Supporting Information

Nickel-catalyzed synthesis of Zn(I)-Zn(I) bonded compounds

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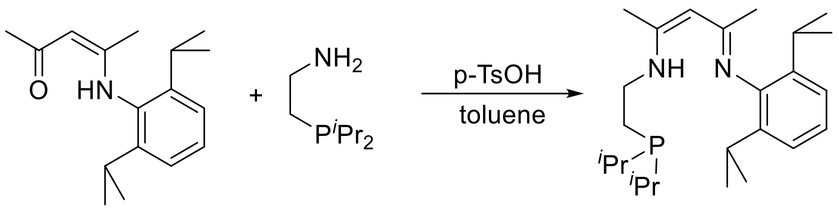
General procedures: All experiments were carried out under a dry Argon atmosphere using standard Schlenk techniques or in a glovebox. Solvents (including deuterated solvents used for NMR) were dried and distilled prior to use. NMR spectra were recorded on a Bruker 400 MHz spectrometer. Chemical shifts were reported as δ units with reference to the residual solvent resonance or an external standard. The assignments of NMR data were supported by 1D and 2D NMR experiments. Elemental analysis data was recorded on a Carlo-Erba EA-1110 instrument. High resolution mass spectrometry was measured with a Bruker micrOTF-Q III. Fourier transform infrared spectroscopy were measured with a Bruker VERTEX70. EPR spectra were collected using X-band frequency on a Bruker Elexsys E500 spectrometer. 2-(Diisopropylphosphino)ethanamine[1], zinc hydrides (**1a** and **1b**)[2], and complex **6**[2] were synthesized following the literature procedures. $Ni(CO)_2(PPh_3)_2$, $Pd_2(dba)_3$, $(C_3H_5)PdCl$, $Ni(COD)_2$, and $NiCl_2(PPh_3)_2$ were purchased from TCI.

Preparation of HL^c



HL^c

Scheme S1.

2-((2,6-Diisopropylphenyl)imido)-2-penten-4-one (2.59 g, 10.0 mmol), 2-(diphenylphosphino)ethanamine (1.61 g, 10.0 mmol) and a catalytic amount of *p*-toluenesulfonic acid (0.17 g, 1.0 mmol) were mixed in toluene (40 mL) and heated at reflux for 60 h. The water produced during the reaction was removed using a Dean-Stark trap. After the reaction was complete, the volatiles were removed under vacuum and the residue was recrystallized in hexane at -30 ^{o}C to remove solid impurities. The solvent in the supernatant was removed under vacuum to afford **HL^c** as a yellow oil (3.26 g, 81%).

HRMS (ESI) m/z calcd. for $C_{25}H_{44}N_2P$ $[M + H]^+$: 403.3242; found: 403.3255.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 11.13 (br s, 1H, N*H*), 7.20 (m, 2H, *m*-N*Ar*), 7.11 (m, 1H, *p*-N*Ar*), 4.71 (s, 1H, MeC(N)C*H*), 3.26 (m, 2H, NCH_2), 3.18 (m, 2H, ArC*H*Me_2), 1.71 (s, 3H, *Me*C), 1.68 (s, 3H, *Me*C), 1.49 (m, 2H, PCH_2), 1.47 (m, 2H, PC*H*Me_2), 1.26 (d, $^3J_{HH}$ = 6.9 Hz, 6H, ArCHMe_2), 1.23 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCHMe_2), 0.91 (dd, $^3J_{PH}$ = 14.0 Hz, $^3J_{HH}$ = 7.1 Hz, 6H, PCHMe_2), 0.89 (dd, $^3J_{PH}$ = 10.9 Hz, $^3J_{HH}$ = 6.9 Hz, 6H, PCHMe_2).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 166.6 (Me*C*), 155.0 (Me*C*), 147.6 (*i*-N*Ar*), 138.2 (*o*-N*Ar*), 123.4 (*p*-N*Ar*), 123.3 (*m*-N*Ar*), 94.1 (MeC(N)*C*H), 43.1 (d, $^2J_{PC}$ = 31.6 Hz, N*C*H_2), 28.6 (Ar*C*HMe_2), 24.4 (ArCHMe_2), 24.3 (d, $^2J_{PC}$ = 21.4 Hz, P*C*H_2), 23.6 (d, $^1J_{PC}$ = 13.5 Hz, P*C*HMe_2), 23.1 (ArCHMe_2), 21.8 (*Me*C), 20.1 (d, $^2J_{PC}$ = 16.6 Hz, PCHMe_2), 19.3 (*Me*C), 18.7 (d, $^2J_{PC}$ = 9.8 Hz, PCHMe_2).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K): δ = -1.5.

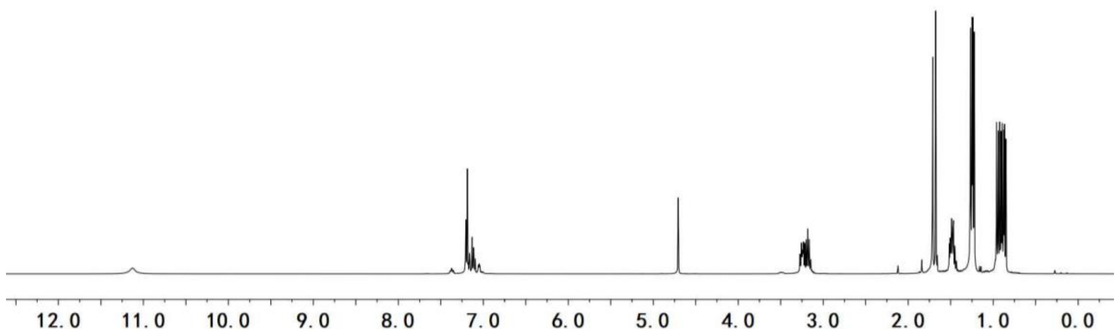


Figure S1. [1]H NMR (400 MHz, C_6D_6, 298 K).

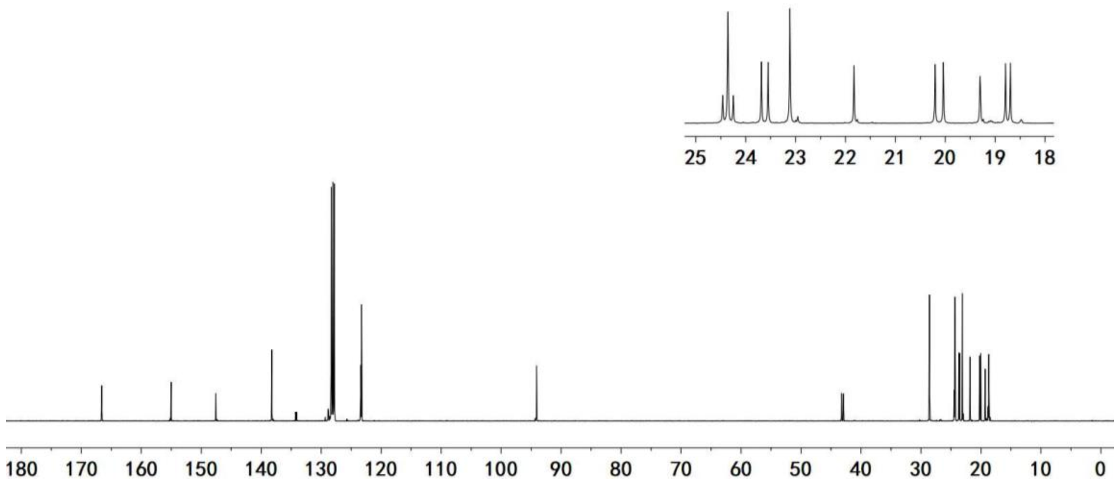


Figure S2. $^{13}C\{^1H\}$ NMR (101 MHz, C_6D_6, 298 K).

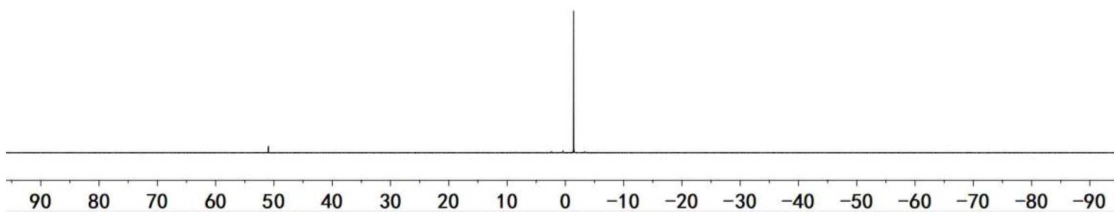
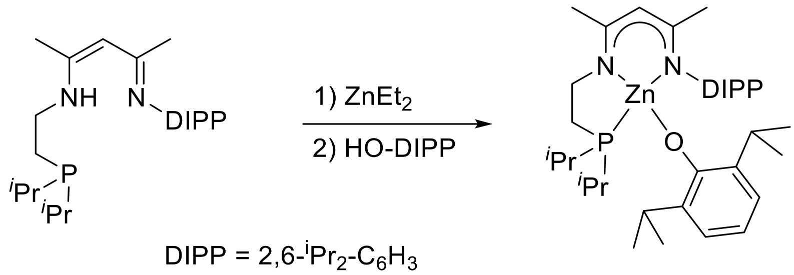


Figure S3. $^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6, 298 K).

Preparation of complex L^cZnOAr



DIPP = 2,6-^{i}Pr$_2$-C_6H_3

HL^c

Scheme S2.

$ZnEt_2$ (2.6 mL, 1.0 M in n-hexane) was slowly added to a solution of **HL^c** (1.01 g, 2.5 mmol) in 15 mL of toluene at -35 ^{o}C. After stirring at room temperature overnight, 2,6-di-*iso*-propylphenol (446 mg, 2.5 mmol) was added. The reaction mixture was stirred at room temperature for 8 h. The volatiles were removed under vacuum and then the residue was washed with hexane (3 * 2 mL) to eventually give **L^cZnOAr** as a colorless solid (902 mg, 56%).

Elemental Analysis: calcd. for $C_{37}H_{59}N_2OPZn$: C, 68.98; H, 9.23; N, 4.35%. Found: C, 69.10; H, 9.38; N, 4.12%.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.14 (m, 1H, *p*-N*Ar*), 7.13 (m, 2H, *m*-N*Ar*), 7.12 (m, 2H, *m*-O*Ar)*, 6.84 (m, 1H, *p*-O*Ar*), 4.58 (s, 1H, MeC(N)C*H*), 3.49 (m, 2H, NC*H*$_2$), 3.34 (m, 2H, NArC*H*Me$_2$), 3.33 (m, 2H, OArC*H*Me$_2$), 1.62 (s, 3H, *Me*C), 1.59 (s, 3H, *Me*C), 1.58 (overlapped with *Me*C, 2H, PC*H*Me$_2$), 1.24 (overlapped with ArCH*Me*$_2$, 2H, PC*H*$_2$)[1], 1.21 (m, 12H, NArCH*Me*$_2$), 1.20 (overlapped with NArCH*Me*$_2$, 12H, OArCH*Me*$_2$), 0.82 (dd, $^3J_{PH}$ = 15.7 Hz, $^3J_{HH}$ = 7.1 Hz, 6H, PCH*Me*$_2$), 0.71 (dd, $^3J_{PH}$ = 12.8 Hz, $^3J_{HH}$ = 7.0 Hz, 6H, PCH*Me*$_2$). [[1]from the ^{1}H, ^{1}H GCOSY experiment]

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 167.8 (Me*C*), 166.4 (Me*C*), 161.3 (*i*-O*Ar*), 145.7 (*i*-N*Ar*), 142.5 (*o*-N*Ar*), 137.4 (*o*-O*Ar*), 125.8 (*p*-N*Ar*), 124.0 (*m*-N*Ar*), 122.7 (*m*-O*Ar*), 115.2 (*p*-O*Ar*), 95.1 (MeC(N)*C*H), 45.4 (N*C*H$_2$), 28.4 (NAr*C*HMe$_2$), 27.1 (OAr*C*HMe$_2$), 24.6 (NArCH*Me*$_2$), 24.3 (NArCH*Me*$_2$), 24.2 (*Me*C), 24.1 (OArCH*Me*$_2$), 21.8 (d, $^1J_{PC}$ = 6.5 Hz, P*C*HMe$_2$), 21.2 (*Me*C), 20.1 (d, $^1J_{PC}$ = 14.7 Hz, P*C*H$_2$), 18.9 (d, $^2J_{PC}$ = 8.0 Hz, PCH*Me*$_2$), 17.4 (d, $^2J_{PC}$ = 1.7 Hz, PCH*Me*$_2$).

$^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6, 298 K): δ = -11.6.

^1H, ^1H GCOSY (400 MHz / 400 MHz, C_6D_6, 298 K) [selected traces]: δ ^1H / δ ^1H = 7.12 / 6.84 (*m*-O*Ar* / *p*-O*Ar*), 3.49 / 1.24 (NCH_2 / PCH_2), 3.34, 3.33 / 1.21 (ArC*H*Me_2 / ArCHMe_2), 1.58 / 0.82, 0.71 (PC*H*Me_2 / PCHMe_2).

^1H, ^{13}C GHSQC (400 MHz / 101 MHz, C_6D_6, 298 K): δ ^1H / δ ^{13}C = 7.14 / 125.8 (*m*-N*Ar*), 7.13 /124.0 (*p*-N*Ar*), 7.12 / 122.7 (*m*-O*Ar*), 6.84 / 115.2 (*p*-O*Ar*), 4.58 / 95.1 (MeC(N)*CH*), 3.49 / 45.4 (NCH_2), 3.34 / 28.4 (NAr*CH*Me_2), 3.33 / 27.1 (OAr*CH*Me_2), 1.62 / 21.2 (*Me*C), 1.59 / 24.2 (*Me*C), 1.58 / 21.8 (P*CH*Me_2), 1.24 / 20.1 (PCH_2), 1.21 / 24.6, 24.3, 24.1 (ArCHMe_2), 0.82, 0.71 / 18.9, 17.4 (PCHMe_2).

^1H, ^{13}C GHMBC (400 MHz / 101 MHz, C_6D_6, 298 K) [selected traces]: δ ^1H / δ ^{13}C = 7.13 / 145.7 (m-N*Ar* / *i*-N*Ar*), 7.12 / 161.3 (*m*-O*Ar* / *i*-O*Ar*), 3.49 / 20.1 (NCH_2 / PCH_2), 3.34 / 145.7, 142.5, 124.0, (NArC*H*Me_2 / *i*-N*Ar*, *o*-N*Ar*, *m*-N*Ar*), 3.33 / 161.3, 137.4, 122.7 (OArC*H*Me_2 / *i*-O*Ar*, *o*-O*Ar*, *m*-O*Ar*).

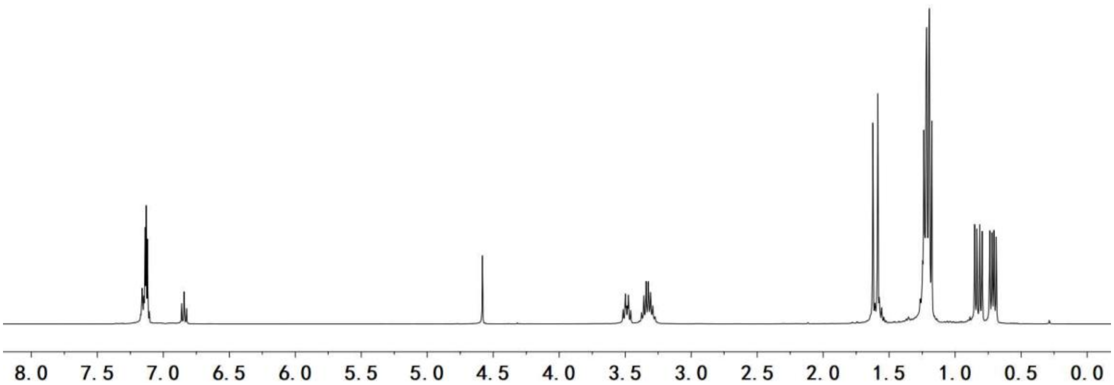


Figure S4. ^1H NMR (400 MHz, C_6D_6, 298 K).

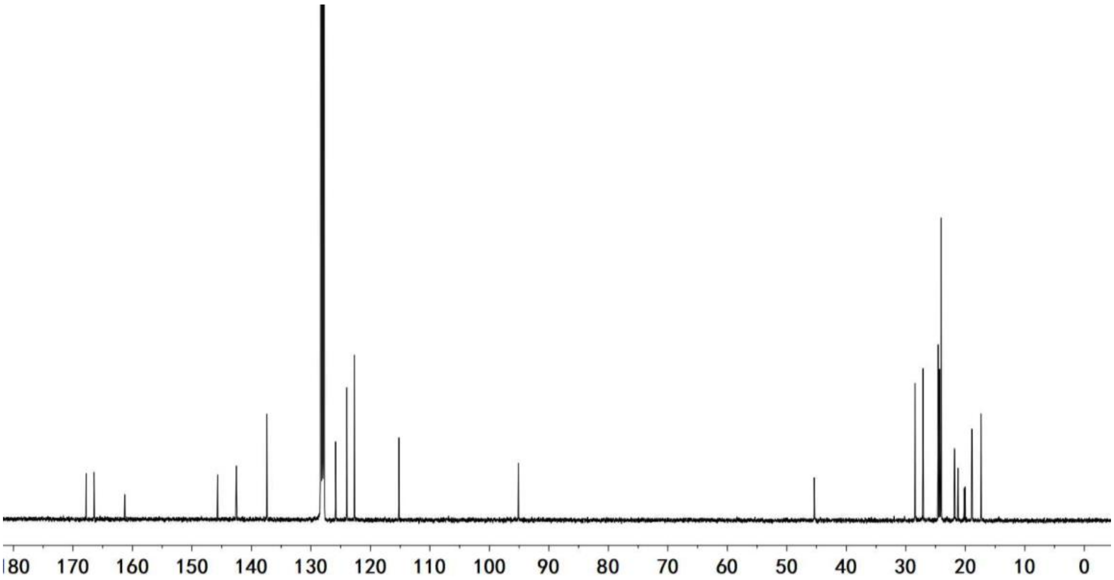


Figure S5. $^{13}C\{^{1}H\}$ NMR (101 MHz, C_6D_6, 298 K).

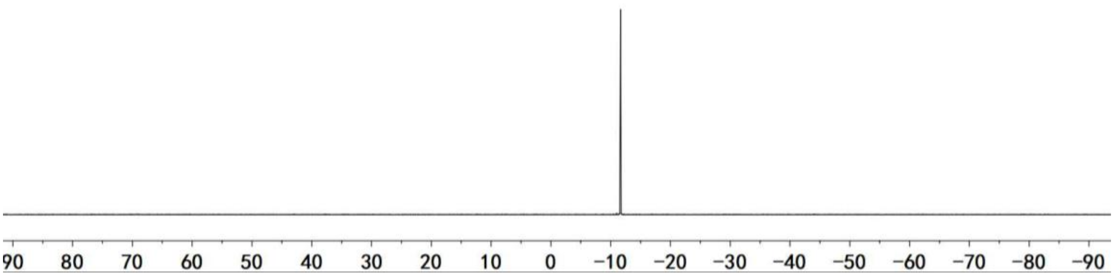
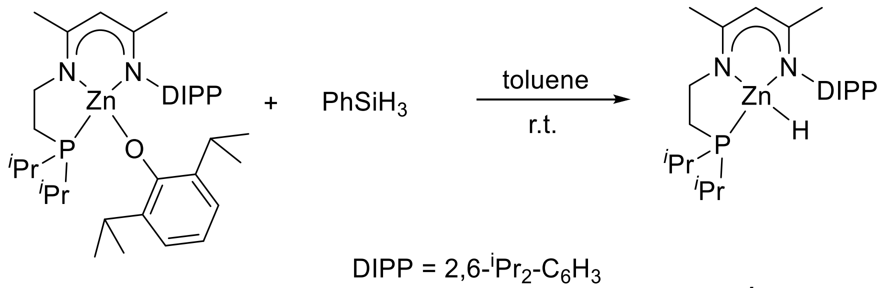


Figure S6. $^{31}P\{^{1}H\}$ NMR (162 MHz, C_6D_6, 298 K).

Preparation of complex 1c



1c

Scheme S3.

$PhSiH_3$ (119 mg, 1.1 mmol) was added to a solution of **L^{c}ZnOAr** (644 mg, 1.0 mmol) in toluene (10 mL). The reaction mixture was stirred at room temperature for 4 h. The volatiles were removed under vacuum, and then the residue was washed with hexane (3 * 2 mL) to eventually give **1c** as a colorless solid (327 mg, 70%). Crystals suitable for the X-ray crystal structure analysis were grown from a layered toluene/hexane (v/v: 1:2) solution at -30 ^{o}C.

Elemental Analysis: calcd. for $C_{25}H_{43}N_2PZn$: C, 64.16; H, 9.26; N, 5.99%. Found: C, 64.66; H, 9.36; N, 5.84%.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.16 (m, 3H, *m*, *p*-N*Ar*), 4.69 (s, 1H, MeC(N)C*H*), 4.39 (s, 1H, Zn*H*), 3.43 (m, 2H, NCH_2), 3.43 (overlapped with NCH_2, 2H, ArC*H*Me$_2$), 1.74 (s, 3H, *Me*C), 1.66 (s, 3H, *Me*C), 1.62 (m, 2H, PC*H*Me$_2$), 1.34 (d, $^3J_{HH}$ = 6.9 Hz, 6H, ArCHMe_2),1.30 (m, 2H, PCH_2), 1.22 (d, $^3J_{HH}$ = 7.0 Hz, 6H, ArCHMe_2), 0.92 (m, 12H, PCHMe_2).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 165.9 (Me*C*), 165.8 (Me*C*), 146.4 (*i*-N*Ar*), 142.5 (*o*-N*Ar*), 125.4 (*p*-N*Ar*), 123.8 (*m*-N*Ar*), 95.1 (MeC(N)*C*H), 47.2 (d, $^2J_{PC}$ = 9.2 Hz, N*C*H$_2$), 28.1 (Ar*C*HMe$_2$), 25.2 (ArCHMe_2), 23.9 (ArCHMe_2), 23.7 (*Me*C), 22.6 (d, $^1J_{PC}$ = 4.5 Hz, P*C*HMe$_2$), 22.2 (br, P*C*H$_2$), 20.9 (*Me*C), 19.4 (d, $^2J_{PC}$ = 12.7 Hz, PCHMe_2), 18.1 (d, $^2J_{PC}$ = 4.1 Hz, PCHMe_2).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K): δ = -14.6.

^{1}H, ^{1}H GCOSY (400 MHz / 400 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{1}H = 3.43 / 1.30 (NCH_2 / PCH_2), 3.43 / 1.34, 1.22 (ArC*H*Me$_2$ / ArCHMe_2), 1.62 / 0.92 (PC*H*Me$_2$ / PCHMe_2).

^{1}H, ^{13}C GHSQC (400 MHz / 101 MHz, C_6D_6, 298 K): δ ^{1}H / δ ^{13}C = 7.16 / 125.4, 123.8 (*p*, *m*-N*Ar*), 4.69 / 95.1 (MeC(N)*CH*), 3.43 /47.2 (N*CH*$_2$), 3.43 / 28.1 (Ar*CH*Me$_2$), 1.74 / 20.9 (*Me*C), 1.66 / 23.7 (*Me*C), 1.62 / 22.6 (P*CH*Me$_2$), 1.34 / 25.2 (ArCH*Me*$_2$), 1.30 / 22.2 (P*CH*$_2$), 1.22 / 23.9 (ArCH*Me*$_2$), 0.92 / 19.4, 18.1 (PCH*Me*$_2$).

^{1}H, ^{13}C GHMBC (400 MHz / 101 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{13}C = 4.69 / 146.4, 47.2 (MeC(N)C*H* / *i*-N*Ar*, N*C*H$_2$), 3.43 / 25.2, 23.9 (ArC*H*Me$_2$/ ArCH*Me*$_2$), 1.34, 1.22 / 142.5 (ArCH*Me*$_2$ / *o*-N*Ar*), 1.30 / 47.2 (PC*H*$_2$ / N*C*H$_2$).

