Electronic Supplementary Information (ESI)

C_1 and C_s 2-Pyridylethylanilido Zirconium (IV), Yttrium (III) and Lutetium (III) complexes: Synthesis, Characterization and Catalytic Activity in the Isoprene Polymerization

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Table S1. Crystal data and structure refinement for complexes **11-12** and **14**.

	11	**12**	**14 · C_7H_8**
CCDC number	1508420	1508421	1508422
Empirical formula	C_{32} H_{49} N_5 Zr	C_{39} H_{55} N_5 Zr	C_{52} H_{75} N_2 O Si_2 Y
Formula weight	594.98	685.10	889.23
Temperature [K]	150(2)	150(2)	100(2)
Wavelength [Å]	1.5418	0.71069	0.71069
Crystal system space group	Orthorhombic $Pca2_1$	Monoclinic $P2_1/c$	Monoclinic $P2_1/n$
a [Å]	21.595(3)	11.693(8)	10.2449(7)
b [Å]	11.459(18)	17.076(11)	18.0995(12)
c [Å]	26.335(4)	18.712(15)	26.6375(19)
α [°]	90	90	90
β [°]	90	91.569(6)	95.6850(10)
γ [°]	90	90	90
V [$Å^3$]	6517(17)	3735(5)	4915.0(6)
Z, Dc [g m^{-3}]	8, 1.213	4, 1.218	4, 1.202
Absorption coefficient [mm^{-1}]	2.955	0.327	1.273
F(000)	2528	1456	1904
Crystal size [mm]	0.01 × 0.01 × 0.02	0.01 × 0.01 × 0.03	0.11 x 0.15 x 0.21
Θ Range for data collection [°]	4.37 ÷ 61.60	4.12 ÷ 26.48	7.60 ÷ 30.00
Limiting indices	$-24 \le h \le 22$ $-11 \le k \le 12$ $-29 \le l \le 25$	$-14 \le h \le 13$ $-19 \le k \le 21$ $-23 \le l \le 22$	$-14 \le h \le 14$ $-25 \le k \le 25$ $-37 \le l \le 37$
Reflections collected/unique	27300/8972	24058/6459	55550/14055
GOF on F^2	1.062	0.968	1.030
Data/restraints/parameters	8972 / 1 / 707	6459 / 0 / 416	14055 / 0 / 535
Final R indices [I>2σ(I)]	R1=0.0846 wR2= 0.1838	R1=0.0836 wR2= 0.1058	R1=0.0411 wR2= 0.0966
R indices (all data)	R1=0.1195 wR2= 0.2115	R1=0.2270 wR2= 0.1490	R1=0.0575 wR2= 0.1015
Flack parameter	0.10(2)	---	---
Largest diff. peak and hole [e $Å^{-3}$]	4.244 and –0.750	0.653 and −0.459	0.873 and −0.565

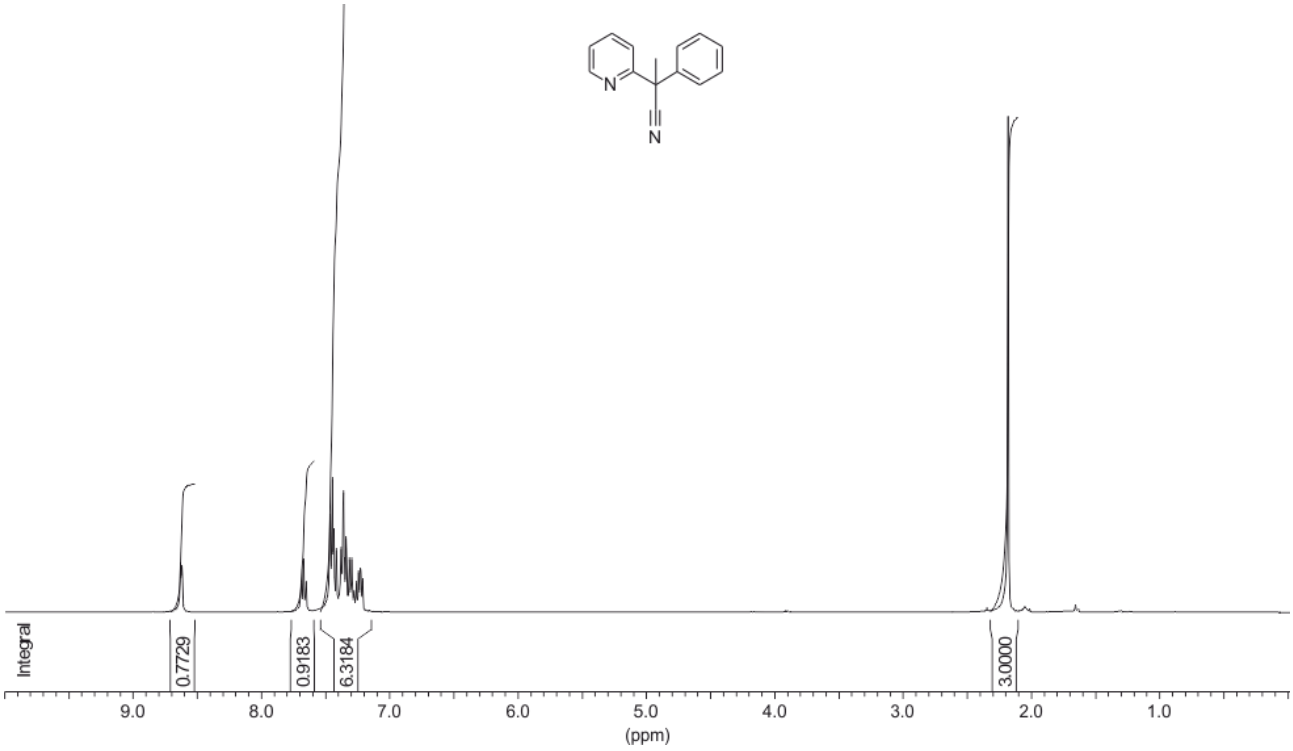

Figure S1. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$, 298K) of **3**.

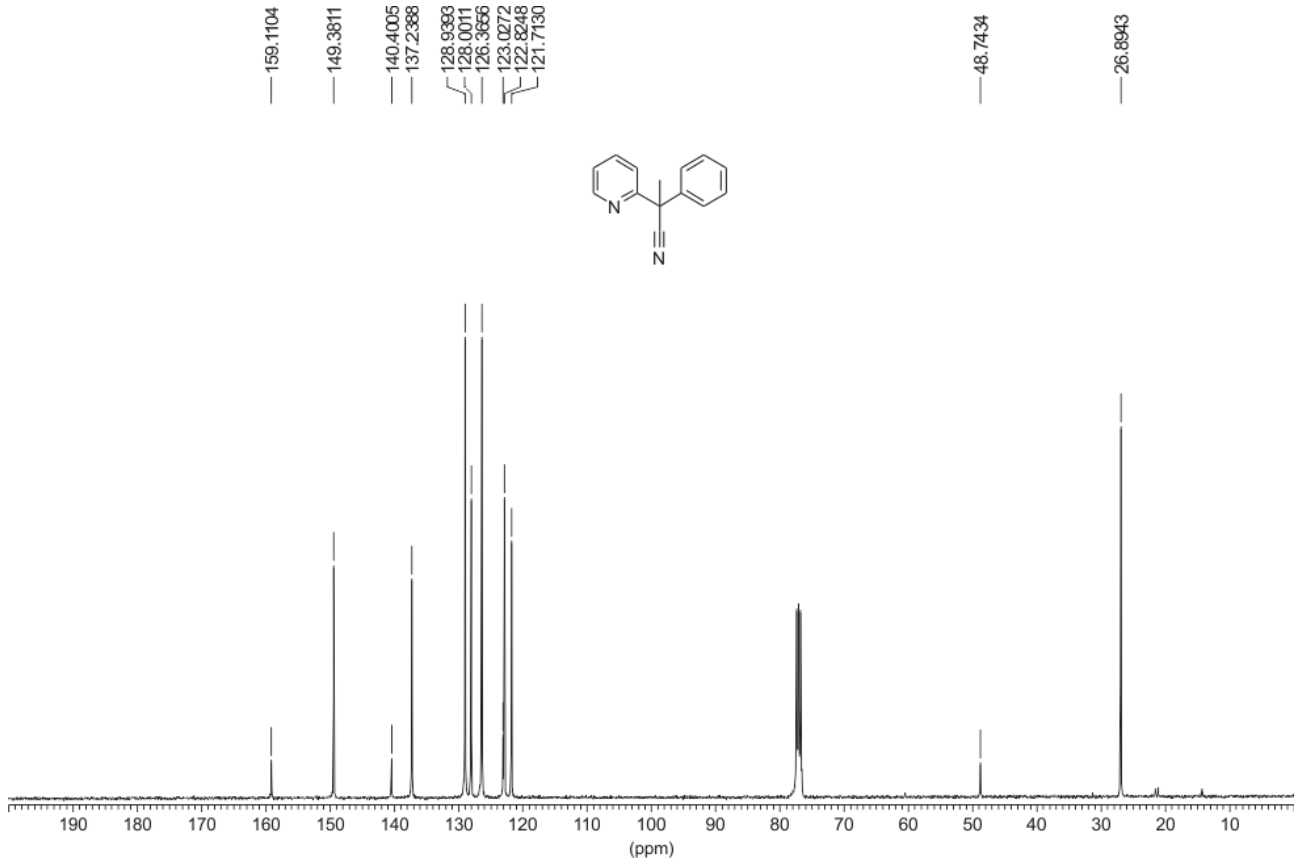

Figure S2. $^{13}C\{^{1}H\}$-NMR spectrum (100 MHz, $CDCl_3$, 298K) of **3**.

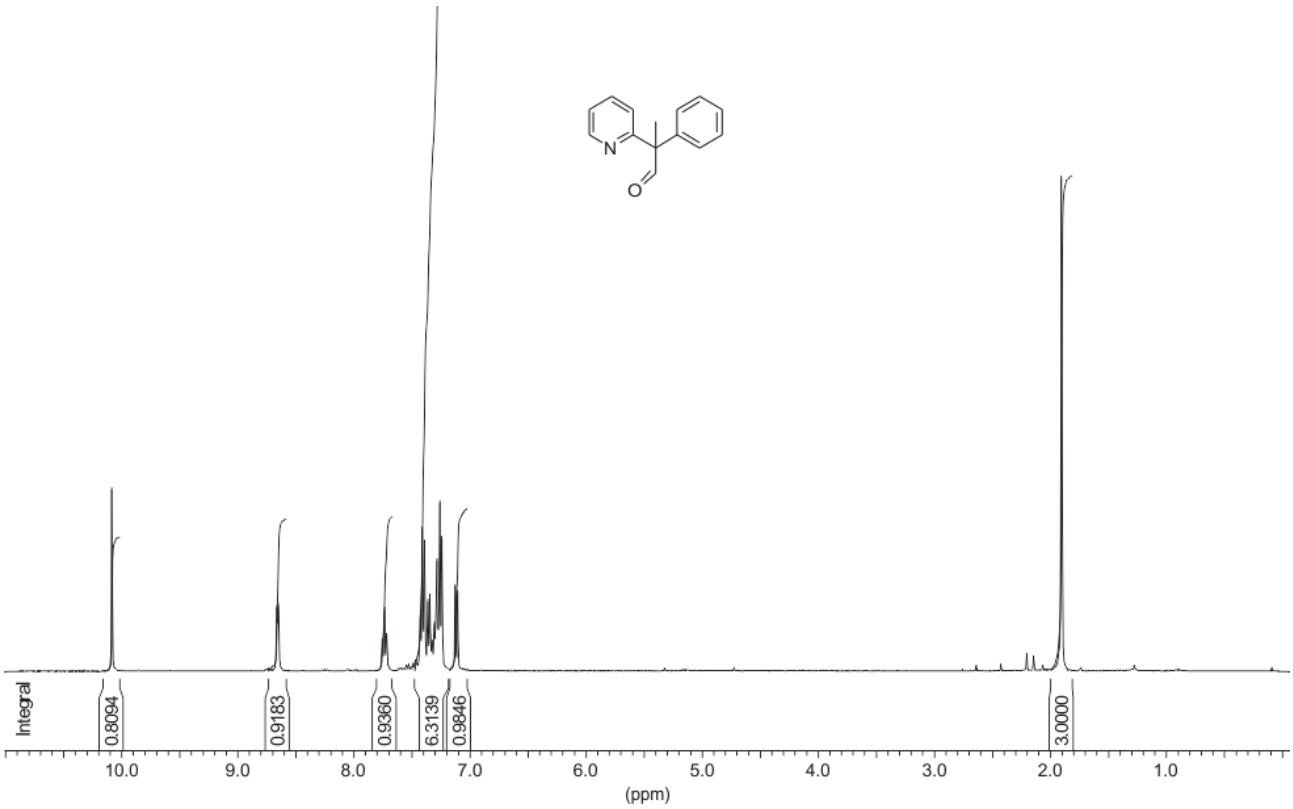

Figure S3. ^{1}H-NMR spectrum (400 MHz, $CDCl_3$, 298K) of **4**.

