

Supplementary Information

Effects of Anionic Structure and Lithium Salts Addition on the Dissolution of Cellulose in 1-Butyl-3-methylimidazolium-Based Ionic Liquids Solvent Systems

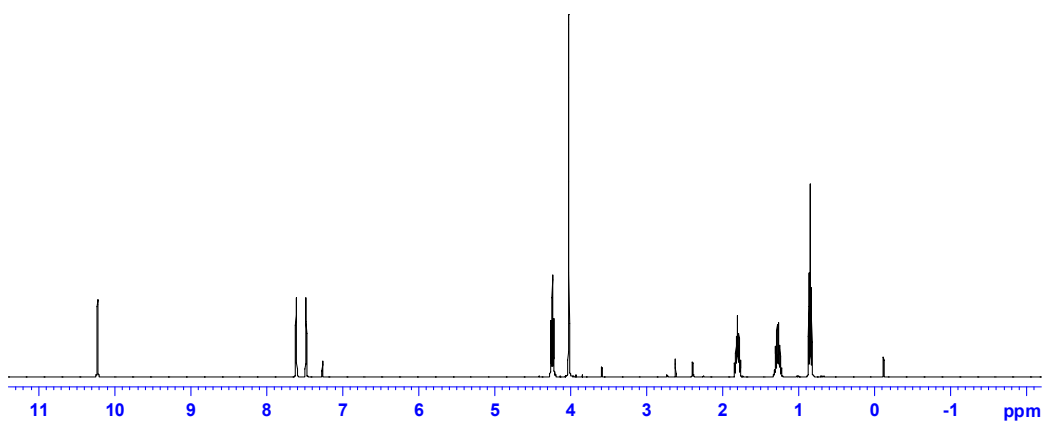
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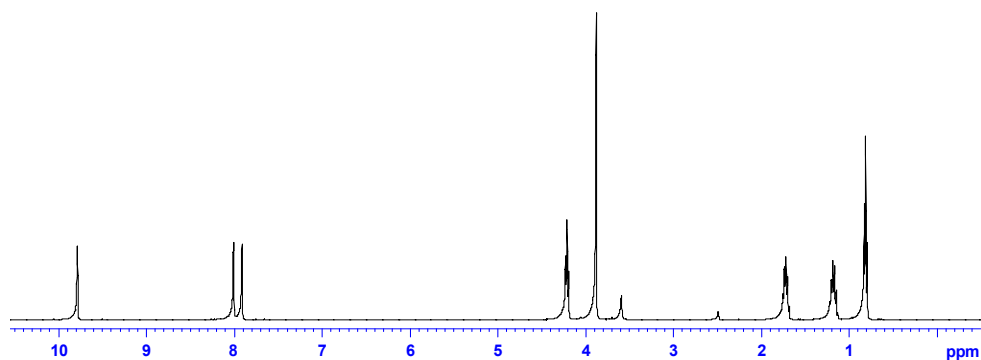
¹H-NMR Data of the ILs

- 1-butyl-3-methylimidazolium bromide ([C₄mim]Br): ¹H NMR(400MHz: CDCl₃; δ/ppm relative to TMS): 0.85(3H, t, but-CH₃), 1.29(2H, m, CH₂), 1.81(2H, m, CH₂), 4.03(3H, s, NCH₃), 4.24(2H, t, NCH₂), 7.48(1H, s, NCH), 7.61(1H, s, NCH), 10.23(1H, s, NCHN).

