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Catalytic and mechanistic studies of a highly active and *E*-selective Co(II) PNN^{H} pincer catalyst system for transfer-semihydrogenation of internal alkynes

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Experimental Section

General considerations

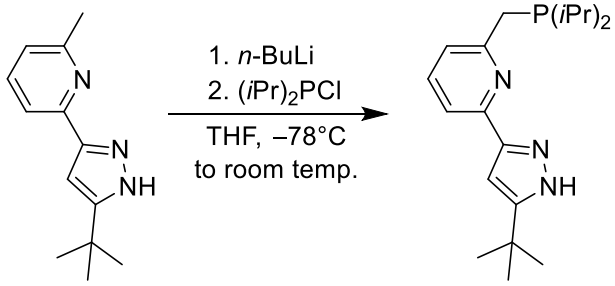
All experiments, unless otherwise stated, were performed under oxygen- and moisture-free conditions under an inert atmosphere of argon using standard Schlenk and glovebox techniques.

Methanol (99.8%, Extra Dry over Molecular Sieve, AcroSeal^{TM}), 2-Propanol (99.5%, Extra Dry over Molecular Sieve, AcroSeal^{TM}) were purchased from Acros Organics, transferred to a Schlenk flask and stored over molecular sieve (3 Å). Ammonia borane was purchased from Sigma-Aldrich and stored in the glovebox. 2-Methyl-6-[5(3)-(*tert*-butyl)-1*H*-pyrazol-3(5)-yl]pyridine and P$^{t\text{Bu}}$NNCoCl$_2$ complex **1a** were synthesised according to the literature.[1] Deuterated educts were synthesized according to literature.[2]

^{1}H, ^{11}B, ^{11}B{^{1}H}^{13}C{^{1}H} and ^{31}P{^{1}H} NMR spectra were recorded at room temperature on Bruker AV300, AV400 or Fourier300 spectrometers. All ^{1}H and ^{13}C NMR spectra were referenced using the chemical shifts of residual proton solvent resonances (CD_2Cl_2: δ_H 5.32 ppm, δ_C 53.84 ppm, $CDCl_3$: δ_H 7.26 ppm, δ_C 77.16 ppm, C_6D_6: 7.16 ppm).

Synthesis of ligands and precatalysts

*Synthesis of 2-(5-(tert-butyl)-1H-pyrazol-3-yl)-6-((diisopropylphosphaneyl)methyl)pyridine (**2**)*



At −78°C a solution of *n*-BuLi (2.5 eq., 2.1 mL, 2.5 M in hexane) were added dropwise over a period of 10 min to a solution of 2-methyl-6-pyrazolylpyridine (451 mg, 2.09 mmol) in THF (10 mL). A colour change to red was observed immediately. The reaction mixture was stirred overnight and slowly warmed to room temperature. A red precipitation formed overnight. Then the solution was cooled again to −78°C and ClP*i*Pr$_2$ (1.2 eq., 368 µL, 353 mg, 2.55 mmol) was slowly added. The mixture was stirred overnight and allowed to warm to room temperature. The reaction mixture was diluted with EtO_2 (15 mL). Then degassed water (5 mL) was added and the solution was stirred for 10 min. The organic layer was separated, and the solvent was removed in vacuum. The product was obtained as yellow oil (512 mg, 1.57 mmol, 75%). The purity of the crude product was high enough for metalation. Further purification steps failed due the high solubility. Two pyrazole H tautomers were observed. – ^{1}H NMR (400 MHz, $CDCl_3$): *δ*(isomer 1) 10.60 (br s, 1 H, NH), 7.27 (d, *J* = 7.1 Hz, 1H), 7.54−7.49 (m, 2H), 6.46 (s, 1H), 2.92 (br s, 2H, CH_2), 1.80−1.73 (m, 2H), 1.30 (s, 9H), 1.10−1.00 (m, 12H). *δ*(isomer 2) 9.82 (br s, 1 H, NH), 7.71 (*d*, *J* = 7.1 Hz, 1H), 7.12−7.09 (m, 2H), 6.57 (s, 1H)), 2.97 (d, *J* = 2.1 Hz, 2H, CH_2), 2.54−2.46 (m, 2H), 1.43 (s, 9H), 1.12−1.07 (m, 12H). ^{31}P NMR (400 MHz, $CDCl_3$): *δ*(isomer 1) 13.38; *δ*(isomer 2) 12.08. MS (ESI): *m*/*z* 332.37 (100) $[M+H]^+$. HRMS (ESI): Calcd. $C_{19}H_{30}N_3P$ $[M+H]^+$: *m*/*z* 332.2256. Found: 332.2256.

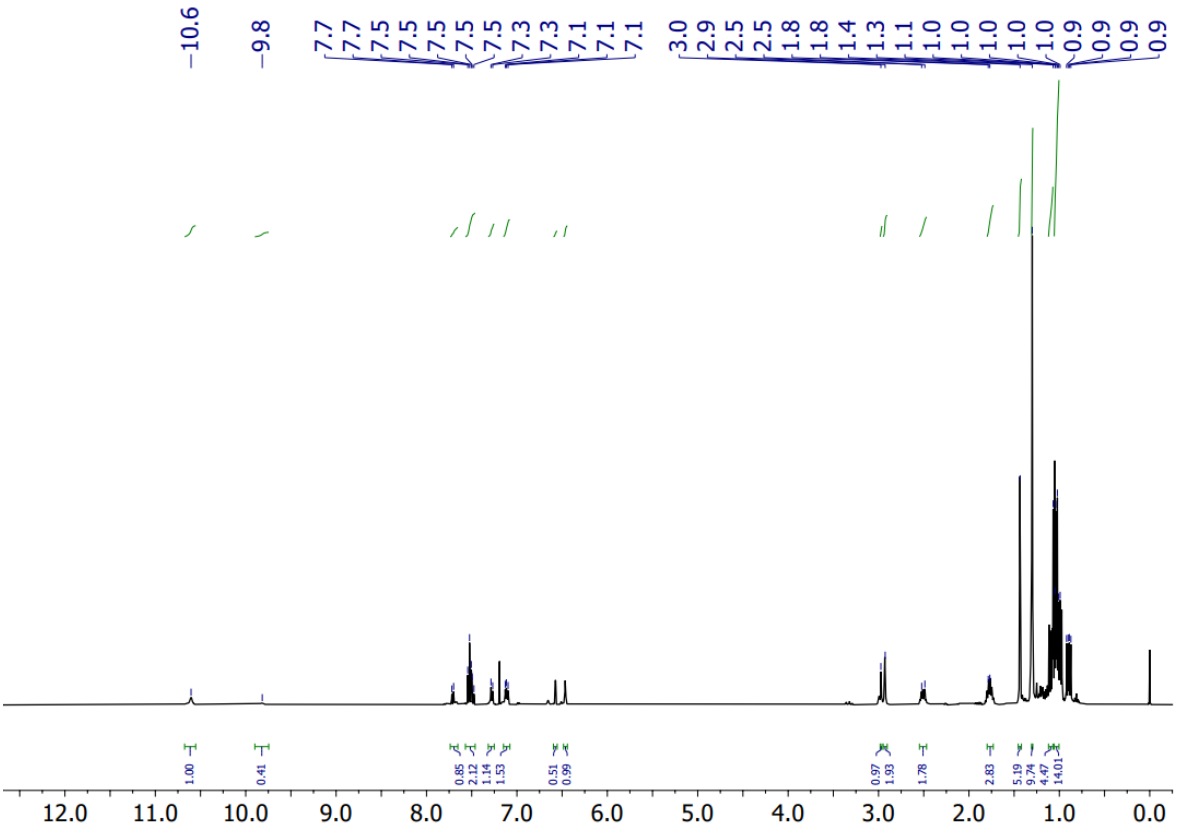


Figure S 1. ^{1}H NMR spectrum of **2** ($CDCl_3$, 25 °C).

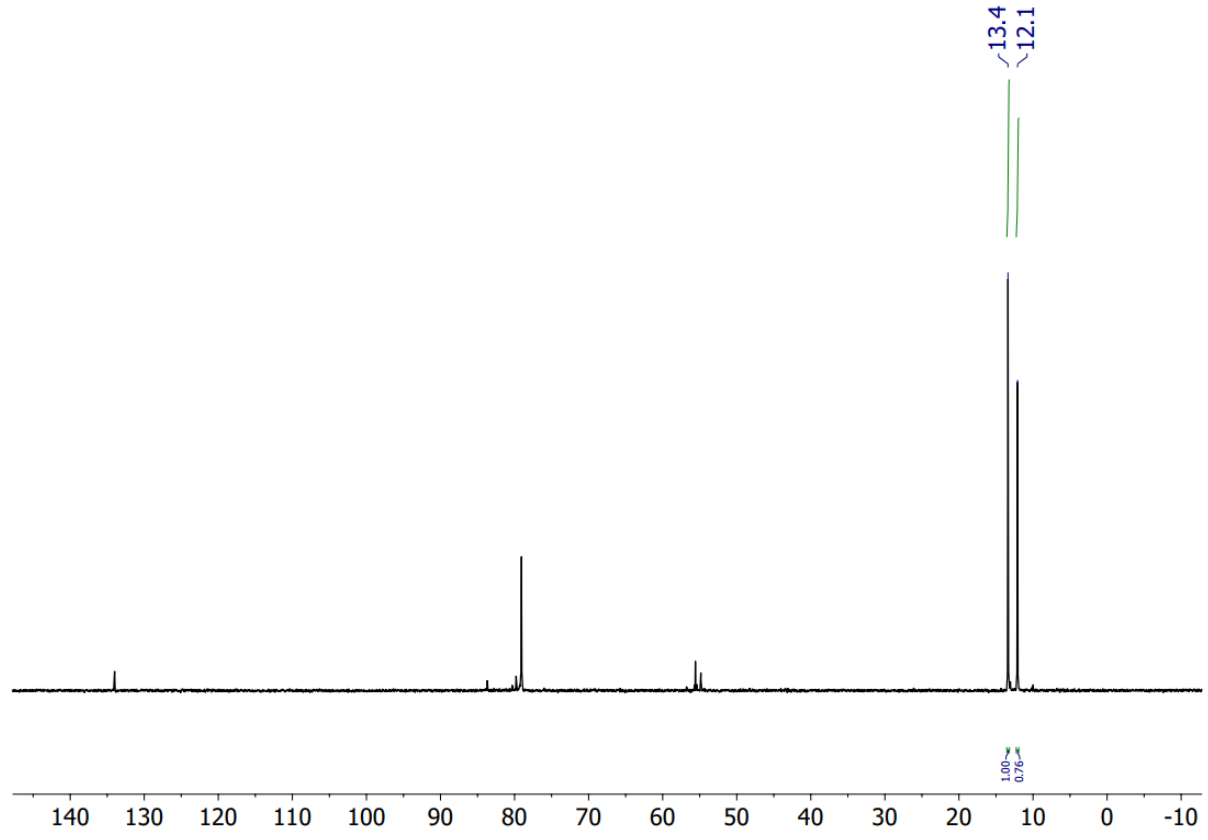
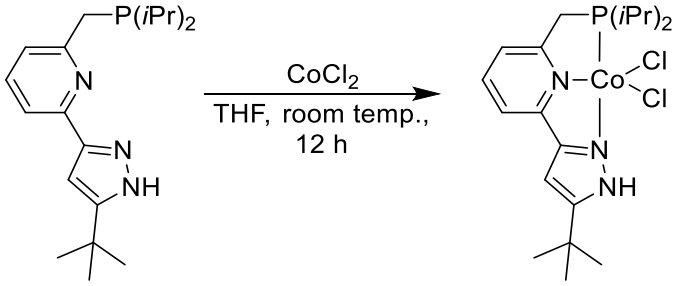


Figure S 2. ^{31}P-NMR spectrum of **2** ($CDCl_3$, 25 °C).

*$P^{iPr}NNCoCl_2$ (**1b**)*



To a suspension of $CoCl_2$ (43.1 mg, 332 µmol) in THF (15 mL) was added a solution of ligand **2** (110 mg, 332 µmol) in THF (5 mL). The reaction mixture was stirred for 12 h at room temperature. The solvent was removed in vacuum and the corresponding residue was extracted with benzene (3x10 mL) and filtered. The solvent was removed in vacuum to ≈ 1 mL and then pentane (20 mL) was added. The precipitation was filtered and washed withEt_2O (2x 10 mL) and pentane (2x 10 mL). The product was obtained as a green solid (97.3 mg, 258 µmol, 78%). – ^{1}H NMR (300 MHz, $CDCl_3$): δ 79.81 (br s, 2 H), 61.27 (br s, 1 H), 54.14 (br s, 1 H), 42.20 (br. s, 1 H), 18.33 (br s, 2 H), 4.86 (br s), −11.14 (br s). MS (ESI): *m/z* 332 [M-$CoCl_2$]$^+$, *m/z* 216 [$C_{13}H_{17}N_3$+H]$^+$.

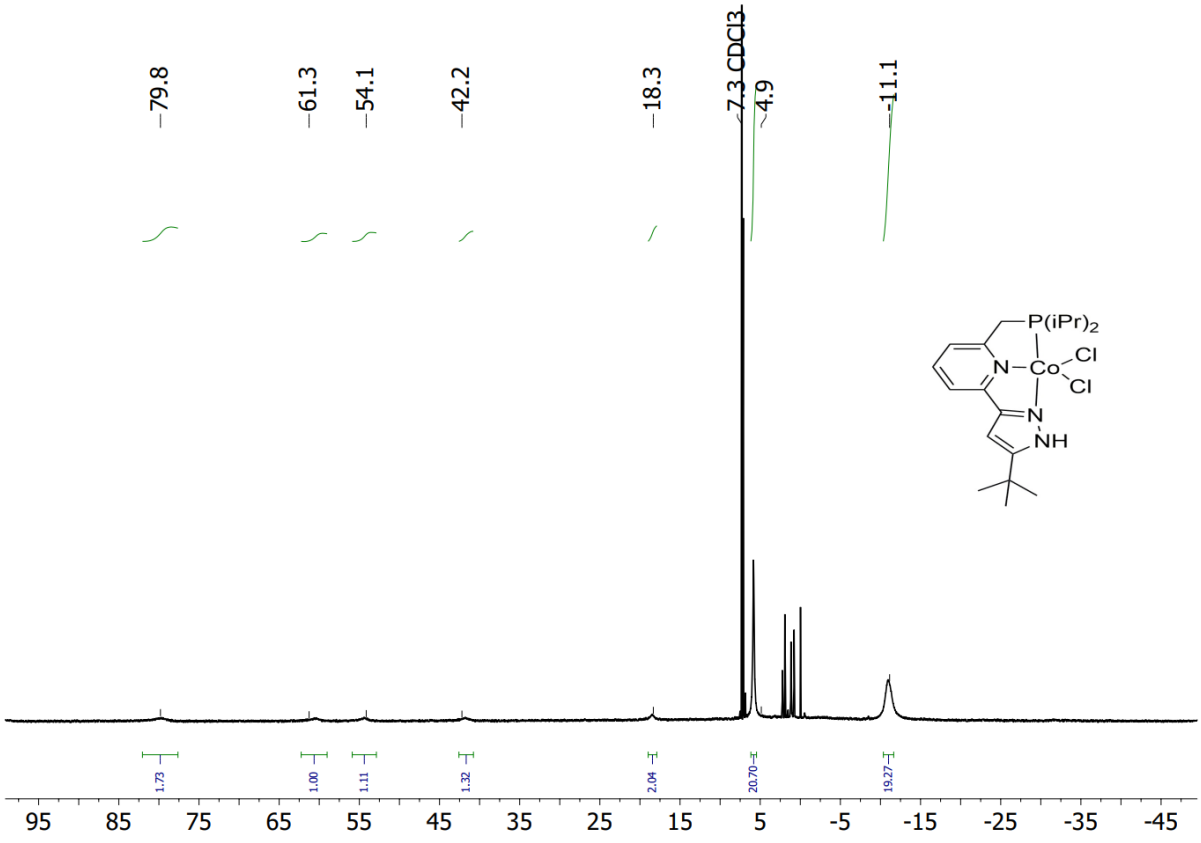
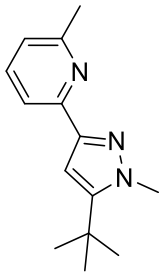


Figure S 3. ^{1}H NMR spectrum of **1b** ($CDCl_3$, 25 °C).



Synthesis of 2-(5-(tert-butyl)-1-methyl-1H-pyrazol-3-yl)-6-methylpyridine[3] ***(3)***

To a suspension of NaH (35.8 mg, 1.45 mmol, 1.25 eq.) in THF (10 mL) was added dropwise a solution of 2-methyl-6-pyrazolylpyridine (250 mg, 1.16 mmol) in THF (8 ml). Then, solid $[Me_3O][BF_4]$ (189 mg, 1.28 mmol, 1.1 eq.) was added in small portions at 0°C. After addition, the reaction mixture was stirred overnight and slowly warmed to room temperature. The reaction mixture was filtered, and the solvent was removed in vacuum. The residue was redissolved in CH_2Cl_2 (15 mL) and washed with H_2O (4x10 mL). The combined organic layers were dried over Na_2SO_4, filtered and the solvent was removed in vacuum. The compound was recrystallized from EtOAc, resulting in colorless needles of the product (221 mg, 964 µmol, 83%). – ^{1}H NMR (300 MHz, $CDCl_3$): δ = 7.70−7.62 (m, 1 H), 7.55 (t, J = 7.7 Hz, 1 H), 7.04−6.97 (m, 1 H), 6.62 (s, 1 H), 3.99 (s, 3 H), 2.52 (s, 3 H), 1.41 (s, 9 H). – ^{13}C NMR (75 MHz, CD_2Cl_2) δ = 157.88, 152.57, 152.01, 149.31, 136.47, 121.33, 116.30, 102.15, 53.84, 39.68, 31.20, 29.42, 24.32. El. Anal. for $C_{14}H_{19}N_3$ (229.33), calcd (%): C 73.32, H 8.35, N 18.32, found (%): C 73.36, H 8.83, N 18.00.– MS (ESI): *m/z* 230.28 (100) $[M+H]^+$.

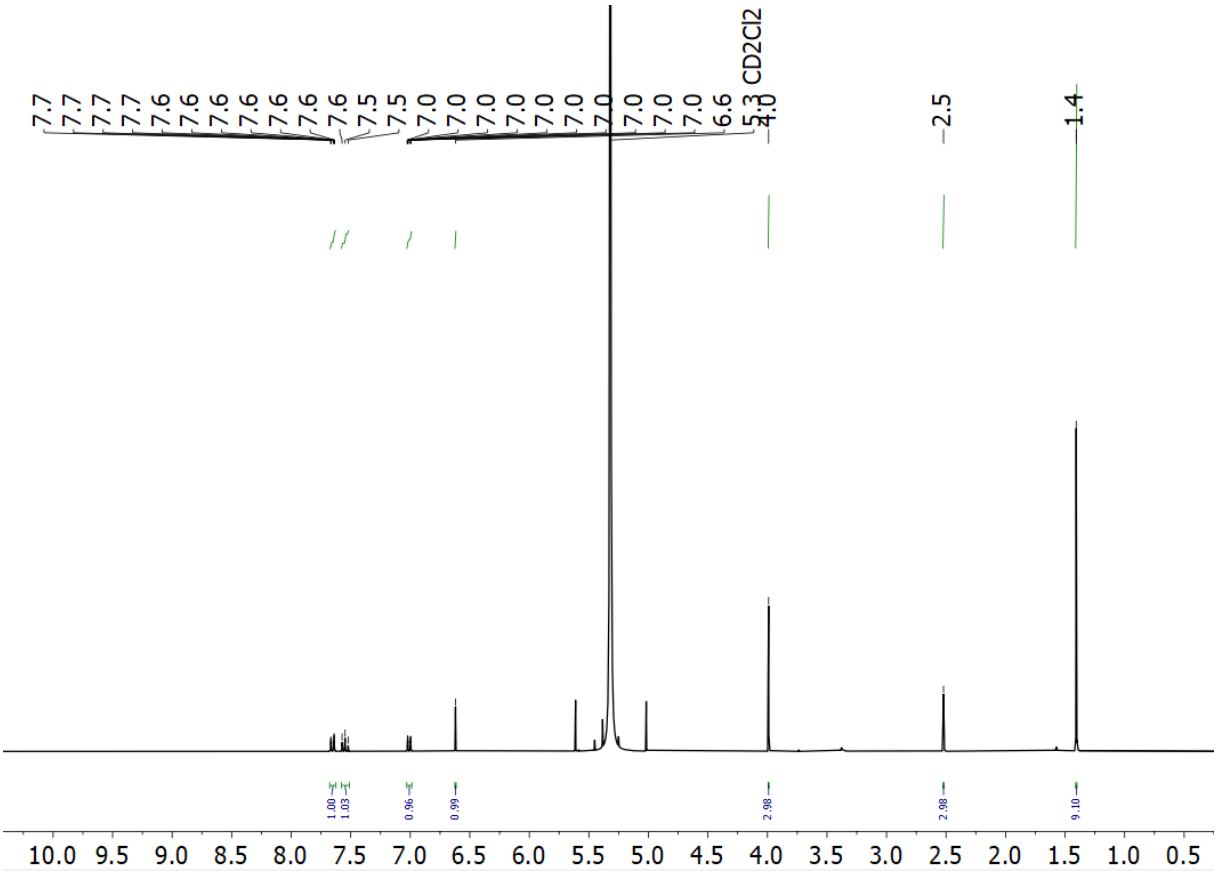


Figure S 4. ^{1}H NMR spectrum of **3** (CD_2Cl_2, 25 °C).

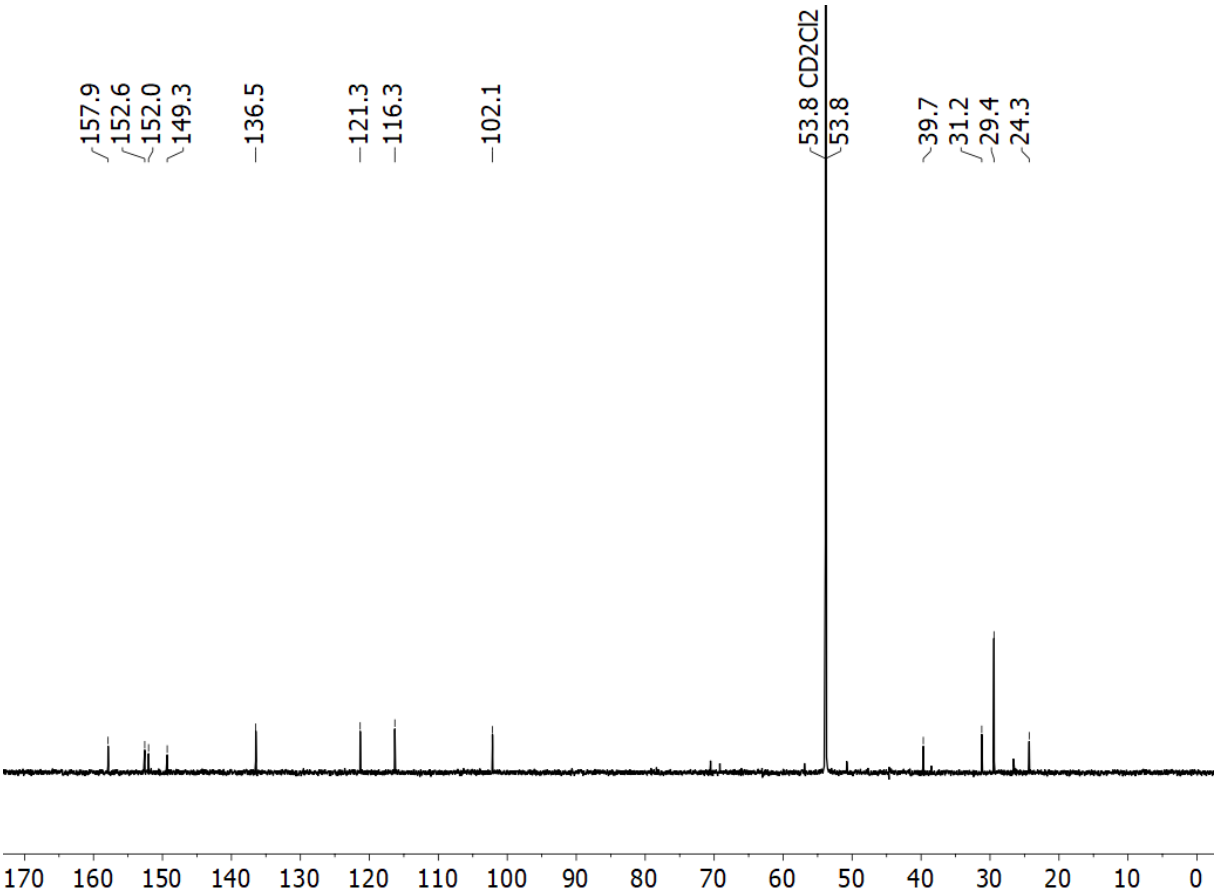
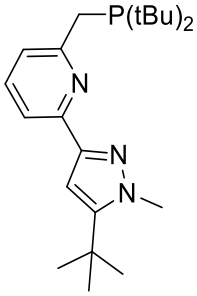


Figure S 5. ^{13}C NMR spectrum of **3** (CD_2Cl_2, 25 °C).



*Synthesis of 2-(5-(tert-butyl)-1-methyl-1H-pyrazol-3-yl)-6-((di-tert-butylphosphaneyl)methyl)pyridine (**4**)*

At −78°C a solution of *n*-BuLi (1.10 eq., 191 µL, 2.5 M in hexane) was added dropwise to a solution 2-(5-(tert-butyl)-1-methyl-1H-pyrazol-3-yl)-6-methylpyridine (99.7 mg, 435 µmol) in THF (10 mL) over a period of 10 min. A colour change to purple was observed immediately. The reaction mixture was stirred overnight and slowly warmed to room temperature. Then the solution was cooled again to −78°C and Cl*P*t*Bu*$_2$ (1.10 eq., 90.1 µL, 86.4 mg, 478 µmol) was slowly added. The mixture was stirred overnight and allowed to warm to room temperature. The reaction mixture was diluted with Et_2O (15 mL). Then degassed water (5 mL) was added and the solution was stirred for 10 min. The organic layer was separated, and the solvent was removed in vacuum. The product was obtained as yellow oil (132.4 mg, 354 µmol, 82%). The purity of the crude product was high enough for subsequent metalation. Further purification steps failed due the high solubility. – ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.67–7.58 (m, 1 H), 7.56 (t, *J* = 7.6 Hz, 1 H), 7.32–7.23 (m, 1 H), 6.62 (s, 1 H), 4.00 (s, 3 H), 3.06 (d, *J* = 3.1 Hz, 2 H), 1.42 (s, 9 H), 1.18 (s, 9 H), 1.14 (s, 9 H). ^{31}P NMR (400 MHz, CD_2Cl_2): δ = 35.9 (s). MS (ESI): *m*/*z* 374.49 (100) $[M+H]^+$. HRMS (ESI): Calcd. $C_{22}H_{36}N_3P$ $[M+H]^+$: *m*/*z* 374.2725. Found: 374.2732.

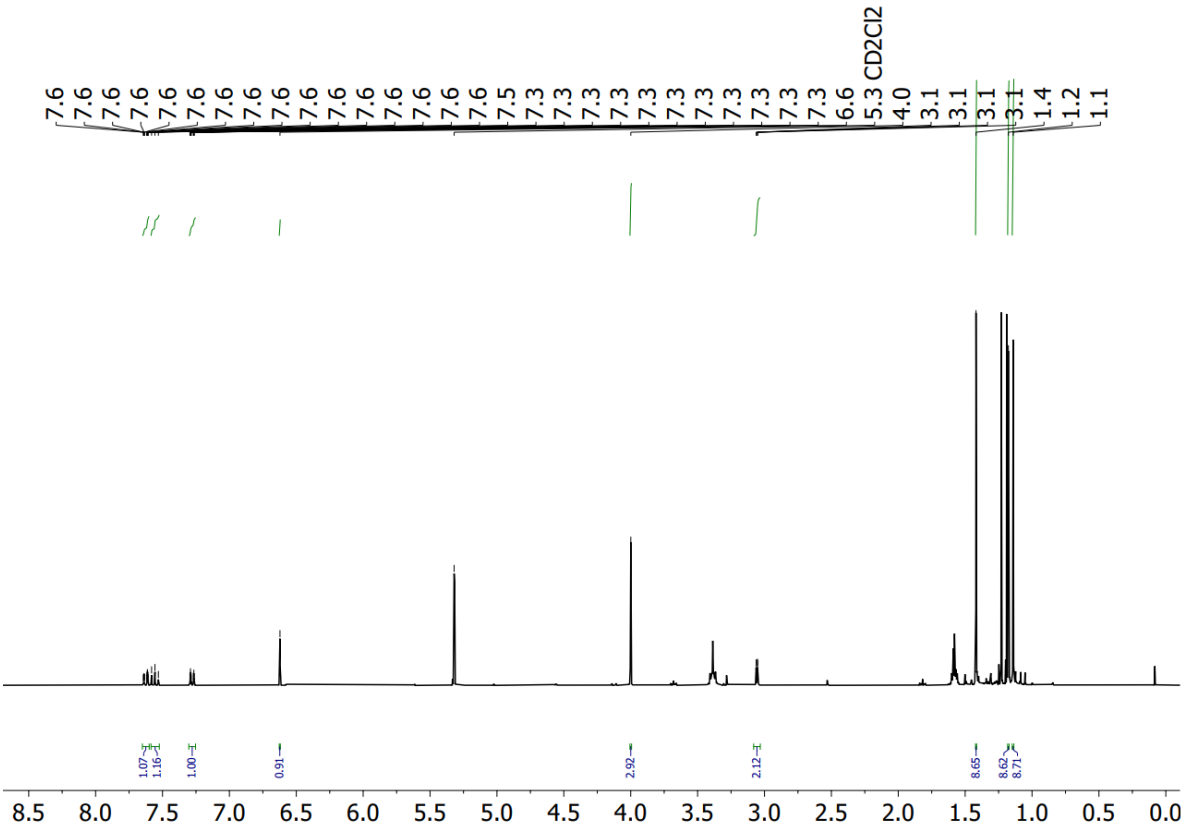


Figure S 6. ^{1}H NMR spectrum of **4** (CD_2Cl_2, 25 °C).

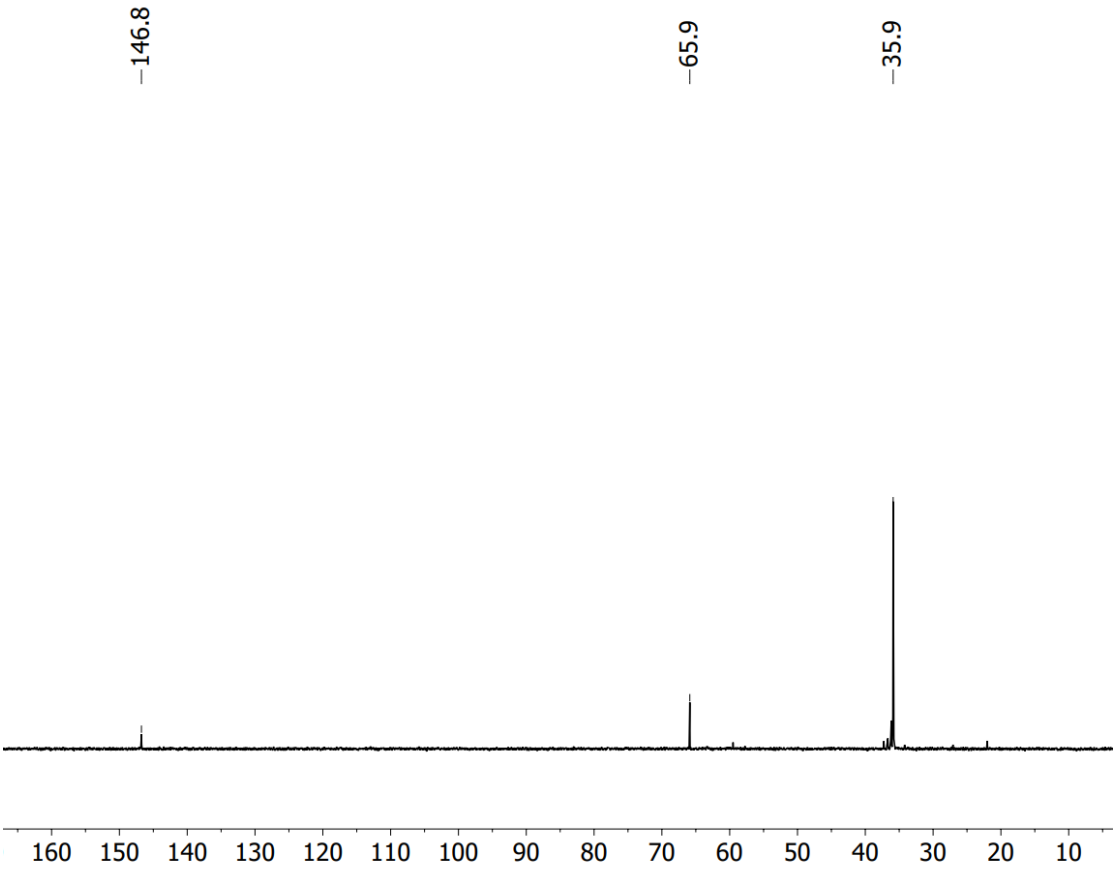
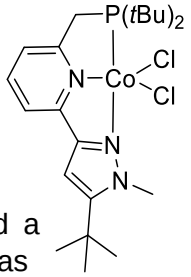


Figure S 7. ^{31}P NMR spectrum of **4** (CD_2Cl_2, 25 °C).

*$P^{tBu}NN^{Me}CoCl_2$ (**1a-Me**)*



To a suspension of $CoCl_2$ (29.6 mg, 228 µmol) in THF (10 mL) was added a solution of ligand **4** (85 mg, 228 µmol) in THF (5 mL). The reaction mixture was stirred for 12 h at room temperature. A colour change to turquoise-blue was observed. The solvent was removed in vacuum and the corresponding residue was extracted with benzene (3x10 mL) and filtered. The solvent was removed in vacuum and the residue was washed with pentane (3x10 mL). After removing of the solvent, the product was obtained as dark blue solid (94.5 mg, 188 µmol, 83%). – ^{1}H NMR (400 MHz, C_6D_6): δ = 66.34 (s, 1 H), 61.40 (s, 2 H), 57.61 (s, 1 H), 24.58 (s, 1 H), 5.38 (s, 2 H), -11.65 (s, 18 H), -12.82 (br s), −42.06 (s, 3 H). MS (ESI): *m*/*z* 374 $[M\text{-}CoCl_2]^+$, *m*/*z* 216 $[C_{14}H_{19}N_3+H]^+$.

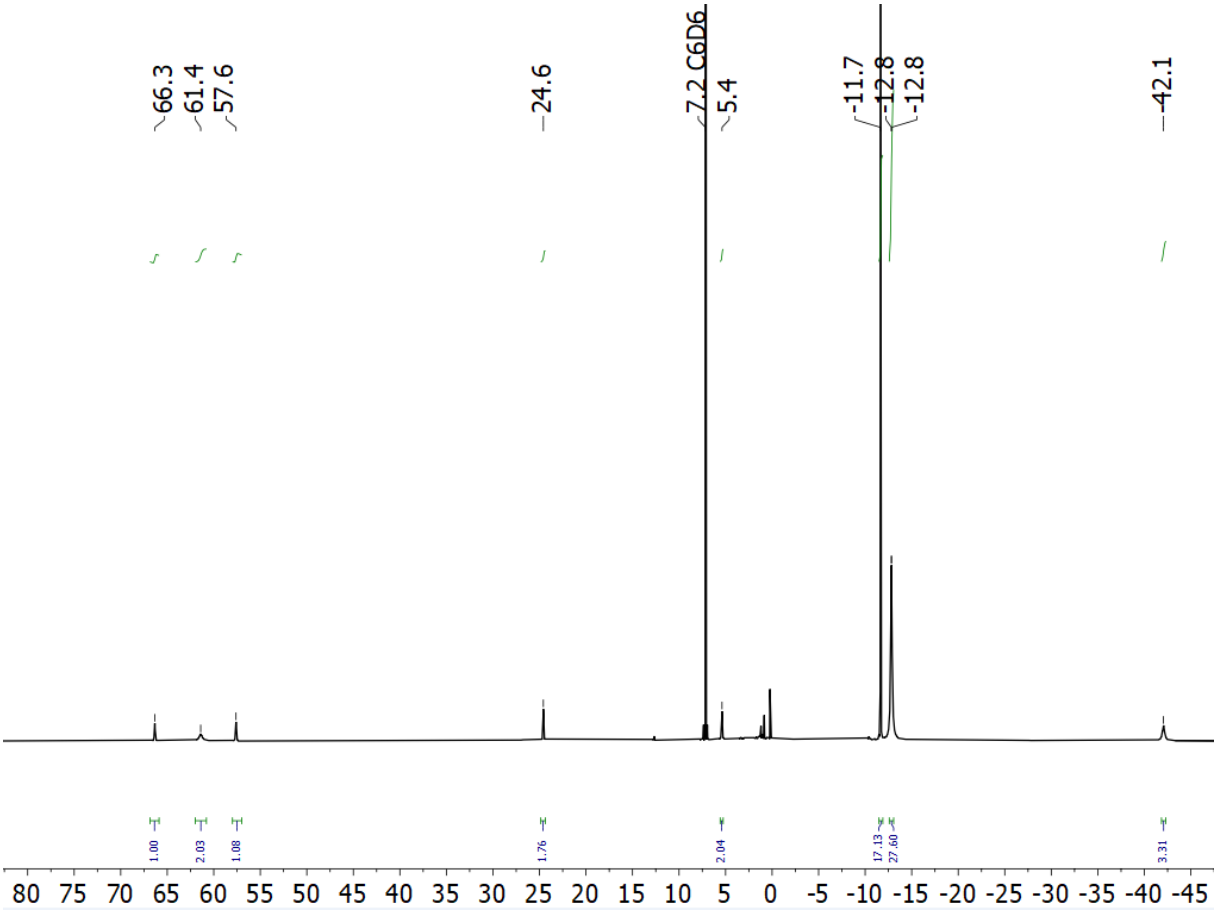
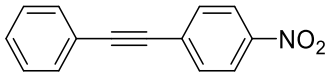


Figure S 8. ^{1}H NMR spectrum of **1a-Me** (C_6D_6, 25 °C).

Synthesis of alkynes[4]

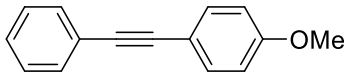
General procedure (GP1)

The corresponding aryl iodide (1 eq.), phenylacetylene (1 eq.), $Pd(PPh_3)_2Cl_2$ (1 mol%), PPh_3 (1 mol%) and CuI (1 mol%) were stirred together over night in THF and NEt_3 under an atmosphere of Ar. Afterwards H_2O (15 mL) were added and the reaction mixture was extracted with EtOAc (3 x 15 mL). The combined organic phases were washed with brine (3 x 10 mL) and dried over Na_2SO_4, filtered and the solvent was removed under reduced pressure. The residue was then purified by column chromatography.



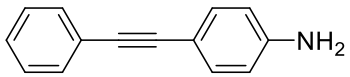
1-nitro-4-(phenylethynyl)benzene

According to GP 1, 1-iodo-4-nitrobenzene (1.22 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by column chromatography (SiO_2; eluent: hexane/EtOAc 10/1, R_f =0.26) the product was obtained as yellow solid (625 mg, 2.80 mmol, 57%). mp.: 118−120 °C (lit.: 120−122 °C[5]). – ^{1}H NMR (300 MHz, $CDCl_3$): δ 8:22 (d, *J* = 9.0 Hz, 2 H, Ar-H), 7.67 (d, *J* = 9.0 Hz, 2 H, Ar-H), 7.60−7.52 (m, 2 H, Ar-H), 7.44−7.34 (m, 3 H, Ar-H).



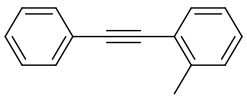
1-methoxy-4-(phenylethynyl)benzene

According to GP 1, 1-iodo-4-methoxybenzene (1.15 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by column chromatography (SiO_2; eluent: hexane/EtOAc 10/1, R_f = 0.38) the product was obtained as white solid (754 mg, 3.62 mmol, 74%). − mp.: 56−58 °C (lit.: 57−59 °C[6]). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.55−7.45 (m, 4 H, Ar-H), 7.40−7.32 (m, 3 H, Ar-H), 6.90 (d, *J* = 9.0 Hz, 2 H, Ar-H), 3.82 (s, 3 H, OCH_3).



4-(phenylethynyl)aniline

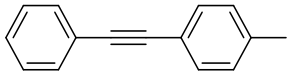
According to GP 1, 4-iodoaniline (1.15 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by column chromatography (SiO_2; eluent: pentane/EtOAc 4/1, R_f = 0.42) the product was obtained as brown solid (736 mg, 3.81 mmol, 78%). − mp.: 125−127 °C (dec.). (lit.: 126−128 °C[7]). – ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56–7.47 (m, 2 H, Ar-H), 7.38–7.28 (m, 5 H, Ar-H), 6.64 (d, *J* = 8.7 Hz, 2 H, Ar-H), 3.81 (s, 2 H, NH_2).



1-methyl-2-(phenylethynyl)benzene

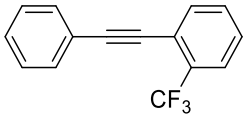
According to GP 1, 1-iodo-2-methylbenzene (1.07 g, 4.90 mmol, 626 µL), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work

up by vacuum distillation (bp.: 84 °C, 1.0 µbar) the product was obtained as colorless liquid (714 mg, 3.72 mmol, 76%). – ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.56−7.43 (m, 3 H, Ar-H), 7.37−7.25 (m, 3 H, Ar-H), 7.23−7.09 (m, 3 H, Ar-H), 2.54 (s, 3 H, CH_3).



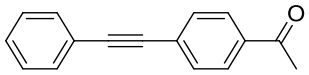
1-methyl-4-(phenylethynyl)benzene

According to GP 1, 1-iodo-4-methylbenzene (1.07 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by column chromatography (SiO_2; eluent: pentane/CH_2Cl_2 6/4, R_f = 0.30) the product was obtained as pale yellow solid (825 mg, 4.29 mmol, 87%). − mp.: 68–71 °C (dec.). (lit.: 70−72 °C[8]). – ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.61–7.50 (m, 2 H, Ar-H), 7.44 (d, *J* = 8.1 Hz, 2 H, Ar-H), 7.39−7.30 (m, 3 H, Ar-H), 7.17 (d, *J* = 7.9 Hz, 2 H, Ar-H), 2.38 (s, 3 H, CH_3).



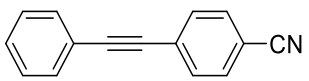
1-(phenylethynyl)-2-(trifluoromethyl)benzene

According to GP 1, 1-iodo-2-(trifluoromethyl)benzene (686 µL, 1.33 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by column chromatography (SiO_2; eluent: pentane, R_f = 0.91) the product was obtained as colorless liquid (1.06 g, 4.30 mmol, 88%). – ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74–7.66 (m, 2 H, Ar-H), 7.61−7.56 (m, 2 H, Ar-H), 7.56−7.49 (m, 1 H, Ar-H), 7.46−7.41 (m, 1 H, Ar-H), 7.41−7.35 (m, 3 H, Ar-H).



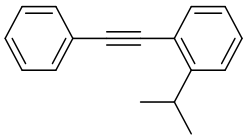
1-(4-(phenylethynyl)phenyl)ethan-1-one

According to GP 1, 1-(4-iodophenyl)ethan-1-one (1.21 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by column chromatography (SiO_2; eluent: hexane/CH_2Cl_2 6/4, R_f = 0.56) the product was obtained as off white solid (965 mg, 4.39 mmol, 89%). − mp.: 94−96 °C. (lit.: 95−97 °C[9]). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.94 (d, *J* = 8.7 Hz, 2 H, Ar-H), 7.63 (d, *J* = 8.7 Hz, 2 H, Ar-H), 7.60−7.53 (m, 2 H, Ar-H), 7.44−7.33 (m, 3 H, Ar-H), 2.59 (s, 3 H, CH_3).



4-(phenylethynyl)benzonitrile

According to GP 1, 4-iodobenzonitrile (1.12 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by column chromatography (SiO_2; eluent: hexane/CH_2Cl_2 6/4, R_f = 0.56) the product was obtained as white solid (901 mg, 4.44 mmol, 91%). − mp.: 104−106 °C. (lit.: 103−105 °C[10]). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.71−7.60 (m, 4 H, Ar-H), 7.59−7.52 (m, 2 H, Ar-H), 7.45−7.36 (m, 3 H, Ar-H).



1-isopropyl-2-(phenylethynyl)benzene

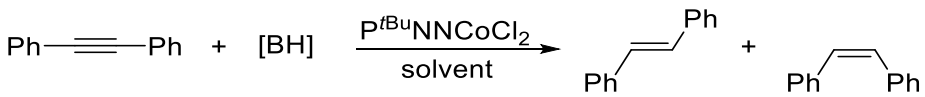
According to GP 1, 1-iodo-2-isopropylbenzene (763 µL, 1.21 g, 4.90 mmol), $Pd(PPh_3)_2Cl_2$ (34.4 mg, 1 mol%), PPh_3 (12.8 mg, 1 mol%) and CuI (9.32 mg, 1 mol%) made to react with phenylacetylene (500 mg, 4.90 mmol, 538 µL) in THF (10 mL) and NEt_3 (10 mL). After work up and purification by vacuum distillation the product was obtained as colorless liquid (757 mg, 3.44 mmol, 70%). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.74−7.49 (m, 3 H, Ar-H), 7.45−7.30 (m, 5 H, Ar-H), 7.28−7.08 (m, 1 H, Ar-H), 3.58 (hept, *J* = 6.9 Hz 1 H, C-H), 1.33 (d, *J* = 6.9 Hz, 6 H, CH_3).