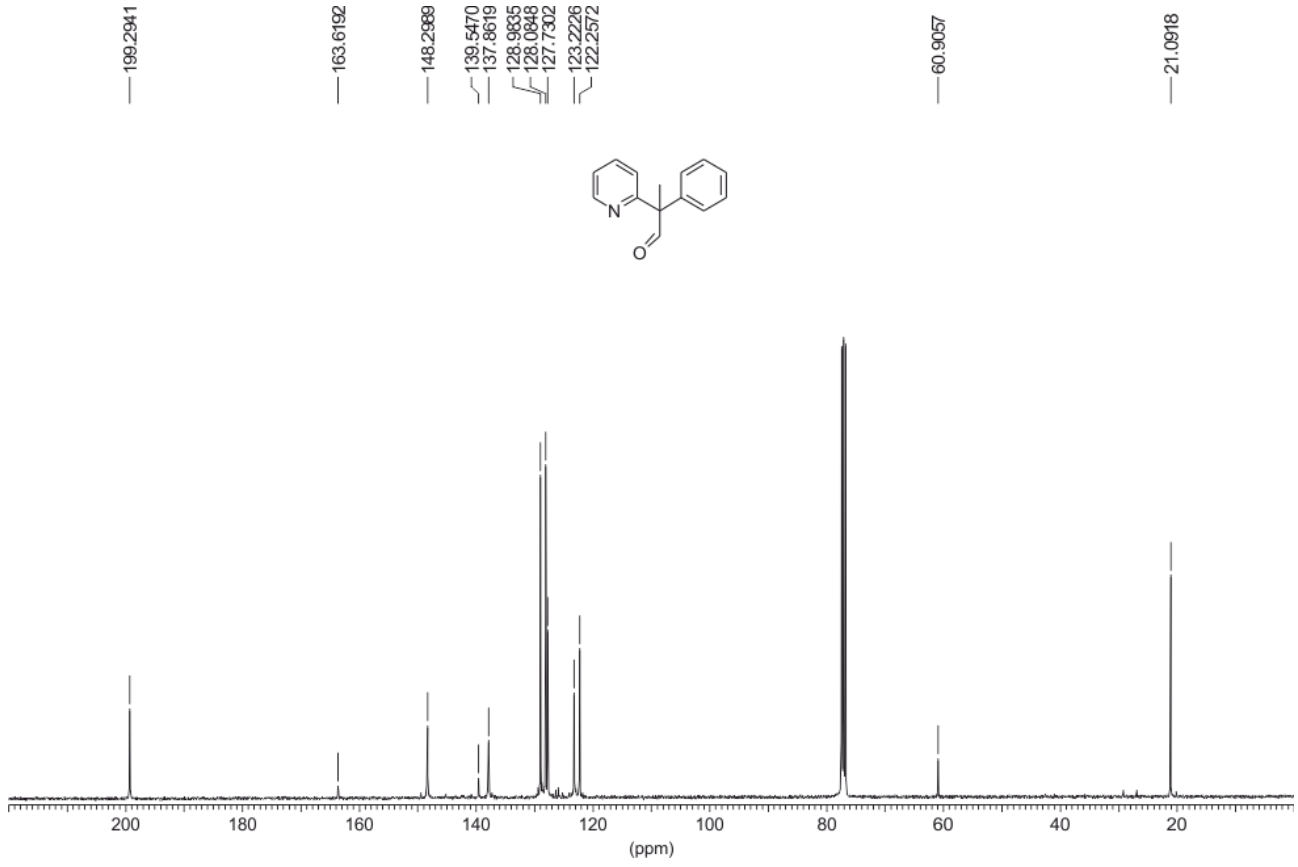

Figure S4. $^{13}C\{^{1}H\}$-NMR spectrum (100 MHz, $CDCl_3$, 298K) of **4**.

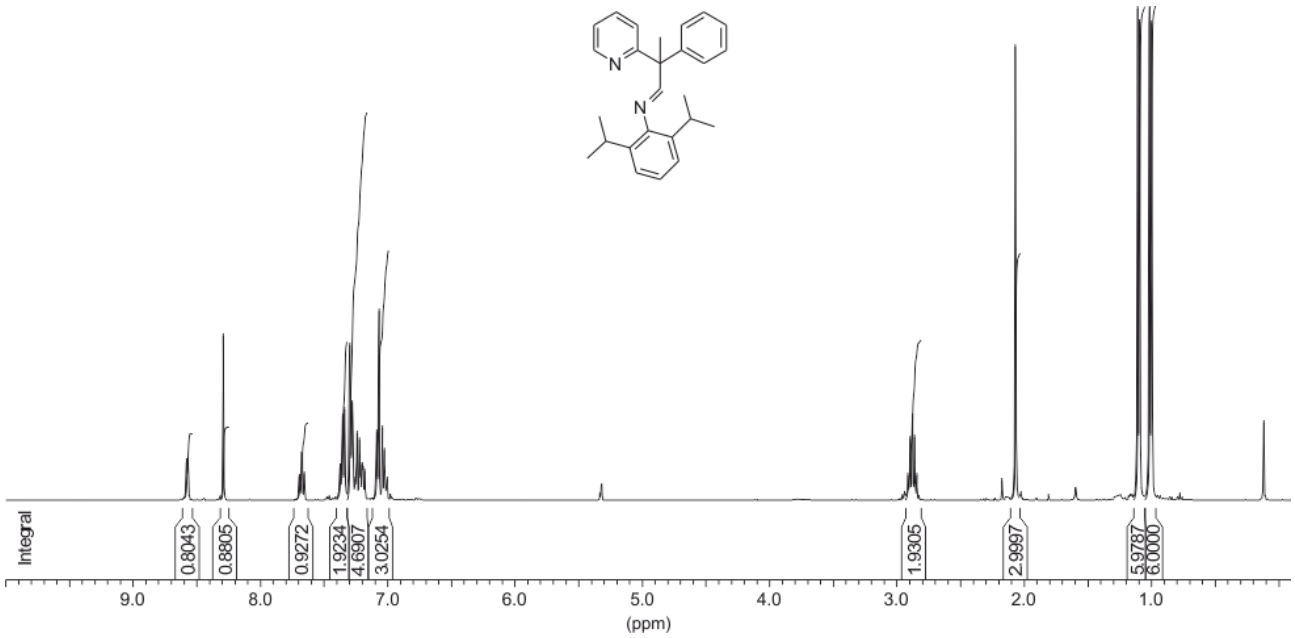

Figure S5. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2, 298K) of **5**.

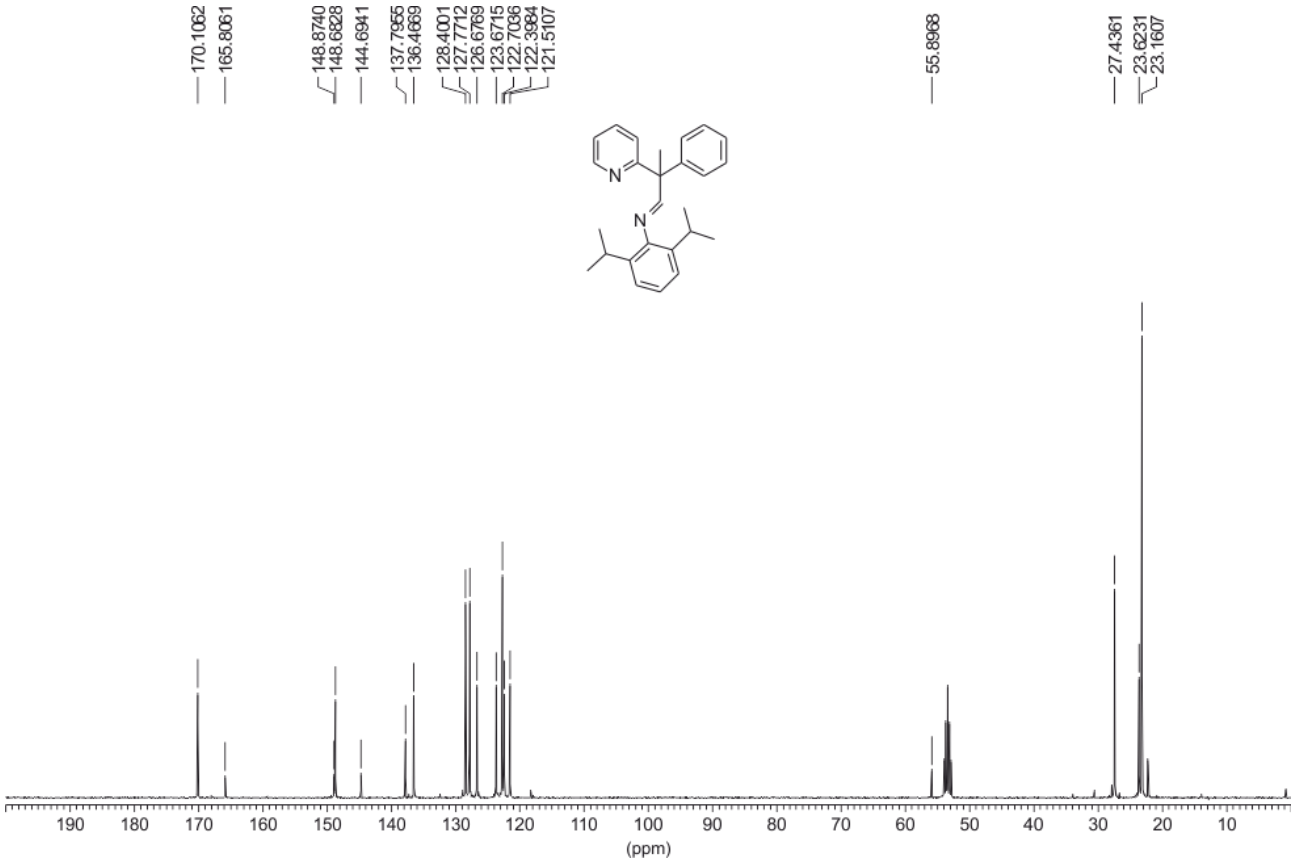

Figure S6. $^{13}C\{^{1}H\}$-NMR spectrum (100 MHz, CD_2Cl_2, 298K) of **5**.

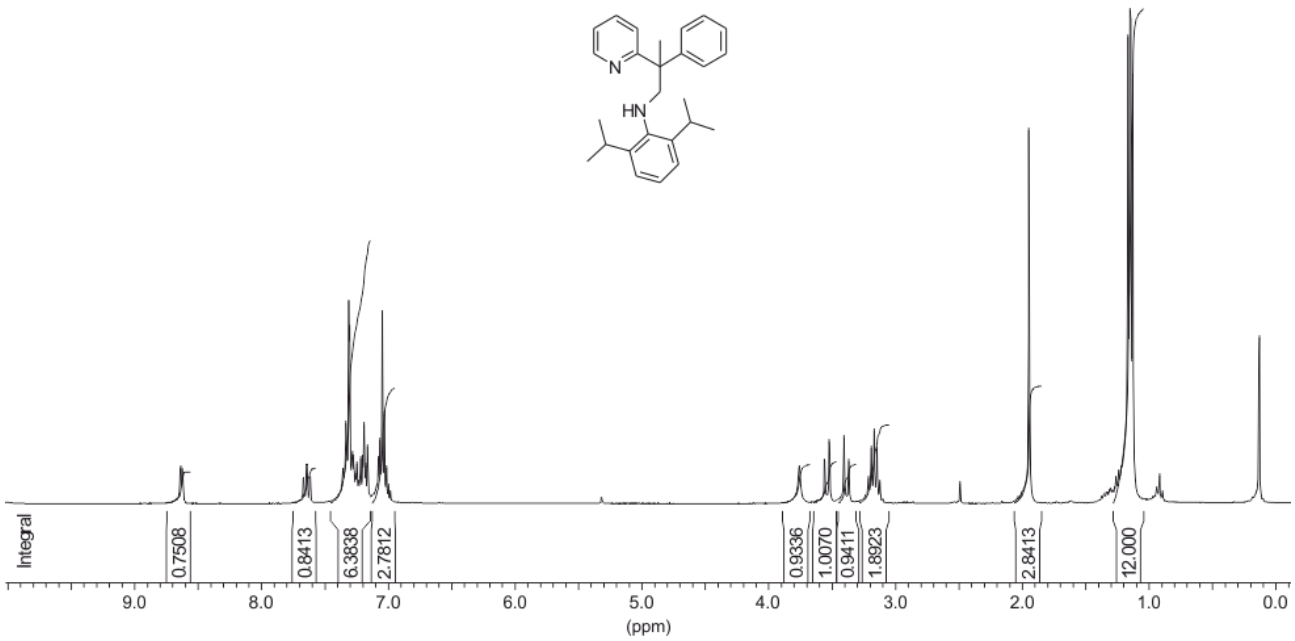

Figure S7. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2, 298K) of **HNC$_1$**.

