Reductive Elimination of Alkylamines from Low-Valent, Alkyl-Palladium(II) Amido Complexes

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Supporting Information

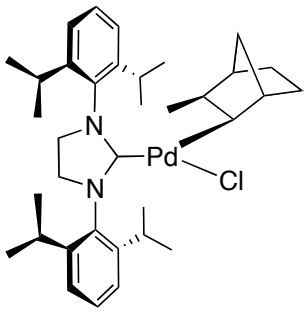
Table of Contents

General Experimental Details

Unless otherwise noted, all manipulations were carried out under an inert atmosphere in a nitrogen-filled glovebox or by standard Schlenk techniques. THF, benzene, toluene and pentane were degassed by purging with argon for 45 minutes and dried with a solvent purification system containing a 1 m column of activated alumina. Potassium anilide salts were prepared by addition 1.1 equiv of HMDS to 1 equiv of arylamine in toluene. The precipitated anilide was collected by filtration and washed with toluene and pentane. (COD)Pd(2-CH_3-norbornyl)Cl was prepared according to literature procedure.

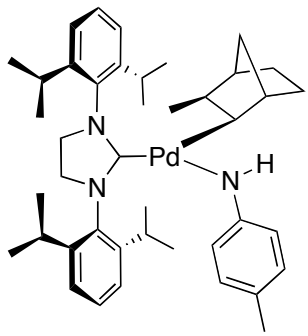
Analytical gas chromatography (GC) was performed using a Hewlett-Packard 5890 Gas Chromatograph fitted with a flame ionization detector and a Hewlett-Packard HP5 (30m x 0.32 mm) capillary column. NMR spectra were acquired on 500 MHz or 400 MHz Varian Unity or 500 MHz Innova instruments at the University of Illinois VOICE NMR facility. Chemical shifts are reported in ppm relative to residual chloroform (7.26 ppm for ^{1}H; 77.0 ppm for ^{13}C), toluene (2.09 ppm for ^{1}H; 20.4 ppm for ^{13}C), benzene (7.15 ppm for ^{1}H; 128.0 ppm for ^{13}C), or THF (3.58 ppm for ^{1}H) or to an external standard (85% H_3PO_4 = 0 ppm for ^{31}P or $CFCl_3$ = 0 ppm for ^{19}F). Coupling constants are reported in Hertz. Elemental analyses were performed by Roberston-Microlit Laboratories, Inc. (Ledgewood, NJ).

Preparation of (SiPr)Pd(2-CH$_3$-norbornyl)Cl (1)



(COD)Pd(2-CH$_3$-norbornyl)Cl (0.150 g, 0.418 mmol) and SiPr (0.177g, 0.459 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of THF. The reaction was stirred at room temperature for 2 h. After 2 h, 15 mL of pentane was added to precipitate an orange solid. The orange solid was collected by filtration and washed with (5 × 3 mL) pentane and dried by vacuum. Collected 0.245 g; 92 %. ^{1}H NMR ($CDCl_3$, 500 MHz): δ 7.42 (t, *J* = 7.5 Hz, 2H), 7.28 (d, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 7.5 Hz, 2H), 4.07-4.00 (m, 4H), 3.23 (hept, *J* = 7.0 Hz, 2H), 3.16 (hept, *J* = 7.0 Hz, 2H), 3.10 (d, *J* = 7.5 Hz, 1H), 2.07 (d, *J* = 10.0 Hz, 1H), 1.99 (d, *J* = 3.5 Hz, 1H), 1.56 (d, *J* = 6.5 Hz, 6H), 1.47 (d, *J* = 3.0 Hz, 1H), 1.44 (d, *J* = 6.5 Hz, 6H), 1.30 (d, *J* = 7.0 Hz, 6H), 1.28 (d, *J* = 6.5 Hz, 6H), 1.22-1.18 (m, 1H), 0.85-0.79 (m, 4H), 0.71-0.66 (m, 2H), 0.56- 0.42 (m, 2H). ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz): δ 200.5, 146.9, 146.6, 134.1, 129.8, 124.8, 124.6, 57.9, 53.6, 47.8, 46.1, 45.9, 34.9, 29.1, 29.0, 28.7, 28.4, 26.1, 26.0, 23.9, 23.8, 23.3. Anal. Calc'd. for $C_{35}H_{51}N_2ClPd$: C, 65.51; H, 8.01; N, 4.37; found, C, 65.39; H, 8.20; N, 4.11.

