

Supporting Information

**Co(I) complexes with a tetradentate phenanthroline-based PNNP ligand
as a potent new metal-ligand cooperation platform**

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General Information

All experiments were carried out under nitrogen atmosphere using Schlenk techniques or a glovebox. All organic solvents were dried with a solvent purification system (MBraun SPS-800 or Glass Contour Ultimate Solvent System). Benzene- d_6 was dried over sodium benzophenone ketyl and distilled. DMSO- d_6 was dried over CaH_2 and distilled. PNNP ligand (2,9-bis((diphenylphosphino)methyl)-1,10-phenanthroline) was synthesized according to the literature procedure.¹ TEMPO-H (1-hydroxy-2,2,6,6-tetramethylpiperidine)² and TEMPO- CH_2SiMe_3 (2,2,6,6-tetramethyl-1-((trimethylsilyl)methoxy)piperidine)³ were synthesized according to the literature procedures. H_2 gas was passed through a Dryclean column (4A molecular sieves, Nikka Seiko Co.) and a Gasclean GC-XR column (Nikka Seiko Co.) prior to use. All other reagents were purchased from commercial suppliers and used without further purification unless otherwise mentioned. ^1H , $^{13}\text{C}\{^1\text{H}\}$, $^{29}\text{Si}\{^1\text{H}\}$, and $^{31}\text{P}\{^1\text{H}\}$ NMR spectra (^1H , 600 MHz; ^{13}C , 150 MHz; ^{29}Si , 119 MHz; ^{31}P , 243 MHz) were recorded on a Bruker AVANCE 600 spectrometer. Chemical shifts are reported in δ (ppm) and referenced to the residual solvent signals for ^1H and ^{13}C , 85% H_3PO_4 for ^{31}P , and 1,4-bis(trimethylsilyl)benzene for ^{29}Si as external standards. The abbreviations designated for multiplicities are as follows: s = singlet, d = doublet, t = triplet, m = multiplet, br = broad, vt = virtual triplet, vq = virtual quartet. High-resolution ESI mass spectra were measured on a Bruker microTOF II. Elemental analyses were performed on a Yanaco CHN CORDER MT-6.

Experimental Details

Synthesis of $[\text{CoCl}(\text{PNNP})]$ (**1**)

$[\text{CoCl}(\text{PPh}_3)_3]$ (198.1 mg, 0.225 mmol) and 2,9-bis((diphenylphosphaneyl)methyl)-1,10-phenanthroline (PNNP) (129.6 mg, 0.225 mmol) were charged in a 50 mL Schlenk tube and dissolved in THF (10 mL). After stirring for 24 h at room temperature, green precipitates formed. The solution was concentrated to dryness in vacuo and the resulting residue was washed with diethyl ether (three times) to give **1** as a green solid (106.8 mg, 0.159 mmol, 71%). A slow diffusion of C_6H_6 to a saturated acetonitrile solution of **1** at room temperature gave single crystals of **1**.

^1H NMR (C_6D_6 , 25 °C) δ 8.06 (d, 2H, Phen- H , $^3J_{\text{HH}} = 7.3$ Hz), 7.94 (br, 4H, PPh_2), 7.37 (d, 2H, Phen- H , $^3J_{\text{HH}} = 7.3$ Hz), 7.08-7.14 (m, 4H, Phen- H (2H) + PPh_2 (2H)), 7.05 (br, 4H, PPh_2), 6.66 (m, 6H, PPh_2), 6.48 (m, 4H, PPh_2), 5.23 (m, 2H, PCH_2), 4.17 (m, 2H, PCH_2). $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6 , 25 °C) δ 55.57 (s). $^{13}\text{C}\{^1\text{H}\}$ NMR could not be measured due to the extremely low solubility of **1** in organic solvents. Anal. Calcd for $\text{C}_{38}\text{H}_{30}\text{N}_2\text{P}_2\text{Co}\cdot 0.5\text{C}_6\text{H}_6$: C, 69.35; H, 4.68; N 3.95. Found: C, 69.40; H, 4.79; N, 4.08.

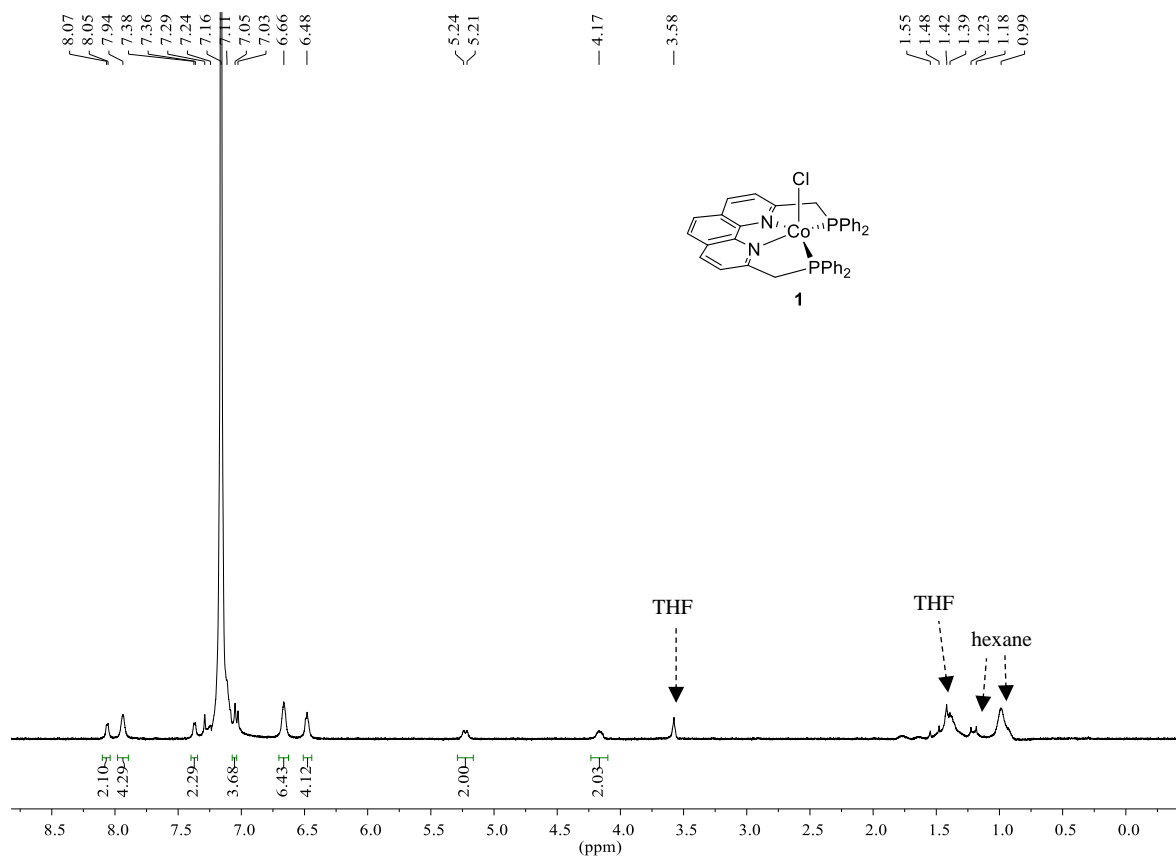


Figure S1. ^1H NMR spectrum of **1** in C_6D_6 .

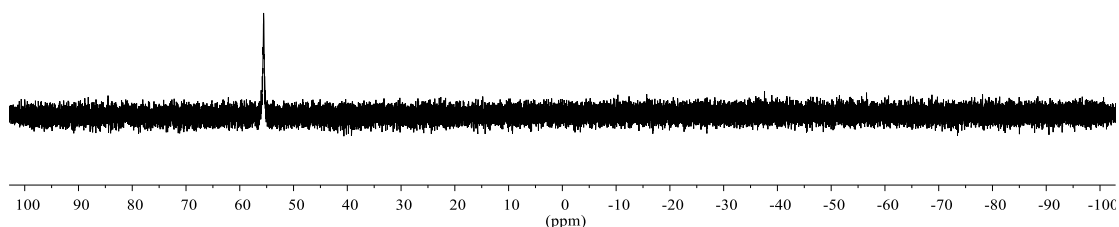


Figure S2. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **1** in C_6D_6 .

Synthesis of [CoMe(PNNP)] (**2**)

[CoCl(PNNP)] (**1**) (50.0 mg, 0.074 mmol) was dissolved in benzene (5 mL) and stored in a 30 mL Schlenk tube. Methylmagnesium bromide (29 μL of 3.0 M Et_2O solution, 0.090 mmol) was added dropwise at room temperature. The mixture was stirred at room temperature for 1 h. The resulting solution was dried under vacuum, and the residue was extracted with ether. The solution was filtered using a Celite pad, and the filtrate was concentrated to dryness under vacuo to afford **2** as a purple solid (23.2 mg, 0.036 mmol, 49 %).

^1H NMR (C_6D_6 , 25 $^\circ\text{C}$) δ 7.69 (br, 2H), 7.29 (br, 4H, PPh_2), 7.12 (m, 2H, Phen- H), 7.08 (s, 2H, Phen- H), 7.02 (brm, 4H, PPh_2), 6.91 (m, 6H, PPh_2), 6.73 (t, 2H, PPh_2 , $^3J_{\text{HH}} = 7.0$ Hz), 6.61 (t, 4H, PPh_2 , $^3J_{\text{HH}} = 7.3$ Hz), 4.42 (d, 2H, PCH_2 , $^3J_{\text{HH}} = 16.3$ Hz), 3.93 (m, 2H, PCH_2), -0.36 (t, 3H, CoCH_3 , $^3J_{\text{PH}} = 3.3$ Hz). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 25 $^\circ\text{C}$) 156.4, 140.8, 138.0, 133.7, 133.4, 131.9, 131.8, 129.3, 128.6, 126.3, 116.3, 112.5, 45.4, -15.2. Two Ar signals were obscured in a residual benzene signal. $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6 , 25 $^\circ\text{C}$) δ 76.92. HRMS (ESI) Calculated: ($\text{C}_{39}\text{H}_{33}\text{CoN}_2\text{P}_2$) 651.1524 ($[\text{M}+\text{H}]^+$), Found: 651.1511.

