Electronic supplementary information

Synthesis of magnesium complexes of ionic liquids with highly coordinating anion

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Table 1. Crystallographic data of $[C_4mim][Mg(hfac)_3]$, $[C_4Pip][Mg(hfac)_3]$, $[C_4Pyr][Mg(hfac)_3]$ and $[C_6Morp][Mg(hfac)_3]$.

	$[C_4mim][Mg(hfac)3]$	**$[C_6Morp]$ $[Mg(hfac)3]$.**	**$[C_4Pip]$ $[Mg(hfac)_3]$**	**$[C_4Pyr]$ $[Mg(hfac)_3]$**
Crystal data				
Chemical formula	$C_{15}H_3F_{18}MgO_6 \cdot C_8H_{15}N2$	$C_{15}H_3F_{18}MgO_6 \cdot C_{11}H_{24}NO$	$C_{15}H_3F_{18}MgO_6 \cdot C_{10}H_{22}N$	$C_{15}H_3F_{18}MgO_6 \cdot C_9H_{14}N$
M_r	784.7	831.79	801.77	781.7
Crystal system, space group	Triclinic, P	Monoclinic, $P2_1/n$	Monoclinic, $P2_1/n$	Triclinic, P
Temperature (K)	100	100	100	100
a, b, c (Å)	9.0058 (8) 17.6783 (15) 20.1473 (17)	9.4523 (8) 18.8574 (16) 18.6567 (16)	18.549 (2) 18.597 (2) 20.171 (2)	9.5379 (7) 10.9322 (8) 15.1147 (10)
α, β, γ (°)	74.180 (2) 86.894 (2) 89.008 (2)	90 91.129 (2) 90	90 111.444 (2) 90	81.617 (1) 86.002 (1) 72.564 (1)
V ($Å^3$)	3081.6 (5)	3324.8 (5)	6476.4 (12)	1486.97 (18)
Z	4	4	8	2
Radiation type	Mo Kα	Mo Kα	Mo Kα	Mo Kα
μ (mm^{-1})	0.21	0.2	0.2	0.21
Crystal size (mm)	0.25 × 0.09 × 0.06	0.33 × 0.13 × 0.06	0.27 × 0.19 × 0.09	0.77 × 0.58 × 0.11
Data collection				
Diffractometer	Bruker D8 Venture diffractometer, CMOS detector			
Absorption correction	Multi-scan (SADABS 2016/2)			
	wR2(int) was 0.1156 before and 0.0532 after correction. The Ratio of minimum to maximum transmission is 0.9295.	wR2(int) was 0.1109 before and 0.0482 after correction. The Ratio of minimum to maximum transmission is 0.8727.	wR2(int) was 0.0882 before and 0.0422 after correction. The Ratio of minimum to maximum transmission is 0.9114.	wR2(int) was 0.1307 before and 0.0464 after correction. The Ratio of minimum to maximum transmission is 0.9337.
T_{min}, T_{max}	0.693, 0.745	0.650, 0.745	0.680, 0.746	0.697, 0.747
No. of measured, independent and observed $[I > 2\sigma_{(I)}]$ reflections	77620, 11140, 7954	24991, 6109, 4551	54735, 16076, 11802	44959, 11358, 9339
R_{int}	0.061	0.038	0.027	0.03
(sin θ/λ)max ($Å^{-1}$)	0.6	0.604	0.668	0.77
Refinement				
$R[F^2 > 2\sigma(F^2)]$, $wR(F^2)$, S	0.054, 0.124, 1.02	0.045, 0.119, 1.03	0.066, 0.204, 1.02	0.039, 0.108, 1.05
No. of reflections	11140	6109	16076	11358
No. of parameters	968	599	1082	479
No. of restraints	84	92	61	24
H-atom treatment	H-atom parameters constrained			
$\Delta\rho_{max}$, $\Delta\rho_{min}$ (e $Å^{-3}$)	0.91, −0.67	0.47, −0.30	1.33, −0.50	0.90, −0.54

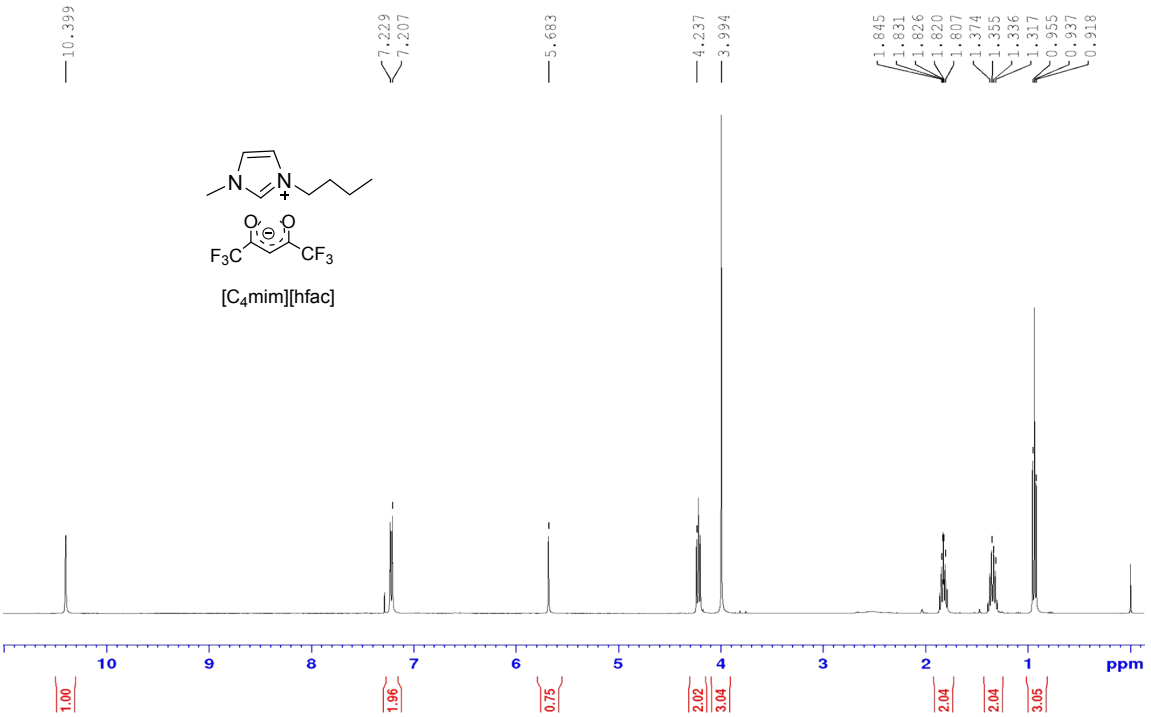

Figure 1. ^{1}H NMR spectrum of [C_4mim][hfac]