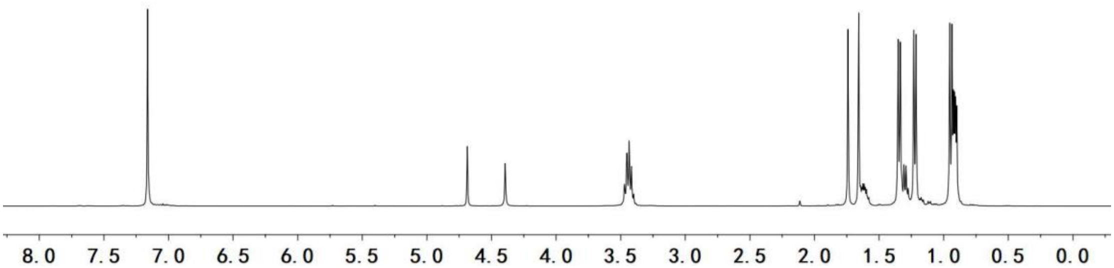


Figure S7. ^{1}H NMR (400 MHz, C_6D_6, 298 K).

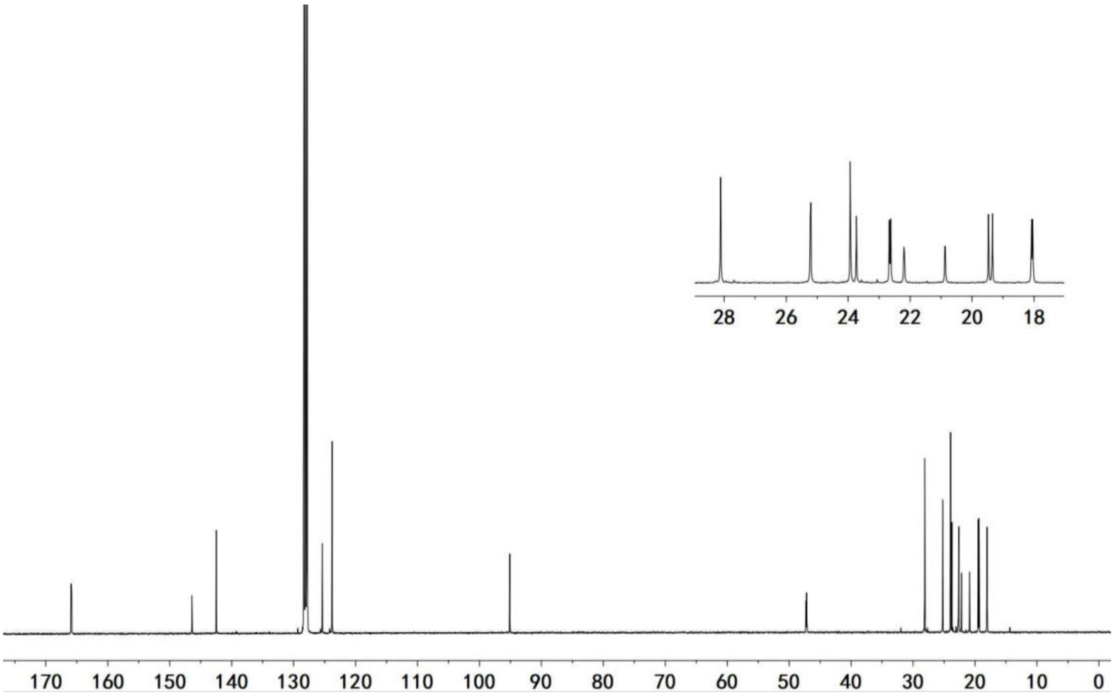


Figure S8. ^{13}C {^{1}H} NMR (101 MHz, C_6D_6, 298 K).

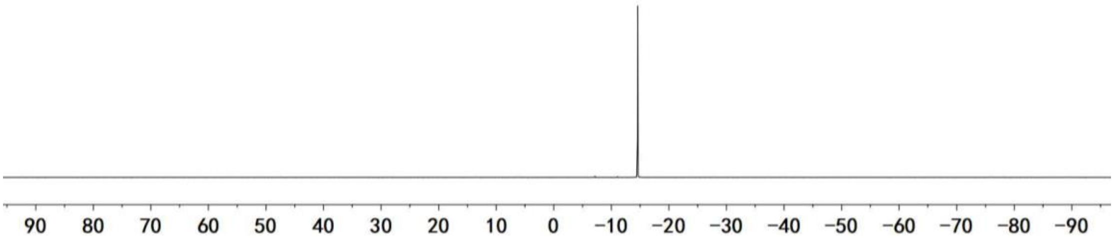


Figure S9. ^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K).

X-ray crystal structure analysis of complex 1c: formula $C_{25}H_{43}N_2PZn$, M = 467.95 gmol^{-1}, colorless, 0.22 × 0.15 × 0.12 mm, Monoclinic, space group $P2_1/c$, a = 17.8843(11), b = 10.2159(5), c = 15.6744(9) Å, β = 114.562(7)°, V = 2604.6(3) Å^3, ρ_{calc} = 1.193 gcm^{-3}, μ = 1.017 mm^{-1}, empirical absorption correction (0.76993 ≤ T ≤ 1.00000), Z = 4, λ = 0.71073 Å, T = 223 K, 17437 reflections collected (-24 ≤ h ≤ 17, -14 ≤ k ≤ 12, -14 ≤ l ≤ 22), 6825 independent (R_{int} = 0.0285) and 5260 observed reflections [I>2σ(I)], 276 refined parameters, the final R_1 was 0.0397 (I > 2σ(I)) and wR_2 was 0.1073 (all data), max. (min.) residual electron density 0.35 (-0.25) e.Å^{-3}, hydrogen atoms except for hydrides were placed in calculated positions and refined using a riding model, the hydride atom in this structure was located in a Fourier difference map and was refined with isotropic displacement parameters.

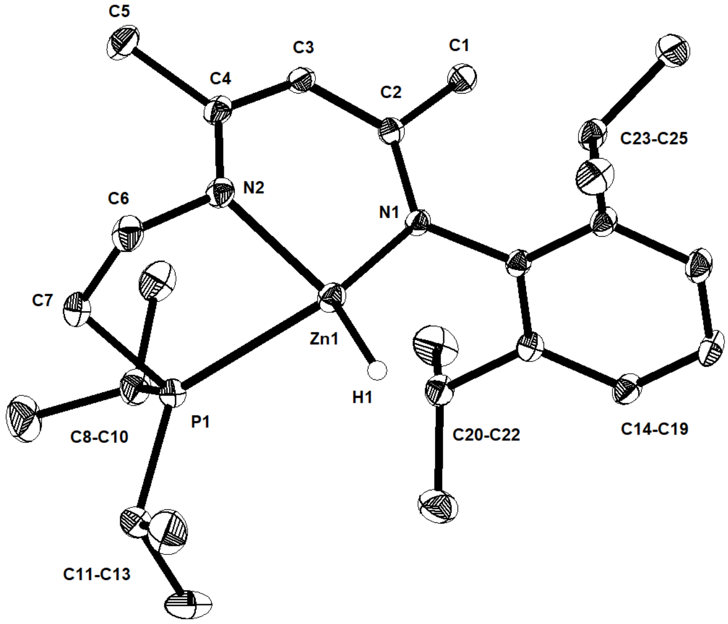
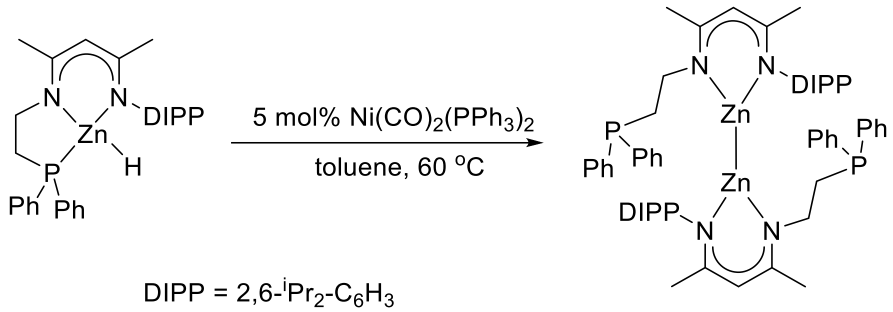


Figure S10. Molecular structure of complex **1c**.

Preparation of complex 2a



1a **2a**

Scheme S4.

$Ni(CO)_2(PPh_3)_2$ (32 mg, 0.05 mmol) was added to a solution of complex **1a** (536 mg, 1.0 mmol) in 5 mL of toluene. After stirring at 60 °C for 24 h, the reaction mixture was filtered through Celite and the solvent was removed in vacuum. The residue was washed with hexane (3 * 2 mL) to eventually give **2a** as a pale-yellow solid (455 mg, 85%). Crystals suitable for the X-ray crystal structure analysis were grown from a layered toluene/hexane (v/v: 1:2) solution at room temperature.

Elemental Analysis: calcd. for $C_{62}H_{76}N_4P_2Zn_2\cdot C_7H_8$: C, 71.31; H, 7.29; N, 4.82%. Found: C, 70.62; H, 7.46; N, 4.87%.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.45 (m, 8H, *o-Ph*$_2$P), 7.17 (m, 8H, *m-Ph*$_2$P), 7.09 (m, 4H, *p-Ph*$_2$P), 7.04 (m, 2H, *p*-N*Ar*), 7.02 (m, 4H, *m*-N*Ar*), 4.84 (s, 2H, MeC(N)C*H*), 3.68 (m, 4H, NC*H*$_2$), 3.10 (sp, $^3J_{HH}$ = 6.9 Hz, 4H, ArC*H*Me$_2$), 2.28 (m, 4H, PC*H*$_2$), 1.76 (s, 6H, *Me*C), 1.59 (s, 6H, *Me*C), 1.09 (d, $^3J_{HH}$ = 6.9 Hz, 12H, ArCH*Me*$_2$), 0.84 (d, $^3J_{HH}$ = 6.9 Hz, 12H, ArCH*Me*$_2$).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 166.8 (Me*C*), 165.0 (Me*C*), 146.4 (*i*-N*Ar*), 142.0 (*o*-N*Ar*), 139.1 (d, $^1J_{PC}$ = 14.3 Hz, *i-Ph*$_2$P), 133.2 (d, $^2J_{PC}$ = 18.6 Hz, *o-Ph*$_2$P), 128.9 (d, $^3J_{PC}$ = 6.5 Hz, *m-Ph*$_2$P), 128.7 (*p-Ph*$_2$P), 125.4 (*p*-N*Ar*), 123.5 (*m*-N*Ar*), 96.9 (MeC(N)*C*H), 49.2 (d, $^2J_{PC}$ = 22.6 Hz, N*C*H$_2$), 32.1 (d, $^1J_{PC}$ = 16.0 Hz, P*C*H$_2$), 28.1 (Ar*C*HMe$_2$), 25.0 (ArCH*Me*$_2$), 24.0 (*Me*C), 23.5 (ArCH*Me*$_2$), 21.5 (*Me*C).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K): δ = -20.5.

^{1}H, ^{1}H GCOSY (400 MHz / 400 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{1}H = 7.45 / 7.17 (*o-Ph*$_2$P / *m-Ph*$_2$P), 3.68 / 2.28 (NC*H*$_2$ / PC*H*$_2$), 3.10 / 1.09, 0.84

(ArC*H*Me$_2$ / ArCH*Me$_2$*).

^{1}H, ^{13}C GHSQC (400 MHz / 101 MHz, C_6D_6, 298 K): δ ^{1}H / δ ^{13}C = 7.45 / 133.2 (*o-Ph$_2$*P), 7.17 / 128.9 (*m*-N*Ar*), 7.09 / 128.7 (*p*-N*Ar*), 7.04 / 125.4 (*p-Ph$_2$*P), 7.02 / 123.5 (*m-Ph$_2$*P), 4.84 / 96.9 (MeC(N)*CH*), 3.68 / 49.2 (N*CH$_2$*), 3.10 / 28.1 (Ar*CH*Me$_2$), 2.28 / 32.1 (P*CH$_2$*), 1.76 / 21.5 (*Me*C), 1.59 / 24.0 (*Me*C), 1.09 / 23.5 (ArCH*Me$_2$*), 0.84 / 25.0 (ArCH*Me$_2$*).

^{1}H, ^{13}C GHMBC (400 MHz / 101 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{13}C = 7.45 / 128.7 (o-*Ph$_2$*P / *p-Ph$_2$*P), 4.84 / 146.4, 49.2 (MeC(N)C*H* / *i*-N*Ar*, N*C*H$_2$), 3.68 / 32.1 (NC*H$_2$* / P*C*H$_2$), 3.10 / 25.0, 23.5 (ArC*H*Me$_2$/ ArCH*Me$_2$*), 2.36 / 139.1 (PC*H$_2$* / *i-Ph$_2$*P), 1.09, 0.84 / 142.0 (ArCH*Me$_2$* / *o*-N*Ar*).

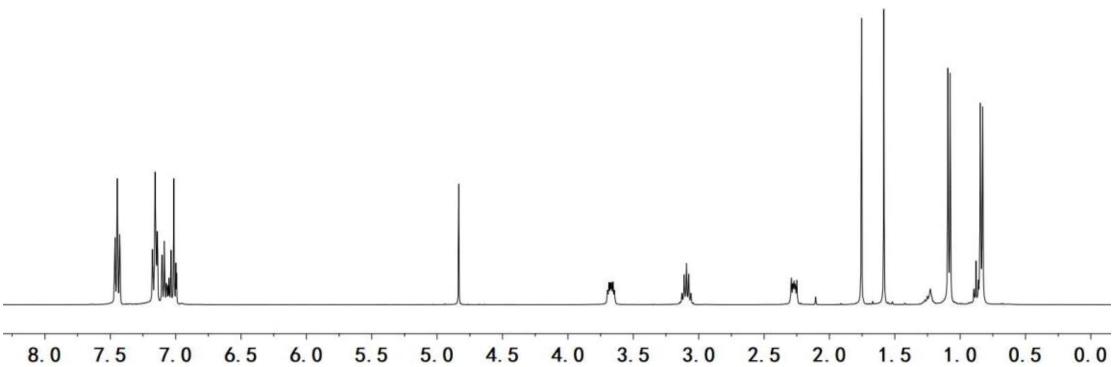


Figure S11. ^{1}H NMR (400 MHz, C_6D_6, 298 K).

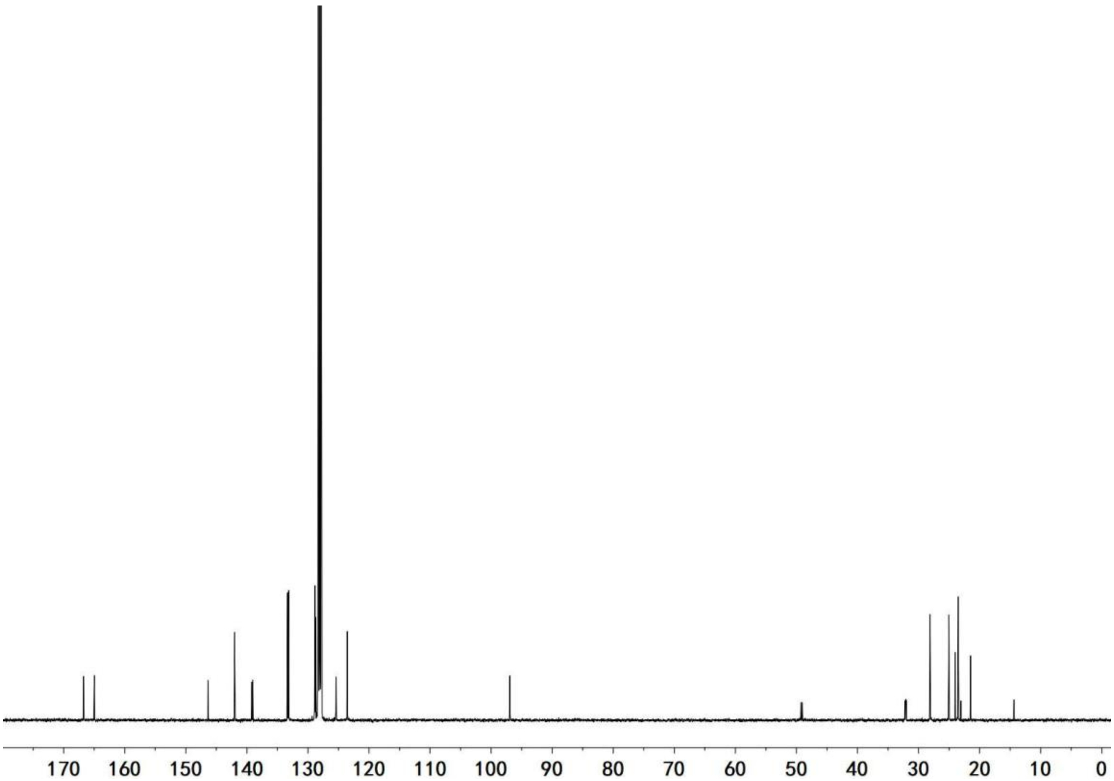


Figure S12. ^{13}C {^{1}H} NMR (101 MHz, C_6D_6, 298 K).

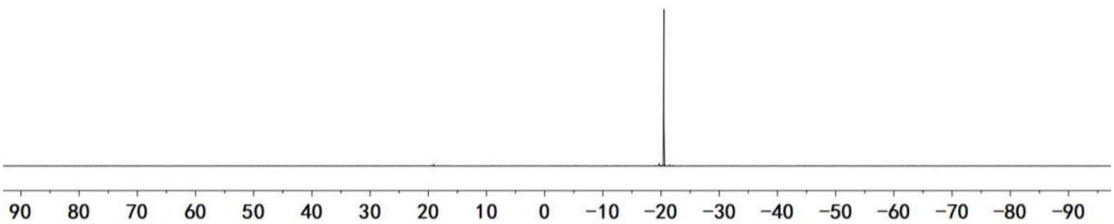


Figure S13. ^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K).

EPR spectroscopic study of complex 2a:

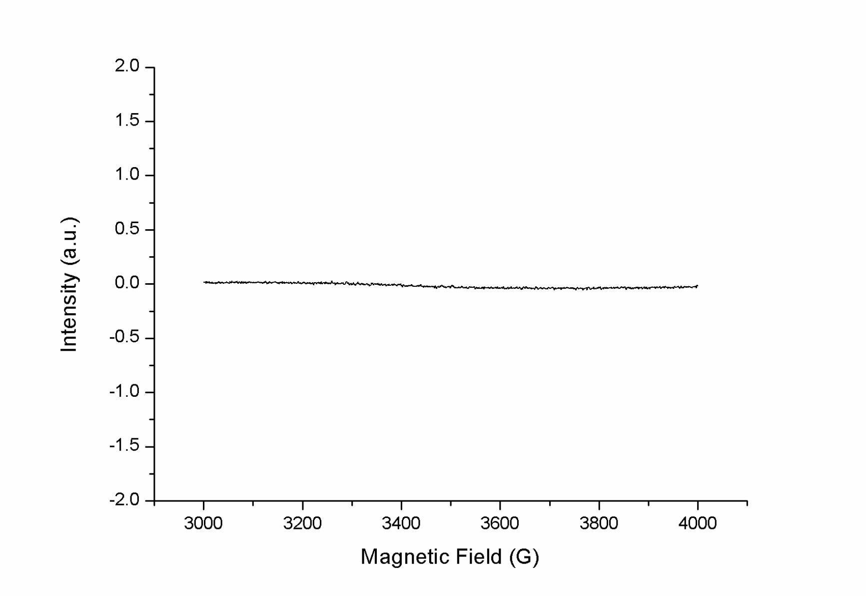


Figure S14. X-band EPR spectrum of a solid sample of **2a** at 25 °C. (υ = 9.839 GHz; P = 2.000 mW; modulation amplitude = 1.000 G)

X-ray crystal structure analysis of complex 2a: formula $C_{62}H_{76}N_4P_2Zn_2 \cdot C_7H_8$, M = 1162.08 gmol^{-1}, colorless, 0.18 × 0.15 × 0.10 mm, triclinic, space group P-1, a = 12.5584(5), b = 13.8088(5), c = 21.0026(9) Å, α = 103.7740(10), β = 93.3920(10), γ = 114.9870(10)°, V = 3153.1(2) Å^3, ρ_{calc} = 1.224 gcm^{-3}, μ = 0.854 mm^{-1}, empirical absorption correction (0.6533 ≤ T ≤ 0.7456), Z = 2, λ = 0.71073 Å, T = 120(2) K, 108875 reflections collected (-16 ≤ h ≤ 16, -17 ≤ k ≤ 17, -27 ≤ l ≤ 27), 14487 independent (R_{int} = 0.0677) and 11444 observed reflections [I>2σ(I)], 695 refined parameters, the final R_1 was 0.0480 (I > 2σ(I)) and wR_2 was 0.1448 (all data), max. (min.) residual electron density 2.38 (-1.07) e.Å^{-3}, hydrogen atoms were placed in calculated positions and refined using a riding model.

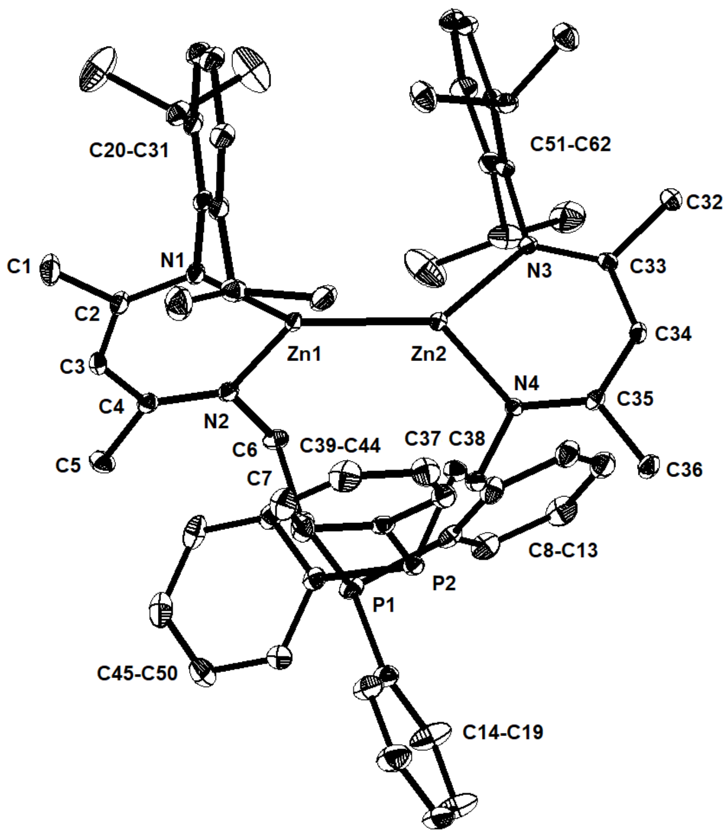
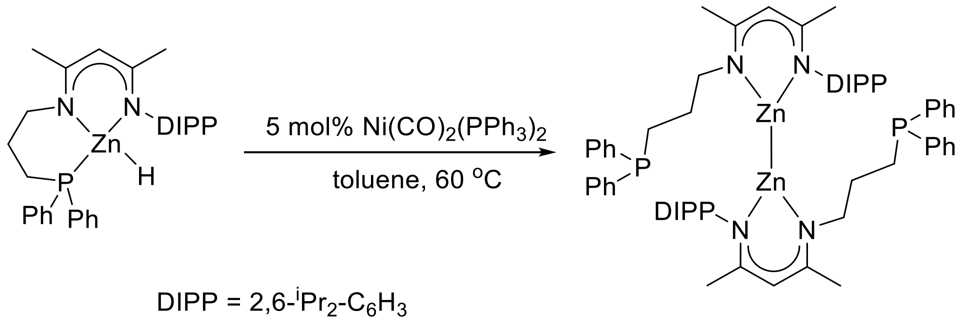


Figure S15. Molecular structure of complex **2a**.

Preparation of complex 2b



1b **2b**

Scheme S5.