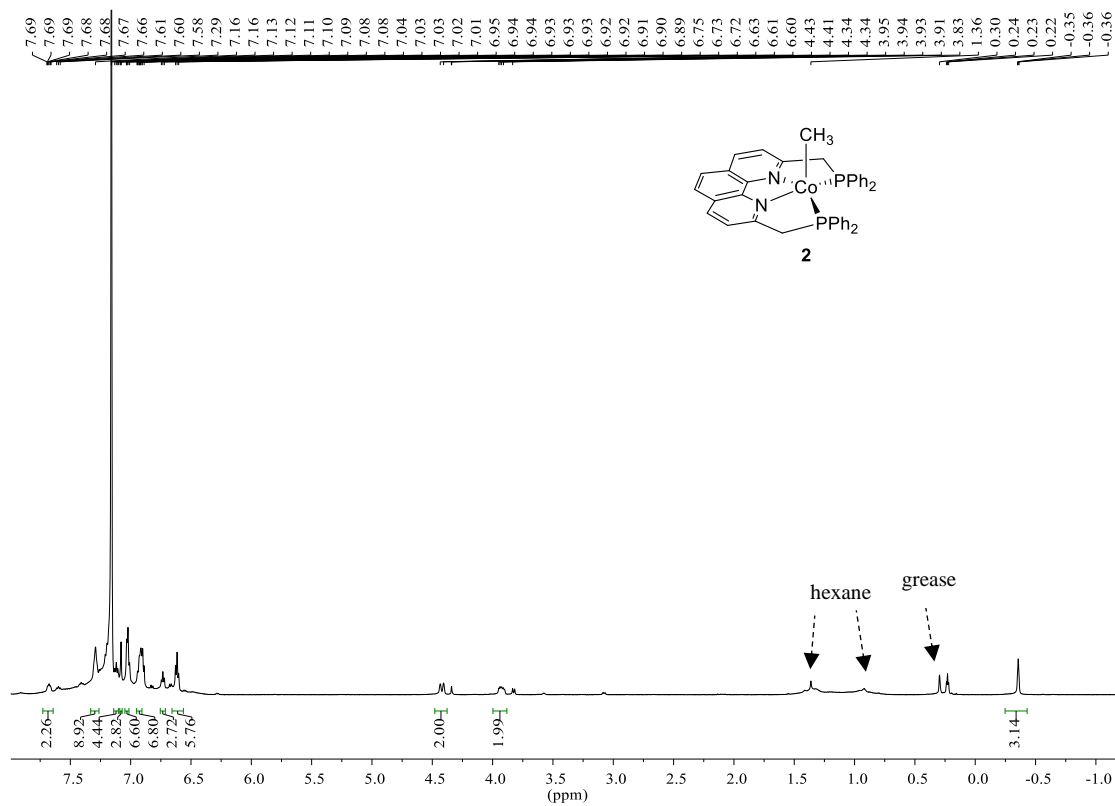


Figure S3. ¹H NMR spectrum of **2** in C₆D₆.

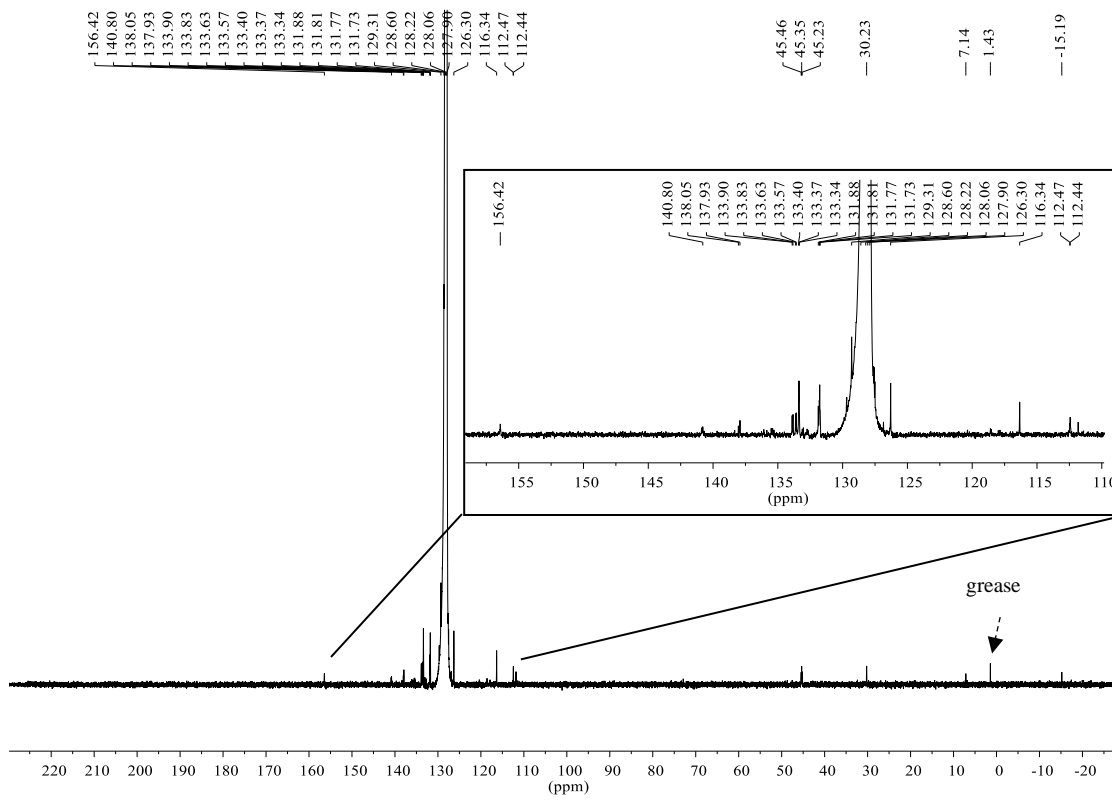


Figure S4. $^{13}\text{C}\{^1\text{H}\}$ NMR spectrum of **2** in C_6D_6 .

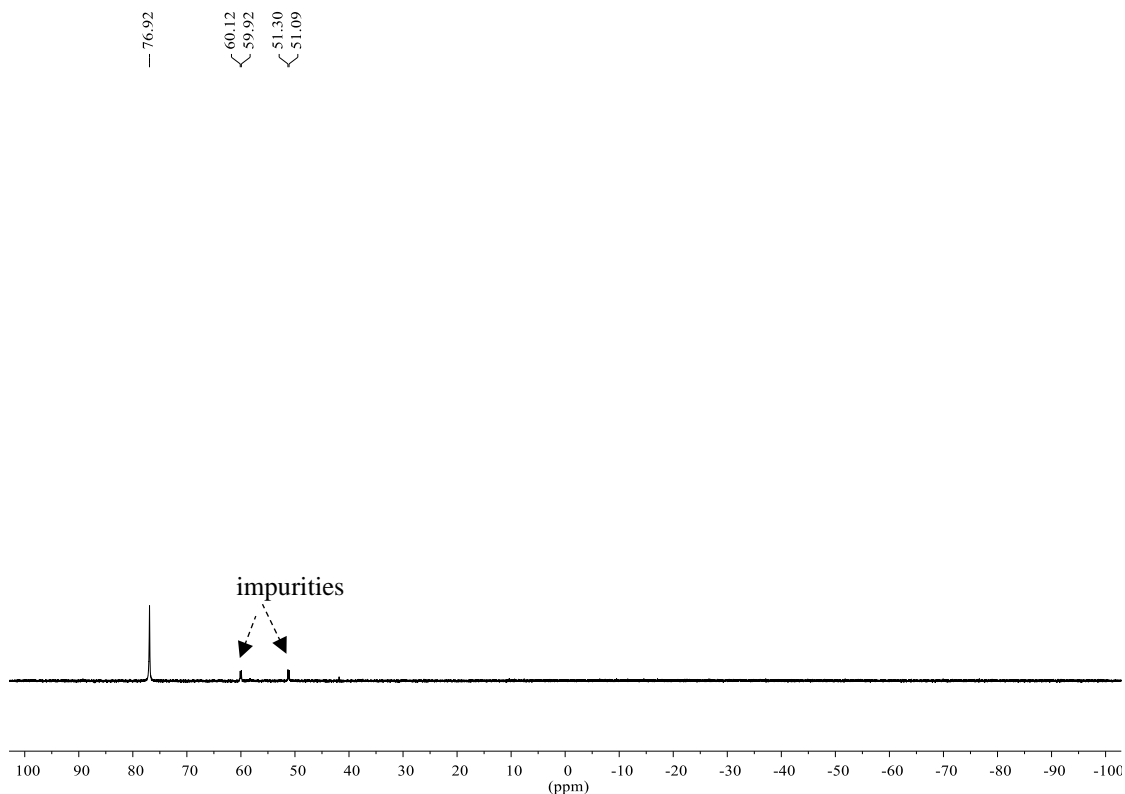


Figure S5. $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of **2** in C_6D_6 .

Synthesis of $[\text{Co}(\text{CH}_2\text{SiMe}_3)(\text{PNNP})]$ (**3**)

$[\text{CoCl}(\text{PNNP})]$ (**1**) (19.9 mg, 0.030 mmol) was dissolved in benzene (35 mL) and stored in a 50 mL Schlenk tube. Trimethylsilylmethylmagnesium chloride (30.0 μL of 1 M THF solution, 0.030 mmol) was added dropwise. The mixture was stirred at room temperature for 1 h. The resulting solution was dried under vacuum. The residue was extracted with Et_2O and filtered using a Celite pad. The filtrate was concentrated to dryness under vacuo to afford **3** as a purple solid (18.7 mg, 0.026 mmol, 87 %).

^1H NMR (C_6D_6 , 25 $^\circ\text{C}$) δ 7.35 (d, 2H, Phen-*H*, $^3J_{\text{HH}} = 7.0$ Hz), 7.32 (m, 4H, *PPh*₂), 7.13 (vt, 4H, Phen-*H* (2H) + *PPh*₂ (2H)), 7.04 (vq, 6H, Phen-*H* (2H) + *PPh*₂ (4H)), 6.75 (m, 4H, *PPh*₂), 6.64 (t, 2H, *PPh*₂, $^3J_{\text{HH}} = 7.4$ Hz), 6.49 (t, 4H, *PPh*₂, $^3J_{\text{HH}} = 7.7$ Hz), 4.81 (d, 2H, *PCH*₂, $^3J_{\text{HH}} = 15.8$ Hz), 3.95 (m, 2H, *PCH*₂), -0.57 (s, 9H, CH_2SiMe_3), -0.60 (t, 2H, CH_2SiMe_3 , $^3J_{\text{PH}} = 4.4$ Hz). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 25 $^\circ\text{C}$) 157.0, 140.0, 138.7, 134.2, 133.5, 131.7, 131.4, 129.5, 128.6 ($\times 2$), 128.3, 126.3, 117.2, 113.7, 45.4, 2.9, -22.2. $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6 , 25 $^\circ\text{C}$) δ 75.72. $^{29}\text{Si}\{^1\text{H}\}$ NMR (C_6D_6 , 25 $^\circ\text{C}$) δ 7.46 (t, $^3J_{\text{SiP}} = 3.6$ Hz). HRMS (ESI) Calculated: ($\text{C}_{42}\text{H}_{42}\text{CoN}_2\text{P}_2\text{Si}$) 723.1919 ($[\text{M}+\text{H}]^+$), Found: 723.1907.