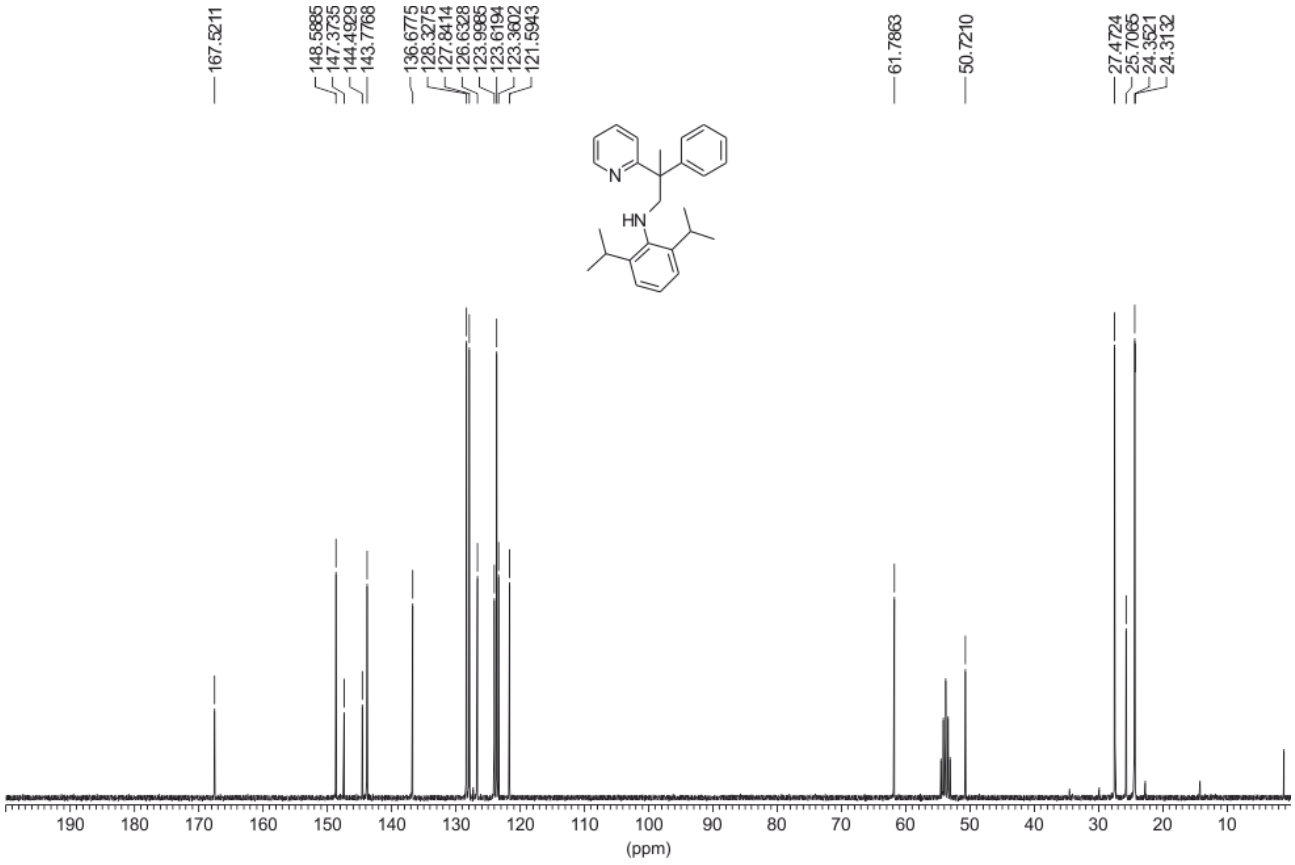

Figure S8. ^{13}C{^{1}H}-NMR spectrum (100 MHz, CD_2Cl_2, 298K) of **HNC$_1$**.

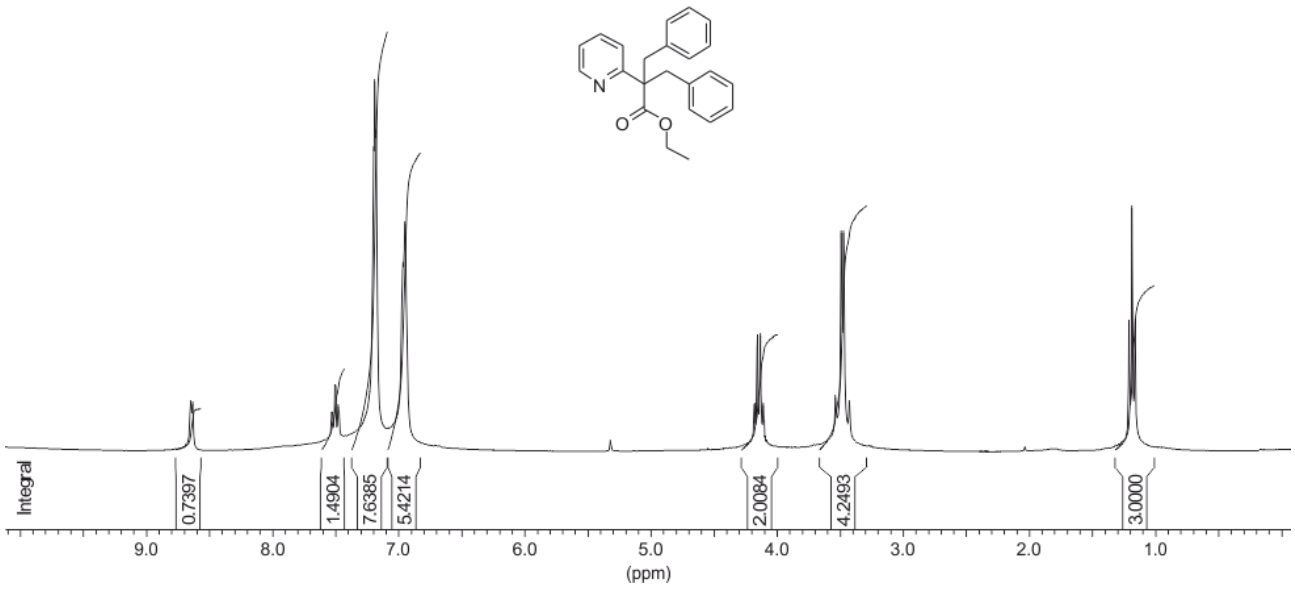

Figure S9. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298K) of **7**.

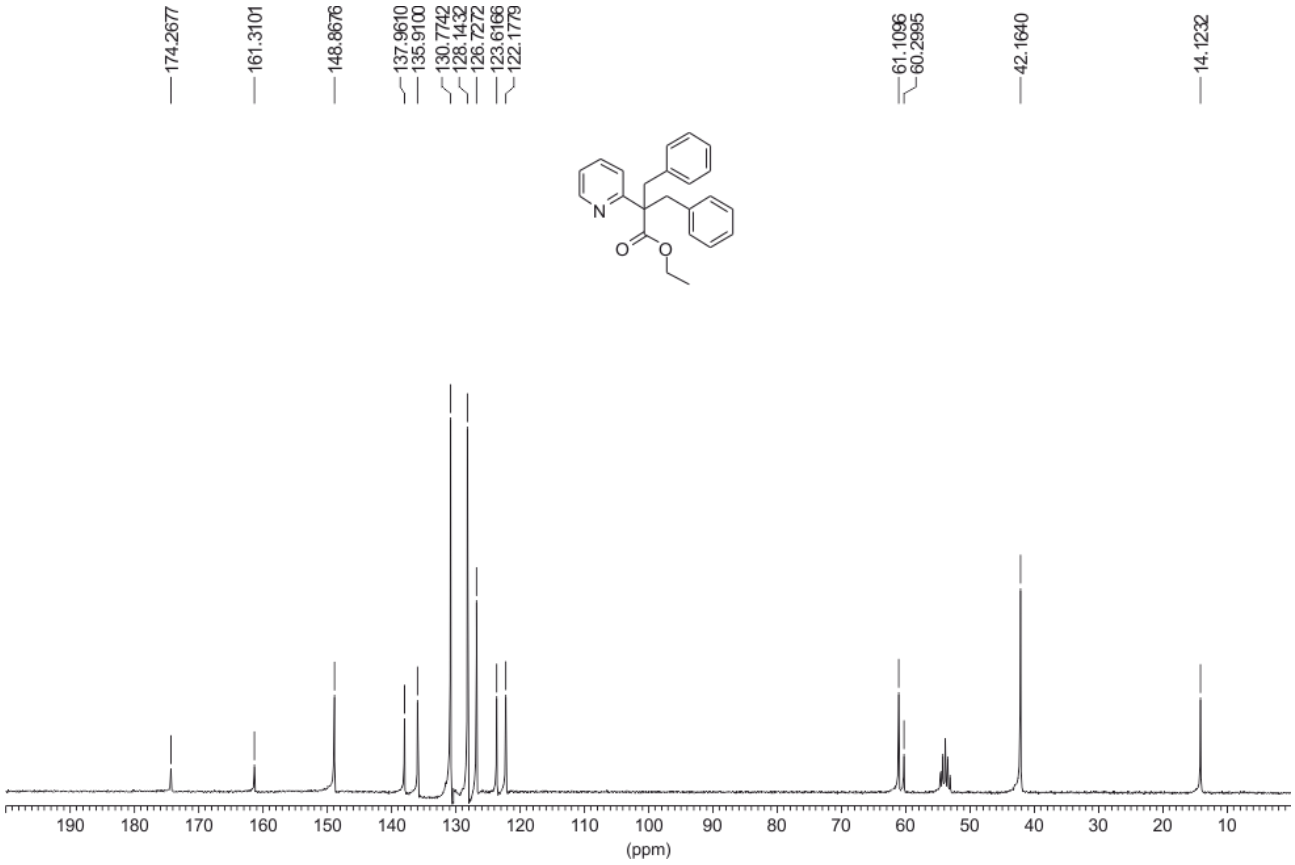

Figure S10. ^{13}C{^{1}H}-NMR spectrum (75 MHz, CD_2Cl_2, 298K) of **7**.

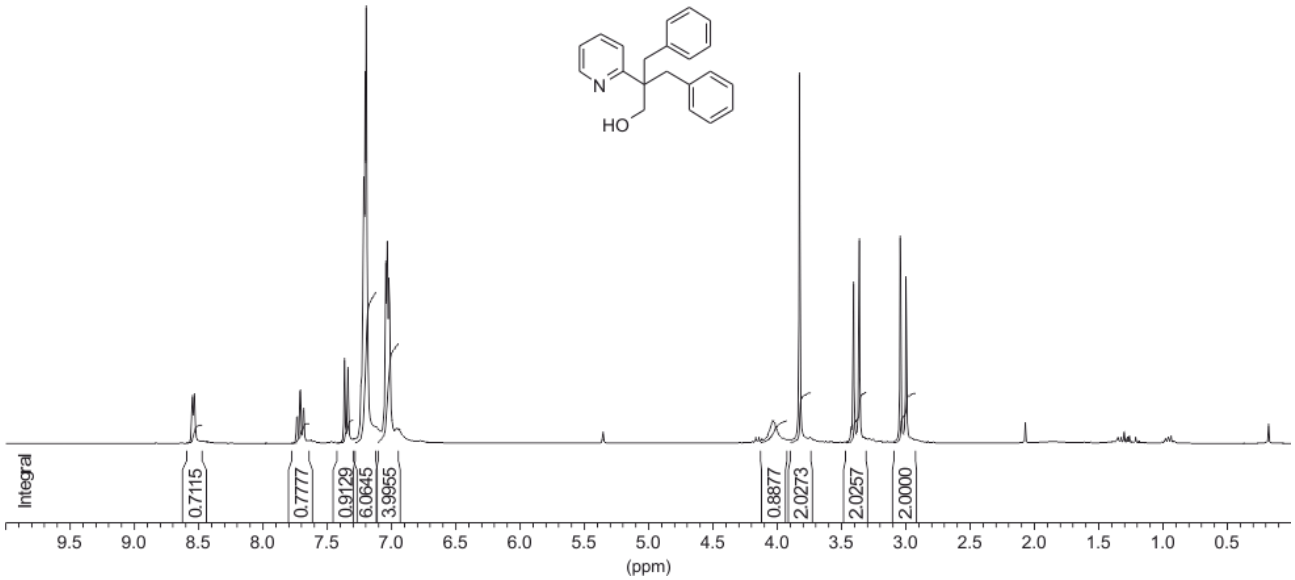

Figure S11. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298K) of **8**.