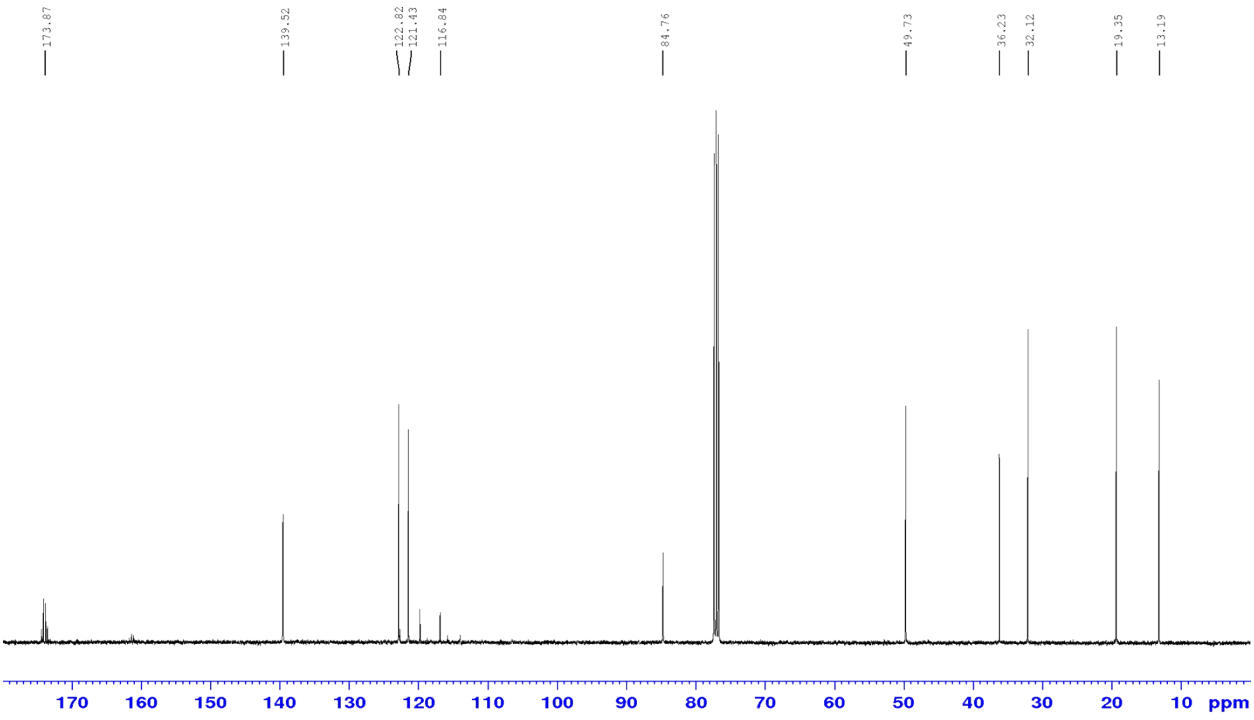

Figure 2. ^{13}C NMR spectrum of [C_4mim][hfac]

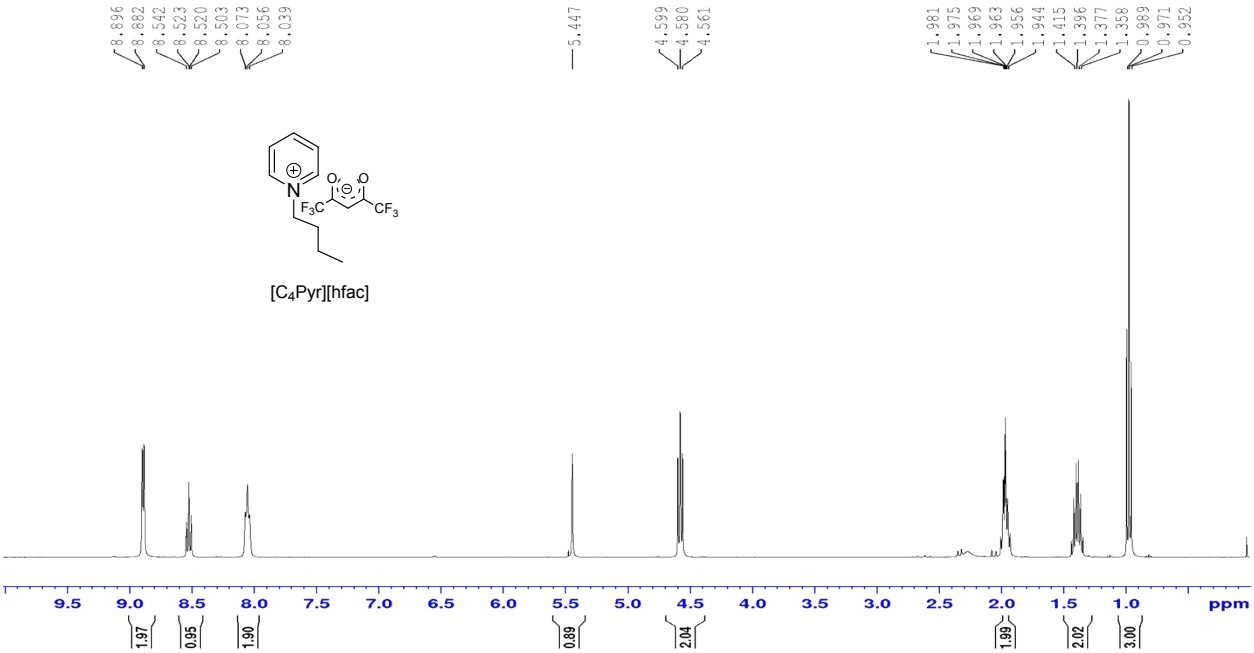

Figure 3. ^{1}H NMR spectrum of [C_4Pyr][hfac]

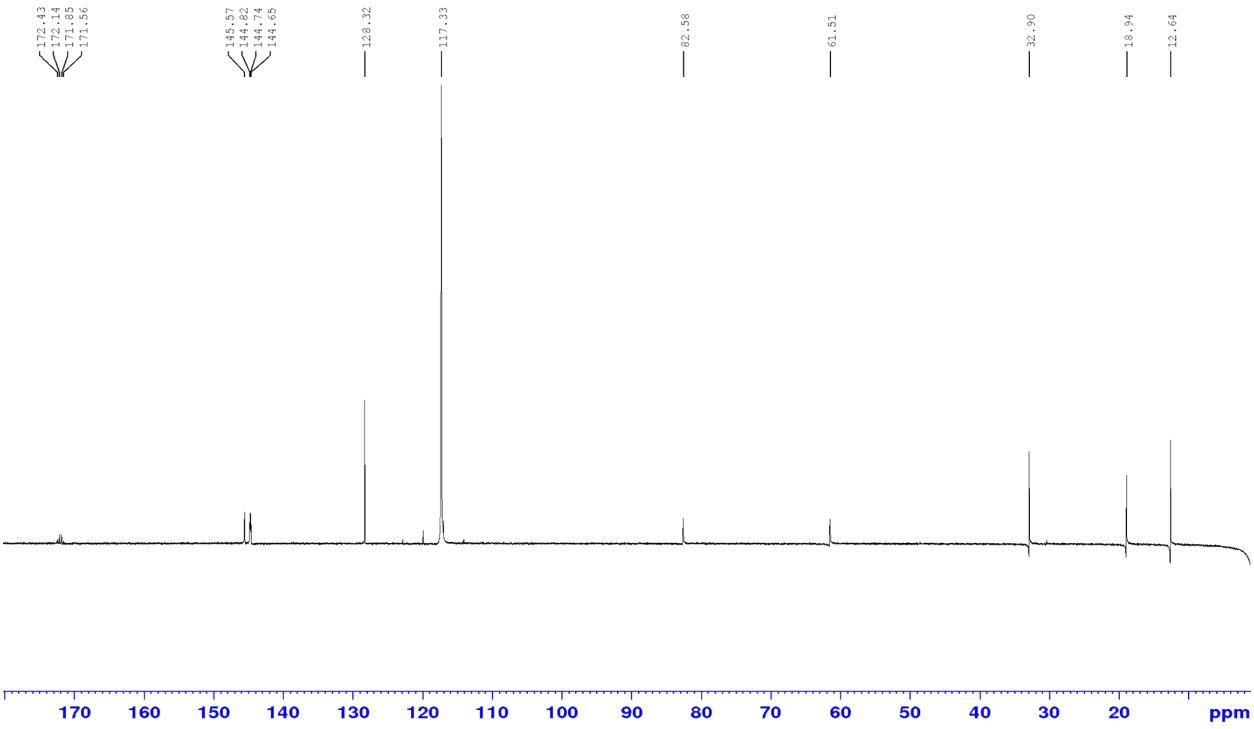

Figure 4. ^{13}C NMR spectrum of [C_4Pyr][hfac]