Following the procedure described for **2a**, reaction of $Ni(CO)_2(PPh_3)_2$ (10 mg, 0.015 mmol) with **1b** (165 mg, 0.30 mmol) for 13 h gave **2b** as a colorless solid (137 mg, 83%). Crystals suitable for the X-ray crystal structure analysis were grown from a layered toluene/hexane (v/v: 1:2) solution at room temperature.

Elemental Analysis: calcd. for $C_{64}H_{80}N_4P_2Zn_2$: C, 70.00; H, 7.34; N, 5.10%. Found: C, 70.34; H, 7.24; N, 4.92%.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.50 (m, 8H, *o-Ph*$_2$P), 7.14 (m, 8H, *m-Ph*$_2$P), 7.12 (m, 6H, *m*, *p*-N*Ar*), 7.08 (m, 4H, *p-Ph*$_2$P), 4.74 (s, 2H, MeC(N)C*H*), 3.24 (sp, $^3J_{HH}$ = 6.9 Hz, 4H, ArC*H*Me$_2$), 3.02 (m, 4H, NC*H*$_2$), 1.99 (m, 4H, PC*H*$_2$), 1.78 (s, 6H, *Me*C), 1.67 (s, 6H, *Me*C), 1.51 (m, 4H, NCH$_2$C*H*$_2$), 1.19 (d, $^3J_{HH}$ = 6.9 Hz, 12H, ArCH*Me*$_2$), 1.15 (d, $^3J_{HH}$ = 6.9 Hz, 12H, ArCH*Me*$_2$).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 166.6 (Me*C*), 164.1 (Me*C*), 147.1 (*i*-N*Ar*), 142.4 (*o*-N*Ar*), 139.7 (d, $^1J_{PC}$ = 14.0 Hz, *i-Ph*$_2$P), 133.2 (d, $^2J_{PC}$ = 18.3 Hz, *o-Ph*$_2$P), 128.8 (d, $^3J_{PC}$ = 6.5 Hz, *m-Ph*$_2$P), 128.7 (*p-Ph*$_2$P), 125.1 (*p*-N*Ar*), 123.7 (*m*-N*Ar*), 96.6 (MeC(N)*C*H), 51.9 (d, $^3J_{PC}$ = 11.5 Hz, N*C*H$_2$), 29.7 (d, $^2J_{PC}$ = 14.7 Hz, NCH$_2$*C*H$_2$), 28.3 (Ar*C*HMe$_2$), 26.4 (d, $^1J_{PC}$ = 11.9 Hz, P*C*H$_2$), 25.1 (ArCH*Me*$_2$), 23.7 (ArCH*Me*$_2$), 23.6 (*Me*C), 21.4 (*Me*C).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K): δ = -16.9.

^{1}H, ^{1}H GCOSY (400 MHz / 400 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{1}H = 7.50 / 7.14 (*o-Ph*$_2$P / *m-Ph*$_2$P), 3.02 / 1.51 (NC*H*$_2$ / NCH$_2$C*H*$_2$), 1.99 / 1.51 (PC*H*$_2$ / NCH$_2$C*H*$_2$), 3.24 / 1.19, 1.15 (ArC*H*Me$_2$ / ArCH*Me*$_2$).

^{1}H, ^{13}C GHSQC (400 MHz / 101 MHz, C_6D_6, 298 K): δ ^{1}H / δ ^{13}C = 7.50 / 133.2

(*o*-*Ph*$_2$P), 7.14 / 128.7 (*m*-*Ph*$_2$P), 7.12 / 125.1 (*p*-N*Ar*), 7.12 / 123.7 (*m*-N*Ar*), 7.08 / 128.7 (*p*-*Ph*$_2$P), 4.74 / 96.6 (MeC(N)*CH*), 3.24 / 28.3 (Ar*CH*Me$_2$,), 3.02 / 51.9 (N*CH*$_2$), 1.99 / 26.4 (P*CH*$_2$), 1.78 / 21.4 (*Me*C), 1.67 / 23.6 (*Me*C), 1.51 / 29.7 (NCH$_2$*CH*$_2$), 1.19 / 23.7 (ArCH*Me*$_2$), 1.15 / 25.1 (ArCH*Me*$_2$).

^{1}H, ^{13}C GHMBC (400 MHz / 101 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{13}C = 7.50 / 128.7 (o-*Ph*$_2$P / *p*-*Ph*$_2$P), 4.74 / 147.1, 51.9 (MeC(N)C*H* / *i*-N*Ar* , N*C*H$_2$), 3.02 / 29.7, 26.4 (NC*H*$_2$ / P*C*H$_2$, NCH$_2$*C*H$_2$), 3.24 / 25.1, 23.7 (ArC*H*Me$_2$/ ArCH*Me*$_2$), 1.99 / 139.7 (PC*H*$_2$ / *i*-*Ph*$_2$P), 1.19, 1.15 / 142.4 (ArCH*Me*$_2$ / *o*-N*Ar*).

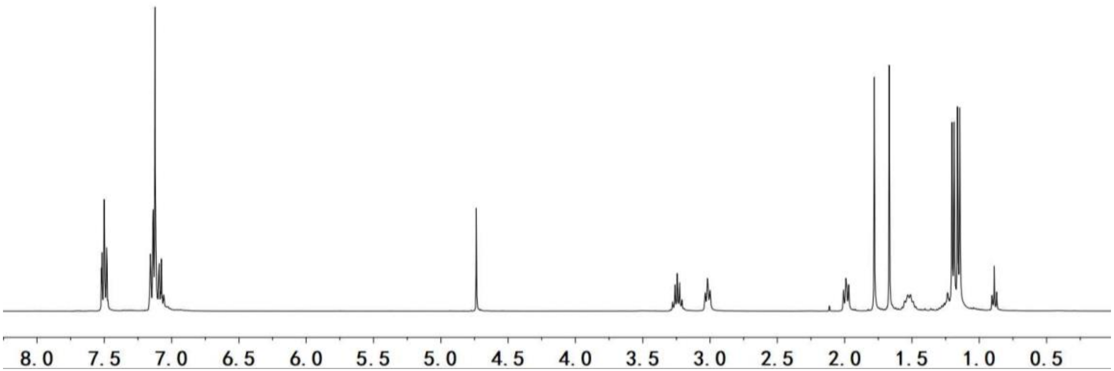


Figure S16. ^{1}H NMR (400 MHz, C_6D_6, 298 K).

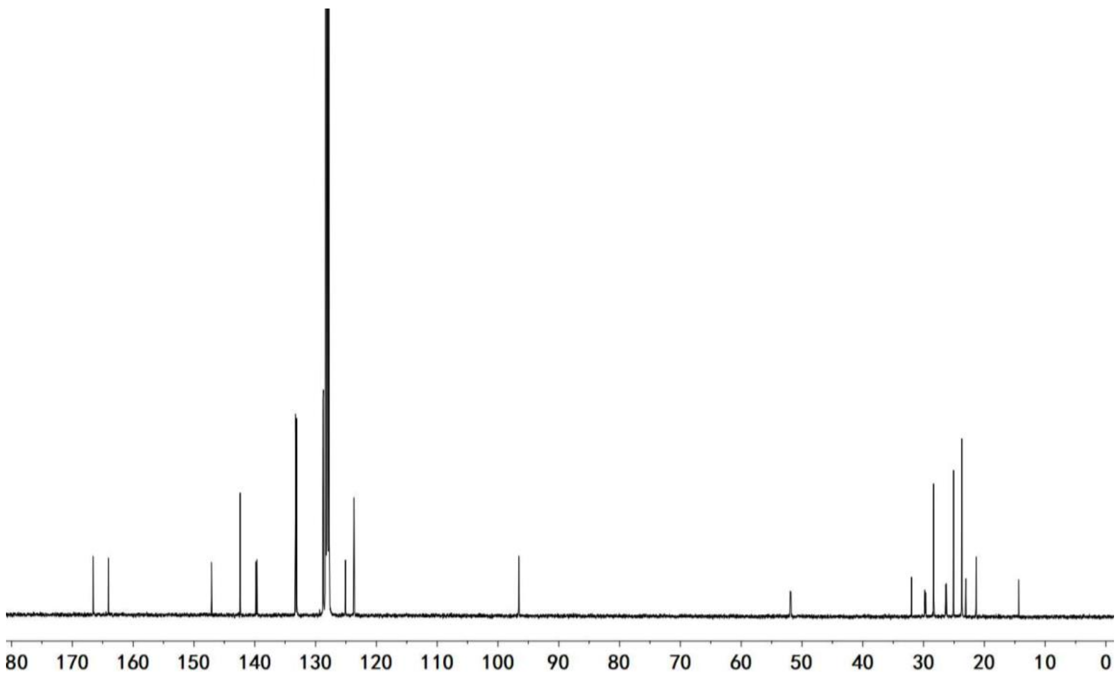


Figure S17. $^{13}C\ \{^1H\}$ NMR (101 MHz, C_6D_6, 298 K).

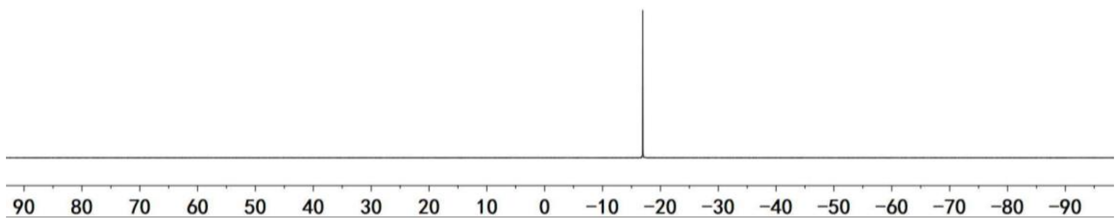


Figure S18. $^{31}P\{^1H\}$ NMR (162 MHz, C_6D_6, 298 K).

EPR spectroscopic study of complex 2b:

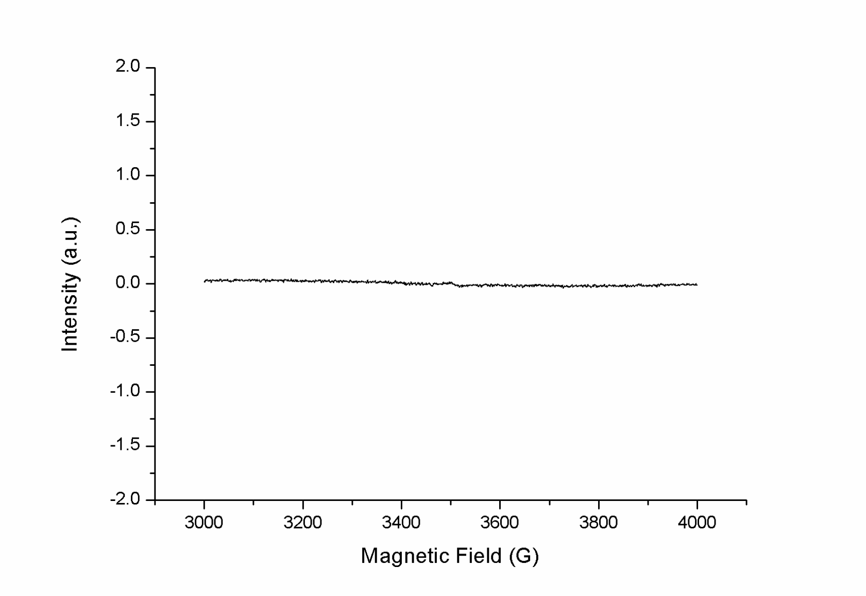


Figure S19. X-band EPR spectrum of a solid sample of **2b** at 25 °C. (υ = 9.839 GHz; *P* = 2.000 mW; modulation amplitude = 1.000 G)

X-ray crystal structure analysis of complex 2b: formula $C_{64}H_{80}N_4P_2Zn_2$, *M* = 1098.04 gmol^{-1}, colorless, 0.25 × 0.18 × 0.15 mm, triclinic, space group *P*-1, *a* = 13.1045(13), *b* = 13.5153(12), *c* = 16.9765(16) Å, α = 95.494(3), β = 97.853(3), γ = 92.241(3)°, *V* = 2960.7(5) Å^3, ρ_{calc} = 1.229 gcm^{-3}, μ = 0.905 mm^{-1}, empirical absorption correction (0.6361 ≤ T ≤ 0.7456), *Z* = 2, λ = 0.71073 Å, T = 120(2) K, 133429 reflections collected (-17 ≤ h ≤ 17, -17 ≤ k ≤ 17, -22 ≤ l ≤ 22), 13608 independent (R_{int} = 0.0729) and 10228 observed reflections [I>2σ(I)], 640 refined parameters, the final R_1 was 0.0476 (I > 2σ(I)) and wR_2 was 0.1028 (all data), max. (min.) residual electron density 1.05 (-0.66) e.Å^{-3}, hydrogen atoms were placed in calculated positions and refined using a riding model.

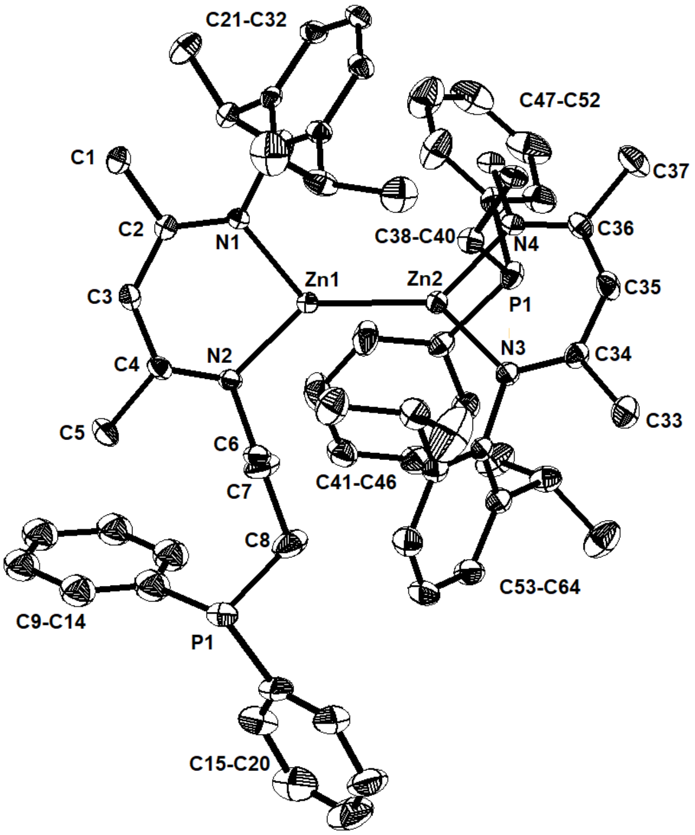
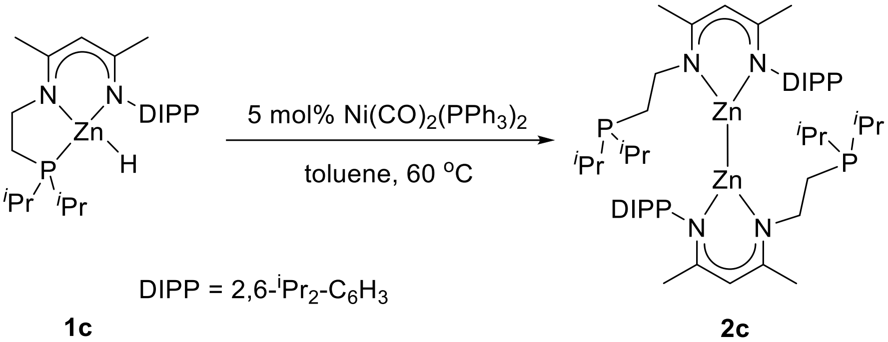


Figure S20. Molecular structure of complex **2b**.

Preparation of complex 2c



Scheme S6.

Following the procedure described for **2a**, reaction of $Ni(CO)_2(PPh_3)_2$ (16 mg, 0.025 mmol) with **1c** (234 mg, 0.50 mmol) gave **2c** as a colorless crystalline solid (149 mg, 64%). Crystals suitable for the X-ray crystal structure analysis were grown from a layered toluene / hexane (v/v: 1:2) solution at -30 °C.

Elemental Analysis: calcd. for $C_{50}H_{84}N_4P_2Zn_2$: C, 64.30; H, 9.07; N, 6.00%. Found: C, 64.66; H, 8.89; N, 5.86%.

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.10 (m, 2H, *p*-N*Ar*), 7.06 (m, 4H, *m*-N*Ar*), 4.79 (s, 2H, MeC(N)C*H*), 3.83 (m, 4H, NCH_2), 3.17 (sp, $^3J_{HH}$ = 6.8 Hz, 4H, ArC*H*Me$_2$), 1.98 (s, 6H, *Me*C), 1.74 (m, 4H, PCH_2), 1.73 (overlapped with PCH_2, 4H, PC*H*Me$_2$), 1.61 (s, 6H, *Me*C), 1.17 (d, $^3J_{HH}$ = 6.9 Hz, 12H, ArCHMe_2), 1.11 (m, 24H, PCHMe_2), 1.04 (d, $^3J_{HH}$ = 6.9 Hz, 12H, ArCHMe_2).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 166.1 (Me*C*), 164.5 (Me*C*), 146.5 (*i*-N*Ar*), 142.1 (*o*-N*Ar*), 125.3 (*p*-N*Ar*), 123.5 (*m*-N*Ar*), 96.8 (MeC(N)*C*H), 51.6 (d, $^2J_{PC}$ = 29.1 Hz, N*C*H$_2$), 28.2 (Ar*C*HMe$_2$), 26.9 (d, $^1J_{PC}$ = 22.1 Hz, P*C*H$_2$), 25.4 (ArCHMe_2), 23.9 (d, $^1J_{PC}$ = 4.0 Hz, P*C*HMe$_2$), 23.7 (*Me*C), 23.6 (ArCHMe_2), 21.9 (*Me*C), 20.3 (d, $^2J_{PC}$ = 16.5 Hz, PCHMe_2), 19.2 (d, $^2J_{PC}$ = 10.1 Hz, PCHMe_2).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K): δ = 0.6.

^{1}H, ^{1}H GCOSY (400 MHz / 400 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{1}H = 3.83 / 1.74 (NCH_2 / PCH_2), 3.17 / 1.17, 1.04 (ArC*H*Me$_2$ / ArCHMe_2), 1.73 / 1.11 (PC*H*Me$_2$ / PCHMe_2).

^{1}H, ^{13}C GHSQC (400 MHz / 101 MHz, C_6D_6, 298 K): δ ^{1}H / δ ^{13}C = 7.10 / 125.3 (*p*-N*Ar*), 7.06 / 123.5 (*m*-N*Ar*), 4.79 / 96.8 (MeC(N)*CH*), 3.83 / 51.6 (N*C*H_2), 3.17 /

28.2 (Ar*CH*Me$_2$), 1.98 / 21.9 (*Me*C), 1.74 / 26.9 (P*CH*$_2$), 1.73 / 23.9 (P*CH*Me$_2$), 1.61 / 23.7 (*Me*C), 1.17 / 23.6 (ArCH*Me*$_2$), 1.11 / 20.3, 19.2 (PCH*Me*$_2$), 1.04 / 25.4 (ArCH*Me*$_2$).

^{1}H, ^{13}C GHMBC (400 MHz / 101 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{13}C = 4.74 / 146.5, 51.6 (MeC(N)C*H* / *i*-N*Ar*, N*C*H$_2$), 3.83 / 26.9 (NC*H*$_2$ / P*C*H$_2$), 3.17 / 25.4, 23.6 (ArC*H*Me$_2$ / ArCH*Me*$_2$), 1.17, 1.04 / 142.1 (ArCH*Me*$_2$ / *o*-N*Ar*).

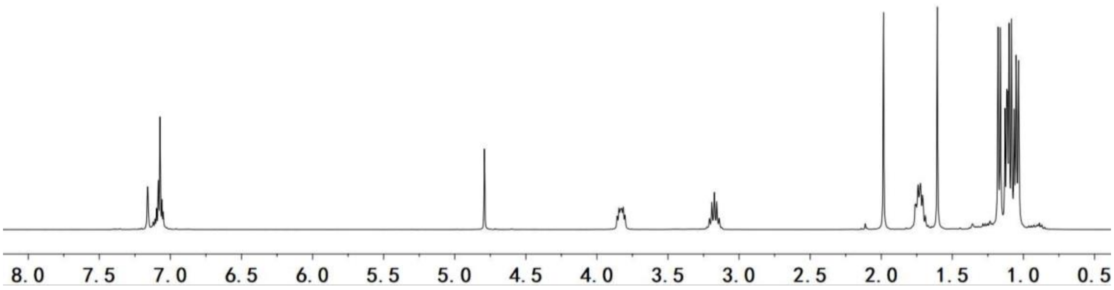


Figure S21. ^{1}H NMR (400 MHz, C_6D_6, 298 K).

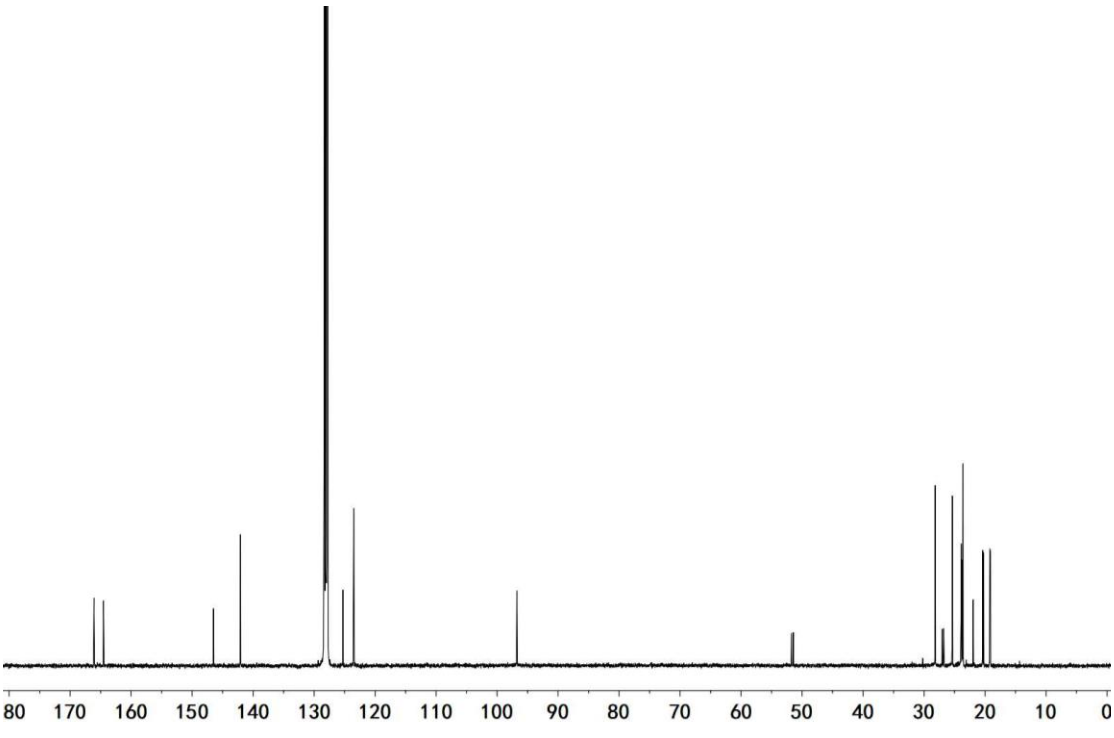


Figure S22. ^{13}C {^{1}H} NMR (101 MHz, C_6D_6, 298 K).

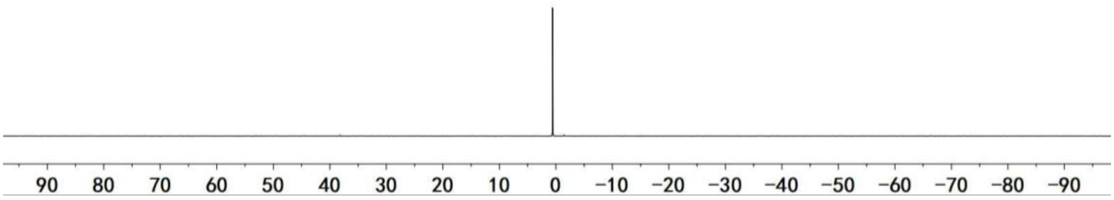


Figure S23. ^{31}**P{**^{1}**H} NMR** (162 MHz, C_6D_6, 298 K).