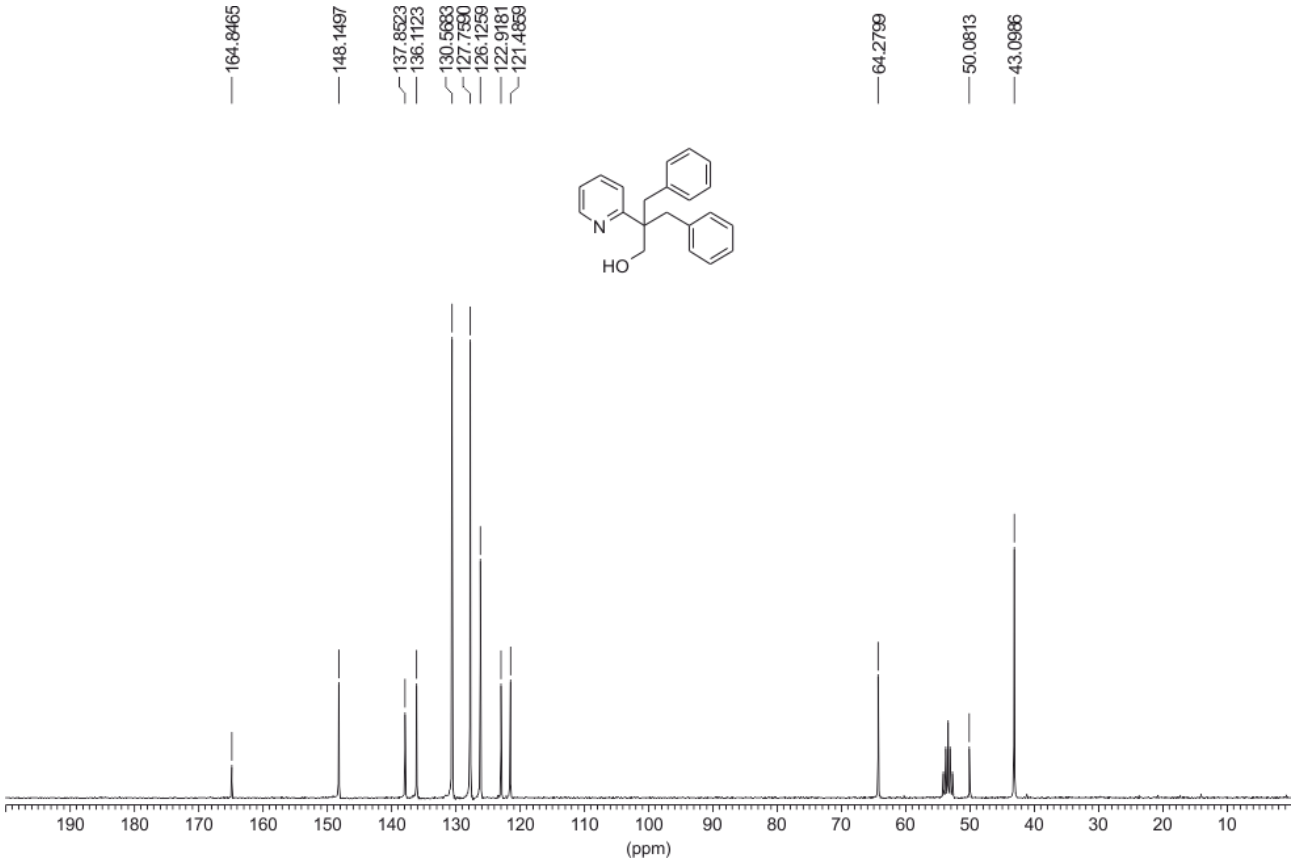

Figure S12. ^{13}C{^{1}H}-NMR spectrum (75 MHz, CD_2Cl_2, 298K) of **8**.

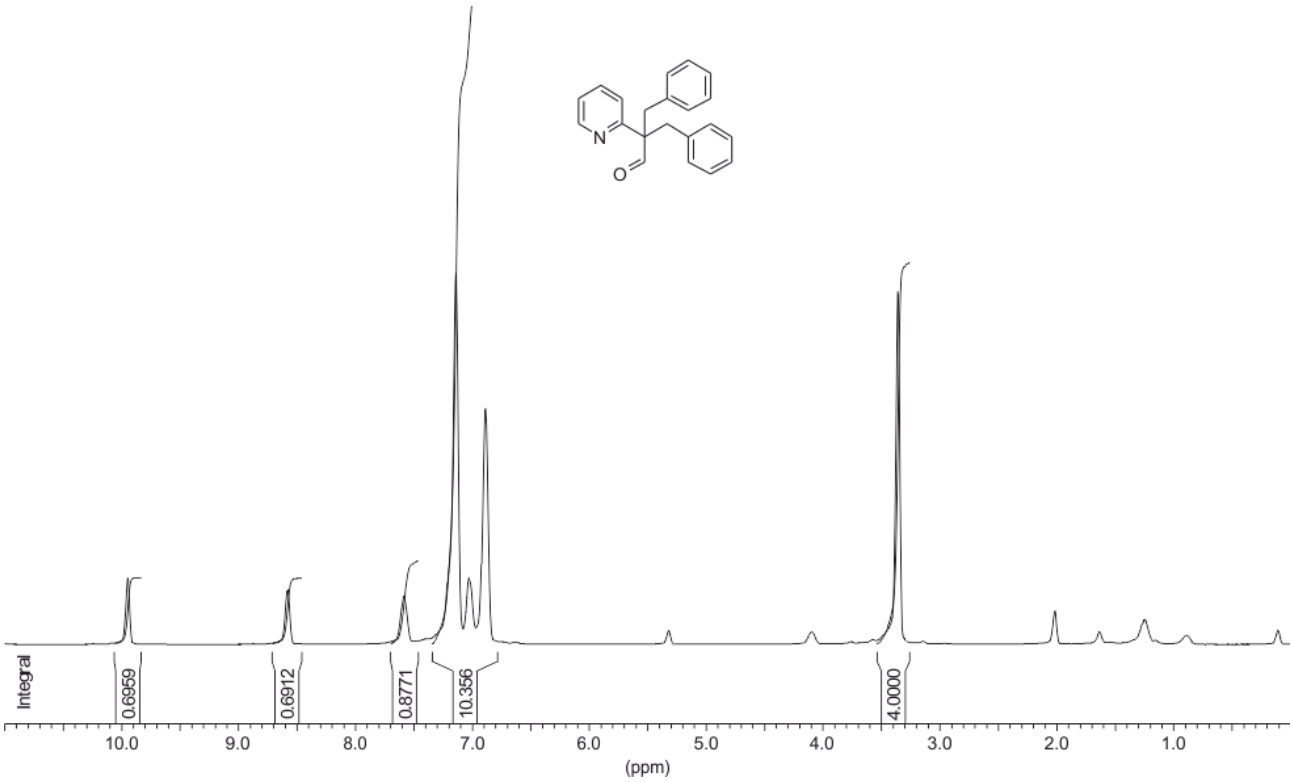

Figure S13. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298K) of **9**.

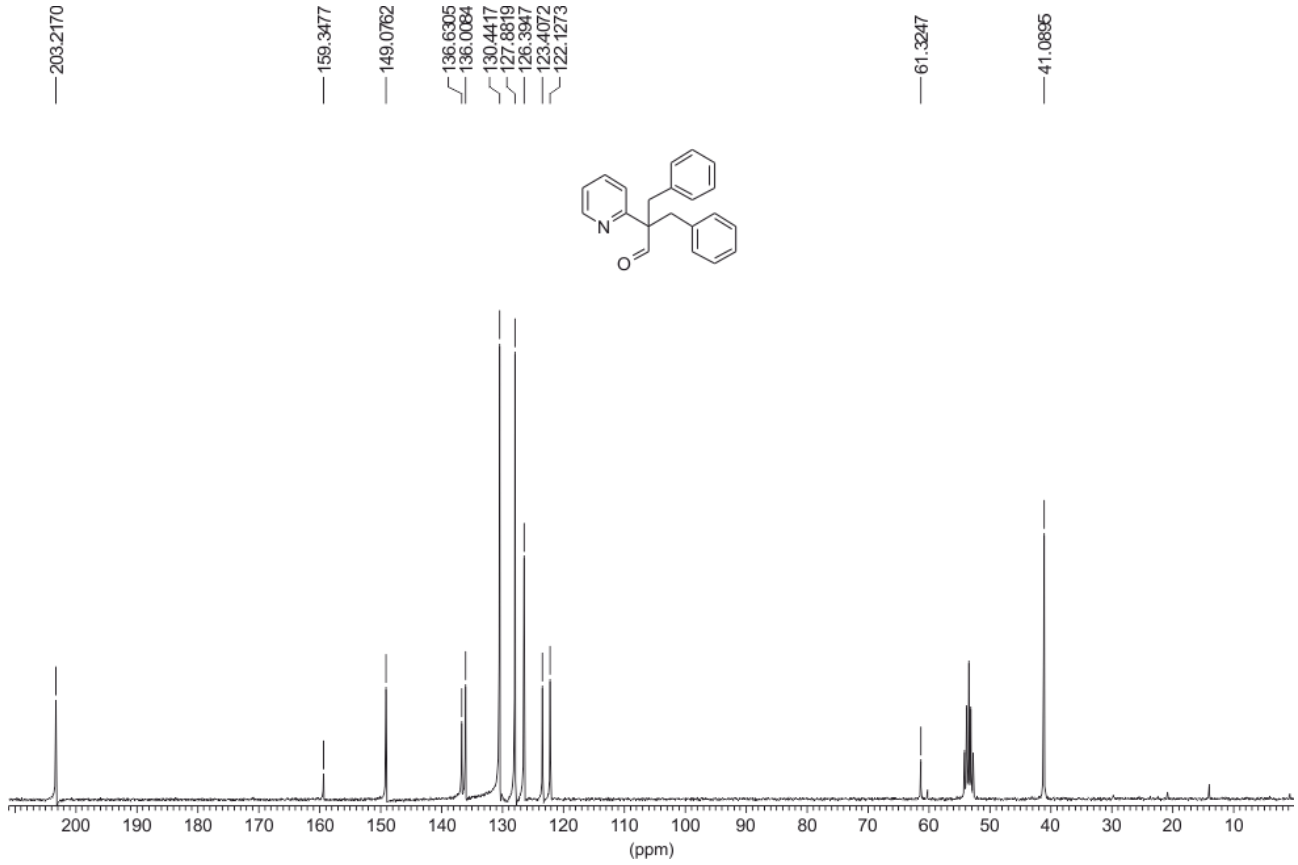

Figure S14. $^{13}C\{^{1}H\}$-NMR spectrum (75 MHz, CD_2Cl_2, 298K) of **9**.

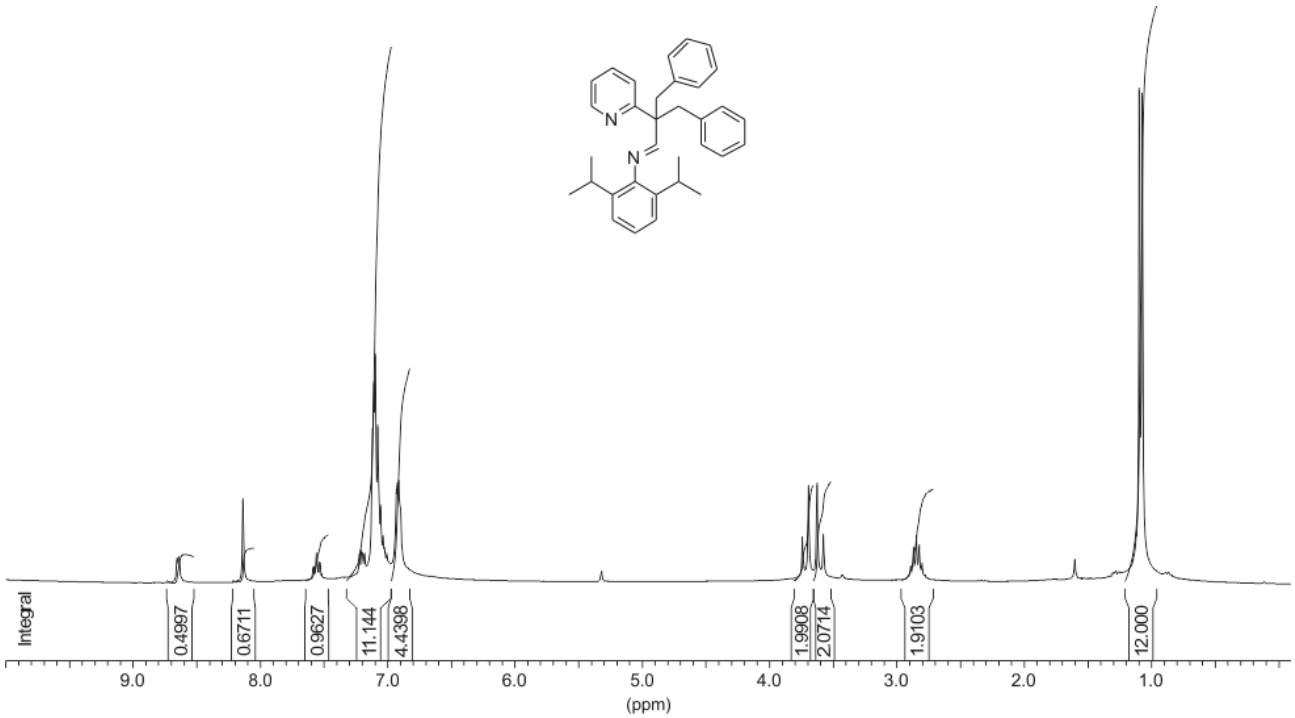

Figure S15. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298K) of **10**.