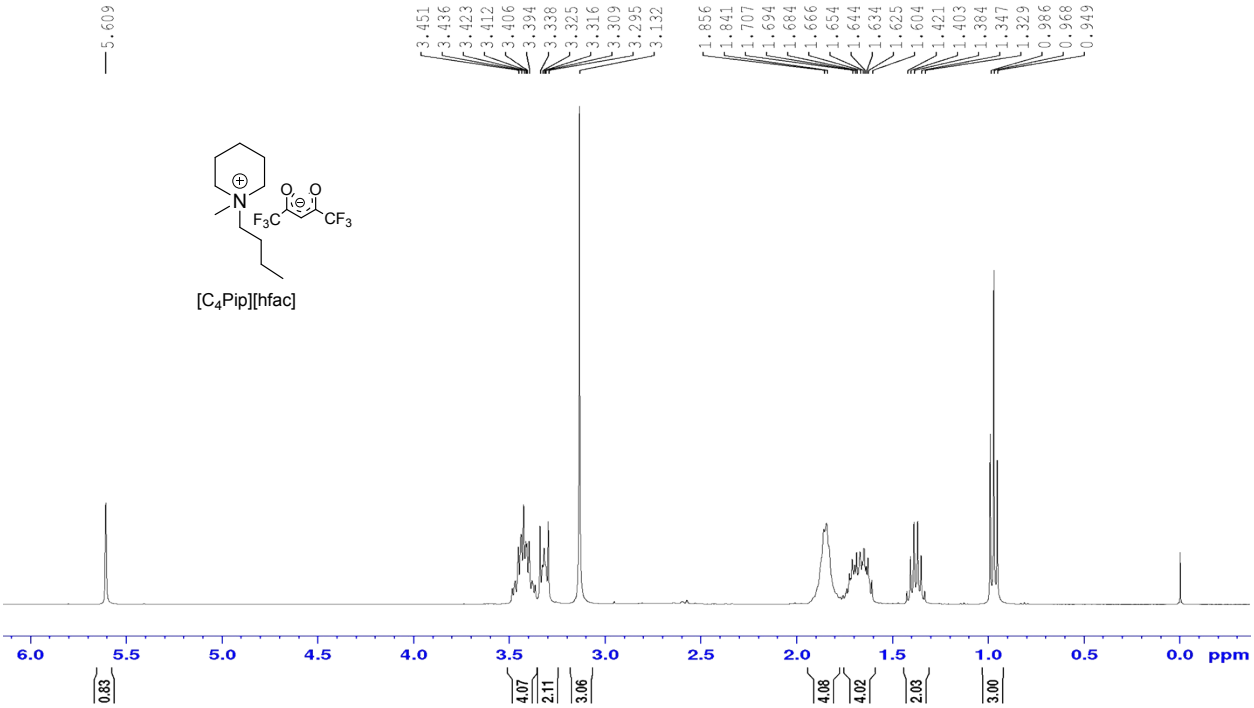

Figure 5. ^{1}H NMR spectrum of [C_4Pip][hfac]

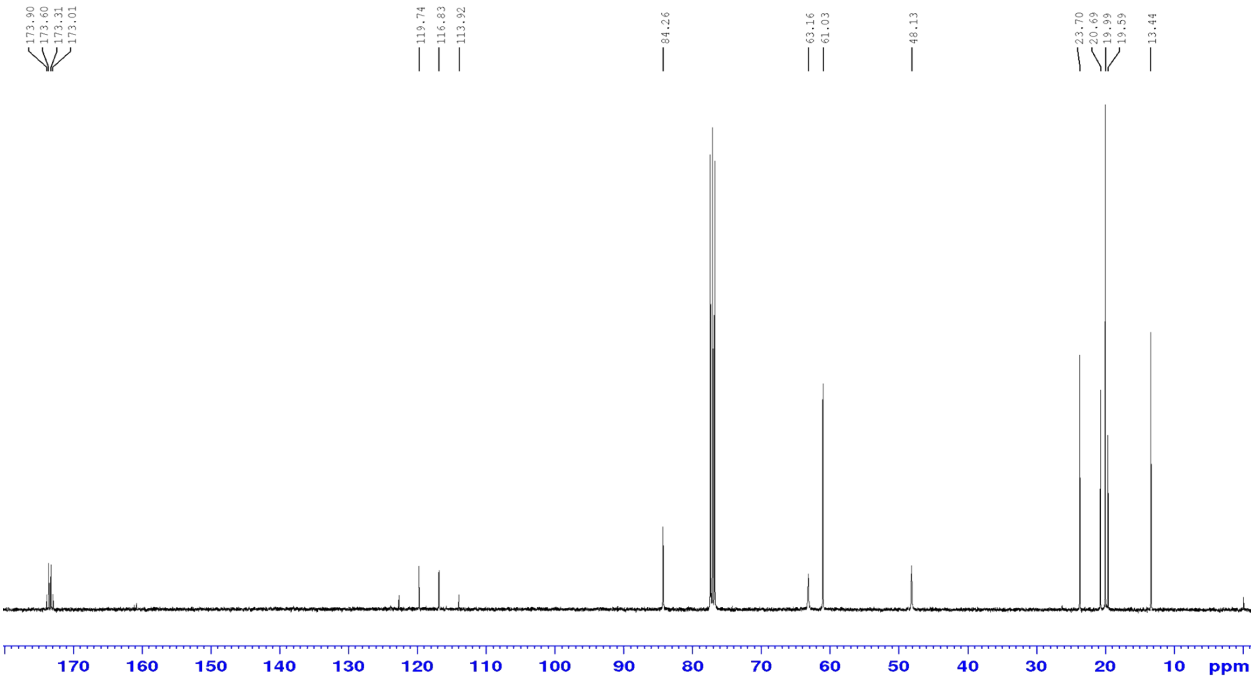

Figure 6. ^{13}C NMR spectrum of [C_4Pip][hfac]

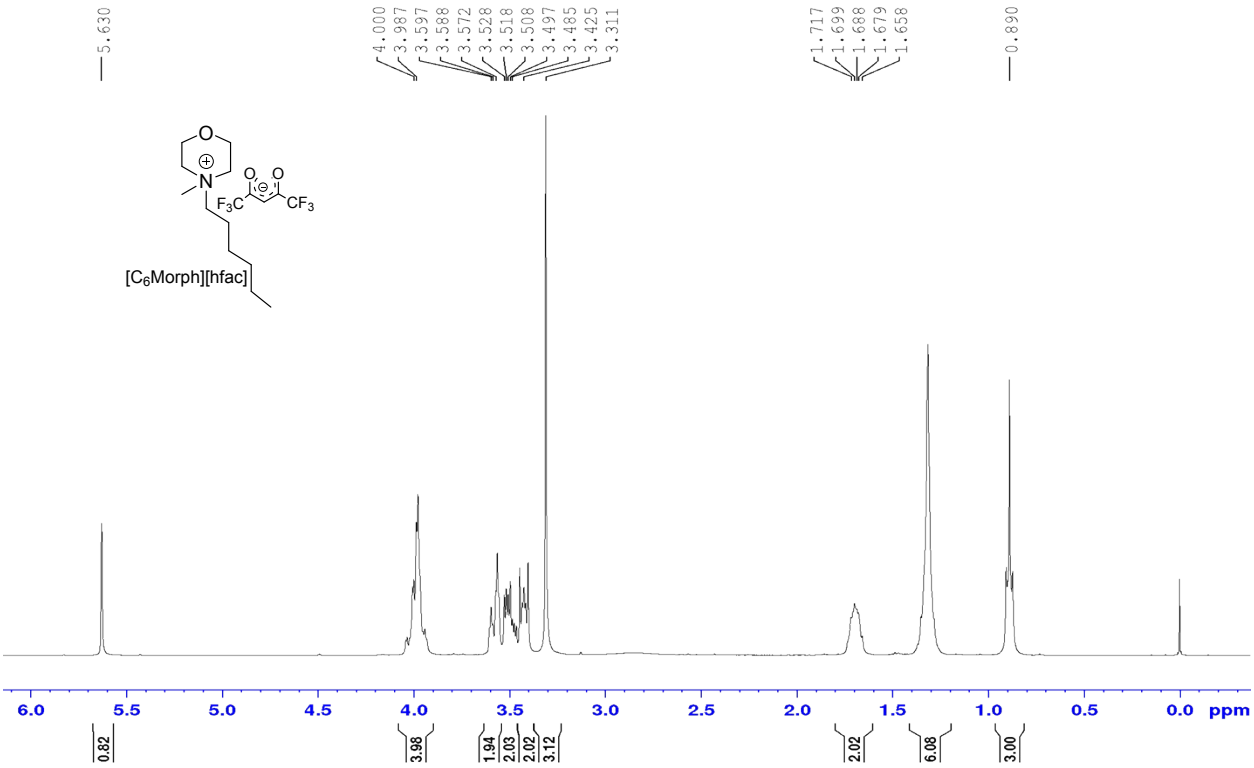

Figure 7. ^{1}H NMR spectrum of [C_6Morph][hfac]