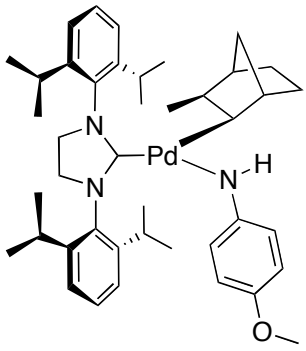
Preparation of (SiPr)Pd(2-CH$_3$-norbornyl)NH(4-CH$_3$C$_6$H$_4$) (2a)



(SiPr)Pd(2-CH$_3$-norbornyl)Cl (0.120 g, 0.187 mmol) and KNH(*p*-CH$_3$) (0.0272 g, 0.187 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of benzene. The reaction mixture was stirred for 2 h and the color changed to dark red/purple. After 2h, the reaction mixture was filtered through a syringe filter and the volatiles were removed by vacuum. A 1.5 mL aliquot of pentane was added to the residue and after 2 minutes dark crystals appeared. The reaction mixture was placed into a freezer (-35 °C) overnight to increase the yield of crystallized product. The supernatant liquid was removed with a pipette and the crystals were dried vacuum. Yield 0.107 g, 80%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.34 (t, *J* = 7.5 Hz, 2H), 7.25 (d, *J* = 7.5 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.85 (d, *J* = 8.0 Hz, 2H), 6.19 (d, *J* = 8.0 Hz, 2H), 3.86 (s, 1H), 3.48-3.34 (m, 6H), 3.11- 3.03 (m, 3H), 2.28 (s, 3H), 2.11 (s, 1H), 1.77 (d, *J* = 9.5 Hz, 1H), 1.66 (d, *J* = 6.5 Hz, 6H), 1.56 (s, 1H), 1.33- 0.95 (m, 22H), 0.80 (bs, 4H), 0.65 (d, *J* = 9.5 Hz, 1H). ^{13}C{^{1}H} NMR (C_6D_6, 126 MHz): δ 210.5, 157.8, 147.5, 146.9, 136.4,

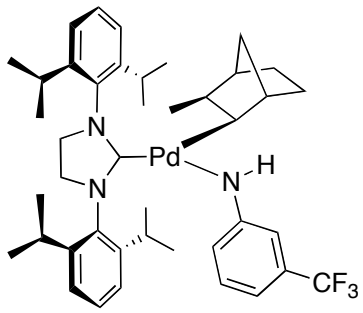
129.5, 129.3, 124.9, 124.8, 120.8, 117.8, 53.4, 48.1, 47.2, 45.4, 44.5, 35.0, 29.8, 29.5, 29.3, 29.1, 26.3, 25.8, 24.4, 24.1, 23.6, 21.0. Anal. Calc'd. for $C_{42}H_{59}N_3Pd$: C, 70.81; H, 8.35; N, 5.90; found, C, 70.58; H, 8.31; N, 5.72.

Preparation of (SiPr)Pd(2-CH_3-norbornyl)NH(4-$OCH_3C_6H_4$) (2b)



