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Electronic Supplementary Information

Bis(alkyl) Scandium and Yttrium Complexes Coordinated by an Amidopyridinate Ligand: Synthesis, Characterization and Catalytic Performance in Isoprene Polymerization, Hydroelementation and Carbon Dioxide Hydrosilylation

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Contents:

Table S1. Crystal data and structure refinement details for $\mathbf{1_{Sc}}$, $\mathbf{1_Y}$ and $\mathbf{1_Y^{THF}}$.

	$\mathbf{1_{Sc}}$	$\mathbf{1_Y}$	$\mathbf{1_Y^{THF}}$
Formula	$C_{36}H_{55}N_4OScSi_2$, C_7H_8	$C_{36}H_{55}N_4OSi_2Y$, 1½C_7H_8	$C_{40}H_{63}N_4O_2Si_2Y$, ½C_6H_{14}
M	753.11	843.13	820.12
T, K	120	100	120
Crystal system	Monoclinic	Monoclinic	Triclinic
Space group	$P2_1/c$	$C2/c$	$P\text{-}1$
a, Å	19.191(2)	22.2860(10)	11.6694(6)
b, Å	16.3197(18)	15.6506(7)	13.2058(7)
c, Å	14.8442(16)	26.8173(12)	17.2330(9)
α, deg	90	90	112.2250(10)
β, deg	108.715(3)	90.9180(10)	104.7190(10)
γ, deg	90	90	91.7040(10)
V, Å^3	4403.3(8)	9352.4(7)	2354.1(2)
Z	4	8	2
d_{calc}, g/cm^3	1.136	1.198	1.157
μ, mm^{-1}	0.257	1.335	1.325
F_{000}	1624	3592	878
Crystal dimensions, mm	0.35×0.25×0.18	0.34×0.18×0.10	0.31×0.12×0.07
θ range for data collection, deg	1.12–26.02	1.77–29.13	1.68–30.03

HKL indices	$-23 \leq h \leq 23$ $-20 \leq k \leq 20$ $-18 \leq l \leq 18$	$-30 \leq h \leq 30$ $-21 \leq k \leq 21$ $-36 \leq l \leq 36$	$-16 \leq h \leq 16$ $-18 \leq k \leq 18$ $-24 \leq l \leq 24$
Reflns. collected	56077	50513	31664
Reflns. unique	8683	12580	13779
R_{int}	0.1155	0.0822	0.0508
Data / restraints / parameters	56077 / 99 / 513	12580 / 291 / 552	13779 / 42 / 500
$S(F^2)$	1.010	1.056	1.007
R_1/wR_2 ($I > 2\sigma(I)$)	0.0535 / 0.1280	0.0590 / 0.1200	0.0474 / 0.0981
R_1/wR_2 (all data)	0.0876 / 0.1490	0.1029 / 0.1383	0.0845 / 0.1101
Largest diff. peak and hole, e/Å^3	1.12 / –0.45	1.10 / –0.58	0.97 / –0.63

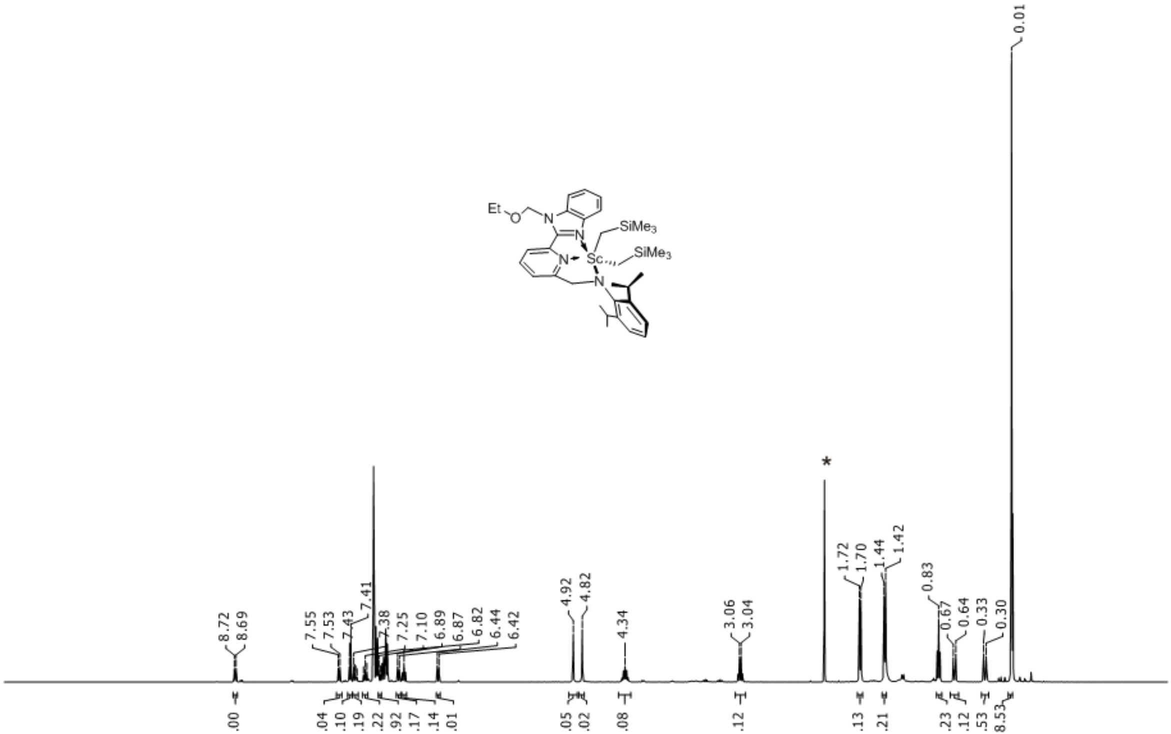

Fig. S1. ^{1}H NMR spectrum (400 MHz, C_6D_6, 293 K) of **1$_{Sc}$**. *signal of toluene solvate.