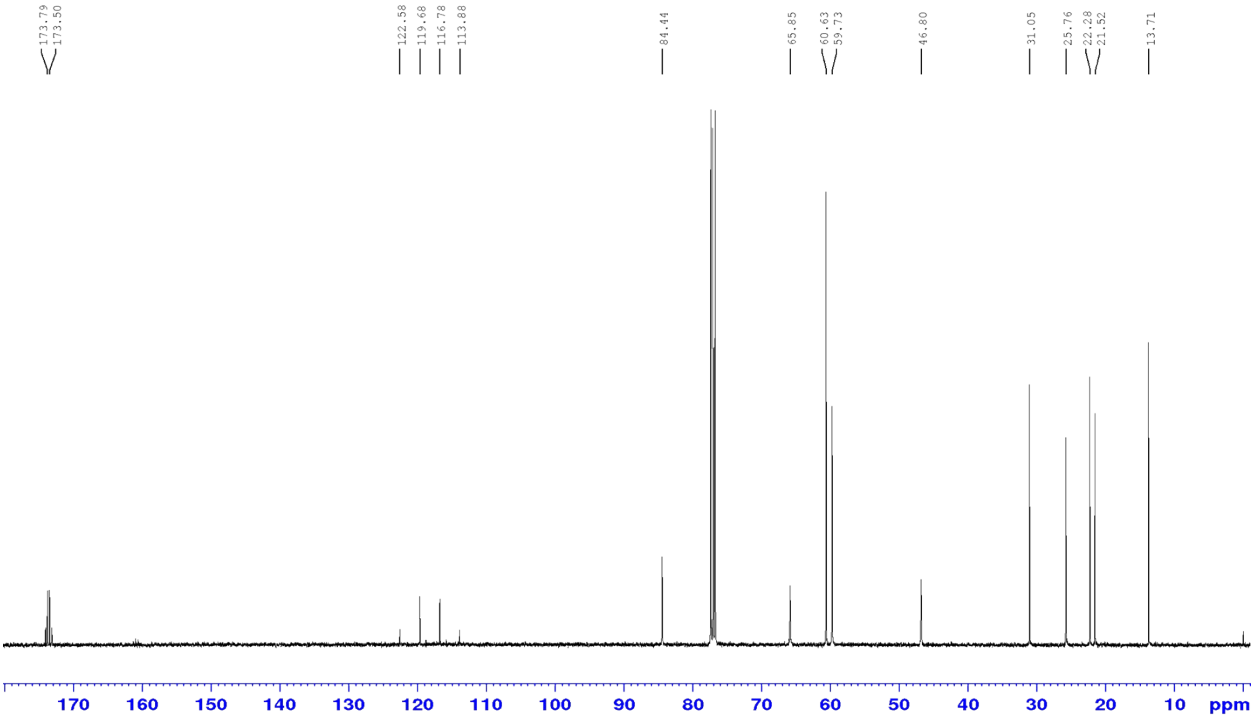

Figure 8. ^{13}C NMR spectrum of [C_6Morph][hfac]

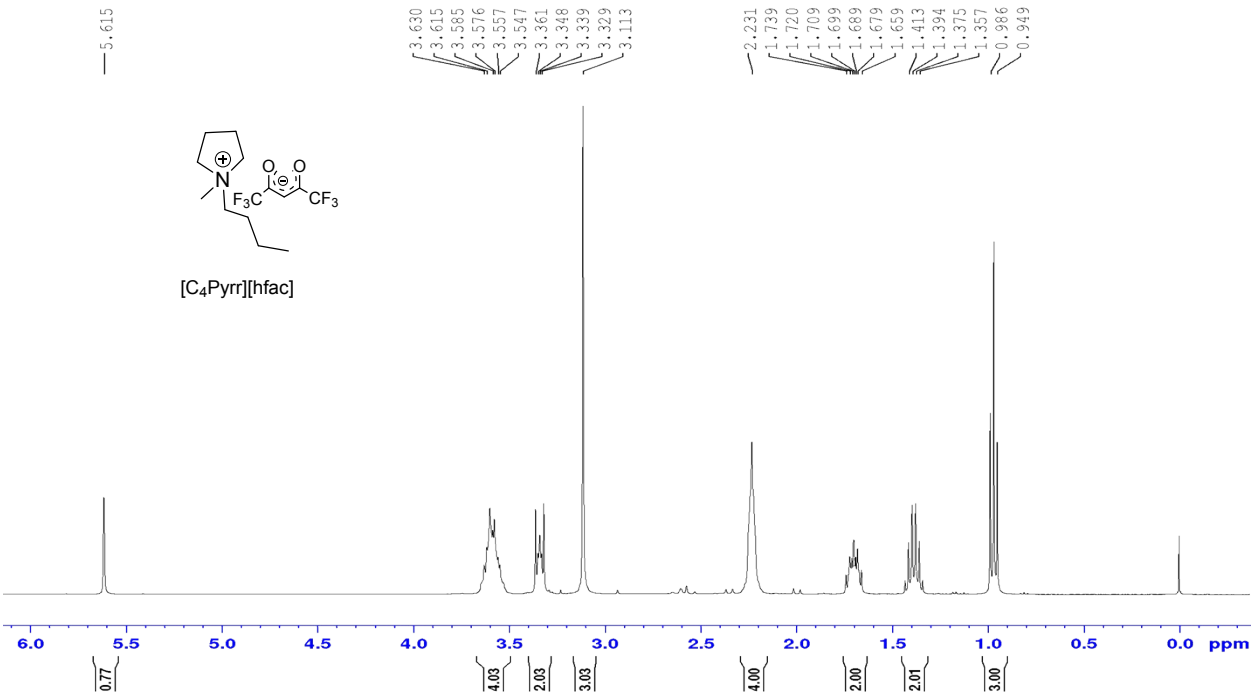

Figure 9. [1]H NMR spectrum of [C4Pyrr][hfac]