General protocol for the transfer semihydrogenation of alkynes

General procedure (GP 2)

Under an atmosphere of argon, cobalt complex **1a** or **1b** (1−0.01 mol%), ammonia borane (15.4 mg, 0.50 mmol), diphenylacetylene (89.1 mg, 0.50 mmol) and alcohol (2 mL) were added sequentially to a preheated Schlenk tube equipped with a magnetic stir bar. The reaction mixture was stirred for 1−118 h at room temperature or 50 °C. Subsequently the reaction mixture was exposed to air and CH_2Cl_2 (5 mL) was added. An aliquot of this solution was analysed by gas chromatography with biphenyl as the internal standard.

Table S 1. Influence of the catalyst loading, solvents, and boron source on the transfer hydrogenation.



entry	[BH]	*c*(catalyst) / mol%	solvent	time / h	Conversion / %	*E*-yield / %	*Z*-yield / %
1	$H_3B{\cdot}NH_3$	1	MeOH	0.5	≥ 95	100	−
2[a]	$H_3B{\cdot}NH_3$	0.5	MeOH	0.5	≥ 95	100	−
3	$H_3B{\cdot}NH_3$	0.1	MeOH	0.5	≥ 95	99	1
4	$H_3B{\cdot}NH_3$	0.01	MeOH	12	65	32	68
5[a]	$H_3B{\cdot}NH_3$	1	EtOH	0.5	≥ 95	99	1
6	$H_3B{\cdot}NH_3$	1	*i*-PrOH	1	≥ 95	38	62
7	$H_3B{\cdot}NH_3$	1	*i*-PrOH	2	≥ 95	99	1
8	$H_3B{\cdot}NMeH_2$	1	MeOH	0.5	≥ 95	100	−
9	$H_3B{\cdot}NMe_2H$	1	MeOH	1.25	≥ 95	100	−
10	$H_3B{\cdot}THF$	1	MeOH	19	≤ 5	38	62
11	$H_3B{\cdot}NH_3$	1	MeOH/H_2O	2	≤ 5	90	10
12	$H_3B{\cdot}NH_3$	1	H_2O	2	12	46	54

Reaction conditions: Diphenylacetylene (0.50 mmol), [BH] (0.50 mmol), *V*(solvent) = 2.0 mL, *T* = room temperature, Yields were determined by GC-Analysis using biphenyl as the internal standard. [a]*T* = 50 °C.

Characterisation data for alkene products

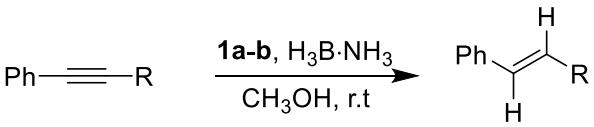
General procedure (GP3)

Under an atmosphere of argon, cobalt complex **1a** or **1b** (1 mol%), ammonia borane (15.4 mg, 0.50 mmol), alkyne (0.50 mmol) and MeOH (2 mL) were added sequentially to a preheated Schlenk tube equipped with a magnetic stir bar. The reaction mixture was stirred for 0.5−40 h at room temperature. Subsequently the reaction mixture was exposed to air and CH_2Cl_2 (5 mL) were added. An aliquot part of this solution was analyzed by gas chromatography.

Note: Liquid substrates were dissolved in MeOH (2 mL) before the addition to the reaction mixture.

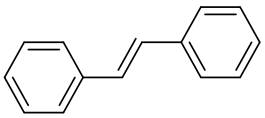
Substrate scope

Table S 2. Substrate scope.



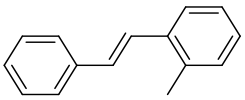
		1a			1b		
entry	***R***	**time/h**	**Conv./%**	***E/Z***	**time/h**	**Conv./%**	***E/Z***
1	-C_6H_5	0.5	≥ 95	100/0	1	≥ 95	100/0
2	2-CH_3-C_6H_4-	0.5	≥ 95	99/1	0.5	≥ 95	100/0
3	4-CH_3-C_6H_4	0.5	≥ 95	100/0	1	≥ 95	100/0
4	*2-i*-Pr-C_6H_4	0.5	≥ 95	95/5	0.5	≥ 95	99/1
5	4-OMe-C_6H_4	0.5	≥ 95	100/0	1.5	81	100/0
6	4-NH_2-C_6H_4	0.5	≥ 95	100/0	1.5	≥ 95	100/0
7[a]	4-C(O)CH_3-C_6H_4	0.5	≥ 95	[b]	0.5	80	[b]
8[a]	4-NO_2-C_6H_4	1	≥ 95	crude mixture (35%)[c]	1	39	crude mixture (2%)[c]
9[a]	4-CN-C_6H_4	1	≥ 95	100/0 (90%)[c]	1	79	25/75 (2%)[c]
10	2-CF_3-C_6H_4	1	≥ 95	99/1	6	≥ 95	97/3
11	CH_3	1	≥ 95	97/3 (3%)[c]	1.5	≥ 95	97/3 (6%)[c]

Reaction conditions: Alkyne (0.50 mmol), $H_3B{\cdot}NH_3$ (0.50 mmol), *V*(MeOH) = 2.0 mL, Yields were determined by GC-Analysis. [a] Formation of the alkane product was observed. [b] In these cases, the reactions were not chemoselective for the alkyne reduction, producing a mixture of several products, containing the alcohol-alkene, the acyl-alkene, as well as the acyl-alkane (Figure S24). The exact composition of these mixtures could not be determined by GC-MS. [c] Yield of the alkane product.



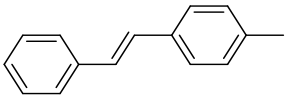
(*E*)-1,2-diphenylethene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 1,2-diphenylethyne (89.1 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as white solid (79 mg, 0.44 mmol, 88%). ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.59−7.46 (m, 4 H), 7.43−7.31 (m, 4 H), 7.30−7.22 (m, 2 H), 7.12 (s, 2 H).



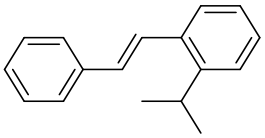
(*E*)-1-methyl-2-styrylbenzene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 1-methyl-2-(phenylethynyl)benzene (96.1 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as colourless liquid (87 mg, 0.45 mmol, 90%). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.67 (d, *J* = 6.3 Hz, 1 H), 7.61 (d, *J* = 8.1 Hz, 2 H), 7.49−7.39 (m, 3 H), 7.37−7.22 (m, 4 H), 7.09 (d, *J* = 16.2 Hz, 1 H), 2.50 (s, 3 H).



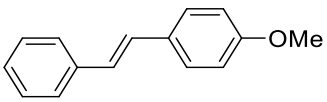
(*E*)-1-methyl-4-styrylbenzene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 1-methyl-4-(phenylethynyl)benzene (96.1 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as yellow solid (80 mg, 0.41 mmol, 82%). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.55−7.49 (m, 2 H), 7.43 (d, *J* = 8.2 Hz, 2 H), 7.40−7.31 (m, 2 H), 7.30−7.21 (m, 1 H), 7.18 (d, *J* = 7.8 Hz, 2 H), 7.10 (d, *J* = 1.4 Hz, 2 H), 2.36 (s, 3 H, CH_3).



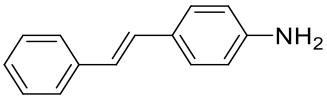
(*E*)-1-isopropyl-2-styrylbenzene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 1-isopropyl-2-(phenylethynyl)benzene (120 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as colorless liquid (93 mg, 0.42 mmol, 84%). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.76−7.49 (m, 4 H), 7.49−7.19 (m, 6 H), 7.03 (d, *J* = 16.0 Hz, 1 H), 3.43 (hept, *J* = 6.8 Hz, 1 H), 1.33 (d, *J* = 6.9 Hz, 6 H).



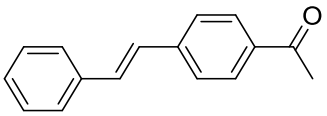
(*E*)-1-methoxy-4-styrylbenzene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 1-methoxy-4-(phenylethynyl)benzene (104 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as off white solid (72 mg, 0.34 mmol, 68%). – ^{1}H NMR (400 MHz, CD_2Cl_2): δ 7.51−7.43 (m, 4 H), 7.35 (t, *J* = 7.6 Hz, 2 H), 7.29−7.18 (m, 1 H), 7.09 (d, *J* = 16.4 Hz, 1 H), 6.99 (d, *J* = 16.3 Hz, 1 H), 6.91 (d, *J* = 8.8 Hz, 2 H), 3.81 (s, 3 H).



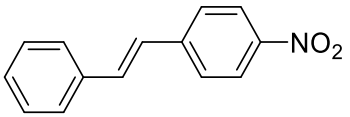
(*E*)-4-styrylaniline

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (89.1 mg, 0.50 mmol) made to react with 4-(phenylethynyl)aniline (96.6 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as yellow solid (82 mg, 0.42 mmol, 84%). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.48 (d, *J* = 7.2 Hz, 2 H), 7.42−7.29 (m, 4 H), 7.25−7.15 (m, 1 H), 7.04 (d, *J* = 16.3 Hz, 1 H), 6.92 (d, *J* = 16.3 Hz, 1 H), 6.67 (d, *J* = 8.5 Hz, 2 H), 3.79 (br. s, 2 H).



(*E*)-1-(4-styrylphenyl)ethan-1-one

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 1-(4-(phenylethynyl)phenyl)ethan-1-one (110 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as off white solid, including several hydrogenation products (see figure S 24) as impurities (107 mg). – GC/MS: *m*/*z* 195, 225, 227.

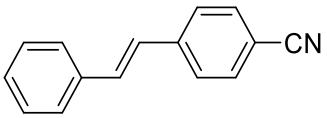


(*E*)-1-nitro-4-styrylbenzene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (89.1 mg, 0.50 mmol) made to react with 1-nitro-4-(phenylethynyl)benzene (111 mg, 0.50 mmol) in MeOH (2 mL). The reaction mixture contains further hydrogenation products. – GC/MS: m/z 195, 205, 225, 227.

In case of precatalyst 1a: Overreduction to the corresponding alkane (30−35%) was observed. The educt decomposed in several runs after the addition of MeOH. **Caution**: Evolution of nitrous gases was observed!

In case of precatalyst 1b: The product was obtained as brown oil (87 mg), containing the (*E*)*/(Z)*-isomer and the full hydrogenation product 1-nitro-4-phenethylbenzene (3−8%).



(*E*)-4-styrylbenzonitrile

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 4-(phenylethynyl)benzonitrile (102.6 mg, 0.50 mmol) in MeOH (2 mL).

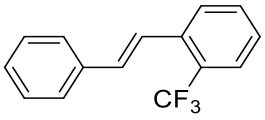
In case of precatalyst 1a: Overreduction to the corresponding alkane was observed (see Figure S 26).

Table S 3. Results of the TSH with **1a** and *p*-CN-$C_6H_4C{\equiv}CPh$.

entry	time / h	Conv. / %	*E*/*Z*	Yield alkane / %
1	0.5	≥ 95	100/0	78
2	0.5	≥ 95	100/0	88
3	1	≥ 95	100/0	90
4	1	≥ 95	100/0	85
5	0.5	≥ 95	100/0	78

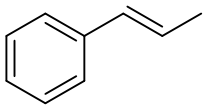
Reaction conditions: Alkyne (0.50 mmol), $H_3B{\cdot}NH_3$ (0.50 mmol), *V*(MeOH) = 2.0 mL.

In case of precatalyst 1b: (*E*)/(*Z*)-mixture of the corresponding product was observed (figure S 27). Overreduction to the corresponding alkane (3−9%) was observed.



(*E*)-1-styryl-2-(trifluoromethyl)benzene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with 1-(phenylethynyl)-2-(trifluoromethyl)benzene (123 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as yellow liquid (106 mg, 0.43 mmol, 85%). – ^{1}H NMR (300 MHz, $CDCl_3$): δ 7.74 (d, *J* = 7.9 Hz, 1 H), 7.63 (d, *J* = 7.8 Hz, 1 H), 7.57−7.40 (m, 4 H), 7.40−7.14 (m, 4 H), 7.04 (d, *J* = 16.1 Hz, 1 H).



(*E*)-prop-1-en-1-ylbenzene

According to GP 4, cobalt catalyst **1a**–**b** (1 mol%) and $H_3B{\cdot}NH_3$ (15.4 mg, 0.50 mmol) made to react with prop-1-yn-1-ylbenzene (62.6 µL, 58.1 mg, 0.50 mmol) in MeOH (2 mL). The product was obtained as colorless oil (39 mg, 0.33 mmol, 66%). – ^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.39–7.25 (m, 4 H), 7.24–7.15 (m, 1 H), 6.51–6.36 (m, 1 H), 6.35–6.20 (m, 1 H), 1.90 (dd, *J*= 6.4, 1.5 Hz, 3 H).

NMR spectra

NMR spectra of alkynes

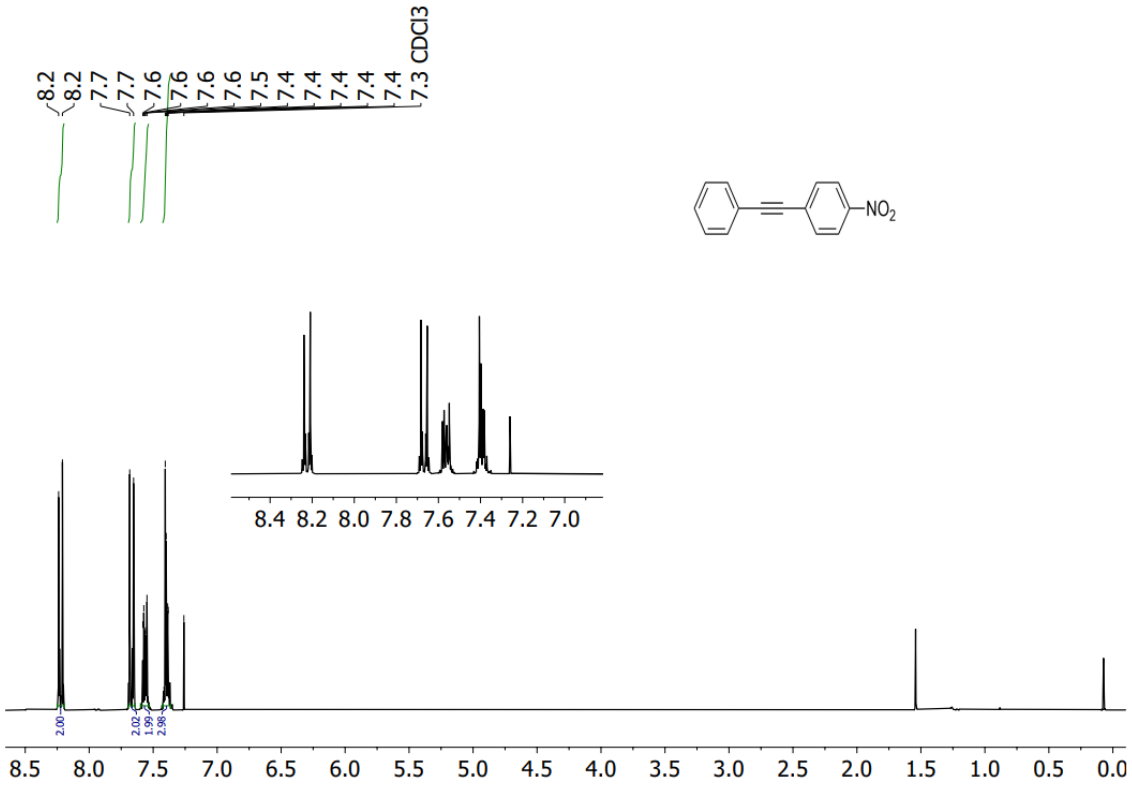


Figure S 9. ^{1}H NMR spectrum of *p*-NO_2-C_6H_4C≡CPh ($CDCl_3$, 25 °C).

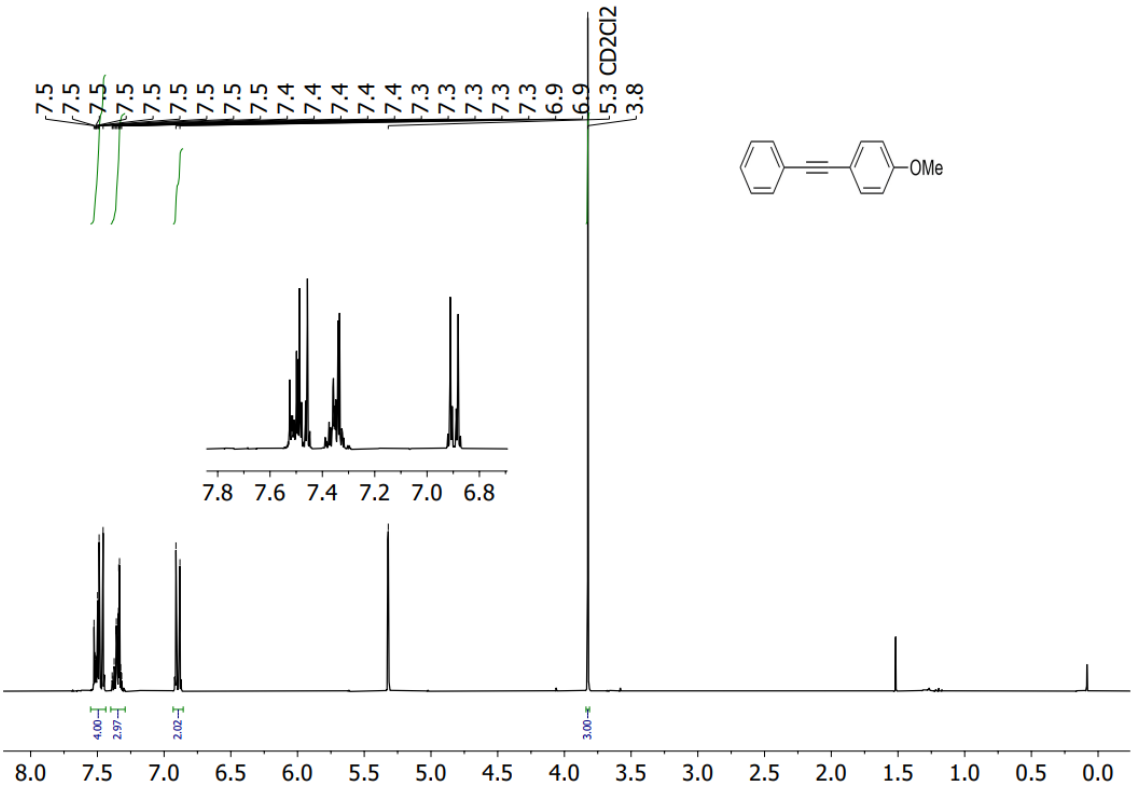


Figure S 10. ^{1}H NMR spectrum of *p*-OMe-C_6H_4C≡CPh ($CDCl_3$, 25 °C).

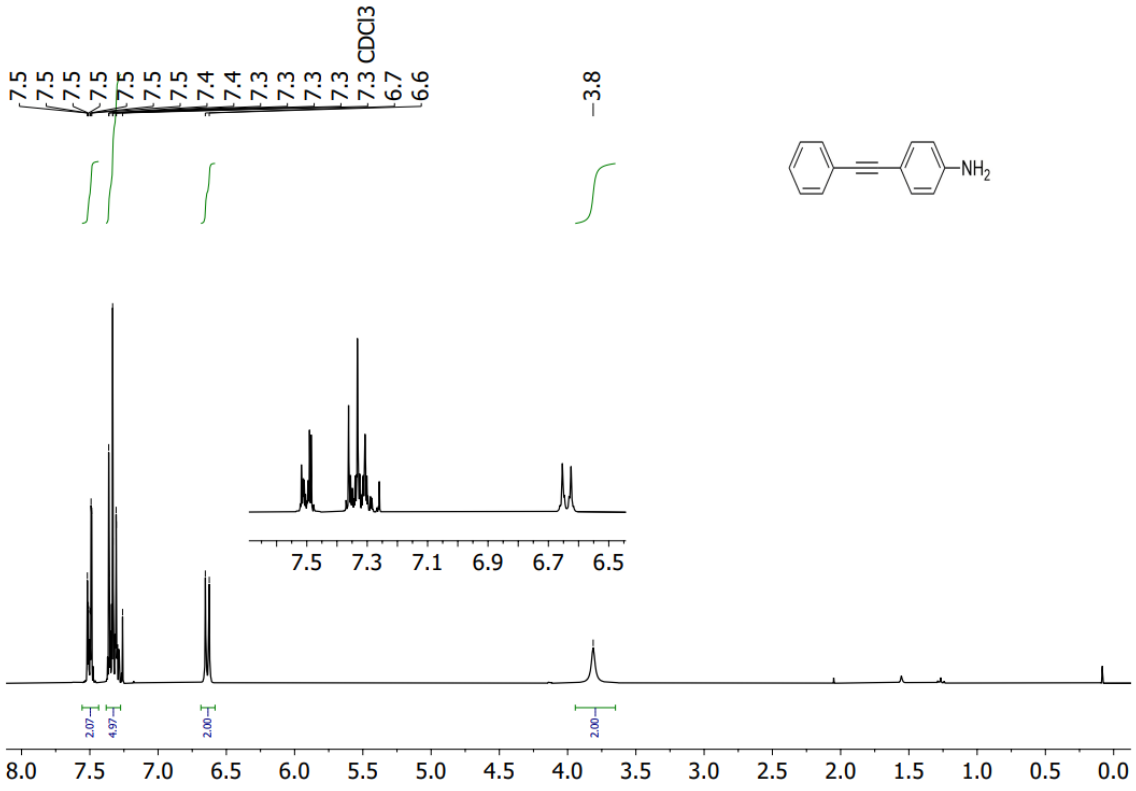


Figure S 11. ^{1}H NMR spectrum of *p*-NH_2-C_6H_4C≡CPh ($CDCl_3$, 25 °C).

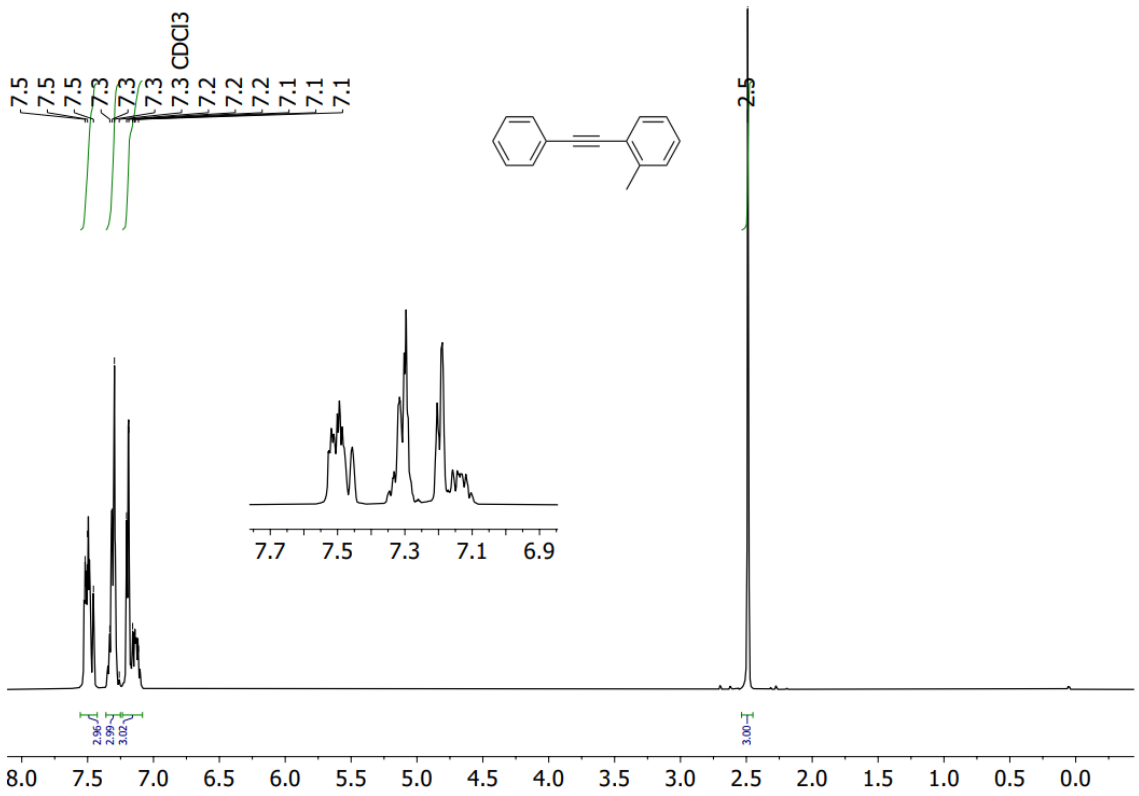


Figure S 12. ^{1}H NMR spectrum of *o*-CH_3-C_6H_4C≡CPh ($CDCl_3$, 25 °C).

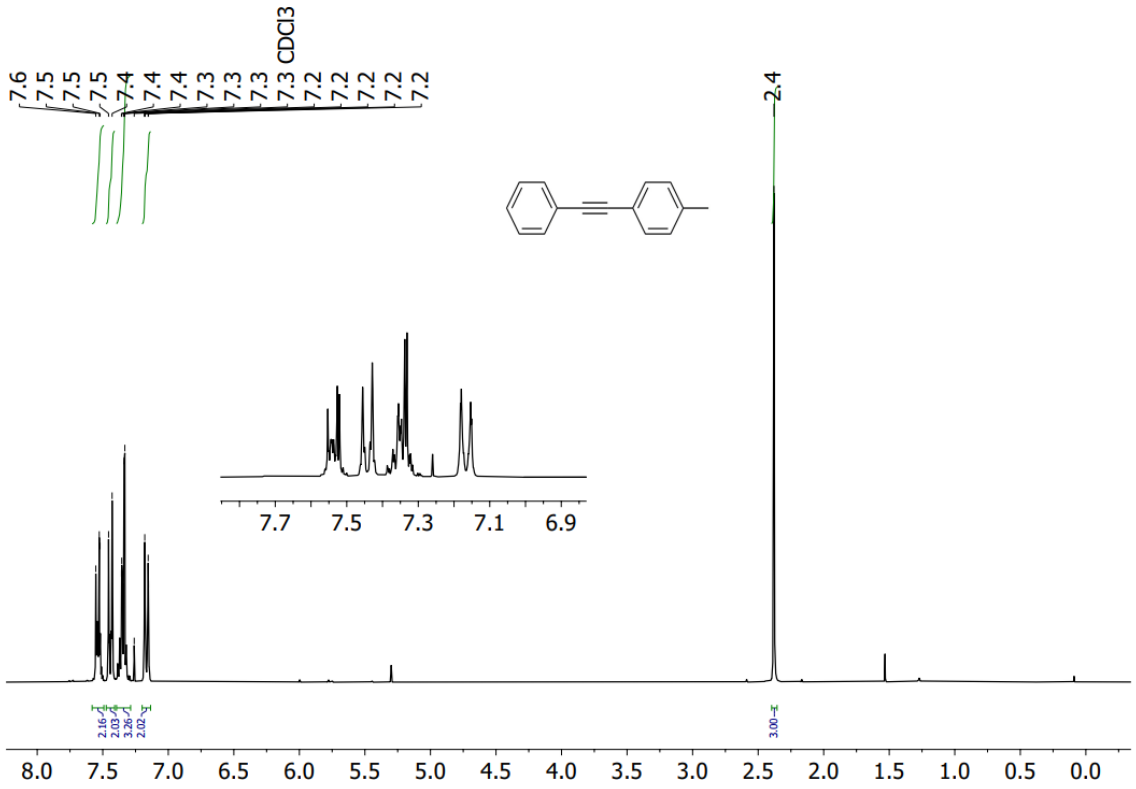


Figure S 13. ^{1}H NMR spectrum of *p*-CH_3-C_6H_4C≡CPh ($CDCl_3$, 25 °C).

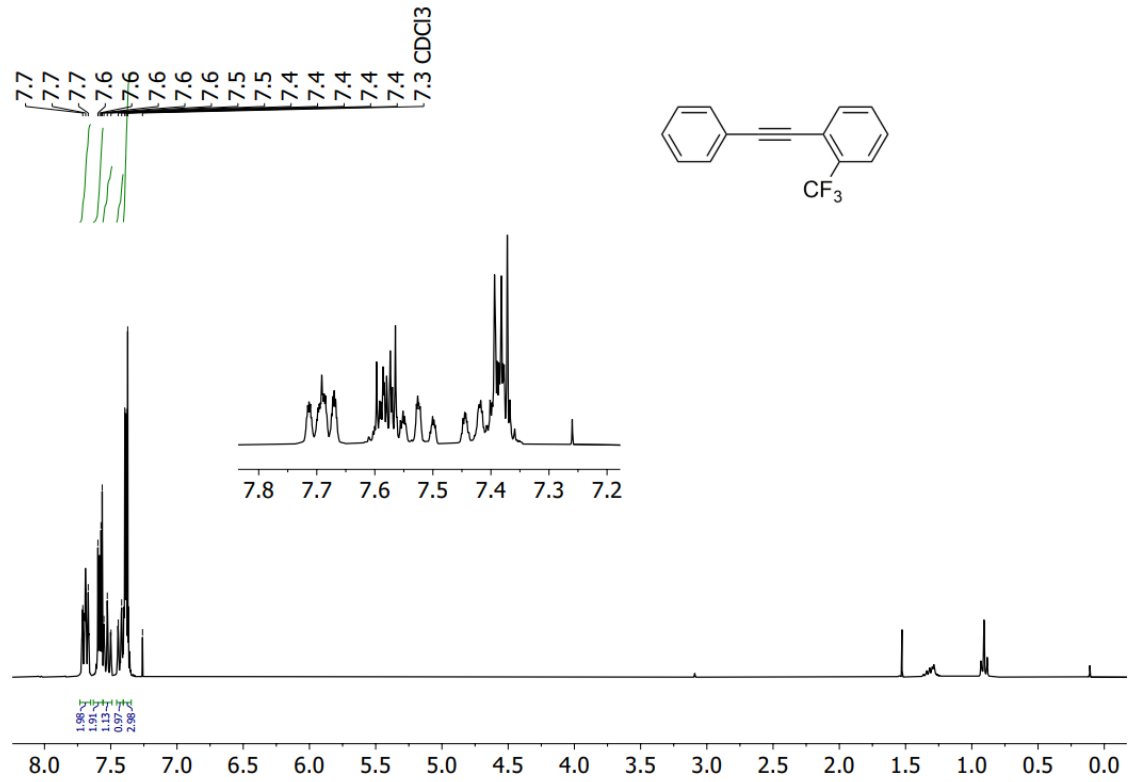


Figure S 14. ^{1}H NMR spectrum of *o*-CF_3-C_6H_4C≡CPh ($CDCl_3$, 25 °C).

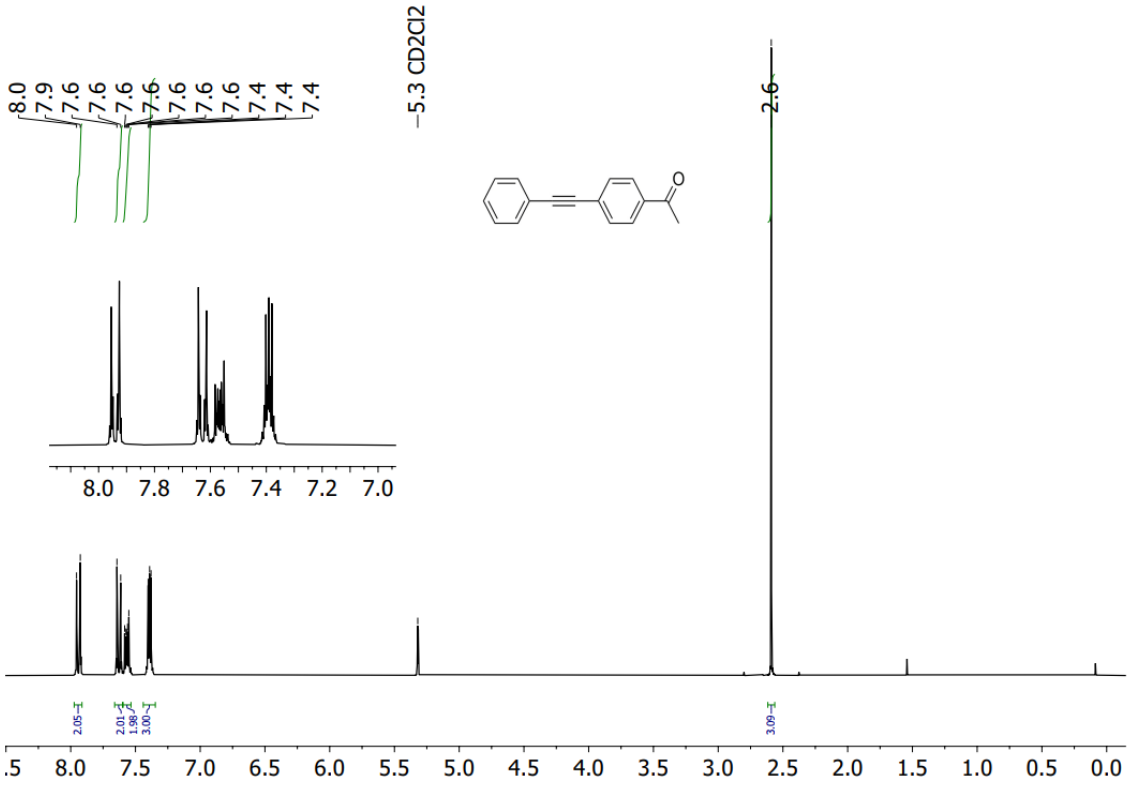


Figure S 15. ^{1}H NMR spectrum of *p*-C(O)CH_3-C_6H_4C≡CPh (CD_2Cl_2, 25 °C).

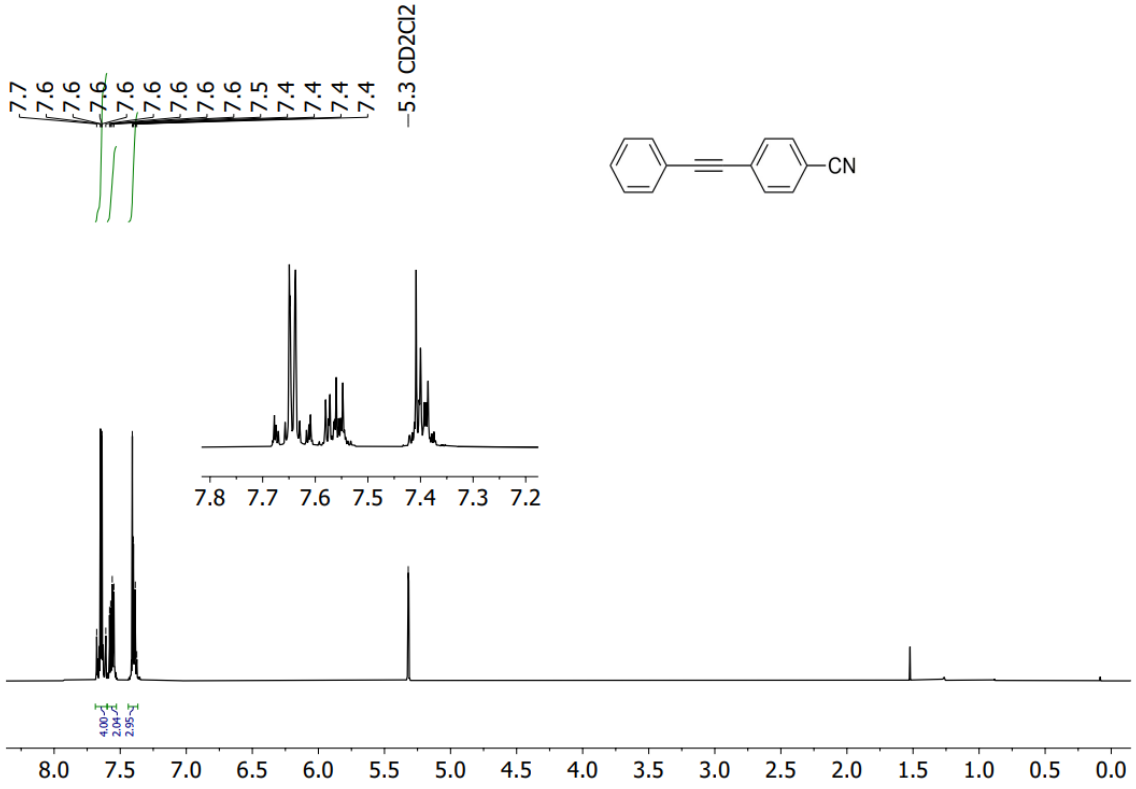


Figure S 16. ^{1}H NMR spectrum of *p*-CN-C_6H_4C≡CPh (CD_2Cl_2, 25 °C).

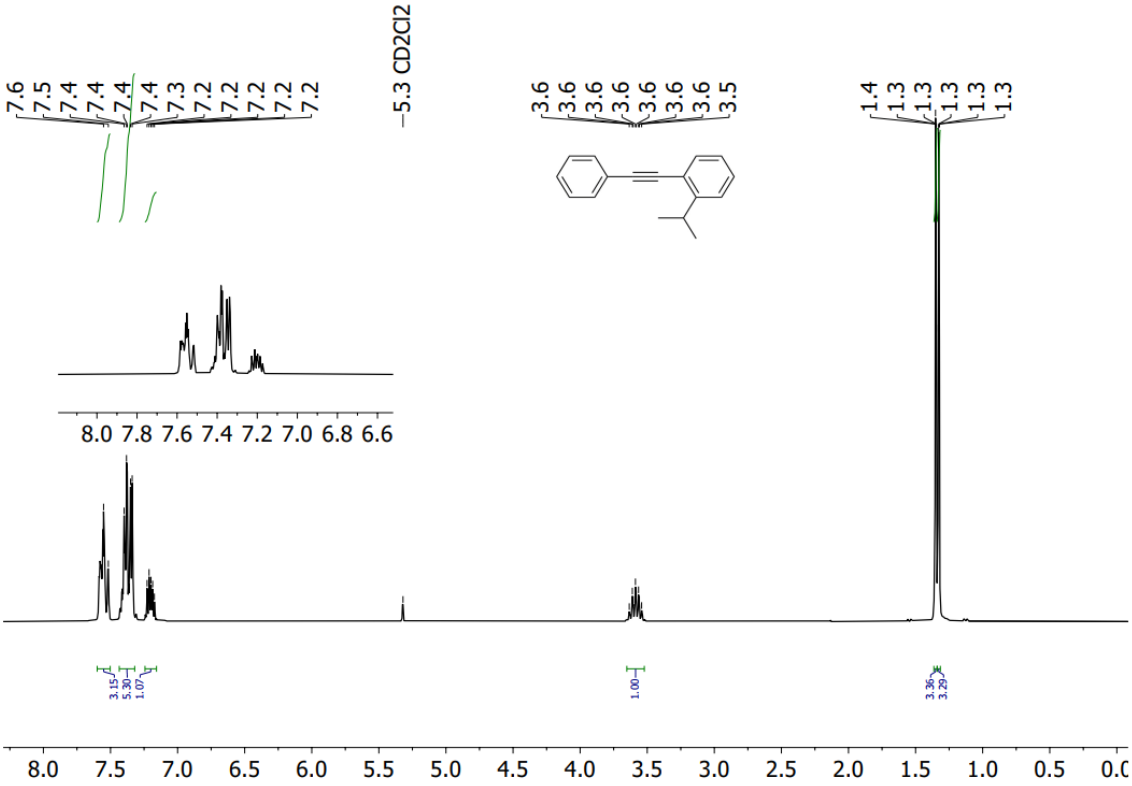


Figure S 17. ^{1}H NMR spectrum of *o-i*-Pr-$C_6H_4C{\equiv}CPh$ (CD_2Cl_2, 25 °C).

NMR spectra of alkenes

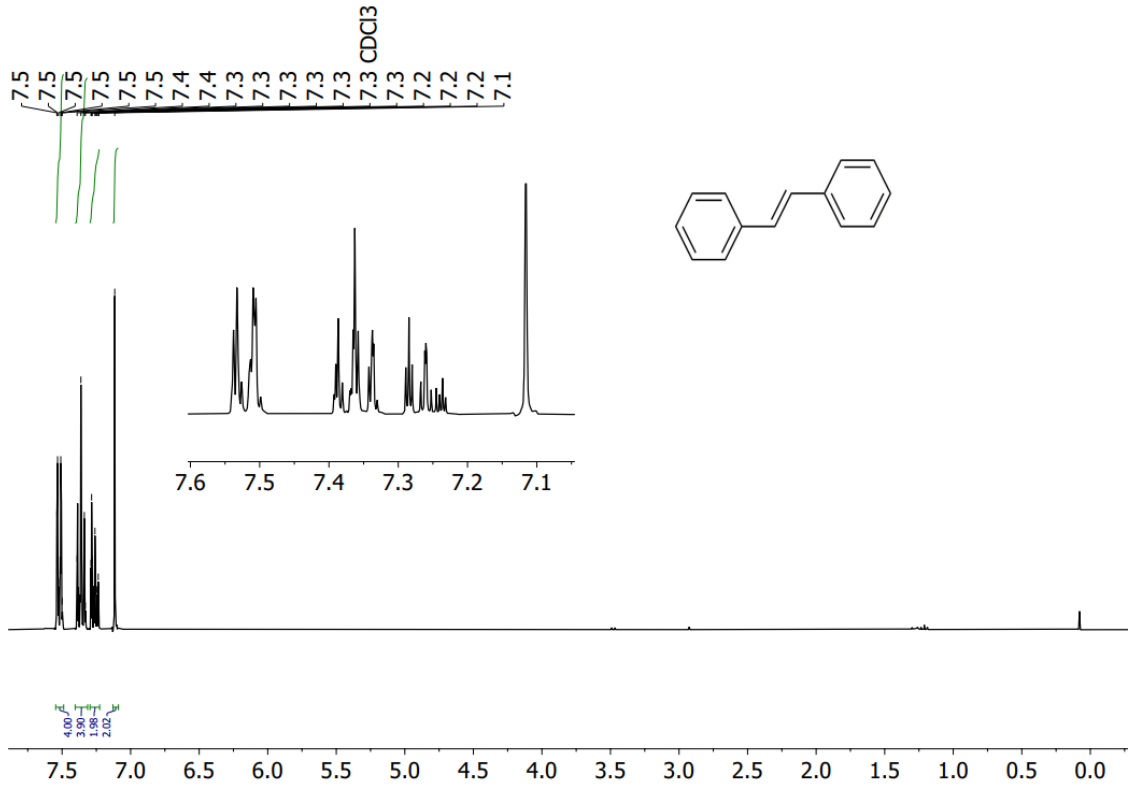


Figure S 18. ^{1}H NMR spectrum of PhCH=CHPh ($CDCl_3$, 25 °C).

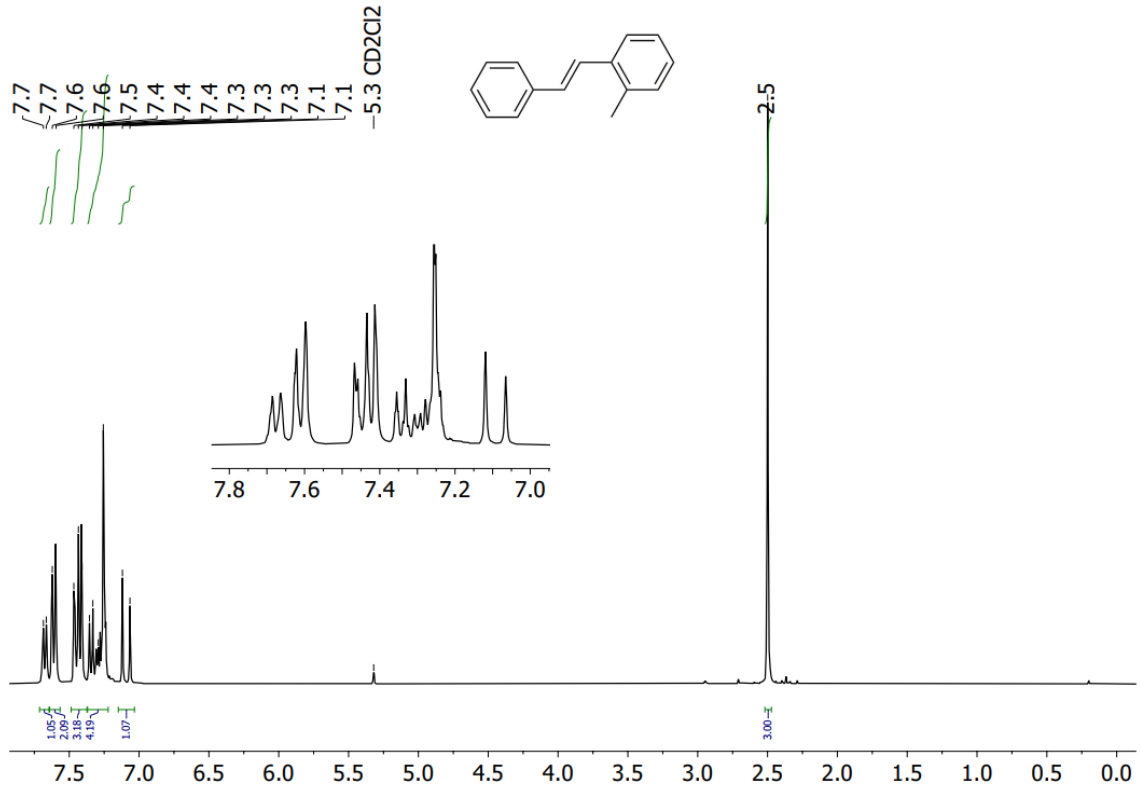


Figure S 19. ^{1}H NMR spectrum of *o*-CH_3-C_6H_4CH=CHPh (CD_2Cl_2, 25 °C).

