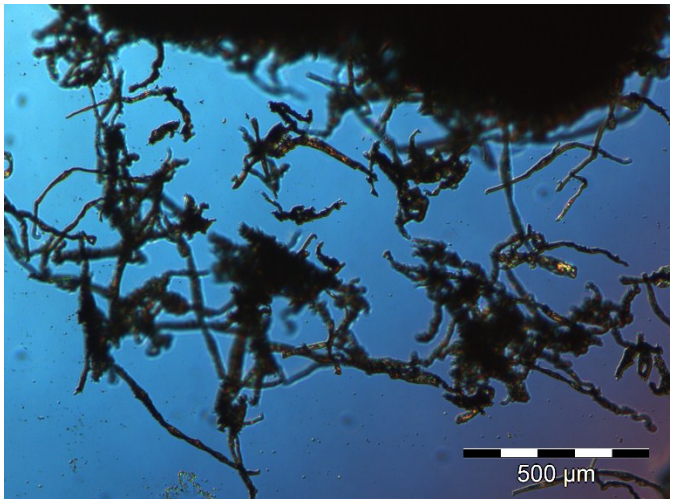

Figure 12: Cellulose 10wt% (Enocell Pulp) treated with [P_{8888}][OAc] and 40wt% DMSO (x5 zoom)

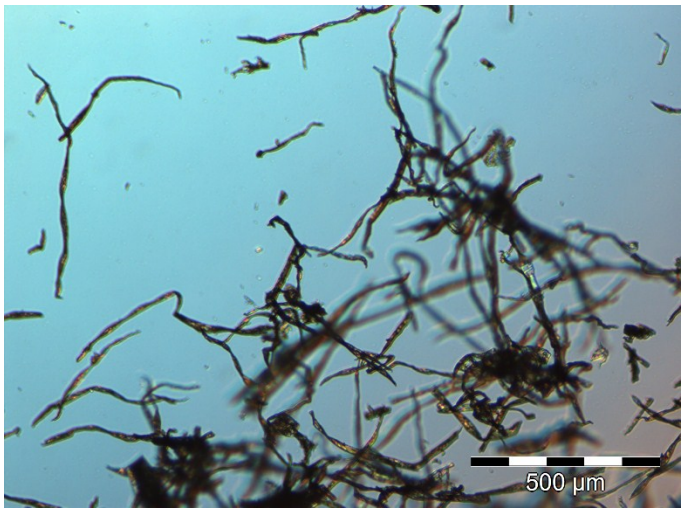

Figure 13: Cellulose 10wt% (Enocell Pulp) treated with [P_{8888}][OAc] and 90wt% DMSO (x5 zoom)