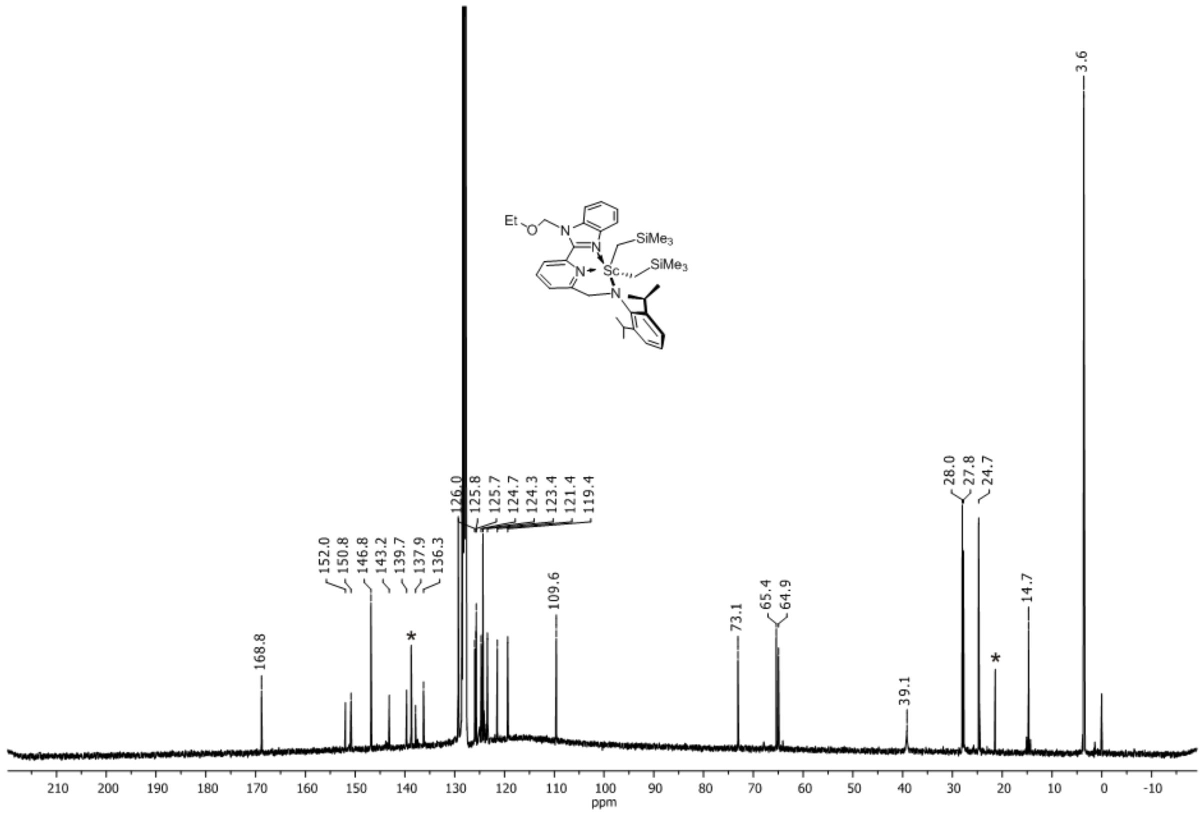

Fig. S2. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, C_6D_6, 293 K) of **1_{Sc}**. *signal of toluene solvate.

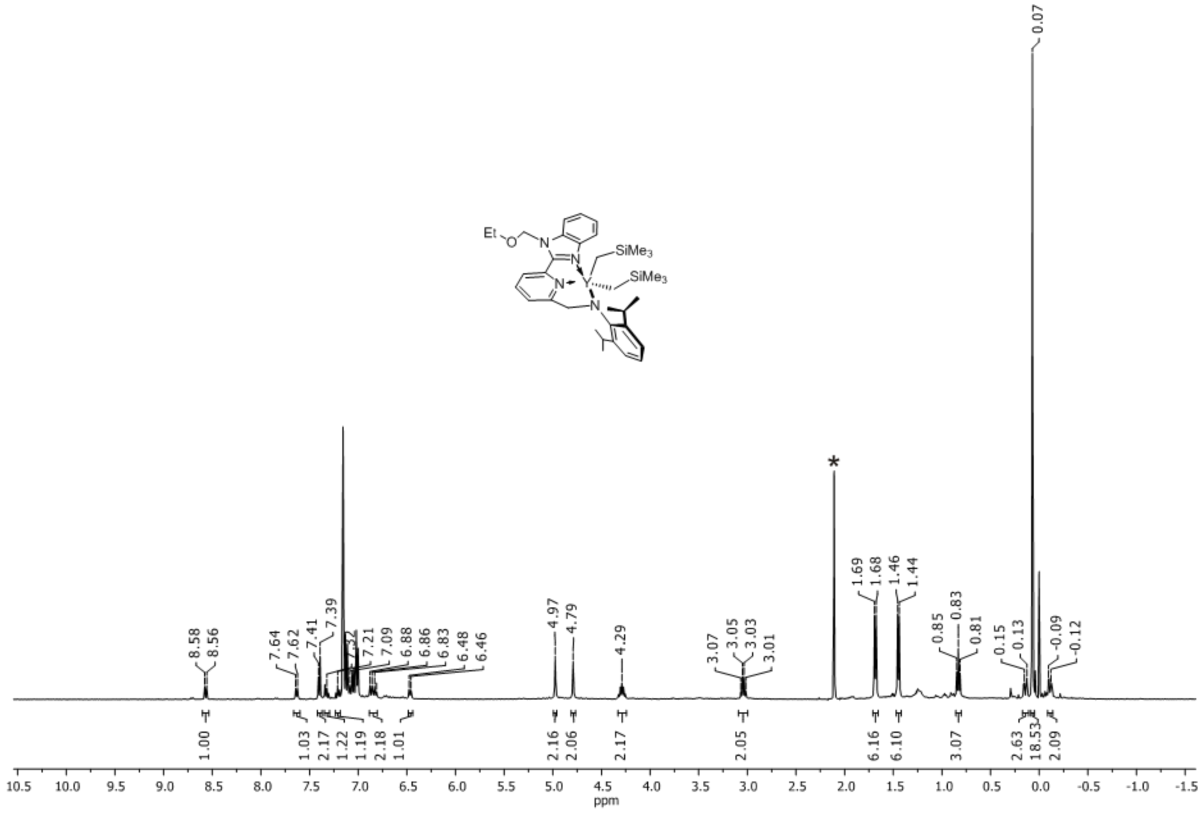

Fig. S3. ^{1}H NMR spectrum (400 MHz, C_6D_6, 293 K) of **1_{Y}**. *signal of toluene solvate.