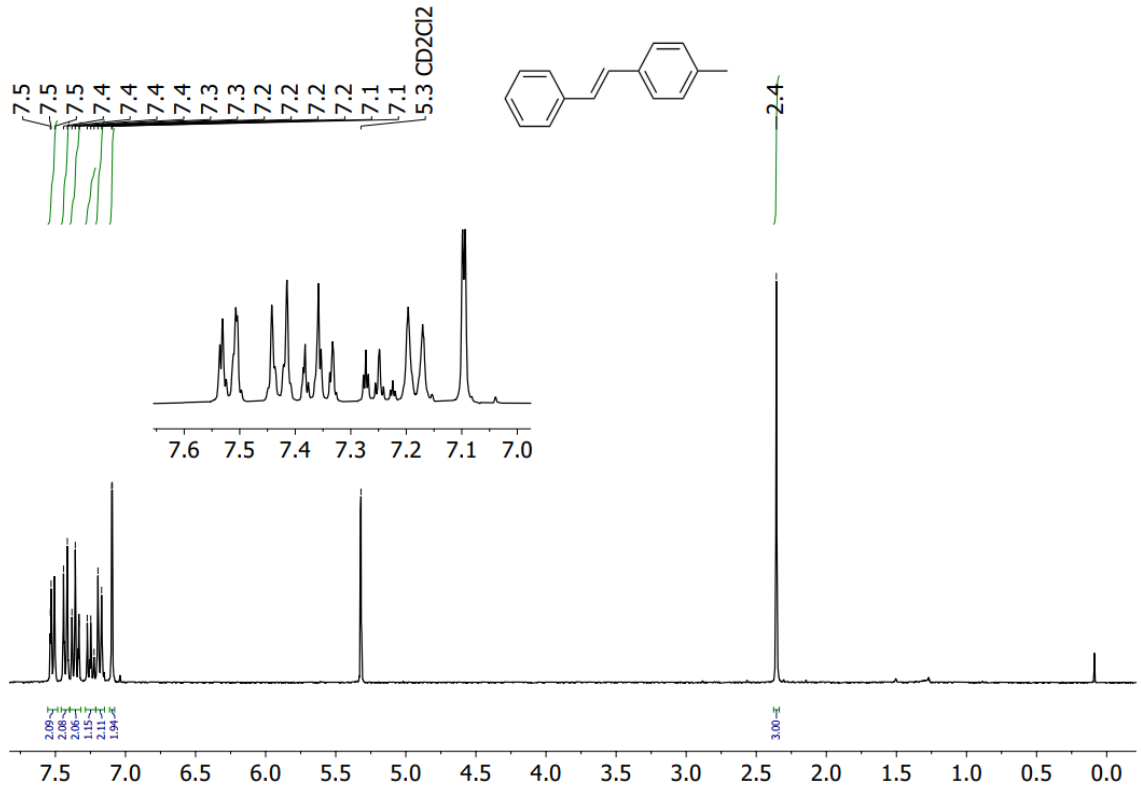


Figure S 20. ^{1}H NMR spectrum of *p*-CH_3-C_6H_4CH=CHPh (CD_2Cl_2, 25 °C).

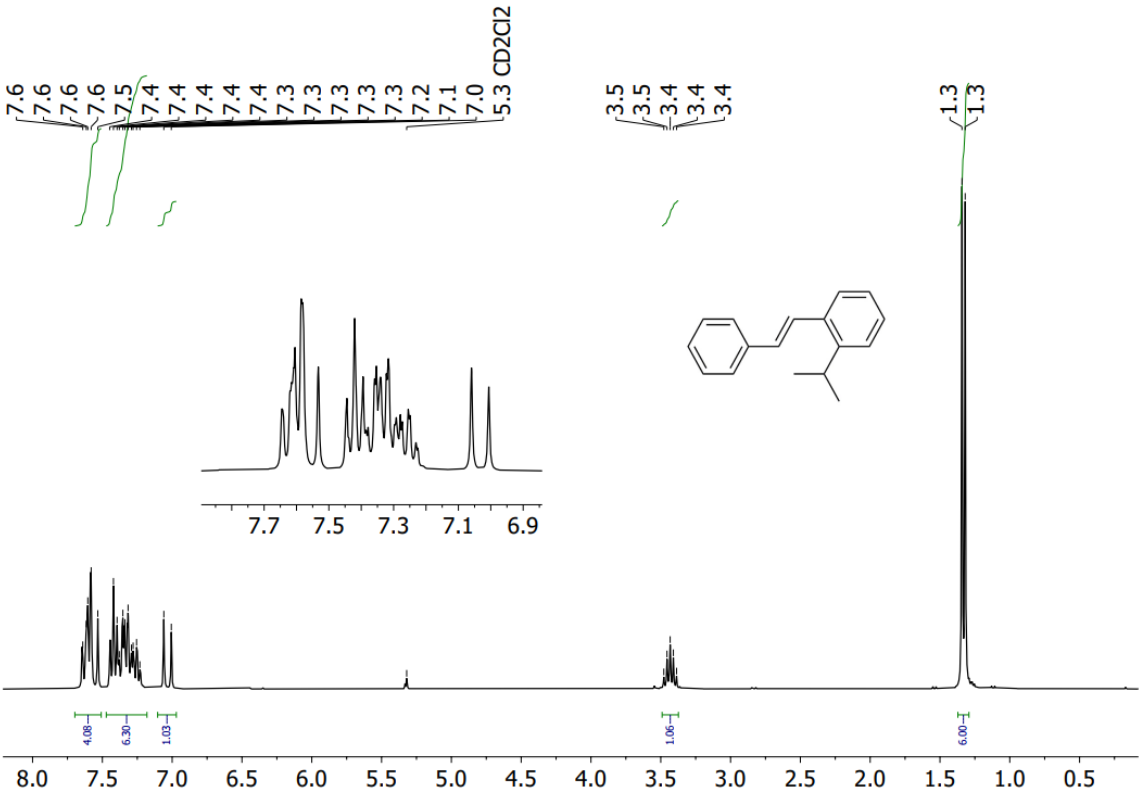


Figure S 21. ^{1}H NMR spectrum of *o-i*-Pr-C_6H_4CH=CHPh (CD_2Cl_2, 25 °C).

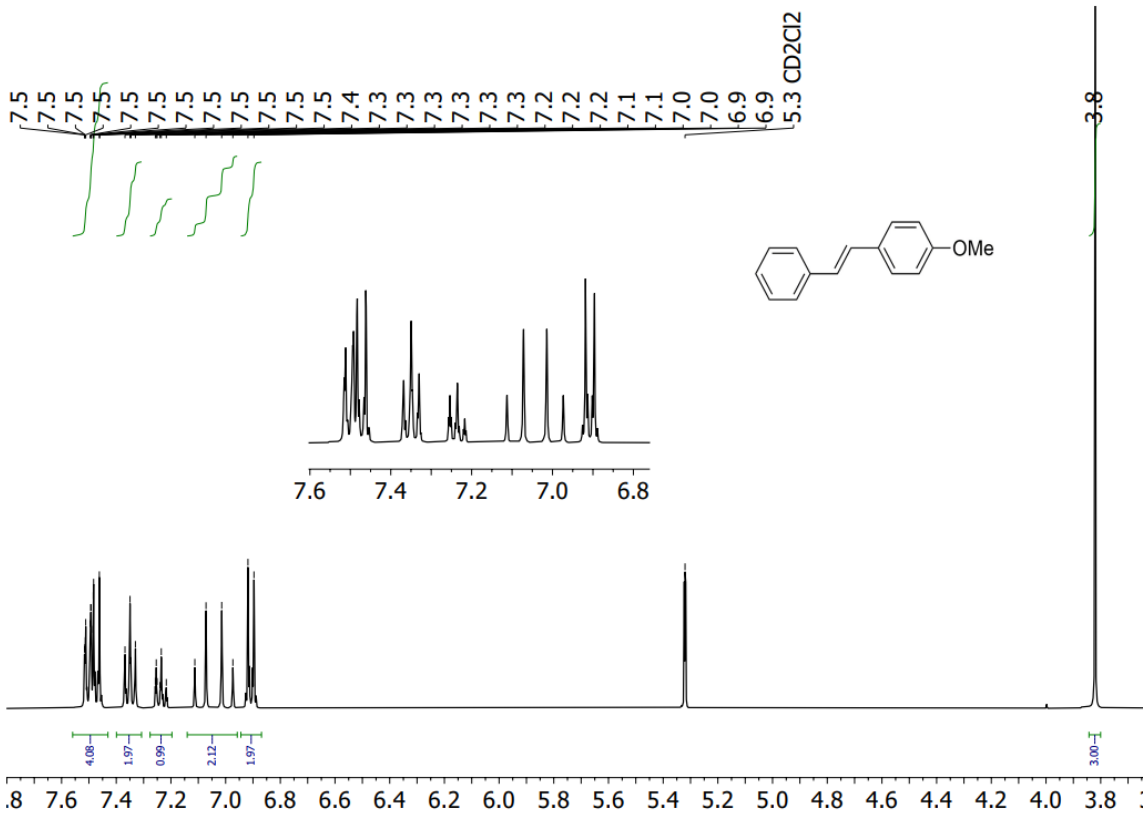


Figure S 22. ^{1}H NMR spectrum of *p*-OMe-C_6H_4CH=CHPh (CD_2Cl_2, 25 °C).

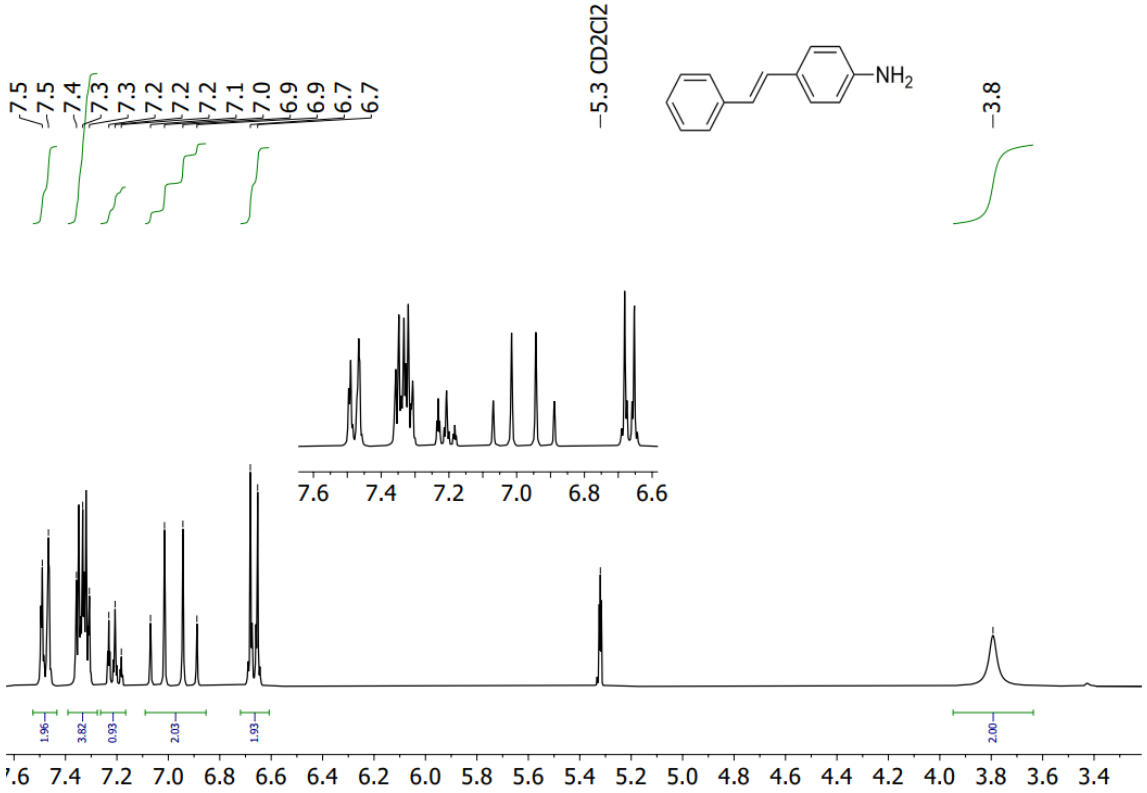


Figure S 23. ^{1}H NMR spectrum of *p*-NH_2-C_6H_4CH=CHPh (CD_2Cl_2, 25 °C).

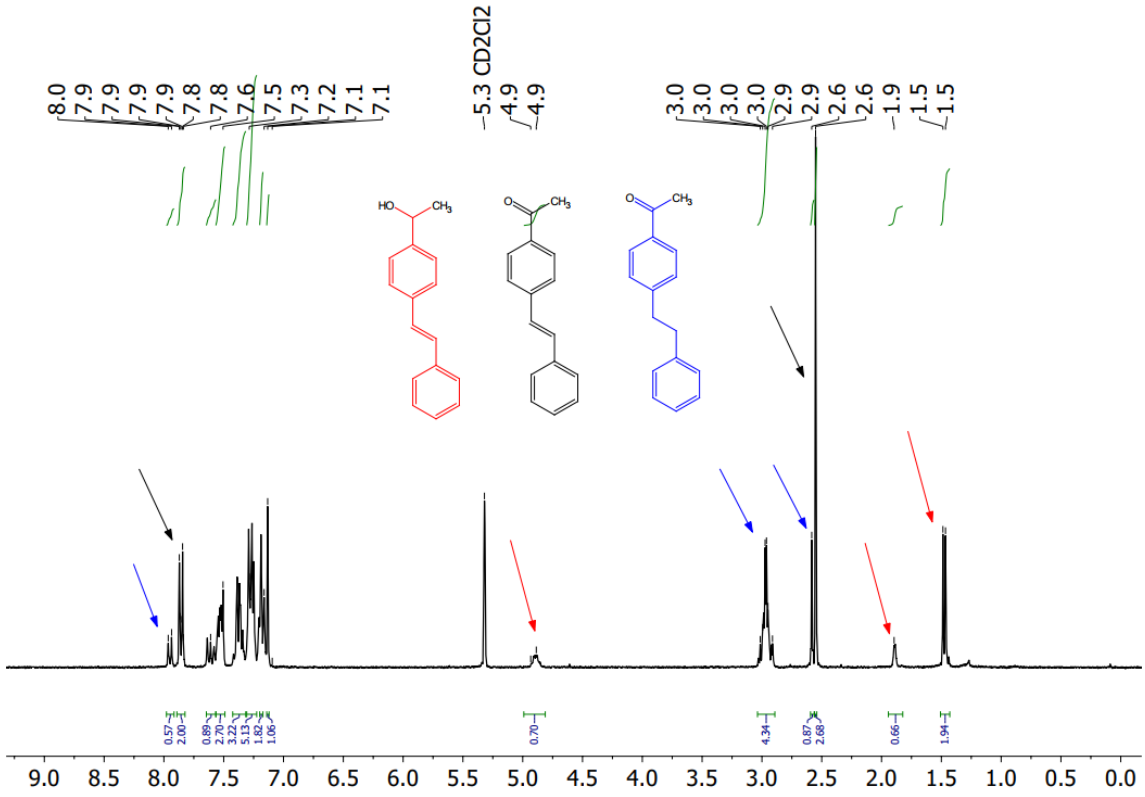


Figure S 24. ^{1}H NMR spectrum of a mixture obtained with **1b** after TSH of *p*-C(O)CH$_3$-C$_6$H$_4$C≡CPh (CD$_2$Cl$_2$, 25 °C).

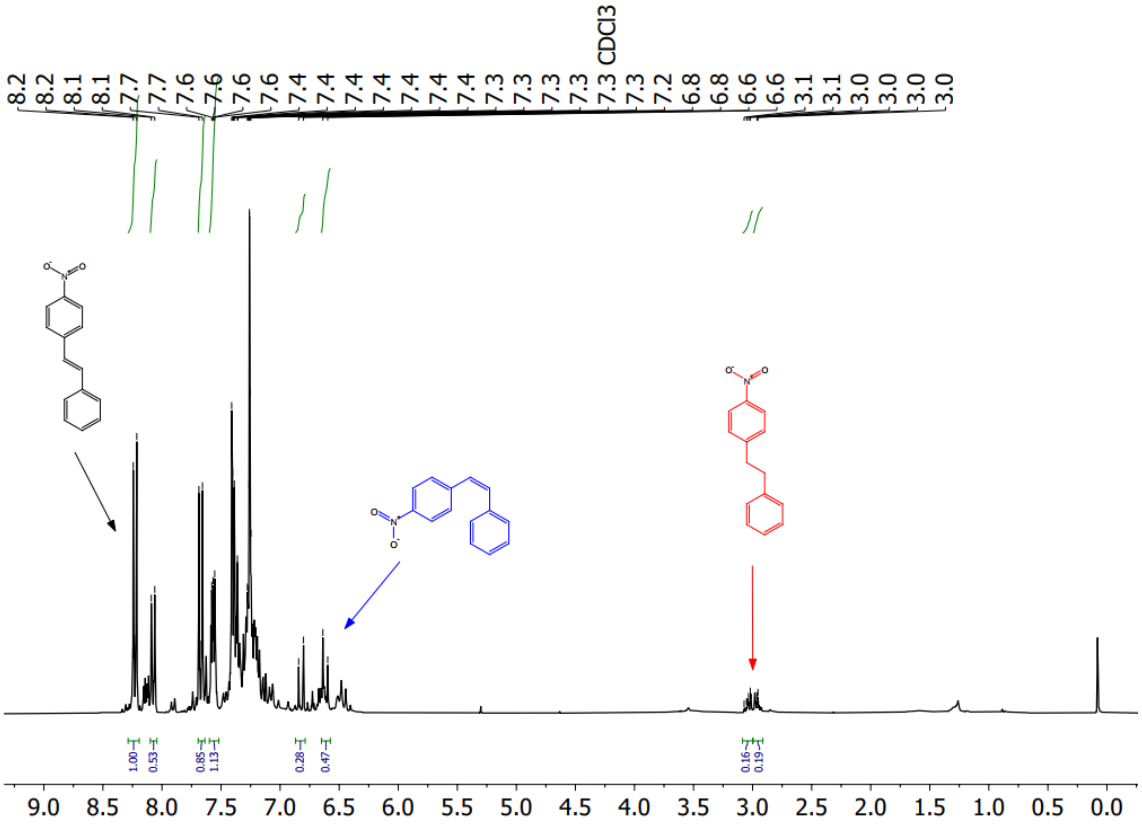


Figure S 25. ^{1}H NMR spectrum of a mixture obtained with **1b** after TSH of *p*-NO$_2$-C$_6$H$_4$C≡CPh (CDCl$_3$, 25 °C). Yield of the corresponding alkane due overreduction: 8%.

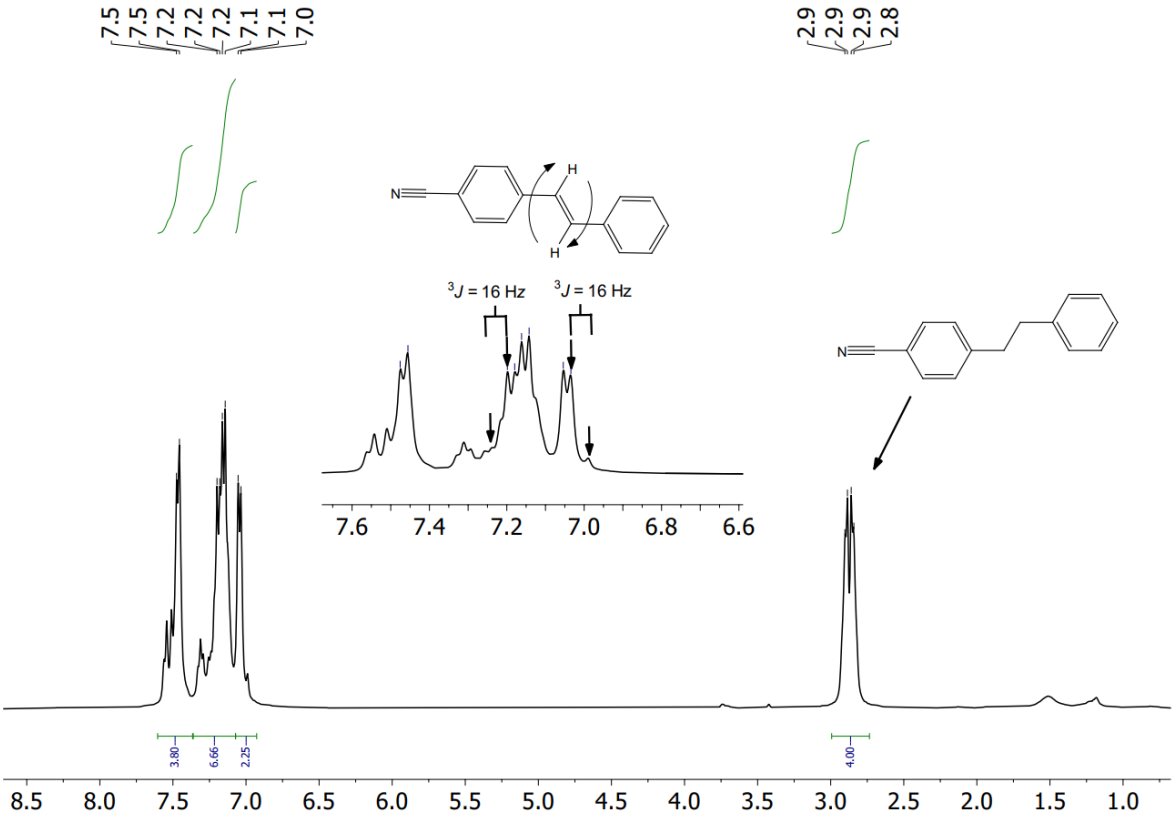


Figure S 26. ^{1}H NMR spectrum of a mixture after TSH with **1a** and *p*-CN-C_6H_4C≡CPh ($CDCl_3$, 25 °C). Yield of the corresponding alkane due overreduction: 78%.

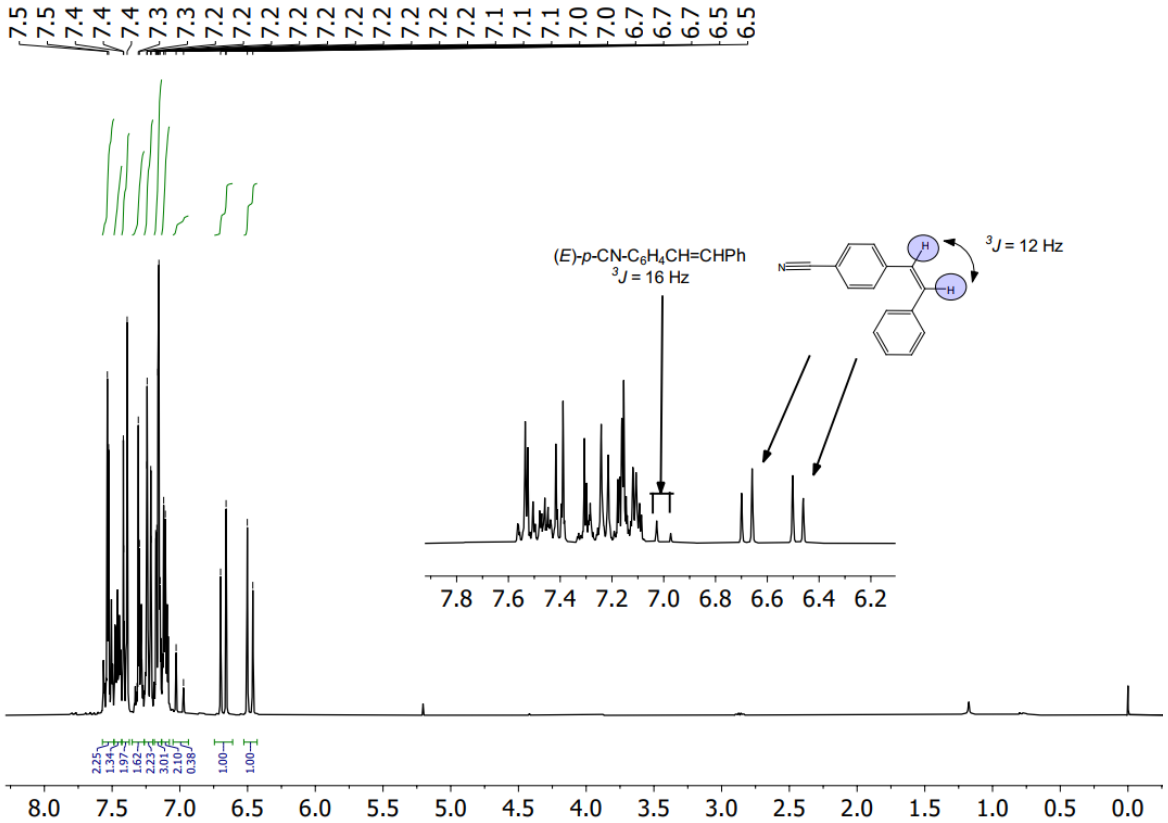


Figure S 27. ^{1}H NMR spectrum of a mixture after TSH with **1b** and p-CN-C_6H_4C≡CPh ($CDCl_3$, 25 °C). Yield of the corresponding alkane due overreduction: 2−3%.

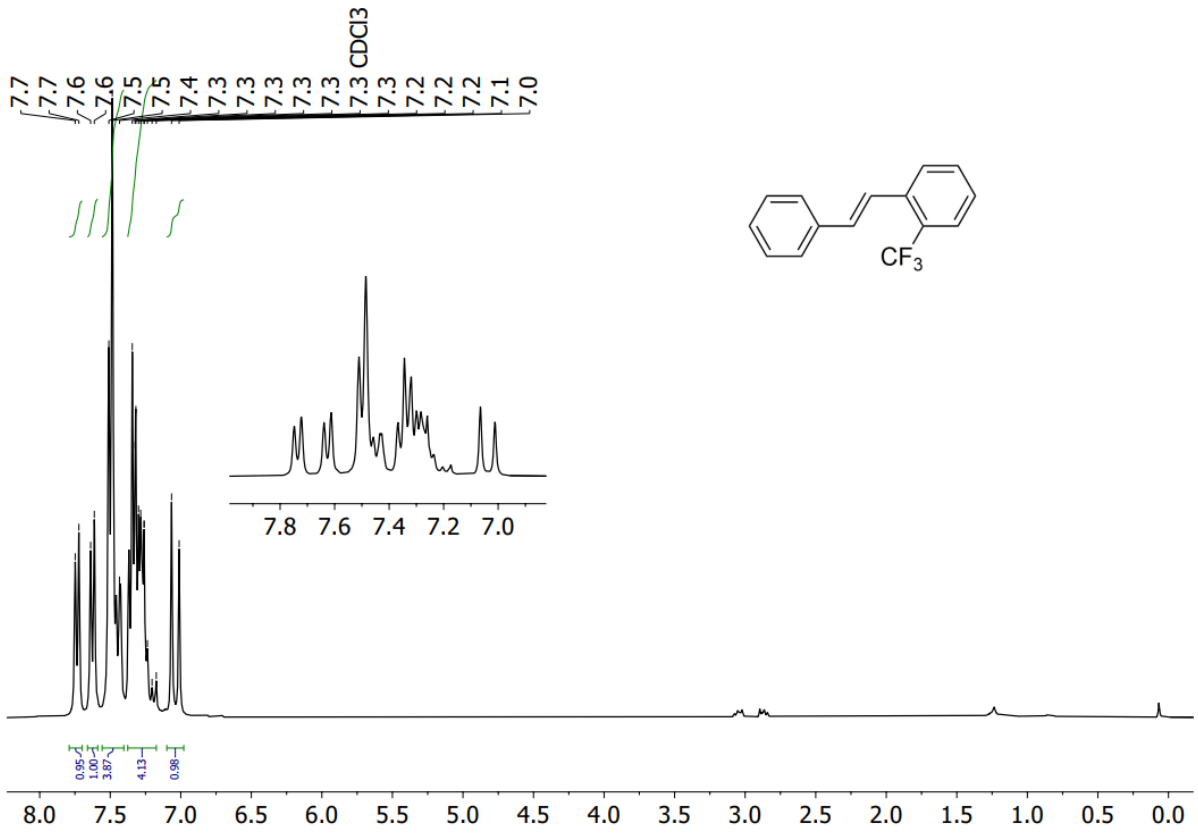


Figure S 28. ^{1}H NMR spectrum of *o*-CF_3-C_6H_4CH=$CHPh$ ($CDCl_3$, 25 °C).

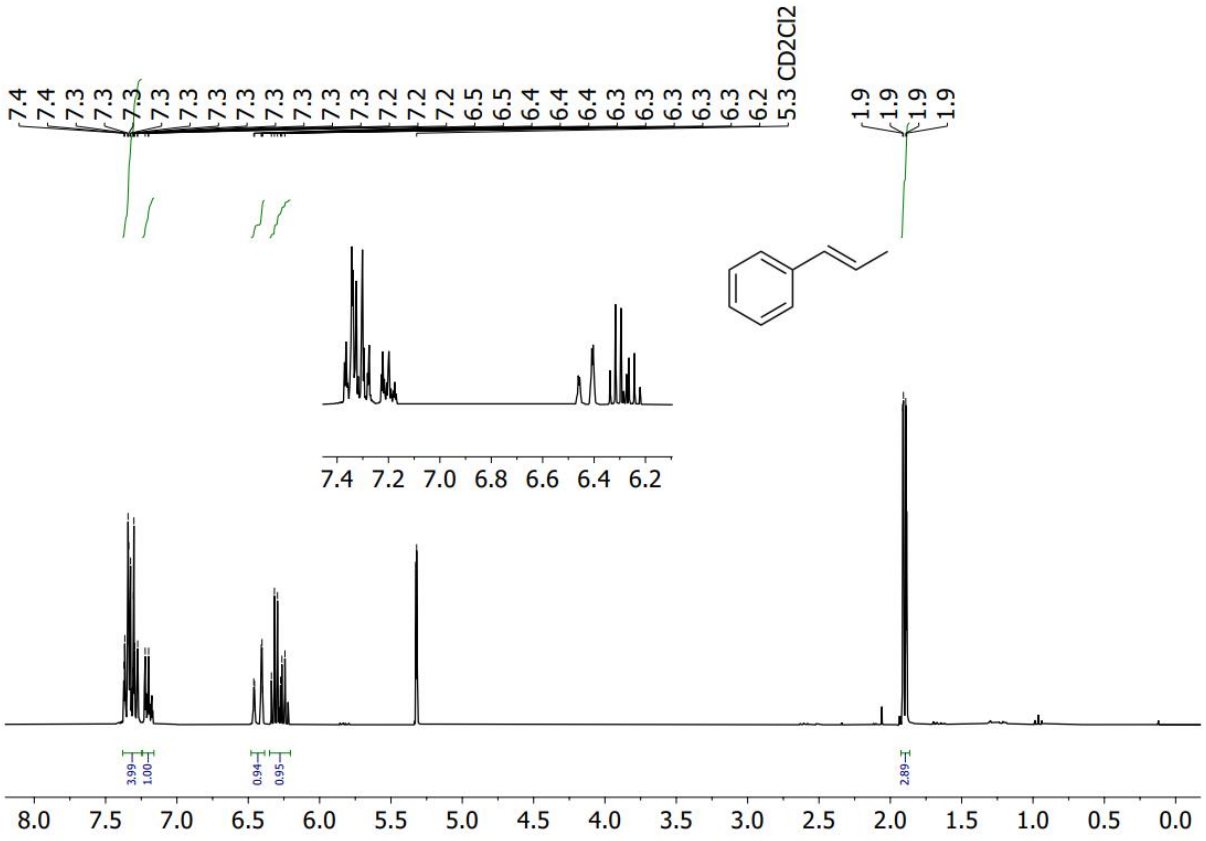


Figure S 29. ^{1}H NMR spectrum of C_6H_5CH=$CHCH_3$ (CD_2Cl_2, 25 °C).

Mechanistic investigations

EPR spectroscopy

EPR measurements were recorded on a Bruker EMX CW-micro X-band spectrometer with a microwave power ≈ 6.9 mW, a modulation frequency of 100 kHz and modulation amplitude up to 5 G. The EPR spectrometer is equipped with a variable temperature control unit including a liquid N_2 cryostat and a temperature controller for recording the EPR spectra at low temperature down to 96K. g values were calculated using the equation $h\nu = g\beta B_0$ with β, B_0 and ν being the Bohr magneton, resonance field and frequency, respectively. Calibration of the g values was performed using a DPPH standard (g = 2.0036 ± 0.0004).

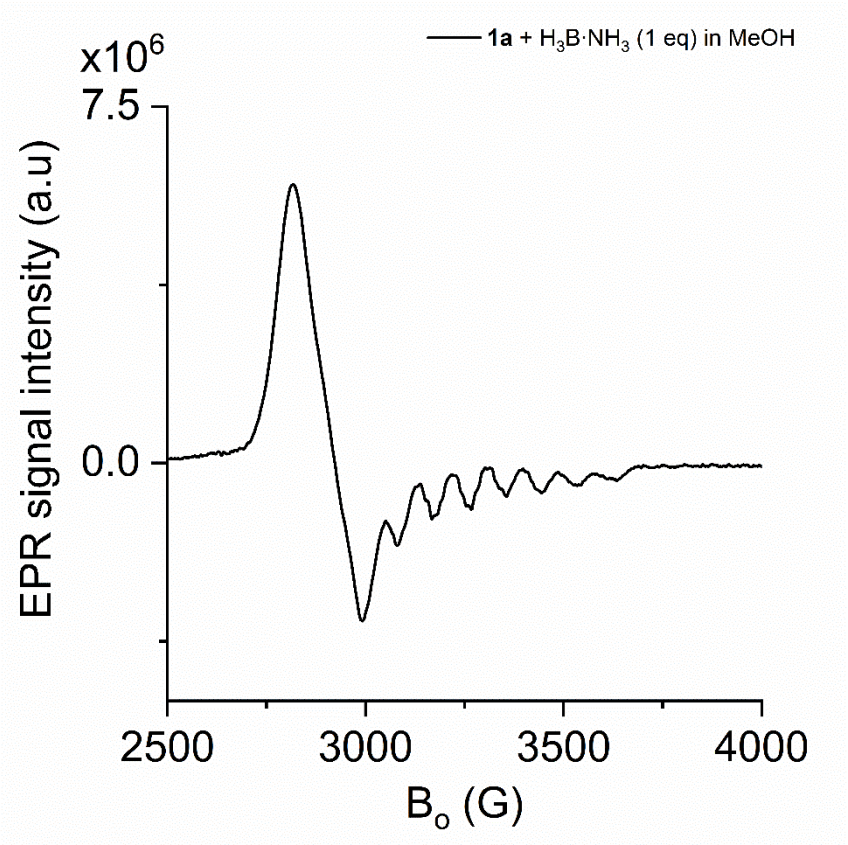


Figure S 30. EPR spectrum of **1a** with $H_3B{\cdot}NH_3$ (1 eq.) measured at 97K.

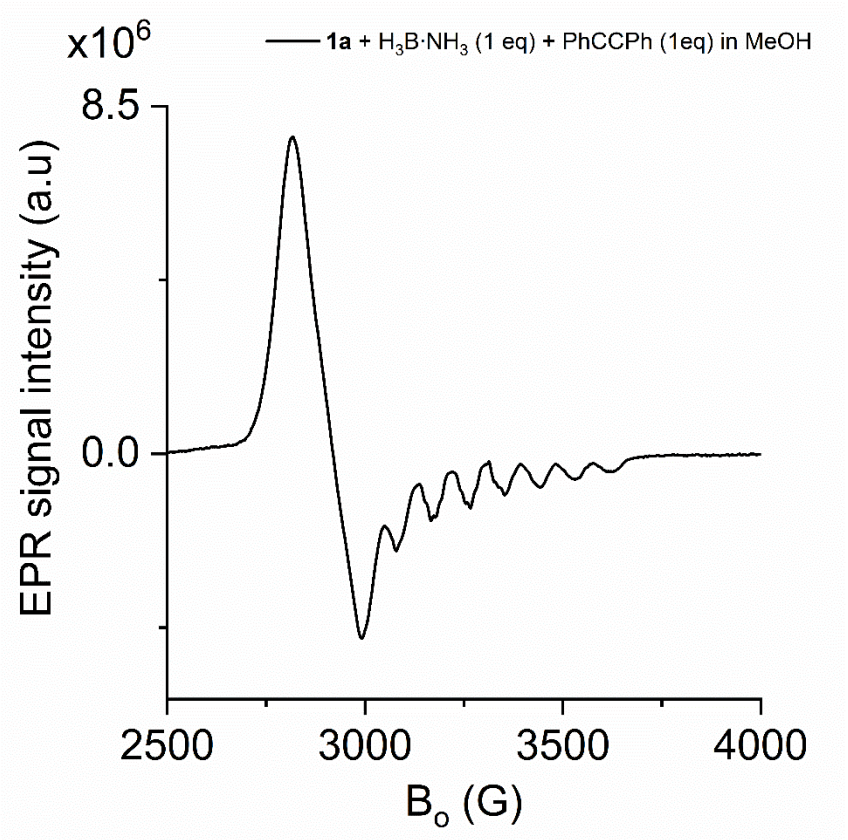


Figure S 31. EPR spectrum of **1a** with $H_3B{\cdot}NH_3$ (1 eq.) and PhCCPh (1 eq.) measured at 97K.

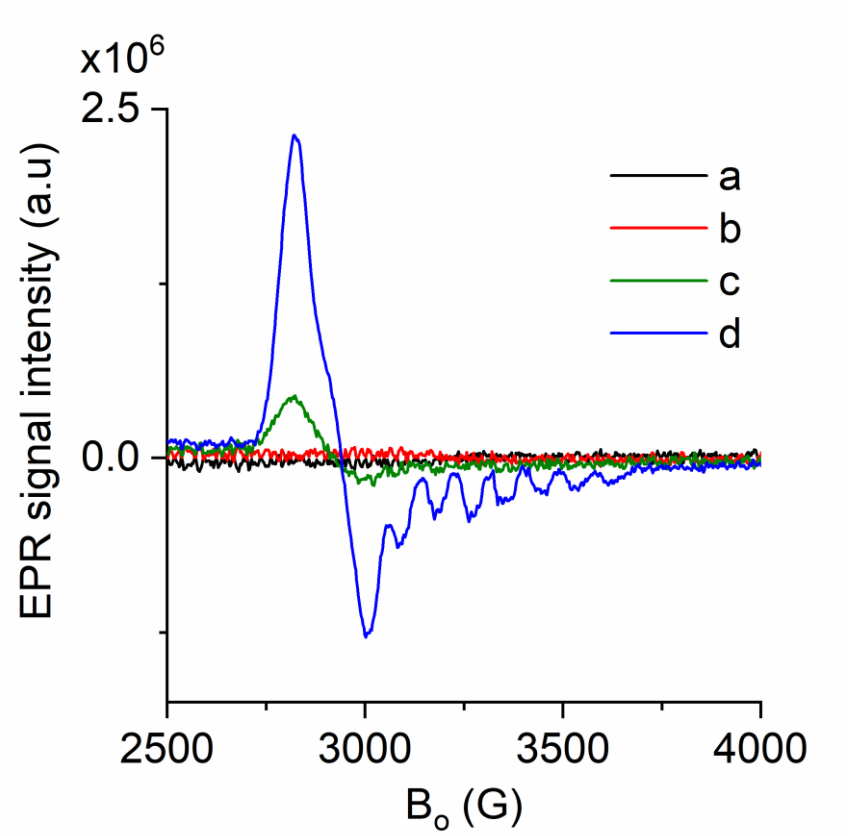
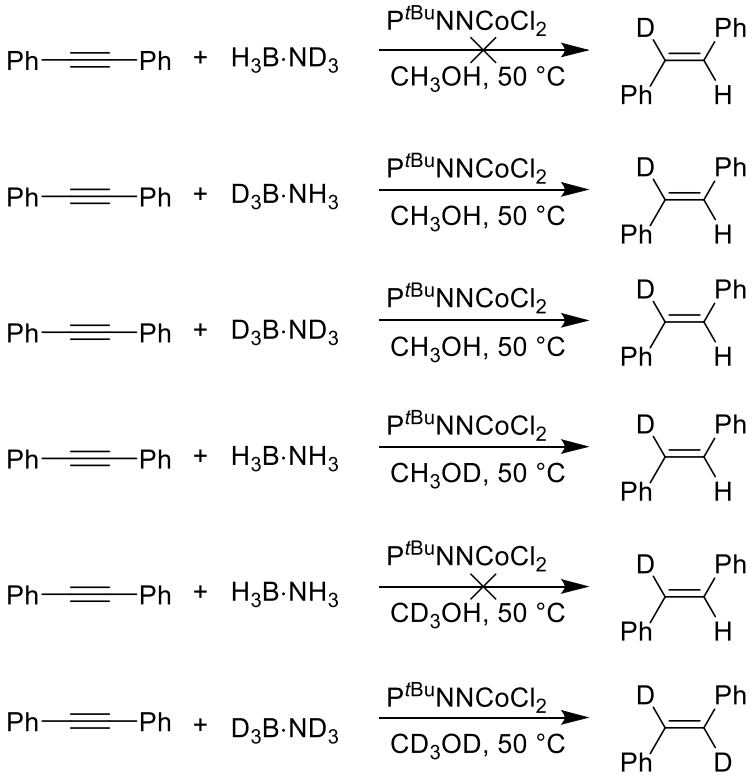


Figure S 32. EPR Spectra measured at 108K of a) **1a** in toluene; b) after addition of 2 equivalents of MeOH to (a); c) after addition of $H_3B{\cdot}NH_3$ to (b); d) after addition an excess of MeOH to (a).

Deuterium labelling studies

General procedure (GP3)

Under an atmosphere of argon, cobalt complex **1a** (2.45 mg, 1 mol%), B-D, N-D or fully deuterated ammonia borane (0.5 mmol) were stirred together with diphenylacetylene (89.1 mg, 0.50 mmol) in methanol (-d_1,-d_3, -d_4) at 50°C overnight. After the reaction, the mixture was exposed to air and CH_2Cl_2 (5 mL) was added. The solution was filtered through a pad of silica and washed with EtOAc (3 x 5 mL). Subsequently the solvent was removed under reduced pressure to give (*E*)-Stilbene, the mono-or di-deuterated product.



Scheme S 1. An overview of the deuterium labeling experiments.

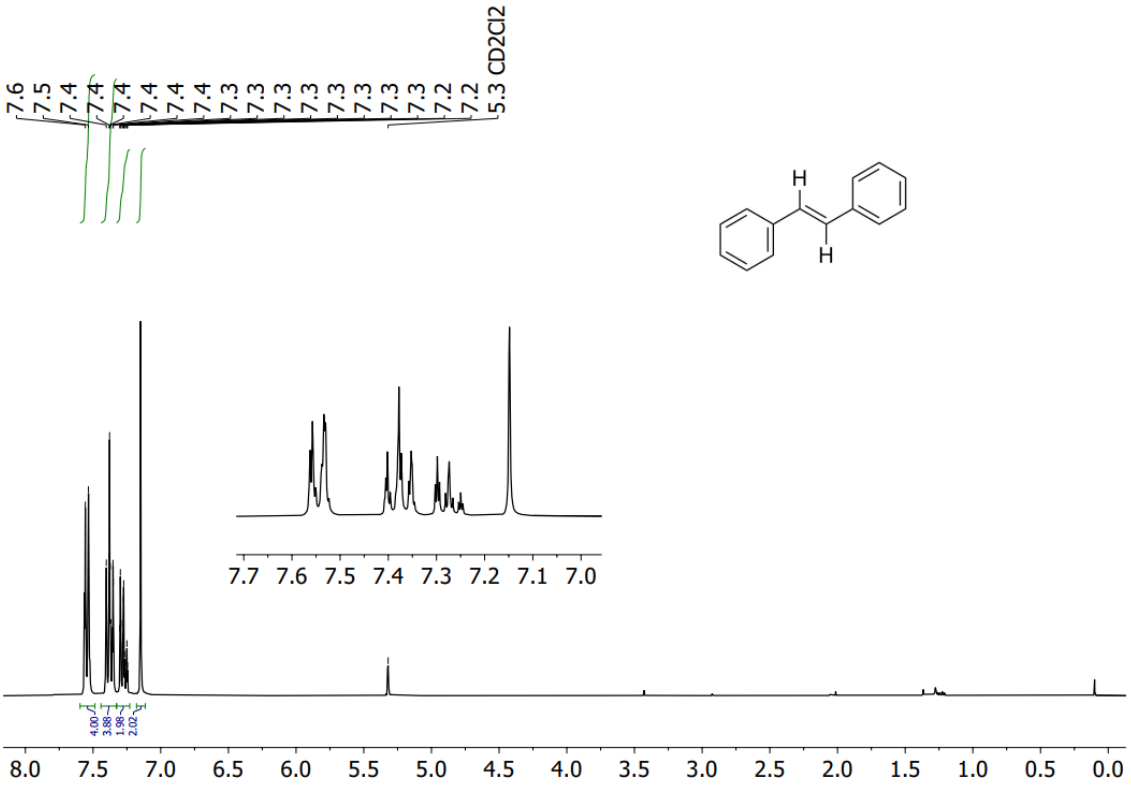


Figure S 33. ^{1}H NMR spectrum (CD_2Cl_2 at 25 °C) of (*E*)-Stilbene after the TSH with $H_3B{\cdot}ND_3$. In CH_3OH.

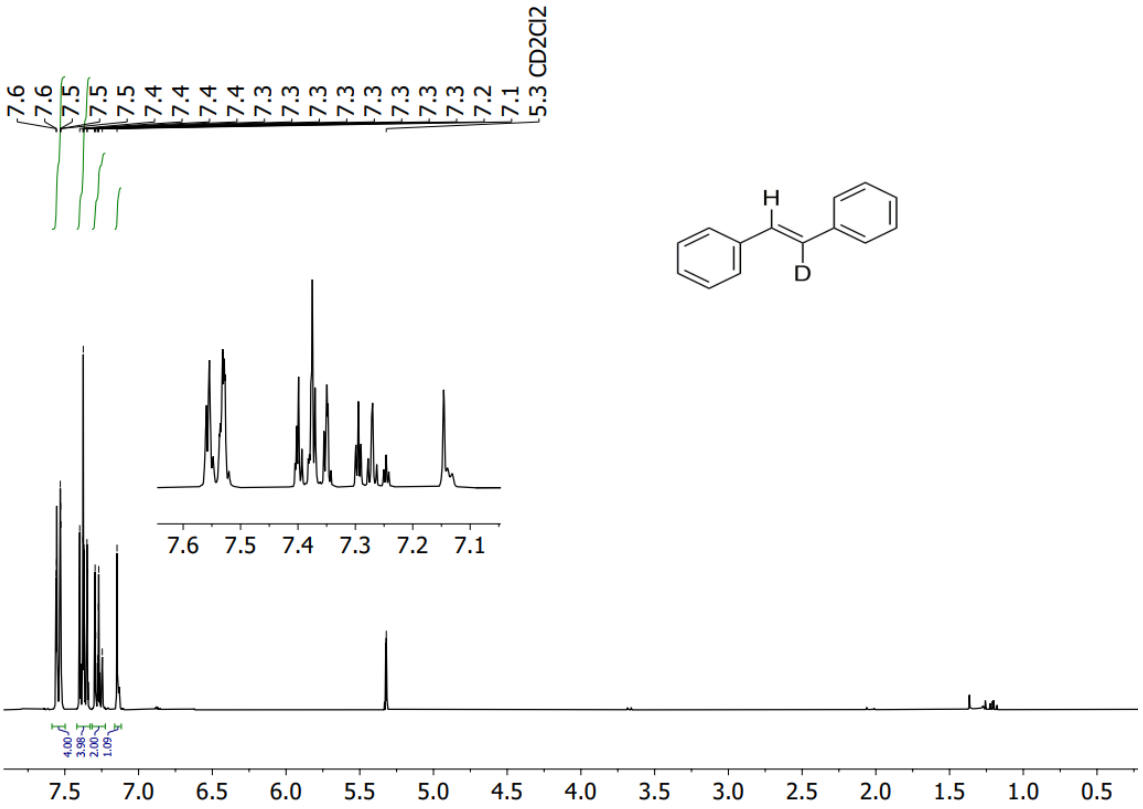


Figure S 34. ^{1}H NMR spectrum (CD_2Cl_2 at 25 °C) of monodeuterated (*E*)-Stilbene after the TSH with $D_3B{\cdot}NH_3$ in CH_3OH.