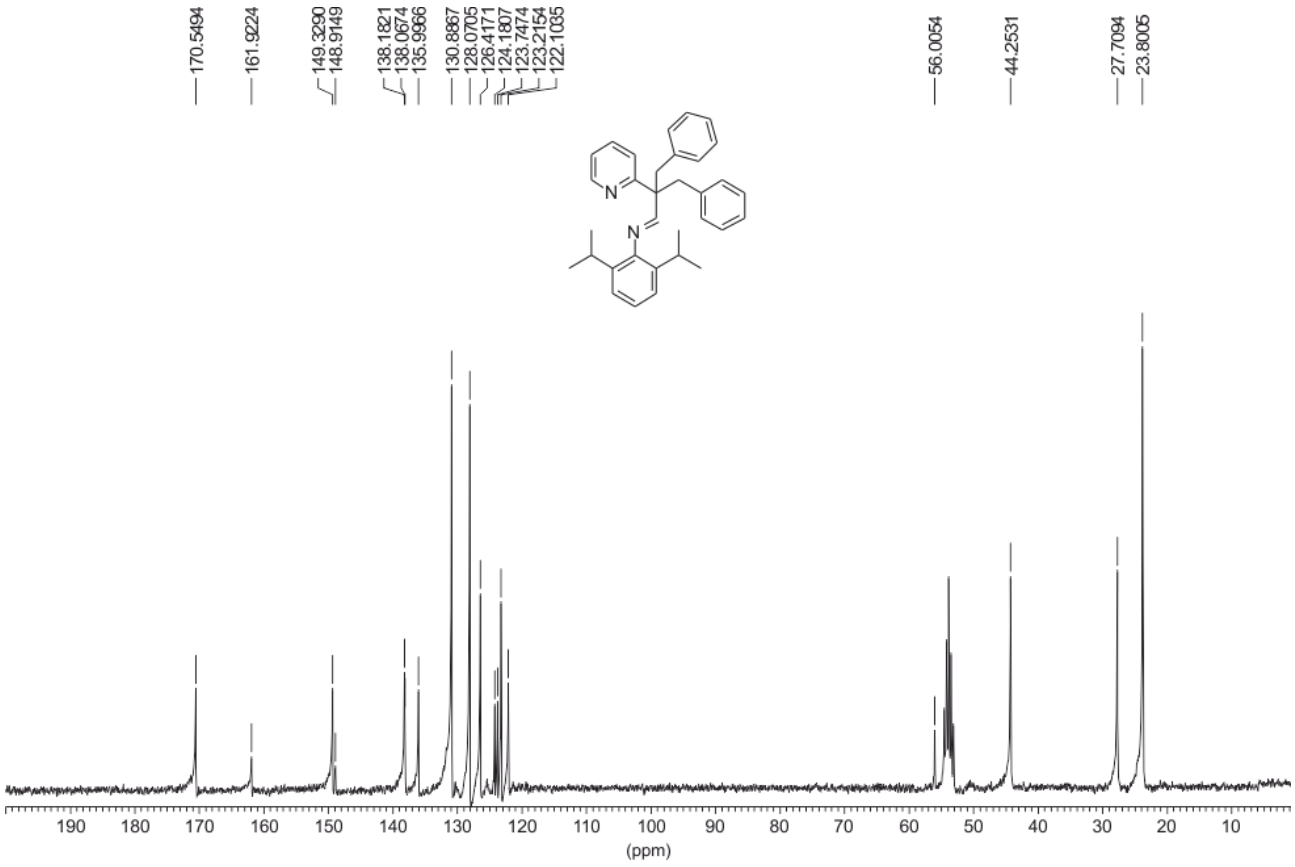

Figure S16. ^{13}C{^{1}H}-NMR spectrum (75 MHz, CD_2Cl_2, 298K) of **10**.

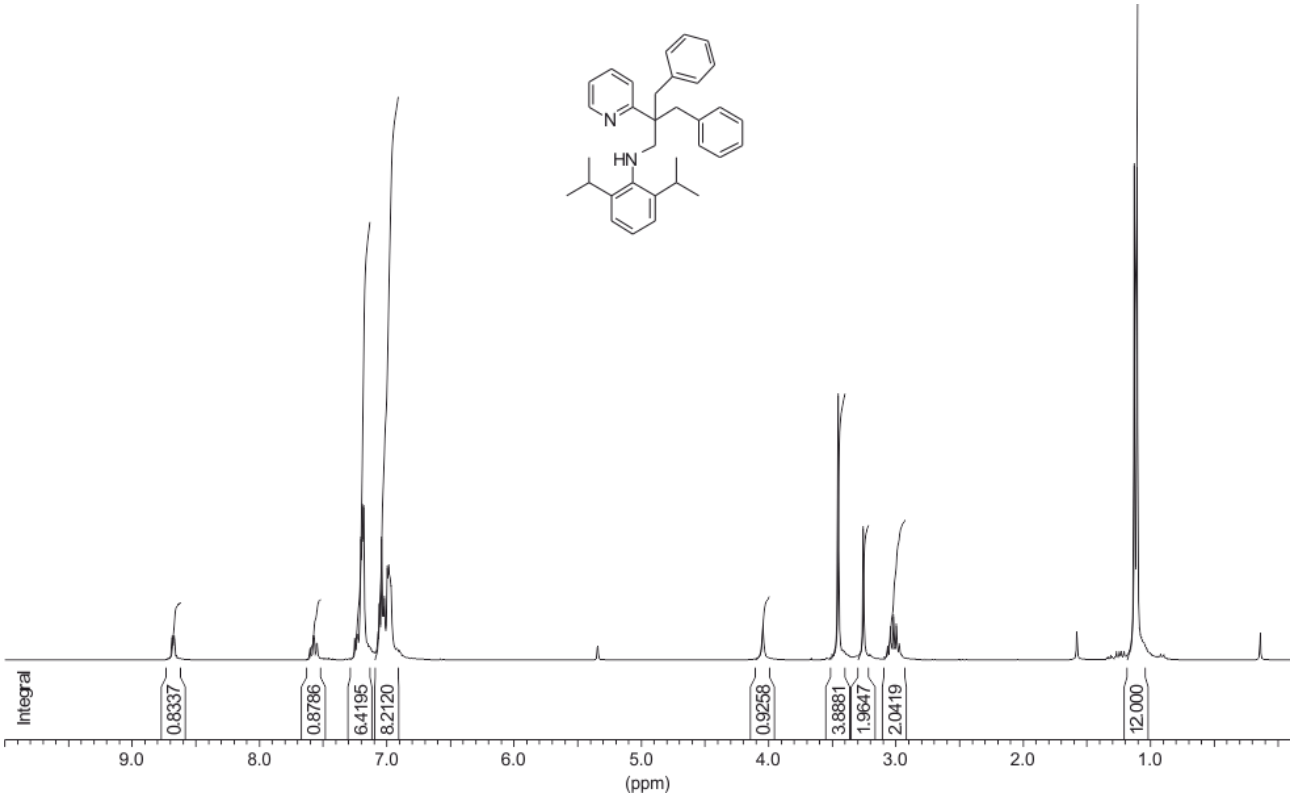

Figure S17. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298K) of **HNC$_S$**.

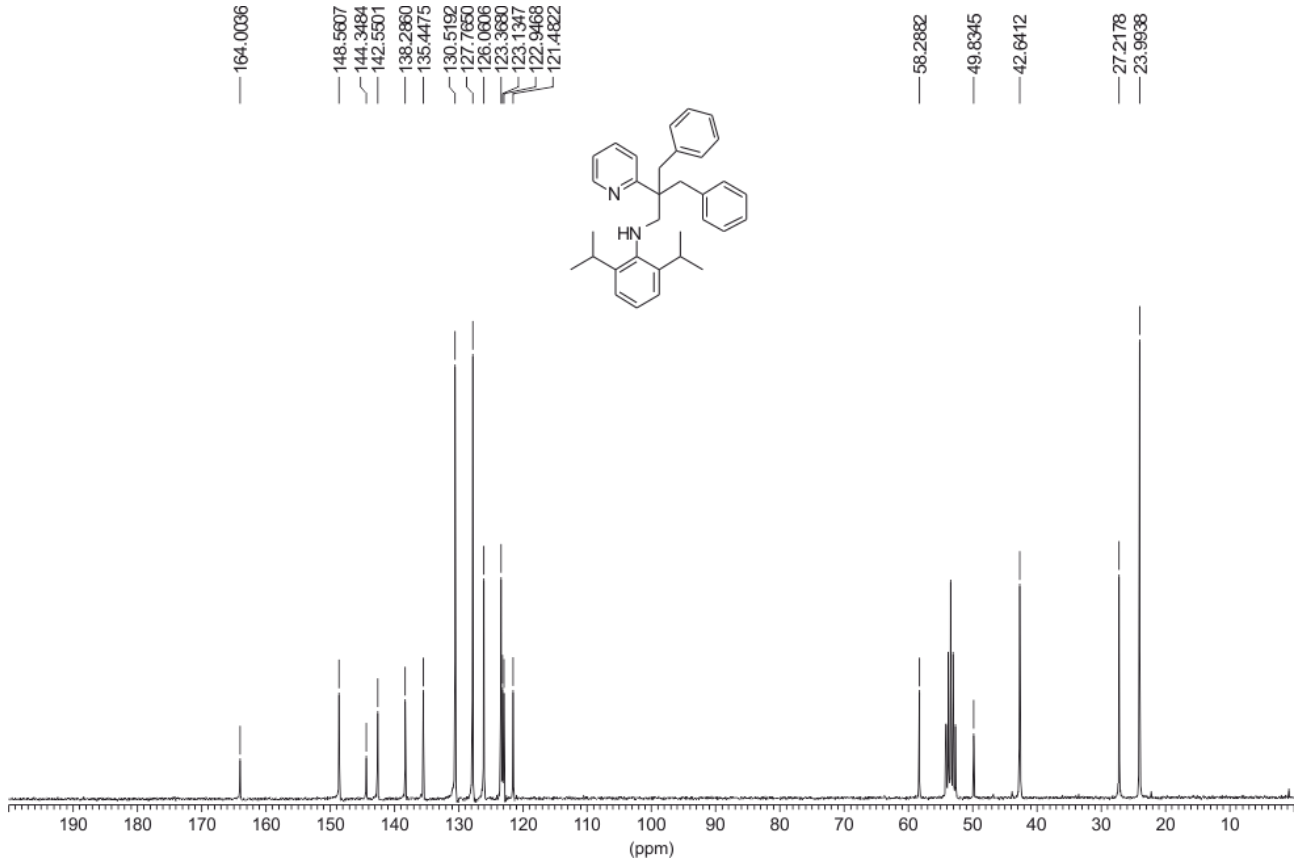

Figure S18. ^{13}C{^{1}H}-NMR spectrum (75 MHz, CD_2Cl_2, 298K) of **HNC$_S$**.