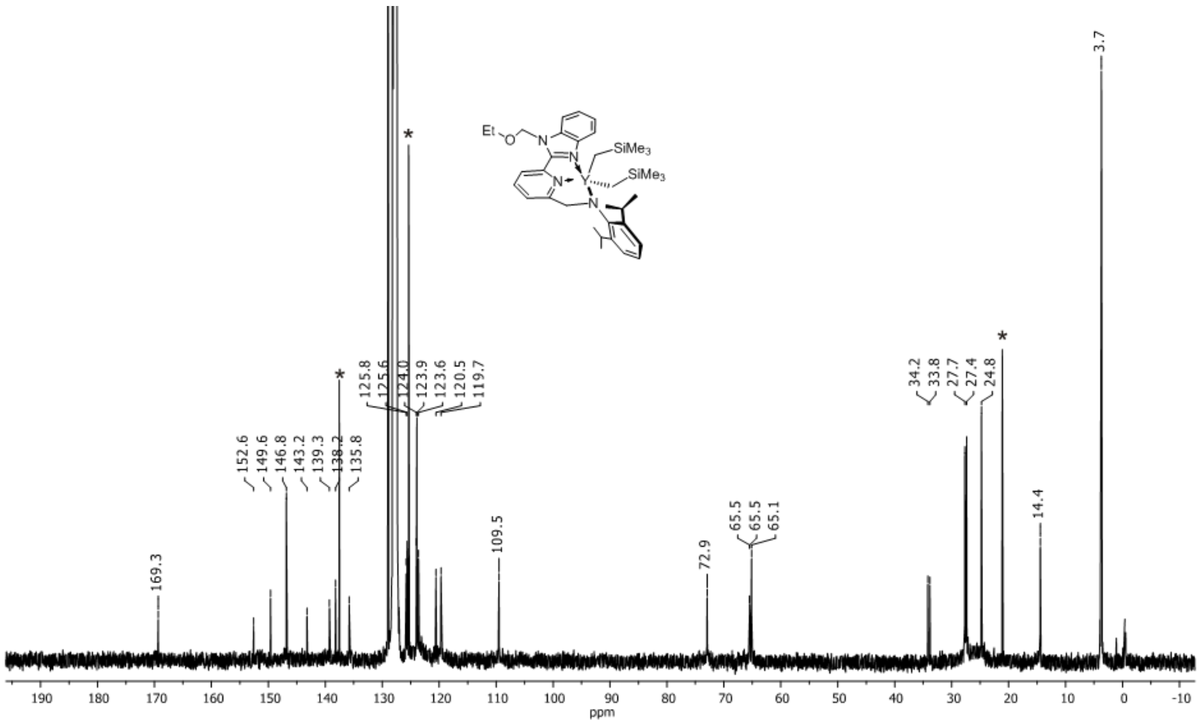

Fig. S4. $^{13}C\{^1H\}$ NMR spectrum (100 MHz, C_6D_6, 293 K) of **1**$_{\mathbf{Y}}$. *signal of toluene solvate.

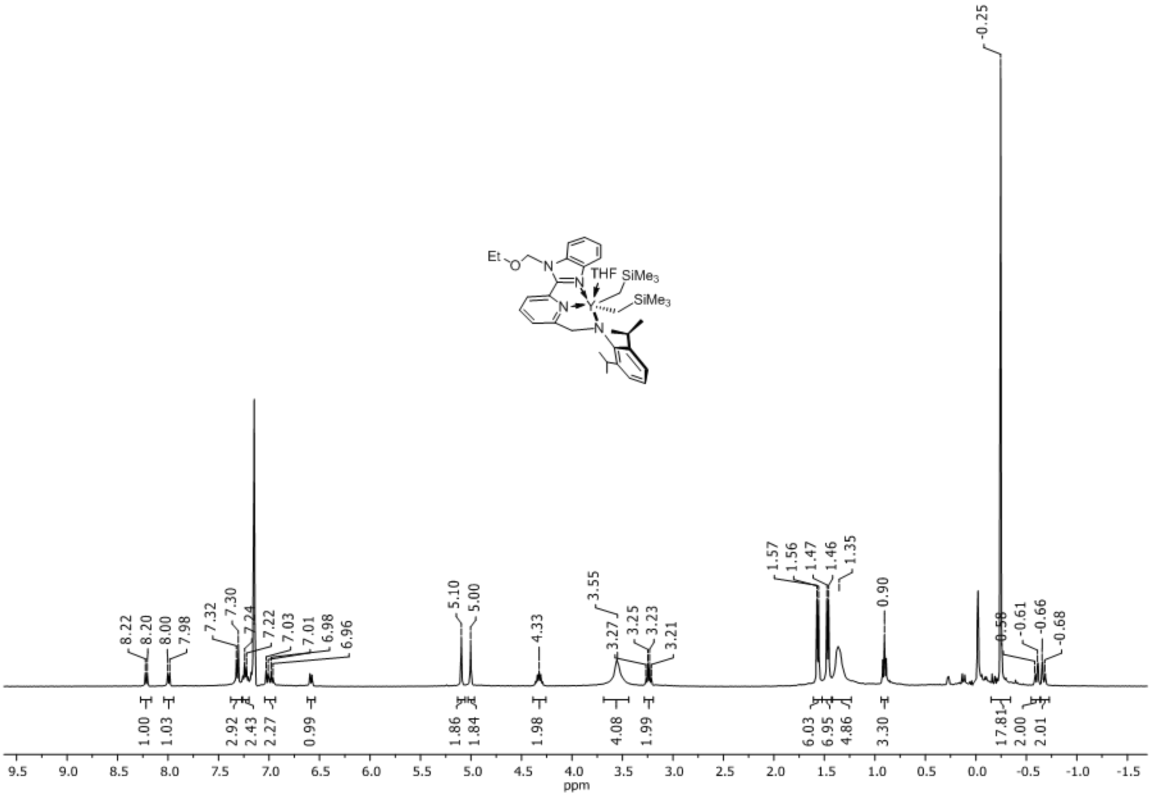

Fig. S5. ^1H NMR spectrum (400 MHz, C_6D_6, 293 K) of **1**$_{\mathbf{Y}}^{\mathbf{THF}}$.