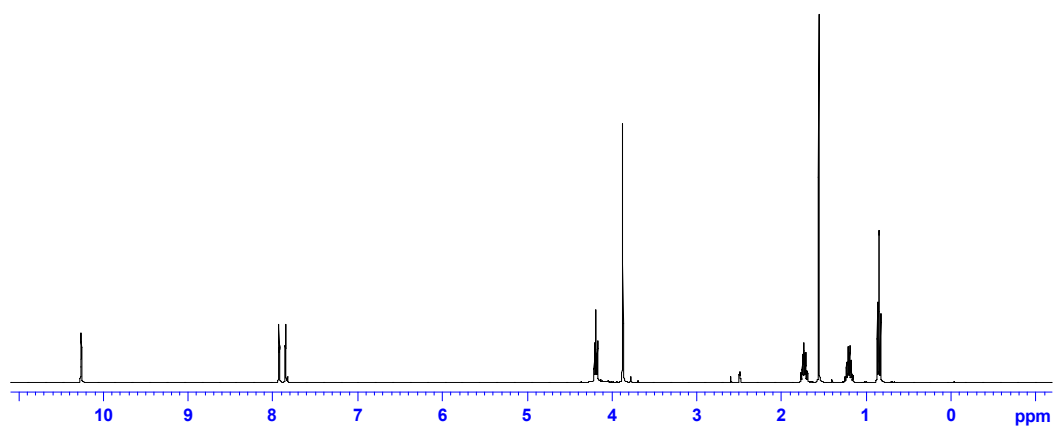


- 1-butyl-3-methylimidazolium chloride ([C₄mim]Cl): ¹H NMR(400MHz: DMSO-d₆; δ/ppm relative to TMS): 0.81(3H, t, but-CH₃), 1.19(2H, m, CH₂), 1.72(2H, m, CH₂), 3.88(3H, s, NCH₃), 4.21(2H, t, NCH₂), 7.91(1H, s, NCH), 8.01(1H, s, NCH), 9.79(1H, s, NCHN).

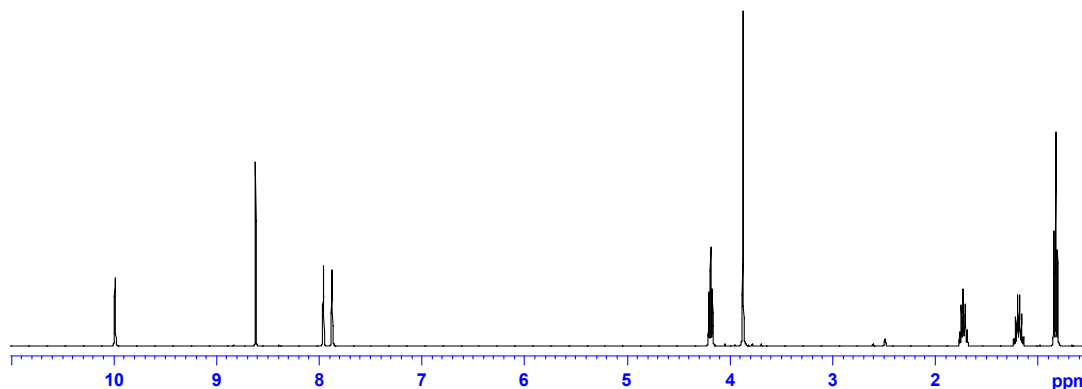
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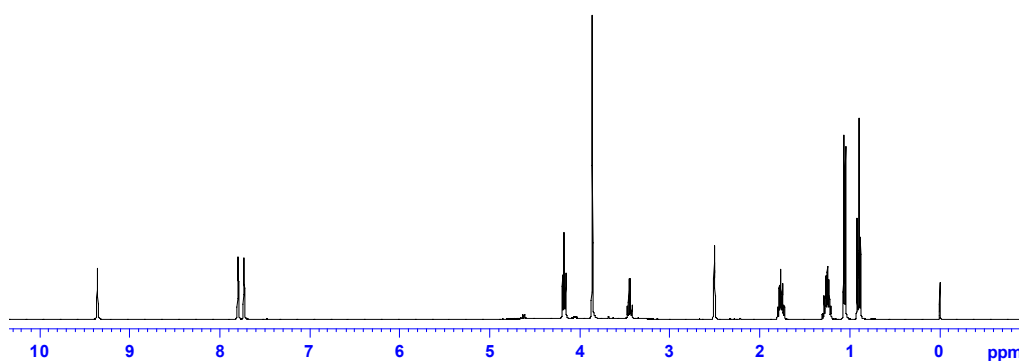
3. 1-butyl-3-methylimidazolium acetate ([C₄mim][CH₃COO]): ¹H NMR(400MHz: DMSO-d₆; δ/ppm relative to TMS): 1.00(3H, t, but-CH₃), 1.21(2H, m, CH₂), 1.56(3H, s, CH₃CO₂), 1.71(2H, m, CH₂), 3.94(3H, s, NCH₃), 4.15(2H, t, NCH₂), 7.85(1H, s, NCH), 7.93(1H, s, NCH), 10.26(1H, s, NCHN).