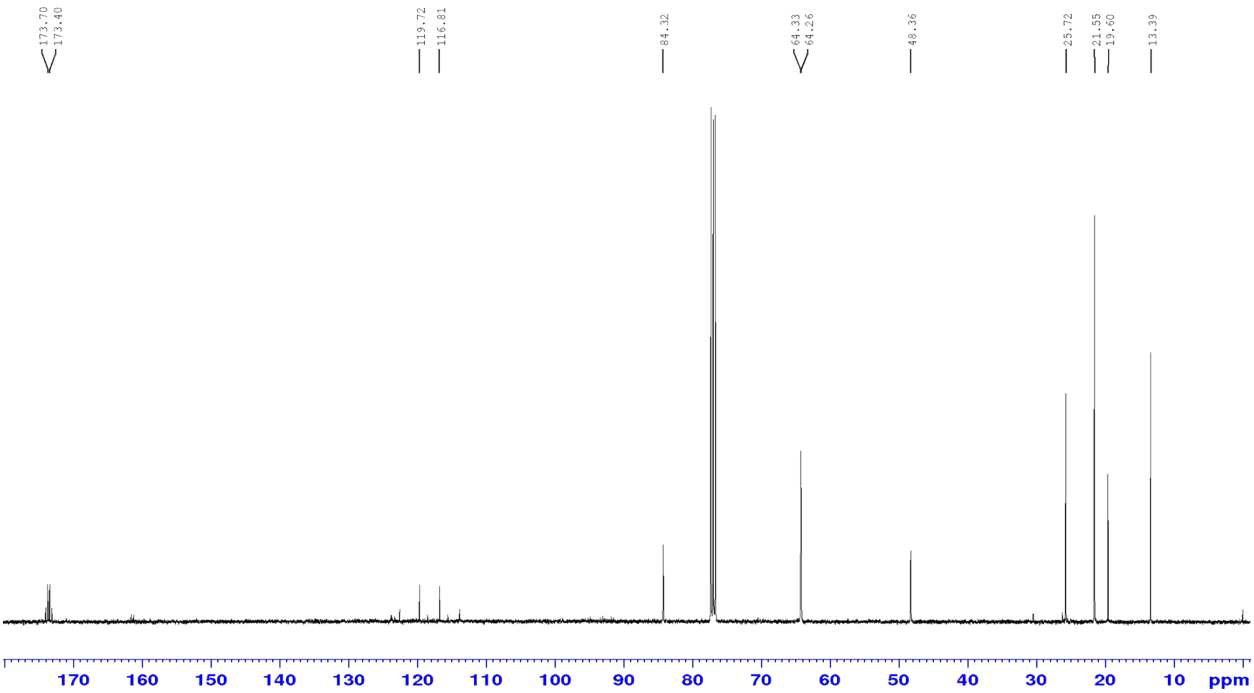

Figure 10. [13] C NMR spectrum of [C4Pyrr][hfac]