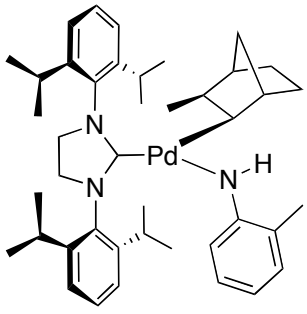
(SiPr)Pd(2-CH_3-norbornyl)Cl (0.100 g, 0.157 mmol) and KNH(*p*-OCH_3) (0.0253 g, 0.157 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of benzene. The reaction mixture was stirred for 2 h and the color changed to dark red/purple. After 2h, the reaction mixture was filtered through a syringe filter and the volatiles were removed by vacuum. A 1.5 mL aliquot of pentane was added to the residue and after 2 minutes dark crystals appeared. The reaction mixture was placed into a freezer (-35 °C) overnight to increase the yield of crystallized product. The supernatant liquid was removed with a pipette and the crystals were dried vacuum. Yield 0.0581 g, 51%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.30 (d, *J* = 8.0 Hz, 2H), 7.22 (d, *J* = 7.5Hz, 2H), 7.08 (d, *J* = 8.0 Hz, 2H), 6.69 (d, *J* = 8.5Hz, 2H), 6.16 (d, *J* = 8.5 Hz, 2H), 3.84 (s, 1H), 3.48 (s, 3H), 3.46-3.35 (m, 6H), 3.09 (hept, *J* = 7.0 Hz, 2H), 3.02 (s, 1H), 2.09 (d, *J* = 3.0 Hz, 1H), 1.77 (d, *J* = 10 Hz, 1H), 1.65 (d, *J* = 7.0 Hz, 6H), 1.61 (d, *J* = 7.0 Hz, 1H), 1.59 (d, *J* = 3.5 Hz, 1H), 1.51 (d, *J* = 7.0 Hz, 1H), 1.35-1.29 (m, 7 H), 1.16 (d, *J* = 7.0 Hz, 6H), 1.11-1.06 (m, 7H), 1.00-0.96 (m, 1H), 0.81 (s, 3H), 0.68 (d, *J* = 7.5Hz, 1H). ^{13}C{^{1}H} NMR (C_6D_6, 126 MHz): δ 210.7, 154.22, 149.9, 147.5, 146.9, 136.3, 129.5, 124.90, 124.8, 118.1, 114.9, 55.7, 53.4, 47.8, 47.2, 45.4, 44.5, 35.0, 29.9, 29.5, 29.3, 29.1, 26.3, 25.8, 24.5, 24.1, 23.6. Anal. Calc'd. for $C_{42}H_{59}N_3OPd$: C, 69.26; H, 8.16; N, 5.77; found, C, 68.97; H, 8.30; N, 5.50.

Preparation of (SIPr)Pd(2-CH$_3$-norbornyl)NH(3-CF$_3$C$_6$H$_4$) (2c)



(SiPr)Pd(2-CH$_3$-norbornyl)Cl (0.100 g, 0.156 mmol) and KNH(3-CF$_3$C$_6$H$_4$) (0.0310 g, 0.156 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of benzene. The reaction mixture was stirred for 2 h and the color changed to dark red/purple. After 2h, the reaction mixture was filtered through a syringe filter and the volatiles were removed by vacuum. A 1.5 mL aliquot of pentane was added to the residue and after 2 minutes dark crystals appeared. The reaction mixture was placed into a freezer (-35 °C) overnight to increase the yield of crystallized product. The supernatant liquid was removed with a pipette and the crystals were dried vacuum. Yield: 0.0662 g; 55%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.31 (t, *J* = 8.0 Hz, 2H), 7.23 (d, *J* = 7.5 Hz, 2H), 7.05 (d, *J* = 7.5Hz, 2H), 6.85 (t, *J* = 8.0 Hz, 1H), 6.74 (d, *J* = 7.0 Hz, 1H), 6.57 (s, 1H), 6.16 (d, *J* = 6.5 Hz, 1H), 3.72 (s, 1H), 3.45-3.22 (m, 6H), 3.14-2.99 (m, 3H), 2.05 (s, 1H), 1.64 (s, 1H), 1.62 (d, *J* = 7.0 Hz, 6H), 1.48 (d, *J* = 3.0 Hz, 1H), 1.30-0.94 (m, 22 H), 0.77 (d, *J* = 7.0 Hz, 3H), 0.72-0.67 (m, 1H), 0.56 (d, *J* = 10.0 Hz, 1H). ^{13}C{^{1}H} NMR (C_6D_6, 126 MHz): δ 208.7, 160.3, 147.2, 146.7, 135.9, 130.8 (q, *J* = 28.2 Hz), 129.8, 128.9, 126.3 (q, *J* = 274 Hz), 125.1, 124.9, 120.6, 113.0, 108.1, 53.4, 49.8, 47.4, 45.5, 44.8, 34.7, 29.5, 29.4, 29.2, 29.1, 26.2, 25.7, 24.1, 24.0, 23.6. ^{19}F NMR (C_6D_6, 470 MHz): δ -61.9. Anal. Calc'd. for $C_{42}H_{56}F_3N_3Pd$: C, 65.83; H, 7.37; N, 5.48; found, C, 65.59; H, 7.46; N, 5.27.