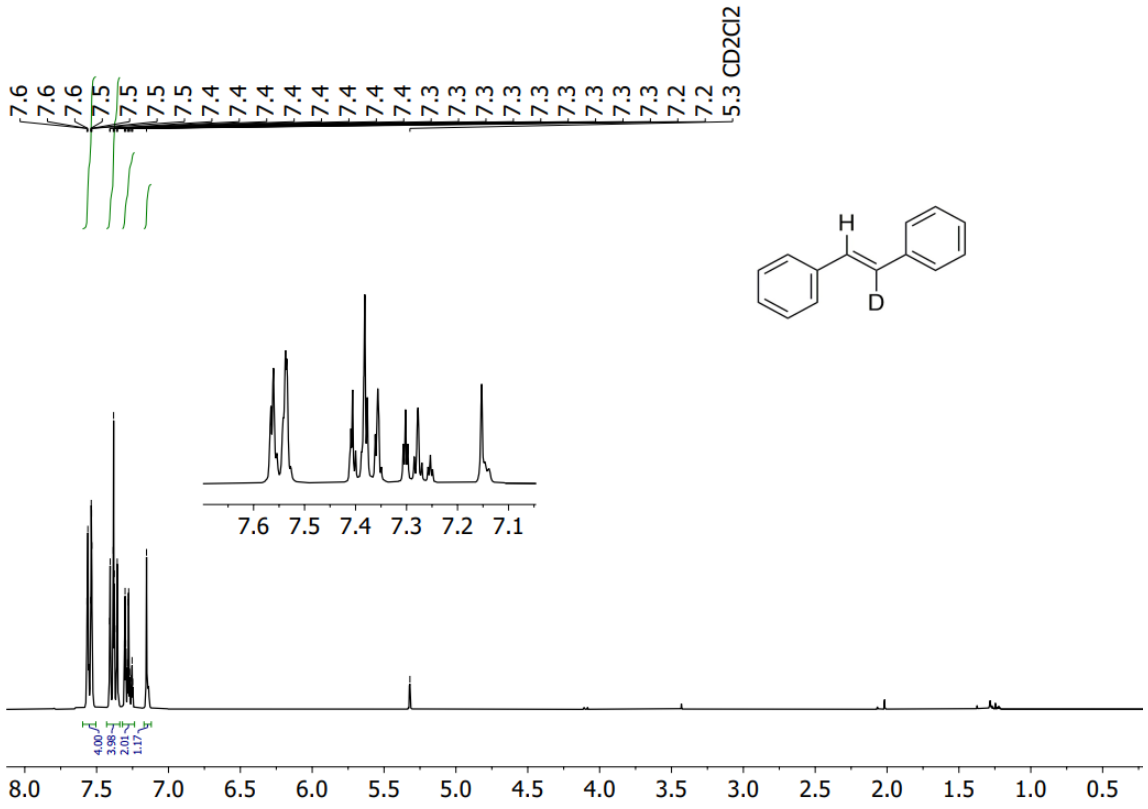


Figure S 35. ^{1}H NMR spectrum (CD_2Cl_2 at 25 °C) of (*E*)-Stilbene after the TSH with $D_3B{\cdot}ND_3$ in CH_3OH.

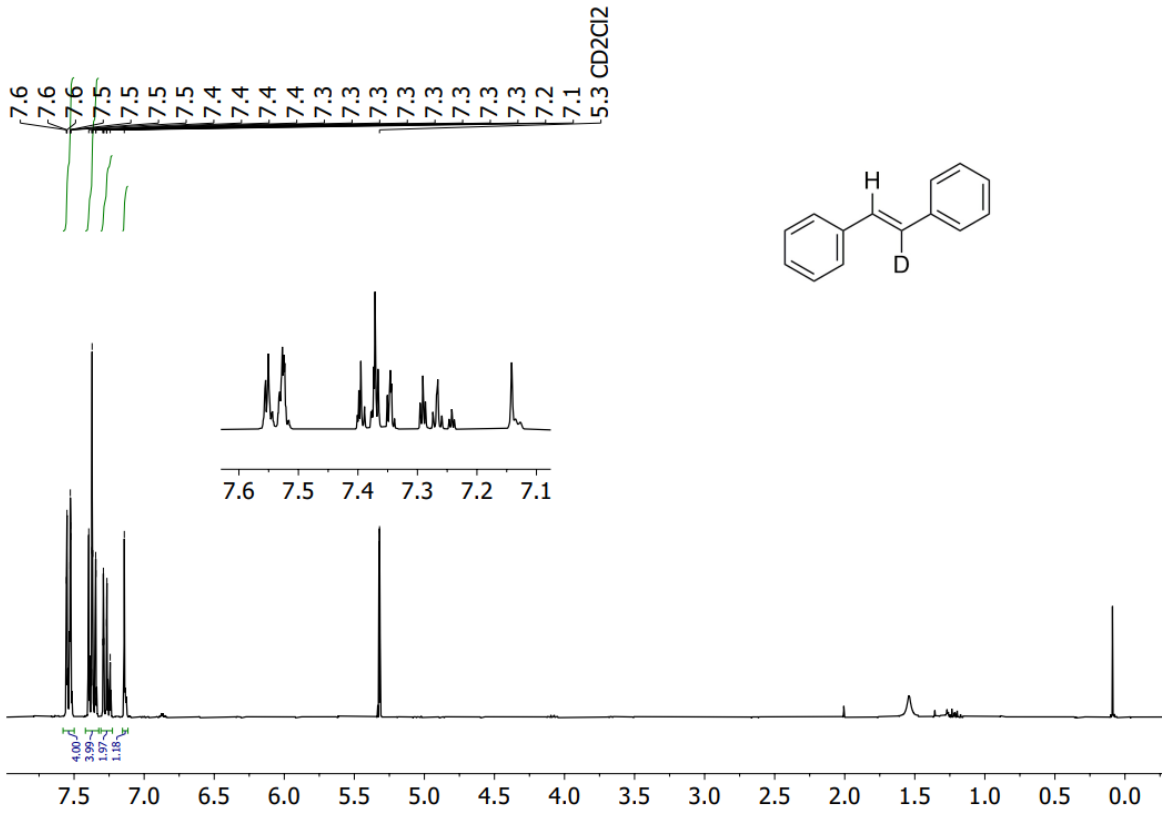


Figure S 36. ^{1}H NMR spectrum (CD_2Cl_2 at 25 °C) of (*E*)-Stilbene after the TSH with $H_3B{\cdot}NH_3$ in CH_3OD.

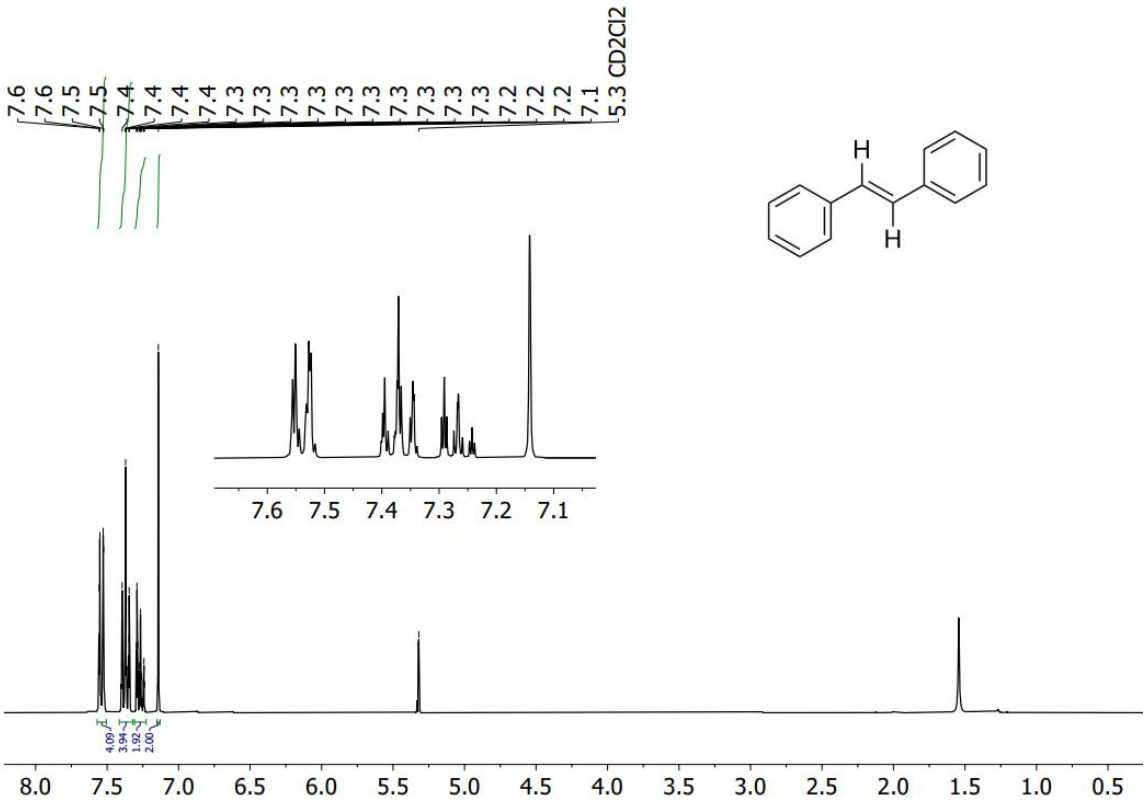


Figure S 37. ^{1}H NMR spectrum (CD_2Cl_2 at 25 °C) of (*E*)-Stilbene after the TSH with $H_3B{\cdot}NH_3$ in CD_3OH.

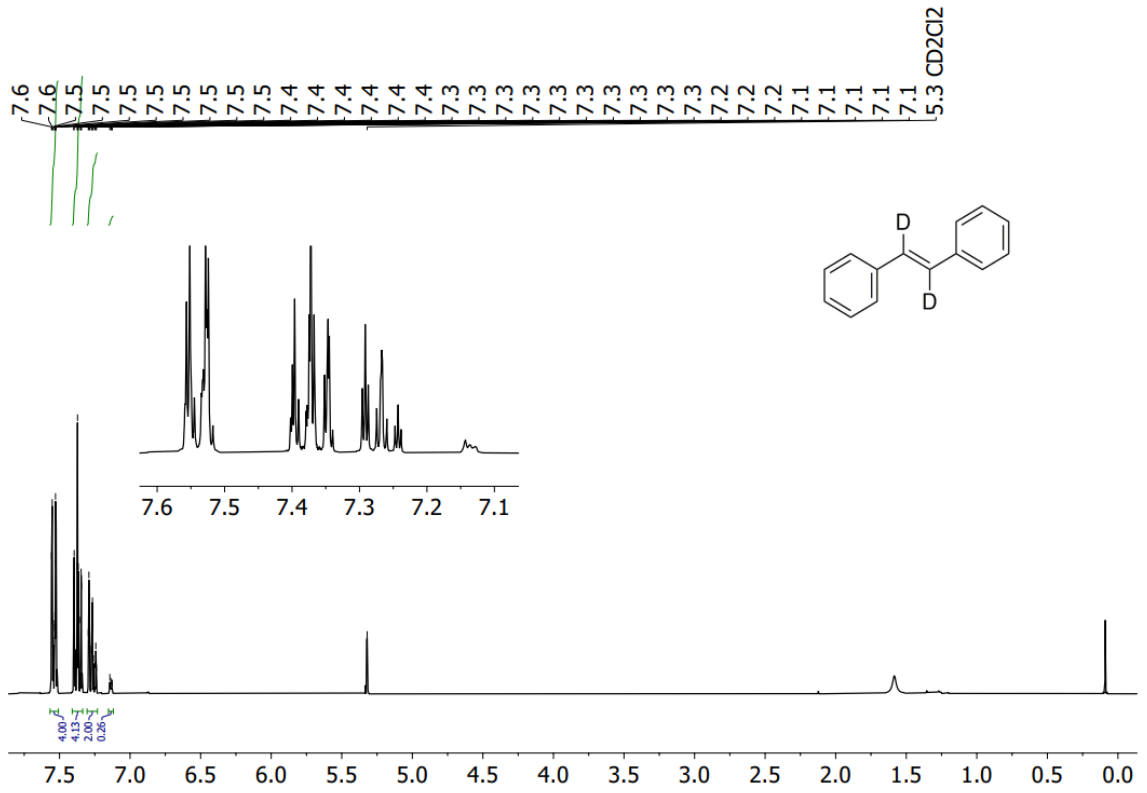


Figure S 38. ^{1}H NMR spectrum (CD_2Cl_2 at 25 °C) of (*E*)-Stilbene after the TSH with $D_3B{\cdot}ND_3$ in CD_3OD.

Control experiments

Mercury poisoning

According to GP 1, cobalt complex **1a** (2.45 mg, 1 mol%), ammonia borane (15.4 mg, 0.50 mmol) and one drop of mercury were made to react with diphenylacetylene (89.1 mg, 0.50 mmol) in methanol (2 mL). The corresponding GC analysis and ^{1}H NMR spectra show full conversion to (*E*)-stilbene.

PMe_3 poisoning

According to GP 1, cobalt catalyst **1a** (2.45 mg, 1 mol%), ammonia borane (15.4 mg, 0.50 mmol) were made to react with diphenylacetylene (89.1 mg, 0.50 mmol) in methanol (2 mL). After a reaction time of 3 min, PMe_3 (0.1 eq or 100 eq) was added and stirred for 12 h. The corresponding GC-analysis and ^{1}H-NMR-spectra shows full conversion to (*E*)-stilbene.

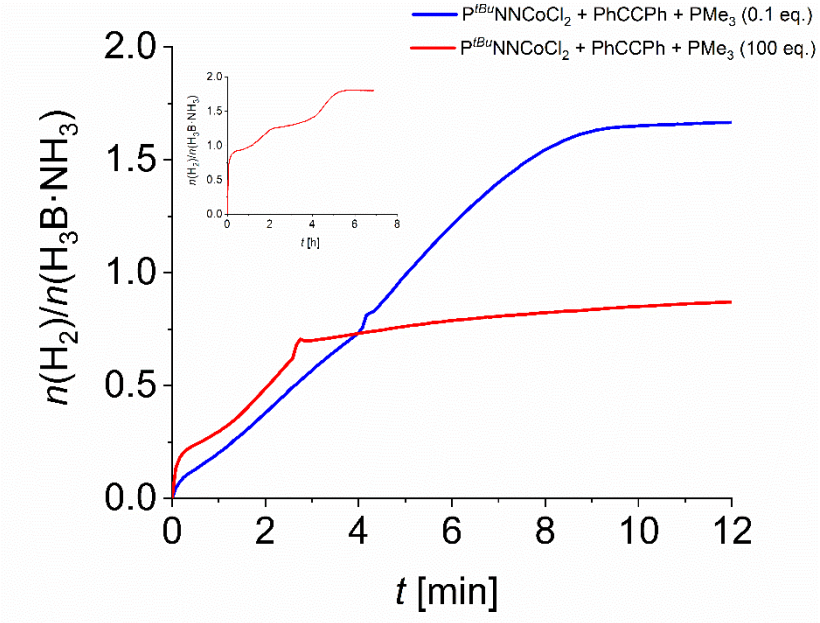


Figure S 39. Comparison of volumetric data from PMe_3 poisoning experiments.

Reaction under H_2 atmosphere

Under an atmosphere of argon, cobalt catalyst **1a** (2.45 mg, 1 mol%) was dissolved in MeOH or THF (2 ml). The reaction mixture was then degassed by using freeze-pump-thaw cycles (3x). Afterwards the Schlenk tube was purged with hydrogen gas and diphenylacetylene (89.1 mg, 0.50 mmol) was added. The reaction mixture was stirred at room temperature for 2 days under an atmosphere of hydrogen. Then CH_2Cl_2 (5 mL) were added, and an aliquot part of this solution was analyzed by gas chromatography. The corresponding GC analysis and ^{1}H NMR spectra shows no conversion to the (*E*)- or (*Z*)-product.

Reaction in the presence of base under H_2 atmosphere

Under an atmosphere of argon, cobalt catalyst **1a** (2.45 mg, 1 mol%) and KOtBu (1−2 eq.) was dissolved in MeOH. The reaction mixture was then degassed by using freeze-pump-thaw cycles (3x). Afterwards the Schlenk tube was purged with hydrogen gas and diphenylacetylene (89.1 mg, 0.50 mmol) was added. The reaction mixture was stirred at room temperature for 2 day under an atmosphere of hydrogen. Then CH_2Cl_2 (5 mL) were added, and an aliquot part of this solution was analyzed by gas chromatography. The corresponding GC analysis shows no conversion to the (*E*)- or (*Z*)-product.

*Reaction of **1a** with MeOH*

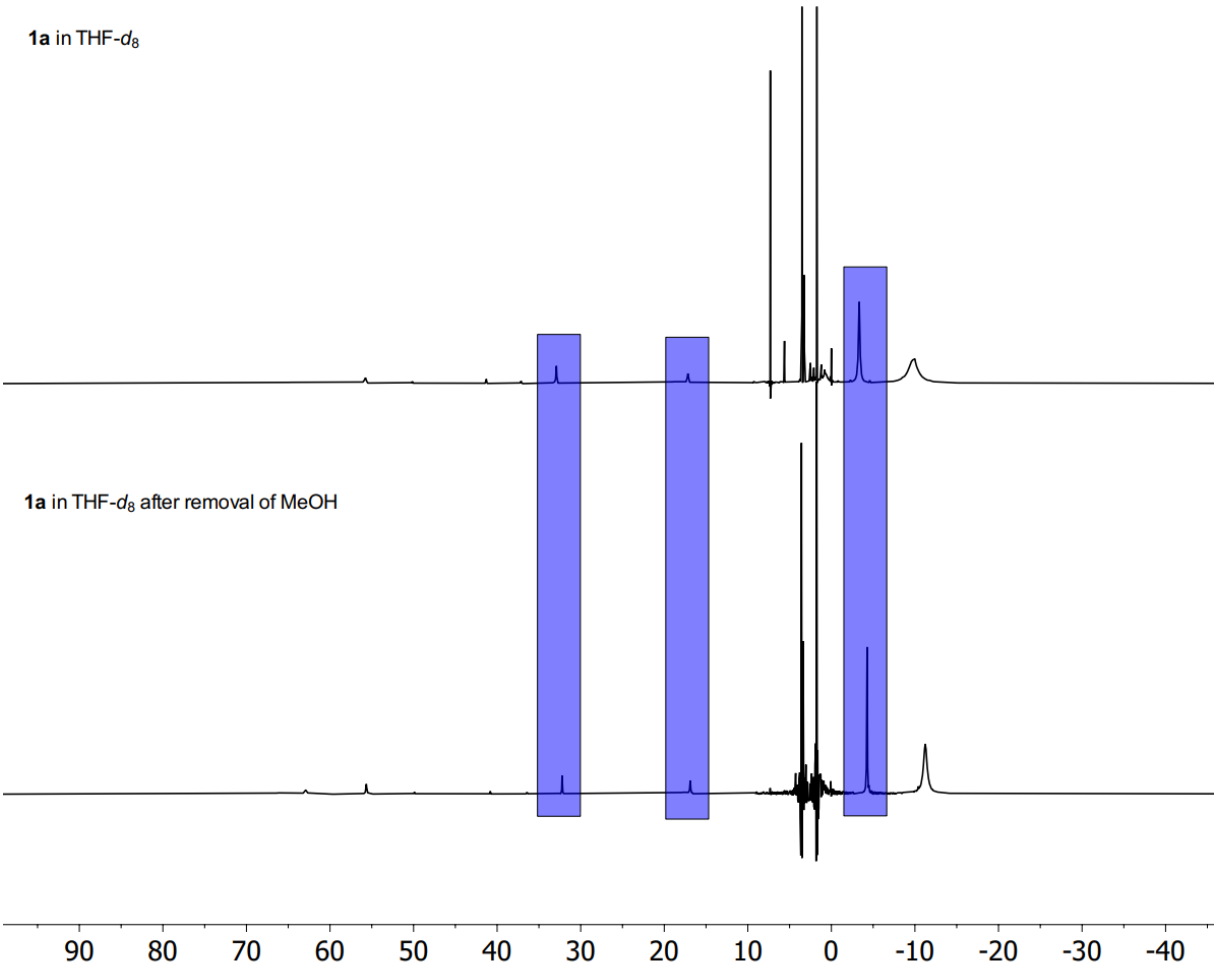


Figure S 40. ^{1}H NMR spectrum (THF-d_8 at 25 °C) of **1a** before the addition of MeOH (above) and **1a** after removal of MeOH (below).

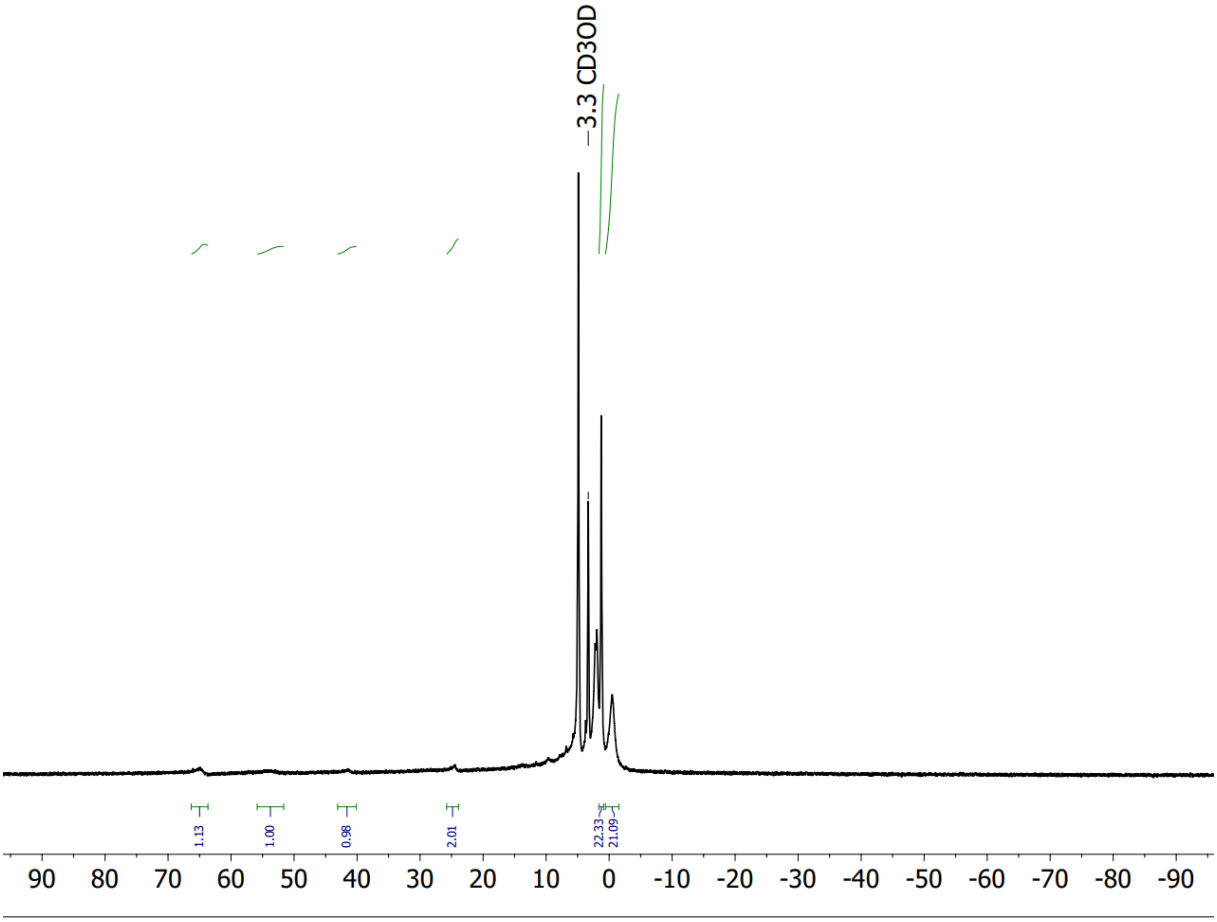


Figure S 41. In situ ^{1}H NMR spectrum (CD_3OD at 25 °C) of catalytic mixtures using complex **1a** as catalyst.

*TSH with **1a** in the presence of Zn*

Under an atmosphere of Ar, cobalt catalyst (2.45 mg, 1 mol%) and Zn (1 eq.) were stirred together in MeOH (2 mL) at ambient temperature for 2 h. Then the reaction mixture was filtered in to an empty Schlenk flask containing diphenylacetylene (89.1 mg, 0.5 mmol) and ammonia borane (15.4 mg, 0.5 mmol). This mixture was stirred for another 2 h. Then CH_2Cl_2 (5 mL) was added, an aliquot of this solution was analysed by gas chromatography (Table S4).

Table S 4. TSH of diphenylacetylene with **1a** in the presence of different additives.

Entry	Cat.	[Co] mol%	Addiditve	T / °C	Conv.	*E*/*Z*
1	—	—	Zn	r.t	51	11/89
2	**1a**	1	Zn	r.t	84	37/63
3	**1a**	1	Zn	40	100	100/0

Yields were determined by GC-Analysis.

*Reaction of **1a** with Zn*

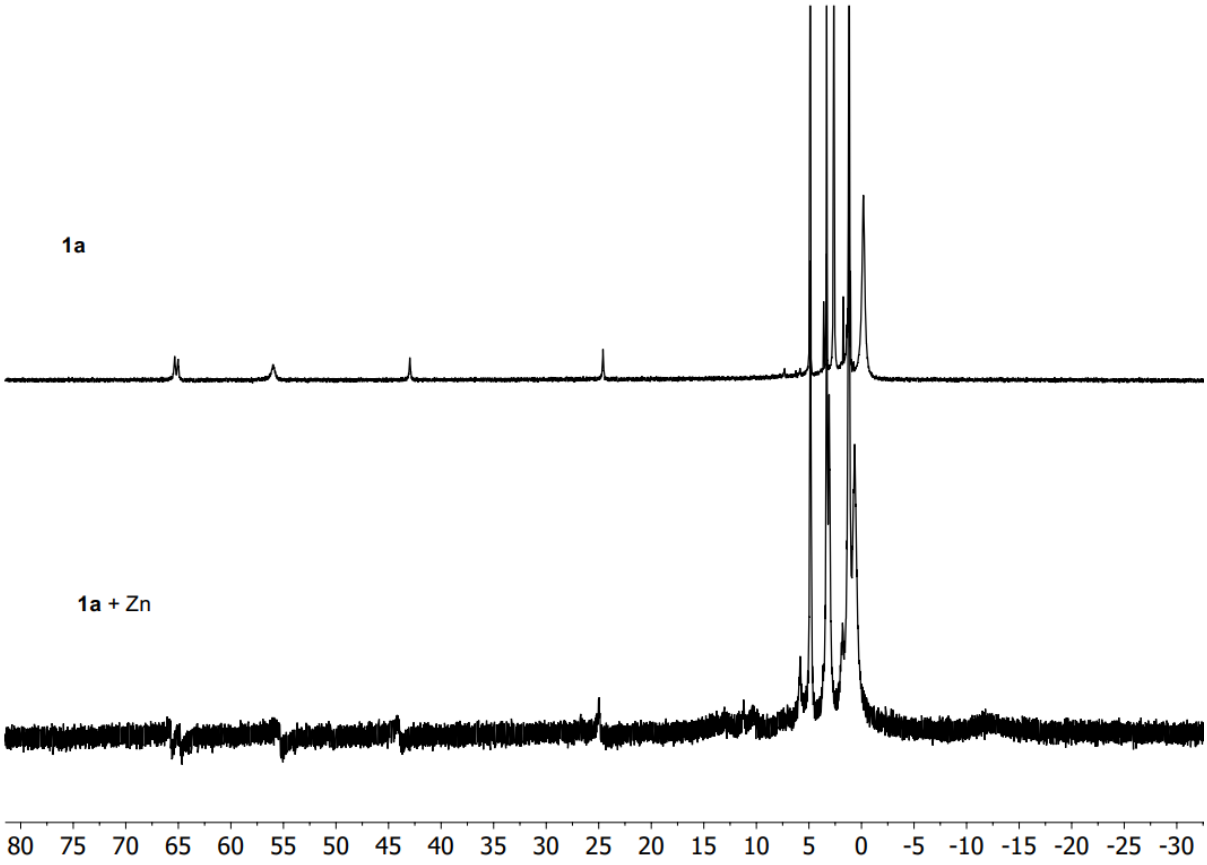


Figure S 42. In situ ^{1}H NMR spectrum (CD_3OD at 25 °C) of complex **1a** (20.4 mmol) in presence of Zn (1 eq.).

*TSH with **1a-Me***

According to GP 3, cobalt complex **1a-Me** (2.52 mg, 1 mol%), ammonia borane (15.4 mg, 0.50 mmol) were reacted with diphenylacetylene (89.1 mg, 0.50 mmol) in methanol (2 mL). Results are shown in Table S 5.

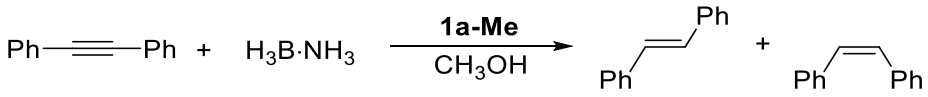


Table S 5. Summary of the TSH experiments with catalyst 1a-Me.

Entry	*c* / mol%	time / h	Conv. / %	*E*/*Z* (GC)
1	1	0.5	58	56/54
2	1	1	70	61/39
3	1	15	99	81/19
4	1	17	94	67/33

Reaction conditions: Alkyne (0.50 mmol), $H_3B{\cdot}NH_3$ (0.50 mmol), *V*(MeOH) = 2.0 mL, Yields were determined by GC-Analysis.

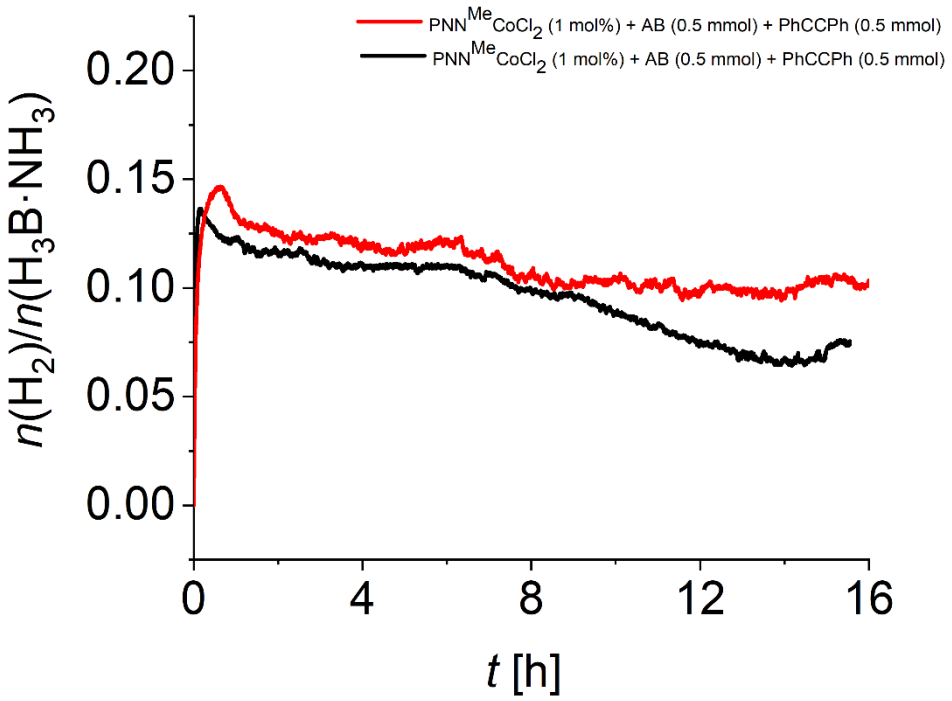


Figure S 43. Volumetric curves of the TSH with **1a-Me** and diphenylacetylene. Red: entry 4 (Table S 5). Black: entry 3 (Table S 5).

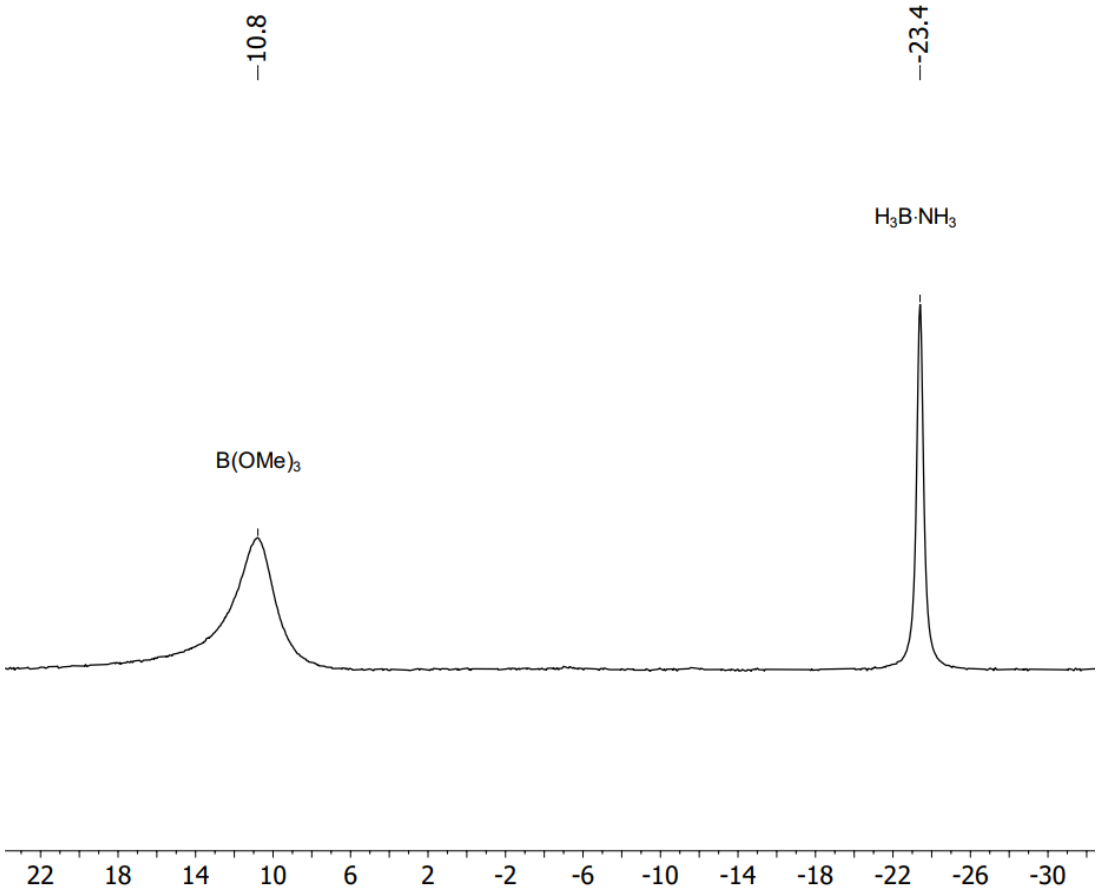


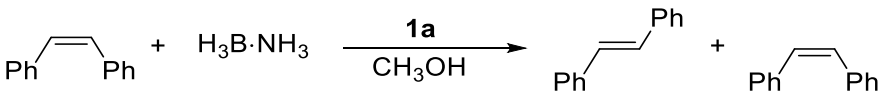
Figure S 44. $^{11}B\{H\}$ NMR spectrum of the reaction mixture of entry 3 (Table S 5) (CD_3OD, 25 °C).

Isomerisation experiments

General procedure (GP2)

Under an atmosphere of argon, cobalt complex **1a** (1 mol%) and ammonia borane (15.4 mg, 0.50 mmol) were added sequentially to a preheated schlenk tube equipped with a magnetic stir bar. (*Z*)-Stilbene (85.7 µL, 89.1 mg, 0.50 mmol) was dissolved in MeOH (2 ml) and added to the Schlenk tube. The reaction mixture was then stirred for 1−3.5 h at given temperature. Subsequently the reaction mixture was exposed to air and CH_2Cl_2 (5 mL) were added. An aliquot of this solution was analysed by gas chromatography with biphenyl as the internal standard.

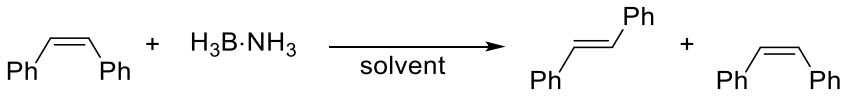
Table S 6. Summary of isomerisation experiments in presence of catalyst and ammonia borane.



entry	*c* / mol%	solvent	*T* / °C	time / h	*E*/*Z* (GC)
1	3	MeOH	50	0.5	100/0
2	1	MeOH	r.t	0.5	97/3
3	1	*i*-PrOH	r.t	0.5	97/3
4	1	THF	r.t	3	82/18

Reaction conditions: (*Z*)-Stilbene (0.50 mmol), $H_3B{\cdot}NH_3$ (0.50 mmol), *V*(solvent)= 2.0 mL, *E*/*Z*-ratio was determined by GC analysis using biphenyl as the internal standard.

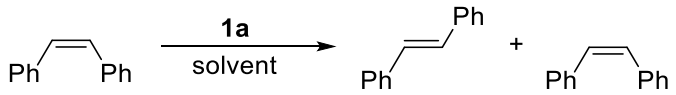
Table S 7. Summary of isomerisation experiments in absence of catalyst.



entry	solvent	*T* / °C	time / h	*E*/*Z* (GC)
1	MeOH	r.t	1	85/15
2	MeOH	r.t	2	82/18
3	MeOH	r.t	3.5	82/18
4	MeOH	50	0.5	86/14
5	*i*-PrOH	r.t	1	88/12
6	*i*-PrOH	50	1	88/12

Reaction conditions: (*Z*)-Stilbene (0.50 mmol), $H_3B{\cdot}NH_3$ (0.50 mmol), *V*(solvent)= 2.0 mL, *E*/*Z*-ratio was determined by GC analysis using biphenyl as the internal standard.

Table S 8. Summary of isomerisation experiments in absence of catalyst and ammonia borane.



entry	solvent	*T* / °C	time / h	*E*/*Z* (GC)
1	MeOH	r.t	0.5	39/61
2	*i*-PrOH	r.t	0.5	29/71

Reaction conditions: (*Z*)-Stilbene (0.50 mmol), *V*(solvent)= 2.0 mL, *E*/*Z*-ratio were determined by GC-Analysis using biphenyl as the internal standard.

Volumetric studies

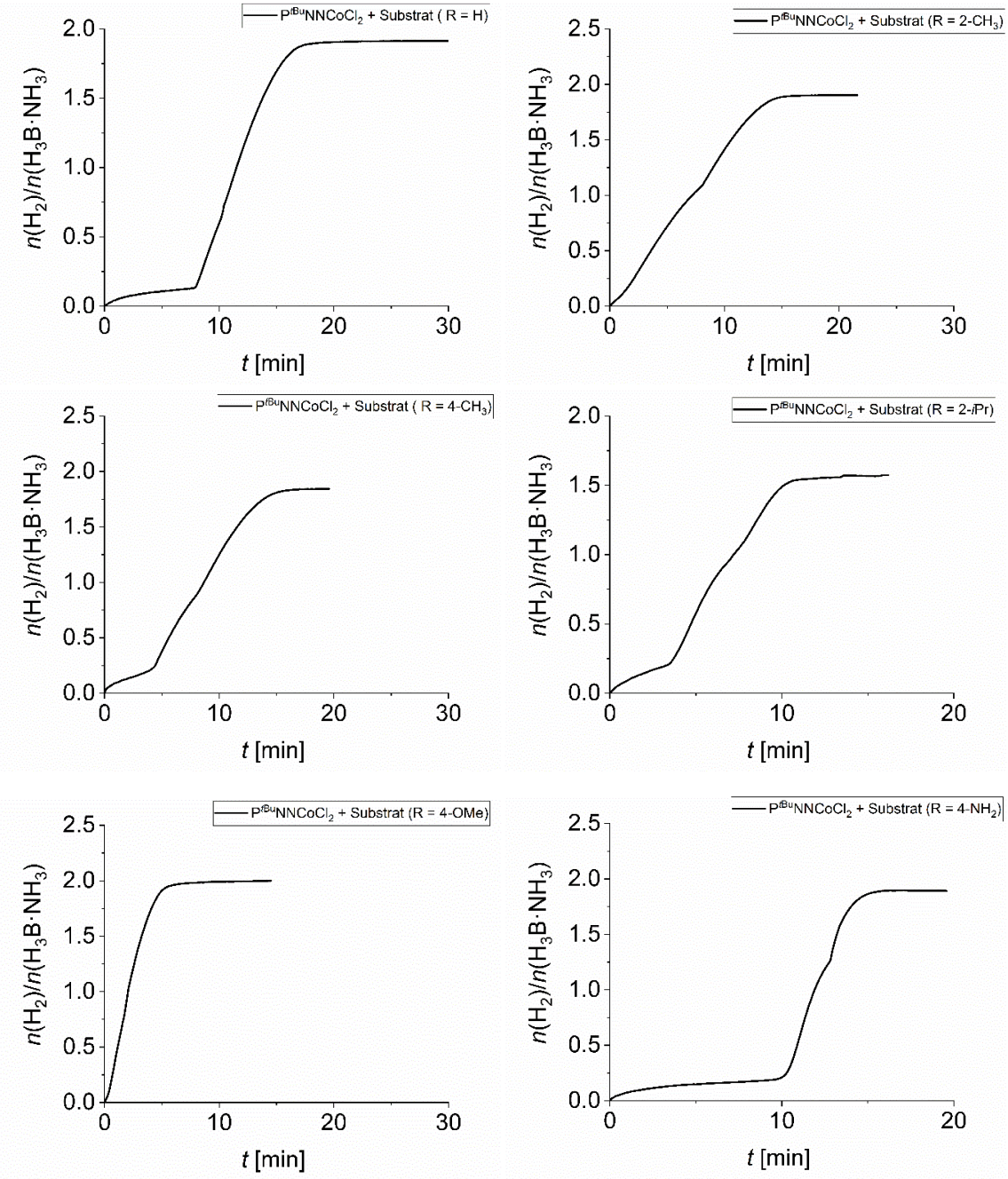


Figure S 45. Volumetric curves of the TSH with **1a** and different substituted alkynes (Part 1).

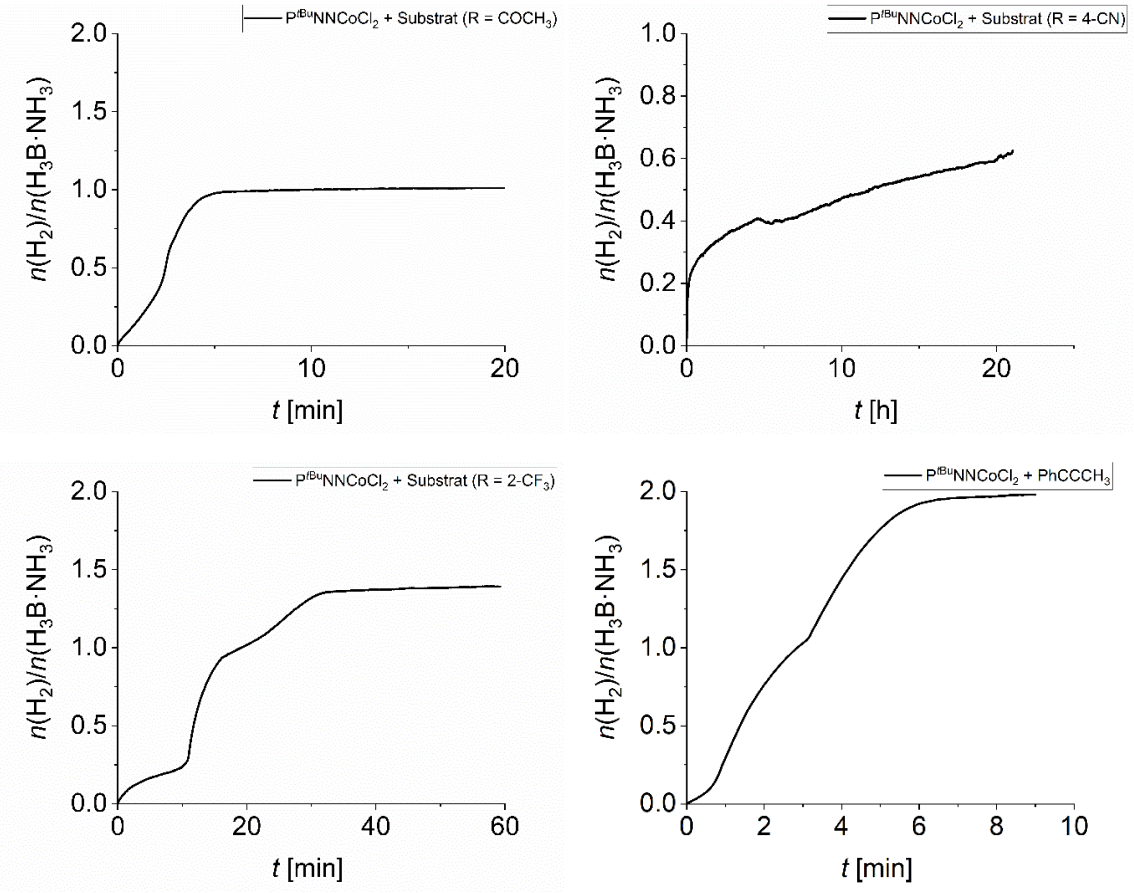


Figure S 46. Volumetric curves of the TSH with **1a** and different substituted alkynes (Part 2).