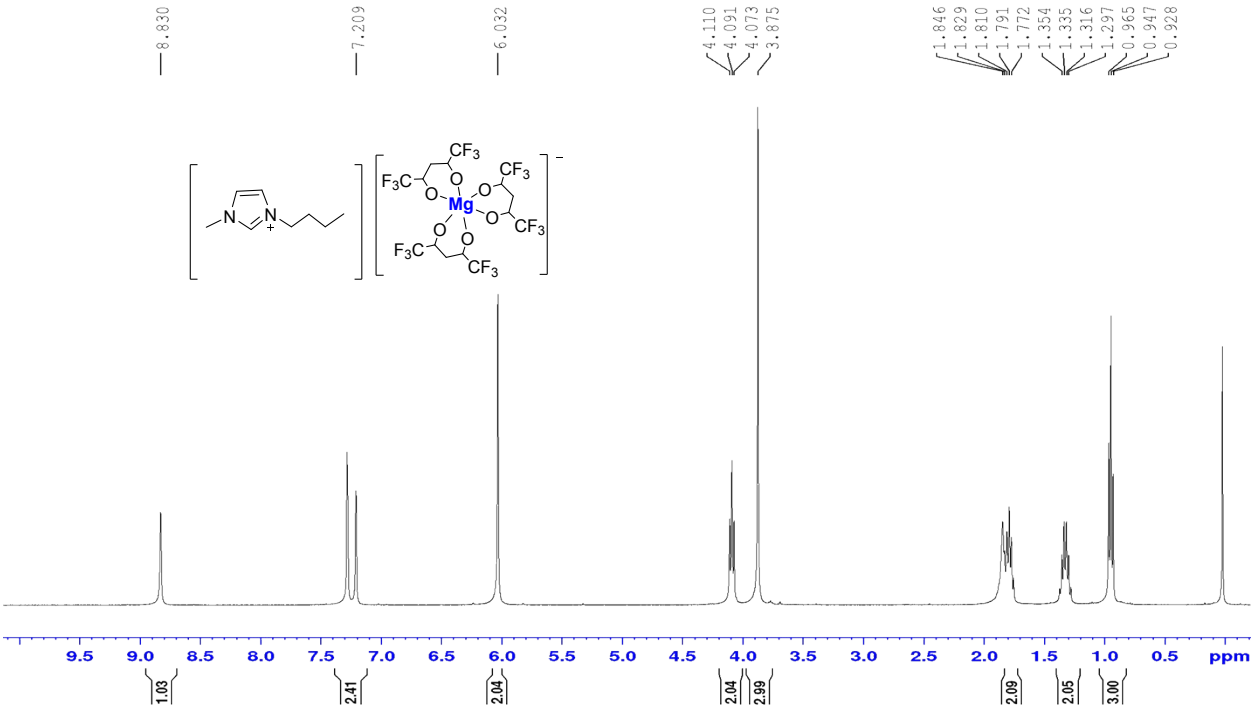

Figure 11. ^{1}H NMR spectrum of $[C_4mim][Mg(hfac)_3]$

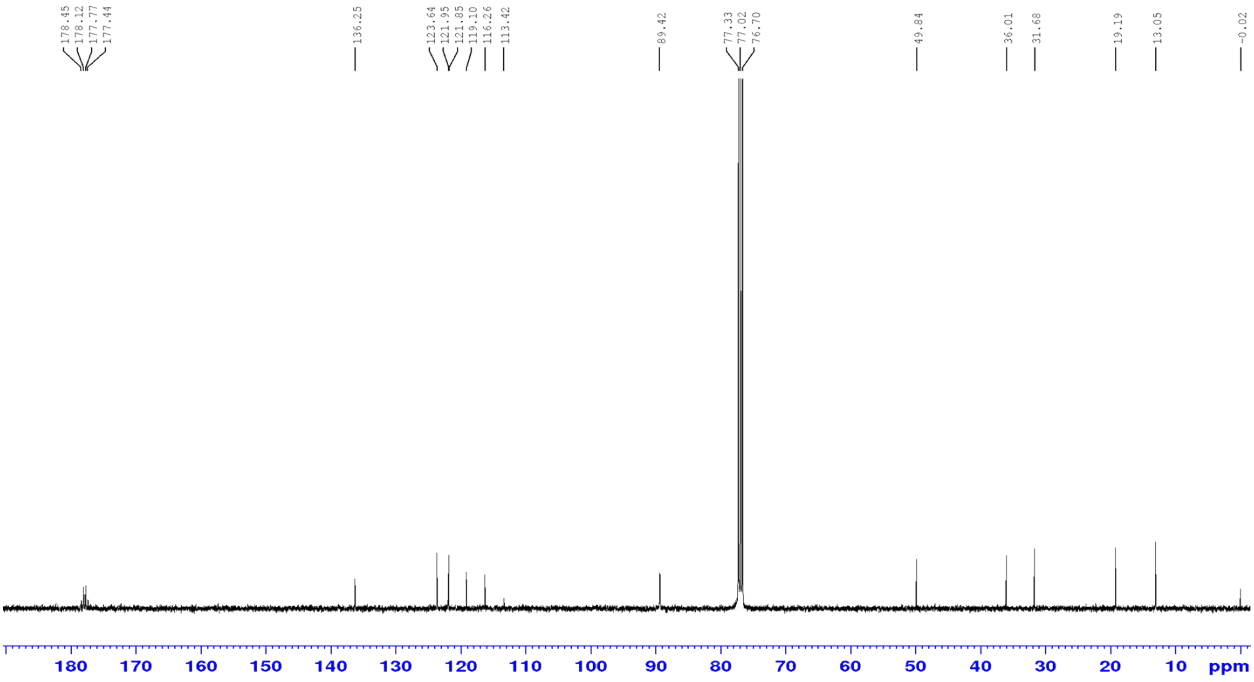

Figure 12. ^{13}C NMR spectrum of $[C_4mim][hfac]$

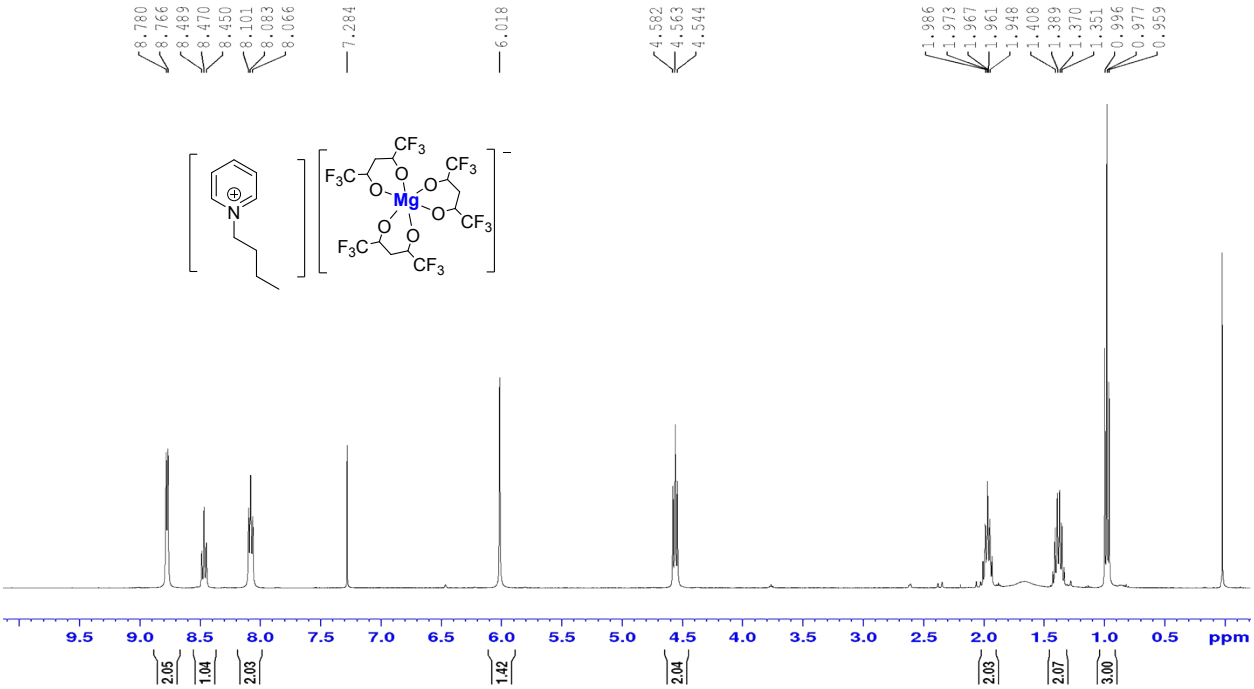

Figure 13. ^{1}H NMR spectrum of $[C_4Pyr][Mg(hfac)_3]$

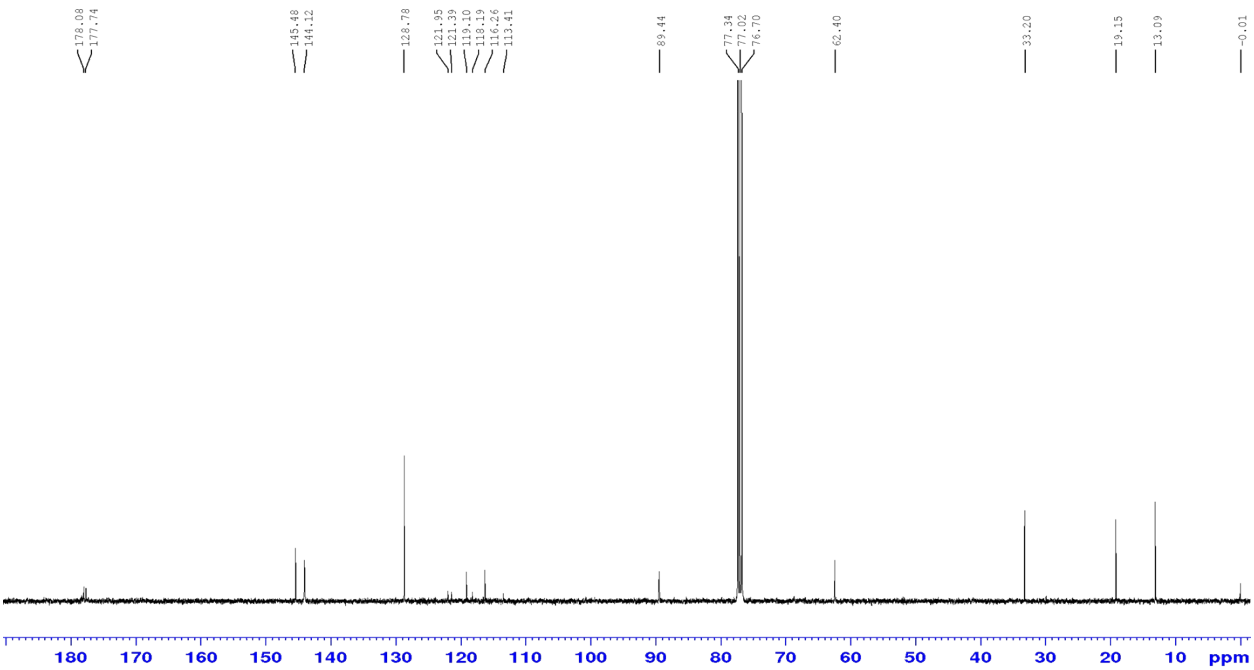