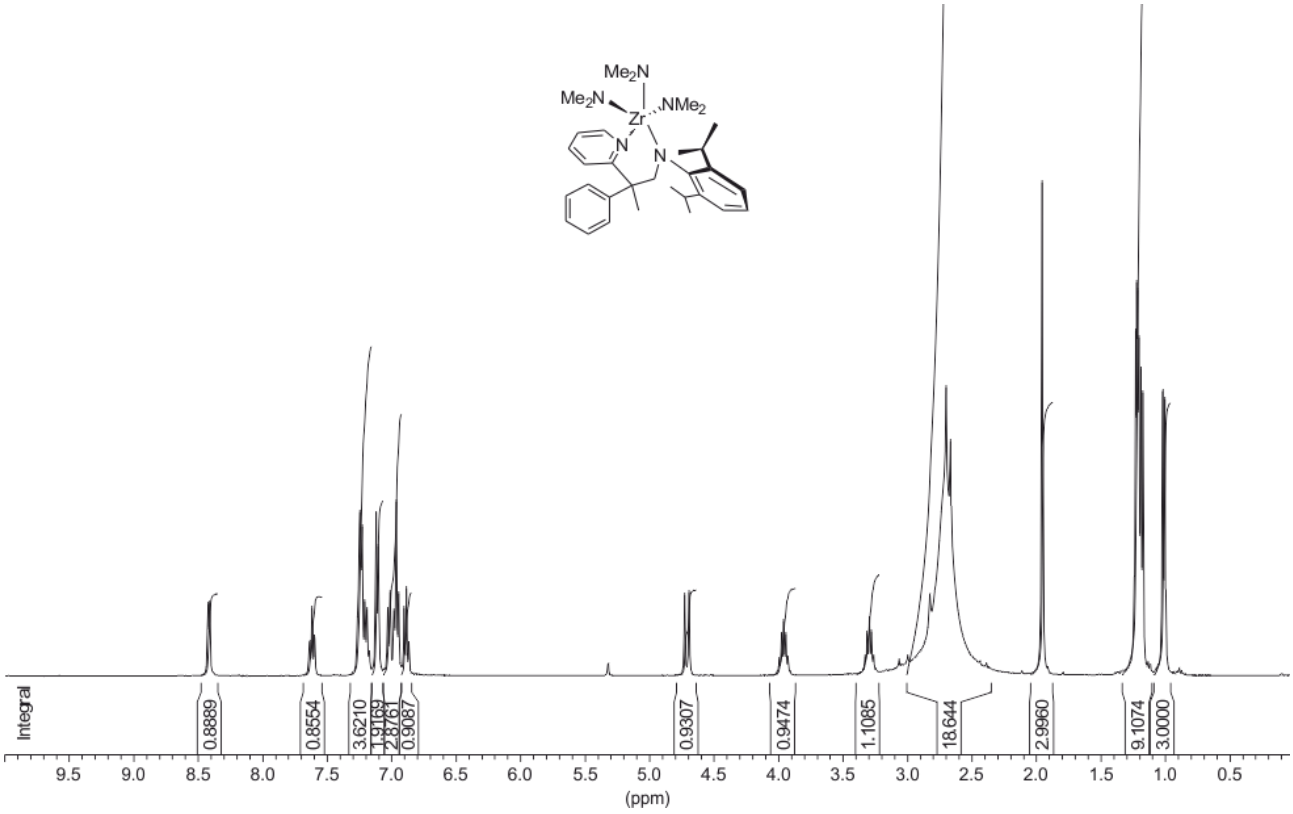

Figure S19. ^{1}H-NMR spectrum (400 MHz, CD_2Cl_2, 298K) of **11**.

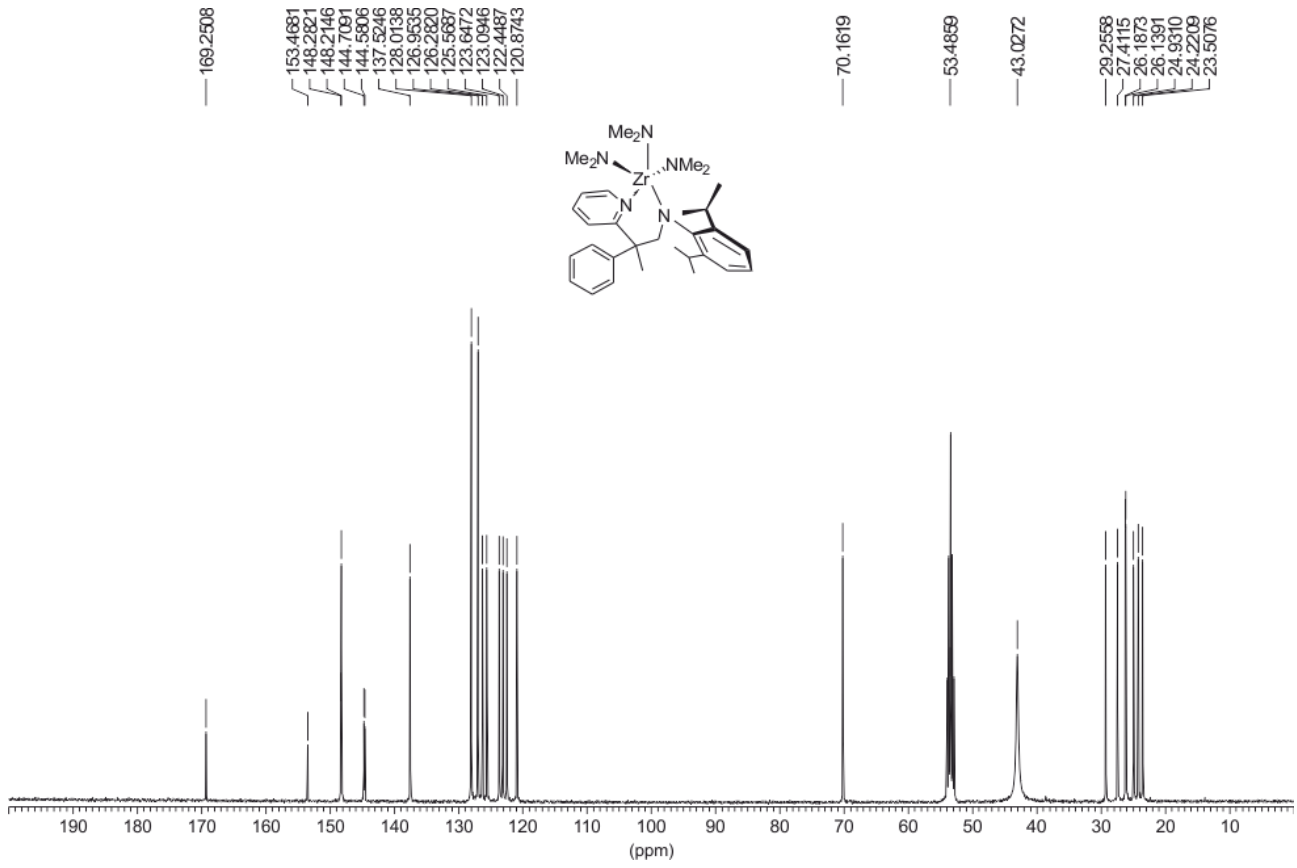

Figure S20. ^{13}C{^{1}H}-NMR spectrum (100 MHz, CD_2Cl_2, 298K) of **11**.

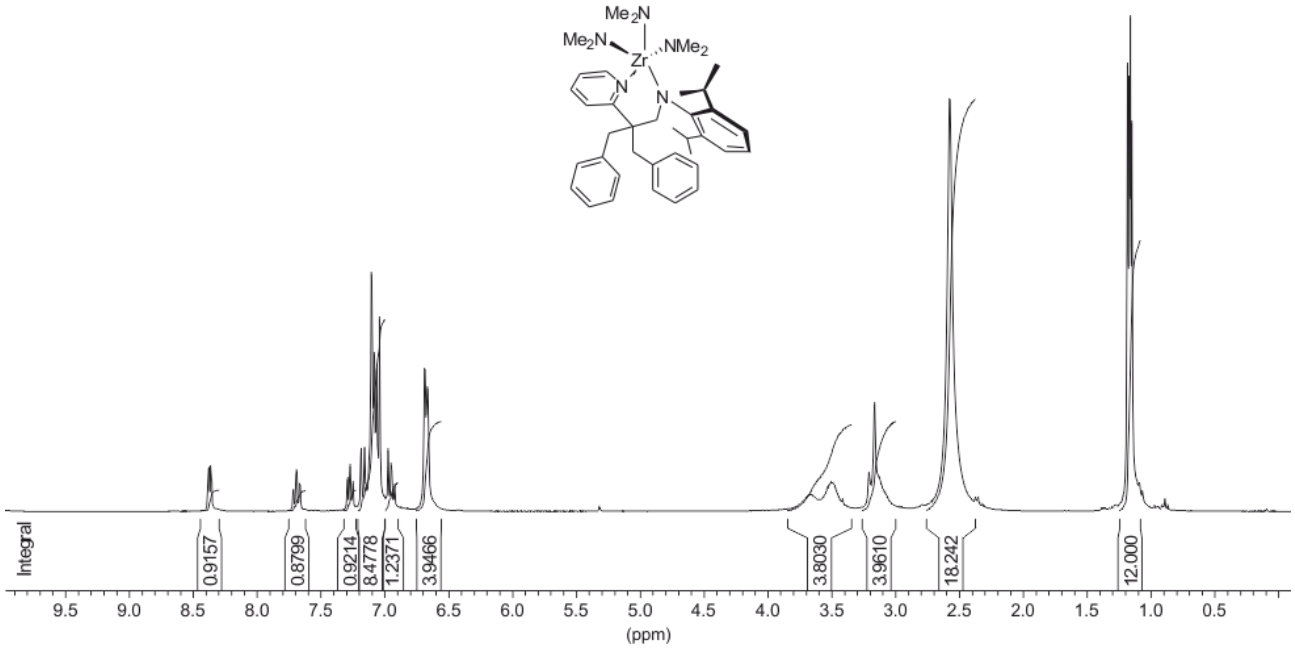

Figure S21. ^{1}H-NMR spectrum (300 MHz, CD_2Cl_2, 298K) of **12**.

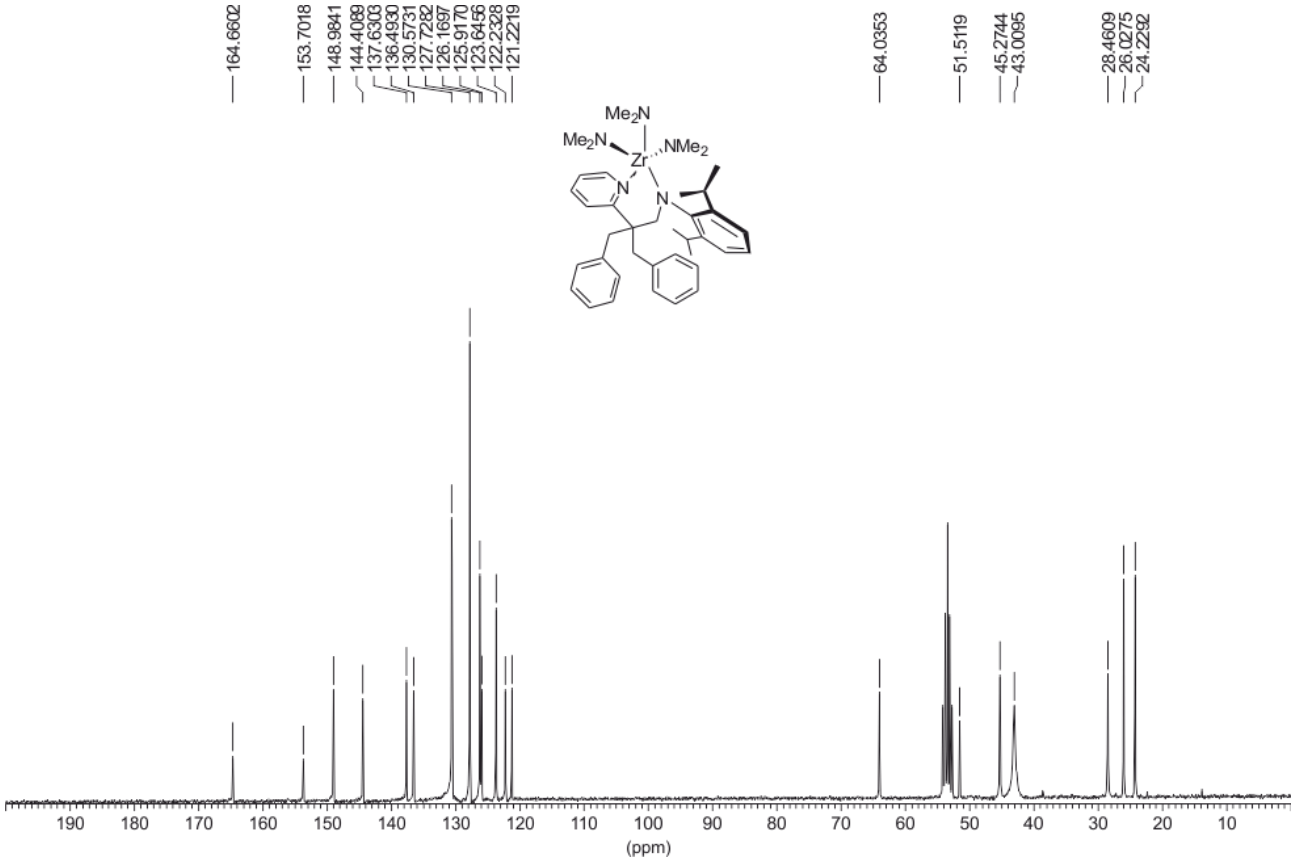

Figure S22. ^{13}C{^{1}H}-NMR spectrum (75 MHz, CD_2Cl_2, 298K) of **12**.