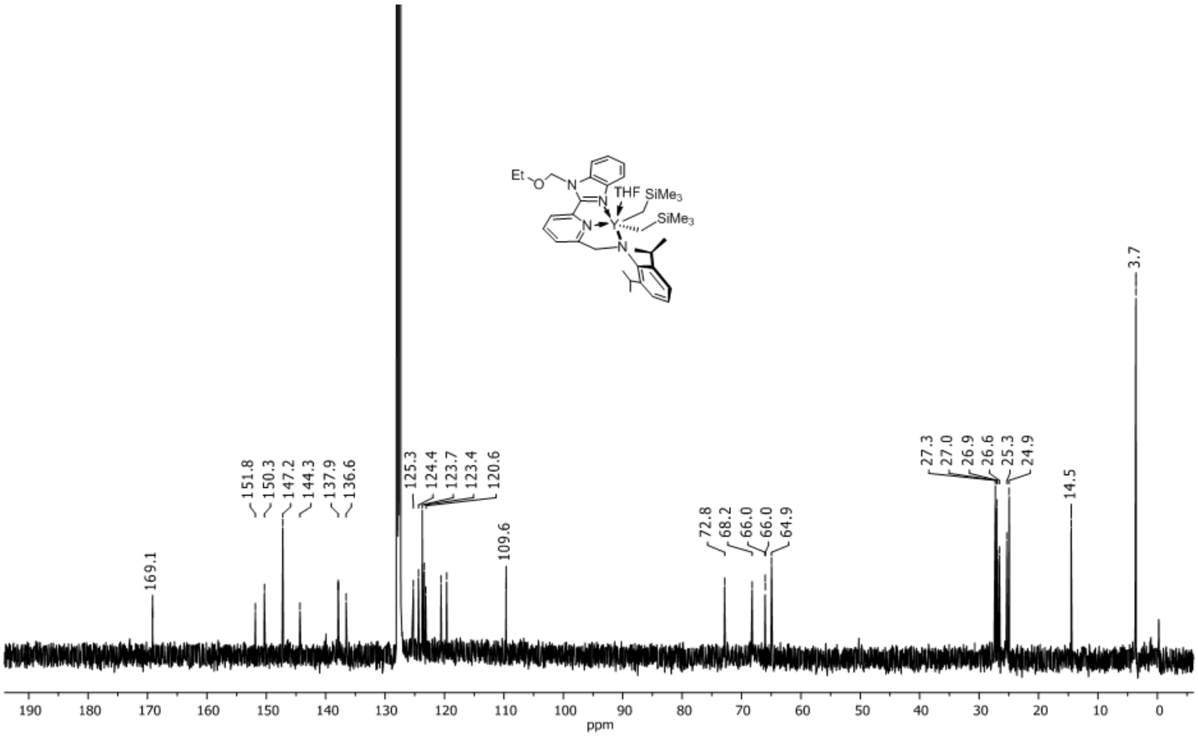

Fig. S6. $^{13}C\{^{1}H\}$ NMR spectrum (100 MHz, C_6D_6, 293 K) of $\mathbf{1_Y}^{\mathbf{THF}}$.

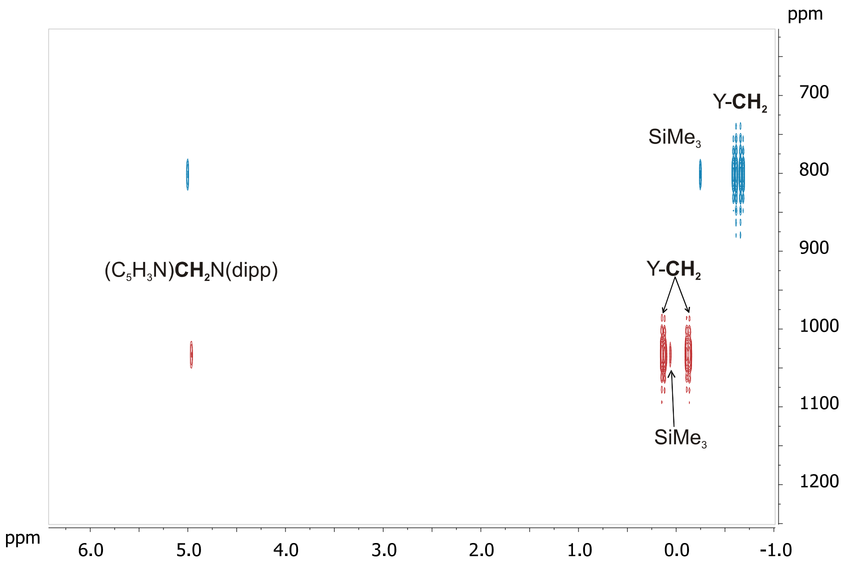

Fig. S7. 2D ^{89}Y-^{1}H *g*-HMQC NMR spectrum (400; 19.6 MHz, C_6D_6, 293 K) of $\mathbf{1_Y}$ (red) and $\mathbf{1_Y}^{\mathbf{THF}}$ (blue).