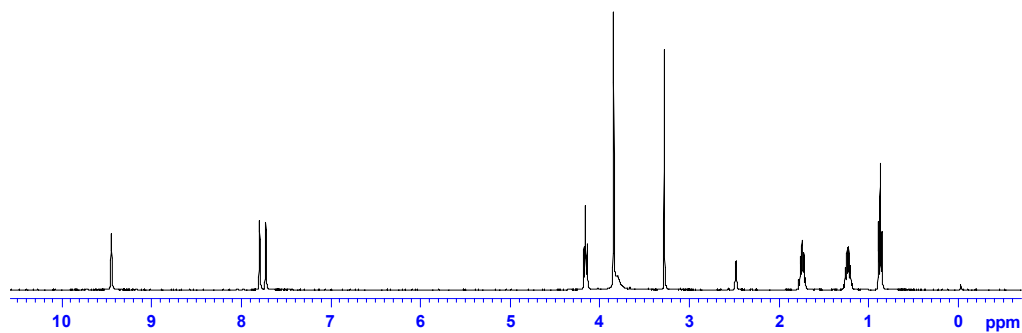
4. 1-butyl-3-methylimidazolium formate ([C₄mim][HCOO]): ¹H NMR(400MHz: DMSO-d₆; δ/ppm relative to TMS): 0.84(3H, t, but-CH₃), 1.20(2H, m, CH₂), 1.73(2H, m, CH₂), 3.87(3H, s, NCH₃), 4.19(2H, t, NCH₂), 7.88(1H, s, NCH), 7.90(1H, s, NCH), 8.62(1H, s, HCOO), 9.99(1H, s, NCHN).



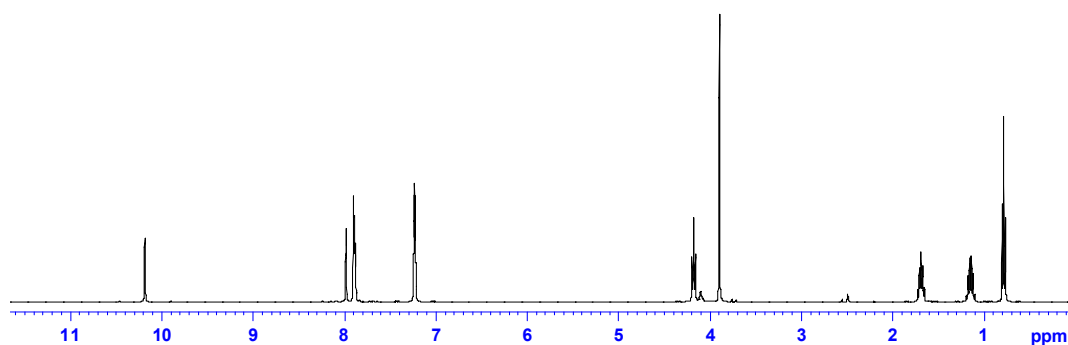
5. 1-butyl-3-methylimidazolium lactate ($[\text{C}_4\text{mim}][\text{CH}_3\text{CHOHCOO}]$): ^1H NMR(400MHz: DMSO- d_6 , δ /ppm relative to TMS): 0.90(3H, t, but- CH_3), 1.05(3H, d, CH_3CHOH), 1.25(2H, m, CH_2), 1.76(2H, m, CH_2), 3.44(1H, m, $\text{CH}_3\text{COHCO}_2$), 3.86(3H, s, NCH_3), 4.17(2H, t, NCH_2), 7.73(1H, s, NCH), 7.80(1H, s, NCH), 9.36(1H, s, NCHN).



