

Electronic Supplementary Information

Acylamido-based Anion-functionalized Ionic Liquids for Efficient Synthesis of Poly(isosorbide carbonate)

Wenjuan Fang,^[a,b] Fei Xu,*^[a,c] Yaqin Zhang,^[a] Heng Wang,^[a] Zhencai Zhang,^[a] Zifeng Yang,^[a]

Weiwei Wang,^[a] Hongyan He,^[a,c] and Yunjun Luo*^[b]

Table S1 The key abbreviations and symbols in the text

No.	Full name	Abbreviation or symbol
1	isosorbide	ISB
2	dimethyl carbonate	DMC
3	ionic liquid	IL
4	polycarbonate	PC
5	bisphenol A	BPA
6	poly(isosorbide carbonate)	PIC
7	diphenyl carbonate	DPC
8	density functional theory	DFT
9	natural population analysis	NPA
10	tetrabutylphosphonium hydroxide	[P ₄₄₄₄][OH]
11	tetrabutylphosphonium phthalimide	[P ₄₄₄₄][Phth]
12	tetrabutylphosphonium 1,8-naphthalimide	[P ₄₄₄₄][Naph]
13	tetrabutylphosphonium glutarimide	[P ₄₄₄₄][Glu]
14	tetrabutylphosphonium 3,3-tetramethylene glutarimide	[P ₄₄₄₄][Tegl]
15	tetrabutylphosphonium 1,2-cyclopentane dicarboximide	[P ₄₄₄₄][Cydi]
16	tetrabutylphosphonium hexahydrophthalimide	[P ₄₄₄₄][Heph]
17	tetrabutylphosphonium succinimide	[P ₄₄₄₄][Suc]
18	hydroxy group	-OH
19	carbonyl group	C=O
20	acylamido group	-N-C=O
21	carboxymethyl group	-OC(O)OCH ₃
22	methoxyl group	-OCH ₃
23	glass transition temperature	T _g
24	the weight average molecular weight	M _w
25	electron spray ionization mass spectrometry	ESI-MS
26	thermogravimetric analysis	TGA
27	differential scanning calorimetry	DSC
28	temperature at 5% weight loss	T _{d-5%}
29	temperature at 95% weight loss	T _{d-95%}

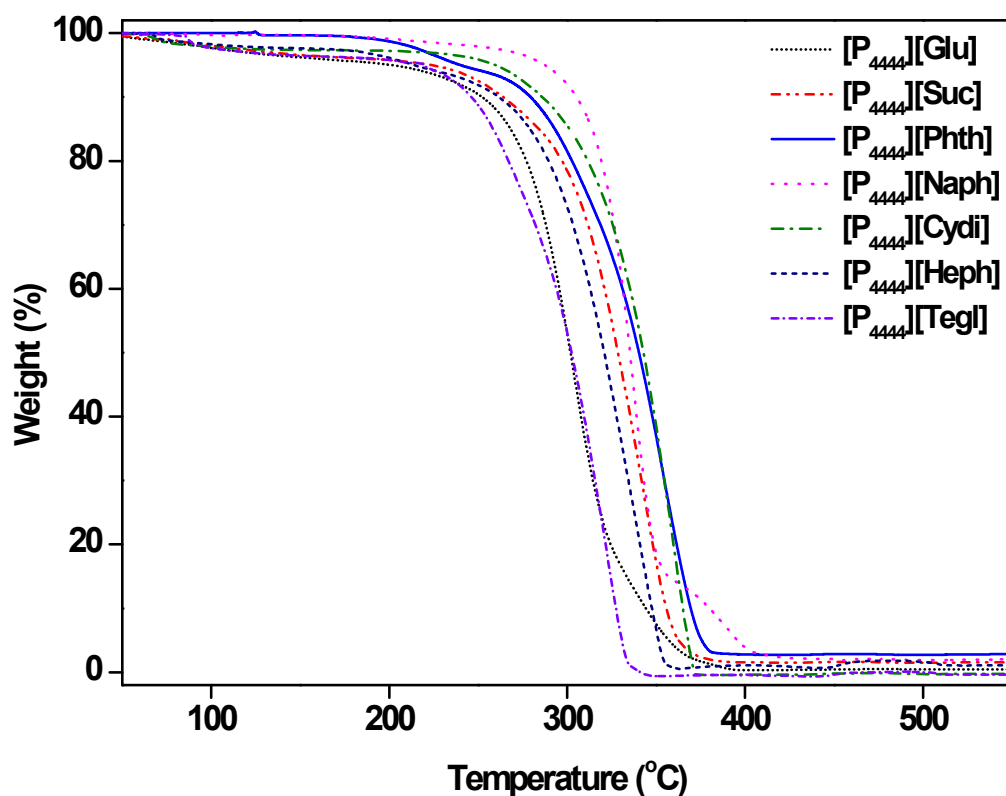


Fig. S1 TGA curves of acylamido-based ILs.

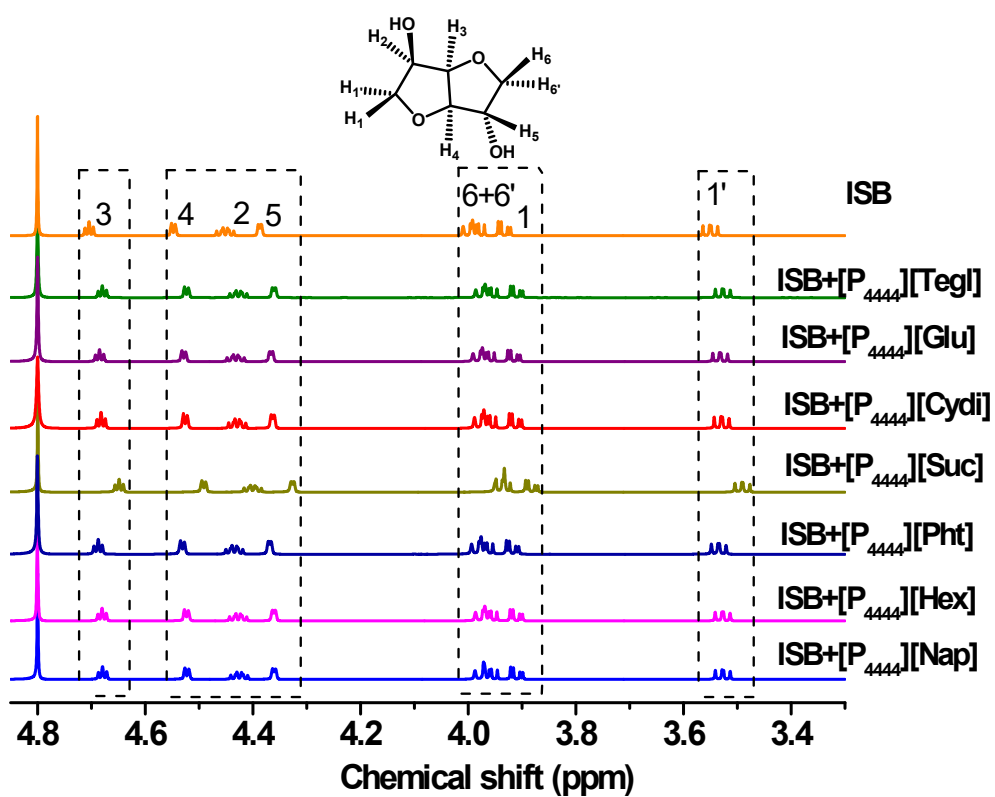


Fig. S2 ¹H NMR spectra of ISB after addition of different acylamido-based ILs.