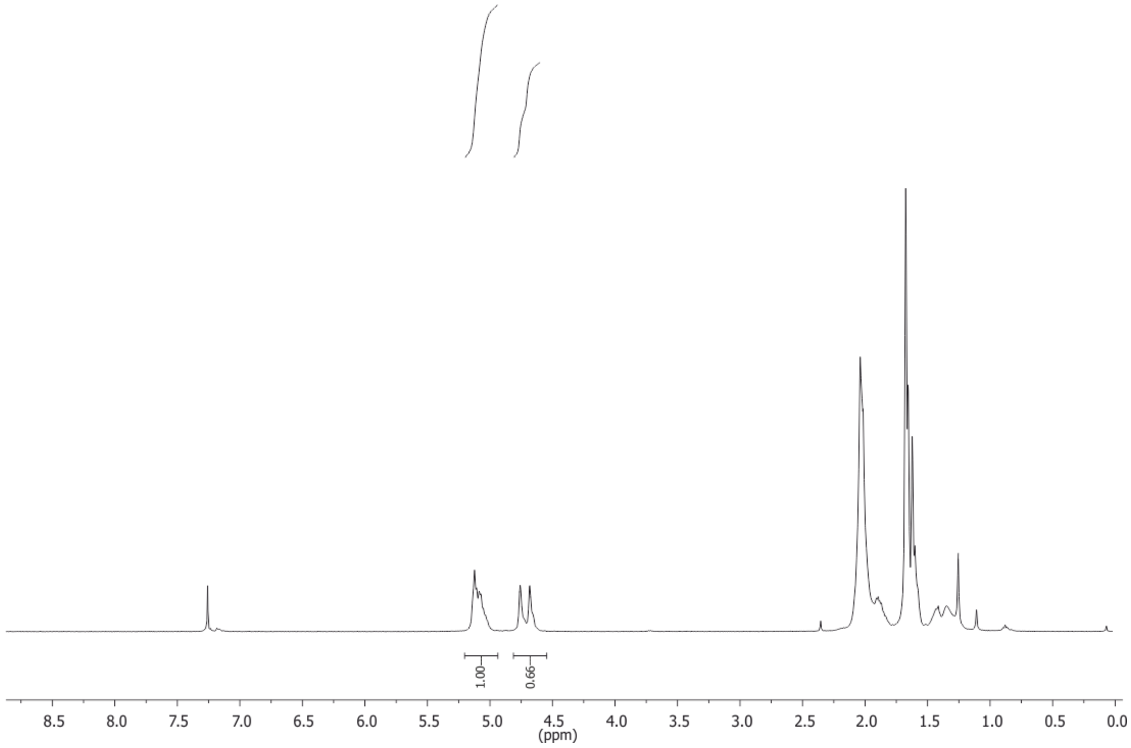

Fig. S8. ^{1}H NMR spectrum (400 MHz, $CDCl_3$, 293 K) of PIP prepared by catalysis with **1**$_{Sc}$/[$PhNHMe_2$] [$B(C_6F_5)_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 5).

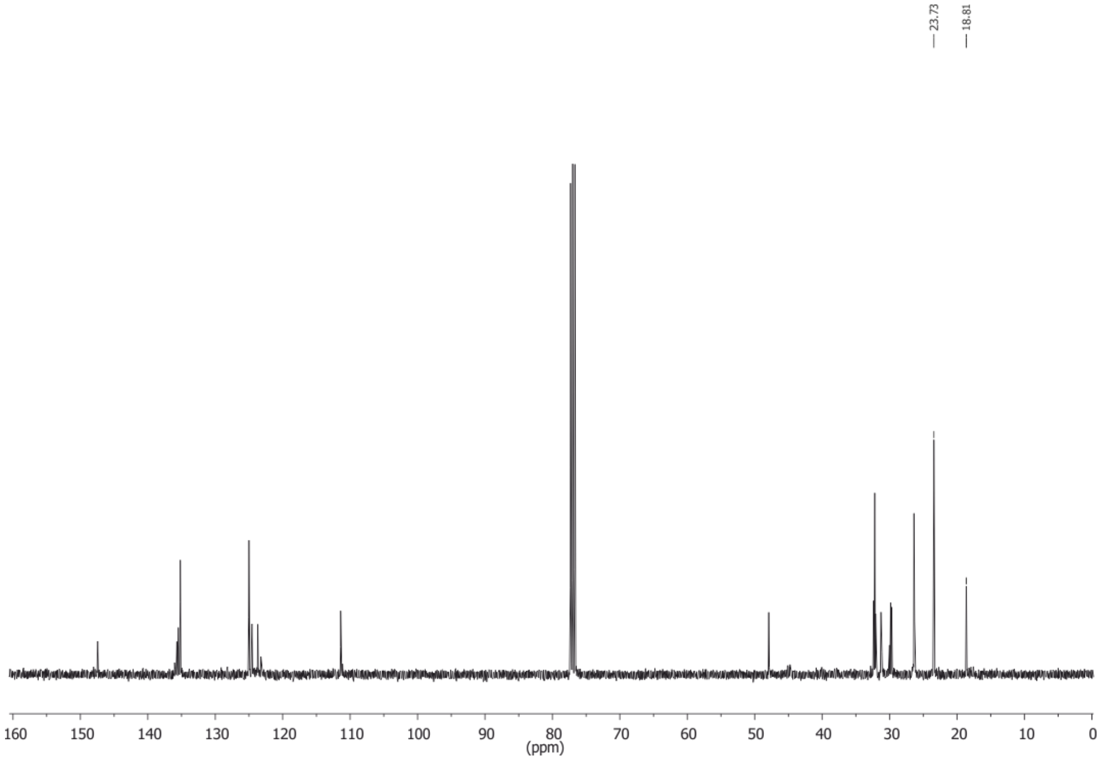

Fig. S9. ^{13}C{^{1}H } NMR spectrum (100 MHz, $CDCl_3$, 293 K) of PIP prepared by catalysis with **1**$_{Sc}$/[$PhNHMe_2$] [$B(C_6F_5)_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 5).

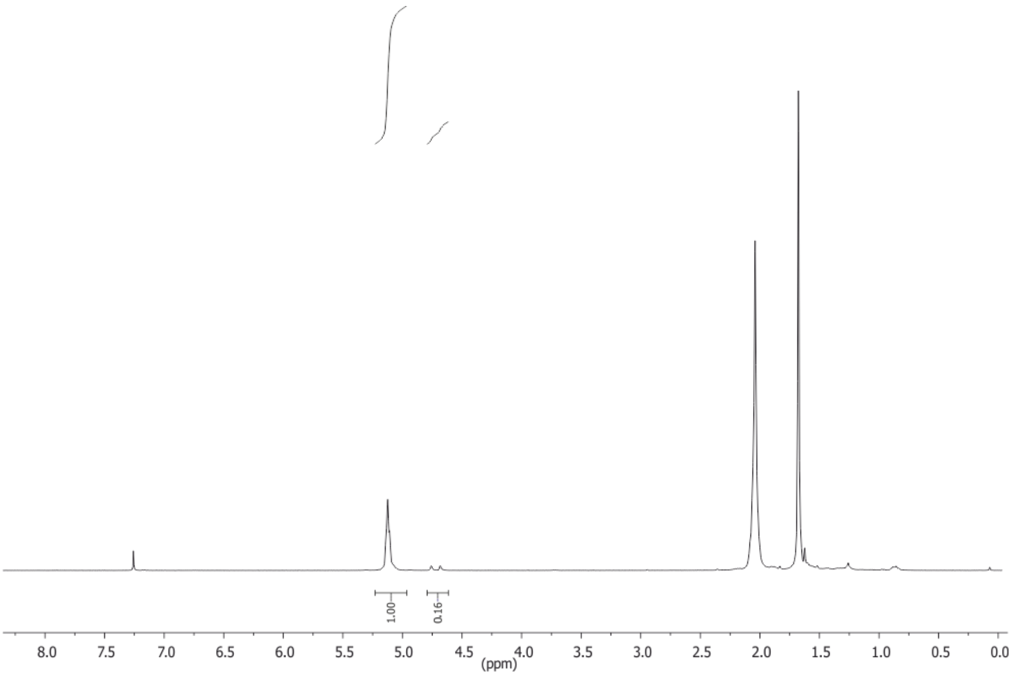

Fig. S10. ^{1}H NMR spectrum (400 MHz, CDCl$_3$, 293 K) of PIP prepared by catalysis with $\mathbf{1}_{\mathrm{Y}}$/[Ph$_3$C][B(C$_6$F$_5$)$_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 9).