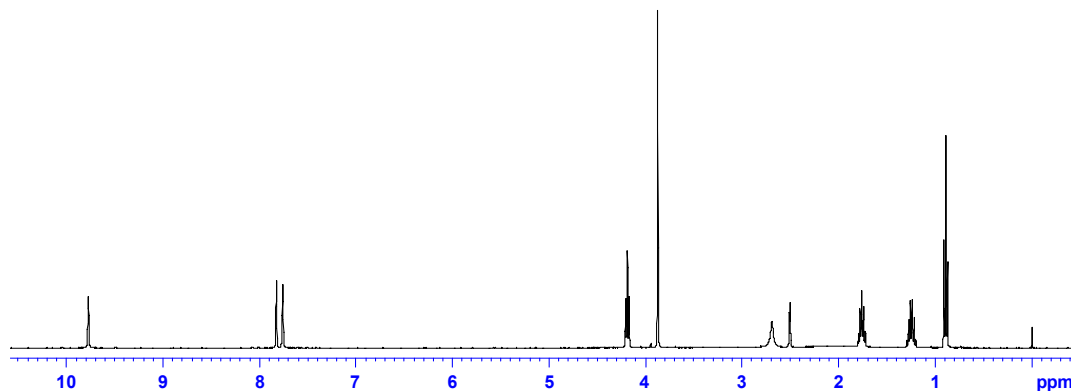
6. butyl-3-methylimidazolium glycollate ($[\text{C}_4\text{mim}][\text{HOCH}_2\text{COO}]$): $[\text{C}_4\text{mim}][\text{HOCH}_2\text{COO}]$ ^1H NMR(400MHz: DMSO- d_6 , δ /ppm relative to TMS): δ = 0.87(3H, t, but- CH_3), 1.24(2H, m, CH_2), 1.74(2H, m, CH_2), 2.48(2H, s, OHCH_2CO_2), 3.81(1H, s, OHCH_2), 3.85(3H, s, NCH_3), 4.16(2H, t, NCH_2), 7.73(1H, s, NCH), 7.79(1H, s, NCH), 9.45(1H, s, NCHN).



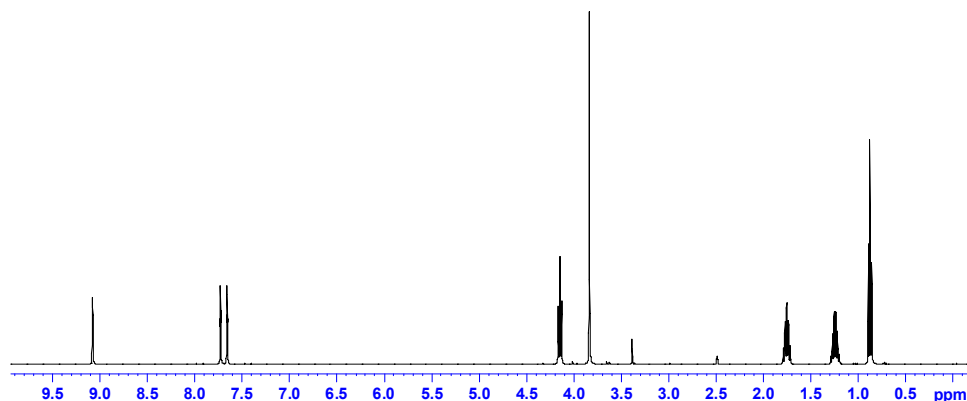
7. 1-butyl-3-methylimidazolium benzoate ($[\text{C}_4\text{mim}][(\text{C}_6\text{H}_5)\text{COO}]$): ^1H NMR(400MHz: DMSO- d_6 , δ /ppm relative to TMS): 0.80(3H, t, but- CH_3), 1.16(2H, m, CH_2), 1.69(2H, m, CH_2), 3.90(3H, s, NCH_3), 4.18(2H, t, NCH_2), 7.23(3H, m, $(\text{CH})_3$), 7.89(2H, m, $(\text{CH})_2$), 7.90(1H, s, NCH), 7.99(1H, s, NCH), 10.19(1H, s, NCHN).