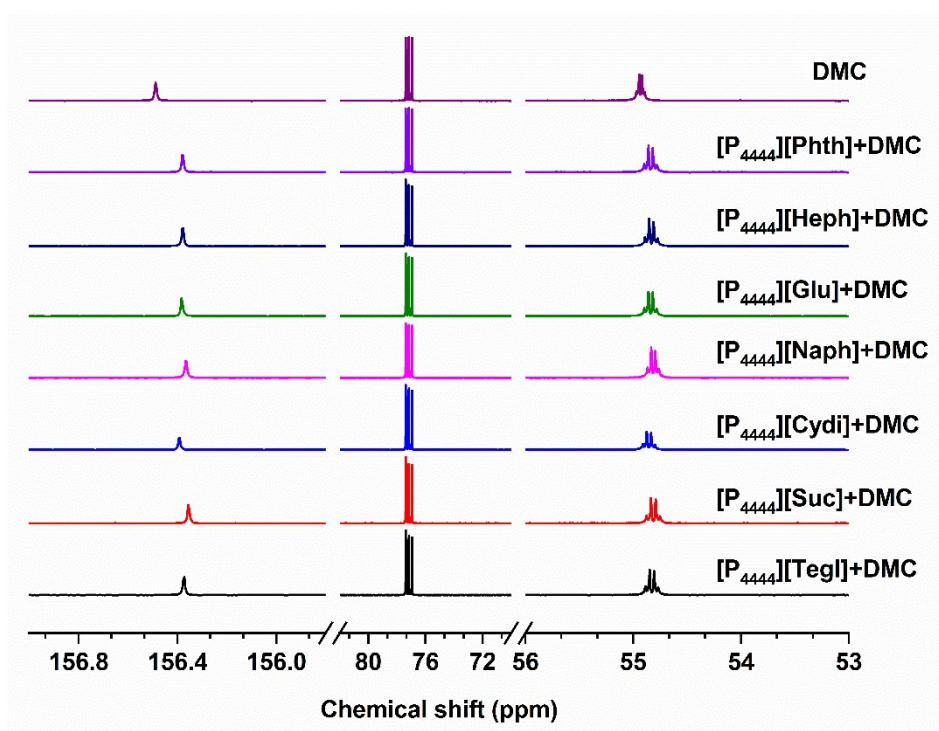


Fig. S3 ^{13}C NMR spectra of DMC after addition of different acylamido-based ILs.

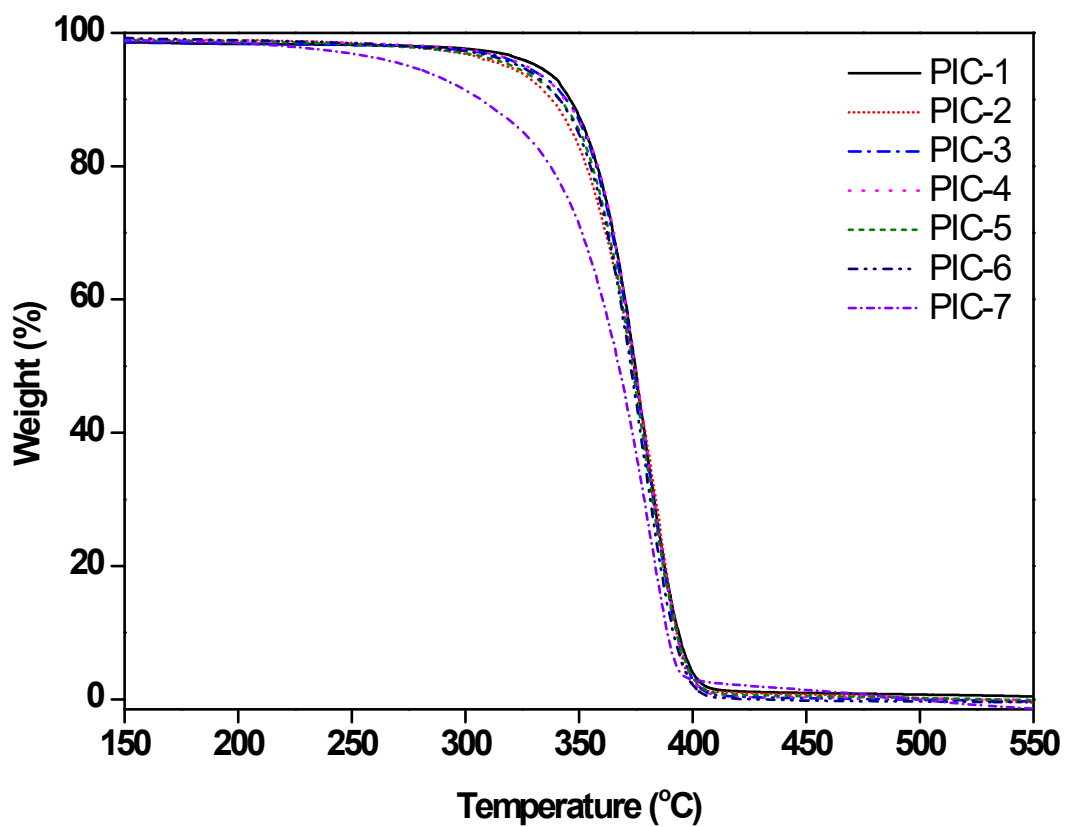


Fig. S4 TGA curves of PIC samples synthesized by acylamido-based ILs.

[P₄₄₄₄][Phth]: ¹H NMR (600 MHz, D₂O): 7.49-7.60 (m, 4H), 2.14-2.19 (m, 8H), 1.44-1.59 (m, 16H), 0.94 (t, 12H); FT-IR (KBr, cm⁻¹): 3058, 2960, 2931, 2870, 1679, 1584, 1564, 1495, 1467, 1397, 1295, 1140, 1093, 1003, 956, 924, 853, 819, 751, 722, 674, 639, 564.