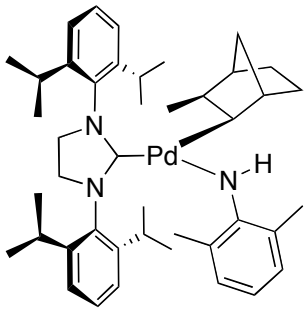
Preparation of (SIPr)Pd(2-CH$_3$-norbornyl)NH(2-CH$_3$C$_6$H$_4$) (2d)



(SiPr)Pd(2-CH$_3$-norbornyl)Cl (0.120 g, 0.187 mmol) and KNH(CH$_3$) (0.0272 g, 0.187 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of benzene. The reaction mixture was stirred for 2 h and the color changed to dark red/purple. After 2h, the reaction mixture was filtered through a syringe filter and the volatiles were removed by vacuum. A 1.5 mL aliquot of pentane was added to the residue and after 2 minutes dark crystals appeared. The reaction mixture was placed into a freezer (-35 °C) overnight to increase the yield of crystallized product. The supernatant liquid was removed with a pipette and the crystals were dried vacuum. Yield 0.100 g, 75%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.32 (t, *J* = 8.0 Hz, 2H), 7.24 (d, *J* = 8.0 Hz, 2H), 7.09-

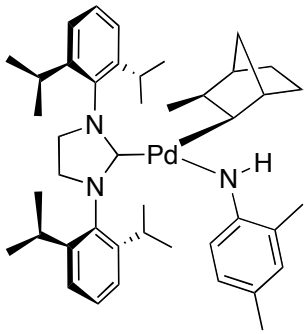
7.05 (m, 3H), 6.99 (t, J = 7.5 Hz, 1H), 6.62 (t, J = 7.5 Hz, 1H), 6.20 (d, J = 8.0 Hz, 1H), 3.96 (s, 1H), 3.48-3.34 (m, 6H), 3.12-3.04 (m, 3H), 2.11 (bs, 4H), 1.66 (d, J = 7.0 Hz, 6H), 1.65 (bs, 1H), 1.56 (d, J = 4.0 Hz, 1H), 1.32- 1.26 (m, 7H), 1.16 (d, J = 7.0 Hz, 6H), 1.10-0.90 (m, 12H), 0.78 (p, J = 7.0 Hz, 1H), 0.57 (d, J = 10.0 Hz, 1H). $^{13}C\{^1H\}$ NMR (C_6D_6, 126 MHz): δ 210.3, 157.9, 147.5, 146.9, 136.3, 129.8, 129.6, 127.1, 125.0, 124.9, 121.7, 118.1, 112.8, 53.4, 48.5, 47.2, 45.6, 44.5, 34.8, 29.7, 29.4, 29.4, 29.2, 26.3, 25.8, 24.6, 24.1, 23.7, 18.8. Anal. Calc'd. for $C_{42}H_{59}N_3Pd$: C, 70.81; H, 8.35; N, 5.90; found, C, 70.89; H, 8.35; N, 5.71.

Preparation of (SIPr)Pd(2-CH_3-norbornyl)NH(2,6-$(CH_3)_2C_6H_4$) (2e)