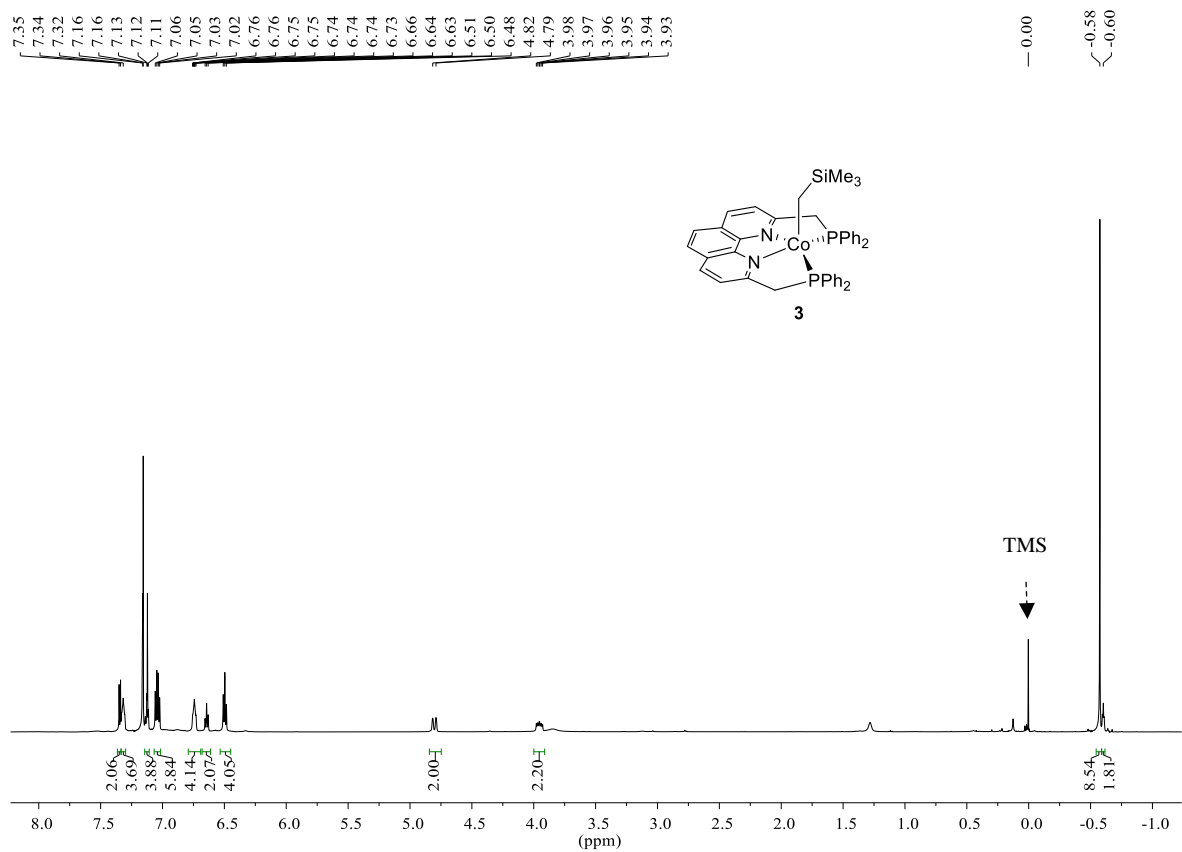


Figure S6. ¹H spectrum of **3** in C₆D₆.

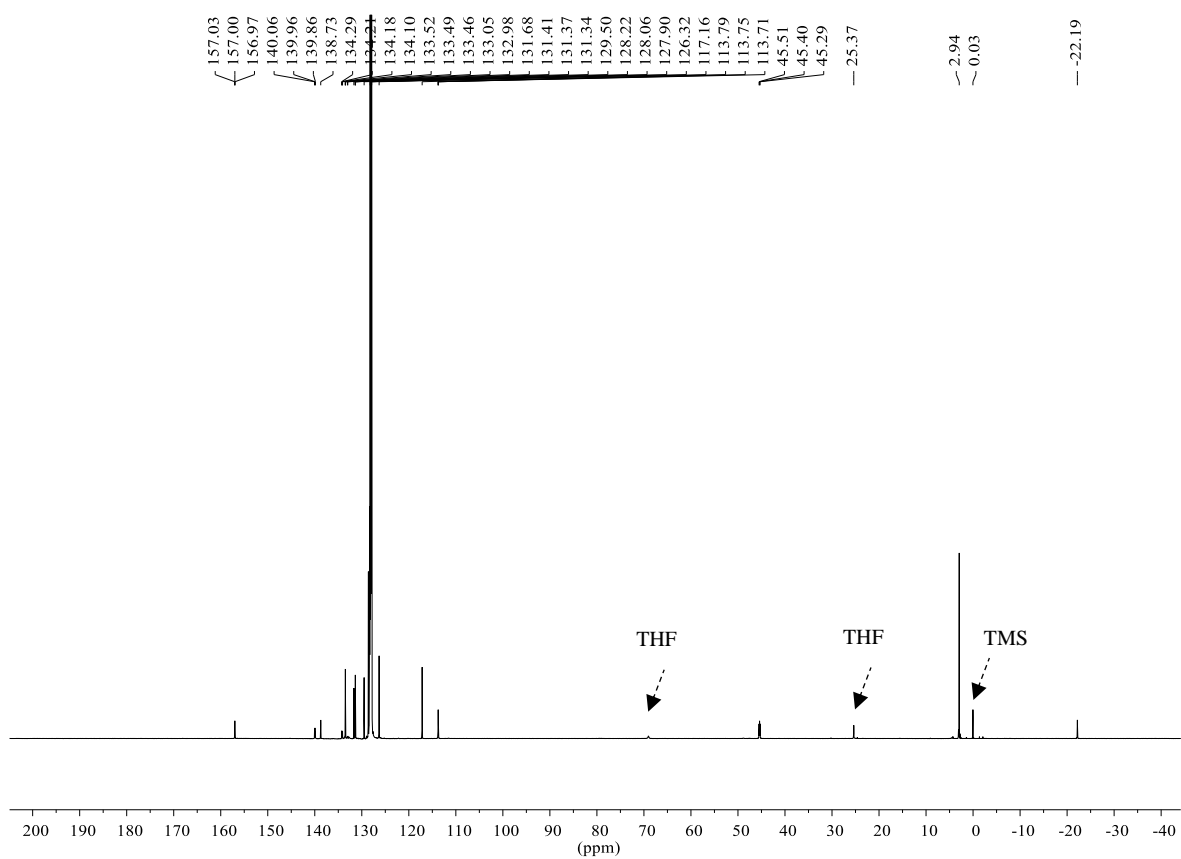


Figure S7. $^{13}\text{C}\{^1\text{H}\}$ spectrum of **3** in C_6D_6 .

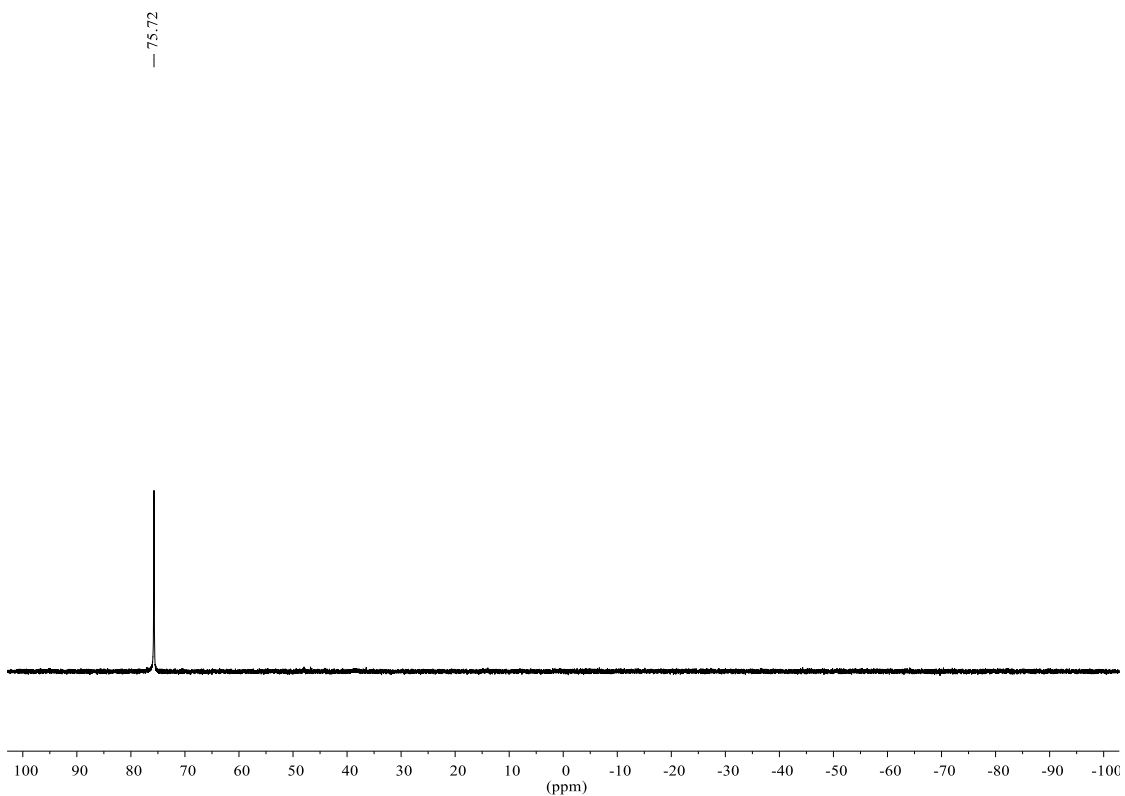


Figure S8. $^{31}\text{P}\{^1\text{H}\}$ spectrum of **3** in C_6D_6 .