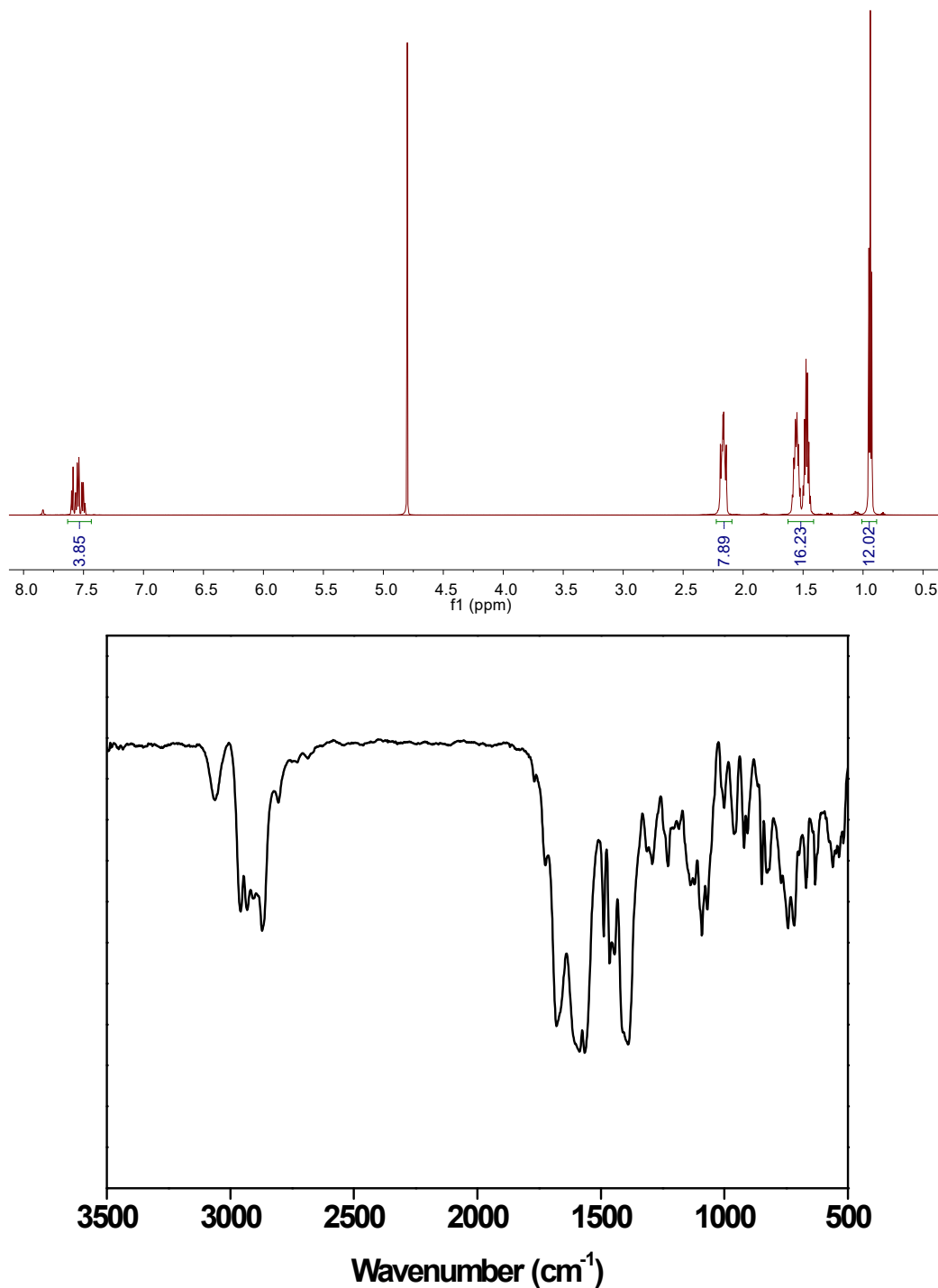


Fig. S5 ¹H NMR and FT-IR spectra of [P₄₄₄₄][Phth].

[P₄₄₄₄][Heph]: ¹H NMR (600 MHz, D₂O): 2.75-2.77 (m, 1H), 2.62-2.65 (m, 1H), 2.16-2.21 (m, 8H), 1.69-2.06 (m, 4H), 1.40-1.64 (m, 20H), 0.95 (t, 12H); FT-IR (KBr, cm⁻¹): 2960, 2930, 2869, 1665, 1609, 1564, 1467, 1352, 1227, 1140, 1093, 1003, 958, 926, 889, 839, 794, 724, 669, 627, 567, 520.

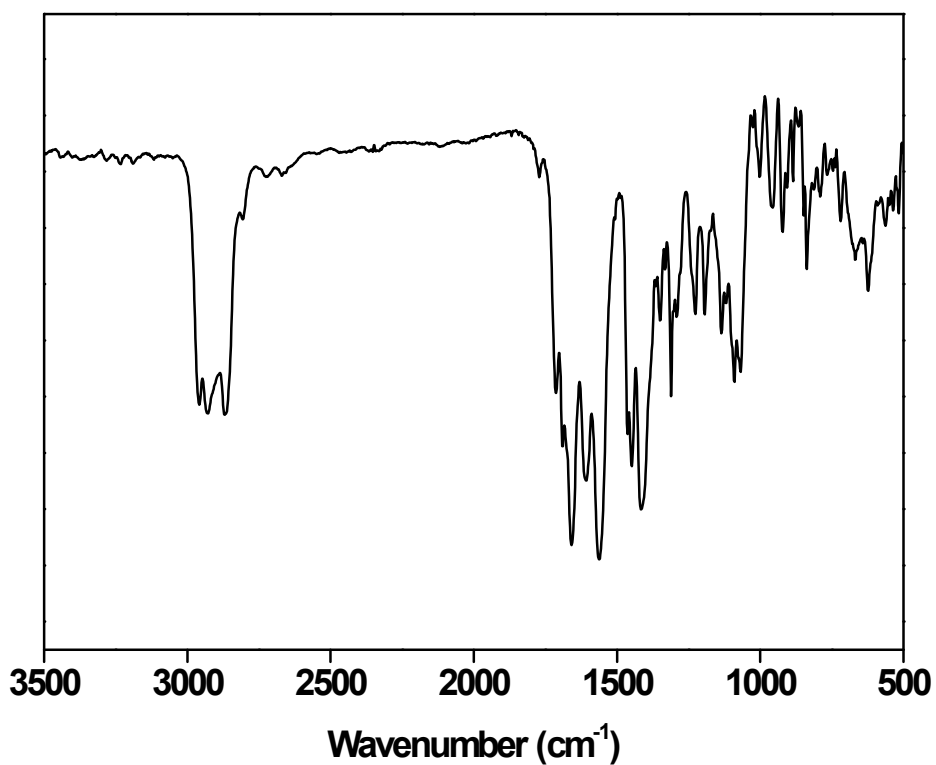
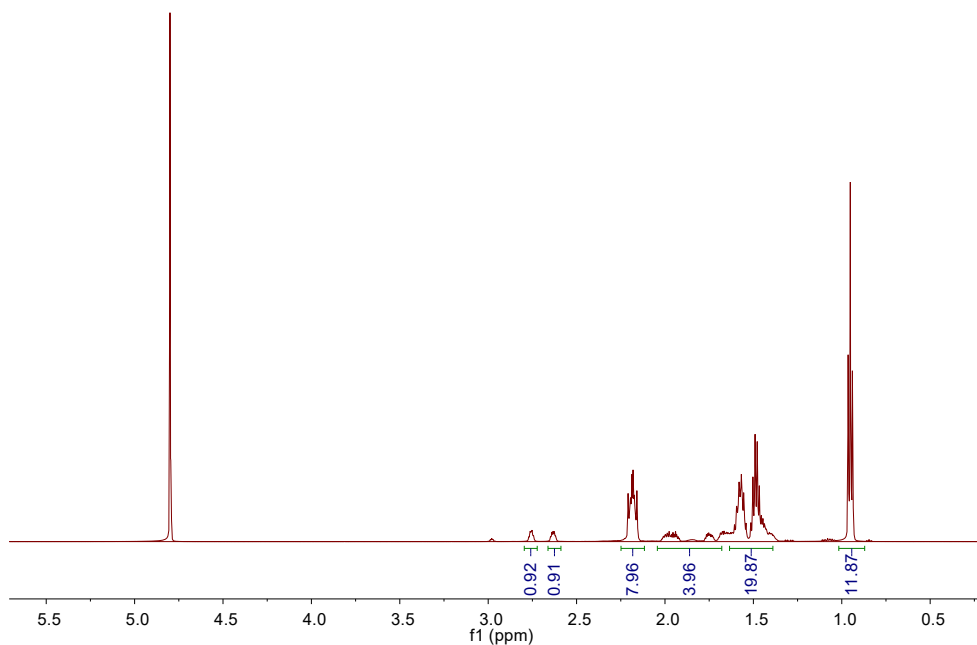


Fig. S6 ¹H NMR and FT-IR spectra of [P₄₄₄₄][Heph].