DFT calculations

All calculations were carried out with Gaussian 16 program.[11] Geometry optimisation was performed in gas phase at the M06L level[12] with the TZVP basis set (M06L/TZVP).[13] The M06L functional has been validated in our recent work[14] in which benchmark calculations have been performed for thermodynamic parameters of the Co(I) and Co(III) PNP complexes by using different density functional methods in conjugation of solvation and van der Waals dispersion correction, and M06L has been found to show the best agreement with experiment. In addition, we also showed that M06L functional can reproduce the difference of the enthalpy of formation between *cis*- and *trans*-stilbene as well as the hydrogenation enthalpy from *trans*-stilbene to 1,2-diphenyl ethane within 1 kcal·mol^{-1} in gas phase.[15] All these show the best performance in calculating the kinetics and thermodynamics. All optimised structures were further characterised either as energy minimums without imaginary frequencies or transition states with only one imaginary frequency by frequency analysis. On the basis of M06L/TZVP geometries in the gas phase, single-point energies were calculated by including the solvation effect of methanol as solvent based on solute electron density (SMD[16]) at the M06L-SCRF (M06L-SCRF/TZVP//M06L/TZVP). The Gibbs free energies were further corrected to standard state in solution with a standard concentration of 1 mol·L^{-1} (p = 24.5 atm) from the standard state in gas phase (p = 1 atm). In our calculations, we used catalyst (**1a**), substrates and intermediates in real-size; this can rule out the effect of oversimplification. The computed energetic data and optimised Cartesian coordinates are listed in Supporting Information.

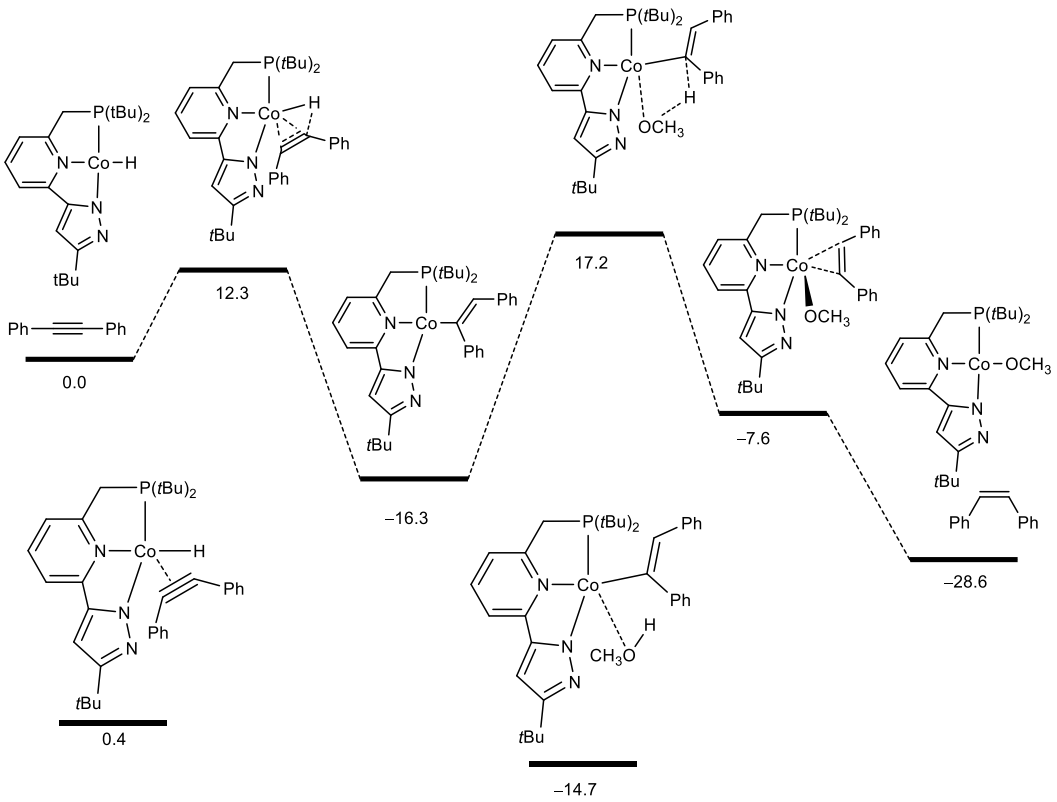


Figure S 47. Full Gibbs free energy profile for the hydrogenation of 1,2-diphenylacetylene to *Z*-stilbene (kcal·mol^{-1}).

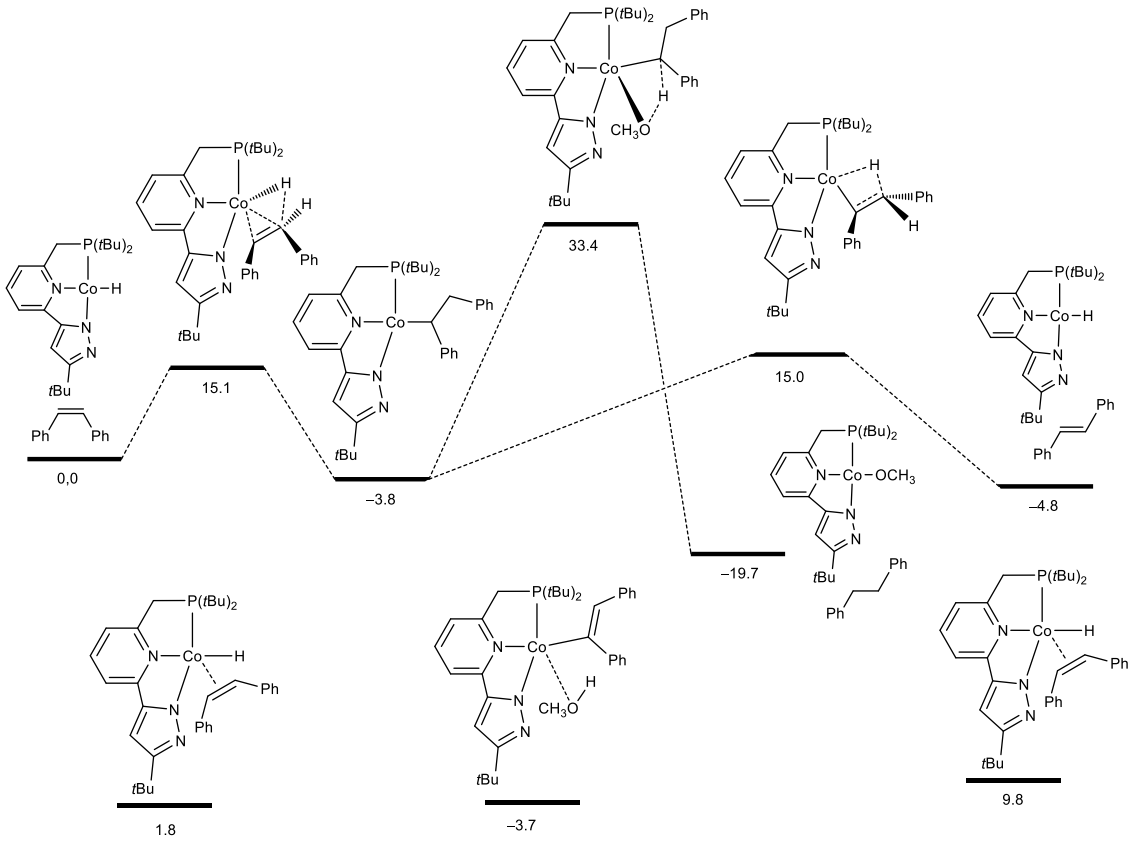
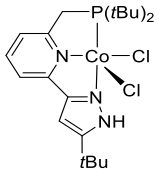
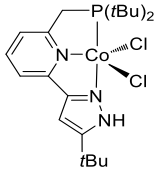
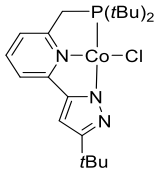
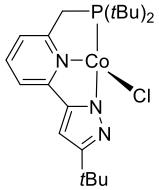
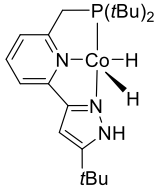
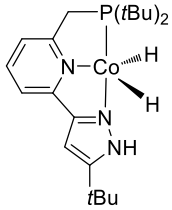


Figure S 48. Full Gibbs free energy profile for isomerization of *Z*-stilbene to *E*-stilbene as well as hydrogenation to 1,2-diphenyl ethane (kcal·mol^{-1}).

Table S 9. M06L/TZVP computed energetic data from structure optimisation in gas phase (M06L/TZVP//FOpt) as well as in methanol solution from single-point calculation on using the gas phase optimised structures (M06L-SCRF/TZVP//M06L/TZVP/SP).

	M06L/TZVP//FOpt	M06L-SCRF/TZVP//M06L/TZVP/SP
 **1a-Doublet**	HF=-3629.8430585 ZPE=0.522884 NImag=0 Htot=-3629.286642 Gtot= -3629.382901	HF=-3629.8873938 ZPE= 0.521854 NImag=0 Htot= -3629.331794 Gtot= -3629.430217
 **1a-Quartet**	HF=-3629.8419592 ZPE=0.521440 NImag=0 Htot=-3629.286079 Gtot= -3629.386989	HF=-3629.8850597 ZPE= 0.520415 NImag=0 Htot= -3629.330060 Gtot= -3629.432122
 **^{PNN}Co-Cl-Doublet**	HF=-3168.9833244 ZPE=0.508132 NImag=0 Htot=-3168.443703 Gtot=-3168.535088	HF=-3169.0275229 ZPE= 0.507125 NImag=0 Htot= -3168.489632 Gtot= -3168.578649
H-Cl	HF=-460.8061245 ZPE=0.006842 NImag=0 Htot=-460.795978 Gtot= -460.817166	HF=-460.8120891 ZPE=0.006839 NImag=0 Htot=-460.801945 Gtot= -460.823133
 **^{PNN}Co-Cl-Quartet**	HF=-3168.9771163 ZPE= 0.508016 NImag=0 Htot= -3168.437346 Gtot= -3168.530838	HF=-3169.0166433 ZPE= 0.506739 NImag=0 Htot= -3168.478663 Gtot= -3168.572275
 **^{PNN}Co(H)2-Doublet**	HF=-2710.4648002 ZPE=0.532207 NImag=0 Htot=-2709.901795 Gtot= -2709.991237	HF=-2710.4985094 ZPE= 0.530898 NImag=0 Htot= -2709.937453 Gtot= -2710.024837
 **^{PNN}Co(H)2-Quartet**	HF=-2710.4334515 ZPE=0.529069 NImag=0 Htot=-2709.872327 Gtot= -2709.966361	HF=-2710.4801352 ZPE= 0.527467 NImag=0 Htot= -2709.921880 Gtot= -2710.011615
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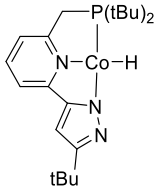
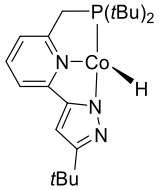
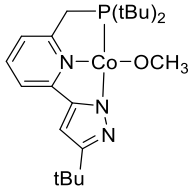
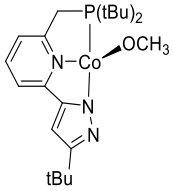
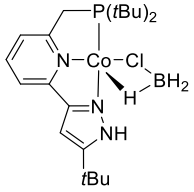
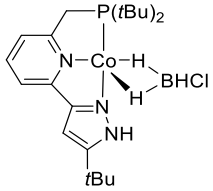
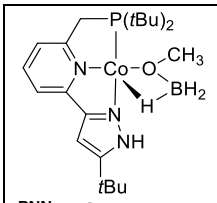
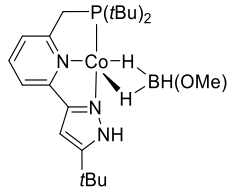
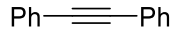
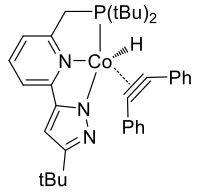
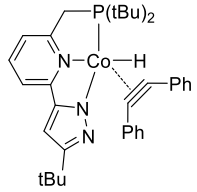
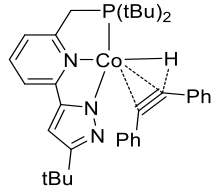
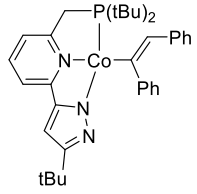
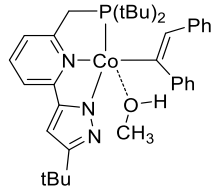
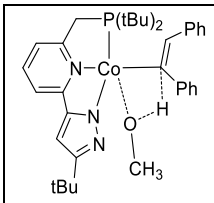
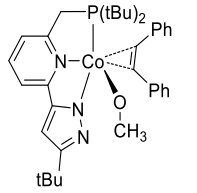
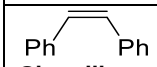
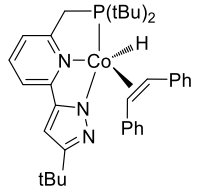
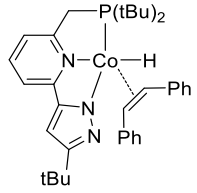
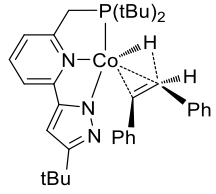
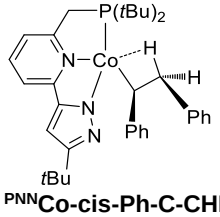
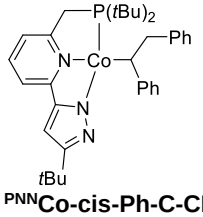
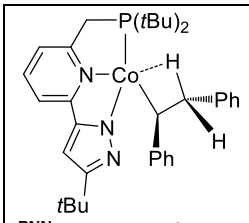
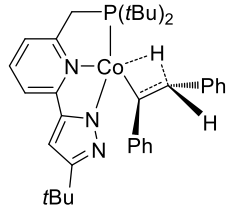
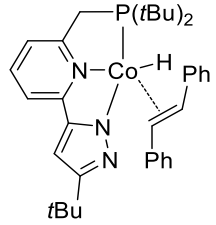
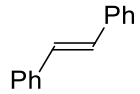
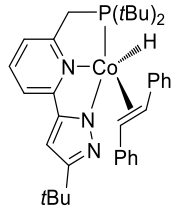
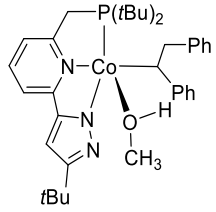
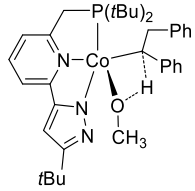
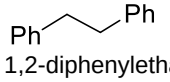
LCoH-OCH3-Anion-Doublet	HF=-2824.5032846 ZPE=0.551899 NImag=0 Htot=-2823.917806 Gtot= -2824.013537	HF=-2824.5954532 ZPE=0.551723 NImag=0 Htot=-2824.012768 Gtot= -2824.100798

LCoH-OCH3-Anion-Q	HF=-2824.4901848 ZPE=0.549642 NImag=0 Htot=-2823.905728 Gtot= -2824.005796	HF=-2824.5887774 ZPE=0.548478 NImag=0 Htot=-2824.008395 Gtot= -2824.100142
LDHCo-H-Anion	HF=-2709.3243999 ZPE=0.509689 NImag=0 Htot=-2708.784475 Gtot= -2708.871971	HF=-2709.4168042 ZPE=0.509711 NImag=0 Htot=-2708.878656 Gtot= -2708.960275
LDHCo-H-Anion-Triplet	HF=-2709.3257488 ZPE=0.508704 NImag=0 Htot=-2708.786474 Gtot= -2708.875866	HF=-2709.416925 ZPE=0.507956 NImag=0 Htot=-2708.879816 Gtot= -2708.965103
LDHCo-Alkynyl-OH-CH3-TS-Anion	HF=-3364.6811203 ZPE=0.755223 NImag= 1 (-1474.2062) Htot=-3363.880551 Gtot= -3364.000229	HF=-3364.7683753 ZPE= 0.754681 NImag=1 (-1588.5016) Htot= -3363.969834 Gtot= -3364.086419
 **^{PNN}CoH-Doublet**	HF=-2709.3010077 ZPE=0.513669 NImag=0 Htot=-2708.757168 Gtot= -2708.846412	HF=-2709.3403456 ZPE= 0.513166 NImag=0 Htot= -2708.797987 Gtot= -2708.883762
 **^{PNN}Co-H_Quartet**	HF=-2709.279053 ZPE=0.511944 NImag= Htot=-2708.736472 Gtot= -2708.826430	HF=-2709.317435 ZPE= 0.508907 NImag=0 Htot= -2708.779311 Gtot= -2708.865446
 **^{PNN}CoOMe-Doublet**	HF=-2823.888669 ZPE=0.547735 NImag=0 Htot=-2823.307654 Gtot= -2823.402919	HF=-2823.9254248 ZPE= 0.546621 NImag=0 Htot= -2823.348042 Gtot= -2823.435414
 **^{PNN}CoOMe-Quartet**	HF=-2823.8820464 ZPE= 0.547311 NImag=0 Htot= -2823.301018 Gtot= -2823.398486	HF=-2823.9201719 ZPE= 0.545739 2823.3744329 Htot= -2823.342056 Gtot= -2823.436132
 **^{PNN}Co(c-H-BH$_2$-Cl)**	HF=-3195.6347416 ZPE=0.540163 NImag=0 Htot=-3195.061006 Gtot= -3195.156997	HF=-3195.6728485 ZPE= 0.538619 NImag=0 Htot= -3195.102086 Gtot= -3195.193023
 **^{PNN}Co(c-H-BHCl-H)**	HF=-3195.6403349 ZPE=0.541240 NImag=0 Htot=-3195.066132 Gtot= -3195.160388	HF=-3195.6817313 ZPE=0.539863 NImag=0 Htot= -3195.108518 Gtot= -3195.206131

 **^{PNN}Co(c-H-BH$_2$-OCH$_3$)**	HF=-2850.5747798 ZPE=0.582570 NImag=0 Htot=-2849.957794 Gtot= -2850.054458	HF=-2850.6089236 ZPE= 0.581399 NImag=0 Htot= -2849.993899 Gtot= -2850.088315
 **^{PNN}Co(c-H-BH(OCH$_3$)-H)**	HF=-2850.5760301 ZPE=0.581776 NImag=0 Htot=-2849.959782 Gtot= -2850.056757	HF=-2850.6131826 ZPE= 0.580416 NImag=0 Htot= -2849.998811 Gtot= -2850.095441
 **1,2-diphenyl acetylene**	HF=-539.5498256 ZPE=0.191224 NImag=0 Htot=-539.346508 Gtot= -539.397315	HF=-539.560954 ZPE=0.191031 NImag=0 Htot= -539.358694 Gtot= -539.405853
 **PNNCo-H + Ph-C$_2$-Ph-trigonal bipyramidal**	HF=-3248.8638408 ZPE=0.706606 NImag= Htot= -3248.114798 Gtot= -3248.230495	HF=-3248.8964235 ZPE= 0.704726 NImag=0 Htot= -3248.149790 Gtot= -3248.264722
 **PNNCo-H + Ph-C$_2$-Ph-tetragonal pyramidal**	HF=-3248.8794302 ZPE=0.706381 NImag=0 Htot=-3248.130241 Gtot= -3248.248521	HF=-3248.9187557 ZPE= 0.704913 NImag=0 Htot= -3248.171698 Gtot= -3248.289055
 **TS1**	HF=-3248.8644769 ZPE=0.705345 NImag=1 (-625) Htot=-3248.116906 Gtot= -3248.234508	HF=-3248.8987255 ZPE= 0.704045 NImag= 1 (-631) Htot= -3248.153121 Gtot= -3248.270071
 **PNNCo-cis-PhC=CHPh**	HF=-3248.9121126 ZPE=0.711217 NImag=0 Htot=-3248.159954 Gtot= -3248.272381	HF=-3248.9565341 ZPE= 0.710959 NImag = 0 Htot= -3248.205618 Gtot= -3248.315513
 **PNNCo-cis-PhC=CHPh + CH$_3$OH**	HF=-3364.6855895 ZPE=0.764568 NImag=0 Htot=-3363.874800 Gtot= -3363.999967	HF=-3364.72324 ZPE= 0.762730 NImag=0 Htot= -3363.915716 Gtot= -3364.036618

 **TS2**	HF=-3364.6371651 ZPE=0.759487 NImag=1 (-1184) Htot=-3363.832465 Gtot= -3363.953350	HF=-3364.669678 ZPE= 0.757530 NImag= 1 (-1303) Htot= -3363.868208 Gtot= -3363.985918
 **PNNCo-OCH_3+cis-Ph-CH=CH-Ph**	HF=-3364.680749 ZPE=0.765329 NImag=0 Htot=-3363.870528 Gtot= -3363.989428	HF=-3364.7140675 ZPE= 0.763155 NImag=0 Htot= -3363.906292 Gtot= -3364.025345
 **Cis-stilbene**	HF=-540.7887551 ZPE=0.214905 NImag=0 Htot=-540.561852 Gtot= -540.611574	HF=-540.7995666 ZPE= 0.214570 NImag=0 Htot= -540.572891 Gtot= -540.623376
 **PNNCo-H + cis-Ph-CH=CH-Ph-trigonal bipyramidal**	HF=-3250.0958269 ZPE=0.730552 NImag=0 Htot=-3249.323398 Gtot= -3249.435939	HF=-3250.1326288 ZPE= 0.729429 NImag=0 Htot= -3249.361116 Gtot= -3249.474823
 **PNNCo-H + cis-Ph-CH=CH-Ph-tetragonal pyramidal**	HF=-3250.1179943 ZPE=0.730134 NImag=0 Htot=-3249.345276 Gtot= -3249.461359	HF=-3250.1595523 ZPE= 0.728942 NImag=0 Htot= -3249.387898 Gtot= -3249.504228
 **TS3**	HF=-3250.105819 ZPE=0.730246 NImag=1 (-662.6301) Htot=-3249.334046 Gtot= -3249.445701	HF=-3250.140871 ZPE= 0.728878 NImag=1 (-680) Htot= -3249.370244 Gtot= -3249.483038
 **^{PNN}Co-cis-Ph-C-CHPh-H-agostic**	HF=-3250.1067169 ZPE=0.732740 NImag=0 Htot=-3249.331980 Gtot= -3249.446307	HF=-3250.1445252 ZPE= 0.731033 NImag=0 Htot= -3249.371109 Gtot= -3249.487533
 **^{PNN}Co-cis-Ph-C-CH_2-Ph**	HF=-3250.1348544 ZPE=0.734860 NImag=0 Htot=-3249.357866 Gtot= -3249.473662	HF=-3250.174805 ZPE= 0.732993 NImag=0 Htot= -3249.401020 Gtot= -3249.513192 DG = -3.80 kcal/mol

 **^{PNN}Co-trans-Ph-C-CHPh-H-agostic**	HF=-3250.1108374 ZPE=0.732920 NImag=0 Htot=-3249.335884 Gtot= -3249.450468	HF=-3250.1501195 ZPE= 0.731760 NImag=0 Htot= -3249.376193 Gtot= -3249.491868
 **TS4**	HF=-3250.1026582 ZPE=0.729522 NImag=1 (-605) Htot=-3249.331290 Gtot= -3249.445503	HF=-3250.1402291 ZPE= 0.727846 NImag=1 (-625) Htot= -3249.371059 Gtot= -3249.483268
 **PNNCo-H + trans-Ph-CH=CH-Ph-tetragonal pyramidal**	HF=-3250.1099403 ZPE=0.729635 NImag=0 Htot=-3249.337792 Gtot= -3249.453406	HF=-3250.1489636 ZPE= 0.728527 NImag=0 Htot= -3249.378665 Gtot= -3249.491554
 **Trans-stilbene**	HF=-540.7960711 ZPE=0.214584 NImag=0 Htot=-540.569251 Gtot= -540.619959	HF=-540.8080128 ZPE= 0.214003 NImag=0 Htot= -540.582458 Gtot= -540.631048
 **PNNCo-H + trans-Ph-CH=CH-Ph-trigonal bipyramidal**	HF=-3250.1066459 ZPE=0.731030 NImag=0 Htot=-3249.333797 Gtot= -3249.445353	HF=-3250.1414281 ZPE= 0.729860 NImag=0 Htot= -3249.369582 Gtot= -3249.482068
 **^{PNN}Co-cis-Ph-C-CH_2-Ph+CH_3OH**	HF=-3365.9100133 ZPE=0.788177 NImag=0 Htot=-3365.075424 Gtot= -3365.200193	HF=-3365.9447167 ZPE= 0.786202 NImag=0 Htot= -3365.112598 Gtot= -3365.236649
 **TS5**	HF=-3365.8508647 ZPE= 0.783491 NImag=0 Htot= -3365.021866 Gtot= -3365.143890	HF=-3365.8846552 ZPE= 0.781390 NImag=0 Htot= -3365.059009 Gtot= -3365.177529
 1,2-diphenylethane	HF=-542.0150722 ZPE=0.238508 NImag=0 Htot=-541.763927 Gtot=-541.816101	HF=-542.0271983 ZPE= 0.238240 NImag=0 Htot= -541.777158 Gtot= -541.826705
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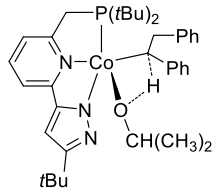
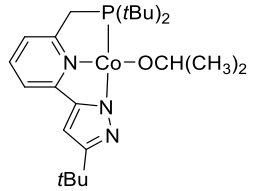
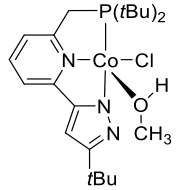
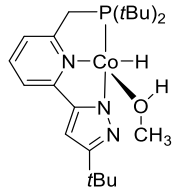
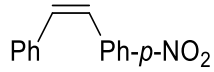
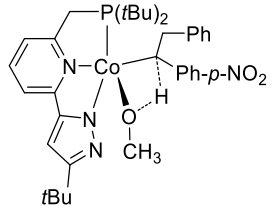
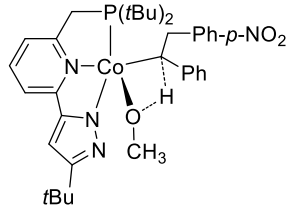
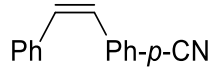
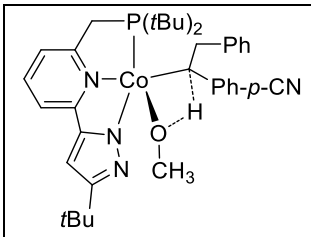
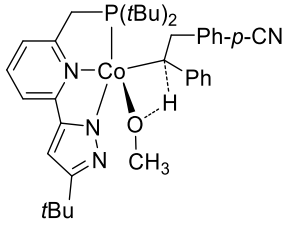
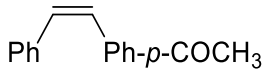
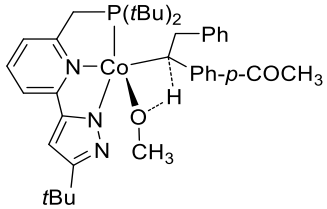
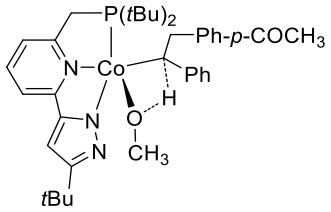
 **TS6**	HF=-3443.2892734 ZPE=0.816249 NImag=1 (-1288) Htot=-3442.425452 Gtot= -3442.551269	HF=-3443.3231864 ZPE= 0.814169 NImag=1 (-1392) Htot= -3442.462773 Gtot= -3442.585069
 ^{PNN}Co-OCH(CH$_3$)$_2$	HF=-2902.5417692 ZPE=0.604048 NImag=0 Htot=-2901.901768 Gtot= -2902.003045	HF=-2902.5787451 ZPE= 0.603017 NImag=0 Htot=-2901.941572 Gtot= -2902.036726
 **^{PNN}Co-Cl+CH$_3$OH**	HF=-3284.7538725 ZPE=0.562282 NImag=0 Htot=-3284.156064 Gtot= -3284.256402	HF=-3284.7901109 ZPE= 0.561137 NImag=0 Htot= -3284.194202 Gtot= -3284.292601
 **^{PNN}Co-H+CH$_3$OH**	HF=-2825.0708278 ZPE=0.567586 NImag=0 Htot=-2824.468966 Gtot= -2824.566995	HF=-2825.1036849 ZPE= 0.566218 NImag=0 Htot= -2824.503812 Gtot= -2824.600746
 (Z)-1-nitro-4-styrylbenzene	HF=-745.3479918 ZPE=0.217238 NImag=0 Htot=-745.116215 Gtot= -745.173392	HF=-745.3607471 ZPE=0.216623 NImag=0 Htot=-745.130334 Gtot= -745.185509
 **TS5-para-NO$_2$-1**	HF=-3570.4134573 ZPE=0.785619 NImag=1 (-1528.1172) Htot=-3569.579620 Gtot= -3569.708831	HF=-3570.449241 ZPE= 0.783532 NImag= 1 (-1621.6943) Htot= -3569.618010 Gtot= -3569.746781
 **TS5-para-NO$_2$-2**	HF=-3570.4121497 ZPE=0.786211 NImag=1 (-1519.4193) Htot=-3569.578009 Gtot= -3569.705936	HF=-3570.4466722 ZPE= 0.783590 NImag=1 (-1597.4319) Htot= -3569.616363 Gtot= -3569.740602
 (Z)-4-styrylbenzonitrile	HF=-633.0538362 ZPE=0.213665 NImag=0 Htot=-632.826395 Gtot= -632.881232	HF=-633.0687026 ZPE=0.213462 NImag=0 Htot=-632.841393 Gtot= -632.896983

 **TS5-para-CN-1**	HF=-3458.1188259 ZPE=0.782268 NImag= 1 (-1498.8733) Htot=-3457.289220 Gtot= -3457.415477	HF=-3458.1561591 ZPE=0.780295 NImag= 1 (-1586.2151) Htot= -3457.328967 Gtot= -3457.454214
 **TS5-para-CN-2**	HF=-3458.1176282 ZPE=0.781951 NImag= 1 (-1526.4252) Htot= -3457.288219 Gtot= -3457.415708	HF=-3458.1546741 ZPE= 0.779962 NImag= 1 (-1634.7201) Htot= -3457.328661 Gtot= -3457.451542
 (Z)-1-(4-styrylphenyl)ethan-1-one	HF=-693.4708321 ZPE=0.252187 NImag=0 Htot=-693.203069 Gtot= -693.262202	HF=-693.4876123 ZPE=0.251714 NImag=0 Htot=-693.221083 Gtot= -693.278130
 **TS5-para-COCH₃-1**	HF=-3518.5342487 ZPE=0.820647 NImag= 1 (-1508.3187) Htot=-3517.664390 Gtot= -3517.795542	HF=-3518.574462 ZPE=0.818776 NImag= 1 (-1600.4532) Htot= -3517.707023 Gtot= -3517.837998
 **TS5-para-COCH₃-1**	HF=-3518.5340399 ZPE=0.820984 NImag=1 (-1511.2896) Htot=-3517.664006 Gtot= -3517.794651	HF=-3518.5732157 ZPE=0.818348 NImag= 1 (-1593.8450) Htot=-3517.706931 Gtot= -3517.835116
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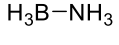
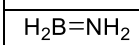
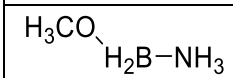
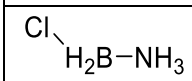
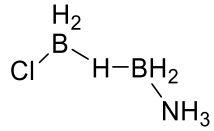
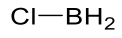
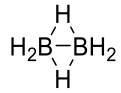
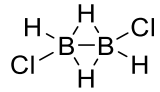
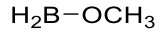
	HF=-83.2338934 ZPE=0.070413 NImag=0 Htot=-83.158727 Gtot= -83.186942	HF=-83.257141 ZPE= 0.070185 Nimag=0 Htot= -83.182179 Gtot= -83.210478
	HF=-82.0552494 ZPE=0.048164 NImag=0 Htot=-82.002907 Gtot= -82.028826	HF=-82.0591652 ZPE= 0.047700 NInag=0 Htot= -82.007254 Gtot= -82.033219
	HF=-197.8224553 ZPE=0.104445 NImag=0 Htot=-197.710799 Gtot= -197.746890	HF=-197.8446269 ZPE= 0.104361 NImag=0 Htot= -197.733124 Gtot= -197.769269
	HF=-542.8918859 ZPE=0.064039 NImag=0 Htot=-542.822491 Gtot= -542.854485	HF=-542.9173884 ZPE= 0.064083 NImag=0 Htot= -542.848047 Gtot= -542.879821

	HF=-569.5342037 ZPE=0.095632 NImag=0 Htot=-569.430762 Gtot= -569.469493	HF=-569.5581873 ZPE= 0.095760 NImag= 0 Htot= -569.454881 Gtot= -569.492459
	HF= -486.2763491 ZPE=0.021290 NImag=0 Htot=-486.251105 Gtot= -486.278337	HF=-486.2787335 ZPE= 0.021132 NImag=0 Htot= -486.253638 Gtot= -486.280882
	HF=-53.3012993 ZPE=0.063984 NImag=0 Htot=-53.232786 Gtot= -53.259113	HF=-53.3030634 ZPE= 0.063708 NImag=0 Htot= -53.234819 Gtot= -53.261151
	HF=-972.5946649 ZPE=0.050149 NImag=0 Htot=-972.538532 Gtot= -972.572862	HF=-972.6029255 ZPE= 0.049830 NImag=0 Htot= -972.547059 Gtot= -972.581527
	HF=-141.2347606 ZPE=0.063780 NImag=0 Htot=-141.165791 Gtot= -141.196199	HF=-141.2366037 ZPE= 0.063547 NImag=0 Htot= -141.167824 Gtot= -141.198368
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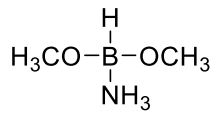
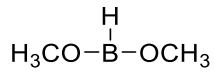
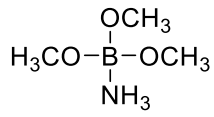
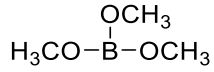
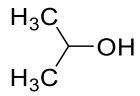
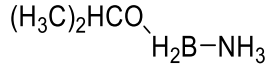
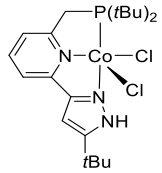
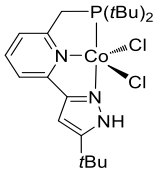
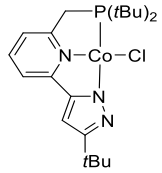
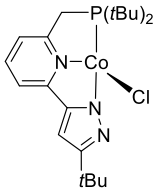
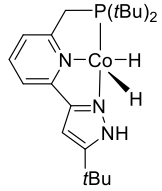
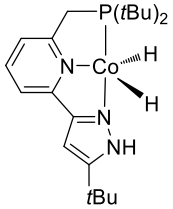
	HF=-312.4209094 ZPE=0.138154 NImag=0 Htot=-312.272847 Gtot= -312.316515	HF=-312.4423422 ZPE= 0.138048 NImag=0 Htot= -312.295308 Gtot= -312.336587
	HF=-255.8495103 ZPE=0.098538 NImag=0 Htot=-255.743156 Gtot= -255.782367	HF=-255.8529767 ZPE= 0.098445 NImag=0 Htot= -255.746753 Gtot= -255.785033
	HF=-427.0217243 ZPE=0.171866 NImag=0 Htot=-426.837425 Gtot= -426.885378	HF=-427.0420082 ZPE= 0.171434 NImag=0 Htot= -426.859736 Gtot= -426.903980
	HF=-370.4574906 ZPE=0.132399 NImag=0 Htot=-370.314306 Gtot= -370.361379	HF=-370.4625145 ZPE= 0.132553 NImag=0 Htot= -370.319392 Gtot= -370.364181
	HF=-194.3945237 ZPE=0.108283 NImag=0 Htot=-194.279872 Gtot= -194.313587	HF=-194.4048783 ZPE= 0.107815 NImag=0 Htot=-194.290543 Gtot= -194.324617
 BH2OIso-NH3	HF=-276.4693244 ZPE=0.161310 NImag=0 Htot=-276.298474 Gtot= -276.340706	HF=-276.4930189 ZPE= 0.161151 NImag=0 Htot = -276.322456 Gtot= -276.364289

Table S 10. M06L/TZVP optimised Cartesian Coordinates in gas phase.

 **1a-Doublet**	 **1a-Quartet**
Co,0,-0.0670756794,-0.1898917832,1.0364216748	Co,0,0.498836086,-0.2828144141,1.2104021084
P,0,0.0451708493,2.0136384156,0.8353025196	P,0,0.2421511532,2.0734982393,0.8439125588
N,0,-1.6063603358,0.1533633143,2.1998854628	N,0,-1.3507402851,0.0853703414,2.3249573351
C,0,-3.7972564097,0.4644948748,3.8507062987	C,0,-3.7274352665,0.466139401,3.6524185618
C,0,-2.3374149592,-0.9311872279,2.5811747746	C,0,-2.1361223508,-0.9714325372,2.6127802119
C,0,-1.9160571168,1.3736223577,2.6751398393	C,0,-1.7066581224,1.3205185507,2.6952703505
C,0,-3.0246962518,1.5589404646,3.4879651193	C,0,-2.9104727804,1.5448064496,3.3575393824
C,0,-3.4412368792,-0.7973463358,3.4091905844	C,0,-3.3392800378,-0.8120058942,3.2879758432
H,0,-3.2630635922,2.5518976965,3.8449075574	H,0,-3.1915907508,2.5520960129,3.6355558785
H,0,-4.0065393233,-1.6742342755,3.6944931869	H,0,-3.9582957371,-1.6710788318,3.5086271658
H,0,-4.6617976522,0.5954251856,4.4882776518	H,0,-4.6663726589,0.6212463431,4.1690150153
C,0,-0.9471947453,2.4603179715,2.3429558161	C,0,-0.7354832635,2.4198844777,2.3949814043
H,0,-0.209406168,2.4749416049,3.1506226657	H,0,0.0186891555,2.4067813034,3.1878416824
H,0,-1.4161143689,3.4449391037,2.3110748932	H,0,-1.2215238311,3.3969188146,2.4247430157
C,0,-1.0058258852,2.5610070598,-0.650991507	C,0,-0.9658019131,2.4541866818,-0.5725766862
C,0,1.6681721043,2.989447616,0.9539084633	C,0,1.6757610378,3.3149969521,0.8924572792
C,0,2.6990669626,2.1882702791,0.1573068727	C,0,2.7593820625,2.740508028,-0.0245122864
H,0,3.6582264336,2.7110288606,0.186907995	H,0,3.6379659024,3.3899323068,0.0021076199
H,0,2.4172293425,2.0588648884,-0.8877727118	H,0,2.4367988989,2.6615090427,-1.0619427848
H,0,2.831090515,1.1939241044,0.5853387833	H,0,3.0620652213,1.744936846,0.3022479375
C,0,2.1172999242,3.0496463204,2.4145052502	C,0,2.2256306886,3.3426949237,2.3201225704
H,0,3.140650965,3.4315463049,2.4386887784	H,0,3.186308701,3.8631438389,2.313498476
H,0,2.1109115997,2.0665564785,2.8869895884	H,0,2.3902517718,2.3402455553,2.7193679342
H,0,1.5074881533,3.7396221141,3.0010047631	H,0,1.5712464997,3.8904317371,3.0002602793
C,0,1.5683747605,4.4196535933,0.4325340224	C,0,1.3207950775,4.7380560556,0.4790691272
H,0,2.5346420459,4.9085087383,0.5802736852	H,0,2.2013960812,5.3750630725,0.6000211713
H,0,0.8272190136,5.0056056557,0.9794977592	H,0,0.5303365384,5.1617776105,1.1014578019
H,0,1.3399091487,4.4792510655,-0.6301018759	H,0,1.0132478681,4.814210277,-0.5632732897
C,0,-0.1681943078,2.4451836812,-1.9237879665	C,0,-0.1697789859,2.4880230032,-1.8764596375
H,0,0.6255484968,3.1892184982,-1.9745147836	H,0,0.4918464642,3.3511831081,-1.9416328137
H,0,-0.8139518108,2.6013245607,-2.7916444304	H,0,-0.8616344915,2.5456234825,-2.7206078402
H,0,0.2820918766,1.4547576802,-2.0131586565	H,0,0.4270005095,1.5810728252,-1.9975615316
C,0,-2.1568323951,1.5540885754,-0.7508325351	C,0,-1.9345337277,1.2676969468,-0.6548207069
H,0,-1.7897743269,0.5358262876,-0.8969356421	H,0,-1.4049609402,0.3180130726,-0.7662540766
H,0,-2.7792393431,1.8092052499,-1.6122851087	H,0,-2.5729635002,1.3917768897,-1.5335128309
H,0,-2.7997747393,1.5660741752,0.1310971904	H,0,-2.5919850927,1.2038641732,0.2131550844
C,0,-1.6024999887,3.958527963,-0.514520058	C,0,-1.7819456438,3.7291564841,-0.3933668296
H,0,-0.8517390922,4.7431967301,-0.4652764232	H,0,-1.1696519769,4.6272229967,-0.3517750917
H,0,-2.2460194023,4.0463636488,0.3626029971	H,0,-2.3953046991,3.6944478648,0.509586624
H,0,-2.2285777704,4.163930637,-1.3867023953	H,0,-2.4686466614,3.8422038925,-1.2368464823
Cl,0,1.0867263912,-0.8415025366,-0.8201402132	Cl,0,1.2223537611,-1.0589915663,-0.8529052517
Cl,0,1.3866784053,-0.3214685569,2.9503131527	Cl,0,1.9185087334,-0.2310316085,2.9905415475
C,0,-1.8253547231,-2.16125773,2.0244492516	C,0,-1.6311313237,-2.2400285287,2.1109655371
N,0,-0.7492478182,-1.9807307927,1.2523837111	N,0,-0.4554340282,-2.187040522,1.4859642985
C,0,-2.13760595,-3.5301274653,2.075205706	C,0,-2.1470967654,-3.5472084767,2.0624880454
H,0,-2.9401313441,-4.0071256628,2.6097643136	H,0,-3.0729130684,-3.9129844252,2.4712886763
C,0,-1.1895340682,-4.160354856,1.2903958249	C,0,-1.2174026031,-4.2858071223,1.3552415397
N,0,-0.3748369328,-3.1788840582,0.8212181172	N,0,-0.2228383885,-3.4163940578,1.0406523738
H,0,0.407274713,-3.1952355634,0.1750319897	H,0,0.584664547,-3.5344757799,0.4418383813
C,0,-0.9762464964,-5.6066333508,0.940073181	C,0,-1.1794650432,-5.7312993873,0.9433553455
C,0,-2.0345740834,-6.456644575,1.636810627	C,0,-2.429296538,-6.437828461,1.4601522335
H,0,-1.9758138468,-6.3580192886,2.7214668981	H,0,-2.4899337771,-6.398233887,2.548544471
H,0,-1.8892516105,-7.5086630899,1.3909533931	H,0,-2.4134743956,-7.487612421,1.1666729658
H,0,-3.0418385939,-6.1788226601,1.3232811755	H,0,-3.3378888189,-5.9930891859,1.0519860942
C,0,-1.0929105009,-5.7909088742,-0.5774622335	C,0,-1.136079855,-5.8270880598,-0.5863020037
H,0,-0.3398284009,-5.2149613468,-1.1168769666	H,0,-0.2469947603,-5.3501168006,-1.0009487053
H,0,-2.0730531497,-5.4804643286,-0.9404556753	H,0,-2.0077369823,-5.352960962,-1.0378630289
H,0,-0.9521197437,-6.8403300974,-0.839862371	H,0,-1.1208835734,-6.8728096053,-0.8964234693