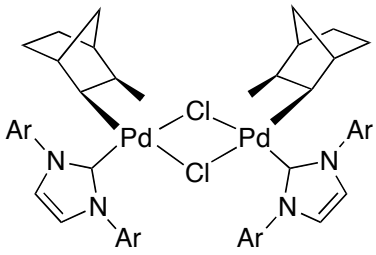
(SiPr)Pd(2-CH_3-norbornyl)Cl (0.120 g, 0.187 mmol) and KNH(2,6-$(CH_3)_2C_6H_3$) (0.0444 g, 0.187 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of benzene. The reaction mixture was stirred for 2 h and the color changed to dark red/purple. After 2h, the reaction mixture was filtered through a syringe filter and the volatiles were removed by vacuum. A 1.5 mL aliquot of pentane was added to the residue and after 2 minutes dark crystals appeared. The reaction mixture was placed into a freezer (-35 °C) overnight to complete the crystallization of the product. The supernatant liquid was removed with a pipette and the crystals were dried vacuum. Yield: 0.108 g, 72%. ^1H NMR (C_6D_6, 500 MHz): δ 7.26 (t, J = 7.5 Hz, 2H), 7.20 (d, J = 8.0 Hz, 2H), 7.10 (d, J = 7.5 Hz, 2H), 7.03 (d, J = 8.0 Hz, 2H), 6.27 (t, J = 7.0 Hz, 1H), 4.62 (s, 1H), 3.52-3.36 (m, 6H), 3.14-3.04 (m, 3H), 2.20 (s, 6H), 2.16 (d, J = 3.0 Hz, 1H), 1.66 (d, J = 7.0 Hz, 6H), 1.51 (d, J = 3.0 Hz, 1H), 1.46 (d, J = 9.0 Hz, 1H), 1.30-0.95 (m, 22H), 0.84 (d, J = 7.0 Hz, 3H), 0.72 (p, J = 6.5 Hz, 1H), 0.55 (d, J = 9.5 Hz, 1H). $^{13}C\{^1H\}$ NMR (C_6D_6, 126 MHz): δ 210.1, 156.3, 147.3, 146.6, 136.8, 129.6, 128.7, 125.2, 125.0, 123.7, 113.1, 53.6, 49.2, 46.8, 46.3, 45.6, 34.5, 30.1, 29.3, 29.2, 29.0, 26.2, 25.9, 25.1, 24.0, 23.8, 20.1. Anal. Calc'd. for $C_{43}H_{61}N_3Pd$: C, 71.10; H, 8.46; N, 5.78; found, C, 70.86; H, 8.55; N, 5.64.

Preparation of (SIPr)Pd(2-CH$_3$-norbornyl)NH(2,4-(CH$_3$)$_2$C$_6$H$_4$) (2f)



(SiPr)Pd(2-CH$_3$-norbornyl)Cl (0.100 g, 0.156 mmol) and KNH(2,4-(CH$_3$)C$_6$H$_3$) (0.0248 g, 0.156 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of benzene. The reaction mixture was stirred for 2 h and the color changed to dark red/purple. After 2h, the reaction mixture was filtered through a syringe filter and the volatiles were removed by vacuum. A 1.5 mL aliquot of pentane was added to the residue and after 2 minutes dark crystals appeared. The reaction mixture was placed into a freezer (-35 °C) overnight to increase the yield of crystallized product. The supernatant liquid was removed with a pipette and the crystals were dried vacuum. Yield: 0.0684 g, 72%. ^{1}H NMR (C$_6$D$_6$, 500 MHz): δ 7.34 (t, *J* = 8.0 Hz, 2H), 7.27 (d, *J* = 8.0 Hz, 2H), 7.09 (d, *J* = 8.0 Hz, 2H), 6.83 (s, 1H), 6.80 (d, *J* = 7.5 Hz, 1H), 6.14 (d, *J* = 8.0 Hz, 1H), 3.99 (s, 1H), 3.49-3.37 (m, 6H), 3.13-3.05 (m, 3H), 2.32 (s, 3H), 2.11 (bs, 4H), 1.68 (d, *J* = 6.5 Hz, 6H), 1.62 (d, *J* = 9.5 Hz, 1H), 1.56 (d, *J* = 5.0 Hz, 1H), 1.33 (d, *J* = 6.5 Hz, 6H), 1.31-0.94 (m, 16 H), 0.90 (d, *J* = 7.0 Hz, 3H), 0.87 (p, *J* = 7.0 Hz, 1H), 0.58 (d, *J* = 9.5 Hz, 1H). ^{13}C{^{1}H} NMR (C$_6$D$_6$, 126 MHz): δ 210.7, 155.5, 147.5, 146.9, 136.4, 130.6, 129.5, 127.6, 124.9, 124.8, 121.7, 120.8, 118.3, 53.4, 48.0, 47.1, 45.5, 44.4, 34.7, 29.8, 29.4, 29.3, 29.2, 26.3, 25.8, 24.8, 24.1, 23.6, 21.1, 18.8. Anal. Calc'd. for C$_{43}$H$_{61}$N$_3$Pd: C, 71.10; H, 8.46; N, 5.78; found, C, 71.37; H, 8.71; N, 5.55.