[P₄₄₄₄][Teg]: ¹H NMR (600 MHz, D₂O): 2.40 (s, 2H), 2.32 (s, 2H), 2.16-2.21 (m, 8H), 1.66-1.73 (m, 4H), 1.45-1.61 (m, 20H), 0.95 (t, 12H); FT-IR (KBr, cm⁻¹): 2960, 2931, 2871, 1665, 1602, 1564, 1410, 1315, 1230, 1188, 1123, 1093, 1003, 958, 924, 908, 871, 831, 771, 749, 722, 699, 647, 622, 565, 542, 522.

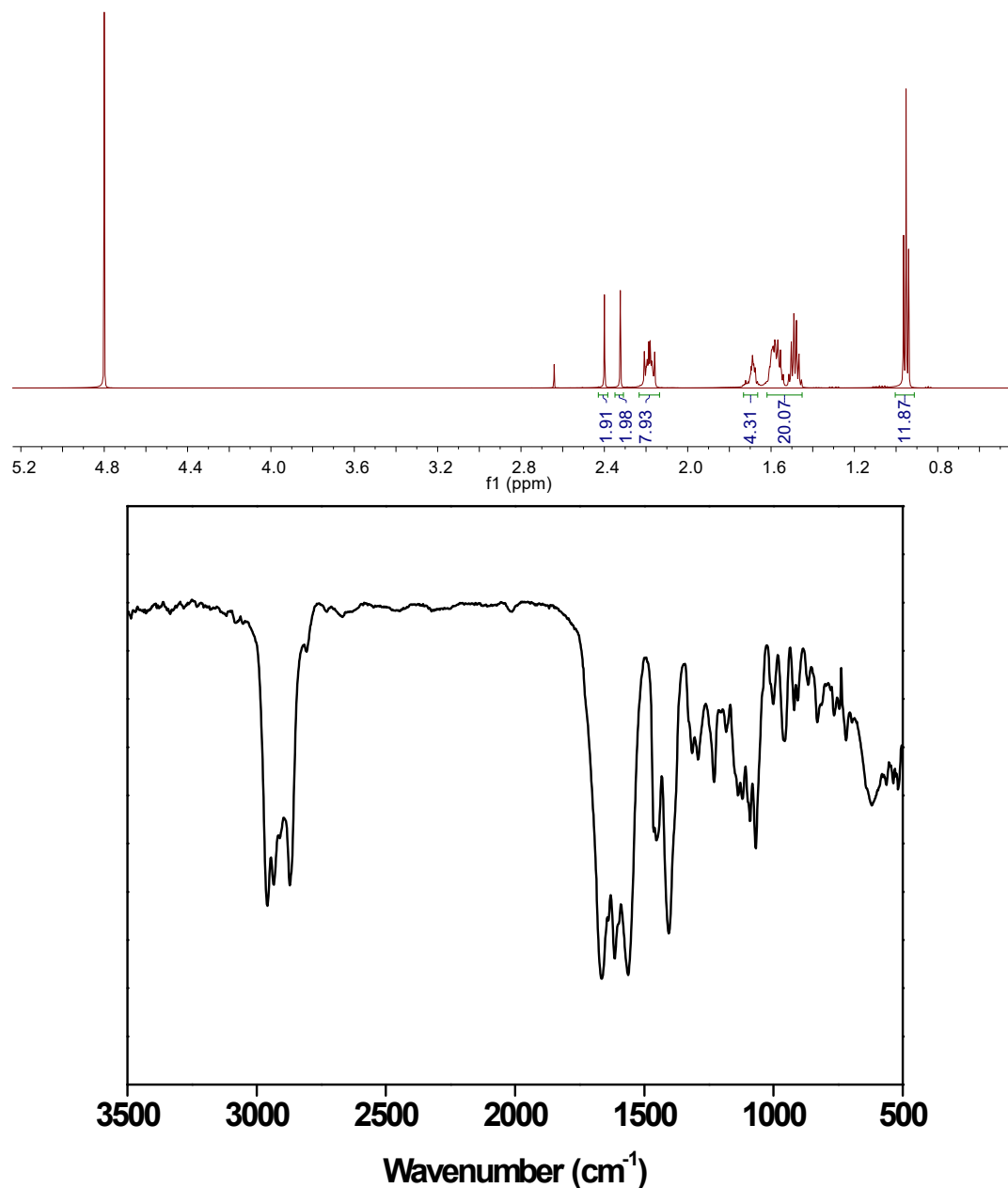


Fig. S7 ¹H NMR and FT-IR spectra of [P₄₄₄₄][Teg].

[P₄₄₄₄][Cydi]: ¹H NMR (600 MHz, D₂O): 3.11-3.12 (m, 2H), 2.16-2.21 (m, 8H), 1.90-1.93 (m, 2H), 1.69-1.79 (m, 3H), 1.45-1.60 (m, 16H), 1.17-1.25 (m, 1H), 0.95 (t, 12H); FT-IR (KBr, cm⁻¹): 2960, 2931, 2871, 1710, 1602, 1564, 1490, 1450, 1387, 1330, 1233, 1185, 1071, 1000, 956, 869, 829, 799, 769, 747, 719, 699, 646, 624, 564, 540, 522.

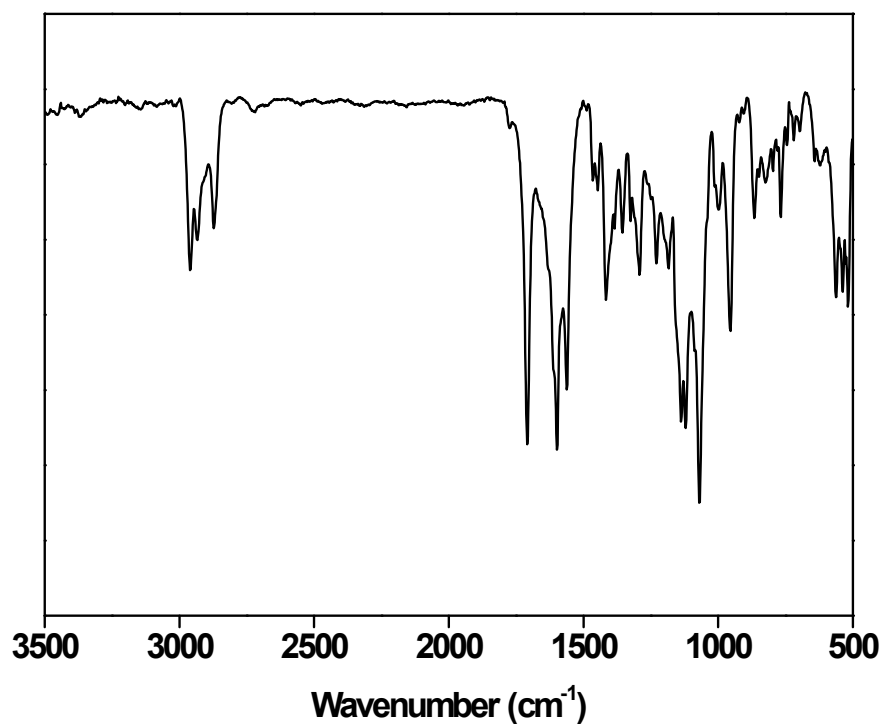
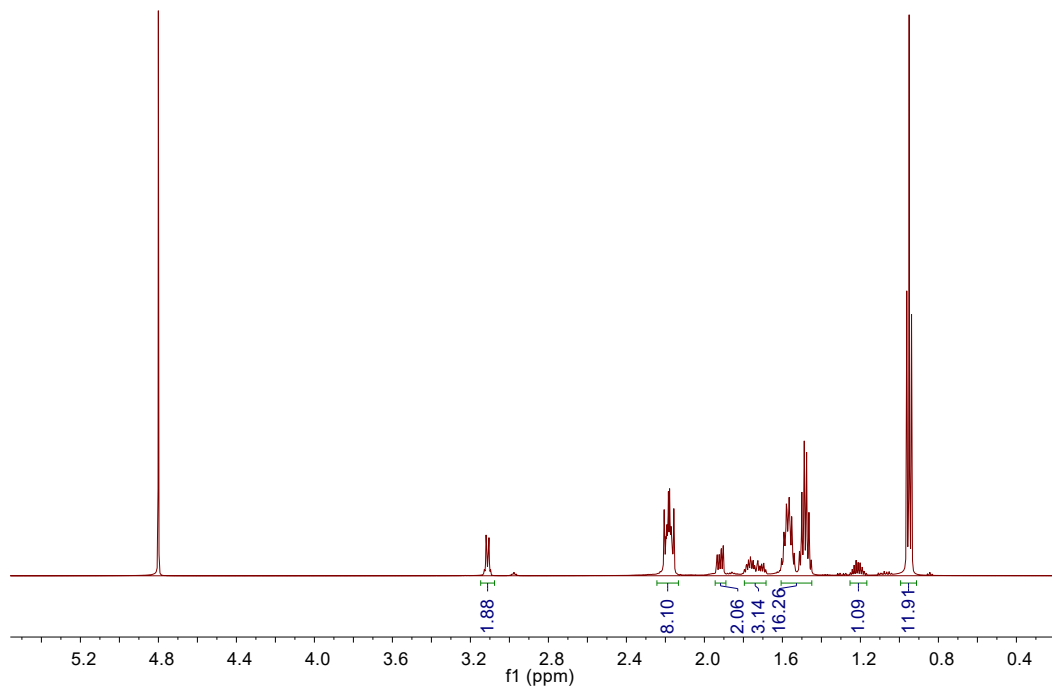