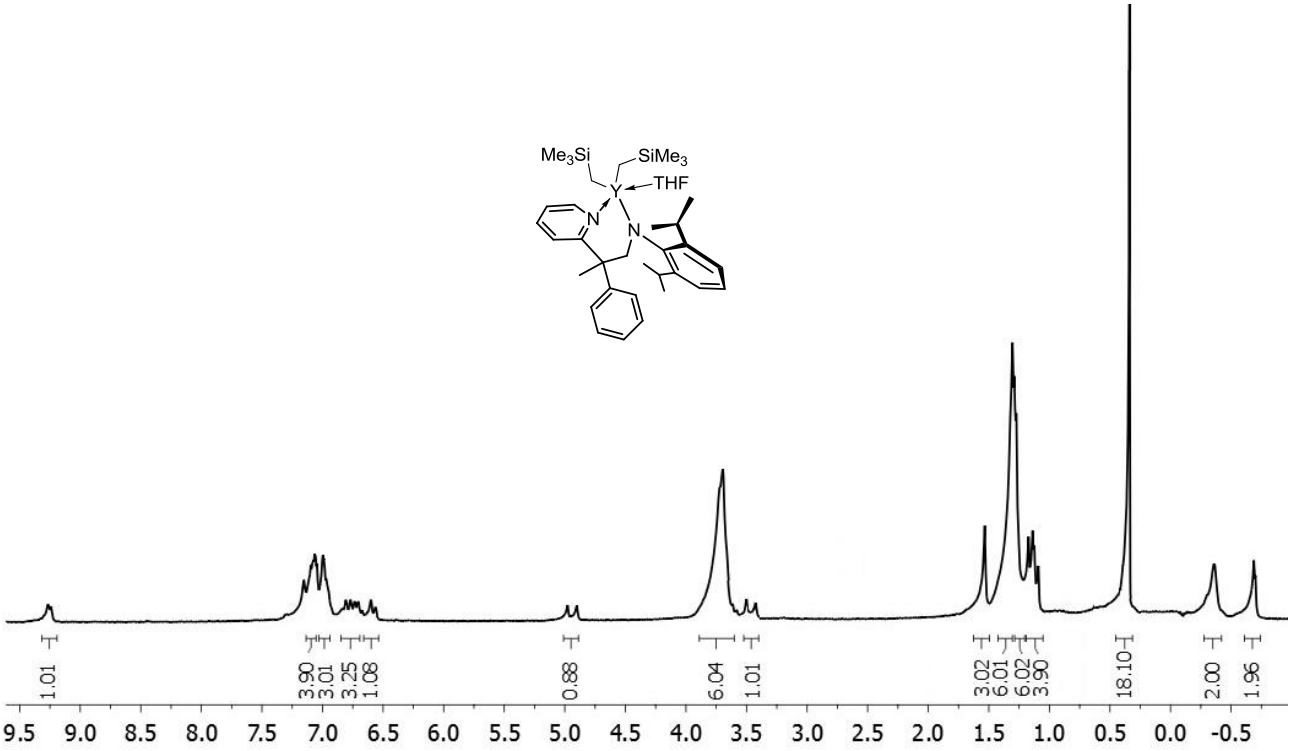

Figure S23. ^{1}H-NMR spectrum (400 MHz, C_6D_6, 298K) of **13**.

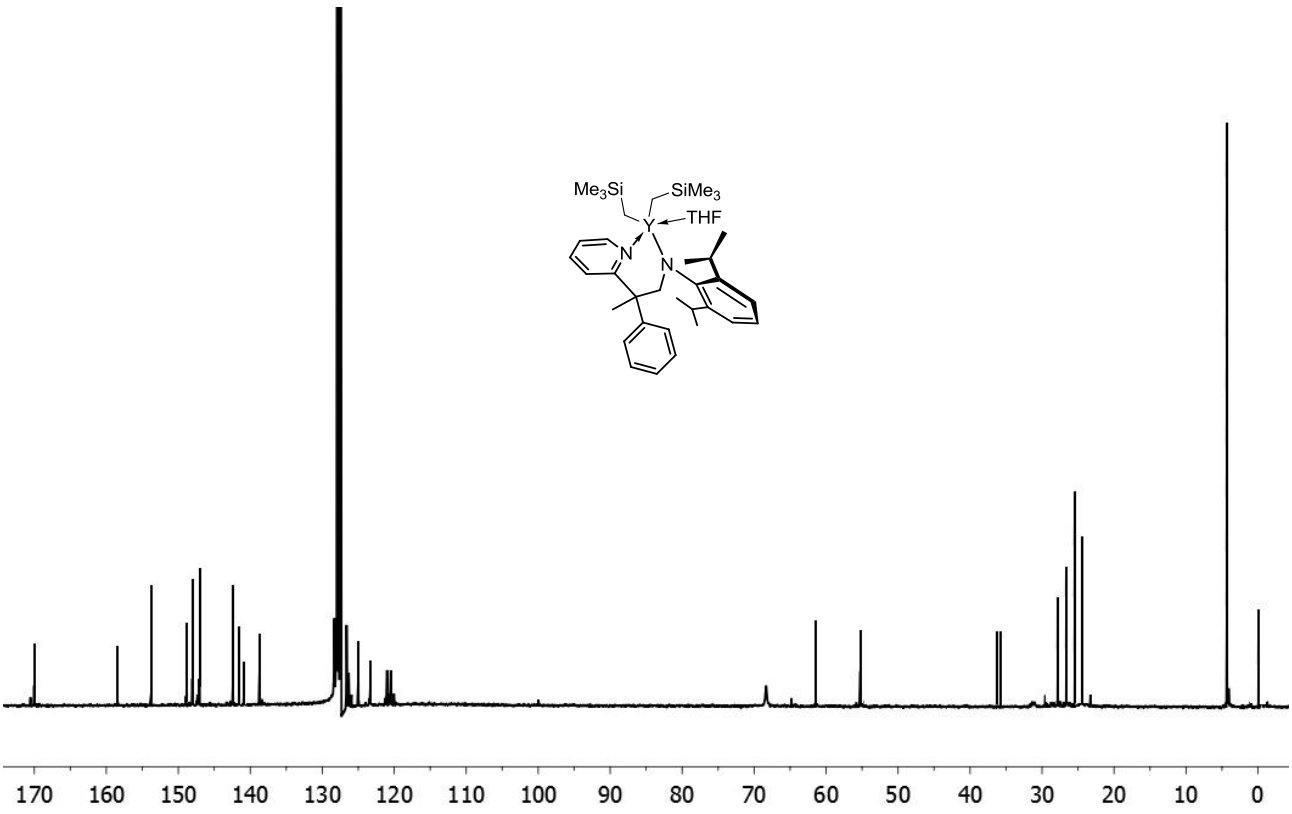

Figure S24. ^{13}C{^{1}H}-NMR spectrum (100 MHz, C_6D_6, 298K) of **13**.

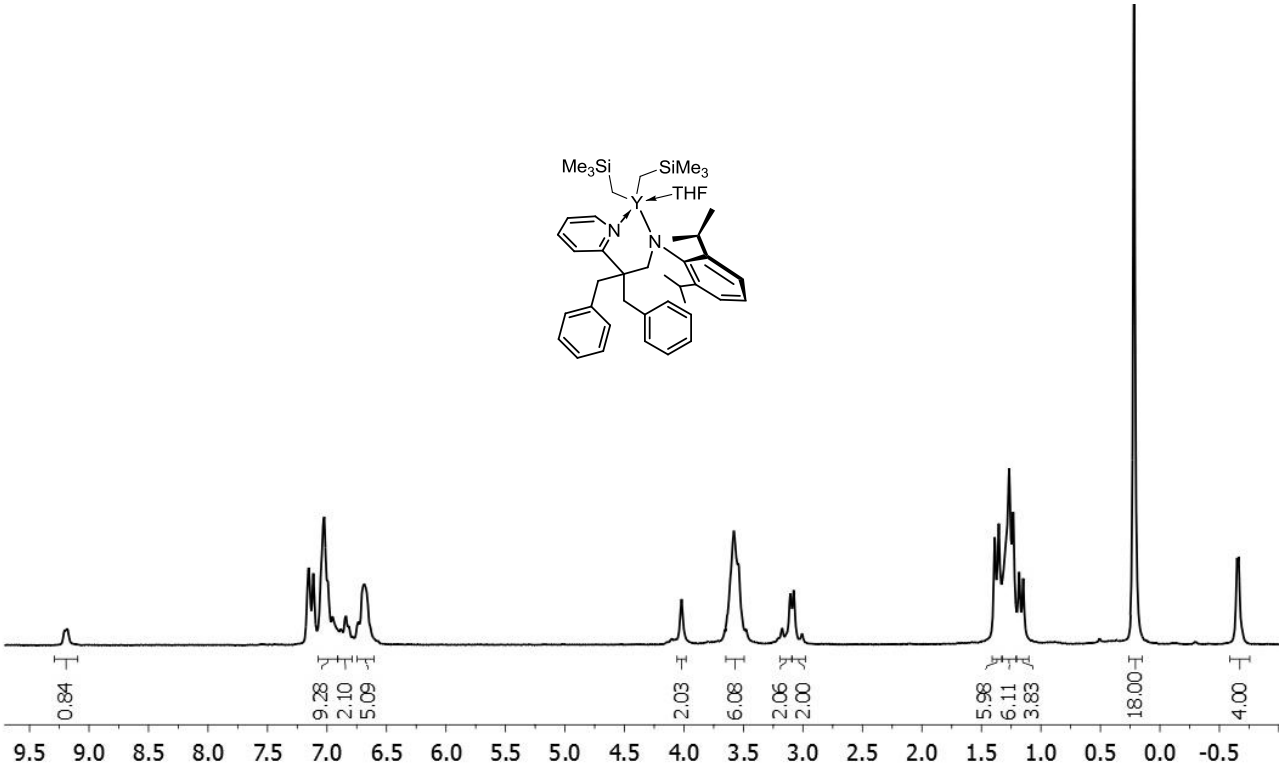

Figure S25. ^{1}H-NMR spectrum (400 MHz, C_6D_6, 298K) of **14**.