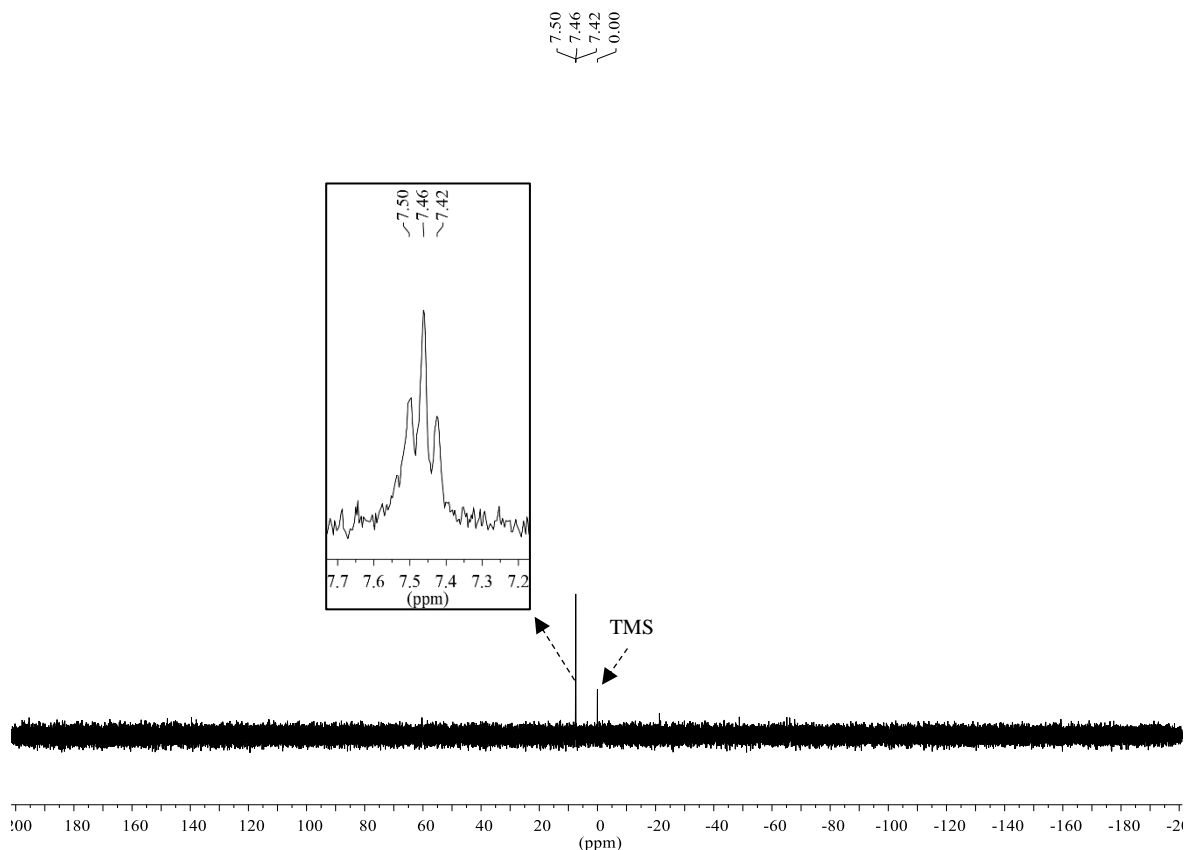


Figure S9. $^{29}\text{Si}\{^1\text{H}\}$ spectrum of **3** in C_6D_6 .

Synthesis of $[\text{Co}(\text{PNNP}')] (\mathbf{4})$

Method 1: $[\text{Co}(\text{CH}_2\text{SiMe}_3)(\text{PNNP})] (\mathbf{3})$ (24.3 mg, 0.034 mmol) was charged in a 50 mL Schlenk tube and dissolved in benzene (10 mL). The solution was stirred at 60 °C for 16 h to form a deep green crystalline precipitate. After filtration, **4** was obtained as an analytically pure form (14.2 mg, 0.029 mmol, 86%). Single crystals of **4** was obtained by slow evaporation of saturated C_6H_6 solution of **4** at room temperature.

Method 2: To a benzene solution (10 mL) of $[\text{CoCl}(\text{PNNP})] (\mathbf{1})$ (15.2 mg, 0.023 mmol), was added sodium *tert*-butoxide (2.2 mg, 0.023 mmol). The solution was stirred at room temperature for a few minutes. The solution was filtered with a Celite pad to give **3** as a deep green solid (13.8 mg, 0.022 mmol, 96%).

^1H NMR (C_6D_6 , 25 °C) δ 7.60 (t, 4H, PPh_2 , $^3J_{\text{HH}} = 8.6$ Hz), 7.56 (d, 1H, Phen-*H*, $^3J_{\text{HH}} = 8.3$ Hz), 7.41 (t, 4H, PPh_2 , $^3J_{\text{HH}} = 8.6$ Hz), 7.00 (m, 4H, PPh_2), 6.88-6.93 (m, 9H, Phen-*H* (1H) + PPh_2 (8H)), 6.65 (m, 2H, Phen-*H*), 6.55 (d, 1H, Phen-*H*, $^3J_{\text{HH}} = 8.0$ Hz), 6.28 (d, 1H, Phen-*H*, $^3J_{\text{HH}} = 8.5$ Hz), 4.33 (brs, 1H, PCH), 3.08 (d, 2H, PCH_2 , $^2J_{\text{PH}} = 12.0$ Hz). $^{13}\text{C}\{^1\text{H}\}$ NMR ($\text{DMSO}-d_6$, 25 °C) δ 165.8, 151.3, 146.0, 143.6, 139.4, 133.9, 132.6, 130.8, 130.7, 129.4, 127.9, 127.7, 127.6, 127.2, 126.1, 124.0, 121.6, 117.1, 114.2, 111.2, 70.9, 46.7. $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6 , 25 °C) δ 52.8 (br), 38.2 (br). HRMS (ESI) Calculated: ($\text{C}_{38}\text{H}_{29}\text{CoN}_2\text{P}_2$) 634.1132 ($[\text{M}+\text{H}]^+$), Found: 634.1148.

Anal. Calcd for $\text{CoN}_2\text{P}_2\text{C}_{38}\text{H}_{29}$: C, 71.93; H, 4.61; N 4.41. Found: C, 72.24; H, 4.96; N, 4.58.

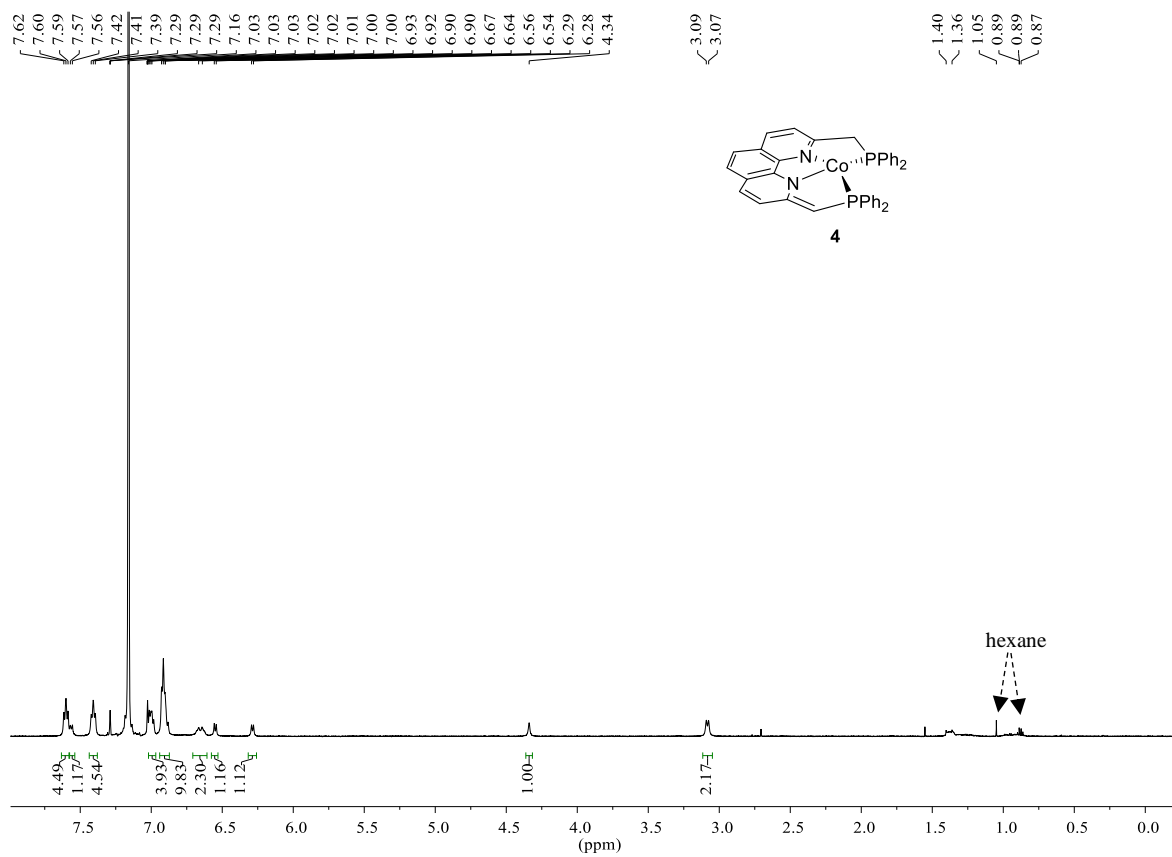


Figure S10. ^1H spectrum of **4** in C_6D_6 .

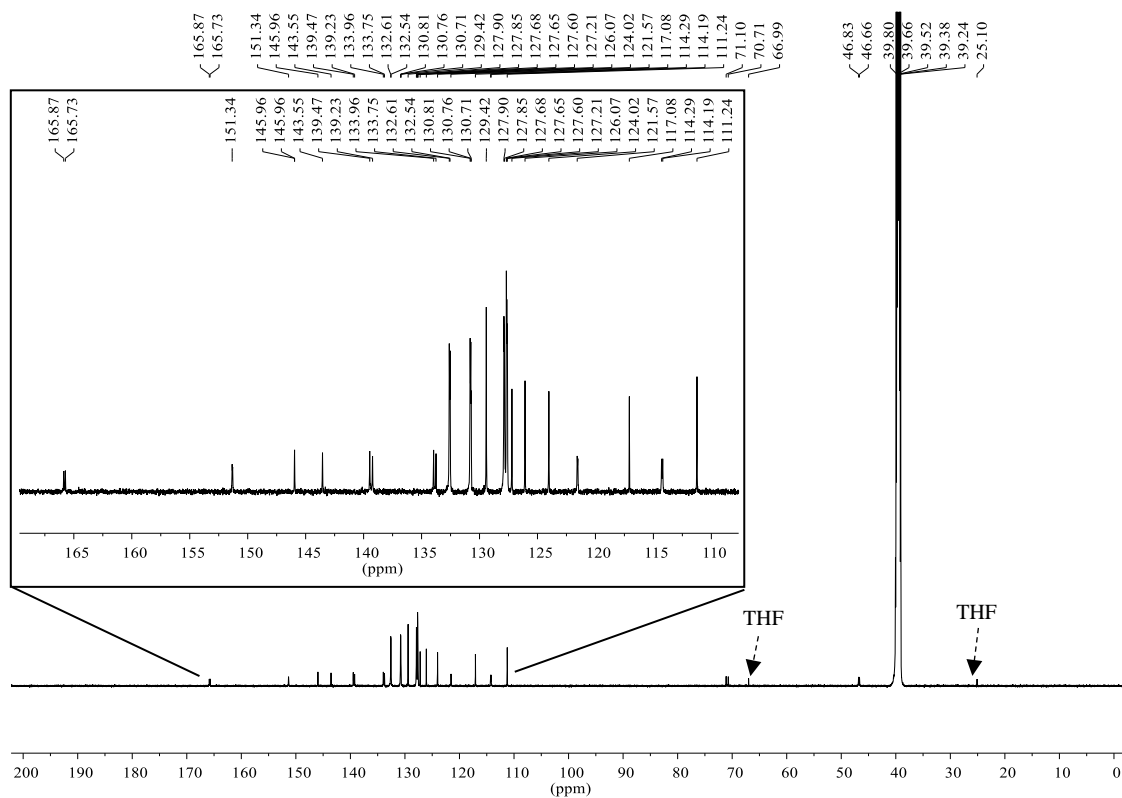


Figure S11. $^{13}\text{C}\{^1\text{H}\}$ spectrum of 4 in $\text{DMSO-}d_6$.