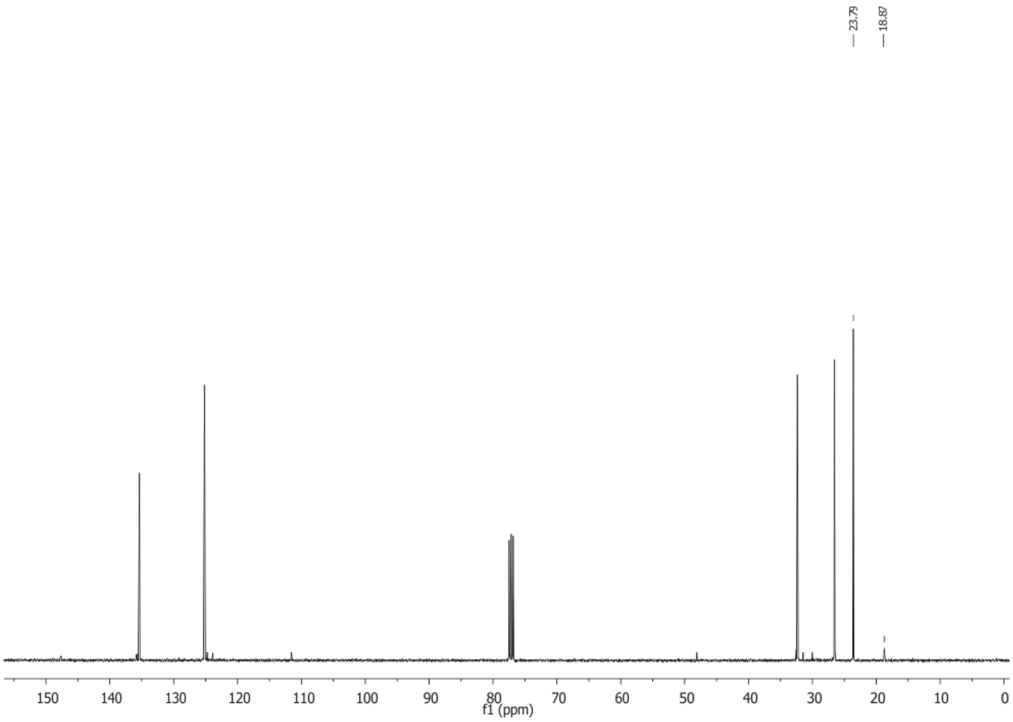

Fig. S11. ^{13}C{^{1}H } NMR spectrum (100 MHz, CDCl$_3$, 293 K) of PIP prepared by catalysis with $\mathbf{1}_{\mathrm{Y}}$/[Ph$_3$C][B(C$_6$F$_5$)$_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 9).

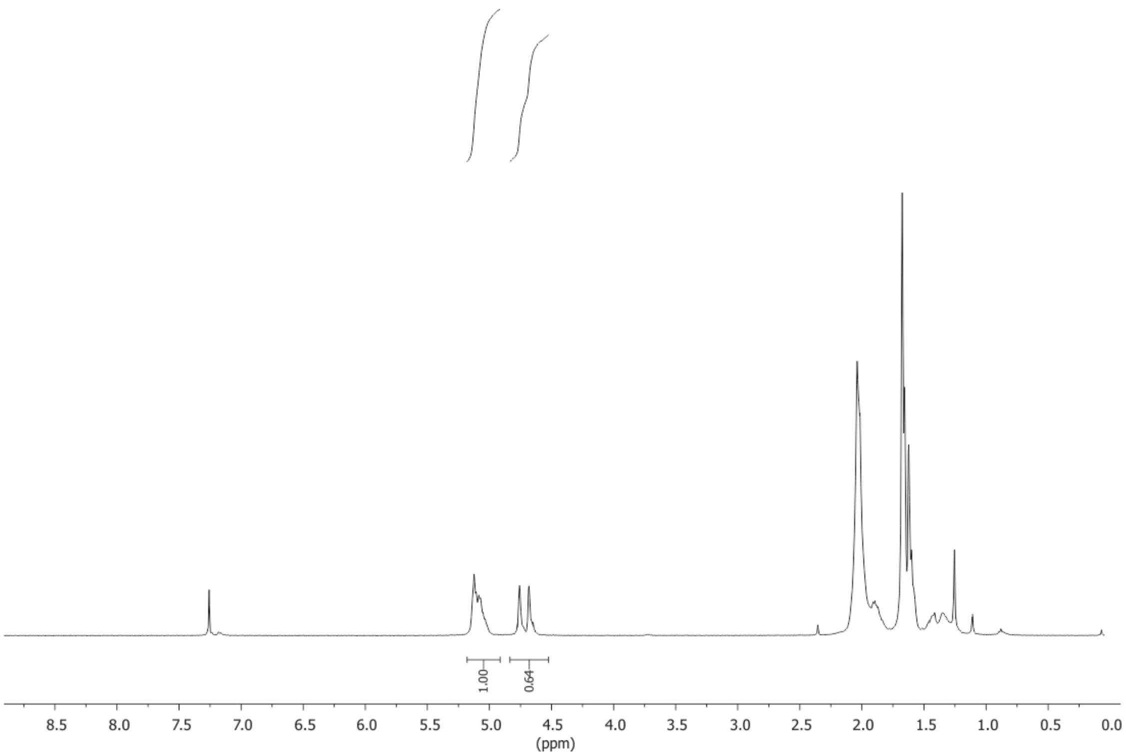

Fig. S12. ^{1}H NMR spectrum (400 MHz, CDCl$_3$, 293 K) of PIP prepared by catalysis with $\mathbf{1_Y^{THF}}$/[PhNHMe$_2$][B(C$_6$F$_5$)$_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 11).