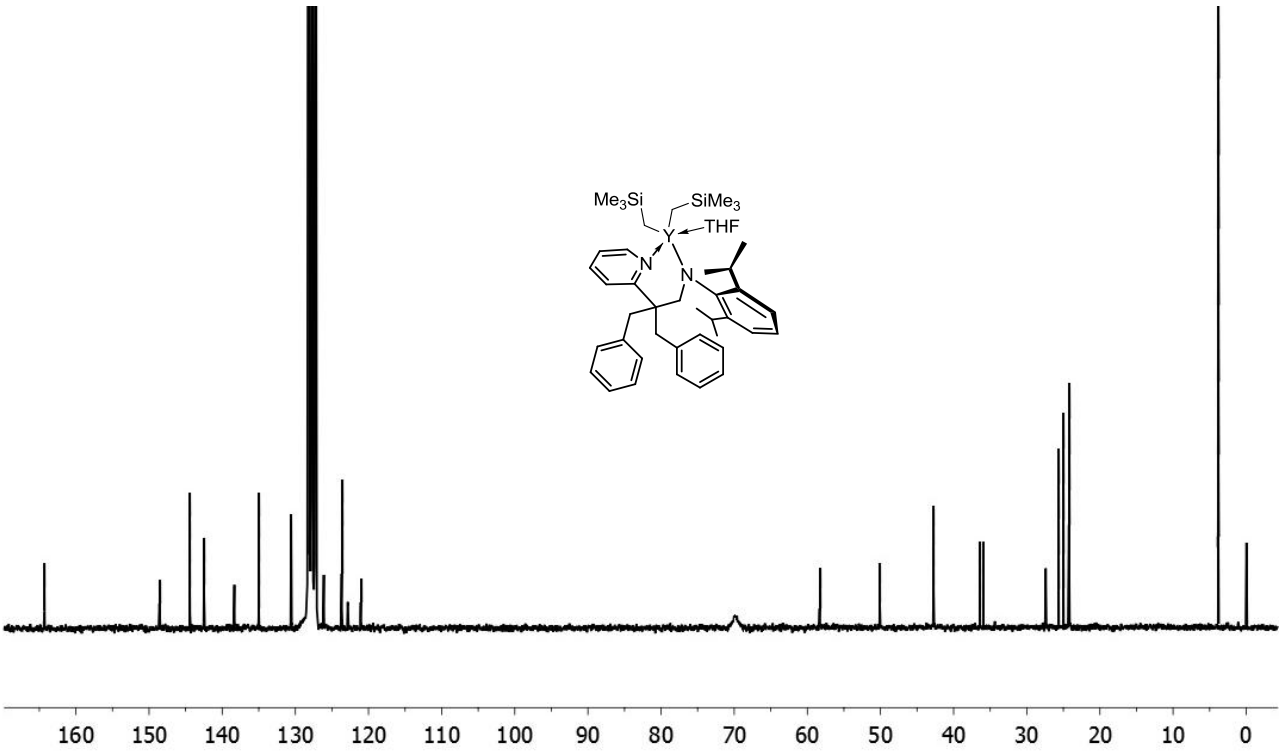

Figure S26. ^{13}C{^{1}H}-NMR spectrum (100 MHz, C_6D_6, 298K) of **14.**

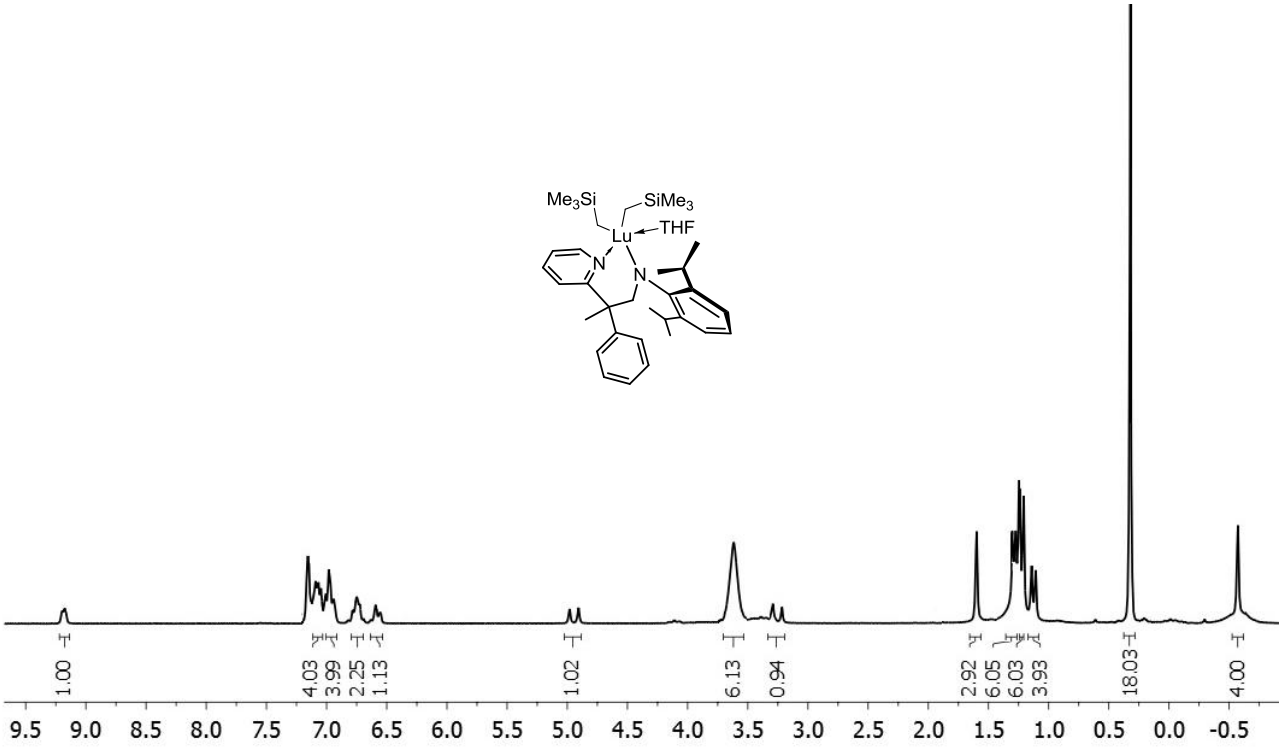

Figure S27. ^{1}H-NMR spectrum (400 MHz, C_6D_6, 298K) of **15**.

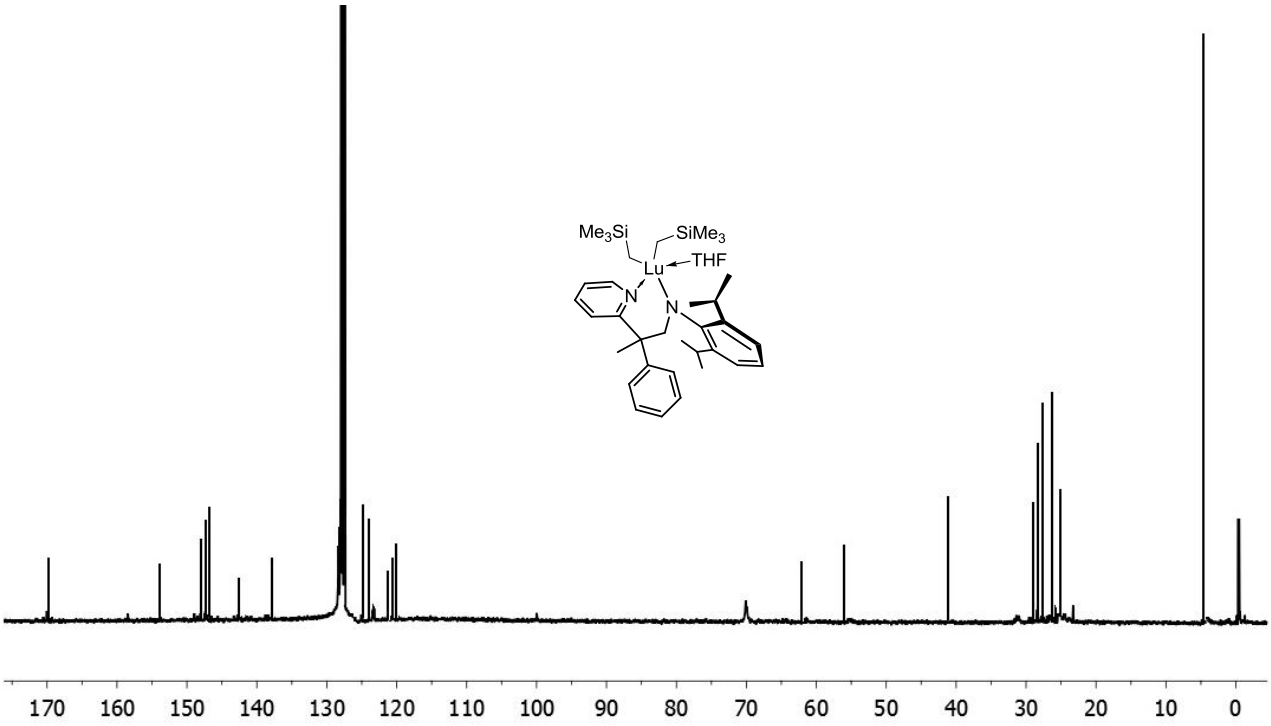

Figure S28. ^{13}C{^{1}H}-NMR spectrum (100 MHz, C_6D_6, 298K) of **15**

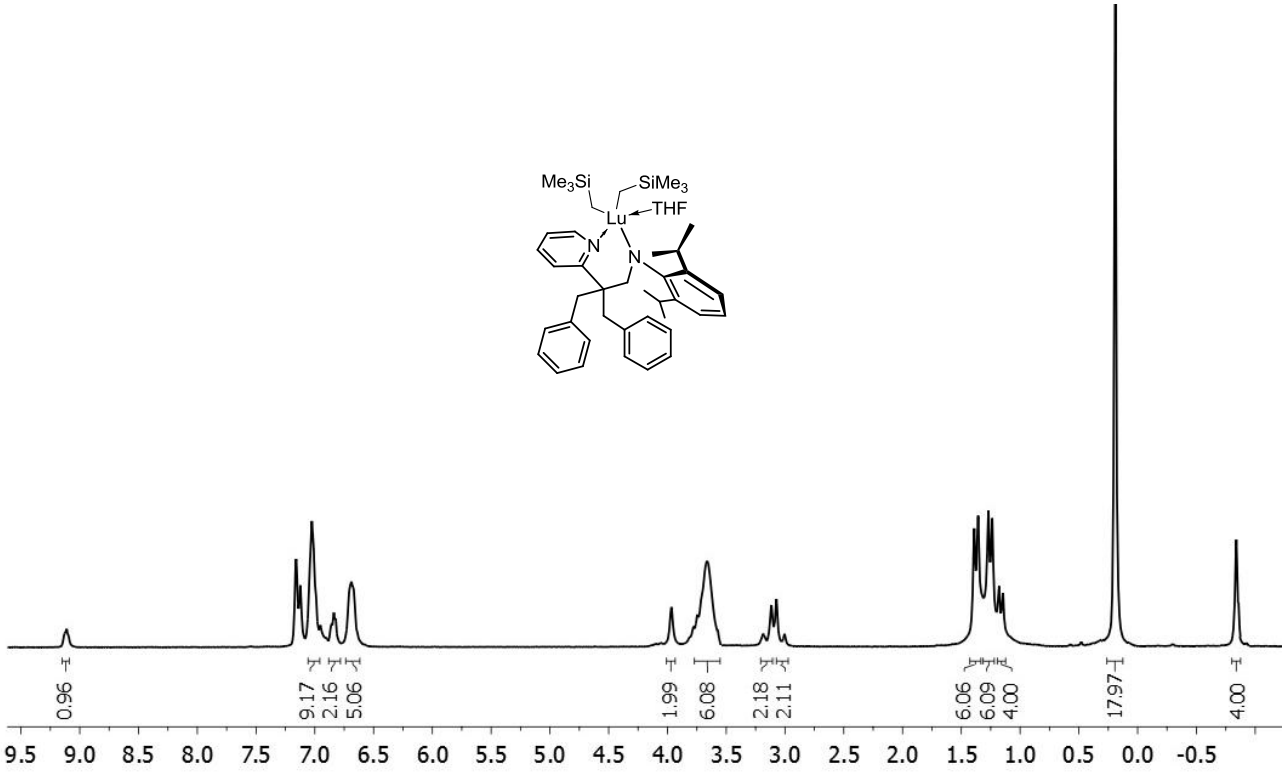

Figure S29. ^{1}H-NMR spectrum (400 MHz, C_6D_6, 298K) of **16**.

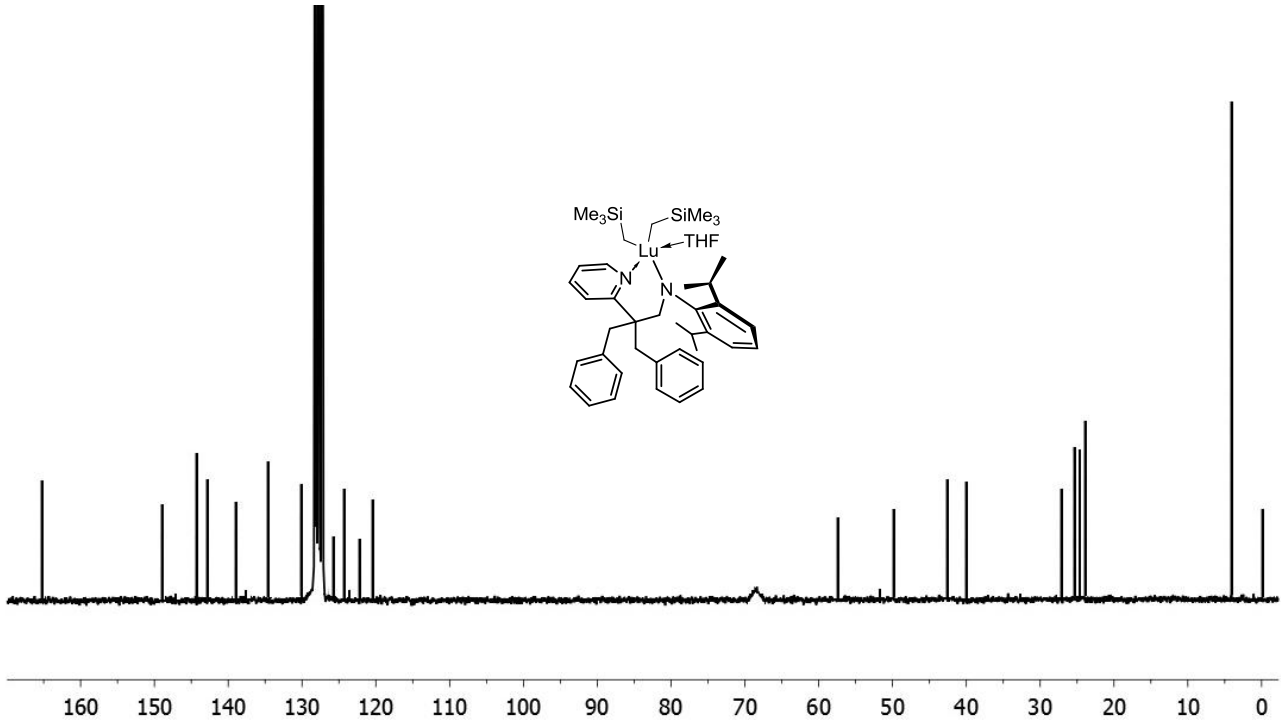

Figure S30. ^{13}C{^{1}H} NMR spectrum (100 MHz, C_6D_6, 298K) of **16.**