C,0,0.4171338121,-6.0465249146,1.4039478725	C,0,0.0657438341,-6.4020909613,1.5342350225
H,0,0.537435804,-5.9136875684,2.4790540189	H,0,0.0714696154,-6.3393849795,2.622545442
H,0,1.2079980104,-5.4811881024,0.9097929526	H,0,0.9860044549,-5.9439711953,1.169921103
H,0,0.5733336505,-7.1009531037,1.1720838402	H,0,0.0919811744,-7.4563943305,1.2554989506
 **^{PNN}Co-Cl-Double**	 **^{PNN}Co-Cl-Quartet**
Co,0,-0.1370345674,-0.1913640348,0.9719586931	Co,0,0.5082367164,-0.3368387765,1.6552461776
P,0,-0.0400569774,2.0175490111,0.7381293756	P,0,0.226599138,1.9478950748,0.9366887817
N,0,-1.6357966221,0.1750201531,2.1696844485	N,0,-1.3104263417,0.1814945163,2.5806208103
C,0,-3.9146423265,0.4866915094,3.6894514796	C,0,-3.8069596791,0.6494635355,3.5944846685
C,0,-2.3624889018,-0.9266499448,2.5350499441	C,0,-2.1717888299,-0.8523201339,2.7049770601
C,0,-2.0164504641,1.4064120132,2.5617116381	C,0,-1.680545186,1.4346878866,2.8553972554
C,0,-3.1607606546,1.5958736324,3.3181014723	C,0,-2.9350262901,1.7132516126,3.3758607369
C,0,-3.5156677725,-0.7757188654,3.3076403466	C,0,-3.4408374106,-0.6367388655,3.2489591984
H,0,-3.4472030747,2.5951775366,3.615865903	H,0,-3.2236624728,2.7320880447,3.5978070155
H,0,-4.0830150818,-1.6534260667,3.5844481089	H,0,-4.1285300415,-1.4638325799,3.3613294441
H,0,-4.8122489552,0.6164287062,4.2809831552	H,0,-4.78976091,0.8365249741,4.0093562288
C,0,-1.1085243983,2.5307782002,2.1714266002	C,0,-0.6527318505,2.4667305599,2.5043686015
H,0,-0.4272362607,2.7347850281,3.0033234849	H,0,0.1260995027,2.4701193326,3.2713053102
H,0,-1.6610130874,3.4567510728,1.997034561	H,0,-1.0741851678,3.4721745677,2.4565409431
C,0,-0.986271482,2.5885068459,-0.7946212992	C,0,-1.0471577672,2.1805988775,-0.4549655622
C,0,1.5723625369,2.9559080203,1.0165448303	C,0,1.6799771356,3.1579410561,0.7831071535
C,0,2.4016715887,2.9627165412,-0.2646311834	C,0,2.7136066875,2.4998694981,-0.1327942832
H,0,3.3976694732,3.3522232834,-0.0413634944	H,0,3.5913033291,3.1453699443,-0.2118404629
H,0,1.9679779942,3.6083554845,-1.0291569414	H,0,2.3391010035,2.3318779154,-1.141886791
H,0,2.5150010052,1.9568099495,-0.6708133284	H,0,3.0398463762,1.5415526103,0.2739487386
C,0,2.3151672438,2.1511007205,2.086039569	C,0,2.3059724957,3.3211988411,2.1703244641
H,0,3.2554529963,2.6512921213,2.3290168709	H,0,3.2590949094,3.8431430543,2.0602463428
H,0,2.54366608,1.1450640367,1.7315924095	H,0,2.5062245656,2.363083539,2.6513778411
H,0,1.7444226311,2.0689782682,3.0145871417	H,0,1.6844602143,3.9261091356,2.8312277833
C,0,1.3553954189,4.3844651292,1.5100092643	C,0,1.2965087775,4.5389495899,0.2628098066
H,0,2.3290924883,4.8527944191,1.6727817307	H,0,2.1806997235,5.1811798034,0.2793358154
H,0,0.8231965505,4.4242950926,2.4610329794	H,0,0.541381592,5.0175680183,0.8886313375
H,0,0.8158627527,5.0024868553,0.7943429032	H,0,0.9317274377,4.525165038,-0.7631936632
C,0,-0.353692859,1.9530880899,-2.0322336285	C,0,-0.3112513129,2.126133884,-1.7931508198
H,0,0.6535410192,2.3178528253,-2.2228778408	H,0,0.3445677269,2.9806350447,-1.9527124712
H,0,-0.9642873041,2.1906922441,-2.9065923998	H,0,-1.0421337091,2.1217395879,-2.6048785023
H,0,-0.2904779913,0.8683044775,-1.9415572003	H,0,0.2851956342,1.2168005652,-1.8879267973
C,0,-2.4040298681,2.0317189018,-0.6390177886	C,0,-2.01035459,0.9881460508,-0.403262336
H,0,-2.4020415512,0.9484987535,-0.4945861999	H,0,-1.4894116063,0.0279095906,-0.3928825367
H,0,-2.972282416,2.2385471871,-1.5482581867	H,0,-2.6436101,1.0102801662,-1.2934510365
H,0,-2.9468079419,2.4823649251,0.1936033103	H,0,-2.6703031403,1.0226952087,0.4625638673
C,0,-1.0461724474,4.1033964419,-0.9434338339	C,0,-1.8615716759,3.464373122,-0.3359888432
H,0,-0.0683940912,4.5326566452,-1.1613956836	H,0,-1.2543182752,4.3649811968,-0.3954468468
H,0,-1.4459408755,4.5971758127,-0.055361245	H,0,-2.4303376943,3.4954988047,0.5948114091
H,0,-1.7032874657,4.3606024889,-1.7780134186	H,0,-2.587699418,3.5064194318,-1.1518329941
Cl,0,1.6182795534,-0.6114692119,-0.3191940058	Cl,0,2.2384533311,-0.2141876674,3.0333649017
C,0,-1.8187154684,-2.1454554462,2.0427276225	C,0,-1.6757871595,-2.0758335908,2.1358286534
N,0,-0.6831965662,-2.0202109282,1.2914555323	N,0,-0.4946263145,-2.0006799147,1.4418026729
C,0,-2.1326862815,-3.500776746,2.1290983943	C,0,-2.1548987895,-3.372673538,2.0293452354
H,0,-2.9605818579,-3.9576351673,2.6460449276	H,0,-3.0583795868,-3.7805929716,2.4520112848
C,0,-1.1267021004,-4.1230121352,1.3937198124	C,0,-1.192776328,-4.0328594267,1.2545325264
N,0,-0.2612882602,-3.2090494184,0.8934279051	N,0,-0.2020315122,-3.1918484979,0.9083722278
C,0,-0.9036491076,-5.5859164735,1.1066104728	C,0,-1.1480639503,-5.4712345332,0.8032923618
C,0,-1.9822695877,-6.4290666226,1.7788870128	C,0,-2.3743476881,-6.2252702885,1.3080679308
H,0,-1.9752198698,-6.2985388662,2.8628700801	H,0,-2.4255988115,-6.2224879695,2.3984848953
H,0,-1.820841052,-7.4884258925,1.5725535322	H,0,-2.3412719495,-7.2660488978,0.981960199
H,0,-2.9786130457,-6.1699441042,1.4151175674	H,0,-3.2993908621,-5.7885605723,0.9263827408
C,0,-0.9457407951,-5.811619284,-0.4076141621	C,0,-1.1137551734,-5.5174474668,-0.7270201619
H,0,-0.1925193042,-5.2027619291,-0.9065444517	H,0,-0.2507462707,-4.9723101851,-1.1079815973
H,0,-1.9202995547,-5.5424970153,-0.8187431915	H,0,-2.0108809175,-5.0669646378,-1.1553953267
H,0,-0.7570099525,-6.8608976949,-0.6460767883	H,0,-1.0537128588,-6.5495920898,-1.0795200104

C,0,0.473216253,-5.997702352,1.635531758 H,0,0.5350336172,-5.8654590555,2.7170917024 H,0,1.2555860854,-5.392069695,1.1795357229 H,0,0.672984154,-7.0482076739,1.411964809	C,0,0.1201419039,-6.1303687441,1.3532675327 H,0,0.1251654471,-6.1258888734,2.4443020788 H,0,1.0079010311,-5.5976585785,1.0142778685 H,0,0.1898518625,-7.1680571799,1.019228141
 **^{PNN}Co(H)2-Double**	 **^{PNN}Co(H)2-Quartet**
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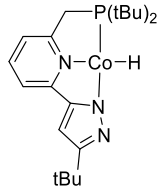
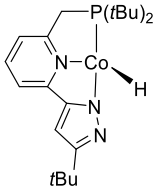
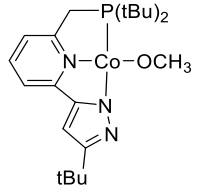
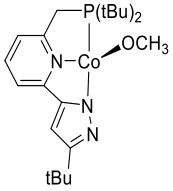
H,0,-0.273054466,-5.3052195889,-1.0359274622	H,0,-0.0316319032,-5.6491747756,-0.7348626015
H,0,-2.0071545069,-5.5666032951,-0.8682357429	H,0,-1.7815941196,-5.6224087938,-0.9283318792
H,0,-0.8852256401,-6.920651797,-0.7051792412	H,0,-0.9484841913,-7.1443350855,-0.5992141995
C,0,0.4570541807,-6.0350835408,1.5211181962	C,0,0.033869191,-6.5116279085,1.8856840666
H,0,0.5632182641,-5.8643301229,2.5925499665	H,0,-0.0531031212,-6.3668904408,2.9627395623
H,0,1.2519136339,-5.4829292983,1.0172744819	H,0,0.9938577252,-6.0991504019,1.5715828024
H,0,0.6239684249,-7.0960770631,1.3281066431	H,0,0.0607460775,-7.5844968198,1.6891115714
 **PNNCoH-Double**	 PNNCo-H_Quartet
Co,0,-0.1657343646,-0.155707932,0.9208898752	Co,0,0.5008669543,-0.3432509909,1.6252279277
P,0,-0.0234900662,2.0065312948,0.7784857773	P,0,0.2039801834,1.9408882452,0.8802226109
N,0,-1.607341572,0.1979486711,2.245962338	N,0,-1.3281257234,0.1656650437,2.5197293252
C,0,-3.8115603115,0.485116567,3.8632311182	C,0,-3.840925064,0.6420330306,3.4968200547
C,0,-2.3135258388,-0.9085146941,2.6198057043	C,0,-2.192629519,-0.8681176619,2.640787024
C,0,-1.9718982456,1.4230621541,2.6594225832	C,0,-1.7001015722,1.4197821218,2.7935798999
C,0,-3.0832378426,1.603694601,3.4689367915	C,0,-2.9604708056,1.7032554601,3.2953130064
C,0,-3.4295252335,-0.7742746137,3.4475767642	C,0,-3.4711516259,-0.6454771159,3.1612902939
H,0,-3.3647277345,2.5973889398,3.7902321317	H,0,-3.2476305556,2.7229199033,3.5158474478
H,0,-3.9868597453,-1.6541774692,3.7384967809	H,0,-4.1621047684,-1.4710185445,3.265798432
H,0,-4.6811735616,0.6044528434,4.4976251761	H,0,-4.8306697332,0.8323386008,3.893421062
C,0,-1.0805332133,2.5514381439,2.2259798987	C,0,-0.6561917216,2.4419302714,2.4666520587
H,0,-0.4022310026,2.7935289246,3.0471649565	H,0,0.1234594236,2.4070128735,3.2315474379
H,0,-1.6517266601,3.4604583056,2.0333974676	H,0,-1.0570560684,3.4564567878,2.4472646117
C,0,-1.0036883193,2.5955816268,-0.7374538051	C,0,-1.0795771284,2.2923984204,-0.4815319798
C,0,1.6207810524,2.9175079512,0.9875617054	C,0,1.690601211,3.1125615423,0.774951408
C,0,2.6177132414,2.3506554296,-0.0247738153	C,0,2.6675169557,2.5188700288,-0.2416949759
H,0,3.6129838166,2.7452947454,0.1926149233	H,0,3.5747653874,3.1268768778,-0.2714584814
H,0,2.3767775622,2.6228041444,-1.049767232	H,0,2.2621409955,2.4876320907,-1.2517047668
H,0,2.658588376,1.2623824233,0.0303732252	H,0,2.9544103118,1.5049195048,0.0404256171
C,0,2.135049386,2.5654962176,2.3860103535	C,0,2.3735413883,3.1000886015,2.1454925799
H,0,3.1715467391,2.8960625181,2.4796042084	H,0,3.3592241312,3.5614464553,2.0525804989
H,0,2.1179385176,1.4879770802,2.5634384318	H,0,2.5107745704,2.0844420467,2.5223597078
H,0,1.5729587755,3.0533760094,3.1822449785	H,0,1.8185140716,3.6759030784,2.8863850516
C,0,1.5103524033,4.4297058193,0.8411103741	C,0,1.341044504,4.5504184734,0.4095879973
H,0,2.4678918675,4.8961218413,1.0869623544	H,0,2.2449454941,5.1636420019,0.454558283
H,0,0.7597000156,4.8592500368,1.5077656905	H,0,0.6218528157,4.9875747385,1.1044074914
H,0,1.265542541,4.7226304735,-0.1802536559	H,0,0.9406592148,4.6454720936,-0.5992044506
C,0,-0.1153568962,2.5193217968,-1.9754135893	C,0,-0.3661910994,2.3314519115,-1.8312459749
H,0,0.6220484472,3.3224247828,-1.9990615025	H,0,0.2818678435,3.2001700511,-1.9414833371
H,0,-0.7319353769,2.6210375087,-2.8717385273	H,0,-1.1098558168,2.3786081879,-2.630192808
H,0,0.4088049986,1.5640867542,-2.0364502807	H,0,0.2333670429,1.4346411398,-1.9978239777
C,0,-2.1311923012,1.5666701187,-0.8756641407	C,0,-2.050009812,1.1049912334,-0.4952320337
H,0,-1.7353877959,0.5572130653,-1.022216133	H,0,-1.5328406018,0.146318143,-0.5724030569
H,0,-2.7473371822,1.8092332889,-1.7451945505	H,0,-2.7106357115,1.1971615027,-1.3609359475
H,0,-2.7868808407,1.5507387531,-0.0026371918	H,0,-2.68209525,1.0745922216,0.3914299008
C,0,-1.6131250061,3.9879734487,-0.6170545574	C,0,-1.8784426335,3.5724165588,-0.2610798864
H,0,-0.8698788231,4.7656130453,-0.4489333164	H,0,-1.2564831618,4.4653991846,-0.2334994853
H,0,-2.3544165719,4.0482403081,0.1801683493	H,0,-2.4585076377,3.5309315859,0.6621208997
H,0,-2.1333431651,4.2324554678,-1.5467227526	H,0,-2.5931946315,3.6978956065,-1.0787227204
H,0,0.8883460968,-0.4438443047,-0.1268081083	H,0,1.8102829403,-0.0770945723,2.508987463
C,0,-1.7921573034,-2.1175305041,2.0649695906	C,0,-1.6824534367,-2.1010101005,2.1088729345
N,0,-0.7168942686,-1.9830400195,1.2273320819	N,0,-0.4862334248,-2.0406327129,1.442616004
C,0,-2.104443694,-3.4718982419,2.1598975258	C,0,-2.1598448949,-3.4033358299,2.0261234288
H,0,-2.8917789052,-3.9308432117,2.7354119033	H,0,-3.0740058021,-3.7996670474,2.4370382106
C,0,-1.1616205061,-4.0917874307,1.3425229085	C,0,-1.1796183109,-4.0813237551,1.2960657162
N,0,-0.3348378075,-3.1783106436,0.7844803744	N,0,-0.1804116401,-3.24622038,0.9511294151
C,0,-0.9700418379,-5.5548652076,1.0316210022	C,0,-1.1199082021,-5.5311830839,0.8847509888
C,0,-2.0069554594,-6.3957249418,1.7693297486	C,0,-2.3593439387,-6.2742426965,1.3734922113
H,0,-1.9255000842,-6.2727731251,2.8511282422	H,0,-2.4417903679,-6.2430211137,2.4616148762
H,0,-1.8687230216,-7.4549648297,1.5453212133	H,0,-2.3170425464,-7.3232027036,1.0752506177
H,0,-3.0234154047,-6.1255230155,1.4763003799	H,0,-3.2731233632,-5.8477869745,0.9549338287
C,0,-1.1155027334,-5.7725938347,-0.4772557899	C,0,-1.040969758,-5.6195009008,-0.6419757164

H,0,-0.3927052444,-5.1665015313,-1.0225419158	H,0,-0.1683716187,-5.0822119083,-1.0121650705
H,0,-2.113010727,-5.4925859367,-0.820424359	H,0,-1.9258039691,-5.1821603625,-1.1078458566
H,0,-0.9522381644,-6.8220404546,-0.7340983447	H,0,-0.9692446622,-6.6606439319,-0.9652157861
C,0,0.4354392072,-5.9820641297,1.4645630443	C,0,0.1320528629,-6.1739695503,1.4885732261
H,0,0.5707972897,-5.8558153552,2.5401534225	H,0,0.1042592318,-6.1412424336,2.5789412292
H,0,1.1905478504,-5.3798258902,0.9603496702	H,0,1.0284794496,-5.6475958664,1.1623394385
H,0,0.6117776486,-7.0330437832,1.2230915028	H,0,0.2141025938,-7.2199713815,1.183957095
 **PNNCoOMe-Double**	 **PNNCoOMe-Quartet**
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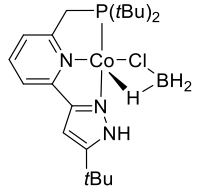
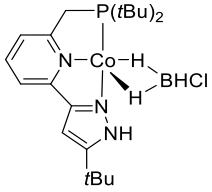
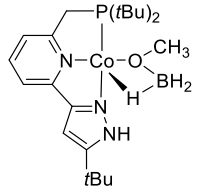
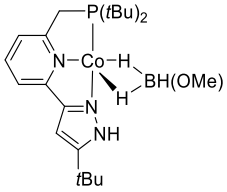
P,0,-0.0586200476,2.0690068962,0.8058812245	P,0,0.2734374541,1.8471647337,0.8295923609
N,0,-1.6309078752,0.2123739137,2.2259599894	N,0,-1.2045336561,0.0597944269,2.5011506469
C,0,-3.9574853856,0.4881356208,3.6862425527	C,0,-3.6539188411,0.5475711365,3.6211178921
C,0,-2.3479019327,-0.8974274491,2.5792777396	C,0,-2.0788531409,-0.9634724093,2.6379485986
C,0,-2.0524121792,1.4387767567,2.5942301839	C,0,-1.5405489769,1.3122766627,2.8255451876
C,0,-3.2185741339,1.6094305447,3.3207727707	C,0,-2.7685446892,1.601112175,3.3993084116
C,0,-3.5216828351,-0.7685386308,3.3220842787	C,0,-3.3240521836,-0.7359329836,3.2330849617
H,0,-3.5359647766,2.6054517579,3.5986546571	H,0,-3.0280376272,2.6187819264,3.6599539939
H,0,-4.0776915537,-1.6562989868,3.5904752055	H,0,-4.0221328209,-1.5533526817,3.3532636768
H,0,-4.8715756327,0.6032425156,4.2550097556	H,0,-4.6178177334,0.7420837122,4.0751965437
C,0,-1.1678866387,2.5851134563,2.20330606	C,0,-0.5006073903,2.3300221011,2.4665518368
H,0,-0.5086754781,2.8254458615,3.0435548371	H,0,0.3154031522,2.2788621966,3.1918386784
H,0,-1.7453673424,3.4900313636,2.0009981122	H,0,-0.8932521026,3.3478233188,2.4847698375
C,0,-0.9635339152,2.593040055,-0.7676976071	C,0,-1.0740856827,2.2372292534,-0.4553339566
C,0,1.5462461809,3.0082135298,1.0956135889	C,0,1.7700696911,2.9984920361,0.6679627636
C,0,2.4127010796,2.9057924548,-0.1572335299	C,0,2.6654632374,2.4453911184,-0.4424869037
H,0,3.4167891836,3.2727744538,0.068798482	H,0,3.580199543,3.0401691121,-0.4975399047
H,0,2.0243730739,3.5148519729,-0.9747108295	H,0,2.1972524817,2.4763998552,-1.4243996719
H,0,2.4924319577,1.8683647403,-0.4877635979	H,0,2.9536658425,1.4138144052,-0.2351824631
C,0,2.2406172074,2.251479488,2.2313991816	C,0,2.5507476065,2.9006303591,1.9819021868
H,0,3.1875255423,2.7428789839,2.4680350315	H,0,3.5239937073,3.3779996325,1.8471254247
H,0,2.4453867822,1.2208644578,1.9380157915	H,0,2.7197036525,1.8615590781,2.271076546
H,0,1.6455449882,2.2390938898,3.1478912422	H,0,2.0514390042,3.4203820718,2.8001137467
C,0,1.3417926579,4.4653146962,1.4977772714	C,0,1.4159384828,4.4560201886,0.3991385915
H,0,2.3151127038,4.9225799623,1.6933233909	H,0,2.3286074981,5.0576197439,0.4103821492
H,0,0.7552361196,4.5657155627,2.4123663142	H,0,0.7523660536,4.8654069832,1.1629134376
H,0,0.858004913,5.0549440745,0.7209857844	H,0,0.9476033561,4.6044021368,-0.5736082487
C,0,-0.2997894064,1.8938585613,-1.9550013978	C,0,-0.4335735459,2.3188399659,-1.8390694035
H,0,0.6968501823,2.278090236,-2.161988654	H,0,0.203176161,3.1948816783,-1.956932157
H,0,-0.9070467156,2.0467611127,-2.8504120819	H,0,-1.2195006699,2.3856119316,-2.5949033928
H,0,-0.2024985885,0.8204798333,-1.7825445532	H,0,0.1600092596,1.4311143226,-2.0647487131
C,0,-2.3878899124,2.0494202642,-0.6267395249	C,0,-2.0492387182,1.0536354087,-0.4549572036
H,0,-2.3947919781,0.9734764519,-0.4359447616	H,0,-1.5406536745,0.0953642071,-0.5808825421
H,0,-2.9321157368,2.2206701985,-1.5579966481	H,0,-2.7494196956,1.1706822076,-1.2858199823
H,0,-2.9486537404,2.5365715553,0.172587656	H,0,-2.6390781431,1.0023790812,0.4593079152
C,0,-1.0105414434,4.0989585628,-0.9883214637	C,0,-1.8546180422,3.5125072505,-0.1548854055
H,0,-0.0241055816,4.5122183978,-1.1988668632	H,0,-1.2255127798,4.4004878117,-0.1209431746
H,0,-1.4280357961,4.6332332722,-0.132247964	H,0,-2.3958422896,3.4402872033,0.7897533246
H,0,-1.6443391393,4.3243590019,-1.8500371621	H,0,-2.6020160962,3.6715850251,-0.9364720765
O,0,1.5135193637,-0.2874339596,0.1442573936	O,0,2.015928516,-0.3357361245,2.5867511089
C,0,-1.7720567199,-2.1106920362,2.1002776283	C,0,-1.6195130394,-2.1871415076,2.042930473
N,0,-0.6229758467,-1.9803431037,1.3711453252	N,0,-0.458340615,-2.1282652256,1.316549482
C,0,-2.0905334607,-3.4650986113,2.1773185541	C,0,-2.124265016,-3.4787580021,1.9509650002
H,0,-2.9296231426,-3.9199712976,2.6777574442	H,0,-3.0219358142,-3.8710584972,2.4002891741
C,0,-1.0741231341,-4.0893835816,1.4587055816	C,0,-1.1968284677,-4.1520584285,1.1519783156
N,0,-0.1998152056,-3.1771592589,0.9770033545	N,0,-0.2008260437,-3.3246091952,0.7784682285
C,0,-0.8483481796,-5.5523592321,1.1726064965	C,0,-1.1857589218,-5.5899141409,0.6964954759
C,0,-1.9451554557,-6.3947624563,1.8157608553	C,0,-2.4032965769,-6.3303551594,1.2408128554
H,0,-1.9638388134,-6.2669534067,2.8998326558	H,0,-2.418048329,-6.328240318,2.3324023254
H,0,-1.7823770331,-7.4541586275,1.6103017141	H,0,-2.3945037222,-7.371073521,0.9123460257
H,0,-2.9314384049,-6.1305590966,1.4292023548	H,0,-3.3349734432,-5.881009016,0.8913338682
C,0,-0.8536769015,-5.775148027,-0.3426249257	C,0,-1.2042127656,-5.6334380932,-0.8342016517

H,0,-0.0852965905,-5.1684262843,-0.8215301294	H,0,-0.3485006529,-5.0968029077,-1.2428405811
H,0,-1.8161325684,-5.5001829821,-0.7775876509	H,0,-2.1098979373,-5.1707780396,-1.230386326
H,0,-0.6634467335,-6.8245445599,-0.5796913619	H,0,-1.1684639699,-6.6652465264,-1.1916180576
C,0,0.5138048114,-5.9706911614,1.7338882359	C,0,0.0916562961,-6.2675300182,1.2006488746
H,0,0.5509355713,-5.8380435387,2.8164580686	H,0,0.1327155782,-6.2678504921,2.2910925945
H,0,1.3098909233,-5.3683628701,1.296606655	H,0,0.9737978434,-5.7434209107,0.8344152779
H,0,0.715399326,-7.021963837,1.515206851	H,0,0.1383076524,-7.3047364479,0.860496896
C,0,2.010228067,-1.5117006864,-0.3005835915	C,0,1.9592664801,-0.2458304756,3.9678069662
H,0,2.9760626576,-1.3384309419,-0.7947616462	H,0,2.5100204546,0.6353885627,4.335419236
H,0,2.1660358177,-2.2402303353,0.5047901695	H,0,0.9316131629,-0.1710948613,4.3595862934
H,0,1.3492180089,-2.0017230736,-1.0297515011	H,0,2.418901518,-1.1231520049,4.4428001484
 **^{PNN}Co(c-H-BH$_2$-Cl)**	 **^{PNN}Co(c-H-BHCl-H)**
Co,0,-0.112773966,-0.2509822185,-0.0811699557	Co,0,-0.552006597,-0.0143938144,0.0985995122
P,0,-0.3335902589,0.4501369677,-2.2073597844	P,0,-0.6296626823,0.6062119285,-2.0682153846
N,0,0.7210621369,1.4776976727,0.2328129814	N,0,0.6424833236,1.5566676301,0.2851544764
C,0,1.550524472,3.9914095008,0.996561538	C,0,2.4274524363,3.6092579938,0.742533162
C,0,1.0583345892,1.7106688175,1.5397355054	C,0,1.3128830424,1.6209170717,1.4767368146
C,0,0.8578488176,2.4454793993,-0.6921302868	C,0,0.8697453464,2.472492667,-0.6718308032
C,0,1.2580914311,3.7226121322,-0.3371632167	C,0,1.7646493099,3.5120476823,-0.4762067035
C,0,1.4695687857,2.9854843697,1.9341415455	C,0,2.2042619403,2.6673044756,1.7225187509
H,0,1.3550785003,4.484337506,-1.098530846	H,0,1.9316859744,4.2313910072,-1.2660841581
H,0,1.7118364601,3.1617997694,2.9729038188	H,0,2.7178377826,2.7096989826,2.6728675786
H,0,1.8578530021,4.9864157986,1.2929982375	H,0,3.1242989209,4.419552546,0.9167282679
C,0,0.6536816155,2.0264782038,-2.113048486	C,0,0.094930321,2.3132491527,-1.9398894243
H,0,1.637403857,1.8198588785,-2.5433978553	H,0,0.6956600902,2.5856435725,-2.8111200961
H,0,0.2253063424,2.8263483521,-2.7189809648	H,0,-0.7530113722,3.0042348814,-1.9292901568
C,0,-2.0028788077,0.9987052879,-2.9003647974	C,0,-2.1644192985,0.9187866499,-3.135878552
C,0,0.6611060677,-0.6137724707,-3.4193338174	C,0,0.685420327,-0.4124779782,-2.9818734918
C,0,-0.1844285261,-1.7983023883,-3.8788720052	C,0,0.3080148621,-1.8907820856,-2.8769057235
H,0,-0.6683623022,-2.305379296,-3.0430240366	H,0,0.1906130747,-2.2003728854,-1.8375346357
H,0,0.4561617253,-2.5242621717,-4.3848050028	H,0,1.1015543363,-2.4981895739,-3.3181997421
H,0,-0.9524338591,-1.4954843492,-4.5911043634	H,0,-0.616211979,-2.1284567864,-3.400578708
C,0,1.8390137554,-1.131601191,-2.5875430353	C,0,1.9957142105,-0.1996609853,-2.2183262383
H,0,2.4933779306,-1.7413054369,-3.2149223546	H,0,2.7688157675,-0.8374368652,-2.6522593654
H,0,1.5011112077,-1.7532025291,-1.755466863	H,0,1.905023137,-0.4701283411,-1.163619023
H,0,2.4464405747,-0.321283751,-2.1763330319	H,0,2.3545551746,0.8295192437,-2.2736684797
C,0,1.1979625263,0.1365582101,-4.635328661	C,0,0.8881936732,-0.0254540298,-4.4407342893
H,0,1.7852257904,-0.5545856484,-5.2449793486	H,0,1.7426888015,-0.5746856038,-4.8440790697
H,0,1.8623635447,0.9584983538,-4.367522221	H,0,1.1012117791,1.0376907369,-4.5674844098
H,0,0.4089200007,0.5345965979,-5.2697267405	H,0,0.0262871104,-0.2781735278,-5.0575493544
C,0,-2.9892044112,-0.1661971856,-2.8434897934	C,0,-2.7175733696,-0.4075463976,-3.6490373134
H,0,-2.7245989811,-0.9711400788,-3.5259446017	H,0,-2.0699457102,-0.8561730122,-4.4031421385
H,0,-3.9789494836,0.1948406392,-3.1332557548	H,0,-3.6878357287,-0.2347834109,-4.1199839491
H,0,-3.0681453935,-0.5817359322,-1.8402152362	H,0,-2.8668083453,-1.1258112919,-2.8425099308
C,0,-2.4961766092,2.1035832772,-1.9624387626	C,0,-3.1982194524,1.5807349371,-2.2216274019
H,0,-2.5422305377,1.7620540512,-0.9277742849	H,0,-3.4943221787,0.9300523621,-1.4028576219
H,0,-3.5055765144,2.3960609072,-2.2588279303	H,0,-4.0878576427,1.8181843062,-2.8093603386
H,0,-1.8754163852,2.9999918606,-2.003171212	H,0,-2.8362264529,2.5188761319,-1.7960560751
C,0,-1.9077764177,1.5336493774,-4.3242282706	C,0,-1.8921119857,1.8570751766,-4.3115292761
H,0,-1.6868490193,0.7433147067,-5.0417494912	H,0,-1.176911333,1.4579180834,-5.0263081492
H,0,-1.1556152533,2.3173847243,-4.4360098048	H,0,-1.5412482209,2.8381992831,-3.990488279
H,0,-2.8692234209,1.9668413457,-4.6108818853	H,0,-2.829587621,2.0192226198,-4.8490317059
C,0,0.9456483301,0.5557605884,2.3605204148	C,0,1.0302441889,0.5272902456,2.3397602808
N,0,0.5407336187,-0.5737061853,1.7098661772	N,0,0.1690131242,-0.404397937,1.8335229321
C,0,1.1704635603,0.2233212999,3.6959798686	C,0,1.4620330778,0.0766791075,3.5862415279
H,0,1.5055476953,0.8673536079,4.4922180134	H,0,2.1455762075,0.5603827765,4.2644334425
C,0,0.8623456341,-1.1334906431,3.7581648671	C,0,0.8057401672,-1.1418042668,3.7481204606
N,0,0.4759120325,-1.594160178,2.5430009836	N,0,0.0311030336,-1.4145745866,2.6717965953
C,0,0.8908458836,-2.0810418429,4.9292660714	C,0,0.8405303927,-2.1186034843,4.8949704489
C,0,1.3426545583,-1.3519041938,6.1904211387	C,0,1.769566072,-1.6129003209,5.9937736818
H,0,2.347989257,-0.940964486,6.0776819952	H,0,2.7931006714,-1.495225576,5.6318594508

H,0,1.3584071365,-2.0360787453,7.0404052109	H,0,1.7925765192,-2.318006985,6.8262182315
H,0,0.6689988741,-0.5299580767,6.440287348	H,0,1.4381592531,-0.649592764,6.386351592
C,0,-0.5166801377,-2.6482780124,5.1391800725	C,0,-0.5774276723,-2.2802811378,5.4515936316
H,0,-0.8648227443,-3.1543796615,4.2391871864	H,0,-1.2602243903,-2.6175699721,4.6722698203
H,0,-1.2296382003,-1.854806248,5.3691654699	H,0,-0.9578098952,-1.3337643264,5.839051114
H,0,-0.5251455917,-3.3624812162,5.9658366701	H,0,-0.5897938288,-3.008543133,6.2657725623
C,0,1.8559312848,-3.2309964585,4.6282076283	C,0,1.3368061497,-3.4753953479,4.3873337983
H,0,2.8738738295,-2.8642451412,4.4845985767	H,0,2.3512740725,-3.4019515199,3.9911377907
H,0,1.5569947526,-3.7539884375,3.720314838	H,0,0.691102493,-3.845672676,3.5916725549
H,0,1.8688570517,-3.9486214671,5.4517430377	H,0,1.3429840877,-4.2095383078,5.1961220197
Cl,0,-1.2215652422,-2.2506072236,-0.2633553214	H,0,-1.3280975179,-1.4535055183,-0.0297101918
B,0,-2.3517183224,-0.9162935103,0.709494683	B,0,-2.4690620774,-0.8970999169,0.2846169003
H,0,-3.4167643013,-0.9156541969,0.1686857318	H,0,-3.1759292033,-1.0388496105,-0.6700322219
H,0,-1.7882854921,0.1788446367,0.4889268723	H,0,-2.2527858157,0.3272567493,0.5191541461
H,0,-2.3046264542,-1.2091961596,1.8601433322	Cl,0,-3.1286998289,-1.7347340718,1.7620909114
	
^{PNN}Co(c-H-BH$_2$-OCH$_3$)	**^{PNN}Co(c-H-BH(OCH$_3$)-H)**
Co,0,-0.5291066277,-0.0864112655,0.0093473637	Co,0,-0.6086417972,0.1712306839,0.0882516625
P,0,-0.5958794922,0.5904269349,-2.1486307722	P,0,-0.6348075943,0.726522931,-2.0805193556
N,0,0.6070385792,1.4900297839,0.2344993755	N,0,0.7384542427,1.6206166318,0.2293468204
C,0,2.4551695215,3.5052753913,0.6185626343	C,0,2.7242506367,3.4918053866,0.6136176949
C,0,1.3850493552,1.4927025803,1.3579615326	C,0,1.4414517862,1.6297280641,1.4028312909
C,0,0.7394070641,2.4672186926,-0.684334739	C,0,1.0309899043,2.4942552602,-0.7481355972
C,0,1.6620071748,3.4865499468,-0.5248475023	C,0,2.0264440226,3.4452676704,-0.5886493119
C,0,2.3149791528,2.5140369563,1.5648061166	C,0,2.4366946813,2.5864548577,1.6121834659
H,0,1.7490634305,4.2526094075,-1.2831316013	H,0,2.245439188,4.1346677625,-1.3925467951
H,0,2.9228637239,2.498377564,2.458766571	H,0,2.9781861612,2.5895446425,2.5480018689
H,0,3.1815331711,4.2953311758,0.7618164321	H,0,3.5005216707,4.232494941,0.760102376
C,0,-0.1862774142,2.3772973501,-1.8510563094	C,0,0.2190058742,2.3794377299,-1.9997899982
H,0,0.1950915445,2.913460317,-2.7208759832	H,0,0.8215485584,2.5937229628,-2.8860685219
H,0,-1.1337720369,2.8462251633,-1.5746477838	H,0,-0.5755205432,3.1314739509,-1.9836745031
C,0,-2.1473353034,0.6263908396,-3.2343451396	C,0,-2.1562035607,1.1172398084,-3.1400678183
C,0,0.9132625361,-0.0914718957,-3.0903848053	C,0,0.5929243736,-0.4049764461,-2.9867204025
C,0,0.5346291813,-1.4217743417,-3.7367414015	C,0,0.1188188767,-1.8508435761,-2.8332683654
H,0,0.0687111869,-2.1007497938,-3.0193225721	H,0,-0.0146431331,-2.1158942006,-1.7833620762
H,0,1.4358175625,-1.9099305967,-4.1151321065	H,0,0.8679210088,-2.523875003,-3.2571111704
H,0,-0.1451047324,-1.2982659146,-4.5790059798	H,0,-0.8217407348,-2.0427392855,-3.3467558362
C,0,2.0016373047,-0.3658200391,-2.0464168977	C,0,1.9275350264,-0.2639511047,-2.2491993999
H,0,2.8615610738,-0.8253072032,-2.5402476187	H,0,2.644907805,-0.9704341855,-2.6725696388
H,0,1.662116916,-1.0542906201,-1.2681562383	H,0,1.8330414879,-0.4918896547,-1.184989869
H,0,2.3538494381,0.5439916722,-1.5597179161	H,0,2.3593248238,0.7337387175,-2.3446707177
C,0,1.4780763591,0.8688543552,-4.1322958361	C,0,0.7987104305,-0.0745732457,-4.4590012999
H,0,2.3250673689,0.3961810734,-4.6361161318	H,0,1.6094039674,-0.6897880767,-4.8578374862
H,0,1.8548443271,1.7853966509,-3.6756365108	H,0,1.0779509848,0.9684860993,-4.6200033413
H,0,0.7563473746,1.1427228082,-4.8991664275	H,0,-0.0872708946,-0.2878844788,-5.0564289808
C,0,-2.761314789,-0.7751079321,-3.2520810319	C,0,-2.8133371798,-0.187405699,-3.580995137
H,0,-2.1259478489,-1.5072482733,-3.7467257007	H,0,-2.2170658537,-0.7166575917,-4.3251309709
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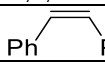
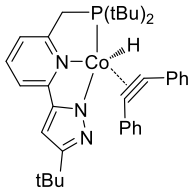
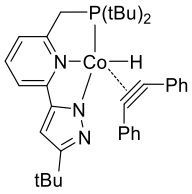
H,0,-2.9691879415,-1.1286671684,-2.2432059055	H,0,-2.9921159696,-0.854164948,-2.7357814204
C,0,-3.143988716,1.5702298314,-2.5553226736	C,0,-3.1264611844,1.8822440918,-2.2367018529
H,0,-3.2599324213,1.3479138505,-1.4939486867	H,0,-3.46224984,1.2773708943,-1.3979789648
H,0,-4.1219497942,1.4392863612,-3.0230355561	H,0,-4.0015344836,2.1705574926,-2.8239216007
H,0,-2.8715158074,2.6192154894,-2.6758926349	H,0,-2.6905228536,2.8005252333,-1.8382610154
C,0,-1.8891151351,1.1137147569,-4.655712097	C,0,-1.8413105617,1.9880380557,-4.3552677022
H,0,-1.2774231009,0.4200385171,-5.2323617551	H,0,-1.1772710618,1.509042372,-5.0702454922
H,0,-1.4109447281,2.0949795504,-4.6797174745	H,0,-1.4040808553,2.9471735277,-4.0755318876
H,0,-2.8440566503,1.2078259952,-5.1792158945	H,0,-2.7751182425,2.2084451583,-4.8785512009
C,0,1.1491066518,0.377357362,2.2097425684	C,0,1.074822443,0.5745933103,2.2863155945
N,0,0.2380919633,-0.5266942549,1.7491320768	N,0,0.1167936564,-0.274737124,1.8119856562
C,0,1.6112996332,-0.0601416514,3.4507752347	C,0,1.4846935782,0.1048319745,3.5338683946
H,0,2.3333881468,0.4152169118,4.0939168627	H,0,2.224778717,0.5303679077,4.1914984003
C,0,0.915586511,-1.2457436371,3.6669821598	C,0,0.7144050412,-1.0398276244,3.7294194936

N,0,0.091608538,-1.5094528894,2.6250408556 C,0,0.9547905524,-2.1946177387,4.8373728599 C,0,1.9703404148,-1.71884775,5.87120713 H,0,2.976550186,-1.6683042206,5.4505033031 H,0,1.9998806066,-2.404435642,6.7197044056 H,0,1.7160718743,-0.7291139679,6.2551690004 C,0,-0.4357127104,-2.2579945444,5.4769003827 H,0,-1.1804305059,-2.5785390602,4.7485567055 H,0,-0.7400163773,-1.2805299686,5.8542251566 H,0,-0.4441567311,-2.9611217563,6.3129858718 C,0,1.3428386518,-3.5915600047,4.3445002586 H,0,2.3351272963,-3.5881822027,3.8901150845 H,0,0.6338988525,-3.946111958,3.5963277396 H,0,1.353120088,-4.3035514177,5.1729002547 O,0,-1.7647019649,-1.5626659647,-0.2016669797 B,0,-2.7583963735,-0.6384549097,0.4974113076 H,0,-3.7405957014,-0.4824827741,-0.1908060494 H,0,-2.1584577934,0.4921153289,0.5244024583 H,0,-2.9645447733,-0.9819155758,1.6291959802 C,0,-1.5749378343,-2.8613396392,0.3372061135 H,0,-2.5084324159,-3.4199588216,0.2333509417 H,0,-0.7970977363,-3.3635250119,-0.24298301 H,0,-1.2793043574,-2.8225189362,1.3873596206	N,0,-0.1042777078,-1.2534182216,2.6729777379 C,0,0.6640613218,-1.9896496371,4.8984660385 C,0,1.6943374154,-1.5944177744,5.9511180676 H,0,2.7087931936,-1.6202502932,5.5481404658 H,0,1.656710429,-2.2814361034,6.7982283124 H,0,1.5099213589,-0.5886616449,6.3335498096 C,0,-0.7401360243,-1.9437653308,5.5100871122 H,0,-1.4916442707,-2.1940738888,4.7610950565 H,0,-0.9709330771,-0.9473159808,5.8900366229 H,0,-0.8244697789,-2.6507321558,6.3388646267 C,0,0.9490871863,-3.412139269,4.4092549587 H,0,1.9466912046,-3.4871829091,3.9729362013 H,0,0.2277708173,-3.7061963485,3.6469033399 H,0,0.8875226932,-4.1237728872,5.235833554 H,0,-1.5274707927,-1.1280722649,0.0135620469 B,0,-2.6129230599,-0.4166388811,0.4838579823 H,0,-3.4106690585,-0.6506275049,-0.4011390598 H,0,-2.2227048375,0.7961438166,0.4880130591 O,0,-2.9677917593,-0.8026178398,1.78129078 C,0,-3.486447311,-2.0891377291,1.9587992904 H,0,-4.007388965,-2.1322202953,2.9172328996 H,0,-4.1950900554,-2.364189467,1.1655705016 H,0,-2.6832402237,-2.8370620244,1.9766238764
Ph—≡—Ph	
C,0,0.0000000022,0.,1.0480113544 C,0,-0.0000000022,0.,2.2581706456 C,0,0.0000000074,0.,-0.365754781 C,0,0.0000000176,0.,-3.1614923685 C,0,0.00000001,1.206020066,-1.0813747423 C,0,0.00000001,-1.206020066,-1.0813747423 C,0,0.0000000151,-1.2007031289,-2.4643176062 C,0,0.0000000151,1.2007031289,-2.4643176062 H,0,0.000000008,2.1409027812,-0.5361678198 H,0,0.000000008,-2.1409027812,-0.5361678198 H,0,0.000000017,-2.140034055,-3.0030346642 H,0,0.000000017,2.140034055,-3.0030346642 H,0,0.0000000216,0.,-4.2440934118 C,0,-0.0000000074,0.,3.671936781 C,0,-0.0000000176,0.,6.4676743685 C,0,-0.00000001,-1.206020066,4.3875567423 C,0,-0.00000001,1.206020066,4.3875567423 C,0,-0.0000000151,1.2007031289,5.7704996062 C,0,-0.0000000151,-1.2007031289,5.7704996062 H,0,-0.000000008,-2.1409027812,3.8423498198 H,0,-0.000000008,2.1409027812,3.8423498198 H,0,-0.000000017,2.140034055,6.3092166642 H,0,-0.000000017,-2.140034055,6.3092166642 H,0,-0.0000000216,0.,7.5502754118	C,0,0.0258916976,-0.3408995022,1.0927043186 H,0,-0.0133384756,0.6341304726,1.5715201569 C,0,0.1151577218,-0.3374178904,-0.2460470074 H,0,0.2270694133,0.63679738,-0.7149472587 C,0,0.0581899929,-1.4527884861,-1.1904582834 C,0,-0.0640168478,-3.5151737717,-3.0859005104 C,0,0.7858604232,-1.3813876496,-2.3828043048 C,0,-0.7588303682,-2.5705126428,-0.9851458813 C,0,-0.8173911026,-3.5876041885,-1.9206957089 C,0,0.7357992123,-2.4053460941,-3.3144886854 H,0,1.4044796272,-0.5106957735,-2.5699486004 H,0,-1.3603195538,-2.6284302607,-0.0865385715 H,0,-1.4621571561,-4.4400629972,-1.7451898923 H,0,1.3170874263,-2.332941357,-4.2254886531 H,0,-0.1114749785,-4.3132364845,-3.8161491576 C,0,-0.0007165414,-1.4669523362,2.0257137304 C,0,-0.0331498912,-3.5518614842,3.900059146 C,0,0.7308776707,-2.6402716079,1.808747053 C,0,-0.7215010019,-1.353678388,3.2189991713 C,0,-0.7481844302,-2.3879340041,4.1402136529 C,0,0.7131800689,-3.6683519652,2.7338933255 H,0,1.3267240589,-2.7336881432,0.9093699237 H,0,-1.2736342124,-0.4412827631,3.4152138286 H,0,-1.3228117988,-2.2817015636,5.0521223274 H,0,1.2927409079,-4.5646314506,2.5494918776 H,0,-0.0455307379,-4.3586199792,4.6221442516
 **PNNCo-H + Ph-C2-Ph-trigonal bipyramidal**	 **PNNCo-H + Ph-C2-Ph-tetragonal pyramidal**
Co,0,0.438919764,0.4852516629,-0.0016240422 P,0,1.1269307444,0.729775933,-2.1112686301 N,0,1.903229986,-0.9632870359,0.0790520975 C,0,3.8833793387,-2.8290576719,0.4204378678 C,0,2.0191895929,-1.5962050582,1.2730598781 C,0,2.8374830402,-1.1106153106,-0.8650402664 C,0,3.8347807119,-2.0667192209,-0.7436439293 C,0,3.0006743192,-2.5737089515,1.4513762468 H,0,4.5689757622,-2.1932616018,-1.5285160985	Co,0,0.1073292663,0.3644730385,-0.3008252627 P,0,0.923949819,0.451049842,-2.3170320593 N,0,1.5434971012,-0.9897250879,0.0111084019 C,0,3.7640851344,-2.4611919402,0.6837758128 C,0,1.8170389266,-1.2242857582,1.3243543139 C,0,2.3441365209,-1.4642182211,-0.9581243566 C,0,3.4742977212,-2.2061346582,-0.6540247275 C,0,2.9386934556,-1.9757720504,1.678300482 H,0,4.1067925927,-2.5825814829,-1.4466712279