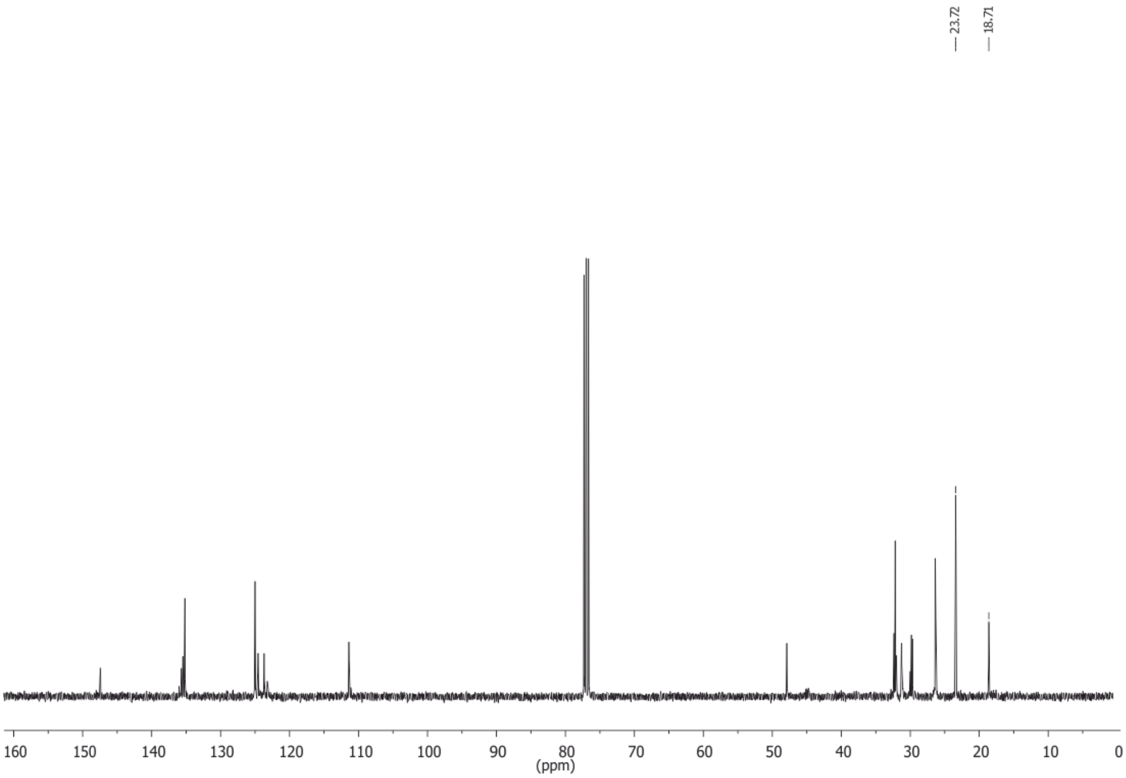

Fig. S13. ^{13}C{^{1}H } NMR spectrum (100 MHz, CDCl$_3$, 293 K) of PIP prepared by catalysis with $\mathbf{1_Y^{THF}}$/[PhNHMe$_2$][B(C$_6$F$_5$)$_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 11).

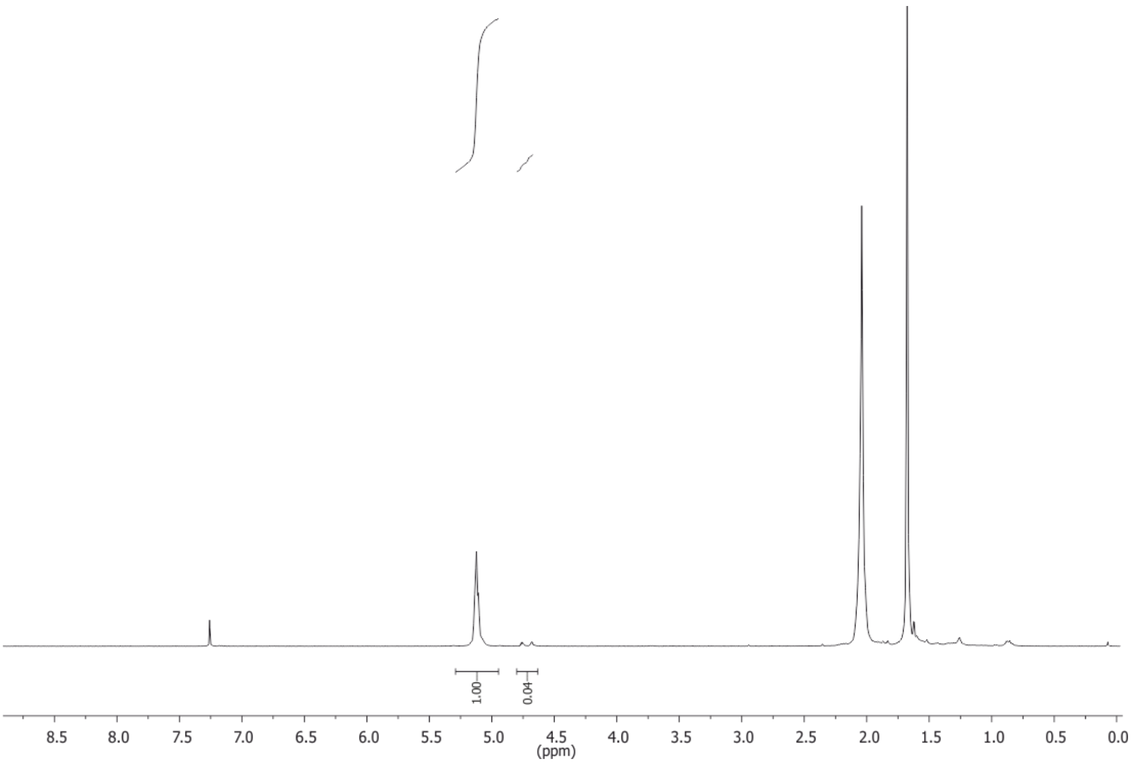

Fig. S14. ^{1}H NMR spectrum (400 MHz, CDCl$_3$, 293 K) of PIP prepared by catalysis with **1**$_{\mathbf{Y}}^{\mathbf{THF}}$/[Ph$_3$C][B(C$_6F_5$)$_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 13).