Figure 14. ^{13}C NMR spectrum of$[C_4Pyr][Mg(hfac)_3]$

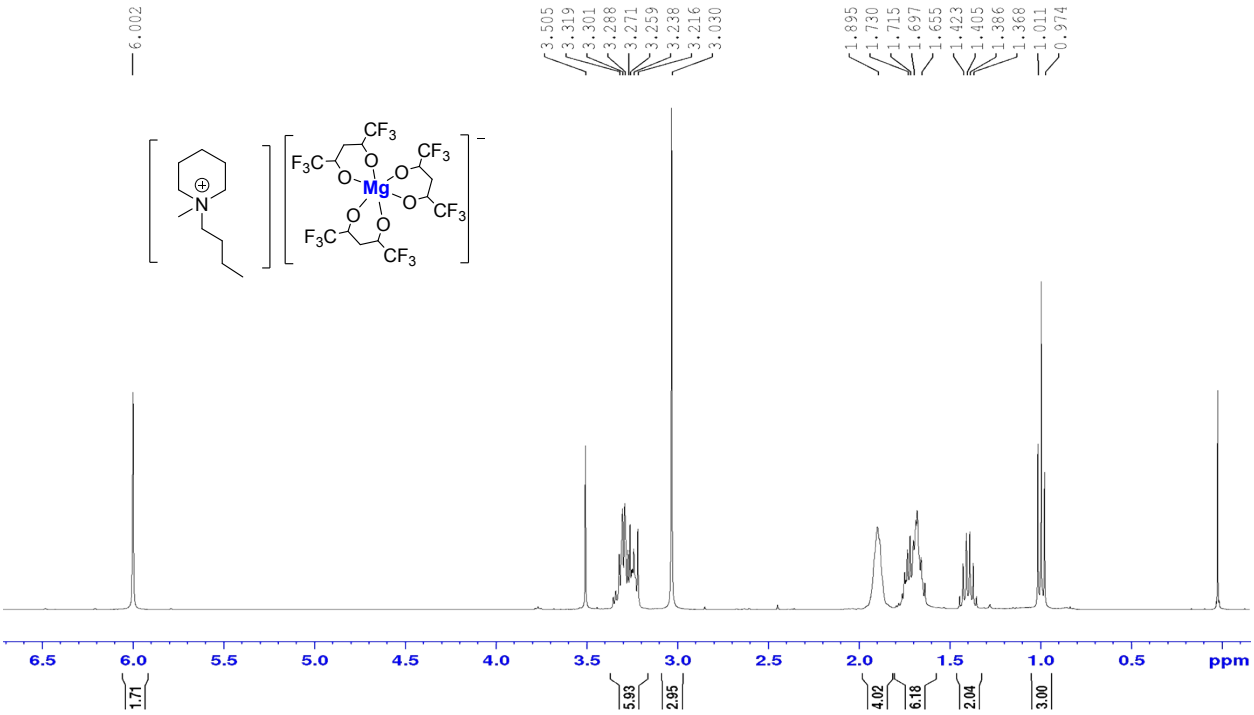

Figure 15. ^{1}H NMR spectrum of $[C_4Pip][Mg(hfac)_3]$

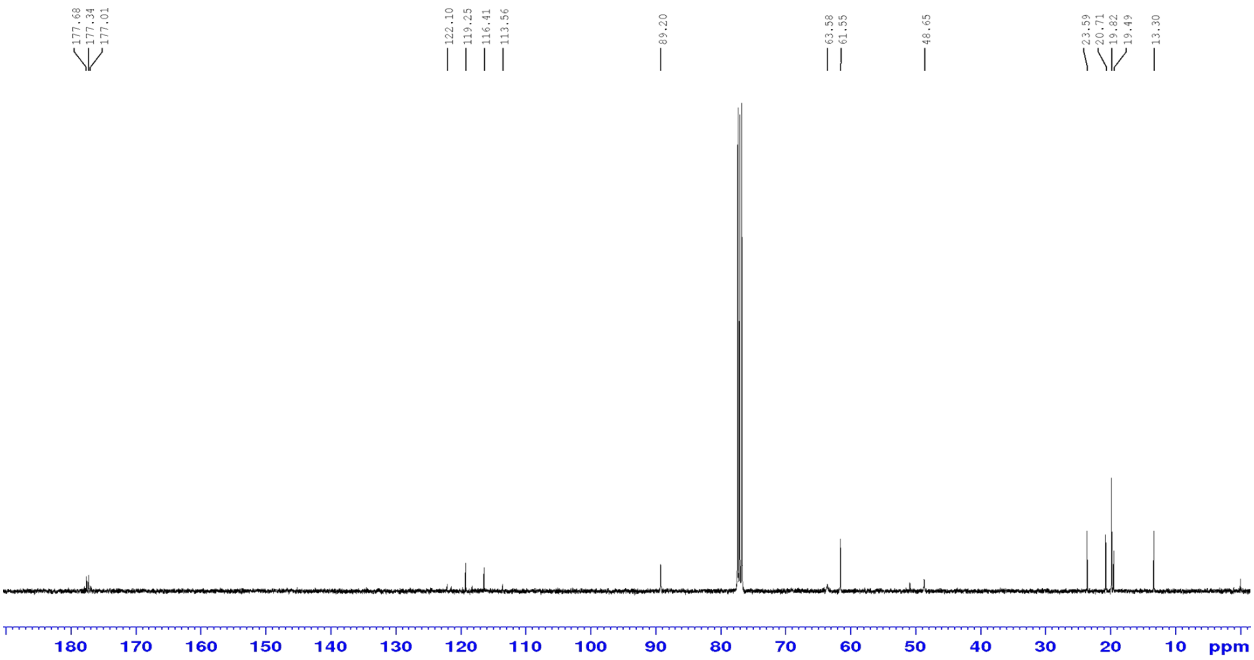

Figure S16. ^{13}C NMR spectrum of $[C_4Pip][Mg(hfac)_3]$

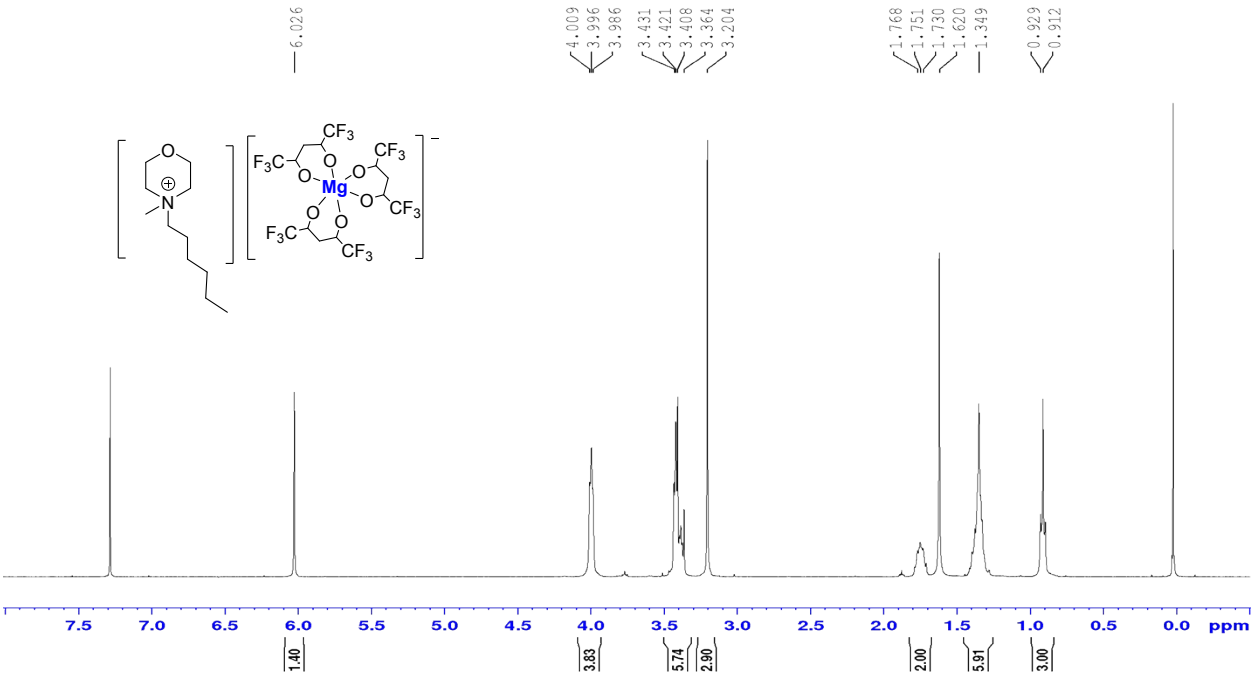