EPR spectroscopic study of complex 2c:

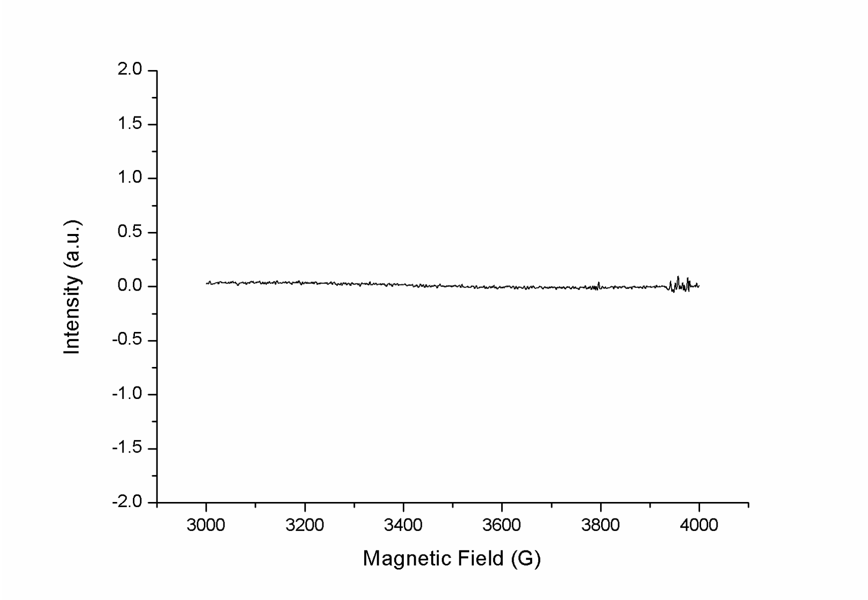


Figure S24. X-band EPR spectrum of a solid sample of **2c** at 25 °C. (υ = 9.839 GHz; P = 2.000 mW; modulation amplitude = 1.000 G)

X-ray crystal structure analysis of complex 2c: formula $C_{50}H_{84}N_4P_2Zn_2$, M = 933.89 gmol^{-1}, colorless, 0.12 × 0.1 × 0.08 mm, monoclinic, space group $P2_1/c$, a = 12.8656(4), b = 9.8087(4), c = 41.6176(12) Å, β = 90.4880(10)°, V = 5251.7(3) Å^3, ρ_{calc} = 1.181 gcm^{-3}, μ = 1.009 mm^{-1}, empirical absorption correction (0.6354 ≤ T ≤ 0.7456), Z = 4, λ = 0.71073 Å, T = 120(2) K, 85103 reflections collected (-16 ≤ h ≤ 16, -12 ≤ k ≤ 12, -54 ≤ l ≤ 54), 12021 independent (R_{int} = 0.0964) and 8212 observed reflections [I>2σ(I)], 543 refined parameters, the final R_1 was 0.0403 (I > 2σ(I)) and wR_2 was 0.1023 (all data), max. (min.) residual electron density 0.65 (-0.47) e.Å^{-3}, hydrogen atoms were placed in calculated positions and refined using a riding model.

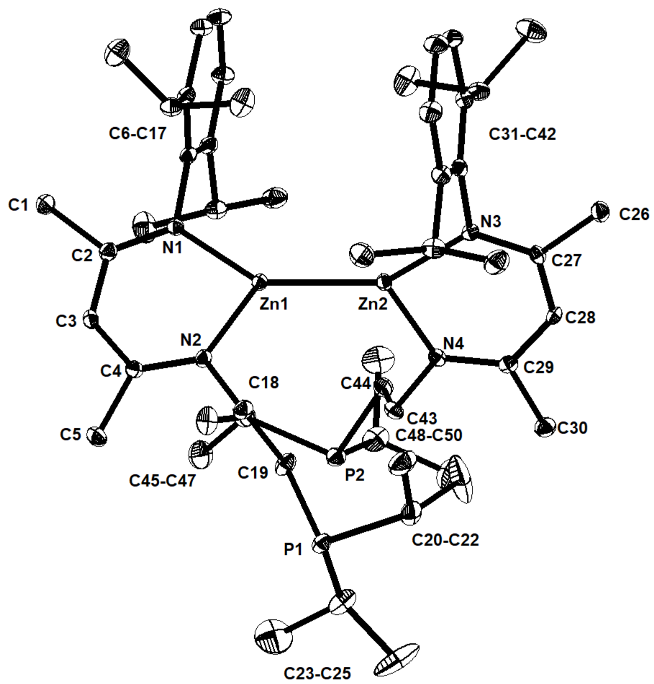
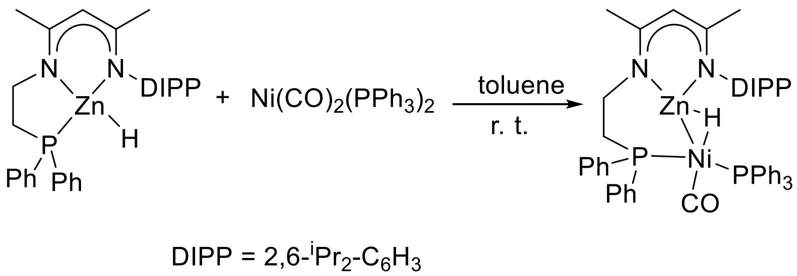


Figure S25. Molecular structure of complex **2c**.

Preparation of complex 3



1a **3**

Scheme S7.

$Ni(CO)_2(PPh_3)_2$ (128 mg, 0.20 mmol) was added to a solution of **1a** (107 mg, 0.20 mmol) in 3 mL of toluene. After stirring at room temperature for 3 days, the reaction solution was concentrated to approximately 1 mL under vacuum and then the residue was recrystallized in hexane at -30 °C to eventually afford **3** as a yellow crystalline solid (108 mg, 61%). Crystals suitable for the X-ray crystal structure analysis were grown from a layered toluene / hexane (v/v: 1:2) solution at room temperature.

Elemental Analysis: calcd. for $C_{50}H_{54}N_2NiOP_2Zn$: C, 67.86; H, 6.15; N, 3.17%. Found: C, 68.05; H, 6.09; N, 3.02%.

FTIR (KBr, cm^{-1}): 1922 (CO).

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.66 (m, 2H, *o-Ph*$_2$P), 7.34 (m, 6H, *o-Ph*$_3$P), 7.25 (m, 1H, *m*-N*Ar*), 7.20 (m, 1H, *p*-N*Ar*), 7.10 (m, 1H, *m*-N*Ar*), 7.08 (m, 2H, *m-Ph*$_2$P), 7.03 (m, 2H, *o-Ph*$_2$P), 6.99 (m, 2H, *p-Ph*$_2$P), 6.94 (m, 9H, *m*, *p-Ph*$_3$P), 6.86 (m, 2H, *m-Ph*$_2$P), 4.81 (s, 1H, MeC(N)C*H*), 3.44 (m, 2H, ArC*H*Me$_2$), 3.39 (m, 2H, NC*H*$_2$), 2.53 (m, 1H, PC*H*$_2$), 2.11 (m, 1H, PC*H*$_2$), 1.71 (s, 3H, *Me*C), 1.63 (s, 3H, *Me*C), 1.42 (d, $^3J_{HH}$ = 6.9 Hz, 3H, ArCH*Me*$_2$), 1.21 (d, $^3J_{HH}$ = 6.9 Hz, 3H, ArCH*Me*$_2$), 1.15 (d, $^3J_{HH}$ = 6.9 Hz, 3H, ArCH*Me*$_2$), 1.07 (d, $^3J_{HH}$ = 6.8 Hz, 3H, ArCH*Me*$_2$), -3.47 (dd, $^2J_{PH}$ = 20.3 Hz, $^2J_{PH}$ = 10.6 Hz, 1H, Zn*H*).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 166.9 (Me*C*), 166.5 (Me*C*), 145.5 (*i*-N*Ar*), 143.1 (*o*-N*Ar*), 142.6 (*o*-N*Ar*), 139.6 (br, *i-Ph*$_2$P), 139.3 (br, *i-Ph*$_2$P), 133.9 (br, *o-Ph*$_3$P), 133.8 (br, *o-Ph*$_2$P), 132.1 (d, $^2J_{PC}$ = 12.1 Hz, *o-Ph*$_2$P), 129.0 (*m-Ph*$_2$P), 128.5 (*p-Ph*$_2$P), 128.2 (overlapped with solvent, *p-Ph*$_3$P), 128.0 (overlapped with solvent, *m-Ph*$_2$P), 127.9 (overlapped with solvent, *m-Ph*$_3$P), 125.9 (*p*-N*Ar*), 124.1

(*m*-N*Ar*), 123.9 (*m*-N*Ar*), 96.0 (MeC(N)*C*H), 46.6 (N*C*H_2), 37.0 (P*C*H_2)[1], 28.6 (Ar*C*HMe$_2$), 28.4 (Ar*C*HMe$_2$), 25.1 (ArCH*Me*$_2$), 24.6 (ArCH*Me*$_2$), 24.2 (ArCH*Me*$_2$), 24.1 (ArCH*Me*$_2$), 23.8 (*Me*C), 22.8 (*Me*C). [Signals of *i-Ph*$_3$P and *C*O were not observed] [[1]from the ^{1}H, ^{13}C GHSQC experiment]

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K): δ = 40.3 (Ph$_3$*P*), 17.4 (Ph$_2$*P*).

^{1}H, ^{1}H GCOSY (400 MHz / 400 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{1}H = 7.66 / 7.08 (*o-Ph*$_2$P / *m-Ph*$_2$P), 7.34 / 6.94 (*o-Ph*$_3$P / *m-Ph*$_3$P), 3.39 / 2.53, 2.11 (NC*H*$_2$ / PC*H*$_2$), 3.44 / 1.42, 1.21, 1.15, 1.07 (ArC*H*Me$_2$ / ArCH*Me*$_2$).

^{1}H, ^{13}C GHSQC (400 MHz / 101 MHz, C_6D_6, 298 K): δ ^{1}H / δ ^{13}C = 7.66 / 133.8 (*o-Ph*$_2$P), 7.34 / 133.9 (*o-Ph*$_3$P), 7.25 / 124.1 (*m*-N*Ar*), 7.20 / 125.9 (*p*-N*Ar*), 7.10 / 123.9 (*m*-N*Ar*), 7.08 / 129.0 (*m-Ph*$_2$P), 7.03 / 132.1 (*o-Ph*$_2$P), 6.99 / 128.5 (*p-Ph*$_2$P), 6.94 / 128.2, 127.9 (*m*, *p-Ph*$_3$P), 6.86 / 128.0 (*m-Ph*$_2$P), 4.81 / 96.0 (MeC(N)C*H*), 3.44 / 28.6, 28.4 (ArC*H*Me$_2$), 3.39 / 46.6 (NC*H*$_2$), 2.53, 2.11 / 37.0 (PC*H*$_2$), 1.71 / 23.8 (*Me*C), 1.63 / 22.8 (*Me*C), 1.42 / 25.1 (ArCH*Me*$_2$), 1.21 / 24.1 (ArCH*Me*$_2$), 1.15 / 24.2 (ArCH*Me*$_2$), 1.07 / 24.6 (ArCH*Me*$_2$).

^{1}H, ^{13}C GHMBC (400 MHz / 101 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{13}C = 7.66 / 128.5 (*o-Ph*$_2$P / *p-Ph*$_2$P), 7.34 / 128.2 (*o-Ph*$_3$P / *p-Ph*$_3$P), 4.81 / 145.5 (MeC(N)C*H* / *i*-N*Ar*), 3.44 / 145.5, 143.1, 142.6 (ArC*H*Me$_2$ / *i*-N*Ar*, *o*-N*Ar*), 3.39 / 166.9 (NC*H*$_2$ / Me*C*).

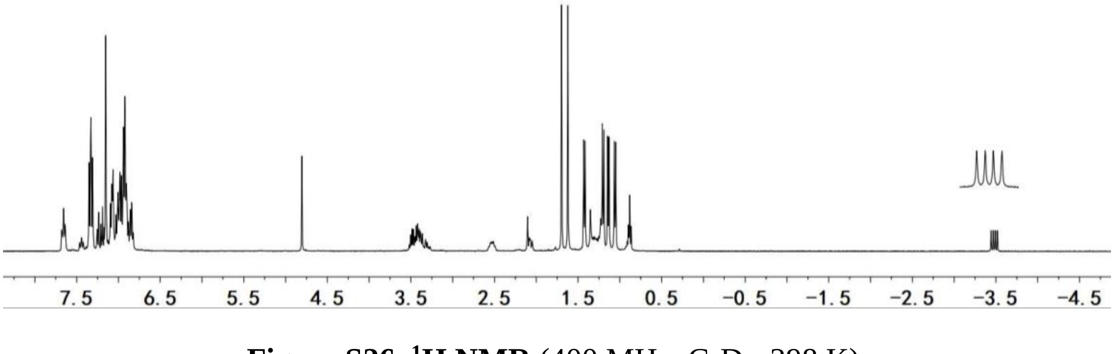


Figure S26. ^{1}H NMR (400 MHz, C_6D_6, 298 K).

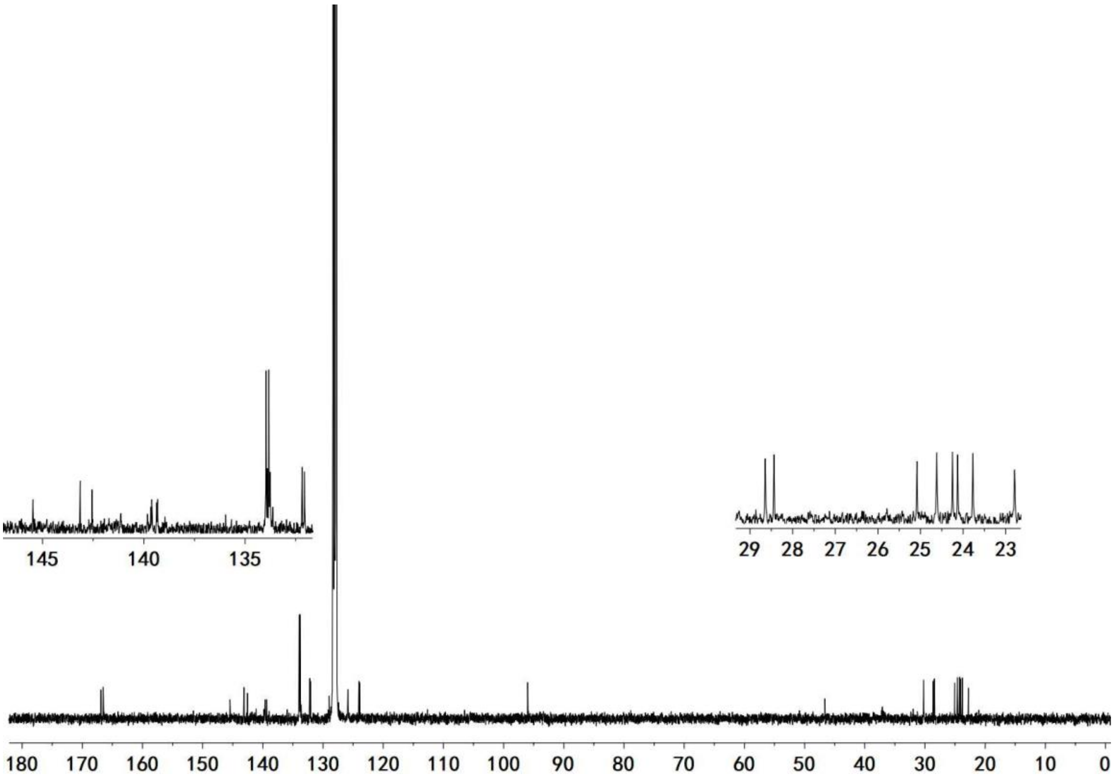


Figure S27. **$^{13}C\{^{1}H\}$ NMR** (101 MHz, C_6D_6, 298 K).

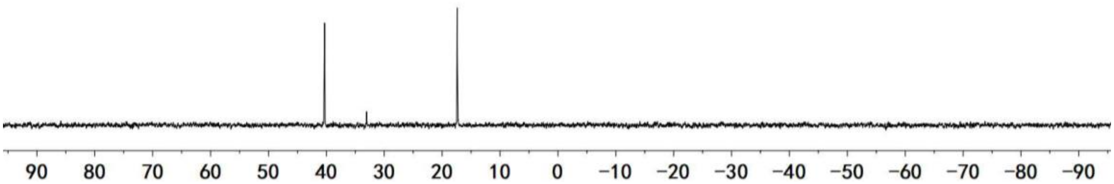


Figure S28. **$^{31}P\{^{1}H\}$ NMR** (162 MHz, C_6D_6, 298 K).

X-ray crystal structure analysis of complex 3: formula $C_{50}H_{54}N_2NiOP_2Zn$, M = 884.97 gmol^{-1}, yellow, 0.18 × 0.15 × 0.12 mm, monoclinic, space group $P2_1/c$, a = 18.6425(15), b = 15.4043(13), c = 16.9677(14) Å, β = 113.062(2), V = 4483.3(6) Å^3, ρ_{calc} = 1.311 gcm^{-3}, μ = 1. 064 mm^{-1}, empirical absorption correction (0.6260 ≤ T ≤ 0.7456), Z = 4, λ = 0.71073 Å, T = 193 K, 54079 reflections collected (-24 ≤ h ≤ 24, -20 ≤ k ≤ 19, -22 ≤ l ≤ 22), 10276 independent (R_{int} = 0.1261) and 6223 observed reflections [I>2σ(I)], 524 refined parameters, the final R_1 was 0.0487 (I > 2σ(I)) and wR_2 was 0.1116 (all data), max. (min.) residual electron density 0.75 (-0.44) e.Å^{-3}, hydrogen atoms except for hydrides were placed in calculated positions and refined using a riding model, the hydride atom in this structure was located in a Fourier difference map and was refined with isotropic displacement parameters.

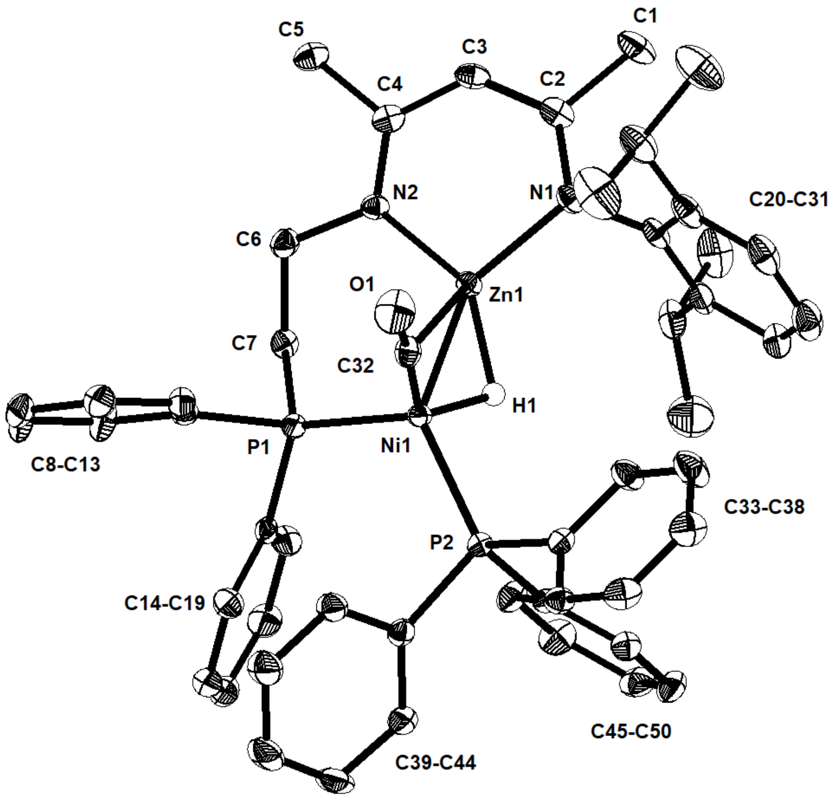
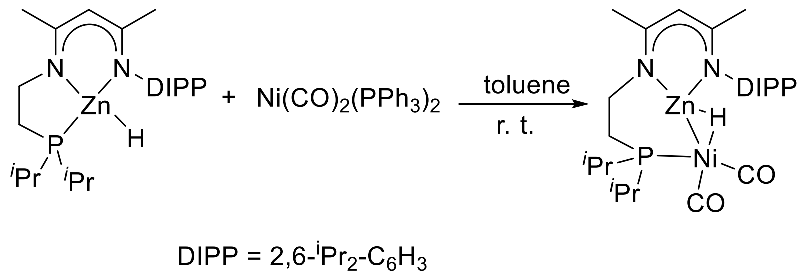


Figure S29. Molecular structure of complex **3**.

Preparation of complex 4



1c **4**

Scheme S8.

$Ni(CO)_2(PPh_3)_2$ (128 mg, 0.20 mmol) was added to a solution of **1c** (94 mg, 0.20 mmol) in 3 mL of toluene. After stirring at room temperature for 10 h, the reaction solution was concentrated to approximately 1 mL under vacuum and then the residue was recrystallized in hexane at -30 °C to eventually afford **4** as a colorless crystalline solid (85 mg, 73%). Crystals suitable for the X-ray crystal structure analysis were grown from a layered toluene / hexane (v/v: 1:2) solution at room temperature.

Elemental Analysis: calcd. for $C_{27}H_{43}N_2NiO_2PZn$: C, 55.65; H, 7.44; N, 4.81%. Found: C, 56.14; H, 7.34; N, 4.71%.

FTIR (KBr, cm^{-1}): 1997, 1927 (CO).

^{1}H NMR (400 MHz, C_6D_6, 298 K): δ = 7.13 (m, 3H, *m*, *p*-N*Ar*), 4.77 (s, 1H, MeC(N)C*H*), 3.39 (m, 2H, NCH_2), 3.21 (sp, $^3J_{HH}$ = 6.9 Hz, 2H, ArC*H*Me$_2$), 1.73 (s, 3H, *Me*C), 1.65 (s, 3H, *Me*C), 1.52 (m, 2H, PC*H*Me$_2$), 1.37 (d, $^3J_{HH}$ = 6.9 Hz, 6H, ArCH*Me*$_2$), 1.18 (m, 2H, PCH_2), 1.16 (d, $^3J_{HH}$ = 6.9 Hz, 6H, ArCH*Me*$_2$), 0.95 (dd, $^3J_{PH}$ = 15.6 Hz, $^3J_{HH}$ = 6.9 Hz, 6H, PCH*Me*$_2$), 0.86 (dd, $^3J_{PH}$ = 13.1 Hz, $^3J_{HH}$ = 6.9 Hz, 6H, PCH*Me*$_2$), -3.25 (d, $^2J_{PH}$ = 17.7 Hz, 1H, Zn*H*).

^{13}C{^{1}H} NMR (101 MHz, C_6D_6, 298 K): δ = 201.4 (d, $^2J_{PC}$ = 3.3 Hz, *C*O), 167.3 (Me*C*), 166.8 (Me*C*), 144.5 (*i*-N*Ar*), 142.2 (*o*-N*Ar*), 126.3 (*p*-N*Ar*), 124.0 (*m*-N*Ar*), 96.2 (MeC(N)*C*H), 47.2 (d, $^2J_{PC}$ = 5.0 Hz, N*C*H$_2$), 28.4 (Ar*C*HMe$_2$), 26.8 (d, $^1J_{PC}$ = 4.5 Hz, P*C*HMe$_2$), 26.2 (d, $^2J_{PC}$ = 14.1 Hz, P*C*H$_2$), 25.0 (ArCH*Me*$_2$), 23.7 (ArCH*Me*$_2$), 23.6 (*Me*C), 22.9 (*Me*C), 18.7 (d, $^2J_{PC}$ = 6.8 Hz, PCH*Me*$_2$), 17.9 (d, $^2J_{PC}$ = 2.6 Hz, PCH*Me*$_2$).

^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K): δ = 38.2.