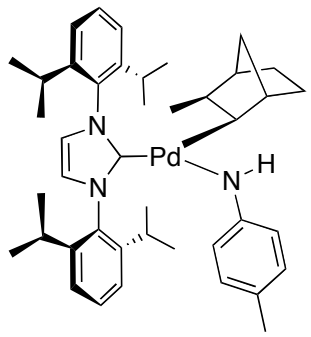
Preparation of (IPr)Pd(2-CH$_3$-norbornyl)Cl (3)



To a 20 mL scintillation vial was added (COD)Pd(2-CH$_3$-norbornyl)Cl (0.130 g, 0.362 mmol) and IPr (0.141 g, 0.363 mmol). The reaction mixture was dissolved in 5 mL benzene and stirred for 3 h. The reaction mixture was filtered through a syringe filter to remove Pd° black, and the volatiles were removed by vacuum. To the yellow residue was added 2 mL and pentane, and the reaction mixture was placed into the freezer (-35 °C) overnight. The supernatant liquid was removed from the light yellow precipitate with a pipette and the solid was dried by vaccum. Yield 0.208 g, 90%. ^{1}H NMR (C$_6$D$_6$, 500 MHz, 90°C): δ 7.24 (t, *J* = 8.0 Hz, 2H), 7.12 (d, *J* = 7.5 Hz, 4H), 6.60 (s, 2H), 2.84 (hept, *J* = 7.0 Hz, 4H), 2.66 (d, *J* = 9.5 Hz, 1H), 2.14 (s, 1H), 1.59 (bs, 1H),

1.42 (d, *J* = 6.5 Hz, 6H), 1.41 (d, *J* = 6.5 Hz, 6H), 1.29-1.24 (m, 4H), 1.03 (d, *J* = 6.5 Hz, 6H), 1.02 (d, *J* = 6.5 Hz, 6H), 0.86-0.77 (m, 4H), 0.63 (p, *J* = 6.5 Hz, 1H), 0.51 (bs, 1H). $^{13}C\{^{1}H\}$ NMR (C_6D_6, 126 MHz, 90°C): δ 146.3, 130.9, 128.6, 124.8, 124.7, 124.1, 48.7, 47.0, 46.9, 34.9, 29.8, 29.6, 25.7, 25.5, 24.5, 23.4. Anal. Calc'd. for $C_{35}H_{49}N_2ClPd$: C, 65.72; H, 7.72; N, 4.38; found, C, 65.80; H, 7.72; N, 4.32.

Preparation of (IPr)Pd(2-CH$_3$-norbornyl)NH(4-CH$_3$C$_6$H$_4$) (4)



(SIPr)Pd(2-CH_3-norbornyl)Cl (0.100 g, 0.156 mmol) and KNH(*p*-CH_3) (0.0227 g, 0.156 mmol) were added to a 20 mL scintillation vial and the reaction mixture was dissolved in 3 mL of benzene. The reaction mixture was stirred for 3 h and the color changed to dark red/purple. After 2h, the reaction mixture was filtered through a syringe filter and the volatiles were removed by vacuum. The residue was dissolved in 15 mL of pentane and was filtered through a syringe filter to remove a small amount of palladium byproduct. The volatiles was removed by vacuum and 1.5 mL of pentane was added to the residue and after 2 minutes dark crystals appeared. The reaction mixture was placed into a freezer (-35 °C) overnight to increase the yield of crystallized product. The supernatant liquid was removed with a pipette and the crystals were dried vacuum. Yield 0.0452 g, 41%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.36 (t, *J* = 8.0 Hz, 2H), 7.26 (d, *J* = 8.0 Hz, 2H), 7.11 (d, *J* = 8.0 Hz, 2H), 6.89 (d, *J* = 8.0 Hz, 2H), 6.48 (s, 2H), 6.35 (d, *J* = 8.5 Hz, 2H), 3.85 (s, 1H), 3.10 (d, *J* = 7.5 Hz, 1H) 3.05 (hept, *J* = 7.0 Hz, 2H), 2.65 (hept, *J* = 2.65 Hz, 2H), 2.31 (s, 3H), 2.11 (d, *J* = 3.0 Hz, 1H), 1.83 (d, *J* = 9.5 Hz, 1H), 1.58 (d, *J* = 3.0 Hz, 1H), 1.55 (d, *J* = 7.0 Hz, 6H), 1.32-1.17 (m, 8H), 1.08-0.96 (m, 14H), 0.94 (d, *J* = 7.0 Hz, 3H), 0.74-0.69 (m, 2H). $^{13}C\{^{1}H\}$ NMR (C_6D_6, 126 MHz): δ 185.7, 157.9, 146.3, 146.0, 136.1, 130.3, 129.4, 124.5, 124.4, 123.2, 120.7, 117.8, 47.6, 47.4, 45.4, 44.4, 35.0, 29.7, 29.6, 29.3, 29.2, 25.8, 25.1, 24.6, 23.4, 23.2, 21.1. Anal. Calc'd. for $C_{42}H_{57}N_3Pd$: C, 70.91; H, 8.22; N, 5.91; found, C, 71.27; H, 8.36; N, 5.65.