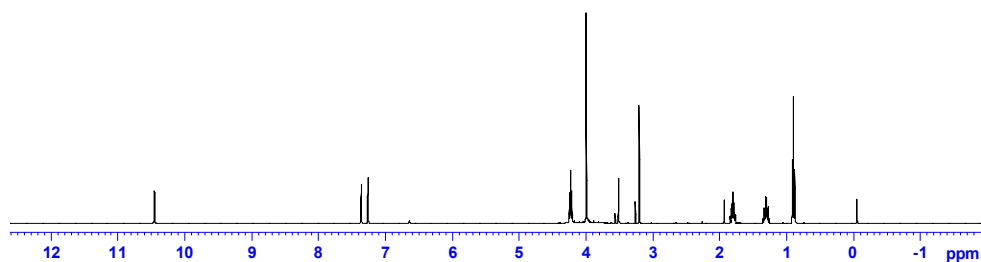
8. 1-butyl-3-methylimidazolium aminoethanic acid salt ($[\text{C}_4\text{mim}][\text{H}_2\text{NCH}_2\text{COO}]$): ^1H NMR(400MHz: DMSO- d_6 , δ /ppm relative to TMS): 0.89(3H, t, but- CH_3), 1.26(2H, m, CH_2), 1.76(2H, m, CH_2), 2.69(2H, s, $\text{CH}_2\text{NH}_2\text{CO}_2$), 3.87(3H, s, NCH_3), 4.19(2H, t, NCH_2), 7.76(1H, s, NCH), 7.82(1H, s, NCH), 9.77(1H, s, NCHN).



9. butyl-3-methylimidazolium dicyanamide ($[\text{C}_4\text{mim}][\text{N}(\text{CN})_2]$): ^1H NMR(400MHz: DMSO-d_6 ; δ/ppm relative to TMS): 0.88(3H, t, but- CH_3), 1.25(2H, m, CH_2), 1.76(2H, m, CH_2), 3.84(3H, s, NCH_3), 4.15(2H, t, NCH_2), 7.66(1H, s, NCH), 7.73(1H, s, NCH), 9.08(1H, s, NCHN).



10. 1-butyl-3-methylimidazolium thioglycollate ($[\text{C}_4\text{mim}][\text{HSCH}_2\text{COO}]$): ^1H NMR(400MHz: CDCl_3 ; δ/ppm relative to TMS): 0.90(3H, t, but- CH_3), 1.30(2H, m, CH_2), 1.80(2H, m, CH_2), 3.26(2H, s, $\text{HSCH}_2\text{CO}_2\text{NCH}_3$), 3.56(1H, s, HSCH_2), 3.99(3H, s, NCH_3), 4.25(2H, t, NCH_2), 7.26(1H, s, NCH), 7.36(1H, s, NCH), 10.45(1H, s, NCHN).



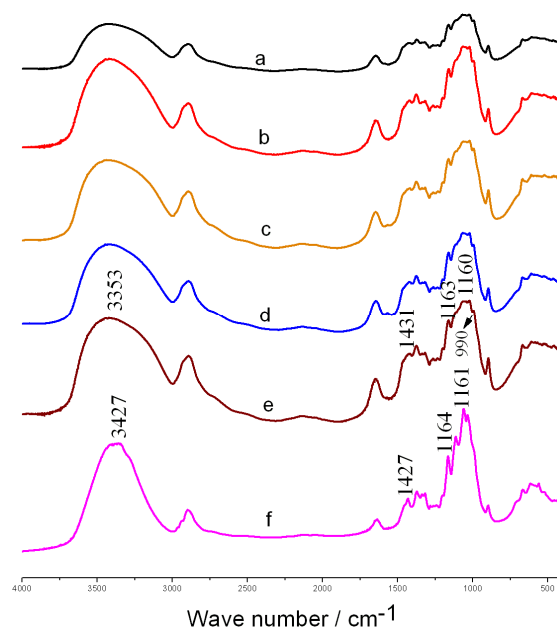


Fig. S1 FT-IR spectra of the original cellulose and the cellulose regenerated from IL/lithium salts systems after 1h of dissolution at 60°C: (a), regenerated from [C₄mim][CH₃COO]/LiCl/cellulose; (b), regenerated from [C₄mim][CH₃COO]/LiClO₄/cellulose; (c), regenerated from [C₄mim][CH₃COO]/LiAc/cellulose; (d), regenerated from [C₄mim][CH₃COO]/LiNO₃/cellulose; (e), regenerated from [C₄mim][CH₃COO]/LiBr/cellulose; (f), the original cellulose.