^{1}H, ^{1}H GCOSY (400 MHz / 400 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{1}H = 3.39 / 1.18 (NC*H₂* / PC*H*₂), 3.21 / 1.37, 1.16 (ArC*H*Me₂ / ArCH*Me*₂), 1.52 / 0.95, 0.86 (PC*H*Me₂ / PCH*Me*₂).

^{1}H, ^{13}C GHSQC (400 MHz / 101 MHz, C_6D_6, 298 K): δ ^{1}H / δ ^{13}C = 7.13 / 126.3, 124.0 (*m*, *p*-N*Ar*), 4.77 / 96.2 (MeC(N)*CH*), 3.39 /47.7 (N*CH*₂), 3.21 / 28.4 (Ar*CH*Me₂), 1.73 / 23.6 (*Me*C), 1.65 / 22.9 (*Me*C), 1.52 / 26.8 (P*CH*Me₂), 1.37 / 25.0 (ArCH*Me*₂),1.18 / 26.2 (P*CH*₂), 1.16 / 23.7 (ArCH*Me*₂), 0.95 / 18.7 (PCH*Me₂*), 0.86 / 17.9 (PCH*Me₂*).

^{1}H, ^{13}C GHMBC (400 MHz / 101 MHz, C_6D_6, 298 K) [selected traces]: δ ^{1}H / δ ^{13}C = 4.77 / 144.5, 47.7 (MeC(N)C*H* / *i*-N*Ar*, N*C*H₂), 3.21 / 25.0, 23.7 (ArC*H*Me₂/ ArCH*Me*₂), 1.37, 1.16 / 142.2 (ArCH*Me*₂ / *o*-N*Ar*), 1.18 / 47.7 (PC*H*₂ / N*C*H₂).

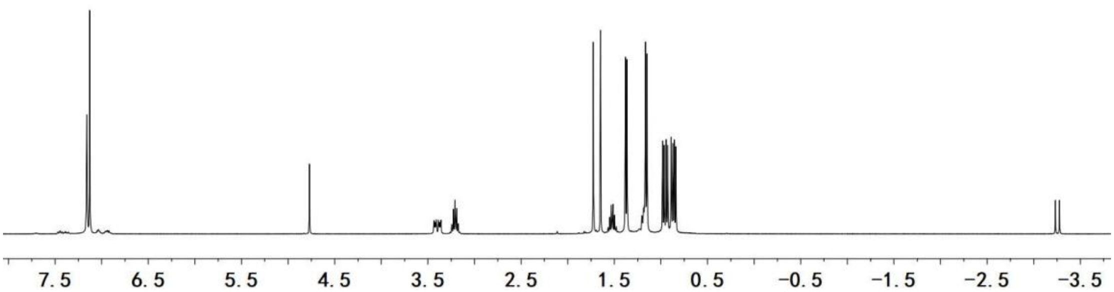


Figure S30. ^{1}H NMR (400 MHz, C_6D_6, 298 K).

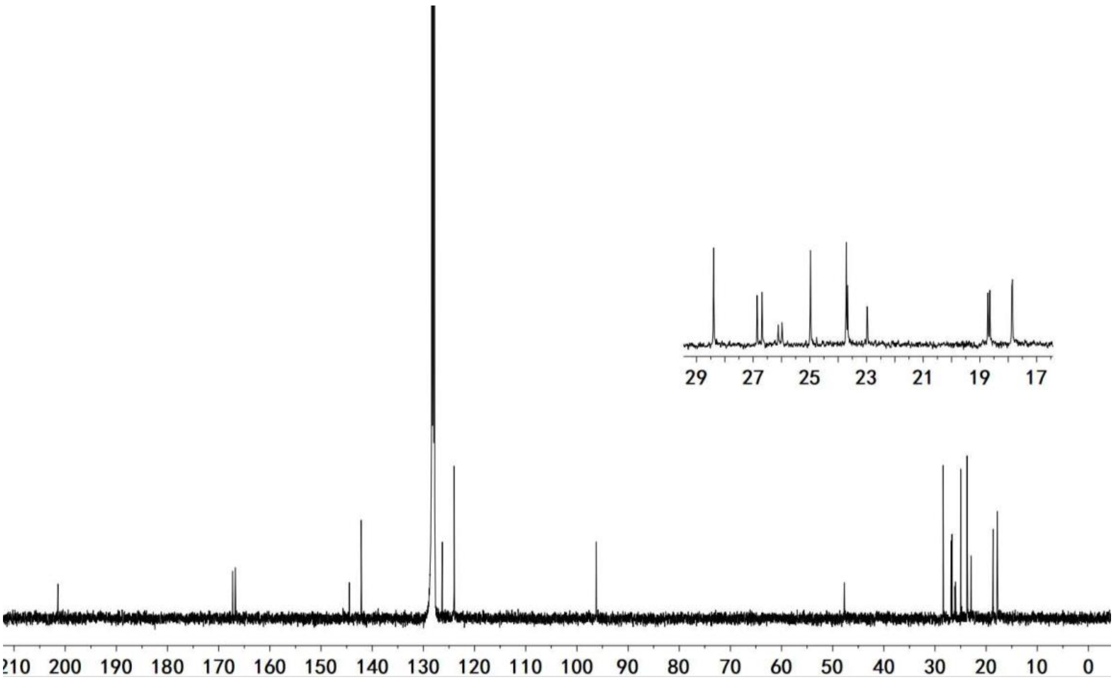


Figure S31. ^{13}C {^{1}H} NMR (101 MHz, C_6D_6, 298 K).

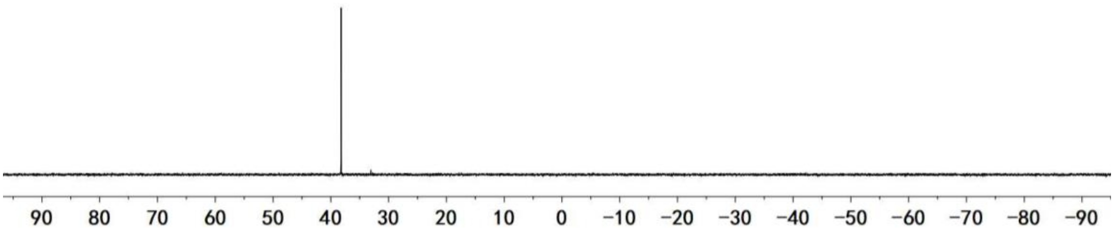


Figure S32. ^{31}P{^{1}H} NMR (162 MHz, C_6D_6, 298 K).

X-ray crystal structure analysis of complex 4: formula $C_{27}H_{43}N_2NiO_2PZn$, M = 582.68 gmol^{-1}, colorless, 0.45 × 0.25 × 0.03 mm, triclinic, space group P-1, a = 8.3843(8), b = 8.4994(8), c = 22.612(2) Å, α = 95.649(3)°, β = 90.677(3)°, γ = 113.428(3)°, V = 1469.0(2) Å^3, ρ_{calc} = 1.317 gcm^{-3}, μ = 1.536 mm^{-1}, empirical absorption correction (0.5276 ≤ T ≤ 0.7456), Z = 2, λ = 0.71073 Å, T = 193 K, 31692 reflections collected (-10 ≤ h ≤ 10, -11 ≤ k ≤ 10, -29 ≤ l ≤ 29), 6735 independent (R_{int} = 0.0746) and 5387 observed reflections [I>2σ(I)], 321 refined parameters, the final R_1 was 0.0643 (I > 2σ(I)) and wR_2 was 0.2007 (all data), max. (min.) residual electron density 1.31 (-1.39) e.Å^{-3}, hydrogen atoms except for hydrides were placed in calculated positions and refined using a riding model, the hydride atom in this structure was located in a Fourier difference map and was refined with isotropic displacement parameters.

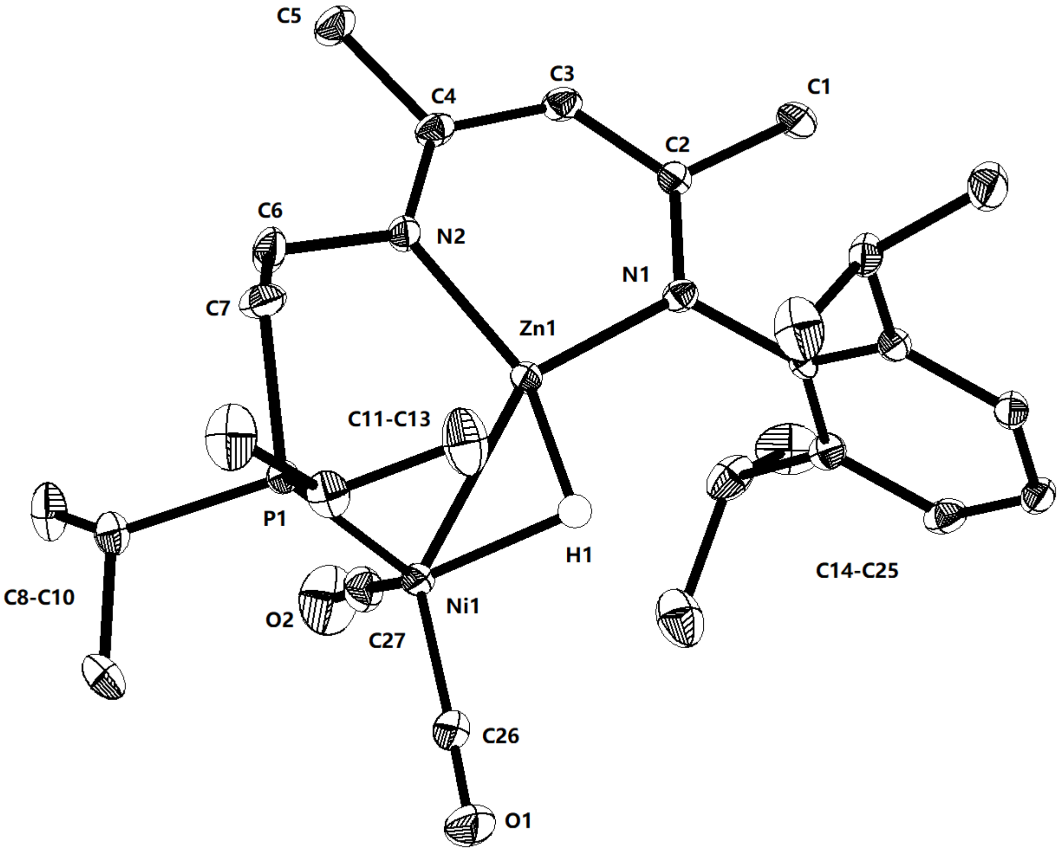
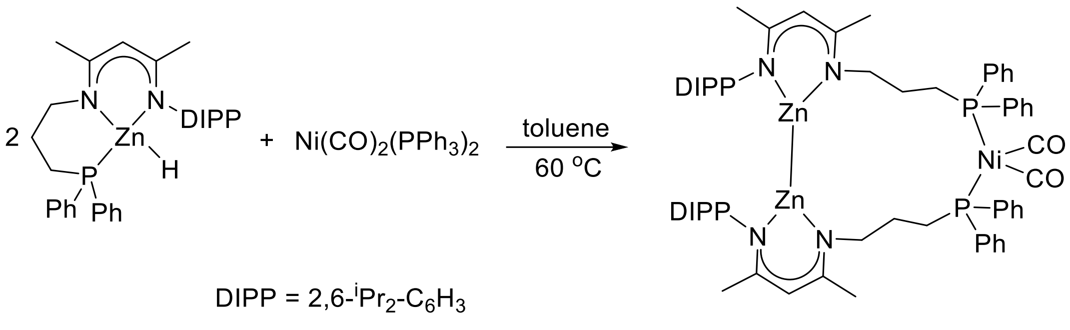


Figure S33. Molecular structure of complex **4**.

Preparation of complex 5



Scheme S9.

$Ni(CO)_2(PPh_3)_2$ (160 mg, 0.25 mmol) was added to a solution of **1b** (275 mg, 0.50 mmol) in 5 mL of toluene. After stirring at 60 °C for 4 h, the reaction mixture was filtered through Celite and the solvent was removed in vacuum. The residue was washed with hexane (5 * 0.5 mL) to eventually give **5** as a colorless solid (203 mg, 67%). Crystals suitable for the X-ray crystal structure analysis were grown from a layered toluene / hexane (v/v: 1:2) solution at room temperature.

Elemental Analysis: calcd. for $C_{66}H_{80}N_4NiO_2P_2Zn_2{\cdot}C_6H_{14}$: C, 66.58; H, 7.29; N, 4.31%. Found: C, 66.65; H, 6.86; N, 4.04%.

FTIR (KBr, cm^{-1}): 1997, 1939 (CO).

^{1}H NMR (400 MHz, Tol-d_8, 243 K): δ = 7.56 (m, 4H, *o-Ph*$_2$P), 7.30 (m, 4H, *o-Ph*$_2$P), 7.01 (m, 2H, *p*-N*Ar*), 6.98 (m, 2H, *p-Ph*$_2$P), 6.97 (m, 4H, *m-Ph*$_2$P), 6.92 (m, 2H, *p-Ph*$_2$P), 6.91 (m, 4H, *m*-N*Ar*), 6.89 (m, 4H, *m-Ph*$_2$P), 4.73 (s, 2H, MeC(N)C*H*), 3.94 (m, 2H, NCH_2), 3.61 (sp, $^3J_{HH}$ = 6.8 Hz, 2H, ArC*H*Me$_2$), 3.34 (m, 2H, NCH_2), 2.77 (sp, $^3J_{HH}$ = 6.8 Hz, 2H, ArC*H*Me$_2$), 2.09 (overlapped with solvent, 2H, PCH_2), 1.99 (m, 2H, NCH$_2$CH_2), 1.98 (m, 2H, PCH_2), 1.61 (s, 6H, *Me*C), 1.56 (s, 6H, *Me*C), 1.49 (d, $^3J_{HH}$ = 6.9 Hz, 6H, ArCH*Me*$_2$), 1.41 (m, 2H, NCH$_2$CH_2), 1.25 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me*$_2$), 1.09 (d, $^3J_{HH}$ = 7.0 Hz, 6H, ArCH*Me*$_2$), 0.37 (d, $^3J_{HH}$ = 6.8 Hz, 6H, ArCH*Me*$_2$).

^{13}C{^{1}H} NMR (101 MHz, Tol-d_8, 243 K): δ = 200.9 (*C*O), 166.8 (Me*C*), 166.4 (Me*C*), 146.1 (*i*-N*Ar*), 142.1 (*o*-N*Ar*), 141.0 (*o*-N*Ar*), 140.3 (d, $^1J_{PC}$ = 35.7 Hz, *i-Ph*$_2$P), 138.2 (d, $^1J_{PC}$ = 30.7 Hz, *i-Ph*$_2$P), 134.3 (*m-Ph*$_2$P), 134.1 (*m-Ph*$_2$P), 132.9 (br, *o-Ph*$_2$P), 131.5 (br, *o-Ph*$_2$P), 129.4 (*p-Ph*$_2$P), 128.8 (*p-Ph*$_2$P), 125.3 (*p*-N*Ar*), 123.6

(m-NAr), 123.3 (m-NAr), 97.4 (MeC(N)CH), 53.3 (d, $^3J_{PC}$ = 16.7 Hz, NCH$_2$), 28.8 (br, NCH$_2$$CH_2$), 28.7 (Ar$CHMe_2$), 28.6 (br, P$CH_2$), 27.7 (Ar$CHMe_2$), 25.1 (ArCH$Me_2$), 24.7 (ArCH$Me_2$), 24.6 (ArCH$Me_2$), 24.0 ($Me$C), 22.5 (ArCH$Me_2$), 21.2 ($Me$C)

^{31}P{^{1}H} NMR (162 MHz, Tol-d_8, 243 K): δ = 22.0.

^{1}H, ^{1}H GCOSY (400 MHz / 400 MHz, Tol-d_8, 243 K) [selected traces]: δ ^{1}H / δ ^{1}H = 7.56 / 6.97 (o-Ph_2P / m-Ph_2P), 7.30 / 6.89 (o-Ph_2P / m-Ph_2P), 3.94 / 3.34, 1.98, 1.41 (NCH_2 / NCH_2, PCH_2), 3.61 / 1.49, 1.25 (ArCHMe$_2$ / ArCHMe_2), 2.77 / 1.09, 0.37 (ArCHMe$_2$ / ArCHMe_2).

^{1}H, ^{13}C GHSQC (400 MHz / 101 MHz, Tol-d_8, 243 K): δ ^{1}H / δ ^{13}C = 7.56 / 131.5 (o-Ph_2P), 7.30 / 132.9 (o-Ph_2P), 7.01 / 125.3 (p-NAr), 6.98 / 128.8 (p-Ph_2P), 6.97 / 134.3 (m-Ph_2P), 6.92 / 129.4 (p-Ph_2P), 6.91 / 123.6, 123.3 (m-NAr), 6.89 / 134.1 (m-Ph_2P), 4.73 / 97.4 (MeC(N)CH), 3.94, 3.34 / 53.3 (NCH_2), 3.61 / 28.6 (ArCHMe$_2$), 2.77 / 27.7 (ArCHMe$_2$), 2.09, 1.98 / 28.6 (PCH_2), 1.99, 1.41 / 28.8 (NCH$_2$$CH_2$), 1.61 / 21.2 ($Me$C), 1.56 / 24.0 ($Me$C), 1.49 / 25.1 (ArCH$Me_2$), 1.25 / 24.6 (ArCH$Me_2$), 1.09 / 22.5 (ArCH$Me_2$), 0.37 / 24.7 (ArCH$Me_2$).

^{1}H, ^{13}C GHMBC (400 MHz / 101 MHz, Tol-d_8, 243 K) [selected traces]: δ ^{1}H / δ ^{13}C = 7.56 / 129.4 (o-Ph_2P / p-Ph_2P), 7.30 / 128.8 (o-Ph_2P / p-Ph_2P), 6.91 / 146.1 (m-NAr / i-NAr), 4.73 / 146.1 (MeC(N)CH / i-NAr), 3.61 / 146.1, 141.0 (ArCHMe$_2$ / i-NAr, o-NAr), 2.77 / 146.1, 142.1 (ArCHMe$_2$ / i-NAr, o-NAr).

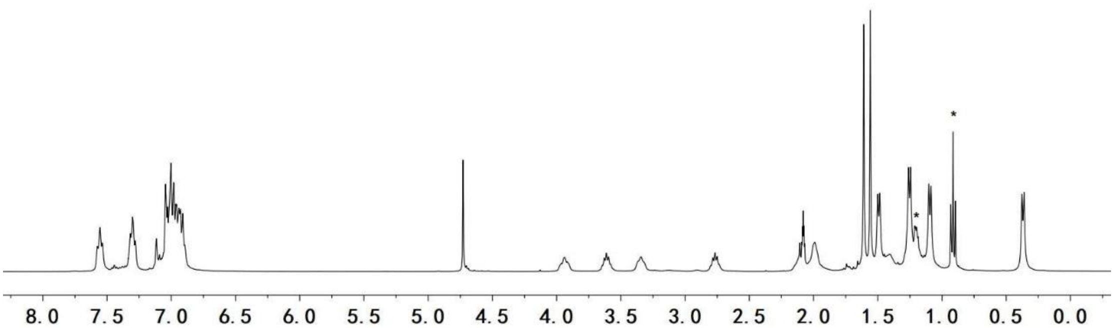


Figure S34. ^{1}H NMR (400 MHz, Tol-d_8, 243 K) [*: Hexane].

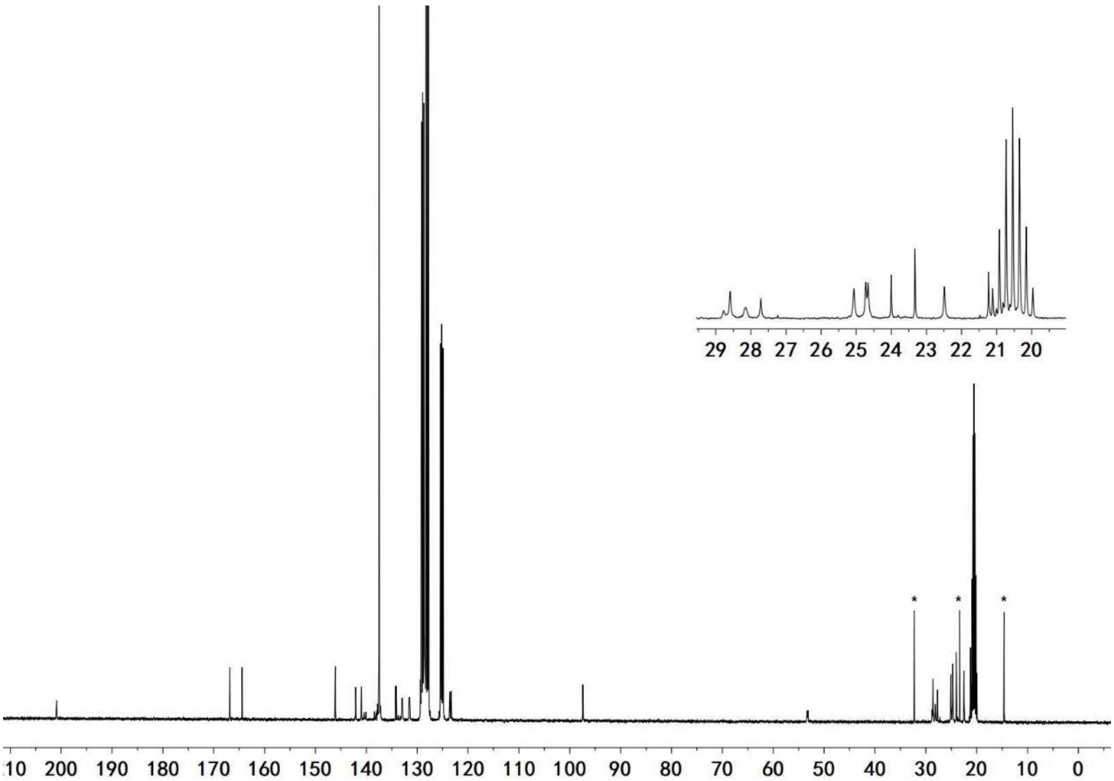


Figure S35. ^{13}C{^{1}H} NMR (101 MHz, Tol-d_8, 243 K) [*: Hexane].

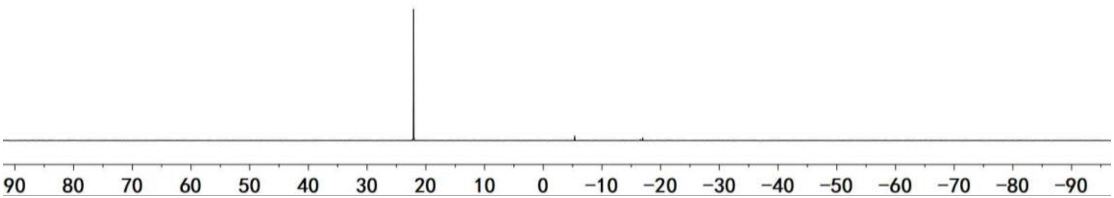


Figure S36. ^{31}P{^{1}H} NMR (162 MHz, Tol-d_8, 243 K).