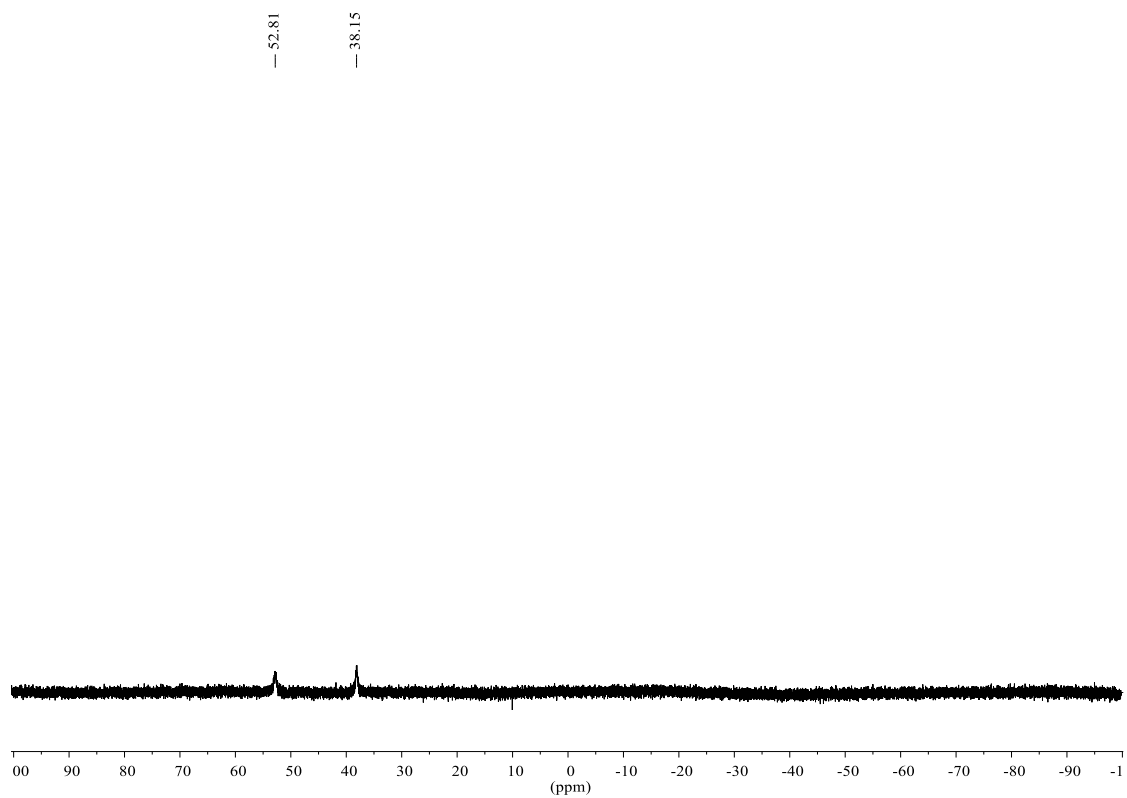


Figure S12. $^{31}\text{P}\{^1\text{H}\}$ spectrum of **4** in C_6D_6 .

Reaction of **3** with TEMPO

A C₆D₆ solution (0.4 mL) of [Co(PNNP)(CH₂SiMe₃)] (**3**) (5.5 mg, 0.0076 mmol) was charged in a J-Young NMR tube, and TEMPO (2,2,6,6-tetramethylpiperidin-1-yl)oxyl) (4.9 mg, 0.031 mmol) was then added to the solution. The solution was left to stand at 60 °C for 1 h, and the resulting solution was analyzed by ¹H NMR. TEMPO-H² and TEMPO-CH₂SiMe₃³ were identified by comparison of their spectral data with those of authentic samples. The molar ratio of the formed TEMPO-H, TEMPO-CH₂SiMe₃ and **5** was determined by ¹H NMR to be 7 : 1 : 1. After removal of all the volatiles, the resultant was extracted with hexane. The extract was concentrated to dryness to give **5** (trace amount).

TEMPO-H: ¹H NMR (C₆D₆, 25 °C) δ 3.74 (br, 1H, OH), 1.39 (m, 4H, CH₂), 1.30 (m, 2H, CH₂), 1.15 (s, 12H, CH₃).

TEMPO-CH₂SiMe₃: ¹H NMR (C₆D₆, 25 °C) δ 3.54 (s, 2H, OCH₂), 1.48 (m, 4H, CH₂), 1.33 (m, 2H, CH₂), 1.16 (br, 6H, CH₃), 1.08 (br, 6H, CH₃), 0.06 (s, 9H, Si(CH₃)₃).

5: ¹H NMR (C₆D₆, 25 °C) δ 7.44 (m, 4H, PPh₂), 7.40 (m, 4H, PPh₂), 7.07 (t, 2H, PPh₂, ³J_{HH} = 7.3 Hz), 7.00 (t, 4H, PPh₂, ³J_{HH} = 7.4 Hz), 6.89 (t, 2H, PPh₂, ³J_{HH} = 7.3 Hz), 6.72 (d, 2H, Phen-H, ³J_{HH} = 9.2 Hz), 6.67-6.63 (m, 6H, Phen-H (2H) + PPh₂ (4H)), 6.62 (d, 2H, Phen-H, ³J_{HH} = 9.2 Hz), 4.68 (s, 2H, PCH), -0.17 (s, 9H, SiMe₃), -0.29 (t, 2H, CH₂SiMe₃, ³J_{PH} = 9.2 Hz). ¹³C{¹H} NMR (C₆D₆, 25 °C) δ 167.5, 146.8, 133.7, 132.7, 132.1, 132.0, 131.9, 131.7, 129.9, 129.4, 128.5, 121.1, 121.0, 117.7, 82.7, 0.60 (× 2). HSQC (C₆D₆, 25 °C) δ_H-δ_C -0.17 (δ_H), -0.29 (δ_H) - 0.60 (δ_C). ³¹P{¹H} NMR (C₆D₆, 25 °C) δ 33.9 (br). ²⁹Si{¹H} NMR (C₆D₆, 25 °C) δ 9.24 (t, ³J_{SiP} = 1.2 Hz). HRMS (ESI) Calculated: (C₄₂H₃₉CoN₂P₂Si) 721.1763 ([M]⁺), Found: 721.1764. Single crystal of **5** was obtained from cold hexane solution at -35 °C.

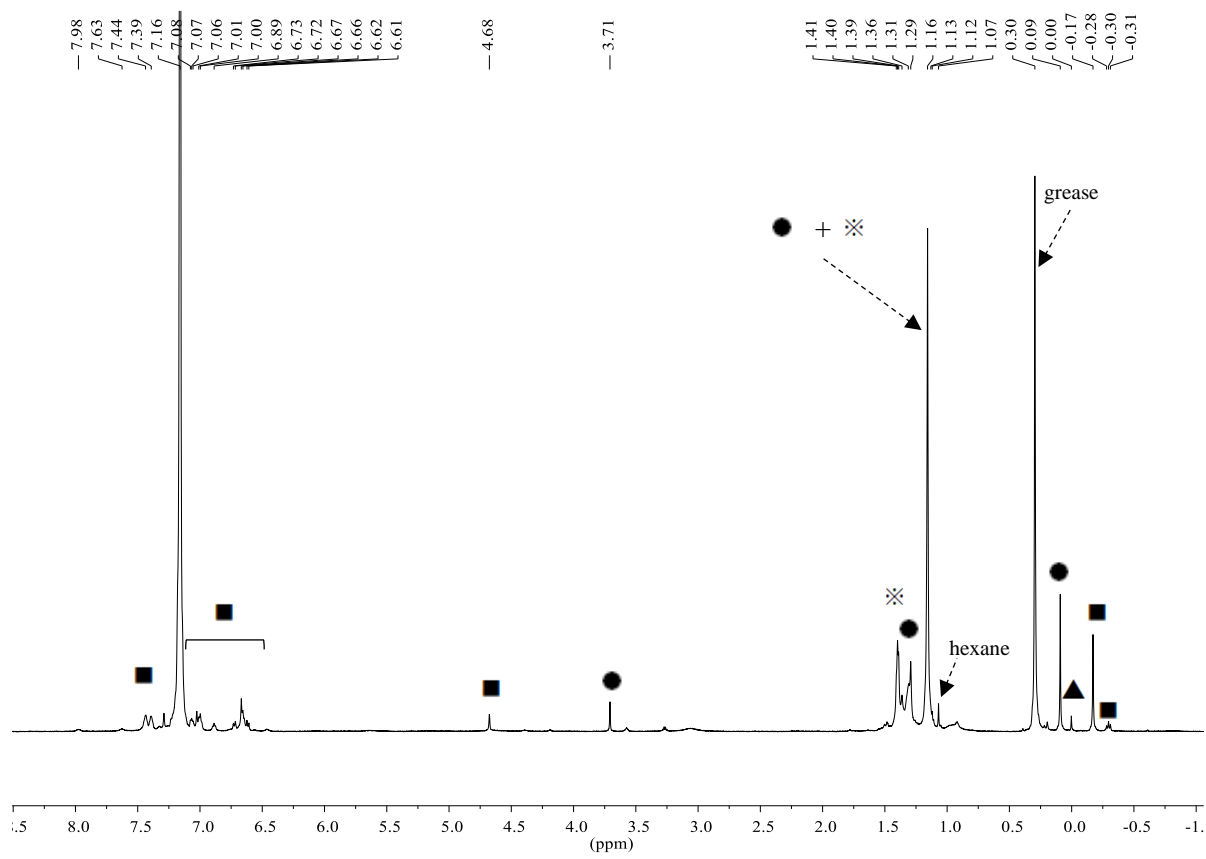


Figure S13. ^1H NMR spectrum of the reaction mixture in C_6D_6 ; ■ : **5**; ● : TEMPO- CH_2SiMe_3 ; ▲ : TMS; ※: TEMPO-H.