Figure 17. ^{1}H NMR spectrum of $[C_6Morph][Mg(hfac)_3]$

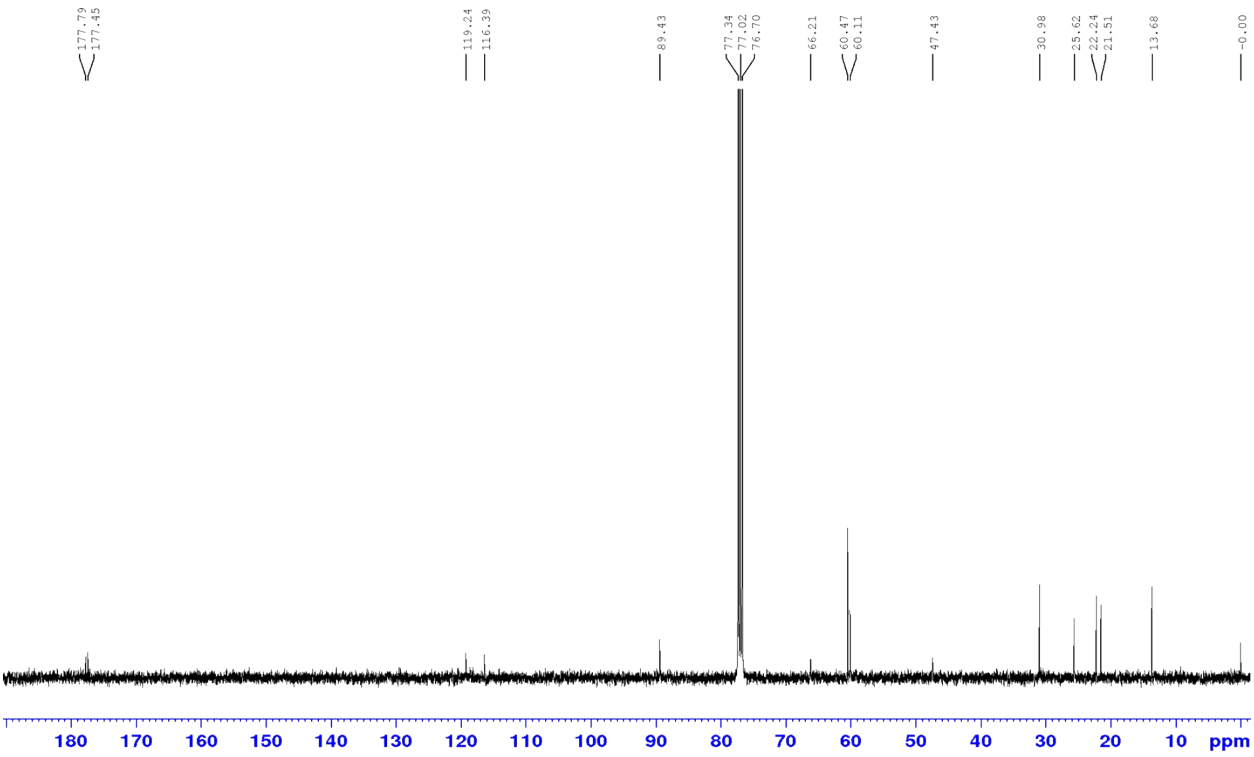

Figure 18. ^{13}C NMR spectrum of $[C_6Morph][Mg(hfac)_3]$

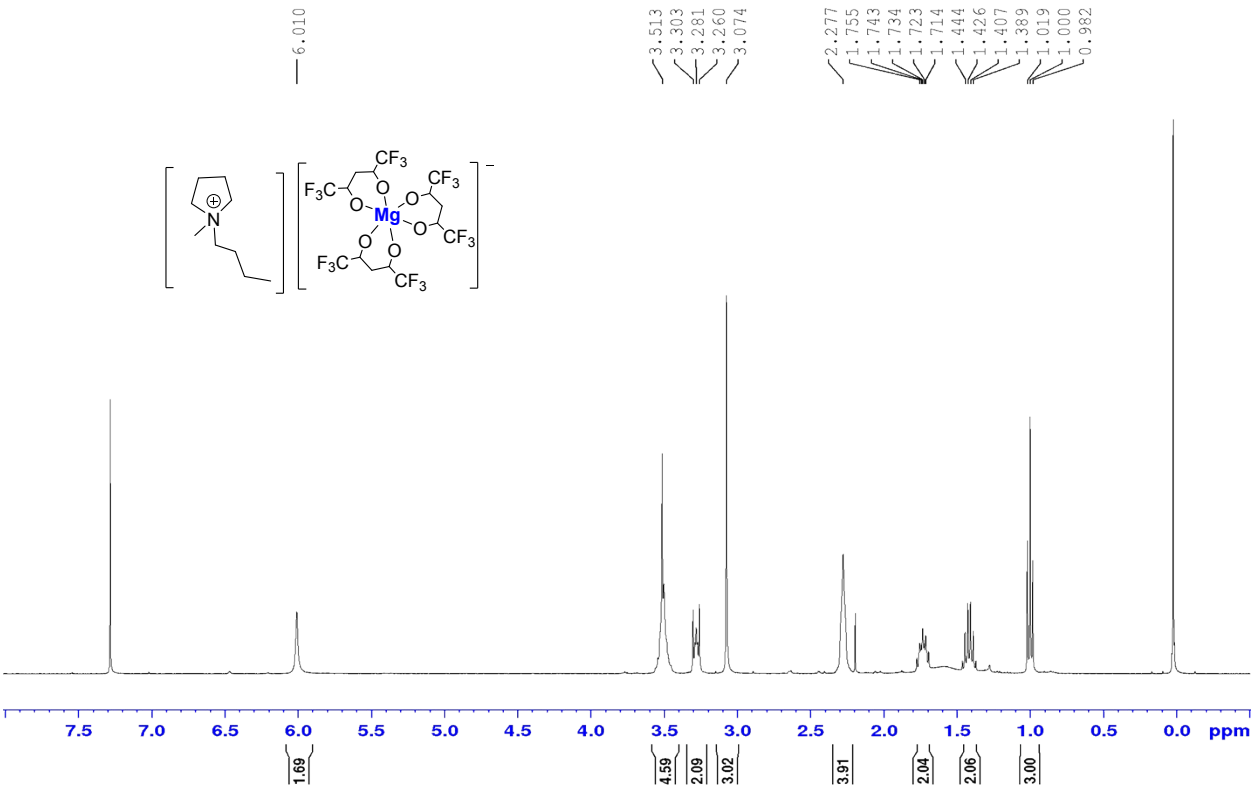

Figure 19. ^{1}H NMR spectrum of $[C_4Pyrr][Mg(hfac)_3]$

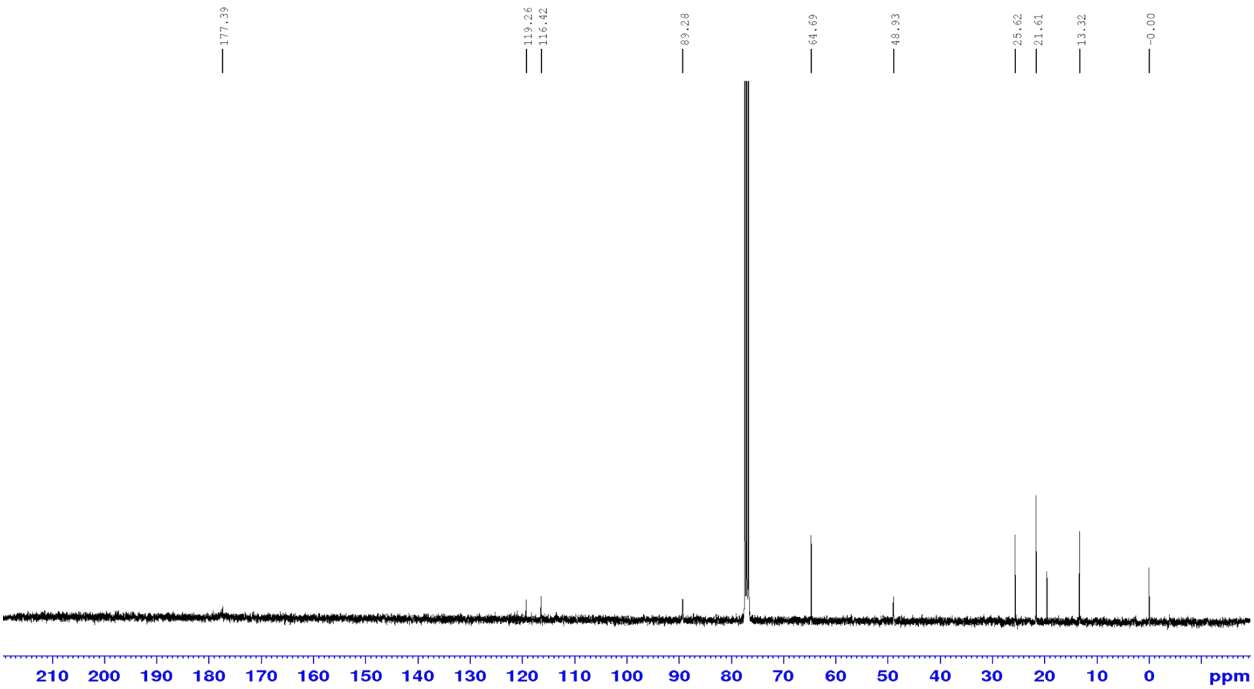

Figure 20. ^{13}C NMR spectrum of $[C_4Pyrr][Mg(hfac)_3]$