EPR spectroscopic study of complex 5:

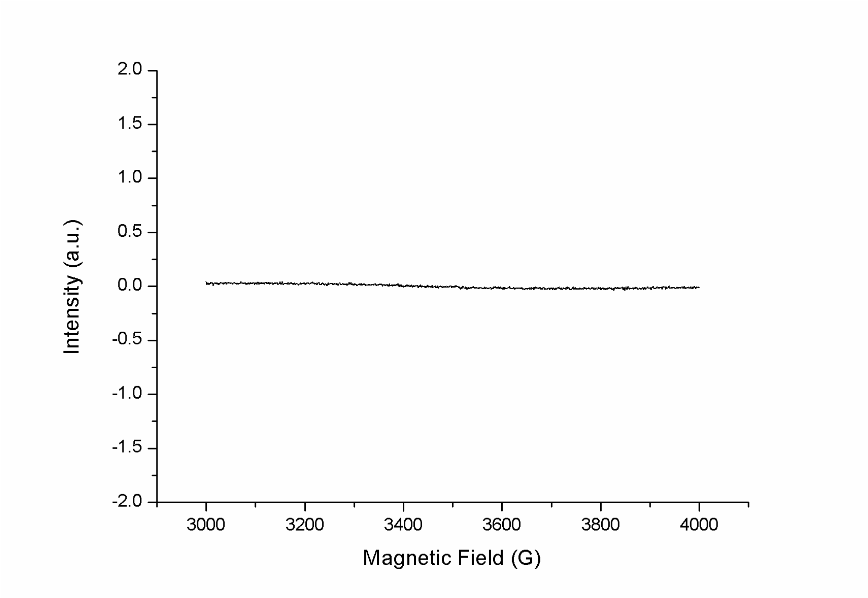


Figure S37. X-band EPR spectrum of a solid sample of **5** at 25 °C. (υ = 9.839 GHz; *P* = 2.000 mW; modulation amplitude = 1.000 G)

X-ray crystal structure analysis of complex 5: formula $C_{66}H_{80}N_4NiO_2P_2Zn_2$, *M* = 1212.76 gmol^{-1}, colorless, 0.18 × 0.12 × 0.08 mm, monoclinic, space group $P2_1/n$, *a* = 8.8752(4), *b* = 14.3633(6), *c* = 48.0556(19) Å, β = 90.0240(10)°, *V* = 6126.0(4) Å^3, ρ_{calc} = 1.315 gcm^{-3}, μ = 1.179 mm^{-1}, empirical absorption correction (0.6188 ≤ T ≤ 0.7456), *Z* = 4, λ = 0.71073 Å, T = 120(2) K, 127462 reflections collected (-10 ≤ h ≤ 11, -18 ≤ k ≤ 18, -62 ≤ l ≤ 62), 14051 independent (R_{int} = 0.0841) and 10765 observed reflections [I>2σ(I)], 706 refined parameters, the final R_1 was 0.0366 (I > 2σ(I)) and wR_2 was 0.0869 (all data), max. (min.) residual electron density 0.74 (-0.62) e.Å^{-3}, hydrogen atoms were placed in calculated positions and refined using a riding model.

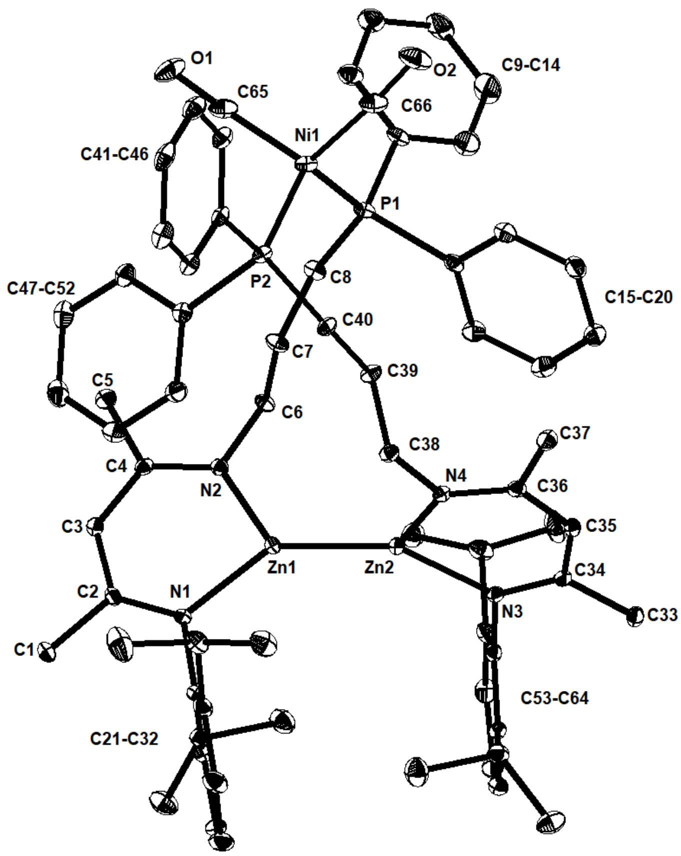
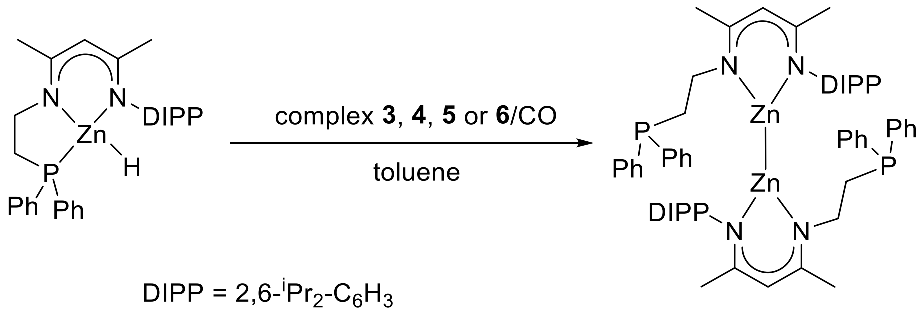


Figure S38. Molecular structure of complex **5**.

Dehydrocoupling of 1a catalyzed by Zn/Ni heterometallic complex



1a **2a**

Scheme S10.

(a) Complex **3** (18 mg, 0.02 mmol) was added to a solution of **1a** (107 mg, 0.20 mmol) in 5 mL of toluene. After stirring at 60 °C for 24 h, the reaction mixture was filtered through Celite. The solvent was removed under vacuum and the residue was recrystallized in hexane at -30 °C to afford **2a** as a pale-yellow solid (87 mg, 81%).

(b) Following the procedure described above, complex **4** (6 mg, 0.01 mmol) catalyzed the dehydrocoupling of **1a** (107 mg, 0.20 mmol) to give **2a** (91 mg, 85%).

(c) Following the procedure described above, complex **5** (12 mg, 0.01 mmol) catalyzed the dehydrocoupling of **1a** (107 mg, 0.20 mmol) to give **2a** (86 mg, 80%).

(d) An oven-dried Schlenk tube was charged with complex **6** (11 mg, 0.01 mmol) and **1a** (107 mg, 0.20 mmol) in 5 mL of toluene. The mixture was degassed by a freeze-pump-thaw cycle and placed under 1 atm CO at room temperature. After stirring at 60 °C for 24 h, the reaction mixture was filtered through Celite. The solvent was removed under vacuum and the residue was recrystallized in hexane at -30 °C to afford **2a** (76 mg, 71%).

Experiments to investigate the role of carbon monoxide concentration on the catalytic reaction

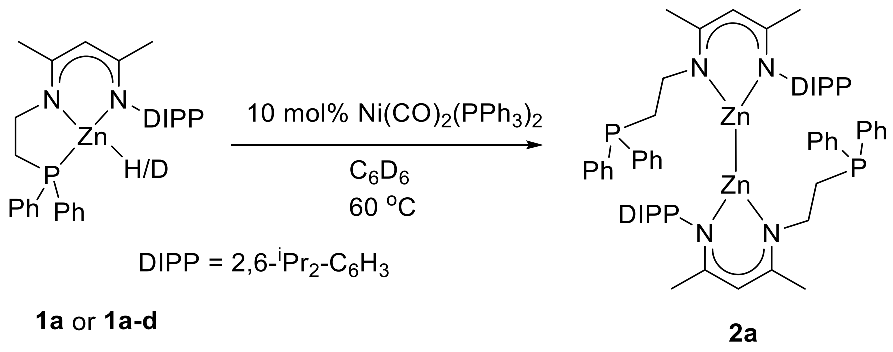
In a glove box, a C_6D_6 solution (1 mL) of **1a** (64.3 mg, 0.12 mmol), $Ni(CO)_2(PPh_3)_2$ (3.8 mg, 0.006 mmol) and hexamethylbenzene (1.1 mg, 0.0067 mmol, as internal standard) was divided equally into two NMR tubes (Samples A and B).

(a) *Sample A*: The tube was sealed and removed from the glove box. After heating at 60 °C for 15 h, the aliquots were analyzed by ^1H NMR. The conversion of **1a** was

63%.

(b) *Sample B*: The J-Young tube was sealed and removed from the glove box. The mixture was degassed by a freeze-pump-thaw cycle and placed under 1 atm CO at room temperature. After heating at 60 ^{o}C for 15 h, the aliquots were analyzed by ^{1}H NMR. The conversion of **1a** was 72%.

Details of kinetics



Scheme S11.

In a glovebox, a C_6D_6 solution (1.0 mL) of complex **1a** (160.8 mg, 0.30 mmol) was added to a C_6D_6 solution (1.0 mL) of $Ni(CO)_2(PPh_3)_2$ (19.2 mg, 0.03 mmol) and internal standard hexamethylbenzene (2.7 mg, 0.017 mmol) in a 25-mL Schlenk tube. The Schlenk tube was sealed, removed from the glovebox and heated at 60 °C. After the measured time interval, a 100 μL aliquot was taken from the reaction mixture and added into an NMR tube containing 400 μL C_6D_6 in the glovebox. The aliquots were immediately analyzed by ^{1}H NMR. The dehydrocoupling of **1a-d** was also carried out and monitored under the exactly same conditions.

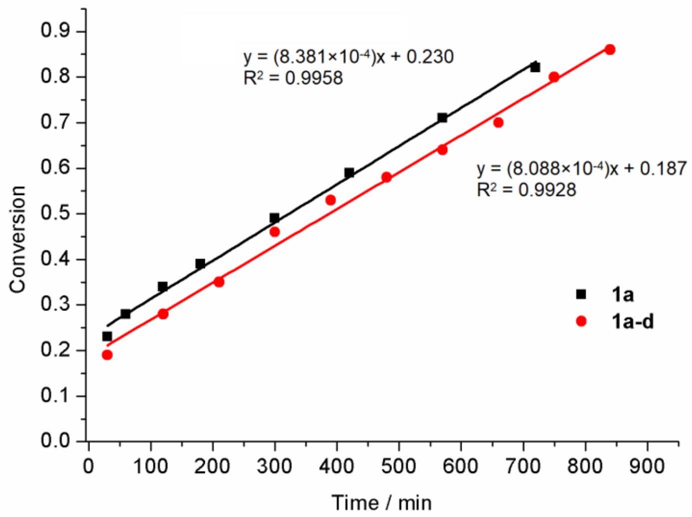
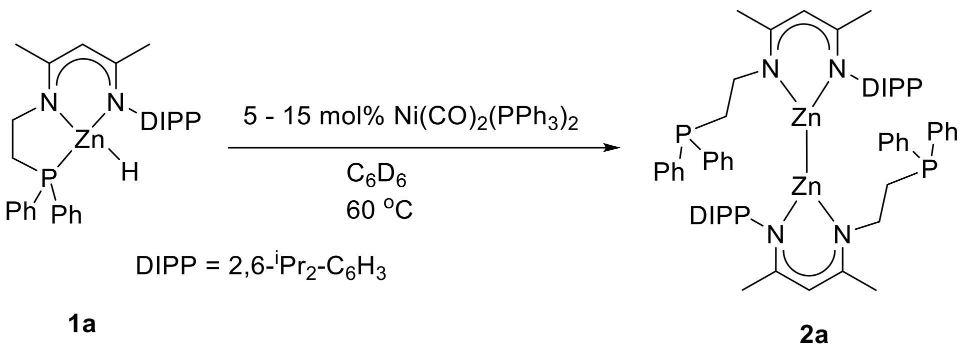


Figure S39. Plot of zinc hydride conversion versus time (min) for the dehydrocoupling of **1a** (black squares) and **1a-d** (red dots) catalyzed by $Ni(CO)_2(PPh_3)_2$.



Scheme S12.

The dehydrocoupling of **1a** (0.30 mmol) with 5 - 15 mol% catalyst loading [$Ni(CO)_2(PPh_3)_2$, 0.015 - 0.045 mmol] in C_6D_6 (2.0 mL) at 60 °C was carried out and the reaction was monitored by ^{1}H NMR spectroscopy.

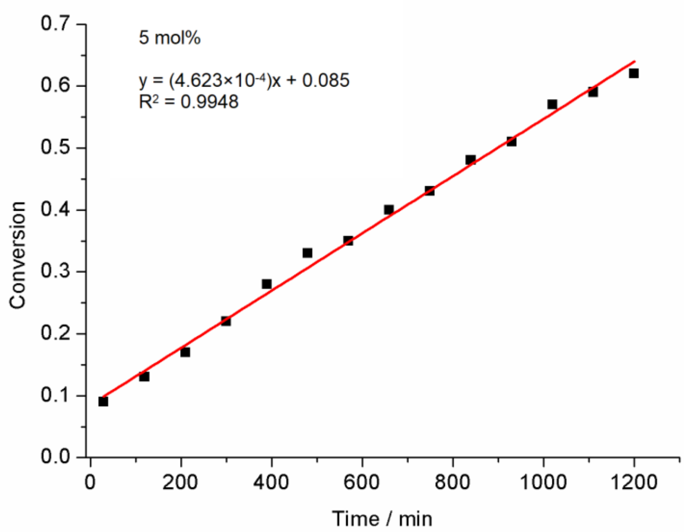


Figure S40. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$. Initial conditions: **1a** (0.15 M), $Ni(CO)_2(PPh_3)_2$ (0.0075 M).

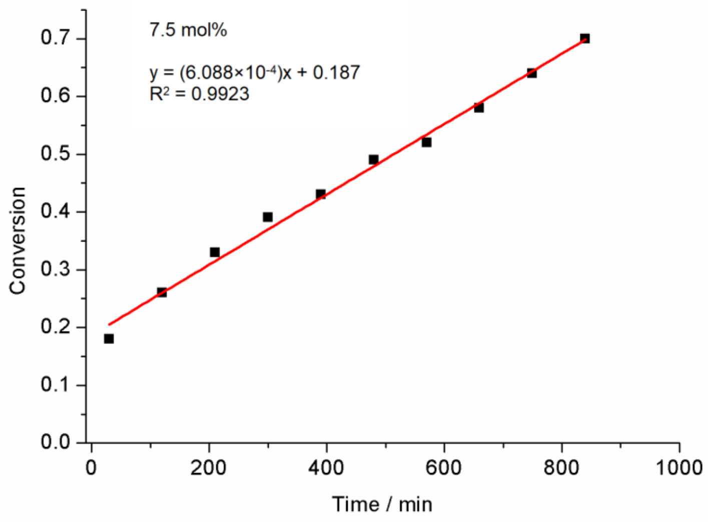


Figure S41. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$. Initial conditions: **1a** (0.15 M), $Ni(CO)_2(PPh_3)_2$ (0.01125 M).

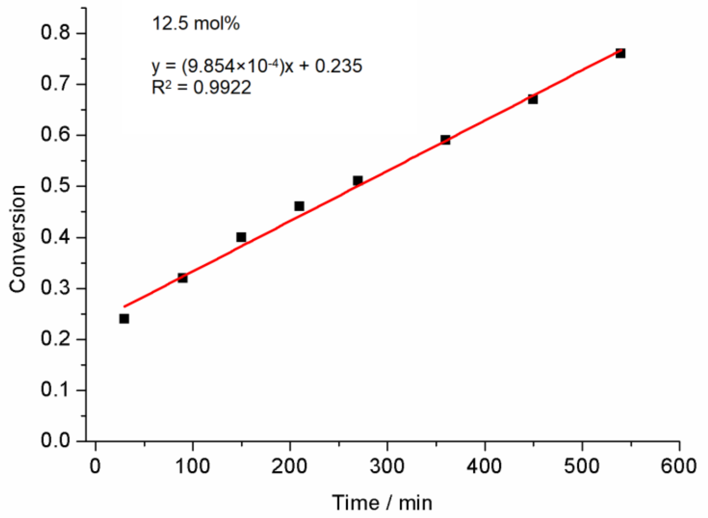


Figure S42. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$. Initial conditions: **1a** (0.15 M), $Ni(CO)_2(PPh_3)_2$ (0.01875 M).

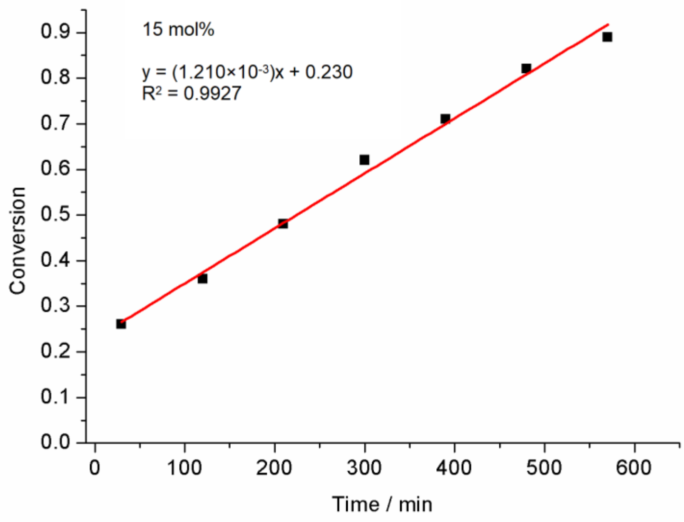


Figure S43. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$. Initial conditions: **1a** (0.15 M), $Ni(CO)_2(PPh_3)_2$ (0.0225 M).

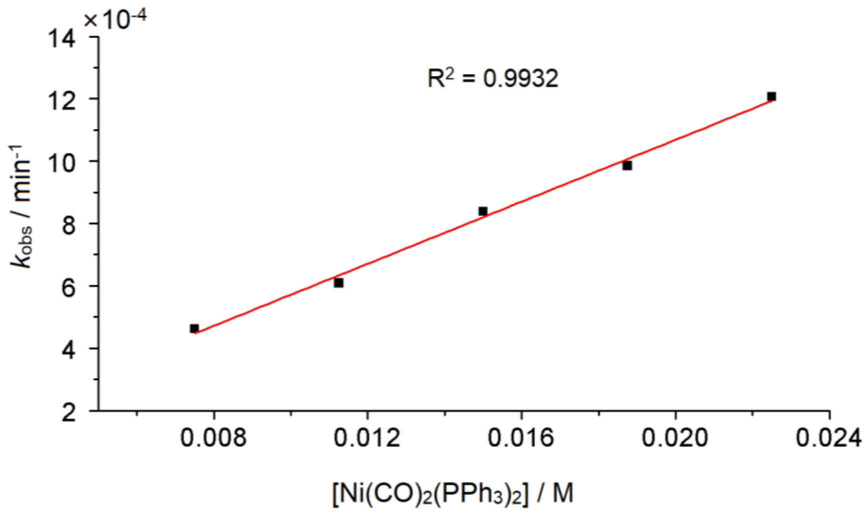
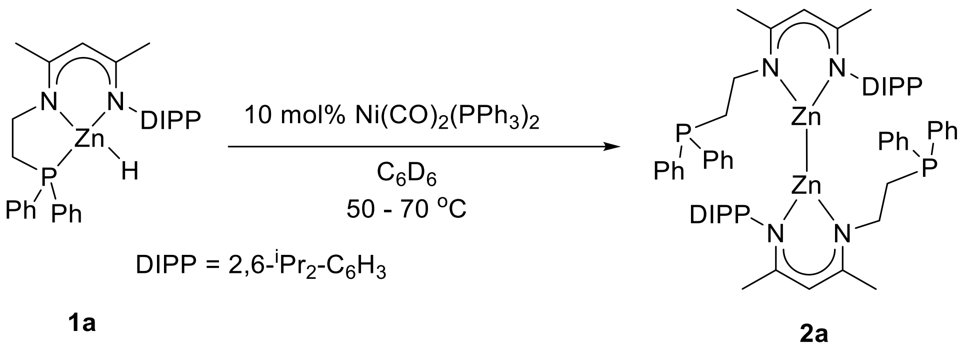


Figure S44. Plot showing first order relationship for the dehydrocoupling of **1a** at different catalyst loadings (5 mol%, 7.5 mol%, 10 mol%, 12.5 mol%, 15 mol%). Conditions: 0.3 mmol **1a**, 2.0 mL C_6D_6, 60 °C.

Eyring analysis



Scheme S13.

The dehydrocoupling of **1a** (0.30 mmol) with 10 mol% catalyst loading [$Ni(CO)_2(PPh_3)_2$, 0.03 mmol] in C_6D_6 (2.0 mL) at various reaction temperatures (50 - 70 °C) was carried out and monitored by ^{1}H NMR spectroscopy.

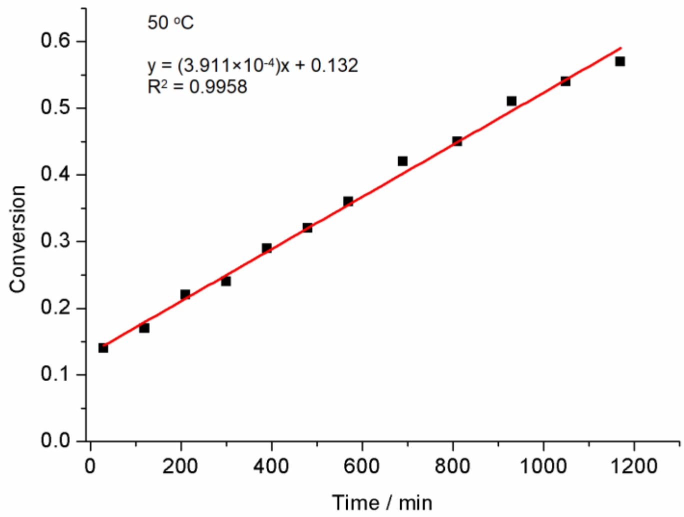


Figure S45. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$ at 50 °C.

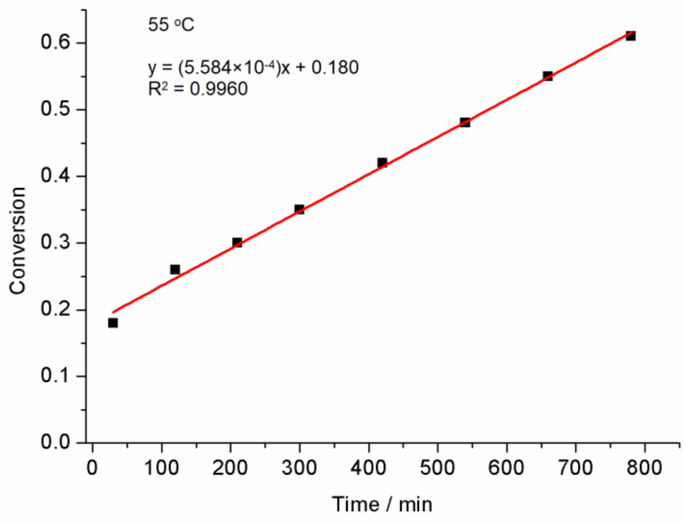


Figure S46. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$ at 55 °C.

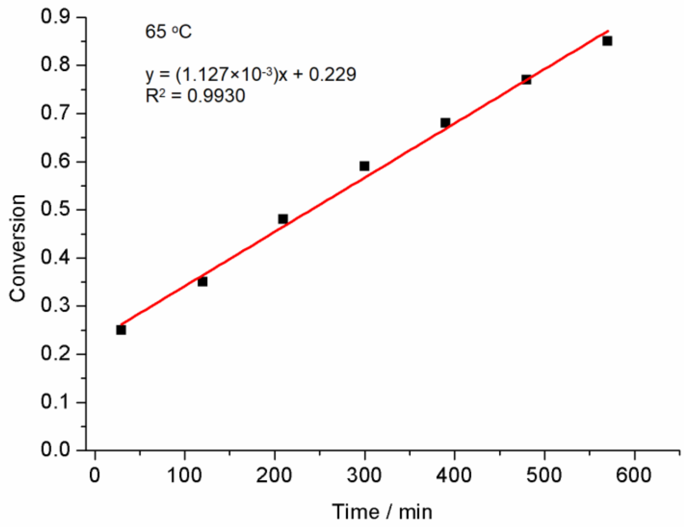


Figure S47. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$ at 65 °C.