Fig. S8 ¹H NMR and FT-IR spectra of [P₄₄₄₄][Cydi].

[P₄₄₄₄][Glu]: ¹H NMR (600 MHz, DMSO): 2.17-2.22 (m, 8H), 1.98 (t, 2H), 1.78 (t, 2H), 1.55-1.60 (m, 2H), 1.37-1.49 (m, 16H), 0.91 (t, 12H); FT-IR (KBr, cm⁻¹): 2960, 2932, 2872, 1680, 1564, 1462, 1417, 1352, 1225, 1140, 1073, 1001, 958, 924, 869, 831, 771, 724, 699, 562, 540, 520.

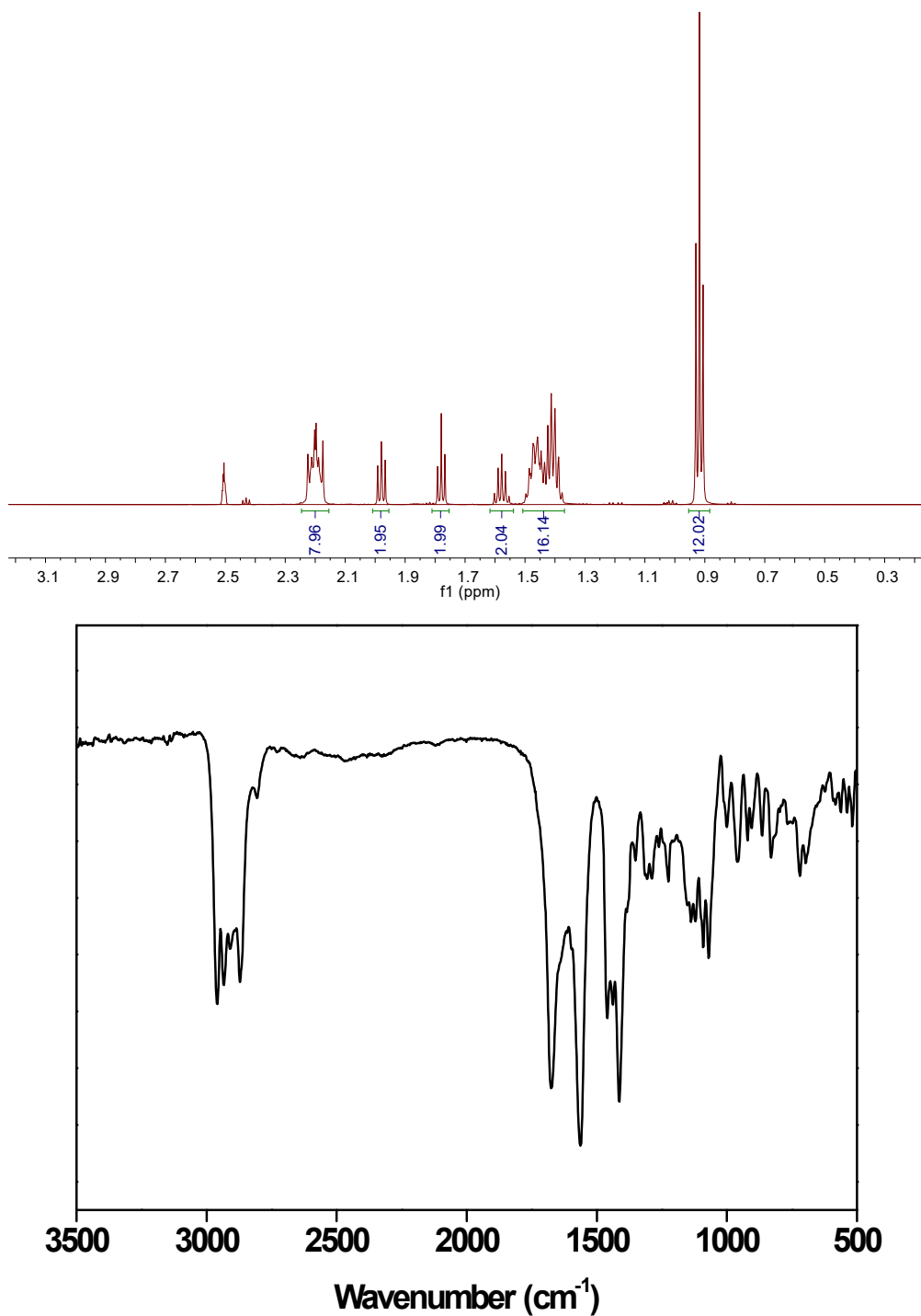


Fig. S9 ¹H NMR and FT-IR spectra of [P₄₄₄₄][Glu].

[P₄₄₄₄][Suc]: ¹H NMR (600 MHz, DMSO): 2.17-2.22 (m, 8H), 2.09-2.11 (t, 2H), 1.96-1.99 (t, 2H), 1.37-1.49 (m, 16H), 0.92 (t, 12H); FT-IR (KBr, cm⁻¹): 2960, 2932, 2872, 1668, 1602, 1569, 1467, 1295, 1185, 1125, 1093, 1003, 958, 924, 909, 873, 831, 769, 739, 722, 699, 647, 567, 539, 520.