H,0,3.0714837959,-3.0993735149,2.3941302274	H,0,3.1533186346,-2.1549420657,2.7232547492
H,0,4.6448567318,-3.5905550877,0.5356927013	H,0,4.6421172448,-3.0392511907,0.9442728079
C,0,2.7996701808,-0.0847138,-1.9592282154	C,0,1.8954490062,-1.1494897775,-2.3528662045
H,0,3.1678506586,-0.473049333,-2.9113494767	H,0,1.1843215549,-1.9227264713,-2.6573178652
H,0,3.4867477285,0.7161355065,-1.6654651763	H,0,2.7180392328,-1.1744847088,-3.0688308265
C,0,1.5531317809,2.4432076623,-2.8305342054	C,0,2.2662156598,1.7985720928,-2.3871440629
C,0,0.3310392432,-0.3597378488,-3.4664492659	C,0,-0.1433648073,0.4399470349,-3.8809742719
C,0,-1.15926528,-0.0501838907,-3.5880750534	C,0,-1.1836255664,1.5543082692,-3.7458849104
H,0,-1.6710013227,-0.1854745841,-2.6367384487	H,0,-1.7140911002,1.4878311138,-2.7945163414
H,0,-1.6119686919,-0.7347704908,-4.3111271883	H,0,-1.9168906844,1.4622736391,-4.5512297789
H,0,-1.3524531508,0.9634447154,-3.9358984671	H,0,-0.7464520071,2.5481314194,-3.8137373695
C,0,0.4877334369,-1.7980736925,-2.965345308	C,0,-0.8909554992,-0.8956589476,-3.8934374348
H,0,-0.1150557793,-2.4669929605,-3.5849666956	H,0,-1.6793490512,-0.8557906131,-4.6487428265
H,0,0.1558013849,-1.9104189715,-1.9317634113	H,0,-1.3653984659,-1.1022732256,-2.9313541577
H,0,1.5191283795,-2.1473919704,-3.0243337045	H,0,-0.2438922741,-1.7350335148,-4.1516410932
C,0,0.9813237046,-0.2515304261,-4.8408165126	C,0,0.6433465743,0.58971172,-5.1772259706
H,0,0.556003603,-1.0164877805,-5.4966525222	H,0,-0.0323961457,0.4781939041,-6.0293449921
H,0,2.0589273549,-0.4206403047,-4.8123066781	H,0,1.4199643279,-0.1710458331,-5.2792301322
H,0,0.7985961413,0.7120075308,-5.3156412136	H,0,1.1121802141,1.5694364764,-5.2680506849
C,0,0.3091545148,3.0304299385,-3.4936789703	C,0,1.6238636268,3.1334002545,-2.7544139343
H,0,0.054345799,2.5256271618,-4.4255555703	H,0,1.3175927358,3.1735725807,-3.7997812494
H,0,0.4891951944,4.0809360408,-3.7348985165	H,0,2.3476893578,3.9371680973,-2.5988980333
H,0,-0.5589017672,2.9927977515,-2.8318743711	H,0,0.7536336158,3.3445776911,-2.1306878415
C,0,1.9378049473,3.347224325,-1.659699973	C,0,2.8183943172,1.910204511,-0.9615698783
H,0,1.1144288179,3.4715138742,-0.9565331074	H,0,2.0317278965,2.1486622259,-0.2404207475
H,0,2.2138512403,4.3313082697,-2.0481872708	H,0,3.5572542968,2.7149157894,-0.9224327384
H,0,2.7881215704,2.9590076378,-1.0970972021	H,0,3.3144915888,0.9956481636,-0.6338442544
C,0,2.7152005861,2.4268431591,-3.8228068846	C,0,3.419723366,1.4861285388,-3.3344907103
H,0,2.5290008786,1.8076552446,-4.6967231009	H,0,3.0992965364,1.3360067856,-4.3641999059
H,0,3.6448622536,2.0912516749,-3.3628132111	H,0,3.9776677964,0.6034552106,-3.0190664598
H,0,2.8899888003,3.4451269146,-4.1797568794	H,0,4.1244650954,2.3217092715,-3.3318235934
C,0,1.119803585,-1.083071527,2.2636856454	C,0,0.8562625265,-0.6347369848,2.207906652
N,0,0.3698908496,-0.0041383909,1.8978189715	N,0,-0.1017895272,0.1397241163,1.6167404009
C,0,0.8266052277,-1.3837101608,3.5958494353	C,0,0.556673309,-0.739962321,3.566418041
H,0,1.2401704082,-2.1750883974,4.1993807309	H,0,1.0991043129,-1.282750986,4.3235708228
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H,0,-0.8843061583,-1.1055337576,7.2461052418	H,0,-1.4410388737,-0.2143864225,7.0457264567
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H,0,0.2824168542,1.4248890066,5.9302670512	H,0,-0.7522907563,2.2336563568,5.3171883214
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H,0,1.5081379923,1.5041450945,0.2413086538	H,0,-0.7978858252,1.5628974943,-0.4765607748
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H,0,-3.6251955476,4.0870566804,-2.2218414123	H,0,-5.7971829602,3.3435060121,-1.2515231455
H,0,-2.8280476733,5.6094517675,-0.4430534297	H,0,-4.1986645261,-0.3894707807,-2.6121959632
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C,0,-1.6651429207,-4.0322660995,1.6920901522	C,0,-0.8022560545,-3.2074908165,1.2858610758
C,0,-2.1208012942,-4.4464999758,-0.631033064	C,0,0.0247608132,-4.2747645764,1.5868782805
H,0,-2.201849803,-2.7166660095,-1.897571451	H,0,-0.7633240066,-3.4495024743,-2.0995011293
H,0,-1.3994494868,-1.9740293512,2.2464965719	H,0,0.7175024611,-5.349011456,-1.5482084229
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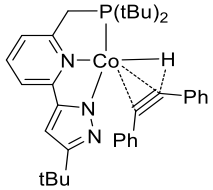
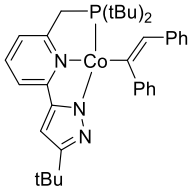
 **TS1**	 **PNNCo-cis-PhC=CHPh**
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C,0,1.4376999714,-1.1823566653,1.5370878074	P,0,1.8178450906,-0.466087548,-2.0308325985
C,0,2.4917899252,-1.9877167907,1.9784374431	N,0,2.8919760222,-0.1363795323,0.5635459233
C,0,3.3198593009,-2.5863818506,1.0529342394	C,0,5.1645271493,1.1577525311,1.4259216705
C,0,3.110144977,-2.3813231489,-0.3093010347	C,0,3.0004539283,0.2337777725,1.8711986702
C,0,2.0494541809,-1.5853764187,-0.7059983083	C,0,3.8808428577,0.1294830957,-0.3061606217
Co,0,-0.2299777202,0.2101500657,-0.2894696819	C,0,5.0339734109,0.7874592486,0.0905004444
P,0,0.9509376747,0.4159670433,-2.1955813084	C,0,4.154292261,0.8781118413,2.3225249717
N,0,-0.3641482039,0.3395823208,1.6699662996	H,0,5.8141793142,0.9954694157,-0.6291795425
N,0,-1.1698202093,0.9599641043,2.5228680778	H,0,4.2293672293,1.1683026122,3.3615063638
C,0,-0.8091563882,0.5671462137,3.7691170123	H,0,6.0586478709,1.6695662513,1.7596230258
C,0,0.2557162597,-0.3279423595,3.7135389597	C,0,3.6521937209,-0.3711056049,-1.6976064608
C,0,0.5143645178,-0.4577672359,2.3476191525	H,0,4.0169296993,-1.3994817261,-1.7530240438
C,0,-1.6793847375,-1.1208213783,-0.8431622781	H,0,4.2134510243,0.1994005944,-2.4387641728
C,0,-2.2345655422,0.0151759654,-0.7230221449	C,0,1.3433569457,1.3274397992,-2.4835272386
C,0,-3.4565300365,0.7646491745,-0.6021518455	C,0,1.6924018896,-1.6066786342,-3.5420001981
C,0,-3.5154987755,1.9875962315,0.0730585491	C,0,0.232560512,-2.0380232323,-3.6953991044
C,0,-4.7175527191,2.6621643815,0.1952540992	H,0,0.1510514585,-2.7391145564,-4.5294515413
C,0,-5.8774432022,2.1382643045,-0.3595165574	H,0,-0.4374376969,-1.2047205687,-3.8983637425
C,0,-5.8296559622,0.9235782411,-1.0326584558	H,0,-0.1360830686,-2.5354831058,-2.7978839041
C,0,-4.6337581382,0.2400833837,-1.1543394964	C,0,2.5380794308,-2.8506965104,-3.2525010907
C,0,-1.7122580551,-2.5262594409,-1.0872806409	H,0,2.2665551162,-3.6389505068,-3.9574213358
C,0,-0.9913003369,-3.4224184457,-0.2812260731	H,0,2.3792141993,-3.2455501221,-2.2480733527
C,0,-1.0196800012,-4.7820757264,-0.532306748	H,0,3.6045706203,-2.6622093527,-3.3770640423
C,0,-1.7458782093,-5.2874361507,-1.6035787745	C,0,2.2048735038,-0.9778463228,-4.8341452239
C,0,-2.4628282758,-4.4158761621,-2.4125678551	H,0,2.1846399464,-1.7268170523,-5.6301268557
C,0,-2.453911018,-3.0558235508,-2.1579887715	H,0,3.2369394079,-0.6339233271,-4.7431801682
H,0,3.7546322592,-2.8311311694,-1.0521063046	H,0,1.5946073645,-0.1408368141,-5.1688336665
H,0,2.6503036873,-2.1164662243,3.0403728429	C,0,0.0289472864,1.339700263,-3.2614471083
H,0,4.1426633424,-3.2073410264,1.3848129218	H,0,0.1368272735,0.9519000942,-4.2733328021
C,0,1.71554274,-1.2860214006,-2.1318836883	H,0,-0.3241587609,2.3702259033,-3.3479944879
H,0,0.9187772294,-1.9668532475,-2.4476532451	H,0,-0.7494581916,0.7656970252,-2.7581717345
H,0,2.5664159167,-1.4454844977,-2.7963411413	C,0,1.1195576922,2.0529143827,-1.1514866963
C,0,2.4377144525,1.6033039219,-2.0173790928	H,0,0.3512034728,1.5679948773,-0.5416353732
C,0,0.1852696979,0.5579629051,-3.9270614439	H,0,0.7800496531,3.0730795733,-1.3481012019
C,0,-0.7936962086,1.7343978276,-3.9049886272	H,0,2.0308267024,2.1213390897,-0.5564128646
H,0,-1.5525859503,1.6022190856,-3.1322623428	C,0,2.4224712241,2.0716638964,-3.2635284785
H,0,-1.3052860168,1.7956531412,-4.8686140927	H,0,2.6826815164,1.5858068301,-4.2025325441
H,0,-0.3051852309,2.6914047845,-3.732974903	H,0,3.3348596808,2.1987817341,-2.6791606397
C,0,-0.6275978546,-0.7131390987,-4.1739620739	H,0,2.0607711683,3.0740755485,-3.5062220157
H,0,-1.2194486107,-0.5830070799,-5.0831823697	C,0,1.8366156848,-0.0712320463,2.6420912649
H,0,-1.3173623716,-0.9132392966,-3.3556590478	N,0,0.7925749449,-0.619965641,1.9521655079
H,0,-0.0020234766,-1.5939194651,-4.3209000073	C,0,1.4580363401,0.0548090206,3.9750538095
C,0,1.1918070378,0.7190019832,-5.0607190207	H,0,2.0406049006,0.4444319974,4.7947342356
H,0,0.6609570577,0.6994681651,-6.0164301762	C,0,0.1561489739,-0.449377582,4.0046533528
H,0,1.920650709,-0.0931892743,-5.08141119	N,0,-0.229275958,-0.8446993267,2.7727794391
H,0,1.7339889757,1.6626709932,-5.0170236593	C,0,-0.7775739309,-0.5555731785,5.1845685431
C,0,2.0054657502,3.0062225527,-2.4382423768	C,0,-0.0580083364,-1.2409276894,6.3491887497
H,0,1.8286022954,3.0909442289,-3.5098175184	H,0,0.2648101726,-2.246173556,6.0751985326
H,0,2.7940506938,3.7182613806,-2.1833924184	H,0,-0.7188339554,-1.3224604776,7.2150155992
H,0,1.1000792779,3.3203716604,-1.9150145176	H,0,0.8257103634,-0.6810953956,6.6602818428
C,0,2.8030495416,1.6572879809,-0.5296530996	C,0,-1.2029491008,0.8514687062,5.6197116826
H,0,1.946706692,1.9164290923,0.0965839864	H,0,-1.7201751426,1.3704368555,4.8116602834

H,0,3.5690173765,2.4228953419,-0.3822501723	H,0,-0.3403263351,1.4561748065,5.9054599586
H,0,3.2137618277,0.7155901912,-0.1662019031	H,0,-1.8778478124,0.8042514006,6.4776179509
C,0,3.6744648791,1.1660969821,-2.7962923027	C,0,-2.0173443423,-1.3635594842,4.8108754778
H,0,3.5064524733,1.0949204314,-3.868744843	H,0,-1.74961855,-2.3696274074,4.4867055158
H,0,4.0520597193,0.2041481387,-2.4460059929	H,0,-2.5620957645,-0.8954157213,3.9916126204
H,0,4.474703244,1.8944388841,-2.6405701435	H,0,-2.6858992755,-1.4436581125,5.6706056636
H,0,0.7578919808,-0.8158414083,4.5328566689	C,0,-0.7119420776,-1.4758690903,-0.2948201839
C,0,-1.5540476045,1.11221474,4.9610177631	C,0,-0.771677078,-2.8588226673,0.1816037921
C,0,-0.9992562499,0.5195280265,6.2522468983	C,0,-0.7583730492,-5.4535523106,1.2634176841
H,0,-1.0972134557,-0.5676312975,6.2673261608	C,0,-1.6787704818,-3.2282500902,1.187292353
H,0,-1.5389617628,0.912684228,7.1156182457	C,0,0.1555719008,-3.8196303144,-0.240268108
H,0,0.0569083241,0.7634076269,6.3828833591	C,0,0.1578949398,-5.1038440906,0.2838294076
C,0,-1.4061831171,2.6363222851,4.9942554534	C,0,-1.6711858095,-4.5055187329,1.7143325576
H,0,-1.7877960602,3.0777802141,4.0737146475	H,0,-2.3728607472,-2.483956791,1.5550109178
H,0,-0.3596096844,2.9285365946,5.0965008141	H,0,0.8750266001,-3.5468766456,-1.0049798128
H,0,-1.9592556532,3.0604136326,5.8357643413	H,0,0.8798534479,-5.8299600659,-0.0709046573
C,0,-3.0384693756,0.7580850052,4.8307714387	H,0,-2.3803134804,-4.7663721885,2.4913283081
H,0,-3.185294786,-0.3231042947,4.8188410971	H,0,-0.7566757666,-6.452578296,1.6813487262
H,0,-3.4490918752,1.1590635863,3.9039933014	C,0,-1.7536553875,-0.7407349503,-0.7236004011
H,0,-3.6084942063,1.1676102547,5.6681498311	H,0,-1.5943780769,0.331224872,-0.8474156364
H,0,-1.2084837331,1.3002355595,-0.6199797823	C,0,-3.1116541033,-1.1554049596,-1.0711516157
H,0,-2.6123040895,2.3715343393,0.5330581397	C,0,-5.7485999271,-1.8349412883,-1.7871507733
H,0,-4.7508356349,3.6021047925,0.7324534027	C,0,-4.1364373522,-0.1988878635,-1.0799137259
H,0,-6.8154805812,2.6709437158,-0.2654971756	C,0,-3.4442209094,-2.4601493365,-1.463829914
H,0,-4.595487216,-0.7100423821,-1.673647353	C,0,-4.742067886,-2.7924942143,-1.8098594202
H,0,-6.7310057104,0.507727677,-1.4662040455	C,0,-5.4351805846,-0.5325723096,-1.4245181895
H,0,-3.0205410037,-2.381525039,-2.7893768522	H,0,-3.8981917373,0.8212986954,-0.7976092988
H,0,-3.0398550678,-4.7995913392,-3.2453306106	H,0,-2.67010605,-3.2161364989,-1.5055404803
H,0,-1.757565554,-6.351489105,-1.8026803339	H,0,-4.9700760038,-3.8085579993,-2.1098389382
H,0,-0.4281534809,-3.0335824183,0.5573186808	H,0,-6.2071291079,0.2278561483,-1.4114102945
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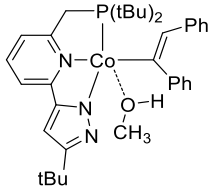
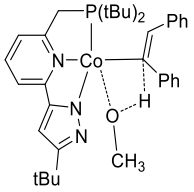
 **PNNCo-cis-PhC=CHPh + CH_3OH**	 **TS2**
Co,0,0.1255421504,0.8827118509,-0.0119335336	Co,0,-0.8027079731,-0.3339825101,0.7198516464
P,0,0.0814275835,1.193197172,-2.2315320545	P,0,-2.7845869628,-1.0267546593,-0.5140875958
N,0,-0.1437928448,2.8782922266,-0.0002854198	N,0,-1.9987865581,1.1448422588,1.1320187956
C,0,-0.2519272259,5.6243770568,0.1340503547	C,0,-3.4495881784,3.3234328437,1.92031501
C,0,0.19466615,3.5063577359,1.1588597598	C,0,-1.3839946636,2.3582796985,1.2043260449
C,0,-0.5529909111,3.5820631186,-1.0682240797	C,0,-3.3265568056,1.0252484898,1.2667168163
C,0,-0.6096600228,4.9666479709,-1.0397074218	C,0,-4.0849458117,2.1058947268,1.6929818612
C,0,0.1425141919,4.8999179749,1.2402919574	C,0,-2.1026495121,3.468433586,1.6455407659
H,0,-0.9335877887,5.5138835557,-1.9147430033	H,0,-5.1547919704,2.0008107927,1.8126052265
H,0,0.4217801539,5.3906584177,2.1626307752	H,0,-1.6105144942,4.4278890381,1.7275369356
H,0,-0.2867527809,6.7058230911,0.179395006	H,0,-4.0247590476,4.1749125531,2.2621564776
C,0,-0.9475699696,2.7504123535,-2.2446818869	C,0,-3.8946339701,-0.2802297655,0.8067111906
H,0,-0.9112974595,3.3126751015,-3.177981204	H,0,-4.9362357282,-0.1580145203,0.5022302977
H,0,-1.9783883958,2.4160193955,-2.1009536173	H,0,-3.86984747,-1.0213798191,1.6127790994
C,0,-0.7862218984,0.0887605529,-3.5048866273	C,0,-3.5432792992,-2.7743210599,-0.671794737
C,0,1.7811303334,1.8007141897,-2.8755547945	C,0,-3.1017332211,-0.0468768325,-2.1158763115
C,0,2.5307597865,0.6700251106,-3.5745725644	C,0,-2.0056771832,-0.4587556296,-3.1051317195
H,0,3.5630250827,0.9828928912,-3.7495712152	H,0,-2.0786665607,0.1593744198,-4.0033977358
H,0,2.0992969618,0.4278367399,-4.5452700991	H,0,-2.07810327,-1.4979970855,-3.4199942182
H,0,2.560134593,-0.2411387065,-2.9756813036	H,0,-1.0125351417,-0.3037044632,-2.6769309165
C,0,2.592862994,2.2275270757,-1.6480722086	C,0,-2.8974731722,1.4411766401,-1.8232525283
H,0,3.6017411127,2.5063907602,-1.963103129	H,0,-2.9754398538,1.9919765341,-2.7640157463
H,0,2.6861010217,1.4217493663,-0.9156820171	H,0,-1.9090449232,1.639377268,-1.4082211802
H,0,2.1585270908,3.0897176306,-1.1424874103	H,0,-3.6515893629,1.8478410925,-1.1478932336
C,0,1.6629400179,2.9920459507,-3.8221575564	C,0,-4.4850298103,-0.2321915156,-2.7269179328
H,0,2.6564090911,3.2552811858,-4.1941889339	H,0,-4.5881745476,0.421820018,-3.597284331
H,0,1.2677453957,3.8758510342,-3.3192565764	H,0,-5.2801819404,0.0371184202,-2.0286771523
H,0,1.0360433818,2.7840807545,-4.6895410335	H,0,-4.6653336514,-1.2497673336,-3.0700570779
C,0,-0.0542058729,-1.249915011,-3.6442873941	C,0,-3.1146324072,-3.4308649464,-1.9820923914

H,0,0.8173516753,-1.1877518362,-4.2905302196	H,0,-2.0316794873,-3.4077482148,-2.1175020532
H,0,-0.7326784452,-1.9811392252,-4.090305037	H,0,-3.5744752617,-2.9756345535,-2.858048588
H,0,0.271210545,-1.639335292,-2.6787591244	H,0,-3.4161532684,-4.481259954,-1.9680339322
C,0,-2.1703367113,-0.2025829347,-2.9189585552	C,0,-2.9670599391,-3.6052617475,0.475597989
H,0,-2.0936039745,-0.6900167586,-1.9466741987	H,0,-1.8806338512,-3.6806351551,0.4182356124
H,0,-2.702390638,-0.8823712854,-3.5886195751	H,0,-3.380857691,-4.6160585751,0.4244581622
H,0,-2.7873045746,0.6879454751,-2.8025709643	H,0,-3.2013324265,-3.1898012825,1.4543420482
C,0,-0.9314394933,0.7525256303,-4.8694922769	C,0,-5.0667739485,-2.7920913687,-0.5617807867
H,0,0.0337654337,0.9296161733,-5.3451199453	H,0,-5.5608656914,-2.1912974529,-1.3228276523
H,0,-1.4656625383,1.7027525361,-4.8176811525	H,0,-5.4080265192,-2.4493674279,0.4150958345
H,0,-1.5009377228,0.0985206846,-5.5351276434	H,0,-5.4213250251,-3.8200698497,-0.6774836971
C,0,0.570566192,2.5995756342,2.1960820439	C,0,-0.0585230532,2.3127113317,0.6620671555
N,0,0.5553670749,1.2729088574,1.8680695952	N,0,0.2628118665,1.123972297,0.0547784868
C,0,0.9198749583,2.7183011725,3.5408025043	C,0,1.0022025913,3.1941313365,0.4644854761
H,0,1.0213881427,3.6210347182,4.1207010825	H,0,1.0799868177,4.2177085884,0.7921835794
C,0,1.1008942496,1.402535898,3.9577569764	C,0,1.9314347555,2.4489175414,-0.2629294489
N,0,0.8838477528,0.5454306484,2.9339324947	N,0,1.4686340181,1.1997076349,-0.4953374338
C,0,1.4712458061,0.8569255913,5.3133823436	C,0,3.3040701049,2.826824284,-0.7598753128
C,0,1.6101005197,1.9921667139,6.3225444223	C,0,3.4076285187,2.5139960408,-2.2547261391
H,0,2.3902665922,2.6961324291,6.0267013086	H,0,3.207745006,1.4590047207,-2.442568441
H,0,1.8755310983,1.599041626,7.3053812708	H,0,4.4067342635,2.7498338704,-2.6282192915
H,0,0.6774909383,2.5498203315,6.4288823495	H,0,2.6860228685,3.095809817,-2.8305685309
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H,0,0.2684574876,-0.9352433346,5.0751883968	H,0,3.5211902658,4.5638404486,0.5346719573
H,0,-0.5873441948,0.3957298977,5.8559048482	H,0,2.8373723784,4.9329156763,-1.050921571
H,0,0.6196776625,-0.5260041044,6.7594828829	H,0,4.5581243533,4.5850820345,-0.8882088907
C,0,2.7974914754,0.0983982193,5.2091406632	C,0,4.3495437575,2.0008222006,-0.0019650188
H,0,3.605823912,0.7614424451,4.8965555102	H,0,4.3193933014,2.2123714348,1.0682476142
H,0,2.7235133543,-0.7051450909,4.4768144837	H,0,5.3560480093,2.2243419929,-0.3634780198
H,0,3.0712944247,-0.3362351402,6.1733589482	H,0,4.1684284558,0.9317335467,-0.1268837153
O,0,-2.2267618468,0.7830265954,0.2800623562	C,0,0.7384051188,-1.7315348647,0.6220254801
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C,0,2.1194237192,-2.9367781688,-0.3509402251	C,0,4.3302460411,-1.2619619935,2.9163709896
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C,0,3.0882530334,-3.3246117551,-1.2871351626	C,0,2.9513533429,-2.5526088972,1.4265600521
C,0,1.6743682757,-3.9078354671,0.5564697643	C,0,4.1052296256,-2.4166148286,2.1776001525
C,0,2.1561618692,-5.2045141096,0.5050015412	C,0,3.3782945139,-0.2531768129,2.9016535532
C,0,3.5672749275,-4.6223738094,-1.3406200463	H,0,1.4955979953,0.415136555,2.1450272316
H,0,3.4628029139,-2.5826500683,-1.9860729248	H,0,2.7804631957,-3.4606544195,0.8601095445
H,0,0.9600270447,-3.6338592511,1.3216316009	H,0,4.8321473048,-3.2199834363,2.1919532722
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C,0,-2.9343582666,-3.2575982566,1.3885836477	C,0,-1.0870748742,-1.2428773689,3.4455152456
C,0,-1.3348193687,-2.7139475148,-0.3273769298	H,0,-1.7707518641,-0.4400357447,3.7448345903
C,0,-1.1455727701,-1.7030920161,1.8428879822	H,0,-0.0628434941,-0.8630340631,3.5405142408
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C,0,-2.4594209921,-3.4077324076,0.0926075987	H,0,-0.3188544626,-2.55634956,-0.9754081855
H,0,-0.9605015742,-2.8550647633,-1.334906246	C,0,2.8646724174,-1.7265111022,-1.6639046865
H,0,-0.6110995032,-1.0481740413,2.5231220206	C,0,3.831428852,-1.9556763886,-2.6251892653
H,0,-2.6153730863,-2.2913272778,3.2799571763	C,0,3.6991888329,-3.0126383104,-3.5186830105
H,0,-2.9640184591,-4.0755878806,-0.5957452905	C,0,1.5971959112,-3.5871977497,-2.5096346234
H,0,-3.8116141354,-3.801120452,1.7164790772	C,0,2.5757433267,-3.8257214003,-3.4604952314
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H,0,-3.7368698609,1.2274954737,1.6468736279	H,0,4.6910408085,-1.2981602159,-2.685337032
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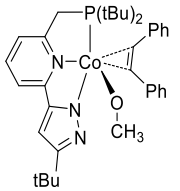	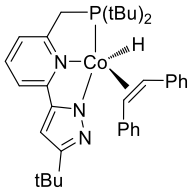

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P,0,-0.2555995184,1.1963782984,-2.6801998942	P,0,-0.3585814414,1.2263160769,-2.4822939256
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C,0,2.4554991027,4.4367161264,0.2372495363	C,0,2.3747563562,4.4845706703,0.192982595
C,0,1.534786304,2.361228541,0.9859669974	C,0,1.4405309973,2.4319147001,1.0009513975
C,0,0.9797755528,3.1664747227,-1.1458724029	C,0,0.7821769855,3.2565300151,-1.0941509103
C,0,1.744806637,4.3067740999,-0.9533024875	C,0,1.5940566071,4.3680875892,-0.9560505787
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H,0,1.7656381797,5.0822027932,-1.7074417113	H,0,1.6044140071,5.1288251214,-1.7249556941
H,0,2.8235639448,3.5966929099,2.1833113932	H,0,2.8386395398,3.626196876,2.107989584
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H,0,0.3399649231,3.5736442658,-3.1714282916	H,0,0.0738325768,3.6206748274,-3.1033316934
H,0,-0.9338580035,3.3866051129,-1.975025168	H,0,-1.1655633503,3.3916300686,-1.8687260513
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C,0,1.1209622156,0.8866638598,-3.9631660133	C,0,1.2414729914,0.8301473754,-3.4777461419
C,0,1.1506424889,-0.6021677455,-4.3039349213	C,0,1.0631681172,-0.3937799409,-4.3724396527
H,0,1.9726950502,-0.8095387066,-4.9935264896	H,0,2.0388483707,-0.6880080043,-4.7675375176
H,0,0.2290903179,-0.9198285778,-4.7949777844	H,0,0.4179323506,-0.1938694327,-5.2276837519
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H,0,0.777320687,2.7413607174,-5.091456327	H,0,2.0276227723,2.8518533422,-3.7323530836
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H,0,-3.4813719263,-0.5340635089,-3.4429178263	H,0,-3.1694472566,-0.4270727438,-4.4232802268
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C,0,-2.0325387061,1.1106833057,-4.9912694772	C,0,-1.7414175928,1.8689730723,-4.89694838
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C,0,1.137528511,1.3668584082,1.9332451877	C,0,1.1121107972,1.4307982425,1.9576978705
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H,0,0.8454126456,-0.5391915239,6.9547104706	H,0,1.2105302266,-0.4554594325,6.985405095
H,0,0.8794322091,1.0331829368,6.1607050714	H,0,1.1898633657,1.1116447944,6.180953834
C,0,-1.3126325771,-0.3601987165,5.2544511298	C,0,-1.0703648455,-0.2895561057,5.4709568911
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H,0,-0.1987330116,-2.5035117416,3.938837828	H,0,-0.0796238314,-2.4380532204,4.0853124169
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H,0,1.9712862929,-0.7134407417,-1.6587217107	H,0,-0.2358325834,-1.5194046709,-1.9693952285
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H,0,3.9468290094,0.0998984255,-1.0157121382	H,0,1.5642047427,-2.7254625301,-2.3488926189
H,0,1.661261876,-2.0085912868,1.931738447	H,0,0.4943124987,-2.1050479255,1.7541766775
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C,0,-0.3188085055,-4.5900442615,1.4808916	C,0,-2.6927776104,-3.3238172444,2.5147039924
H,0,1.3613853324,-3.8392232892,0.3789353615	H,0,-1.3128398935,-3.5770686419,0.8964094095
H,0,-2.1705950131,-1.4376574879,0.2579660396	H,0,-3.207085041,0.2407965231,1.1509466045
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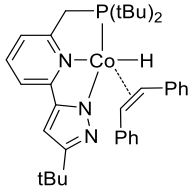	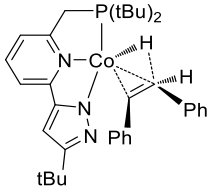
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P,0,1.7227017394,0.5813177644,-2.0551046195	P,0,1.819273672,0.6518751082,-2.0429108688
N,0,1.9621983791,-0.4746755151,0.5331337571	N,0,1.7317329019,-0.6093403435,0.4794681548
C,0,3.6897199437,-2.2783441299,1.6849440516	C,0,3.1054679718,-2.7455966942,1.5431285209
C,0,2.060247075,-0.5380519483,1.8905333225	C,0,1.8018765365,-0.7588204263,1.8334875201
C,0,2.7202255043,-1.2593436175,-0.2475867667	C,0,2.382462212,-1.4540786523,-0.3350896124
C,0,3.601008527,-2.1796172191,0.2999697781	C,0,3.0790349434,-2.5415557786,0.1668063962
C,0,2.9251071984,-1.4563492446,2.4869742224	C,0,2.4789356025,-1.8497244559,2.3820745598
H,0,4.2030880937,-2.80400763,-0.3464563829	H,0,3.5933990295,-3.2103597332,-0.5100337888
H,0,2.9835286393,-1.5097390247,3.565568188	H,0,2.5114057616,-1.9660516228,3.4566002794
H,0,4.3643955458,-2.9973732801,2.132906707	H,0,3.6353915607,-3.5958256998,1.9541266387
C,0,2.5512334949,-1.0623156442,-1.7252348268	C,0,2.3308109832,-1.1263316555,-1.7953731016
H,0,1.8769890546,-1.8298816467,-2.1211571864	H,0,1.5557435471,-1.7288492381,-2.2808369282
H,0,3.4987442778,-1.1884543415,-2.2559377065	H,0,3.2721240813,-1.3846592035,-2.2879760451
C,0,3.159880191,1.8285261031,-2.1450611812	C,0,3.4414162801,1.65093534,-1.909351449
C,0,0.9522332447,0.3186873335,-3.7699273829	C,0,1.2180268212,0.6188289316,-3.8502957113
C,0,0.5482141812,1.668873792,-4.3545968281	C,0,1.0579529231,2.0501839091,-4.3540830604
H,0,-0.0682404167,1.512396847,-5.2430022619	H,0,0.5371164112,2.0461553025,-5.3146372436
H,0,1.4112836317,2.2597950362,-4.6611624409	H,0,2.0174365345,2.543033268,-4.5098448492
H,0,-0.0352725486,2.2567910124,-3.6437406437	H,0,0.4714109874,2.659561424,-3.6630105282
C,0,-0.3114875996,-0.510360166,-3.5450751209	C,0,-0.1586102643,-0.0480239499,-3.8420848292
H,0,-0.8185851521,-0.6679786833,-4.4999781719	H,0,-0.5435329128,-0.0910162607,-4.863944065
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H,0,3.3923923219,3.9653993555,-2.0222669506	H,0,3.9751782177,3.7148797419,-1.5939446945
H,0,1.9126742142,3.3737303308,-1.253385534	H,0,2.3938157885,3.2887945267,-0.9332386687
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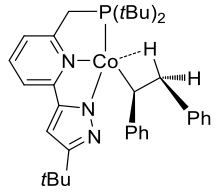
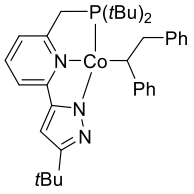
 **PNNCo-cis-Ph-C-CHPh-H-agostic**	 **PNNCo-cis-Ph-C-CH₂-Ph**
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P,0,1.6917667163,0.583626364,-1.9976038857	P,0,1.9158730901,-0.8578811614,-1.8274676903
N,0,1.3170973148,-1.1888749081,0.0831657394	N,0,2.7300272143,-0.4531456894,0.8525538233
C,0,3.0399969022,-3.0524111087,1.1214540171	C,0,5.1369513338,0.4105140808,1.8979160545
C,0,1.4167709207,-1.3163749815,1.4380003966	C,0,2.7789161472,0.0527385852,2.1168401827
C,0,2.2059518461,-1.7916365054,-0.7266415418	C,0,3.8468160088,-0.5037287824,0.1066038495
C,0,3.0683120801,-2.7571648596,-0.2436938564	C,0,5.0697068064,-0.071842382,0.5945128363
C,0,2.2492626111,-2.3093406599,1.9695479659	C,0,3.9931264712,0.4727469411,2.6648885303
H,0,3.7663648005,-3.2446322858,-0.9107071183	H,0,5.9497529301,-0.1219602844,-0.0324943257
H,0,2.2934749279,-2.4432893856,3.041829212	H,0,4.0122055506,0.8665307573,3.6718619279

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H,0,1.5439530358,-1.7000927512,-2.7751301666	H,0,3.8311712001,-2.1627172281,-1.1954508403
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H,0,0.4956131203,2.9142253478,-3.3154260701	H,0,0.3228919983,-2.9339630007,-4.581494084
C,0,-0.0930922115,0.3075842879,-4.0632423025	C,0,2.345333099,-3.4248224624,-2.812012093
H,0,-0.3589509931,0.4011536685,-5.1190979181	H,0,2.0369928108,-4.2017888471,-3.5146794809
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H,0,2.3131569928,-0.7468654005,-4.742400998	H,0,3.6850267484,-1.4405374205,-4.2420424772
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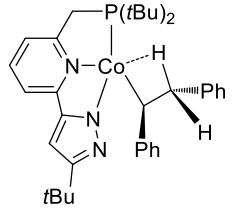
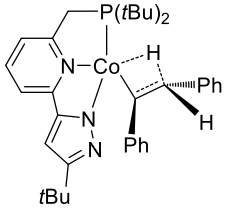
H,0,-1.6030926494,-3.2917009759,0.4322774964	H,0,-0.0215675457,-5.5956893164,0.2975392408
H,0,-2.006227008,-4.3031185434,2.6347026645	H,0,-1.3810879687,-5.7069271247,2.3704214234
 **^{PNN}Co-trans-Ph-C-CHPh-H-agostic**	 **TS4**
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P,0,1.6863938294,0.6364222886,-2.2519297042	C,0,0.0913848645,-1.5611310981,1.8777442732
N,0,1.4606801237,-1.1325371068,-0.1521828718	C,0,-0.2146078427,-2.401600667,2.9547241092
C,0,3.2359650869,-2.9641173054,0.8381795568	C,0,-1.5346757029,-2.7010255153,3.2201675161
C,0,1.5740919455,-1.2753395588,1.1963214116	C,0,-2.5442563456,-2.234317833,2.3778241133
C,0,2.3426017581,-1.7082129433,-0.9846914471	C,0,-2.1943131799,-1.3888809425,1.3398823209
C,0,3.2308521586,-2.6637410914,-0.5242502778	Co,0,-0.3991886647,0.3461974985,-0.1739984241
C,0,2.4436186114,-2.2447360061,1.7080956372	P,0,-2.0490858295,-0.662522301,-1.2978220601
H,0,3.9196734872,-3.1415330899,-1.2076857906	C,0,-3.1087528445,-0.9591987158,0.2331017995
H,0,2.516580635,-2.3817665867,2.7785498898	N,0,1.3530720324,-0.7172315326,0.0584659969
H,0,3.9131159867,-3.7178200836,1.2206728974	N,0,2.5779080315,-0.719844967,-0.4563535057
C,0,2.3538066513,-1.1225567473,-2.3643906853	C,0,3.3956209166,-1.3352390658,0.4353117188
H,0,1.6634864036,-1.6555483433,-3.0265795218	C,0,2.6779289573,-1.7433104697,1.5561991948
H,0,3.3474215739,-1.1974178375,-2.8136643965	C,0,1.3712998883,-1.332293383,1.2856582348
C,0,3.1254934924,1.7314397118,-1.6688530572	C,0,0.0939636501,1.7958396662,1.172571058
C,0,1.2462865974,0.9961902434,-4.0657512577	C,0,-1.3515906792,1.4846725676,3.1531246258
C,0,1.003524996,2.4906376518,-4.2548039959	C,0,-2.5342018136,1.6603909527,3.8467358676
H,0,0.5748548278,2.6694361434,-5.2438960414	C,0,-3.5554385649,2.4367050229,3.3115267174
H,0,1.9228524504,3.0719839277,-4.1913740978	C,0,-3.3639992245,3.046095994,2.0789894928
H,0,0.3011844117,2.8833258401,-3.5161655308	C,0,-2.1787657261,2.8713112551,1.3830435817
C,0,-0.0665029445,0.2591527707,-4.3379381387	C,0,-1.1444470433,2.075855645,1.8961860679
H,0,-0.3684501344,0.4226078983,-5.3754783806	C,0,0.4019889164,2.3065307529,-0.1191899515
H,0,-0.8726164211,0.6188493746,-3.6962233564	C,0,1.9721153157,3.2315591932,-1.7970818664
H,0,0.0228056248,-0.8190283125,-4.1910389346	C,0,3.2361203441,3.5669400576,-2.250078755
C,0,2.2901993865,0.499113499,-5.063540766	C,0,2.9138555028,2.2997751837,0.1974581305
H,0,1.9537973917,0.7234695063,-6.0792449706	C,0,4.3476160007,3.2769258615,-1.4720951725
H,0,2.4274379763,-0.5810456311,-5.0058119591	C,0,4.1792716415,2.6450594393,-0.2489824476
H,0,3.2620262103,0.9693576705,-4.9335861365	C,0,1.7890925692,2.5998574672,-0.5666042168
C,0,2.5252870759,3.0783957334,-1.2572714635	H,0,-3.5725176202,-2.5431534891,2.5072422618
H,0,2.1161179032,3.6366997013,-2.0978765247	H,0,0.5872809119,-2.8393116355,3.5336813395
H,0,3.3050774977,3.695682806,-0.8046028263	H,0,-1.7838462193,-3.3525561888,4.0486977857
H,0,1.7350544968,2.9426170107,-0.5156814571	H,0,-3.5736408147,0.0066138625,0.4613320202
C,0,3.7057151763,1.0871519195,-0.4082326446	H,0,-3.918921843,-1.6782962888,0.0888915966
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H,0,4.6548497634,0.9759564264,-3.0340693404	H,0,-1.6278802984,0.7134992388,-3.8487548061
H,0,5.0541862891,2.489461849,-2.2358285203	C,0,-3.2002187617,1.7773282092,-1.8265239493
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C,0,0.5473424988,-0.064419891,3.2695922206	H,0,-3.5461565719,1.8144559478,-0.7920166104
H,0,0.7753380244,-0.6997121531,4.1112145101	C,0,-4.6556540341,-0.1470018196,-2.3902090941
C,0,-0.1346961735,1.1500223428,3.2674119724	H,0,-5.2650159404,0.4992583682,-3.027352368
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C,0,-0.7360190836,1.8825064073,4.4408318679	H,0,-4.7553868511,-1.1613440263,-2.7695776731
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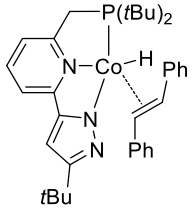
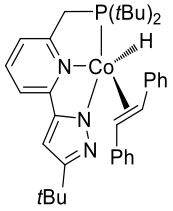
H,0,-0.0508128413,2.7794678372,6.3001619303	H,0,-0.2698347457,-3.1454038213,-3.4762834246
H,0,1.1085664897,2.9071714157,4.9732599778	H,0,0.2845182472,-1.6833914556,-2.6562136413

C,0,-1.4468399456,3.1477209438,3.9710731697	C,0,-1.1424878704,-3.2668013355,-0.9691248518
H,0,-2.2460031963,2.9089378913,3.2694070852	H,0,-0.2460700804,-2.8410291032,-0.5172556495
H,0,-0.7613416211,3.8216799059,3.4572995913	H,0,-0.8640555336,-4.2240712759,-1.4163322747
H,0,-1.8794825784,3.6751426257,4.8243819056	H,0,-1.8693415849,-3.4750460134,-0.1824695283
C,0,-1.7514898386,0.9701693472,5.1370543745	C,0,-2.9118279,-3.0327254607,-2.7023837433
H,0,-1.2829747237,0.0541212592,5.5010962352	H,0,-3.2808816273,-2.4953723523,-3.5755753545
H,0,-2.5512710466,0.6848527226,4.4508984965	H,0,-3.7371162613,-3.1474221013,-1.9967212694
H,0,-2.2047439506,1.476084258,5.9930445972	H,0,-2.6354605052,-4.035692442,-3.0382995101
H,0,-1.209177984,1.0459973511,-1.3303026196	H,0,3.0411803687,-2.2698276406,2.4248666946
C,0,-1.5798699132,-0.7840464506,-0.126525051	C,0,4.8681163593,-1.5124338187,0.1584282537
H,0,-1.7010775058,-0.758635696,0.9522372251	C,0,5.2159888237,-3.0046585406,0.1617072395
C,0,-2.0818031156,0.4020305121,-0.8546000958	H,0,4.9823431415,-3.4668484958,1.1224630179
H,0,-2.6142685512,0.1287442531,-1.7731644632	H,0,6.2811910699,-3.1548985555,-0.0303838398
C,0,-2.8730224336,1.4084677612,-0.0654457581	H,0,4.6563804287,-3.5383092717,-0.6077744026
C,0,-1.4910344228,-2.1034656589,-0.7262831411	C,0,5.2333312823,-0.9128953965,-1.1961868048
C,0,-1.0099249103,-4.64618175,-1.842451086	H,0,4.988338448,0.1484503367,-1.2383230641
C,0,-1.5537014135,-2.3162712533,-2.1134027166	H,0,4.6848152528,-1.3978423919,-2.0031996093
C,0,-1.1999863273,-3.2146813364,0.0844348335	H,0,6.3028908933,-1.0326189918,-1.3834635962
C,0,-0.9624159531,-4.4597940101,-0.4645224952	C,0,5.6765036766,-0.8136722295,1.2566647899
C,0,-1.3147219492,-3.5667155935,-2.6602525919	H,0,5.4574451499,-1.2318831702,2.2406757803
H,0,-1.7988952799,-1.4894343495,-2.7703608797	H,0,5.445371138,0.2522514867,1.2926182201
H,0,-1.1457558398,-3.0727373204,1.1585125819	H,0,6.7493147262,-0.9208295876,1.07900281
H,0,-0.7347925218,-5.2962616257,0.1855586331	H,0,-0.0019295103,1.3108888539,-1.2761824095
H,0,-1.3727200229,-3.7000005531,-3.7346387544	H,0,0.9067644498,1.4119316293,1.7798534554
H,0,-0.8235465277,-5.6227658234,-2.2704887695	H,0,-0.3025926929,3.0389413797,-0.5123590706
C,0,-2.489885851,2.74308696,-0.0017937717	H,0,-2.050866751,3.371899885,0.4309240861
C,0,-3.2623314185,3.6668853341,0.6836725645	H,0,-0.5657971401,0.8647627815,3.5719009922
C,0,-4.4242925287,3.2635868759,1.3249656857	H,0,-2.6637519432,1.1843862463,4.8114605477
C,0,-4.0319547382,1.0072623445,0.5941658358	H,0,-4.1425449813,3.6712291774,1.6571523184
C,0,-4.8032082963,1.9289828966,1.285243635	H,0,-4.4817169289,2.575626901,3.8542352245
H,0,-1.5581171174,3.0500303733,-0.4662967536	H,0,1.1021436733,3.4593557767,-2.4056105919
H,0,-2.9438262156,4.7006214264,0.7361289324	H,0,3.3543187389,4.0576500175,-3.2082971118
H,0,-5.023725839,3.983309796,1.8684686077	H,0,5.3395512186,3.5409433374,-1.8170070339
H,0,-4.3276563414,-0.0357073981,0.5628711948	H,0,2.8073754821,1.7925540896,1.1484380177
H,0,-5.7018651588,1.6038565266,1.7950034135	H,0,5.0433366896,2.4131670013,0.3616296767
 **PNNCo-H + trans-Ph-CH=CH-Ph-tetragonal pyramidal**	 **PNNCo-H + trans-Ph-CH=CH-Ph-trigonal bipyramidal**
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P,0,1.4867887619,0.4864389677,-2.0078972393	P,0,0.3237834482,-1.1415636251,-2.1291599524
N,0,1.3391879305,-1.2143833123,0.1084745976	N,0,-0.9791322704,-1.9874144671,0.3065744042
C,0,3.1765340541,-2.9390359216,1.1793500653	C,0,-2.8354323915,-3.9421458119,0.8094708531
C,0,1.414785179,-1.3386193273,1.4626922785	C,0,-1.5567720798,-2.0560127881,1.5378095987
C,0,2.2662561557,-1.766211541,-0.6890197277	C,0,-1.2105213574,-2.9289373031,-0.6151745018
C,0,3.1963391738,-2.6601005721,-0.1874086311	C,0,-2.1550164273,-3.9209744815,-0.4057696099
C,0,2.3141863727,-2.258887849,2.0143478198	C,0,-2.5230626196,-3.0297050368,1.7969856937
H,0,3.9318471249,-3.1066238139,-0.8425058176	H,0,-2.3380534509,-4.6686025672,-1.1658471603
H,0,2.3519086782,-2.3902269096,3.0872536594	H,0,-3.0035324516,-3.0619184185,2.7652549887
H,0,3.8817354065,-3.6485703822,1.5944259905	H,0,-3.588446092,-4.6987996133,0.9922385341
C,0,2.2659034063,-1.2224649127,-2.0852329675	C,0,-0.2893726375,-2.8755802754,-1.78809596
H,0,1.6135989648,-1.8163084233,-2.7363547968	H,0,-0.7087043938,-3.3559660021,-2.6733993214
H,0,3.2670409693,-1.2485408246,-2.5226171103	H,0,0.6029544001,-3.4492941075,-1.5176640616
C,0,2.813948227,1.6991451758,-1.3965345337	C,0,2.0169104353,-1.5106596445,-2.9411386626
C,0,1.0188178369,0.8305469986,-3.8109611082	C,0,-0.9269630954,-0.6092242882,-3.4841779883
C,0,0.6735751785,2.3056697762,-3.9910513175	C,0,-0.7505651302,0.8598555993,-3.864876843
H,0,0.2338819305,2.4539441191,-4.980258358	H,0,-1.4620407192,1.1081248071,-4.6569024658
H,0,1.5487556489,2.9514989277,-3.9272157696	H,0,0.246649344,1.0916250742,-4.2336870166
H,0,-0.0558537982,2.6394694203,-3.2510567723	H,0,-0.9559182711,1.5278138839,-3.0332201057
C,0,-0.2395430762,0.0071023353,-4.0842766775	C,0,-2.3025273318,-0.7872946223,-2.8364247305
H,0,-0.5727700038,0.1828898399,-5.1102333107	H,0,-3.0650877298,-0.304550706,-3.452451178
H,0,-1.0502349002,0.2858291068,-3.4088133064	H,0,-2.3423389588,-0.3401400107,-1.8409305048