General Procedure for Kinetic Analysis of Reductive Elimination from Norbornylamido Complexes

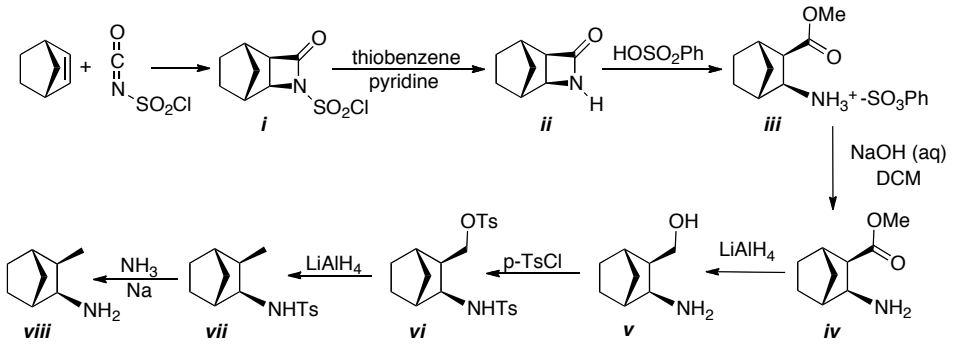
In an N_2 filled glovebox, (SiPr)Pd(2-CH_3-norbornyl)NHAr (0.130 mmol), SiPr (0.130 mmol), and trimethoxybenzene (0.130 mmol) was added to a 4 mL vial and the reaction mixture was dissolved into 0.4 mL toluene-d_8. The reaction mixture was carefully transferred to an NMR tube and inserted into a 500 MHz NMR probe that was pre-warmed to 90 °C. An array was collected with scans every 45 s until the complex had reacted greater than three half-lives. The spectra were integrated and fit to an exponential decay to determine the rate constant for reductive elimination. The yields of the norbornylamine products were determined by comparing the integration of the aryl proton resonances to those of trimethoxybenzene in the ^{1}H NMR spectrum following completion of the reaction.

Effect of Solvent on the Reductive Elimination from Norbornylamido Complexes

In an N_2 filled glovebox, (SiPr)Pd(2-CH_3-norbornyl)NH(4-$CH_3C_6H_4$) (0.130 mmol), SIPr (0.130 mmol), and trimethoxybenzene (0.130 mmol) were added to a 4 mL vial, and the reaction mixture was dissolved in ether 0.4 mL toluene-d_8 or 0.4 mL THF-d_8. The reaction mixture was carefully transferred to an NMR tube, and an initial ^{1}H NMR spectrum was obtained. The NMR tube was placed into an oil bath at 50 °C. ^{1}H NMR spectra were obtained every 45 to 135 minutes by ^{1}H NMR spectroscopy. The spectra were integrated and fit to an exponential decay to determine the rate constant for reductive elimination. The rate constant for reductive elimination was found to be 1.3 x 10^{-4} s^{-1} in THF-d_8 and 7.8 x 10^{-5} s^{-1} in toluene-d_8.