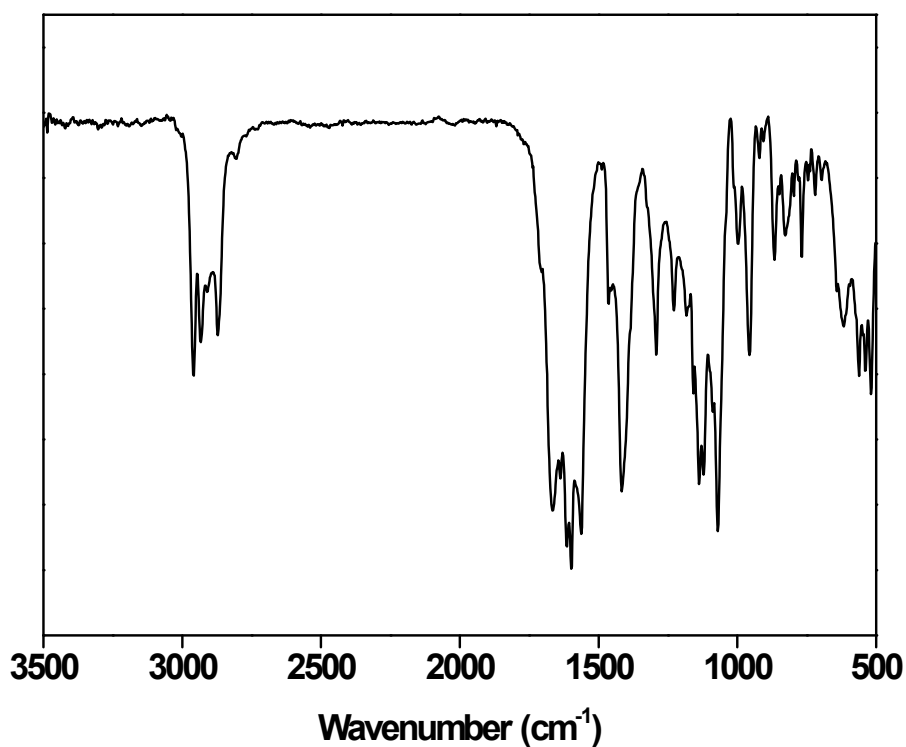
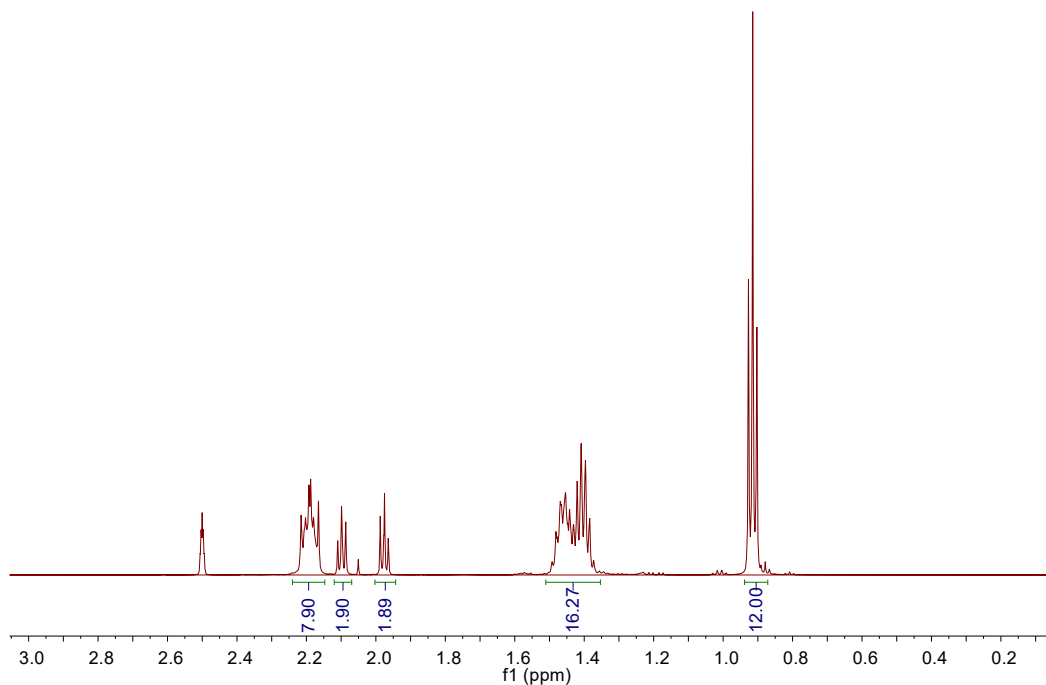


Fig. S10 ¹H NMR and FT-IR spectra of [P₄₄₄₄][Suc].

[P₄₄₄₄][Naph]: ¹H NMR (600 MHz, DMSO): 8.11 (d, 2H), 8.03 (d, 2H), 7.60 (t, 2H), 2.16-2.21 (m, 8H), 1.36-1.48 (m, 16H), 0.89 (t, 12H); FT-IR (KBr, cm⁻¹): 3055, 2960, 2931, 2870, 1683, 1634, 1579, 1539, 1500, 1465, 1437, 1412, 1380, 1337, 1277, 1233, 1208, 1160, 1093, 1071, 1026, 968, 923, 911, 861, 834, 811, 786, 724, 699, 617, 552, 530.