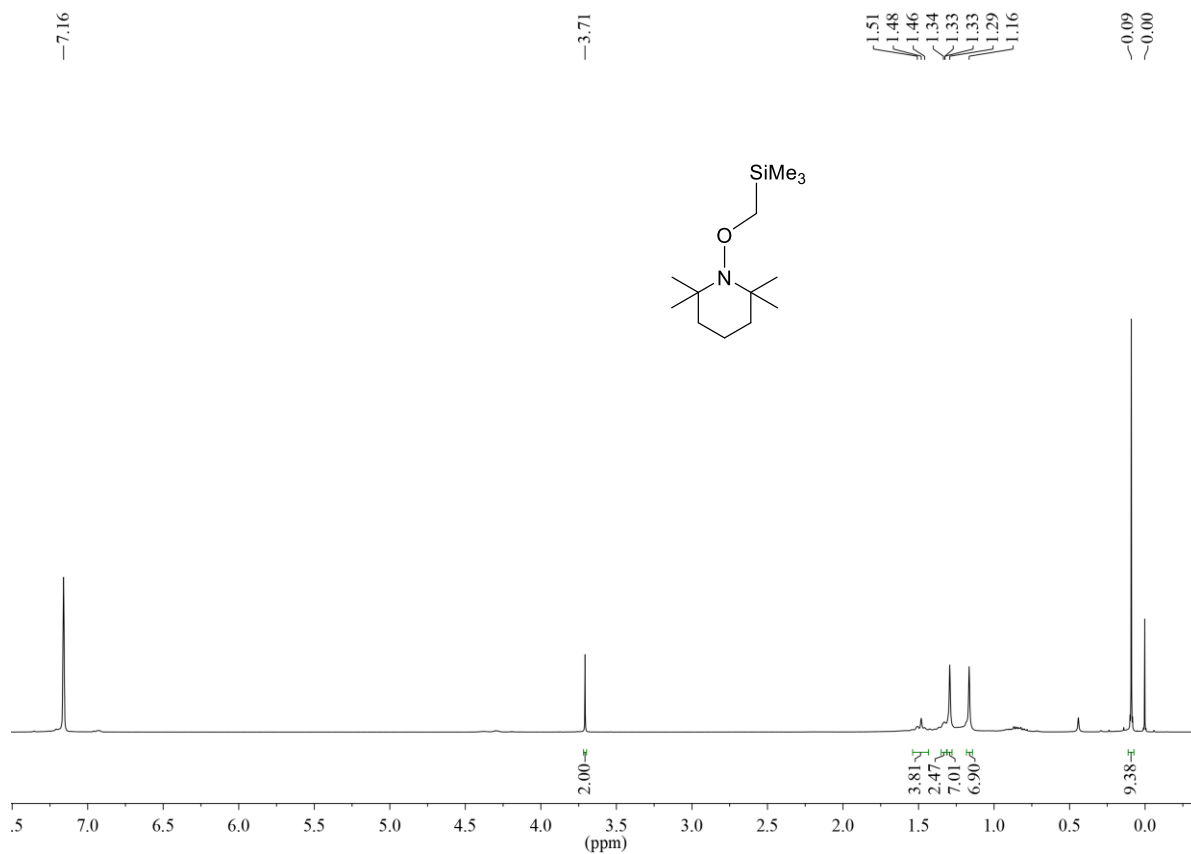


Figure S14. ¹H spectrum of TEMPO-CH₂SiMe₃ in C₆D₆.

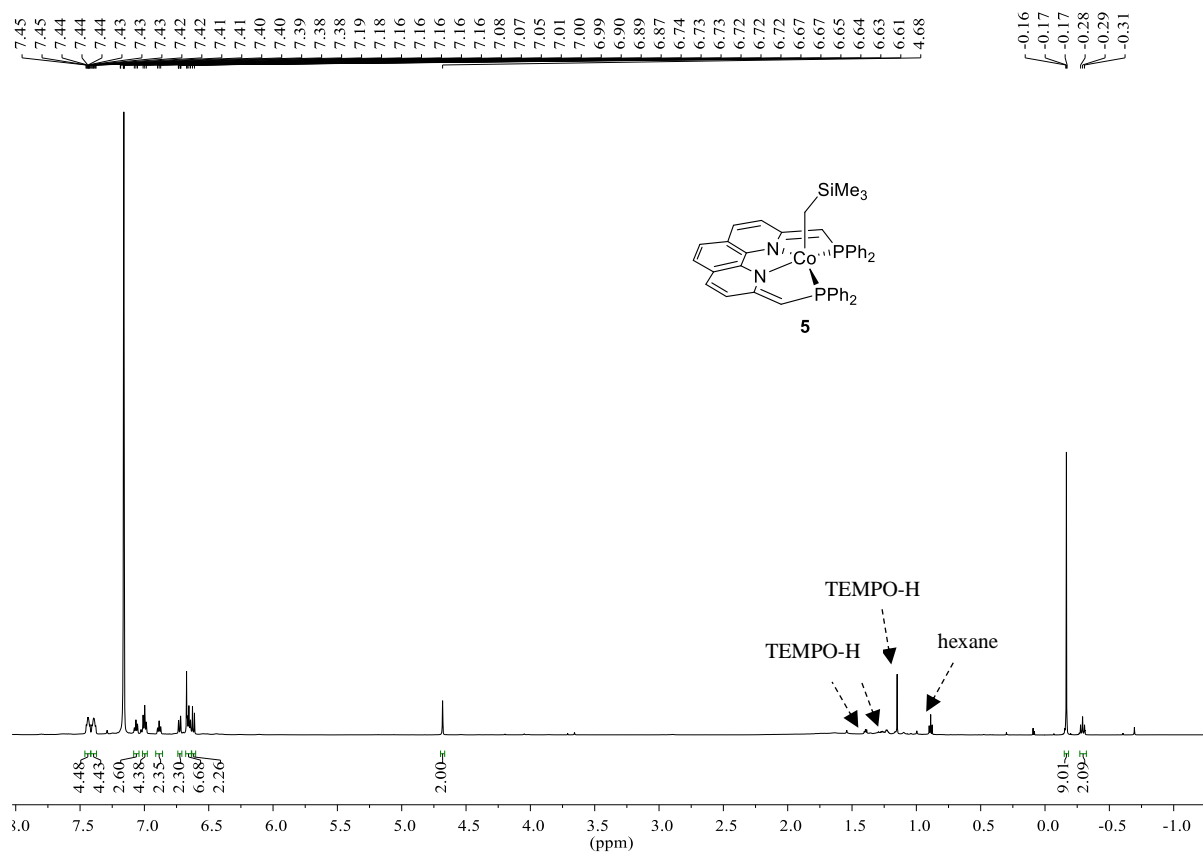


Figure S15. ¹H spectrum of **5** in C₆D₆.

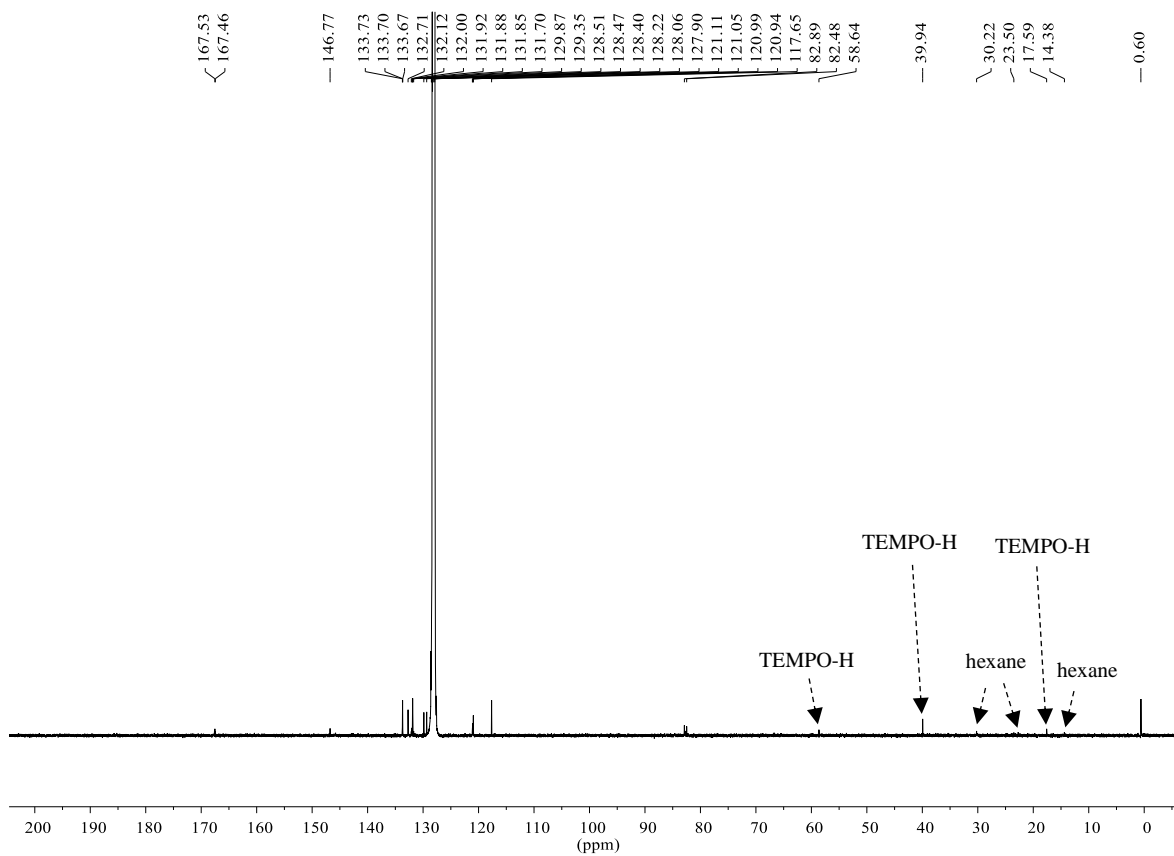


Figure S16. $^{13}\text{C}\{^1\text{H}\}$ spectrum of **5** in C_6D_6 .

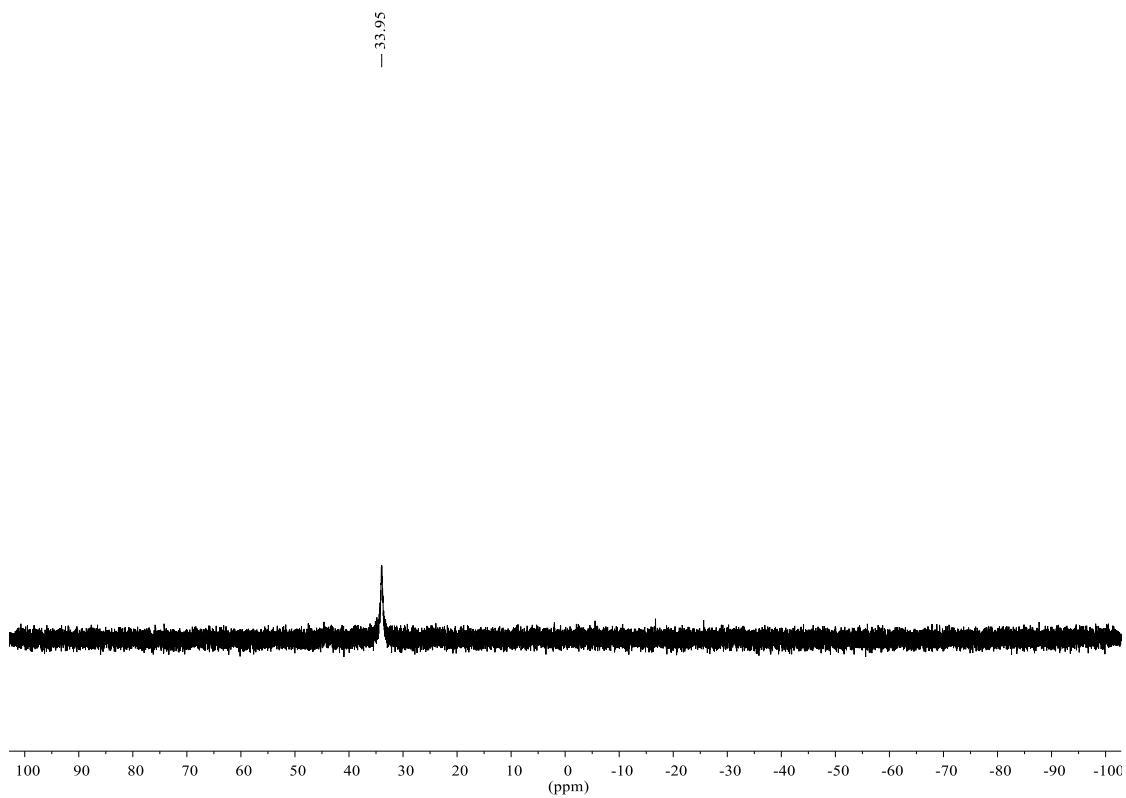


Figure S17. $^{31}\text{P}\{^1\text{H}\}$ spectrum of **5** in C_6D_6 .