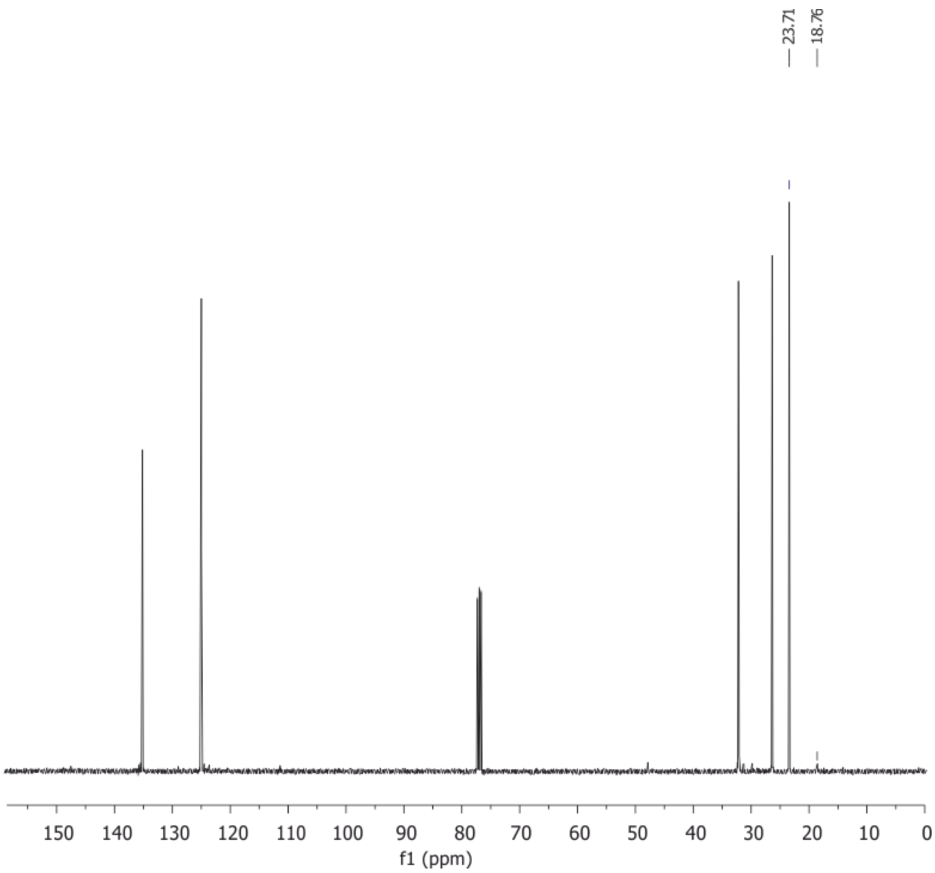

Fig. S15. ^{13}C{^{1}H } NMR spectrum (100 MHz, CDCl$_3$, 293 K) of PIP prepared by catalysis with **1**$_{\mathbf{Y}}^{\mathbf{THF}}$/[Ph$_3$C][B(C$_6F_5$)$_4$]/Al^{i}Bu$_3$ ternary system (from Table 2, entry 13).

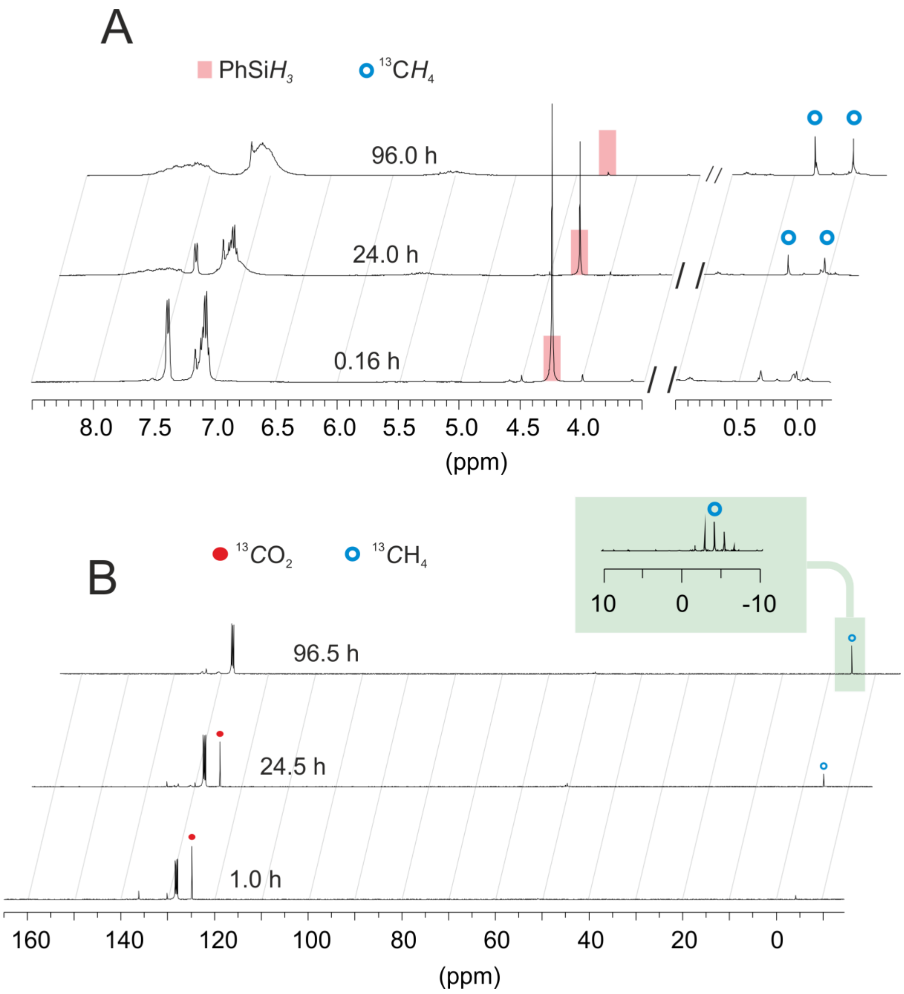

Fig. S16. ^{1}H and ^{13}C{^{1}H} NMR spectra (400 MHz, C_6D_6, 298 K) recorded at variable time for the $^{13}CO_2$ hydrosilylation reaction, using $PhSiH_3$ as reductant. Conditions: r.t., **1Y*** (1.5 mol % vs. $PhSiH_3$); (Y/B = 1/1.1). green inset ^{13}C NMR spectrum