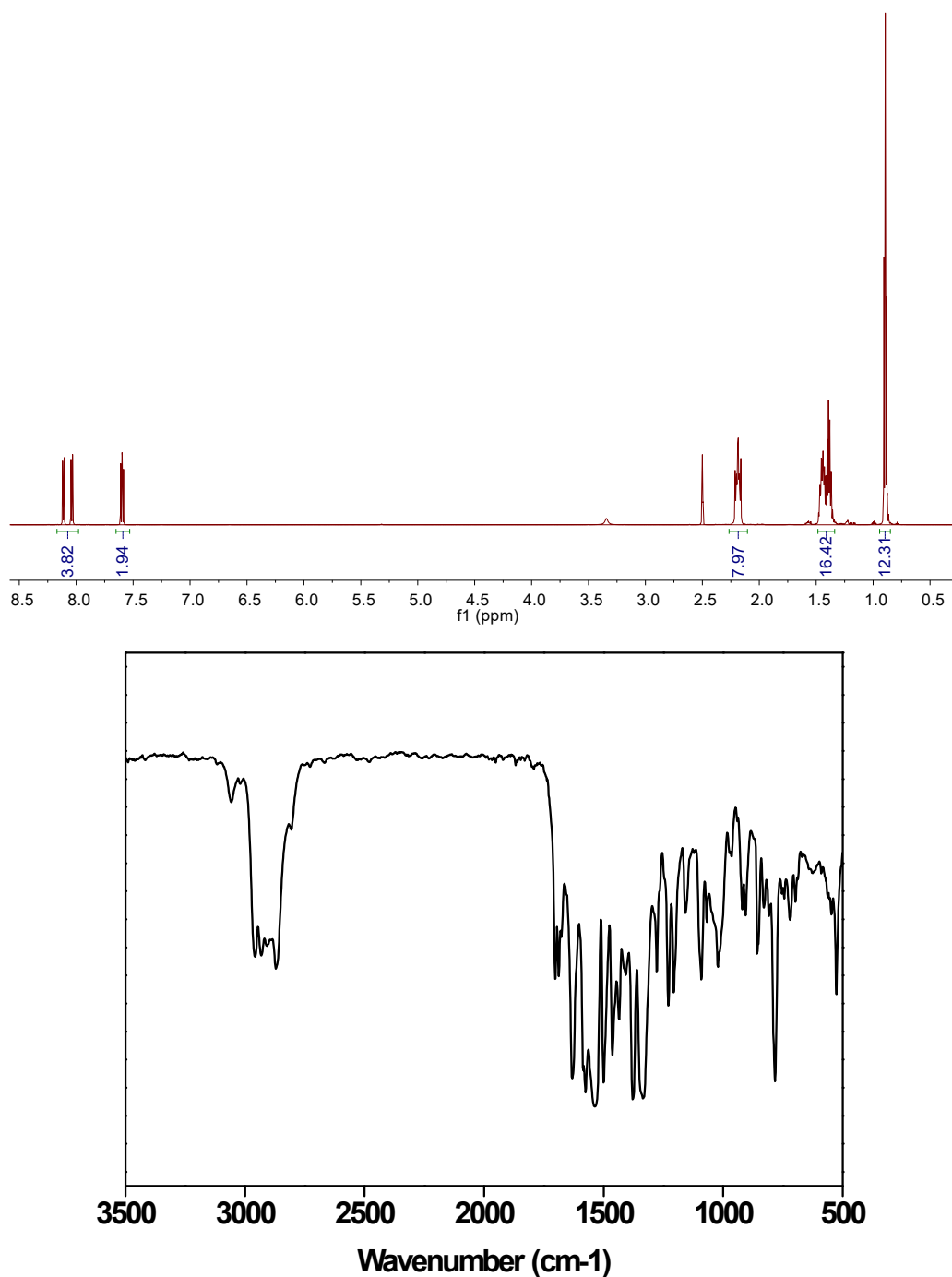


Fig. S11 ¹H NMR and FT-IR spectra of [P₄₄₄₄][Naph].

MC-1: ^1H NMR (600 MHz, CDCl_3): 2.47 (s, 1H), 3.57 (dd, 1 H), 3.81 (s, 3 H), 3.88 (dd, 1 H), 4.00 (dd, 1 H), 4.12 (d, 1H), 4.30 (q, 1H), 4.53 (d, 1H), 4.64 (t, 1H), 5.13 (d, 1 H); ^{13}C NMR (600 MHz, CDCl_3): 55.1, 72.3, 73.3, 73.6, 81.6, 82.0, 85.4, 154.7.

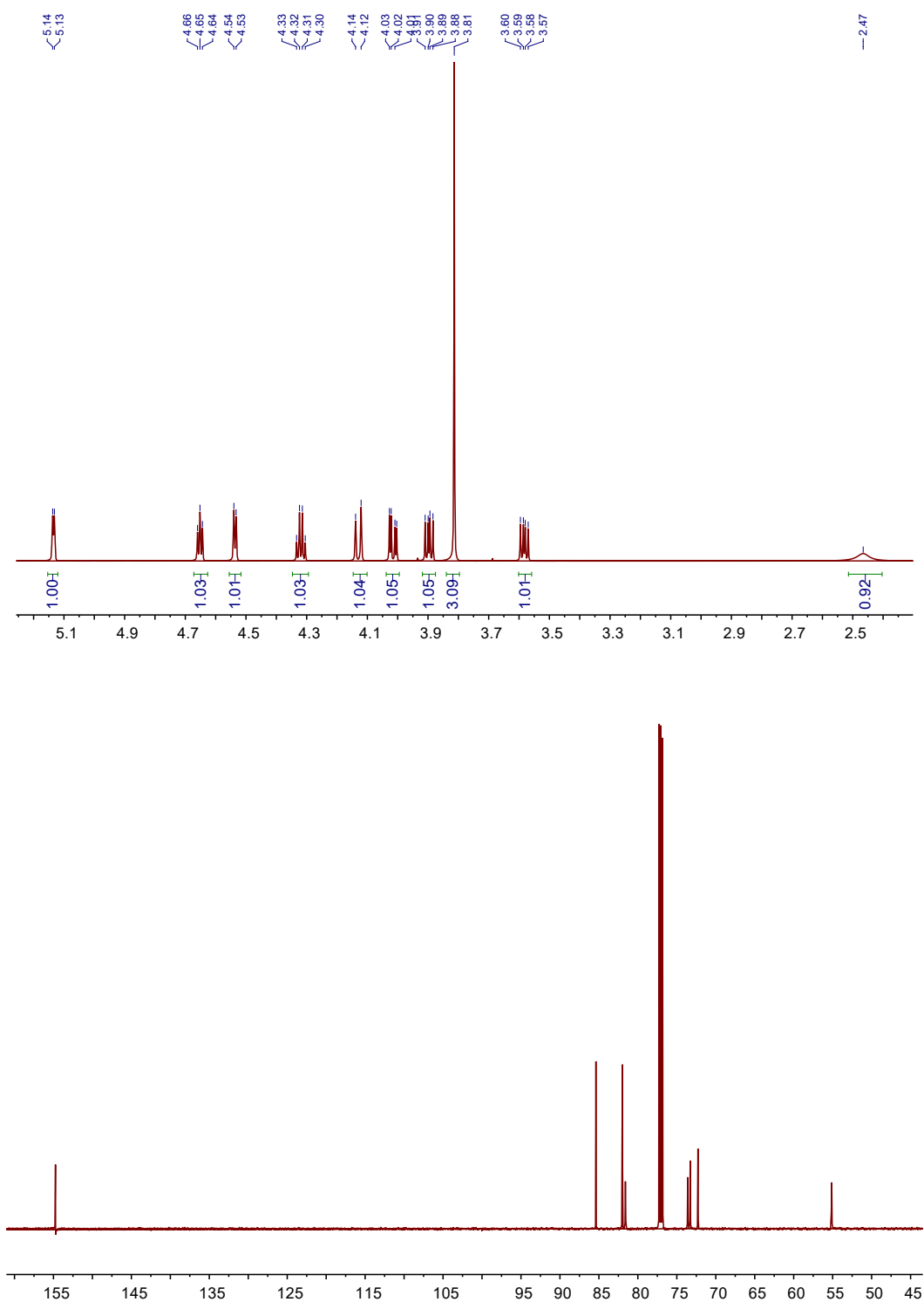


Fig. S12 ^1H NMR and ^{13}C NMR spectra of MC-1.

MC-2: ^1H NMR (600 MHz, CDCl_3): 2.12 (s, 1H), 3.82 (s, 3H), 3.85-3.92 (m, 4H), 4.34 (s, 1H), 4.40 (d, 1H), 4.88(t, 1H), 5.05 (q, 1H); ^{13}C NMR (600 MHz, CDCl_3): 55.3, 70.5, 75.8, 76.3, 77.1, 80.6, 88.5, 155.4.