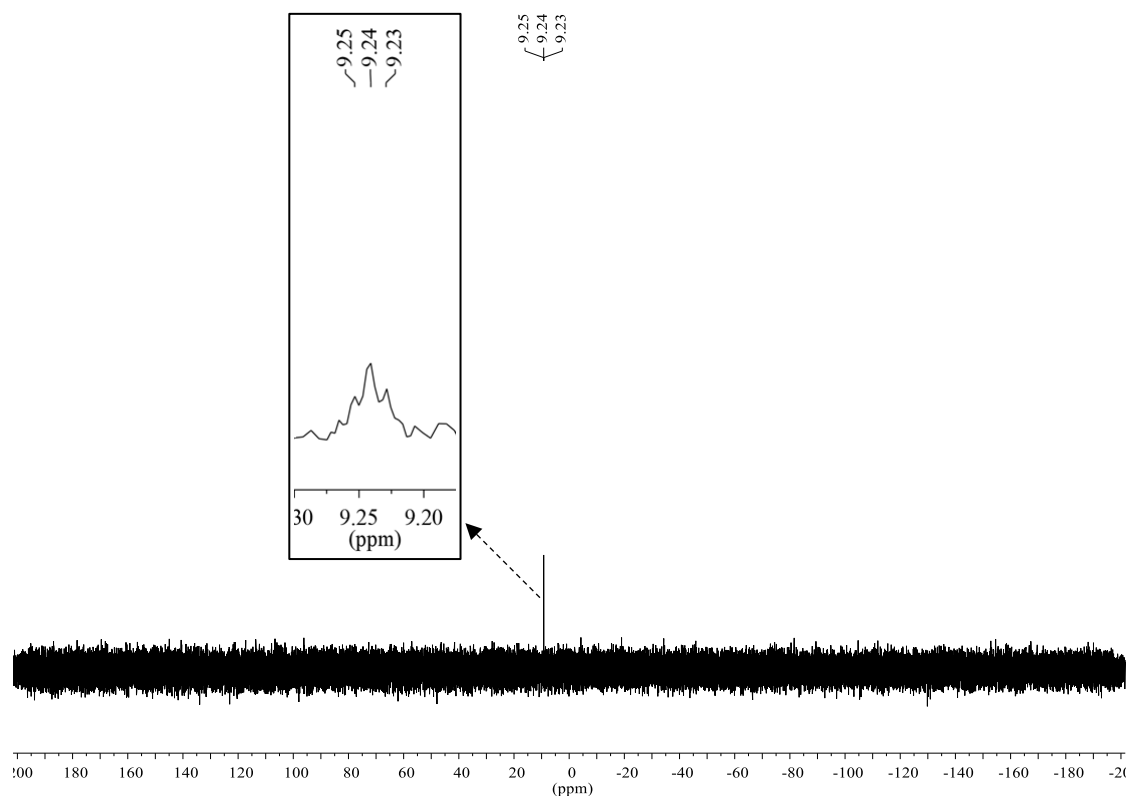
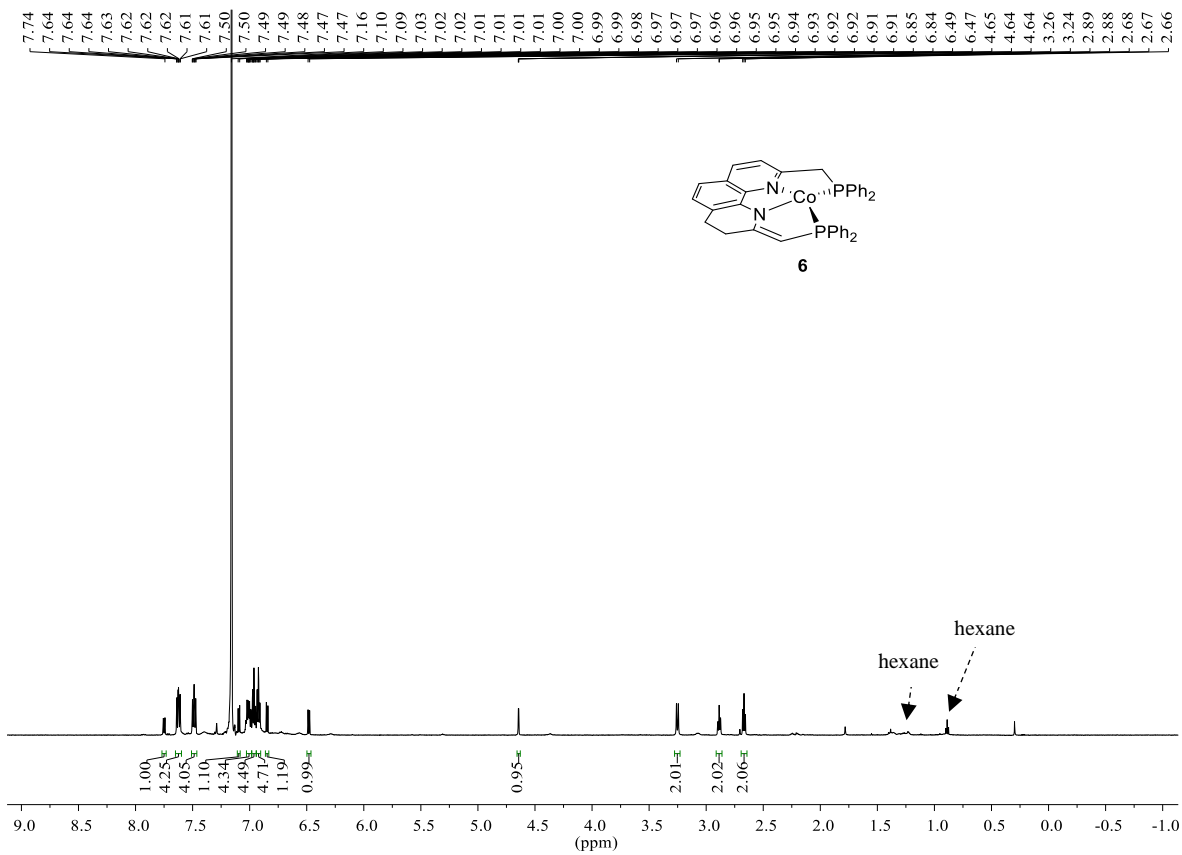


Figure S18. $^{29}\text{Si}\{^1\text{H}\}$ spectrum of **5** in C_6D_6 .

Reaction of **4** with H_2

A C_6D_6 solution (0.5 mL) of $[\text{Co}(\text{PNNP}^*)]$ (**4**) (4.1 mg, 0.0065 mmol) was charged in a J-Young NMR tube. H_2 (1 atm) was introduced to the NMR tube. The solution was kept at room temperature overnight. Full conversion of **4** and clean formation of **6** were confirmed by NMR analysis. The solution was concentrated to dryness under vacuum and washed with hexane to give **6** as a brown solid (2.2 mg, 0.0035 mmol, 53%). Single crystals of **6** was obtained by slow evaporation of saturated C_6H_6 solution of **6** at room temperature.

6: ^1H NMR (C_6D_6 , 25 °C) δ 7.74 (d, 1H, Phen-*H*, $^3J_{\text{HH}} = 8.3$ Hz), 7.62 (m, 4H, *PPh*₂), 7.49 (m, 4H, *PPh*₂), 7.10 (d, 1H, Phen-*H*, $^3J_{\text{HH}} = 7.9$ Hz), 7.00 (m, 2H \times 2, *PPh*₂), 6.96 (m, 4H, *PPh*₂), 6.92 (m, 4H, *PPh*₂), 6.84 (d, 1H, Phen-*H*, $^3J_{\text{HH}} = 7.9$ Hz), 6.48 (d, 1H, Phen-*H*, $^3J_{\text{HH}} = 8.3$ Hz), 4.64 (m, 1H, *PCH*), 3.25 (d, 2H, *PCH*₂, $^2J_{\text{PH}} = 9.4$ Hz), 2.89 (t, 2H, *CH*₂, $^3J_{\text{HH}} = 7.0$ Hz), 2.67 (t, 2H, *CH*₂, $^3J_{\text{HH}} = 7.2$ Hz). $^{13}\text{C}\{^1\text{H}\}$ NMR (C_6D_6 , 25 °C) δ 166.0, 155.7, 149.9, 143.0, 138.8, 137.1, 132.9, 132.8, 130.0, 128.6, 128.3* (\times 2), 128.2*, 127.9*, 119.6, 118.7, 110.5, 89.7, 49.4, 26.9, 25.5. One ipso-carbon was obscured due to low intensity. * signals were determined based on HSQC. HSQC (C_6D_6 , 25 °C) $\delta_{\text{H}}-\delta_{\text{C}}$ 7.00 (δ_{H}) - 128.2 (δ_{C}), 128.3 (δ_{H}) - 128.3 (δ_{C}); 6.96 (δ_{H}) - 128.3 (δ_{C}); 6.92 (δ_{H}) - 127.9 (δ_{C}). $^{31}\text{P}\{^1\text{H}\}$ NMR (C_6D_6 , 25 °C) δ 55.6 (br), 44.5 (br). Anal. Calcd for $\text{CoN}_2\text{P}_2\text{C}_{38}\text{H}_{31}$: C, 71.70; H, 4.91; N 4.40. Found: C, 72.13; H, 4.87; N, 4.28.