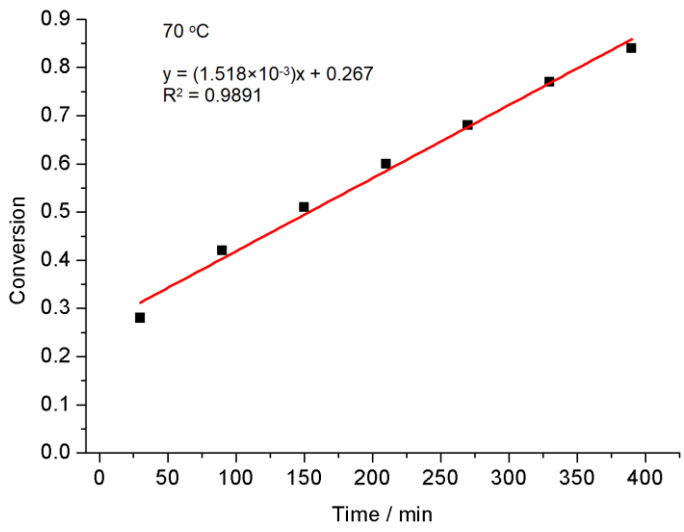


Figure S48. Plot of **1a** conversion versus time (min) for the dehydrocoupling reaction catalyzed by $Ni(CO)_2(PPh_3)_2$ at 70 °C.

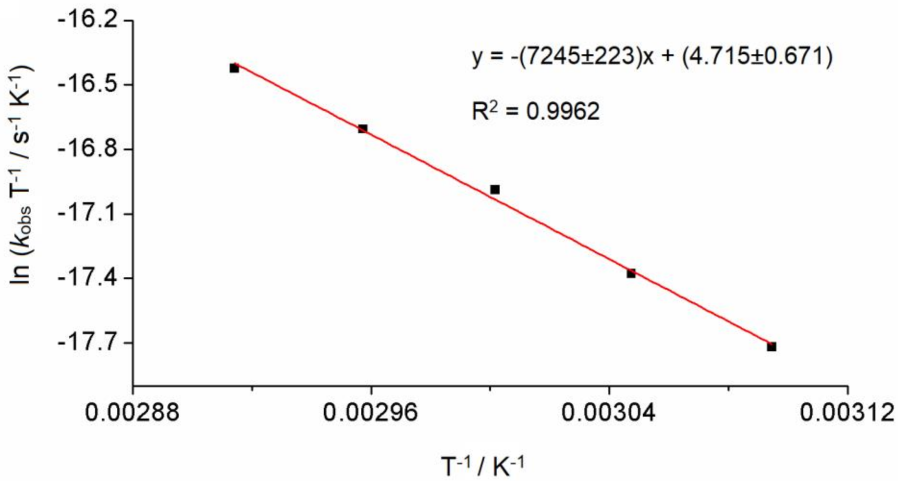
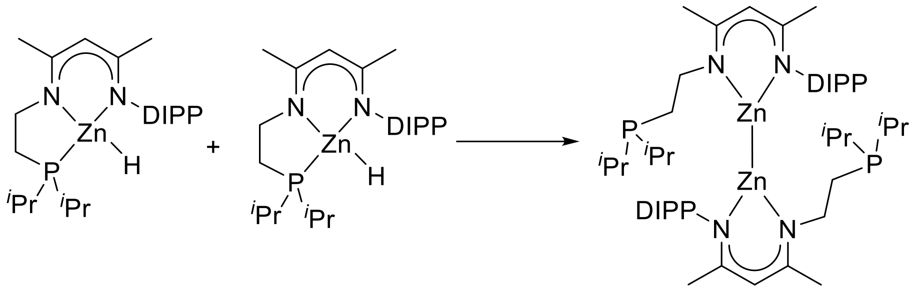


Figure S49. Eyring equation plot for the dehydrocoupling of **1a** at various reaction temperatures (50 ºC, 55 ºC, 60 ºC, 65 ºC, 70 ºC) catalyzed by $Ni(CO)_2(PPh_3)_2$. Conditions: 0.3 mmol **1a**, 2.0 mL of C_6D_6, 10 mol% catalyst loading.

Computational Details

All DFT calculations were performed with Gaussian 09.[3] Geometries were fully optimized in gas phase without symmetry constraints, employing the B3PW91 functional[4] and the Stuttgart effective core potential for Zn.[5] For the other elements (Si, P, N, C and H), Pople's double-ζ basis set 6-31G(d,p) [6] was used. Calculations of vibrational frequencies were systematically done in order to characterize the nature of stationary points. Analytical frequency calculations at 298.15 K and 1 atm were systematically done in order to characterize the nature of stationary points. IRC calculations were carried out in order to confirm the connectivity between reactant(s), transition state and product(s). Dispersion corrections were treated with the D3 version of Grimme's dispersion with Becke-Johnson damping. [7]



1c **1c** **2c**

DIPP = 2,6-^{i}Pr$_2$-C$_6$H$_3$

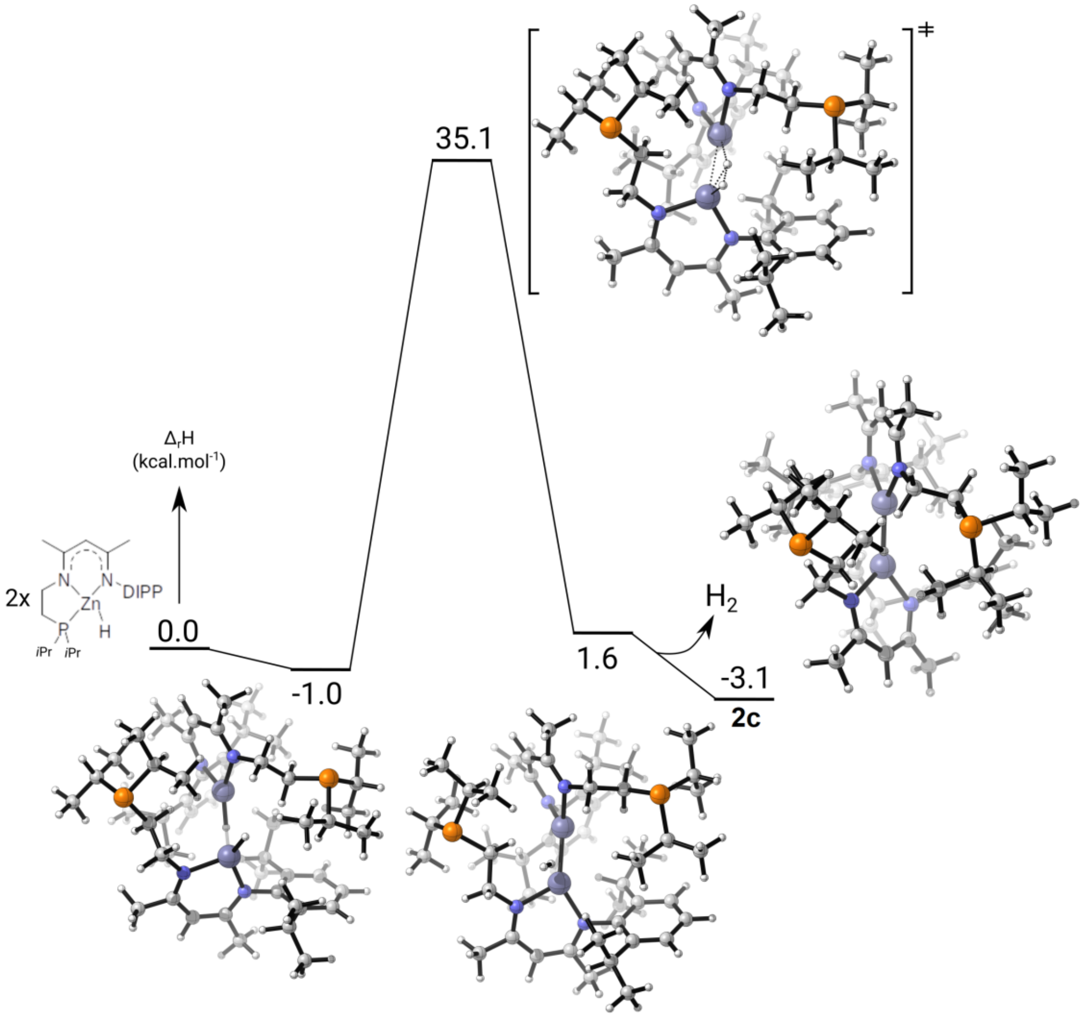
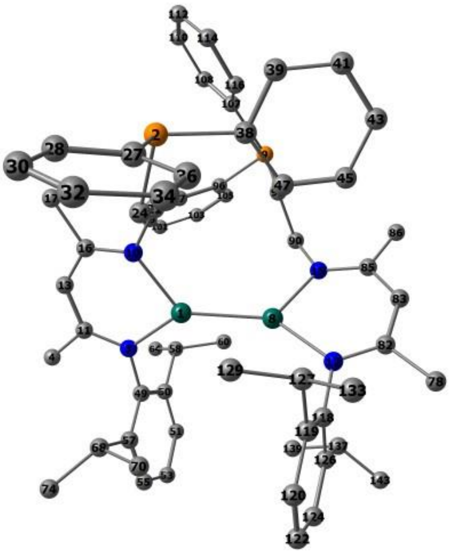


Figure S50. Computed Enthalpy energy profile (kcal.mol^{-1}) of the non-catalyzed formation of **2c** from **1c**.

NBO Information 2a

<table>
<tr><th rowspan="2">Complexes</th><th rowspan="2" colspan="2">Natural Charges</th><th colspan="4">NBO</th><th rowspan="2" colspan="2">WBI</th></tr>
<tr><th>Bond</th><th>Occupancy</th><th>Center (contribution)</th><th>Hybridation (contribution%)</th></tr>
<tr><td rowspan="5">2a_Zn2</td><td rowspan="5">Zn$_1$
Zn$_8$</td><td rowspan="5">0.63
0.63</td><td>Zn$_1$-Zn$_8$</td><td>1.97</td><td>Zn$_1$ (50%) ; Zn$_8$ (50%)</td><td>Zn$_1$ (s78 p21 d1) ; Zn$_8$ (s78 p21 d1)</td><td rowspan="2">Zn$_1$-Zn$_8$</td><td rowspan="2">0.91</td></tr>
<tr><th colspan="4">Second Order</th></tr>
<tr><th>Donor</th><th colspan="2">Acceptor</th><th>Total Energy (kcal.mol^{-1})</th><td rowspan="3">Zn$_1$
Zn$_8$</td><td rowspan="3">1.67
1.66</td></tr>
<tr><td>x</td><td colspan="2">x</td><td>x</td></tr>
</table>

Orbitals and bond length



Atomic labels

LUMO (264) HOMO (263) HOMO-2 (261)

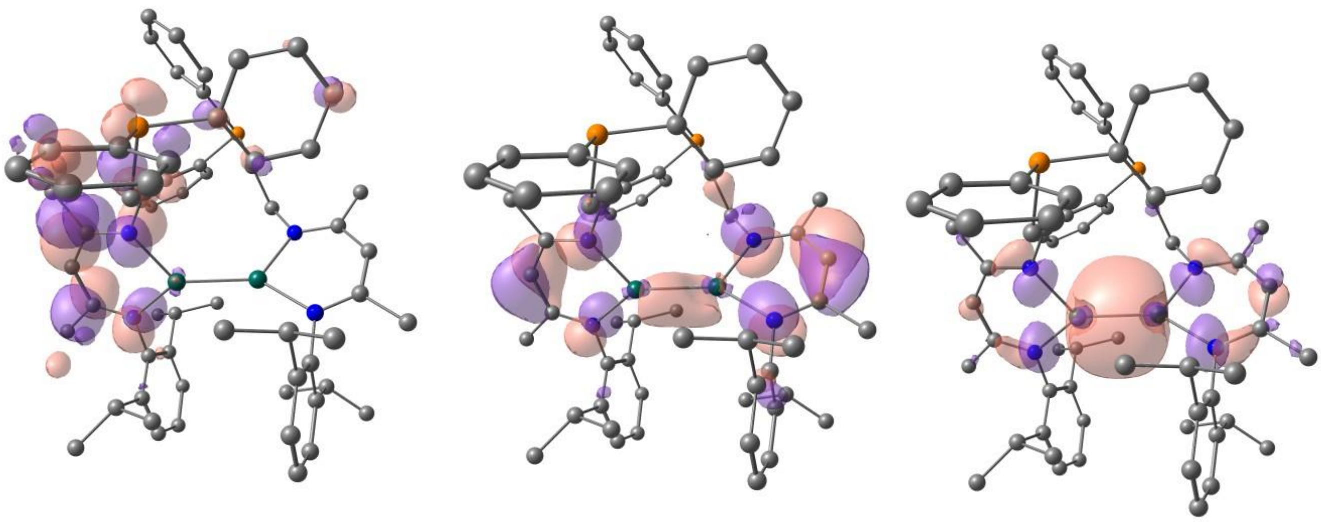


Figure S51. Metal-metal bonding interactions in complex **2a**.

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1c complex

Zn	5.23913	12.42859	4.33900
P	7.15151	11.84587	2.75386
N	4.68551	11.14923	5.75784
N	4.33099	11.42092	2.82419
C	5.09441	11.46668	7.08062
H	5.43324	13.97189	4.49255
C	6.39175	11.10033	7.49655
C	3.83770	10.14685	5.54543
C	7.43622	10.10303	2.14755
C	3.58641	10.34505	3.02096
C	4.24420	12.20749	7.92525
C	8.68449	12.88502	2.55942
C	6.02289	12.57536	1.47387
H	5.88186	13.61707	1.78353
H	6.45899	12.58299	0.46980
C	3.33305	9.78124	4.28666
H	2.66906	8.92514	4.28889
C	5.95633	12.14311	9.64406
H	6.29001	12.40009	10.64547
C	7.30765	10.34763	6.54896
H	7.11652	10.74866	5.54480
C	3.34259	9.33777	6.72274
H	2.97046	8.36483	6.39692
H	2.52056	9.86354	7.22015
H	4.12602	9.19398	7.46956
C	4.69631	12.53149	9.20673
H	4.05336	13.10542	9.86805
C	6.79819	11.43992	8.78824
H	7.78918	11.15965	9.13052
C	4.67627	11.83673	1.47408
H	3.90342	12.49763	1.05404
H	4.74953	10.97468	0.79981
C	2.89945	12.71715	7.44271
H	2.64276	12.17644	6.52722
C	8.79101	10.55206	6.85473
H	9.04061	11.61300	6.94787
H	9.40343	10.12828	6.05234
H	9.08845	10.04995	7.78194
C	2.96825	9.63070	1.83888
H	2.43554	10.32735	1.18392
H	2.26783	8.86324	2.17031
H	3.73772	9.13860	1.23191

C	6.97322	8.85112	6.50965
H	7.03953	8.41444	7.51230
H	7.67509	8.31352	5.86224
H	5.96692	8.67673	6.12402
C	1.77691	12.48216	8.45696
H	1.72233	11.43307	8.76510
H	0.81058	12.76299	8.02552
H	1.91600	13.08482	9.36080
C	3.00725	14.20261	7.07452
H	3.27521	14.79898	7.95403
H	2.05213	14.57568	6.68803
H	3.77462	14.35910	6.31100
C	7.59793	9.90188	0.64112
H	6.49996	9.61886	2.45906
C	8.57822	9.44440	2.92227
H	8.25408	13.89673	2.57690
C	9.47558	12.72119	1.26360
C	9.57510	12.75000	3.79718
H	10.39426	13.47662	3.75851
H	10.02098	11.75348	3.86665
H	9.00401	12.92665	4.71234
H	9.98260	11.75210	1.22857
H	10.24965	13.49429	1.19327
H	8.84151	12.80445	0.37636
H	7.60894	8.83024	0.40952
H	8.53507	10.32640	0.27452
H	6.78110	10.35145	0.07091
H	8.60177	8.36746	2.72346
H	8.46845	9.58480	4.00022
H	9.54797	9.85420	2.62302

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H-H coupling adduct

C	-1.34979	2.64232	-3.33246
C	-0.13239	2.09980	-2.85810
C	0.84971	2.92351	-2.27704
C	0.59512	4.29333	-2.16813
C	-0.59556	4.84158	-2.62733
C	-1.55382	4.01757	-3.21083
N	0.02804	0.68940	-2.84045
C	0.15898	-0.01176	-3.96628
C	-0.06471	-1.39240	-4.04070
C	-0.64549	-2.24004	-3.06826
C	-1.07722	-3.60263	-3.55796
C	2.18055	2.36435	-1.82010

C	3.30303	2.81997	-2.76023
C	-2.45370	1.75083	-3.87932
C	-3.23146	2.39624	-5.02791
Zn	-0.16764	-0.21078	-1.10983
N	-0.83175	-1.90029	-1.80085
C	-1.59847	-2.74125	-0.88451
C	-2.55523	-1.87640	-0.06911
P	-3.83287	-2.86388	0.86854
C	-5.13628	-1.53470	1.11262
C	-5.86467	-1.27943	-0.20878
Zn	0.82211	-0.51439	1.70395
N	2.80404	-0.34033	1.59080
C	3.47742	-1.35705	0.80424
C	3.38105	-1.07122	-0.69474
P	4.13000	-2.44881	-1.70456
C	2.56203	-3.29870	-2.26639
C	2.87003	-4.33560	-3.34426
N	0.54966	1.02841	2.92221
C	1.55563	1.79427	3.34680
C	2.89471	1.63655	2.96621
C	3.48341	0.63617	2.16473
C	4.98680	0.71933	2.00265
C	-0.76466	1.27419	3.40748
C	-1.20059	0.62871	4.58332
C	-2.50975	0.84489	5.01915
C	-3.36336	1.70329	4.33382
C	-2.91791	2.33982	3.18173
C	-1.62639	2.13006	2.69233
C	-0.27326	-0.28787	5.35855
C	-0.56962	-1.75492	5.03199
C	-1.18193	2.81576	1.41564
C	-2.09180	2.44854	0.24518
C	1.25792	2.89121	4.34046
C	-1.09496	4.33814	1.56064
C	-0.32458	-0.03709	6.86779
C	-3.04196	-2.95930	2.56313
C	-1.94704	-4.02675	2.54211
C	-4.08972	-3.27994	3.62789
C	0.55036	0.71056	-5.23109
C	2.50388	2.71714	-0.36929
C	-3.40184	1.31394	-2.75654
C	-4.63573	-0.23630	1.73499
C	4.65283	-1.51941	-3.24991
C	5.85092	-0.62761	-2.91572

C	3.54896	-0.73674	-3.95395
C	1.86628	-3.93742	-1.06417
H	0.98564	2.45486	5.30770
H	0.40567	3.49693	4.02473
H	2.12465	3.53736	4.48535
H	3.58085	2.36544	3.37966
H	5.28249	0.67368	0.94974
H	5.48512	-0.11037	2.51591
H	5.36802	1.65053	2.42317
H	-3.58656	3.00584	2.64283
H	-4.37473	1.86950	4.69359
H	-2.86103	0.34530	5.91743
H	-0.18145	2.44653	1.17866
H	-2.07124	4.77007	1.80753
H	-0.75727	4.78239	0.61848
H	-0.39199	4.63111	2.34552
H	-2.15361	1.36178	0.13467
H	-1.70660	2.86904	-0.68684
H	-3.11174	2.82211	0.38882
H	0.74731	-0.08187	5.02223
H	-0.16288	1.01914	7.10557
H	0.44810	-0.62415	7.37482
H	-1.28855	-0.33092	7.29679
H	-1.59741	-2.01262	5.31125
H	0.10907	-2.42039	5.57708
H	-0.44948	-1.94601	3.96237
H	2.99600	-2.31673	1.02125
H	4.53078	-1.47715	1.07830
H	3.89840	-0.13231	-0.91783
H	2.33008	-0.91685	-0.97689
H	5.01069	-2.30949	-3.92410
H	3.10944	0.01313	-3.29035
H	2.73665	-1.38293	-4.29431
H	3.94654	-0.20761	-4.82854
H	6.25482	-0.16810	-3.82469
H	6.65328	-1.19399	-2.43283
H	5.56619	0.18869	-2.24227
H	1.89292	-2.53850	-2.68650
H	0.99647	-4.51700	-1.39292
H	1.50414	-3.19076	-0.35144
H	2.53634	-4.62223	-0.53216
H	3.58141	-5.08537	-2.98007
H	3.29366	-3.88022	-4.24485
H	1.95482	-4.86127	-3.64039

H	-0.28869	1.28568	-5.63469
H	0.87997	0.00469	-5.99501
H	1.35575	1.42082	-5.02682
H	0.11278	-1.84456	-5.00886
H	-0.68277	-3.79109	-4.55694
H	-2.16959	-3.66874	-3.61177
H	-0.73266	-4.39861	-2.89284
H	-2.48555	4.45102	-3.56040
H	-0.77880	5.90791	-2.53291
H	1.34720	4.93775	-1.72174
H	-1.99991	0.83723	-4.27148
H	-2.86193	0.76322	-1.98265
H	-4.18937	0.66180	-3.14952
H	-3.87491	2.17983	-2.28274
H	-3.84418	3.23711	-4.68643
H	-3.91069	1.66554	-5.47822
H	-2.56038	2.76724	-5.80915
H	2.11404	1.27435	-1.88756
H	2.55822	3.79993	-0.21624
H	3.47118	2.29617	-0.08146
H	1.75693	2.31221	0.31504
H	3.09335	2.54482	-3.79820
H	4.25619	2.36171	-2.47553
H	3.42784	3.90756	-2.72197
H	-0.90723	-3.26034	-0.21151
H	-2.17320	-3.50153	-1.41936
H	-3.10609	-1.23224	-0.76422
H	-1.98945	-1.23254	0.61705
H	-2.58216	-1.98926	2.79069
H	-4.64295	-4.19328	3.37864
H	-4.81339	-2.47003	3.75613
H	-3.60346	-3.44341	4.59636
H	-1.53278	-4.16654	3.54678
H	-1.11716	-3.73732	1.89202
H	-2.34265	-4.99068	2.20297
H	-5.85521	-2.00359	1.79790
H	-3.91949	0.27091	1.08274
H	-4.14250	-0.39011	2.69692
H	-5.46633	0.46031	1.90174
H	-6.71667	-0.60799	-0.05256
H	-6.23712	-2.20801	-0.65251
H	-5.20785	-0.79626	-0.94109
H	0.22547	0.52034	0.20013
H	0.13931	-1.91278	1.57998

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H-H coupling TS

C	0.53211	10.07114	22.71689
C	1.72392	9.63114	23.33914
C	2.55006	10.53956	24.03717
C	2.17279	11.88345	24.08312
C	1.01311	12.33188	23.45980
C	0.20375	11.42737	22.78489
N	2.02976	8.24646	23.34701
C	2.24231	7.61373	22.18492
C	2.06730	6.24080	21.98762
C	1.36722	5.33476	22.82249
C	0.92636	4.03861	22.18137
C	3.82515	10.06589	24.70630
C	4.91971	9.76002	23.68016
C	-0.44594	9.10602	22.06483
C	-0.98652	9.62216	20.72839
Zn	1.85966	7.19649	25.03350
N	1.08652	5.59966	24.08051
C	0.19233	4.77585	24.87790
C	-0.90780	5.66793	25.45349
P	-2.17655	4.77347	26.48592
C	-3.63811	5.93746	26.27889
C	-4.23506	5.76960	24.87998
Zn	3.18962	7.36448	27.19960
N	5.11164	7.68491	27.01824
C	5.91030	6.84654	26.13185
C	5.04001	6.11948	25.11816
P	5.90593	4.69674	24.28490
C	4.39965	3.79467	23.63478
C	4.81729	2.73569	22.61468
N	2.78660	8.60672	28.65309
C	3.73131	9.36942	29.18853
C	5.07371	9.36189	28.77569
C	5.71736	8.55950	27.81234
C	7.21232	8.74384	27.68952
C	1.48044	8.51965	29.19910
C	1.24708	7.73677	30.34841
C	-0.06982	7.59135	30.79296
C	-1.12532	8.21453	30.13658
C	-0.87614	8.99055	29.00842
C	0.42004	9.14525	28.51279
C	2.38093	7.06109	31.09795
C	2.35712	5.54194	30.90492