H,0,-0.0655378156,-1.0644617621,-3.977155415	H,0,-2.5815342784,-1.8373510872,-2.7385027352
C,0,2.1004652281,0.4083547202,-4.8036543504	C,0,-0.8783641292,-1.4373461536,-4.7644639674
H,0,1.7518428014,0.6095492261,-5.8198232796	H,0,-1.737093385,-1.171441523,-5.3871447616
H,0,2.3118472237,-0.6599975,-4.7464735519	H,0,-0.9367676409,-2.5115131941,-4.5859335581
H,0,3.0367436962,0.9457712044,-4.6708238847	H,0,0.0153066436,-1.2348776374,-5.353946845
C,0,2.0988347466,2.9900128491,-0.9899846293	C,0,2.4605253231,-0.3061474626,-3.7653515356
H,0,1.6656923954,3.5203850617,-1.8357815292	H,0,1.8855455719,-0.1992737561,-4.6858191555
H,0,2.820056577,3.6612339006,-0.5175731443	H,0,3.5077804281,-0.4295122841,-4.0523575949
H,0,1.303484721,2.7876669774,-0.2704024768	H,0,2.3881337991,0.6239882179,-3.2009126931
C,0,3.4426648433,1.109311338,-0.1327488989	C,0,3.0347928597,-1.7349391804,-1.8244197551
H,0,2.6955519536,0.9382513947,0.6424673949	H,0,3.2047216059,-0.8285349564,-1.2470328866
H,0,4.16560569,1.8285394031,0.2593578205	H,0,3.9833275307,-2.0426822095,-2.2728818203
H,0,3.9797870723,0.1778338642,-0.3183813246	H,0,2.7269302381,-2.5161126175,-1.1268417992
C,0,3.9122624042,1.9819011236,-2.4140497197	C,0,2.01312448,-2.7623966822,-3.8213075306
H,0,3.5446716625,2.5129886284,-3.2914291125	H,0,1.3074830222,-2.7163721898,-4.6457153315
H,0,4.4124337858,1.071057249,-2.7495753047	H,0,1.8134500327,-3.6711668687,-3.2536568744
H,0,4.674435286,2.6155070063,-1.9531223934	H,0,3.0087087296,-2.8787780915,-4.2567255744
C,0,0.6388875633,-0.3574999297,2.1511880591	C,0,-0.9946871604,-1.1184259695,2.4573975445
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C,0,0.4803906129,0.0241827366,3.4846541302	C,0,-1.0794288849,-0.8744814708,3.8282947513
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H,0,0.4838171131,3.4974972767,5.9086353631	H,0,0.8617152503,2.6885862792,6.0896021686
H,0,1.2324244715,3.379451219,4.3124017662	H,0,-0.4518433663,2.6845233579,4.9116828382
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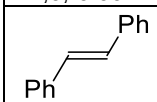	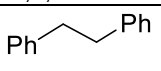
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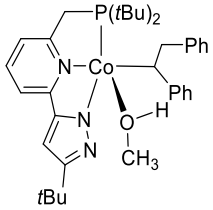
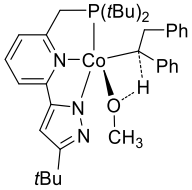
 **^{PNN}Co-cis-Ph-C-CH$_2$-Ph+CH$_3$OH**	 TS5
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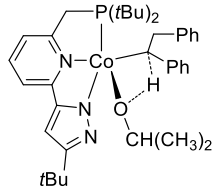
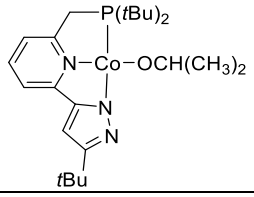
H,0,0.1123242299,2.3431519608,1.1785345877	H,0,-0.5843050818,-0.6492439963,4.3468602041
	
TS6	

	^{PNN}Co-OCH(CH$_3$)$_2$
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P,0,-2.7995581514,-1.0466268446,-0.4979654409	P,0,-0.0734907305,2.0448046346,0.7882589164
N,0,-2.0339471993,1.1847542409,1.0747503724	N,0,-1.6221685603,0.1986890392,2.249831353
C,0,-3.5015513812,3.3636383083,1.8306702919	C,0,-3.9192046979,0.4920773542,3.7519254149
C,0,-1.4277152233,2.4024126635,1.1337854611	C,0,-2.3378864025,-0.9059606862,2.6206046734
C,0,-3.3596126503,1.0566978975,1.2132369497	C,0,-2.0289922771,1.4284904223,2.622484884
C,0,-4.1273307729,2.1382328299,1.6204851873	C,0,-3.180487424,1.6077755741,3.3703240008
C,0,-2.1549069481,3.5138714527,1.5568510467	C,0,-3.4974032907,-0.7683994813,3.3836448855
H,0,-5.19601844,2.0256309786,1.7435047825	H,0,-3.4868963482,2.6063289591,3.6513561914
H,0,-1.6682820506,4.4768526535,1.6298592567	H,0,-4.0532585606,-1.6521514809,3.6652125483
H,0,-4.0831922062,4.2156321124,2.1600619631	H,0,-4.8220649522,0.6140542612,4.3369676861
C,0,-3.9162556979,-0.266998541,0.7953062731	C,0,-1.1455411183,2.5685004925,2.2119470261
H,0,-4.9591390253,-0.1648798212,0.4882884773	H,0,-0.4640862936,2.8014522945,3.0364306171
H,0,-3.8807180462,-0.9789931469,1.6279992536	H,0,-1.7206813751,3.4783049154,2.0255192912
C,0,-3.5572935403,-2.7995077416,-0.6162558557	C,0,-1.0174388817,2.5657806942,-0.7631565029
C,0,-3.108021797,-0.1114163229,-2.1293380016	C,0,1.5408555692,2.9822652457,1.0328475316
C,0,-1.9997806489,-0.5434269849,-3.0963870257	C,0,2.374231817,2.8846403055,-0.2427920985
H,0,-2.076819931,0.0390936647,-4.0178387363	H,0,3.381831459,3.2570268054,-0.0423838829
H,0,-2.052352024,-1.5950244866,-3.3722834946	H,0,1.9619770289,3.4911789212,-1.0503779438
H,0,-1.0124869701,-0.3549307091,-2.6679243955	H,0,2.4519812594,1.8473947958,-0.5743767082
C,0,-2.9153211423,1.3861625922,-1.8804747045	C,0,2.2688645615,2.2265013856,2.1481653307
H,0,-2.9914505009,1.9069523386,-2.8383631874	H,0,3.2182338732,2.7239861984,2.3612046649
H,0,-1.9306723863,1.6037279564,-1.4662873959	H,0,2.4717491843,1.1979278362,1.846013719
H,0,-3.6758870679,1.8082496005,-1.2220821925	H,0,1.697974256,2.2079825868,3.0798850787
C,0,-4.484863761,-0.3208334178,-2.7478889782	C,0,1.3444232705,4.4387763397,1.4420951139
H,0,-4.5815233267,0.3068985572,-3.6381198875	H,0,2.3222143531,4.8983053442,1.6075565399
H,0,-5.2875064958,-0.0333284123,-2.0656037716	H,0,0.7865467769,4.5370635229,2.3746404293
H,0,-4.6593164086,-1.3485034012,-3.0625295201	H,0,0.8351844924,5.0276501054,0.6811512185
C,0,-3.1224889431,-3.4895271947,-1.9073237107	C,0,-0.3910372304,1.8531500554,-1.9624563642
H,0,-2.0381430384,-3.4801844882,-2.0325422708	H,0,0.6147287977,2.2058508183,-2.1824420106
H,0,-3.569603818,-3.0511161966,-2.7981159579	H,0,-1.006032703,2.0270885722,-2.8487591989
H,0,-3.4337116094,-4.5365739947,-1.8716136646	H,0,-0.3255692365,0.7766991416,-1.7946229006
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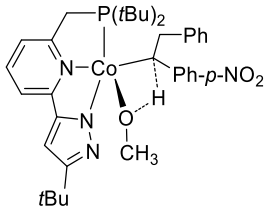
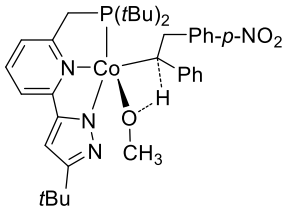
H,0,-1.9050884267,-3.6823795925,0.5081261428	H,0,-2.4505308248,0.9583069444,-0.3860965346
H,0,-3.4074109456,-4.6167311617,0.520196072	H,0,-3.007625311,2.2025785031,-1.5014257326
H,0,-3.234672643,-3.1684553717,1.5211976203	H,0,-2.9789133943,2.5289699132,0.227077872
C,0,-5.0815958628,-2.8124551951,-0.5150858531	C,0,-1.0598949935,4.0707804151,-0.991119922
H,0,-5.5706463603,-2.2283257308,-1.2919766224	H,0,-0.0766798297,4.476756098,-1.2287839477
H,0,-5.4278800702,-2.4481806053,0.4521209074	H,0,-1.4524629743,4.6122269285,-0.1277911482
H,0,-5.4364854404,-3.8424488765,-0.6098478555	H,0,-1.714007006,4.2952210088,-1.8377572335
C,0,-0.0933201919,2.3555707649,0.6140154454	O,0,1.4920788472,-0.2998737356,0.130389163
N,0,0.2433561639,1.1607325632,0.0270638723	C,0,-1.7745436144,-2.1243871781,2.1378203777
C,0,0.9710842049,3.2363878757,0.4345663152	N,0,-0.6355056535,-2.0008280737,1.392779723
H,0,1.0404843253,4.2627966486,0.7552613382	C,0,-2.0968898071,-3.4774765919,2.2254426706
C,0,1.9190435796,2.4848330835,-0.2614555482	H,0,-2.9317539734,-3.9269056786,2.7376798815
N,0,1.4633500769,1.2328497593,-0.492490185	C,0,-1.092710361,-4.1088363028,1.4954506555
C,0,3.3023183297,2.8602337469,-0.7300631216	N,0,-0.2225858362,-3.2015412697,0.9994515638
C,0,3.4316323099,2.5581551622,-2.2252610842	C,0,-0.8761145493,-5.5715858256,1.2023026804
H,0,3.2288269046,1.5059336791,-2.4251355981	C,0,-1.9876686074,-6.4092942862,1.8258784867
H,0,4.4388564077,2.7905259848,-2.5786787777	H,0,-2.0159514252,-6.2923370703,2.9109945387
H,0,2.7243490742,3.1488044083,-2.8098026731	H,0,-1.8334903601,-7.468212352,1.6115930888
C,0,3.5654170262,4.3419724313,-0.4815318914	H,0,-2.9672263002,-6.1309257747,1.4323065432
H,0,3.5031392248,4.5868080047,0.5805378211	C,0,-0.8647901566,-5.7796084581,-0.3152156824
H,0,2.8486573521,4.9699897977,-1.0140201243	H,0,-0.0895716501,-5.1695582929,-0.7794540416
H,0,4.5650713823,4.6145587056,-0.8240444105	H,0,-1.8213021516,-5.4967004262,-0.7582112379
C,0,4.330347614,2.0242994329,0.0405133106	H,0,-0.6754718062,-6.8271476455,-0.5608275419
H,0,4.2813513617,2.2279573886,1.111506652	C,0,0.4758947877,-6.0059841871,1.7757895741
H,0,5.3441755227,2.2464157771,-0.3008040584	H,0,0.5030860983,-5.8799508223,2.8594267835
H,0,4.1471947463,0.9569846684,-0.0960207904	H,0,1.2823751924,-5.4091126762,1.3499554422
C,0,0.7153712066,-1.693769561,0.5759001024	H,0,0.6700739173,-7.0577581535,1.5530194044
C,0,0.664786982,-2.2515499091,-0.658723435	C,0,2.0049830688,-1.5071446929,-0.3816552328
C,0,1.7370040232,-2.5030962769,-1.616343986	C,0,3.4761300287,-1.2759565839,-0.6829606566
C,0,1.9505206662,-1.4957397619,1.3541801646	H,0,1.9139999492,-2.3137740678,0.3597540605
C,0,4.2449169413,-1.2186406007,2.9612328027	C,0,1.2391710589,-1.9318228653,-1.6221606834
C,0,2.1398510224,-0.3697907038,2.1654619481	H,0,3.9558128584,-2.1839092962,-1.052683735
C,0,2.9345375275,-2.4939237532,1.3975237757	H,0,3.5914160406,-0.4985541441,-1.4425805112
C,0,4.0655359609,-2.3548104849,2.1823176471	H,0,4.0059700847,-0.9498693496,0.2128771633

C,0,3.2714798464,-0.2301943774,2.9516777956 H,0,1.3936656701,0.4179141852,2.1651893067 H,0,2.7982611305,-3.3893490884,0.8024192113 H,0,4.8101656034,-3.1418506194,2.1920827409 H,0,3.3938679668,0.6597546123,3.557683967 H,0,5.1286645936,-1.1116342969,3.5777783748 O,0,-1.3757324197,-1.6455746992,2.1383640832 H,0,-0.3743001449,-1.9080905751,1.4333380699 C,0,-0.9795292606,-1.4833027247,3.5004388035 C,0,-1.2302707767,-0.069772885,3.9861490768 H,0,0.0975985056,-1.6923199665,3.5863819696 C,0,-1.7446137151,-2.507883107,4.31478197 H,0,-0.324738216,-2.5111740631,-1.0337105343 C,0,2.8563315589,-1.6650111452,-1.6979075249 C,0,3.8333405628,-1.8906046533,-2.6498933226 C,0,3.7208798403,-2.9559849139,-3.5360958207 C,0,1.6172458872,-3.5470997585,-2.5406188209 C,0,2.6062342081,-3.7813430667,-3.4815537982 H,0,2.9106782751,-0.8085179289,-1.0360376097 H,0,4.6855983962,-1.2234585343,-2.7086509951 H,0,4.4908036248,-3.1315324342,-4.2773695787 H,0,0.7401341672,-4.1853562252,-2.5052162598 H,0,2.5043333602,-4.6030808904,-4.1799479611 H,0,-0.9654588295,0.0371883626,5.0390749759 H,0,-0.6391158608,0.6531577142,3.420107645 H,0,-2.2842424148,0.1963378841,3.8721448589 H,0,-1.4609879426,-2.4745087686,5.3675619377 H,0,-2.818261892,-2.3162561947,4.2463714434 H,0,-1.5591772363,-3.51421005,3.940600813	H,0,1.6061858257,-2.8805854344,-2.0195152474 H,0,0.1825336533,-2.065129423,-1.3842022719 H,0,1.3319920918,-1.1734311253,-2.4046550675
 **TS5-para-NO_2-1**	 **TS5-para-NO_2-2**
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H,0,-2.9786299206,-3.4044229974,-2.3579407136	H,0,-3.0639808552,-3.3811810654,-2.3733376612
H,0,-2.5691240165,-4.6956459897,-1.2407582959	H,0,-2.6513684974,-4.6846732227,-1.2716110402
C,0,-2.2789296272,-3.359297959,1.0176965393	C,0,-2.3029847592,-3.3656785193,0.9889682927
H,0,-1.1947787708,-3.3106689659,0.9122407318	H,0,-1.2203581119,-3.3212408269,0.8645737803
H,0,-2.5527022972,-4.4052567382,1.1780165728	H,0,-2.5799856748,-4.4113944887,1.1455248372
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H,0,-4.6655853877,-4.1622270981,-0.0076787043	H,0,-4.7184487467,-4.1363476596,-0.0028312239
C,0,-0.2614547327,2.818322843,0.195434821	C,0,-0.2471235991,2.7933601249,0.188207526
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H,0,0.4965999249,4.8879976347,-0.0840560316	H,0,0.5239317802,4.8577510015,-0.0965820151
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N,0,1.3879184914,1.8115676331,-0.8733816371	N,0,1.3787504008,1.7761020199,-0.9049913647
C,0,2.8510813416,3.6759222182,-1.5788147651	C,0,2.857306836,3.6290451148,-1.609867507
C,0,2.8860274028,5.1986760063,-1.4952689809	C,0,2.8758012654,5.1540838167,-1.576175054
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H,0,5.0053302681,3.4754835436,-1.3683587744	H,0,5.0106000371,3.4598289059,-1.3566608263
C,0,2.8418645529,3.2427017794,-3.0474511645	C,0,2.8776993545,3.1474260712,-3.0627832469
H,0,2.8053482635,2.1561801849,-3.1290050759	H,0,2.8521103444,2.0585292659,-3.1089586542
H,0,3.7398625109,3.5959234759,-3.5588885728	H,0,3.7811093008,3.4922347616,-3.570418761
H,0,1.9743161578,3.6460634387,-3.5721457555	H,0,2.0155707951,3.5244041034,-3.6151546205
C,0,0.9957180138,-1.4438867104,0.7986673094	C,0,0.9817819633,-1.4604441251,0.7959158927
H,0,0.7723228748,-2.4868104907,1.0717130985	H,0,0.7582589335,-2.5048361962,1.0659811995
C,0,1.24233777,-1.4530403382,-0.7188904293	C,0,1.233707794,-1.469912623,-0.7207748604
H,0,1.4411687867,-0.4471728462,-1.0911876577	H,0,1.4078866785,-0.4618698768,-1.098836377
H,0,0.3234629776,-1.789505255,-1.2093606862	H,0,0.329953622,-1.8410725885,-1.2147610146
C,0,2.3766584396,-2.365935542,-1.100097299	C,0,2.3973671764,-2.3462232856,-1.0888640176
C,0,4.4994285604,-4.0660912837,-1.7567891125	C,0,4.5618575228,-3.9552123893,-1.7103343843
C,0,2.2543780716,-3.7480693633,-0.9624203608	C,0,2.325691438,-3.7320217654,-0.9297374056
C,0,3.5800941213,-1.8516907395,-1.5748118374	C,0,3.5828186535,-1.7895537817,-1.5684401743
C,0,4.6342725694,-2.6935546172,-1.9004772118	C,0,4.6700166088,-2.5853819566,-1.8816603284
C,0,3.3030069327,-4.5928930261,-1.2884433393	C,0,3.3985607578,-4.5445820179,-1.2391277859
H,0,1.3189425815,-4.1650609267,-0.5982761779	H,0,1.4074664226,-4.1776225967,-0.5596196931
H,0,3.6826722866,-0.7773213409,-1.6913522358	H,0,3.6428184128,-0.7142166198,-1.6961993407
H,0,5.5641781577,-2.2756477582,-2.2665173815	H,0,5.596651069,-2.1706539377,-2.2529130768
H,0,3.1884719216,-5.6646753481,-1.1796673943	H,0,3.358465922,-5.6189584714,-1.1273932906
H,0,5.3213137927,-4.7240456488,-2.0100488953	N,0,5.7119944545,-4.8126956783,-2.0445317024
C,0,2.1344663542,-1.0121157954,1.6552480932	C,0,2.1275456985,-1.0324302372,1.6563183472
C,0,4.1792724656,-0.2092492296,3.3552747568	C,0,4.2030968426,-0.2308975692,3.3667362879
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H,0,1.6833792341,-2.4581783665,3.1791452942	H,0,1.6960293422,-2.4971048152,3.1643189728
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H,0,-0.0721644596,-1.2106907071,1.5994593388	H,0,-0.0910702621,-1.2343463381,1.5944477813
C,0,-0.7211674016,-0.0589554803,3.4381314178	C,0,-0.7264452425,-0.0941225443,3.4398232479
H,0,-1.4821714039,0.7079035561,3.6291482142	H,0,-1.4826643097,0.6764140622,3.6356301027
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H,0,-0.603713237,-0.6579757705,4.3477309924	H,0,-0.6143636727,-0.7013348476,4.3445739789
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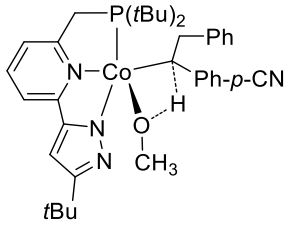	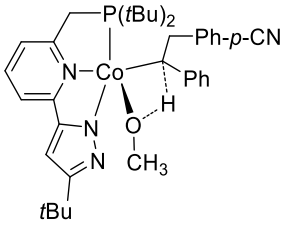
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N,0,-2.0079411293,1.4718194111,0.8831026772	N,0,-2.0155627267,1.4772131057,0.8669237335
C,0,-3.7013097315,3.5298290796,1.4731533117	C,0,-3.7134966976,3.534653909,1.4483297439
C,0,-1.5493504172,2.747635791,0.7902913308	C,0,-1.5609246525,2.7535793203,0.7657475877
C,0,-3.3025920677,1.200870426,1.0983488616	C,0,-3.3088256403,1.2045956377,1.0879409341
C,0,-4.179978462,2.2237166387,1.4260859373	C,0,-4.1886702677,2.2269416937,1.4105308775
C,0,-2.3932883184,3.8063061307,1.1237564589	C,0,-2.4067586552,3.812225422,1.0951990668
H,0,-5.2221561555,2.001188364,1.6103856262	H,0,-5.2298379519,2.0028169252,1.5986827957
H,0,-2.0253147015,4.8217401819,1.0738597672	H,0,-2.0417292275,4.8283735811,1.0382243997
H,0,-4.3709985338,4.3388408749,1.736826278	H,0,-4.38496533,4.3435670431,1.7078341123
C,0,-3.7103832307,-0.2148300756,0.8383296379	C,0,-3.7121802205,-0.2145530385,0.839828197
H,0,-4.7608219935,-0.2624428103,0.5428066223	H,0,-4.7624603738,-0.2689568422,0.5446731594
H,0,-3.5890837307,-0.8208484546,1.7413750479	H,0,-3.5887728303,-0.8121149174,1.7483101667
C,0,-3.0078012078,-2.8351631816,-0.2494656539	C,0,-2.9988140606,-2.8401932366,-0.2245137854
C,0,-3.0345544323,-0.3245978657,-2.1036767601	C,0,-3.0330958302,-0.3473491802,-2.1022105147
C,0,-1.9239938791,-0.7080633905,-3.0856609943	C,0,-1.912722483,-0.7255213216,-3.075274959
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H,0,-1.8227496475,-1.7827533884,-3.2236609582	H,0,-1.7948307211,-1.8003547992,-3.2001749721
H,0,-0.9598239447,-0.3152534099,-2.7564677793	H,0,-0.9563463608,-0.3137337686,-2.7463473926
C,0,-3.0579126381,1.2039226762,-2.0357477714	C,0,-3.0739934974,1.1813084795,-2.0467346331
H,0,-3.2486839709,1.5919873018,-3.0393112189	H,0,-3.2679551169,1.5587183191,-3.0537769431
H,0,-2.1009763826,1.6088561168,-1.704944809	H,0,-2.1220868038,1.5998552645,-1.7185021207
H,0,-3.8454789369,1.5884548111,-1.3862998208	H,0,-3.8664943381,1.5622522519,-1.4011451932
C,0,-4.3897715576,-0.8091243245,-2.6035760964	C,0,-4.3791184319,-0.8506888311,-2.6084253663
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C,0,-2.4955568027,-3.6172165931,-1.4563206467	C,0,-2.4643020209,-3.6302188524,-1.4163753868
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H,0,0.5210201417,4.8695891138,-0.076437999	H,0,0.503780621,4.879613753,-0.099682349
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H,0,1.9973556053,3.5747064569,-3.5781701979	H,0,1.9967091276,3.6059787732,-3.6018493512

C,0,0.9831818542,-1.4616302718,0.8050186823	C,0,0.98664768,-1.4443417295,0.7872289208
H,0,0.760460002,-2.5039912526,1.0813964952	H,0,0.755815543,-2.489700252,1.0466382732
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H,0,3.6125004948,-0.7285357399,-1.7590947491	H,0,3.7054507681,-0.7384333371,-1.621865027
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H,0,5.4154926668,-4.608689749,-2.0073727163	C,0,5.6221827817,-4.8784230148,-2.0710035449
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H,0,4.6655581548,1.221250606,1.8358455664	H,0,4.640407603,1.2440319858,1.9073139224
C,0,5.2438951155,0.2099082848,4.235556963	H,0,5.0015056252,0.0494708877,4.0474627683
O,0,-1.1117272065,-0.8985890681,2.358459578	O,0,-1.0901420106,-0.8757965631,2.3585956259
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H,0,0.2166061236,0.4347093498,3.2777479077	H,0,0.2651906887,0.4477871018,3.2516445591
H,0,-0.6335148921,-0.6823381945,4.3532773123	H,0,-0.5855050092,-0.6493436866,4.3450883298
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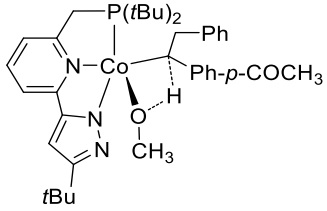
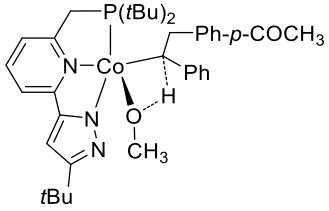
 **TS5-para-COCH$_3$-1**	 **TS5-para-COCH$_3$-1**
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N,0,-2.0165105036,1.4683152083,0.8823264004	N,0,-2.0148662059,1.4715605274,0.8798974901
C,0,-3.7200456448,3.51887168,1.4691371948	C,0,-3.7191445809,3.5191909634,1.4764633196
C,0,-1.5634580438,2.7462291208,0.7894384007	C,0,-1.5652047049,2.7500855513,0.784324003
C,0,-3.3102010424,1.1916575701,1.095677847	C,0,-3.3067438607,1.1928347057,1.1012249226
C,0,-4.1929992309,2.2105112915,1.4211653214	C,0,-4.1897392647,2.2099790345,1.4321172418
C,0,-2.4126459014,3.8012241603,1.1226648274	C,0,-2.4143222909,3.8037298912,1.1215616355
H,0,-5.2346950879,1.9835811765,1.602922873	H,0,-5.2297837904,1.981075884,1.6208169601
H,0,-2.049215094,4.8183301466,1.0730944175	H,0,-2.0535264423,4.8216589604,1.069057438
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C,0,-3.7105464035,-0.2260090329,0.8350089984	C,0,-3.7050341776,-0.2260742823,0.8432506325
H,0,-4.7604345948,-0.2793084149,0.5384911315	H,0,-4.7562150009,-0.2825576654,0.5517907569
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C,0,-2.9948913828,-2.8407227434,-0.2544302461	C,0,-2.9844154192,-2.8403432386,-0.2471615684
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C,0,-1.903662457,-0.7011514683,-3.0815519459	C,0,-1.9191363782,-0.6972022243,-3.0833643091
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H,0,-1.7926150595,-1.7747460199,-3.2210413595	H,0,-1.8012744059,-1.7702435057,-3.2217626804
H,0,-0.9452670163,-0.3012684099,-2.7441565106	H,0,-0.9617194492,-0.2892939869,-2.7526666748
C,0,-3.0603874406,1.199063473,-2.0356554875	C,0,-3.0811768163,1.1966256923,-2.0325536615
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H,0,-4.6042713527,-0.3246911899,-3.564224469	H,0,-4.6245182341,-0.3417131856,-3.5503282674
H,0,-5.1843872962,-0.5921345559,-1.9274241752	H,0,-5.1931567769,-0.6062832578,-1.9088859371
H,0,-4.3842618296,-1.8945051086,-2.8127955944	H,0,-4.3901490865,-1.9071731346,-2.793467806
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H,0,-1.3982105982,-3.4358076726,-1.6200006026	H,0,-1.3939511221,-3.4314785764,-1.6214754822
H,0,-2.9932948042,-3.3920874687,-2.3786694711	H,0,-2.9933618353,-3.3932276089,-2.3715294746
H,0,-2.5814930565,-4.6892913436,-1.2690811097	H,0,-2.5710010059,-4.6881772203,-1.2634323309
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H,0,-1.2026930872,-3.3161547044,0.888318234	H,0,-1.1820378768,-3.3050737585,0.8829129085
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H,0,-4.8836333348,-2.6414239733,0.8206649128	H,0,-4.8669937541,-2.6445343477,0.8392058588
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H,0,0.5057403634,4.8764891775,-0.0611706925	H,0,0.4881943722,4.8870125938,-0.0810421884
C,0,1.6172152815,3.1348257978,-0.8892872914	C,0,1.6035771232,3.1496822318,-0.9137278268
N,0,1.3820893806,1.8033599553,-0.8795472908	N,0,1.3750503596,1.8172495416,-0.9010747476
C,0,2.852587189,3.6670935755,-1.5706113824	C,0,2.8339064908,3.6867439451,-1.6005646109
C,0,2.8874287406,5.1898284695,-1.4864747821	C,0,2.8559924338,5.2104679695,-1.5312329703
H,0,2.0176253284,5.6369759529,-1.9714322061	H,0,1.9824761635,5.6452333073,-2.0204922188
H,0,3.778819372,5.5779536075,-1.9816279449	H,0,3.7441795724,5.6017804089,-2.0298579934
H,0,2.9091482094,5.5329615942,-0.4505535547	H,0,2.8737878473,5.5638398348,-0.4986191223
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C,0,2.8488685463,3.2342362915,-3.0392834222	C,0,2.8358121703,3.2396692517,-3.0648123774
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H,0,1.455477559,-0.4528332678,-1.0914579967	H,0,1.4469644015,-0.4323218247,-1.1078467071
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C,0,2.3780153979,-2.3782777081,-1.0982067854	C,0,2.3875324032,-2.3468022117,-1.1082541221
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H,0,3.1552442159,-5.6848906772,-1.2068297018	H,0,3.218207201,-5.6486451999,-1.2246933216
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C,0,2.1267643996,-1.0244495084,1.6572019069	C,0,2.1420429218,-1.0044667852,1.6416006225
C,0,4.1921467477,-0.216676097,3.3980182936	C,0,4.2142966023,-0.2067959919,3.3587504435
C,0,2.9863067279,0.0264819591,1.3148623636	C,0,2.9892601924,0.0521083399,1.2997264602
C,0,2.3308144571,-1.6636857112,2.8854641655	C,0,2.361960828,-1.6535366437,2.8603989488
C,0,3.3409430115,-1.2691693781,3.7415472779	C,0,3.3822675996,-1.2602007422,3.7109547798
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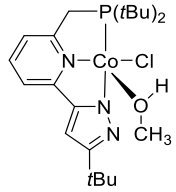
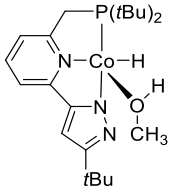
C,0,5.4991070994,-0.4570707161,5.59554977 H,0,6.3360965204,-0.0051046592,6.1194292505 H,0,4.6078086678,-0.3917260423,6.2215684164 H,0,5.7013841978,-1.5187981338,5.4461471583	C,0,6.9558674964,-4.4197993052,-2.5045644444 H,0,7.6553376015,-5.2284762159,-2.6940432639 H,0,6.8390461399,-3.8269985228,-3.4130977718 H,0,7.3724842214,-3.7545146992,-1.7468377289
 Ph Ph-*p*-CN	 Ph Ph-*p*-NO_2
C,0,-0.4932525667,-0.4697327902,1.0253543871 H,0,-0.7205700787,0.4655084675,1.5303179928 C,0,-0.2565642736,-0.3816740071,-0.2930515107 H,0,-0.2258552521,0.6216139279,-0.7089533941 C,0,-0.4643257684,-1.6349497647,1.9073003448 C,0,-0.4177986142,-3.8006485918,3.6837527661 C,0,0.4531083389,-2.6789236052,1.7427994857 C,0,-1.3334269251,-1.687451366,3.0019304623 C,0,-1.3199749258,-2.7642026248,3.8730052837 C,0,0.4745770543,-3.7479603618,2.6202916188 H,0,1.164228472,-2.6363414825,0.9270198808 H,0,-2.0326632815,-0.8739016036,3.1589801819 H,0,-2.0101110703,-2.790400586,4.7070569642 H,0,1.1983276641,-4.5413441677,2.4806436195 H,0,-0.3990270799,-4.6388429769,4.3687504173 C,0,-0.0565327775,-1.4397211784,-1.2788191682 C,0,0.3075504665,-3.3886827818,-3.2676924906 C,0,0.7460631595,-1.1900110218,-2.3985705678 C,0,-0.7009651291,-2.6812280898,-1.1977036564 C,0,-0.5247160768,-3.6409902267,-2.1707700679 C,0,0.9393875754,-2.1470736808,-3.3739563814 H,0,1.2320267813,-0.2261479964,-2.4935928449 H,0,-1.3593222362,-2.8843972359,-0.3633058832 H,0,-1.0350681999,-4.5923346559,-2.0982930509 H,0,1.5732078639,-1.9416929533,-4.2264148577 C,0,0.4955558655,-4.3784915982,-4.2695312793 N,0,0.6504536566,-5.1860788053,-5.0859819581	C,0,-0.4878345548,-0.4736387286,1.0234189246 H,0,-0.7092702061,0.4652705004,1.5242082602 C,0,-0.2507259591,-0.3919713647,-0.2956780226 H,0,-0.2121909472,0.6096305708,-0.7147997384 C,0,-0.4640312195,-1.6346131498,1.9097492328 C,0,-0.4303114767,-3.7956726986,3.6911085749 C,0,0.4424187511,-2.6880105802,1.7431661798 C,0,-1.327102414,-1.6746715277,3.0097660859 C,0,-1.3203505362,-2.7493933632,3.88317667 C,0,0.4572032921,-3.7549422515,2.6229517072 H,0,1.1503719776,-2.6542617574,0.9242515689 H,0,-2.0170041589,-0.8535109647,3.1683704738 H,0,-2.006005582,-2.7661631508,4.7210848877 H,0,1.1716729945,-4.5563475485,2.4818343721 H,0,-0.416758057,-4.6325411295,4.3778091106 C,0,-0.0564306149,-1.4538162303,-1.277686389 C,0,0.2949817836,-3.3841700333,-3.2392886806 C,0,0.7507619221,-1.2071752757,-2.3964811369 C,0,-0.7106960855,-2.6916605916,-1.1930056077 C,0,-0.5394185897,-3.6548589489,-2.1646143342 C,0,0.9408823003,-2.1665770245,-3.3712501346 H,0,1.2420938602,-0.2460958165,-2.489842112 H,0,-1.3712972597,-2.8867800197,-0.3586041461 H,0,-1.0437422983,-4.6096139397,-2.1153608597 H,0,1.5718331834,-1.9918455075,-4.2312219989 N,0,0.4851923278,-4.4127502458,-4.2759387949 O,0,1.2142015567,-4.1375953607,-5.2205381053 O,0,-0.096554003,-5.4800541726,-4.1283661675
 Ph Ph-*p*-$COCH_3$	
C,0,-0.4634003899,-0.4579552201,1.0218243132 H,0,-0.6541845569,0.4884260184,1.5212100489 C,0,-0.2281519966,-0.3896422689,-0.2981718825 H,0,-0.1611212093,0.6091056591,-0.7212749953 C,0,-0.4718056155,-1.617029301,1.9123178609 C,0,-0.4891278733,-3.7703974649,3.7056954958 C,0,0.4006946311,-2.6984982327,1.7447734094 C,0,-1.3275809527,-1.6270656768,3.0187248855 C,0,-1.3459418396,-2.6968075773,3.8984248058 C,0,0.3902690239,-3.7610307829,2.6300217228 H,0,1.1018234454,-2.6907404296,0.9195276866 H,0,-1.9912745193,-0.7846465235,3.1782933779 H,0,-2.0253616014,-2.6883249009,4.7417006601 H,0,1.0798643174,-4.5839354528,2.4875658206 H,0,-0.4951038597,-4.6035811459,4.3970987601 C,0,-0.0683143952,-1.4612123816,-1.2766815279 C,0,0.2283371538,-3.4423194572,-3.2556771964 C,0,0.7542346141,-1.2539000555,-2.3927586697 C,0,-0.766250498,-2.6721805288,-1.1922604552 C,0,-0.6202309033,-3.6422687483,-2.1634685089 C,0,0.9104138163,-2.2287751092,-3.3551654924 H,0,1.281625994,-0.3113138717,-2.4874442426 H,0,-1.4380128022,-2.8396471806,-0.3600041833 H,0,-1.180851961,-4.5648195639,-2.0737382378 H,0,1.5566495855,-2.0771307367,-4.2110077125 C,0,0.4238739861,-4.4597069944,-4.3225508032 O,0,1.170213053,-4.2450936104,-5.2587307529	

C,0,-0.3257639055,-5.7622169604,-4.2120345467 H,0,-0.077859711,-6.3957997183,-5.0581817845 H,0,-1.4037642049,-5.5942761859,-4.1941487568 H,0,-0.0738491784,-6.2839097213,-3.2874472529	
 **^{PNN}Co-Cl+CH_3OH**	 **^{PNN}Co-H+CH_3OH**
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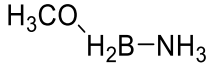
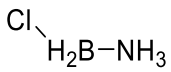
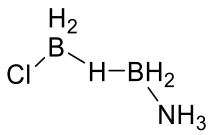
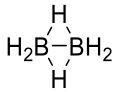
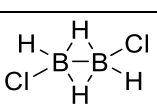
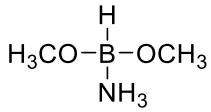
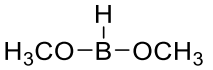
H,0,3.4622516772,0.9173966358,5.0777122824 H,0,2.7110201121,-0.5555059742,4.4689058903 H,0,2.8648159299,-0.2957429526,6.2145373035 O,0,-1.5139798063,0.065378529,0.4702247402 Cl,0,1.3049788983,-0.892817126,-0.1824948806 C,0,-2.1801013412,0.368650854,1.6943380685 H,0,-2.9878108945,-0.3429422529,1.8826327624 H,0,-1.4896411151,0.3715540084,2.5403526651 H,0,-2.6097591106,1.3635254762,1.5882639948 H,0,-0.9472092824,-0.7144681409,0.6034662018	H,0,3.334957284,0.7659869301,5.2424270305 H,0,2.6659283259,-0.6747379379,4.4810399089 H,0,2.6266383766,-0.5054700258,6.2438297436 O,0,-1.1546561824,-0.0509795314,0.7721681844 H,0,1.3176350897,-0.0822801873,-0.3398411919 C,0,-2.0315867953,0.6019727547,1.680362497 H,0,-2.596972042,-0.1192427764,2.2779707692 H,0,-1.4964527662,1.2775089482,2.3537891117 H,0,-2.7348415797,1.1867131464,1.0874363248 H,0,-0.4104483905,-0.3973401506,1.2916075601
H_3C-OH	H_3B-NH_3
C,0,0.0094913835,-0.0164396713,1.0865460649 H,0,1.022670451,0.0055193913,1.5044060773 H,0,-0.5161140454,-0.8828996048,1.5044062447 H,0,-0.5083416623,0.8804721709,1.4205771352 O,0,-0.0003034841,0.0005252454,-0.3248917613 H,0,0.455275848,-0.7885601605,-0.6289923402	N,0,-2.854130811,-0.5383776749,-0.0268748835 B,0,-2.3017748553,0.2427066843,1.3260402068 H,0,-1.1021249851,0.1929728922,1.2401743699 H,0,-2.748327834,1.3572532627,1.2400353713 H,0,-2.7485191264,-0.3888913895,2.2482615395 H,0,-2.5345630274,-1.5002986866,-0.0606891243 H,0,-2.5347388569,-0.0865447116,-0.8768018709 H,0,-3.8675505039,-0.5580013765,-0.0605256088
$H_2B=NH_2$	
B,0,0.,0.,0.7628614846 H,0,-1.039923048,0.,1.3384876598 H,0,1.039923048,0.,1.3384876598 N,0,0.,0.,-0.624364452 H,0,-0.8378898784,0.,-1.1806531261 H,0,0.8378898784,0.,-1.1806531261	C,0,0.4591553169,0.1952434089,1.2777631527 N,0,-2.9522396465,-0.5122721692,0.0269893346 O,0,-0.6581040643,-0.2302179202,0.5586641285 B,0,-1.9271423604,0.157000462,1.1311774084 H,0,-2.7903699915,-1.5129559257,-0.0247858917 H,0,-2.7594996071,-0.1284566488,-0.8926771912 H,0,-3.9285271149,-0.3536860189,0.2452431903 H,0,-2.1698586384,1.348297099,1.1163138694 H,0,-2.2081368432,-0.3671899553,2.1916444265 H,0,0.473146905,-0.2091001846,2.3002375776 H,0,1.363525558,-0.1444107496,0.7686155449 H,0,0.5071404865,1.2907216024,1.3600514499
	
N,0,-2.8468285634,-0.5280955654,-0.0332551554 B,0,-2.2868759489,0.2637785449,1.2898404245 H,0,-1.0951702595,0.1936887579,1.2357758769 H,0,-2.7501605754,1.363979391,1.2357710135 Cl,0,-2.9877293743,-0.7273416052,2.7008327654 H,0,-2.5290591657,-1.4929117006,-0.0311659448 H,0,-2.5405853919,-0.0950191446,-0.8993024459 H,0,-3.8623897074,-0.5500761875,-0.0311700342	N,0,0.4763939836,0.1258557994,0.4913445791 B,0,1.649502746,-0.1923731376,-0.550557404 H,0,2.4181422887,0.7912897485,-0.6909597743 H,0,2.3076538834,-1.0912752417,-0.1362063435 Cl,0,0.8607546347,-0.4859079392,-2.1679442101 H,0,-0.0522582673,0.9367557516,0.1741666278 H,0,0.8665763665,0.3676987193,1.3995628776 H,0,-0.1567817728,-0.6623030105,0.5880949478 B,0,2.3773960417,1.9946182196,-0.0186966288 H,0,3.3452436246,2.4183394092,-0.5688271015 H,0,1.3231393814,2.4720135836,-0.3358690005 H,0,2.5053190895,1.6965797978,1.1372801302
$Cl-BH_2$	
B,0,-2.2085173446,0.3745907299,1.526783746 H,0,-1.1099973313,0.1280142551,1.1680480657 H,0,-2.8071230941,1.3281132774,1.1680312389 Cl,0,-2.9791882657,-0.7152412372,2.6367219494	H,0,1.0325072922,0.,1.4466052489 H,0,-1.0325072922,0.,1.4466052489 H,0,-1.0325072922,0.,-1.4466052489 H,0,1.0325072922,0.,-1.4466052489 B,0,0.,0.,0.8687903321 B,0,0.,0.,-0.8687903321 H,0,0.,0.9758449641,0. H,0,0.,-0.9758449641,0.
	H_2B-OCH_3
H,0,1.4506169292,0.,-1.0380744113	C,0,0.5442981253,0.2885371664,1.3806261088

H,0,-1.4506169292,0.,1.0380744113 B,0,0.8810132765,0.,-0.0054462022 B,0,-0.8810132765,0.,0.0054462022 Cl,0,1.7806202871,0.,1.5181164675 Cl,0,-1.7806202871,0.,-1.5181164675 H,0,0.,0.9773853293,0. H,0,0.,-0.9773853293,0.	O,0,-0.6626939303,0.6658228185,0.7356701188 B,0,-1.8576972446,0.2724956907,1.2036528553 H,0,-2.8131390763,0.63613868,0.5993568134 H,0,-1.9276007344,-0.4100183857,2.1826081425 H,0,0.3534157406,-0.3318304457,2.258987685 H,0,1.1642364742,-0.262820918,0.6741335313 H,0,1.0795186455,1.1887313937,1.6819747448
NH3-M06L	BH3-M06L
H,0,-1.8149030191,0.4672480836,0.8092974206 H,0,-1.8149030191,0.4672480836,-0.8092974206 H,0,-1.8149030191,-0.9344961672,0. N,0,-1.42608436,0.,0.	H,0,-1.7190979128,0.5919770055,1.0253342504 H,0,-1.7190979128,0.5919770055,-1.0253342504 H,0,-1.7190979128,-1.1839540109,0. B,0,-1.7190897693,0.,0.
	
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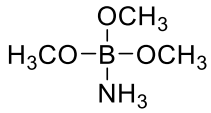	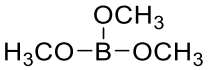
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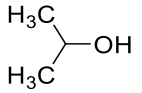	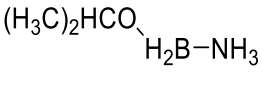
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H-Cl	H2
H,0,0.,0.,0.3432323259 Cl,0,0.,0.,-0.9432323259 H,0,0.,0.,0.3721688168 H,0,0.,0.,-0.3721688168	H,0,0.,0.,0.3721688168 H,0,0.,0.,-0.3721688168

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