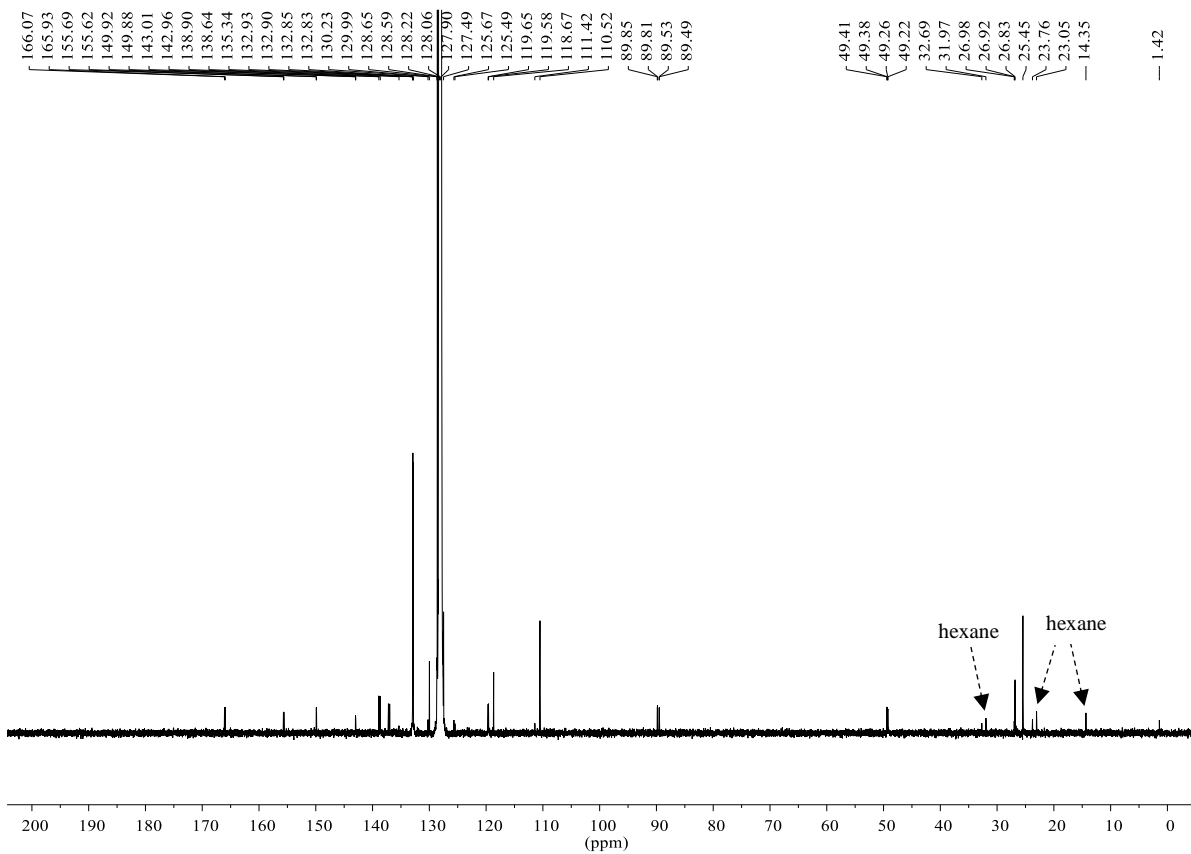


Figure S20. $^{13}\text{C}\{^1\text{H}\}$ spectrum of **6** in C_6D_6 .

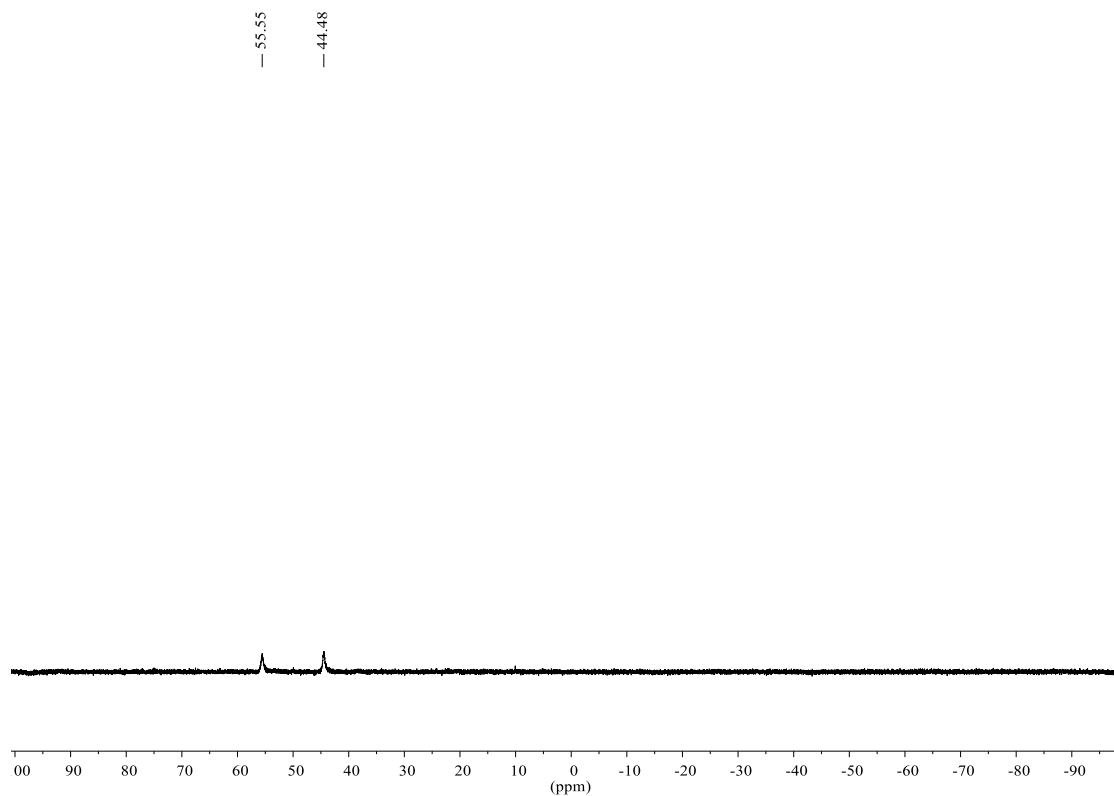


Figure S21. $^{31}\text{P}\{^1\text{H}\}$ spectrum of **6** in C_6D_6 .

X-ray Crystallographic Data

All single-crystal X-ray diffraction measurements of **1**, **4**, **5**, and **6** were performed under a cold nitrogen stream on a Rigaku XtaLAB P200 diffractometer with a Pilatus 200K detector using multi-layer mirror monochromated Mo-K α radiation ($\lambda = 0.71073 \text{ \AA}$, 50 kV/24 mA). The determination of crystal systems and unit cell parameters were performed with the CrystalClear program package. Data processing was performed with the CrystalClear program package or CrysAlisPro program package. All structures were solved by direct methods using SIR2014 program⁴, and refined by full-matrix least squares calculations on F_2 for all reflections (SHELXL-2014/7)⁵, using Yadokari-XG 2009 program⁶. The X-ray crystallographic data for **1**, **4**, **5**, and **6** have been deposited at the Cambridge Crystallographic Data Centre (CCDC) under deposition no. CCDC 2013566, 2013567, 2013568, 2013569. These data can be obtained free of charge from the CCDC (www.ccdc.cam.ac.uk/data_request/cif)

Table S1. Crystallographic parameters

	1	4	5	6
Empirical formula	$C_{38}H_{30}ClCoN_2P_2 \cdot CH_3CN$	$C_{38}H_{29}CoN_2P_2$	$C_{42}H_{39}CoN_2P_2Si$	$C_{38}H_{31}CoN_2P_2$
Formula weight	671.00	634.50	720.71	636.52
Temperature	93(2) K	93(2) K	93(2) K	93(2)
Crystal system	triclinic	monoclinic	monoclinic	orthorhombic
Space group	$P\bar{1}$	$P2_1/n$	$P2_1/c$	$P2_12_12_1$
$a/\text{\AA}$	10.996(5)	9.6072(16) \AA	15.4631(12) \AA	9.1277(13)
$b/\text{\AA}$	12.777(5)	17.588(3) \AA	12.4153(11) \AA	12.3182(18)
$c/\text{\AA}$	13.167(5)	17.717(3) \AA	18.8980(12) \AA	26.862(4)
α/deg	80.538(5) $^\circ$	90 $^\circ$	90 $^\circ$	90 $^\circ$
β/deg	72.079(5) $^\circ$	101.736(3) $^\circ$	103.596(8) $^\circ$	90 $^\circ$
γ/deg	71.390(5) $^\circ$	90 $^\circ$	90 $^\circ$	90 $^\circ$
Volume	1663.6(12) \AA^3	2931.1(9) \AA^3	3526.3(5) \AA^3	3020.3(8) \AA^3
Z	2	4	4	4
Density	1.421	1.438	1.358	1.400
Goodness-of-fit on F^2	1.142	1.073	1.038	0.843
Final R indices	$R1 = 0.0954,$	$R1 = 0.0279,$	$R1 = 0.0577,$	$R1 = 0.0488,$
$[I > 2\sigma(I)]$	$wR2 = 0.2659$	$wR2 = 0.0709$	$wR2 = 0.1107$	$wR2 = 0.1203$
R indices (all data)	$R1 = 0.1191,$ $wR2 = 0.2808$	$R1 = 0.0323,$ $wR2 = 0.0731$	$R1 = 0.1227,$ $wR2 = 0.1564$	$R1 = 0.0734,$ $wR2 = 0.1373$

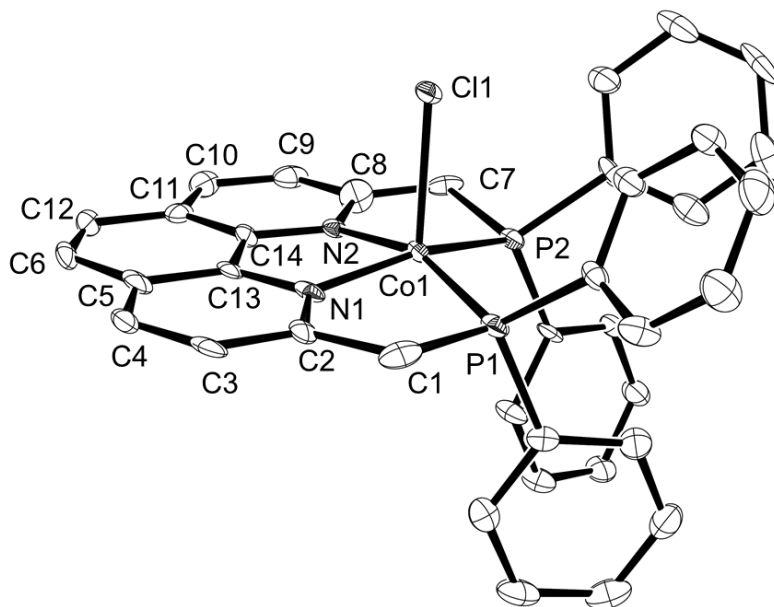


Figure S22. ORTEP drawing of **1** with 50% probability ellipsoids. Hydrogen atoms and CH₃CN molecule are omitted for clarity. Selected bond distances (Å) and angles (deg): Co1–P1, 2.164(2); Co1–P2, 2.164(2); Co1–N1, 1.907(5); Co1–N2, 1.901(5); P1–C1, 1.847(8); P2–C7, 1.856(7); C1–C2, 1.491(10); C2–C3, 1.405(10); C3–C4, 1.397(11); C4–C5, 1.404(12); C7–C8, 1.461(11); P1–Co1–P2, 104.79(8); P1–Co1–N1, 84.3(2); N1–Co1–N2, 82.4(3); N2–Co1–P2 83.79(19).

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