C	0.69636	10.01120	27.29971
C	-0.35501	9.85349	26.20801
C	3.38479	10.28173	30.33995
C	0.85612	11.48278	27.69399
C	2.36749	7.42305	32.58702
C	-1.56701	5.23415	28.19321
C	-0.27895	4.47529	28.50255
C	-2.63452	4.94922	29.24698
C	2.65499	8.41757	20.97218
C	4.34803	11.02443	25.77046
C	-1.59354	8.78122	23.02738
C	-3.36494	7.40615	26.59376
C	6.60161	5.48378	22.72648
C	7.70248	6.47735	23.10473
C	5.58935	6.12882	21.78599
C	3.64083	3.14880	24.79563
H	3.62721	9.79529	31.29061
H	2.32123	10.52490	30.35620
H	3.96709	11.20426	30.28313
H	5.71731	10.05786	29.30059
H	7.48153	9.10747	26.69108
H	7.74019	7.79630	27.83835
H	7.57978	9.46134	28.42337
H	-1.70132	9.48393	28.50464
H	-2.14108	8.09490	30.50222
H	-0.26910	6.98318	31.67107
H	1.65160	9.68081	26.87650
H	-0.05965	11.86141	28.16183
H	1.06486	12.08923	26.80663
H	1.67713	11.61849	28.40358
H	-0.46072	8.79953	25.93170
H	-0.06279	10.41303	25.31759
H	-1.34052	10.21548	26.51940
H	3.32303	7.41805	30.67321
H	2.34397	8.50644	32.73907
H	3.25762	7.02436	33.08468
H	1.49276	7.00074	33.09313
H	1.43708	5.10861	31.31327
H	3.20370	5.07772	31.42278
H	2.42118	5.28730	29.84294
H	6.46055	6.09643	26.72043
H	6.66440	7.44377	25.60739
H	4.60097	6.81856	24.39578
H	4.21622	5.64660	25.66636

H	7.07971	4.64144	22.20819
H	5.04406	6.93454	22.28487
H	4.84589	5.41719	21.42084
H	6.09717	6.56418	20.91664
H	8.26883	6.78243	22.21767
H	8.40597	6.05309	23.82839
H	7.27276	7.38574	23.53977
H	3.74479	4.52772	23.14923
H	2.78291	2.58078	24.41789
H	3.25366	3.88319	25.50735
H	4.28226	2.45283	25.34739
H	5.51846	2.01913	23.05787
H	5.29677	3.17021	21.73249
H	3.94204	2.17260	22.27023
H	1.78725	8.66920	20.35452
H	3.33804	7.82848	20.35508
H	3.14032	9.35318	21.25514
H	2.33260	5.87124	21.00396
H	1.39568	3.91460	21.20449
H	-0.15938	4.02609	22.03490
H	1.18519	3.17608	22.80146
H	-0.71322	11.77574	22.31908
H	0.73866	13.38163	23.50861
H	2.79642	12.59333	24.61479
H	0.06806	8.16334	21.86607
H	-1.20996	8.32308	23.94097
H	-2.30100	8.08339	22.56569
H	-2.14082	9.68686	23.30981
H	-1.64080	10.49034	20.86016
H	-1.57762	8.84401	20.23483
H	-0.17753	9.91777	20.05300
H	3.59238	9.11838	25.21278
H	4.69715	11.96688	25.33338
H	5.19012	10.57153	26.29549
H	3.58464	11.25139	26.51937
H	4.59261	9.00491	22.96316
H	5.81515	9.38175	24.18514
H	5.19778	10.66275	23.12476
H	0.76372	4.31102	25.69146
H	-0.26255	3.96191	24.30545
H	-1.42465	6.14465	24.61444
H	-0.45228	6.47306	26.04812
H	-1.33649	6.30599	28.20433
H	-2.93479	3.89510	29.23352

H	-3.53283	5.55753	29.10247
H	-2.24232	5.17303	30.24530
H	0.03918	4.69064	29.52604
H	0.54601	4.77647	27.85073
H	-0.41740	3.39206	28.40796
H	-4.37400	5.55469	26.99863
H	-2.64063	7.83320	25.89378
H	-2.96957	7.54640	27.60288
H	-4.28589	7.99563	26.50773
H	-5.16134	6.34758	24.78536
H	-4.46138	4.72154	24.66106
H	-3.54944	6.13417	24.10632
H	2.17074	6.26108	26.64540
H	2.72180	5.66539	27.59375

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H-H coupling product

C	-1.44007	2.48857	-3.08415
C	-0.21568	2.00557	-2.56204
C	0.70811	2.89319	-1.97365
C	0.38988	4.25192	-1.90860
C	-0.81161	4.73658	-2.41000
C	-1.71324	3.85485	-2.99664
N	0.02643	0.60881	-2.54561
C	0.17631	-0.05705	-3.69250
C	-0.04286	-1.43353	-3.83238
C	-0.71019	-2.28850	-2.92184
C	-1.27006	-3.56938	-3.49875
C	2.05961	2.41449	-1.48776
C	3.14710	2.76030	-2.51159
C	-2.48558	1.55080	-3.66580
C	-3.14233	2.10218	-4.93354
Zn	-0.08522	-0.36871	-0.78646
N	-0.87171	-1.99442	-1.64676
C	-1.77254	-2.73764	-0.78165
C	-2.98910	-1.86466	-0.46317
P	-4.16140	-2.62975	0.76832
C	-5.76757	-1.77762	0.29007
C	-6.27281	-2.34887	-1.03677
Zn	1.04059	0.13527	1.19878
N	3.03274	-0.11664	1.43333
C	3.71983	-1.16065	0.67913
C	3.01656	-1.50111	-0.62925
P	4.02470	-2.66567	-1.67922
C	2.65216	-3.52943	-2.61062

C	3.23100	-4.30016	-3.79655
N	0.82042	1.23688	2.83669
C	1.83996	1.89470	3.39080
C	3.18098	1.66753	3.06414
C	3.73718	0.66508	2.24022
C	5.24331	0.52806	2.31318
C	-0.45737	1.26834	3.44866
C	-0.64448	0.61761	4.68999
C	-1.92134	0.62351	5.25561
C	-2.99331	1.22865	4.60701
C	-2.79924	1.83767	3.37226
C	-1.53741	1.87368	2.77332
C	0.49350	-0.14154	5.35500
C	0.55959	-1.58029	4.82999
C	-1.31988	2.58908	1.45503
C	-2.54259	2.57028	0.54431
C	1.56857	2.93146	4.45846
C	-0.82551	4.02223	1.67357
C	0.42661	-0.12025	6.88237
C	-3.66744	-1.66007	2.28843
C	-2.23280	-1.99487	2.68468
C	-4.63375	-1.93490	3.43832
C	0.54818	0.70436	-4.94358
C	2.42380	2.95943	-0.10779
C	-3.53671	1.20376	-2.60814
C	-5.73064	-0.25121	0.25903
C	4.68198	-1.46198	-2.96802
C	5.61664	-0.46416	-2.28003
C	3.63017	-0.73596	-3.80271
C	1.90763	-4.47306	-1.66574
H	1.53708	2.47796	5.45451
H	0.60719	3.42340	4.29892
H	2.36141	3.68258	4.46068
H	3.89623	2.29077	3.58797
H	5.70997	0.73870	1.34403
H	5.53595	-0.48749	2.59834
H	5.65922	1.22030	3.04576
H	-3.64077	2.30268	2.86863
H	-3.97983	1.22051	5.06147
H	-2.08511	0.13495	6.21097
H	-0.52812	2.05046	0.92047
H	-1.55742	4.60114	2.24821
H	-0.66948	4.51651	0.70982
H	0.12300	4.03684	2.21668

H	-2.93713	1.55519	0.43658
H	-2.26961	2.93998	-0.44700
H	-3.35156	3.20615	0.92150
H	1.43671	0.32849	5.06734
H	0.32779	0.90034	7.26607
H	1.33707	-0.55780	7.30387
H	-0.41714	-0.70530	7.26376
H	-0.33723	-2.14233	5.10975
H	1.43134	-2.10012	5.24224
H	0.64109	-1.59476	3.74026
H	3.79663	-2.07469	1.28684
H	4.74881	-0.86800	0.44790
H	2.80012	-0.58135	-1.18352
H	2.05142	-1.97592	-0.43241
H	5.29206	-2.08633	-3.63424
H	2.95732	-0.14390	-3.17574
H	3.00956	-1.42294	-4.38276
H	4.11174	-0.04473	-4.50468
H	6.12390	0.16458	-3.02049
H	6.38144	-0.96922	-1.68100
H	5.05568	0.20570	-1.61861
H	1.94705	-2.77405	-2.97875
H	1.14910	-5.03906	-2.21790
H	1.39301	-3.93427	-0.86604
H	2.59162	-5.19531	-1.20591
H	3.96855	-5.03955	-3.46325
H	3.72208	-3.64291	-4.52060
H	2.43628	-4.83878	-4.32587
H	-0.34260	1.09490	-5.44607
H	1.06638	0.04825	-5.64606
H	1.18810	1.55760	-4.70944
H	0.14694	-1.84305	-4.81787
H	-0.88999	-3.73197	-4.50822
H	-2.36323	-3.52223	-3.55696
H	-1.01038	-4.43806	-2.88785
H	-2.65451	4.23428	-3.38298
H	-1.04398	5.79570	-2.34750
H	1.10224	4.94155	-1.46518
H	-1.99907	0.61076	-3.93573
H	-3.06341	0.73904	-1.74109
H	-4.27724	0.50340	-3.01082
H	-4.06419	2.10035	-2.26540
H	-3.77224	2.97310	-4.72451
H	-3.78508	1.34030	-5.38637

H	-2.39475	2.40337	-5.67427
H	2.00500	1.32356	-1.41093
H	2.56312	4.04559	-0.12235
H	3.35474	2.51196	0.24777
H	1.64836	2.73706	0.63044
H	2.92520	2.33003	-3.49195
H	4.12140	2.37820	-2.18952
H	3.23109	3.84582	-2.63377
H	-1.23852	-2.98142	0.14426
H	-2.10443	-3.68603	-1.21452
H	-3.52480	-1.66464	-1.39675
H	-2.64370	-0.89200	-0.08434
H	-3.69665	-0.59007	2.04767
H	-4.65457	-3.00171	3.68819
H	-5.65722	-1.62573	3.20235
H	-4.31717	-1.38413	4.33034
H	-1.98069	-1.46731	3.60652
H	-1.51433	-1.66699	1.92711
H	-2.09647	-3.06985	2.85080
H	-6.47009	-2.09471	1.07277
H	-5.00974	0.11436	-0.47838
H	-5.46235	0.17647	1.22876
H	-6.71251	0.15105	-0.01834
H	-7.27626	-1.97073	-1.26245
H	-6.31624	-3.44222	-1.01416
H	-5.62403	-2.05626	-1.87055
H	0.96919	-2.78269	1.52286
H	1.27043	-3.41588	1.77884

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2c complex

Zn	2.57115	5.91136	25.67926
P	6.23842	3.86435	28.71796
N	1.64578	5.57957	23.94962
C	0.89858	4.22625	22.04071
H	1.25436	3.36310	21.47541
H	0.92373	5.11287	21.40402
H	-0.15320	4.05492	22.29617
Zn	3.10175	7.77364	26.98227
P	7.42826	7.67777	24.18899
N	3.13839	4.01167	25.94041
C	1.70708	4.41346	23.30385
N	2.12127	8.94859	28.24875
C	2.44713	3.30687	23.74108
H	2.45069	2.45702	23.06912

N	4.88691	8.61445	27.30382
C	3.09068	3.10309	24.97893
C	3.71536	1.73931	25.18281
H	3.16670	1.16318	25.93603
H	4.75137	1.81829	25.52579
H	3.70574	1.16920	24.25309
C	0.77250	6.58710	23.45425
C	-0.59868	6.53308	23.77863
C	-1.44911	7.50298	23.24575
H	-2.50880	7.47117	23.47910
C	-0.95944	8.50788	22.41704
H	-1.63623	9.24712	21.99798
C	0.40270	8.58087	22.15225
H	0.78289	9.38746	21.53317
C	1.29178	7.63996	22.67866
C	-1.10828	5.48799	24.75089
H	-0.45204	4.61482	24.67952
C	-2.53391	5.01861	24.46144
H	-3.26760	5.81282	24.63633
H	-2.79683	4.18749	25.12355
H	-2.64536	4.67920	23.42642
C	-0.99284	6.03745	26.17705
H	0.02565	6.37433	26.39917
H	-1.26966	5.28077	26.91818
H	-1.64407	6.90489	26.31352
C	2.77957	7.73960	22.40616
H	3.28480	7.19207	23.20969
C	3.15207	7.06293	21.08223
H	2.91960	5.99537	21.10166
H	4.22287	7.16713	20.87636
H	2.60286	7.51597	20.24939
C	3.28238	9.18276	22.44134
H	2.87864	9.77981	21.61692
H	4.37078	9.20641	22.34733
H	3.01035	9.67192	23.38043
C	3.79398	3.71440	27.20690
H	3.80362	2.64293	27.43451
H	3.20579	4.19302	27.99487
C	5.21255	4.27733	27.22078
H	5.14835	5.36116	27.07894
H	5.75437	3.87783	26.35733
C	5.32104	4.74780	30.10426
H	6.10625	4.92514	30.85150
C	4.70567	6.09407	29.73555

H	3.90008	5.98066	29.00282
H	5.43224	6.78751	29.30635
H	4.27367	6.57907	30.61848
C	4.29959	3.80367	30.74374
H	3.81775	4.28141	31.60518
H	4.77399	2.87923	31.08559
H	3.50912	3.52621	30.03999
C	7.65167	5.06896	28.44125
H	7.24130	6.08715	28.43366
C	8.32905	4.81626	27.09432
H	9.21128	5.45643	26.98631
H	7.67284	5.04471	26.25168
H	8.65772	3.77390	27.00607
C	8.66343	4.95087	29.58192
H	9.08354	3.94013	29.62594
H	8.22137	5.17076	30.55851
H	9.49180	5.65260	29.43080
C	1.87483	10.67013	29.97369
H	2.49514	11.31875	30.59366
H	1.29877	10.00166	30.61993
H	1.14503	11.28825	29.44068
C	2.71545	9.87632	29.00211
C	4.08200	10.18006	28.95161
H	4.40578	10.96798	29.62074
C	5.09408	9.60461	28.15872
C	6.48752	10.16375	28.35566
H	6.46209	11.04753	28.99408
H	6.94907	10.44244	27.40352
H	7.14328	9.42508	28.83057
C	0.70931	8.79058	28.34562
C	-0.13049	9.63203	27.58563
C	-1.51217	9.47074	27.69282
H	-2.17088	10.11421	27.11823
C	-2.06063	8.49757	28.52372
H	-3.13898	8.38970	28.59890
C	-1.22227	7.65468	29.24073
H	-1.64977	6.88235	29.87467
C	0.16749	7.78203	29.16252
C	0.46976	10.64410	26.63021
H	1.43971	10.95161	27.03483
C	0.72582	9.97239	25.27751
H	1.38457	9.10329	25.37718
H	1.18649	10.67241	24.57252
H	-0.20788	9.61160	24.83769

C	-0.37765	11.90473	26.45764
H	-1.31514	11.69680	25.93082
H	0.16801	12.64307	25.86148
H	-0.62621	12.36029	27.42176
C	1.05801	6.83536	29.93930
H	2.08985	7.15366	29.77313
C	0.91756	5.40480	29.41093
H	-0.11196	5.04465	29.51076
H	1.56830	4.72253	29.96636
H	1.18478	5.35273	28.35094
C	0.79325	6.89293	31.44618
H	0.90085	7.91176	31.83078
H	1.49967	6.25025	31.98270
H	-0.21784	6.54967	31.69015
C	5.99259	8.04833	26.55117
H	5.83130	6.96792	26.48890
H	6.95556	8.17410	27.05766
C	6.09093	8.59081	25.12728
H	6.31383	9.66303	25.15010
H	5.12021	8.47991	24.62987
C	6.36719	6.71220	22.98731
H	5.65106	7.40635	22.53316
C	7.22108	6.08673	21.88683
H	7.99605	5.44019	22.31403
H	7.71717	6.84070	21.26773
H	6.60022	5.47114	21.22580
C	5.58326	5.64359	23.74731
H	4.89807	5.10556	23.08343
H	4.97970	6.07317	24.55347
H	6.25850	4.90912	24.19917
C	8.12623	9.04370	23.10814
H	8.83201	8.52277	22.44724
C	7.11634	9.79758	22.24778
H	6.37460	10.31109	22.86869
H	6.58027	9.13203	21.56490
H	7.61820	10.55964	21.63949
C	8.93861	9.99989	23.98509
H	9.45121	10.74776	23.36983
H	9.69118	9.46511	24.57253
H	8.29347	10.54419	24.68437

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H2

H	-3.34787	2.03779	-1.26145
H	-3.43148	2.75279	-1.44740

2a_Zn2
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Zn	1.245614000	2.709692000	4.109369000
P	1.073005000	2.544011000	9.622250000
N	2.564444000	3.632732000	2.895636000
C	4.757530000	4.548971000	2.263750000
H	5.773095000	4.611865000	2.658070000
H	4.412337000	5.562190000	2.034677000
H	4.779700000	4.008605000	1.313261000
Zn	-0.912383000	1.691201000	3.965891000
P	1.809703000	-2.870017000	5.286340000
N	2.495991000	2.638528000	5.703707000
C	3.827939000	3.879241000	3.252367000
N	-2.872573000	2.168792000	3.866039000
C	4.378721000	3.569939000	4.506560000
H	5.425174000	3.826742000	4.621718000
N	-1.233496000	-0.311582000	4.059946000
C	3.770659000	3.010762000	5.648867000
C	4.682580000	2.822511000	6.846957000
H	5.663914000	3.260058000	6.658229000
H	4.827634000	1.758520000	7.067021000
H	4.275272000	3.282246000	7.752107000
C	1.960387000	2.104247000	6.952885000
H	2.706129000	1.508624000	7.494773000
H	1.149493000	1.415179000	6.694473000
C	1.395957000	3.189455000	7.877933000
H	0.505883000	3.654615000	7.442463000
H	2.130193000	3.991762000	8.013690000
C	0.336324000	4.083554000	10.374771000
C	1.238042000	5.039653000	10.863593000
H	2.308241000	4.852671000	10.798942000
C	0.780781000	6.222084000	11.440974000
H	1.494075000	6.954797000	11.809131000
C	-0.588888000	6.455957000	11.560138000
H	-0.948425000	7.372848000	12.019105000
C	-1.493891000	5.502691000	11.096423000
H	-2.562731000	5.674952000	11.193512000
C	-1.036270000	4.324901000	10.505140000
H	-1.750433000	3.587740000	10.149732000
C	-0.420790000	1.455129000	9.412012000
C	-0.703916000	0.573369000	10.466109000
H	-0.066730000	0.573971000	11.347900000
C	-1.787049000	-0.300584000	10.397061000
H	-1.993649000	-0.971936000	11.226275000

C	-2.594069000	-0.322094000	9.259721000
H	-3.431366000	-1.011997000	9.197975000
C	-2.319466000	0.540300000	8.199041000
H	-2.937435000	0.522350000	7.304821000
C	-1.244205000	1.427201000	8.278942000
H	-1.052339000	2.096352000	7.445227000
C	2.119028000	4.044061000	1.599507000
C	2.155266000	3.134093000	0.518219000
C	1.668607000	3.551094000	-0.725070000
H	1.694698000	2.858913000	-1.563126000
C	1.153665000	4.828078000	-0.910370000
H	0.780688000	5.132615000	-1.884638000
C	1.118997000	5.712538000	0.161352000
H	0.711196000	6.709633000	0.017223000
C	1.597434000	5.347160000	1.422717000
C	2.702743000	1.722207000	0.663842000
H	3.089990000	1.617254000	1.682009000
C	1.596826000	0.672859000	0.482755000
H	1.994330000	-0.335274000	0.642927000
H	1.172252000	0.712385000	-0.526882000
H	0.780216000	0.836026000	1.193059000
C	3.862681000	1.448177000	-0.304142000
H	4.270282000	0.446682000	-0.130895000
H	4.675723000	2.170675000	-0.179519000
H	3.536784000	1.496310000	-1.349116000
C	1.518805000	6.343620000	2.570248000
H	2.112109000	5.944502000	3.398839000
C	0.073315000	6.484906000	3.066931000
H	0.022291000	7.163029000	3.926339000
H	-0.342646000	5.519124000	3.369164000
H	-0.576674000	6.886006000	2.281956000
C	2.102653000	7.715728000	2.206907000
H	2.114875000	8.367103000	3.087665000
H	1.508740000	8.221638000	1.437866000
H	3.128620000	7.636422000	1.832567000
C	-5.286910000	1.714630000	4.022134000
H	-5.954735000	0.917728000	4.353650000
H	-5.565980000	1.994072000	3.001114000
H	-5.454134000	2.599450000	4.641575000
C	-3.841246000	1.269834000	4.074466000
C	-3.626889000	-0.095957000	4.313998000
H	-4.525983000	-0.677480000	4.480880000
C	-2.433409000	-0.847027000	4.239448000
C	-2.607577000	-2.351485000	4.333438000

H	-3.626533000	-2.603389000	4.631183000
H	-1.920278000	-2.808846000	5.050579000
H	-2.420346000	-2.823715000	3.361916000
C	-0.065764000	-1.185490000	3.963499000
H	0.668490000	-0.697333000	3.314681000
H	-0.315719000	-2.138373000	3.479845000
C	0.581399000	-1.441457000	5.329887000
H	-0.190107000	-1.724326000	6.054562000
H	1.054716000	-0.526218000	5.699429000
C	3.120589000	-2.198202000	4.140494000
C	3.754527000	-0.963550000	4.338107000
H	3.484461000	-0.346667000	5.190523000
C	4.737326000	-0.521365000	3.456045000
H	5.211877000	0.442432000	3.619700000
C	5.106605000	-1.314592000	2.366878000
H	5.881402000	-0.974559000	1.685017000
C	4.482870000	-2.542808000	2.158948000
H	4.767803000	-3.164098000	1.313967000
C	3.492928000	-2.980302000	3.041339000
H	3.008303000	-3.940518000	2.880945000
C	2.667234000	-2.644120000	6.925783000
C	3.937703000	-3.215740000	7.096185000
H	4.423715000	-3.707293000	6.256804000
C	4.592036000	-3.148446000	8.322764000
H	5.579129000	-3.590572000	8.430673000
C	3.985015000	-2.516400000	9.408786000
H	4.495341000	-2.462880000	10.366509000
C	2.719551000	-1.955771000	9.255515000
H	2.235421000	-1.458826000	10.091661000
C	2.063650000	-2.020275000	8.024949000
H	1.078890000	-1.572041000	7.936521000
C	-3.243714000	3.490121000	3.458135000
C	-3.368344000	4.525616000	4.411668000
C	-3.700220000	5.810479000	3.969029000
H	-3.803924000	6.611369000	4.697064000
C	-3.902262000	6.082904000	2.622011000
H	-4.160577000	7.087751000	2.298604000
C	-3.770043000	5.058738000	1.691637000
H	-3.921287000	5.273063000	0.636737000
C	-3.446358000	3.756670000	2.082619000
C	-3.155213000	4.289438000	5.898862000
H	-2.933387000	3.225444000	6.032266000
C	-1.954561000	5.090264000	6.420749000
H	-1.784374000	4.890399000	7.484341000

H	-2.117874000	6.168113000	6.311249000
H	-1.043197000	4.838118000	5.869803000
C	-4.409379000	4.611744000	6.724948000
H	-4.242123000	4.374289000	7.781209000
H	-5.279764000	4.040970000	6.386583000
H	-4.667381000	5.674718000	6.662214000
C	-3.297511000	2.676380000	1.020903000
H	-3.203284000	1.714514000	1.534084000
C	-2.015774000	2.889918000	0.203705000
H	-1.883804000	2.084285000	-0.527425000
H	-1.128907000	2.917401000	0.843602000
H	-2.049937000	3.838015000	-0.343862000
C	-4.518288000	2.585700000	0.094443000
H	-4.408585000	1.741457000	-0.595060000
H	-4.635677000	3.489157000	-0.513980000
H	-5.447420000	2.443042000	0.655799000

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