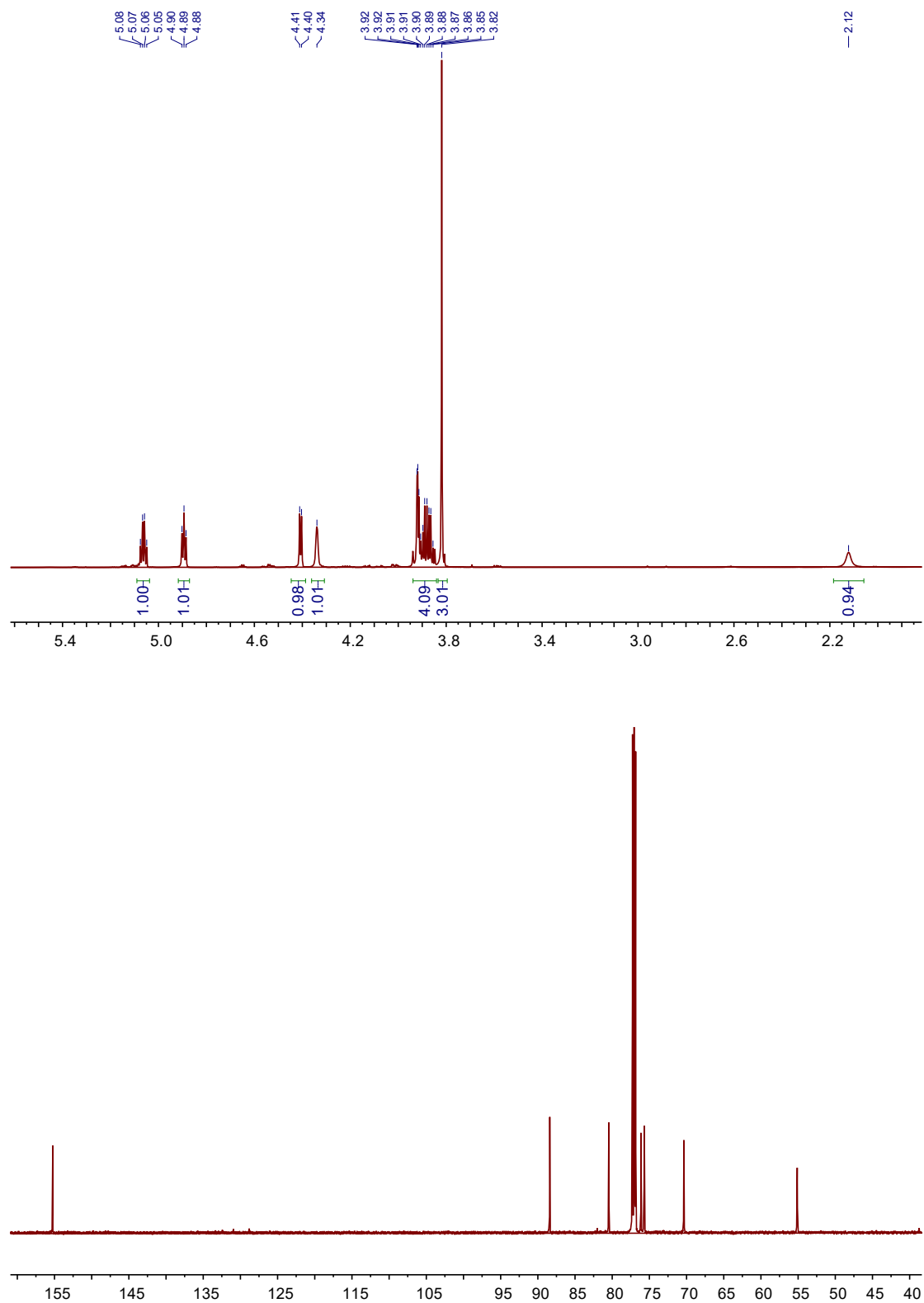


Fig. S13 ^1H NMR and ^{13}C NMR spectra of MC-2.

DC: ^1H NMR (600 MHz, CDCl_3): 3.81 (s, 3H), 3.82 (s, 3H), 3.88-3.94 (m, 2H), 4.01 (dd, 1 H), 4.07 (d, 1H), 4.54 (d, 1H), 4.88 (t, 1 H), 5.05-5.11 (m, 2 H); ^{13}C NMR (600 MHz, CDCl_3): 55.3, 70.6, 73.4, 76.9, 81.0, 81.4, 86.0, 154.9, 155.3.

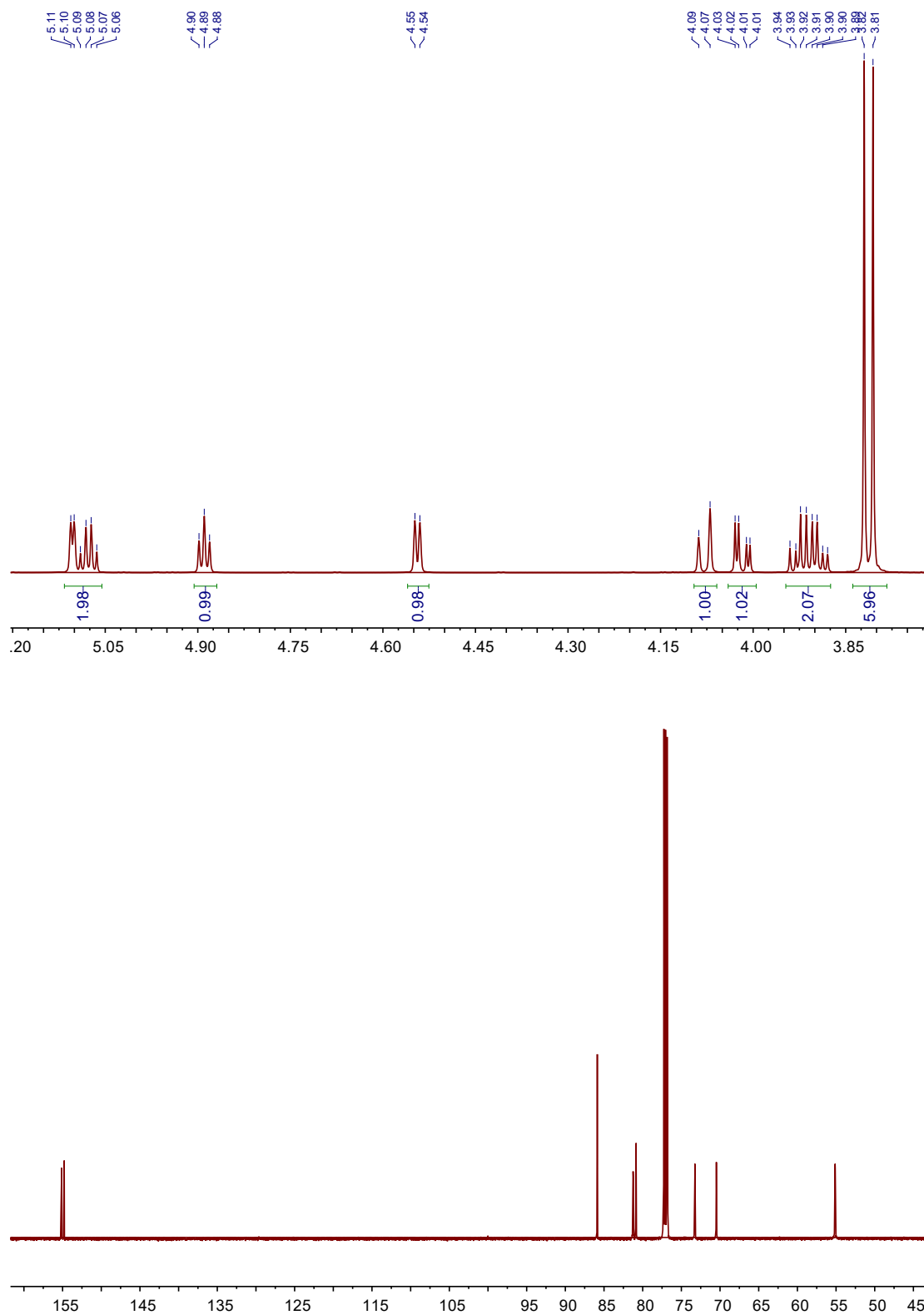


Fig. S14 ^1H NMR and ^{13}C NMR spectra of DC.