Synthesis of syn-exo-3-methyl-exo-2-aminonorbornane

The preparation of the parent norbornylamine, *syn*-*exo*-3-methyl-*exo*-2-aminonorbornane, was conducted by a modified procedure illustrated below. Intermediates ***i-iii*** were prepared from a procedure reported by Moriconi,[1] and the aminoester ***iv*** was revealed by the reaction of ***iii*** with NaOH in dichloromethane. Intermediate ***iv*** was carried on to the parent norbornylamine product by a previously described procedure.[2]



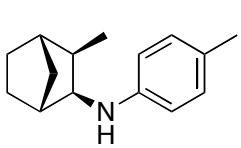
General Procedure for the Preparation of the N-arylnorbornylamine Products

Two different procedures were employed to synthesize the N-arylnorbornylamine products from intermediate ***viii***.[3,4]

1) In an N_2 filled glovebox, 4 mL vial was charged with 3-methylbicyclo[2.2.1]heptan-2-amine (0.069 g; 0.55 mmol), 3-bromobenzotrifluoride (0.113 g; 0.050 mmol), NaO*t*Bu (0.067 g; 0.70 mmol), $Pd(OAc)_2$ (0.0056 g; 0.025 mmol) and Josiphos - CyPF-*t*-Bu (0.014 g; 0.025 mmol). The reaction mixture was dissolved in 0.50 mL anhydrous DME and heated to 100 °C for 18 h. The reaction mixture was cooled to RT and filtered through celite. The product was purified by column chromatography (hexane/ethylacetate).

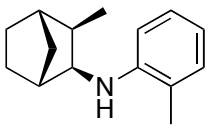
2) In an N_2 filled glovebox, 4 mL vial was charged with 3-methylbicyclo[2.2.1]heptan-2-amine (0.069 g; 0.55 mmol), 1-bromo-2,4-dimethylbenzene (0.0925 g; 0.050 mmol), NaO*t*Bu (0.067 g; 0.70 mmol),Chloro[2-(dicyclohexylphosphino)-3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl][2-(2-aminoethyl)phenyl]palladium(II) (0.0200 g; 0.025 mmol) and 2-(Dicyclohexylphosphino)3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl (0.0134 g; 0.025 mmol). The reaction mixture was dissolved in 0.5 mL Bu_2O and stirred at 110 °C for 4 h. The reaction mixture was cooled to room temperature and filtered through celite. The reaction mixture was purified by column chromatography (hexane/ethylacetate). This procedure is adapated from a method described by Buchwald.

Preparation of anti-exo-3-methyl-endo-2-(4-methylanilino)norbornane



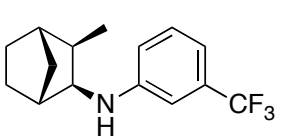
Prepared according to procedure 1 using 3-methylbicyclo[2.2.1]heptan-2-amine (0.090 g; 0.72 mmol), 4-bromotoluene (0.123 g; 0.72 mmol), $Pd(OAc)_2$ (0.0016 g; 0.0072 mmol), Josiphos - CyPF-*t*-Bu (0.0040 g; 0.0072 mmol), and NaO*t*Bu (0.097 g; 1.0 mmol). Collected 0.061 g; 40%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.01 (d, *J* = 8.0 Hz, 2H), 6.45 (d, *J* = 8.5 Hz, 2H), 3.27 (s, 1H), 3.13 (bs, 1H), 2.22 (s, 3H), 1.92 (s, 1H), 1.69-1.64 (m, 2H), 1.38-1.31 (m, 3H), 1.06-1.01 (m, 2H), 0.84 (dt, *J* = 10.5, 1.5 Hz, 1H), 0.80 (d, *J* = 7.5 Hz, 3H). Anal. Calc'd. for $C_{15}H_{21}N$: C, 83.67; H, 9.83; N, 6.50; found, C, 83.66; H, 9.65; N, 6.40.

Preparation of anti-exo-3-methyl-endo-2-(2-methylanilino)norbornane



Prepared according to procedure 1 using 3-methylbicyclo[2.2.1]heptan-2-amine (0.069 g; 0.55 mmol), 2-bromotoluene (0.855 g; 0.050 mmol), NaO*t*Bu (0.067 g; 0.70 mmol), $Pd(OAc)_2$ (0.0056 g; 0.025 mmol) and Josiphos - CyPF-*t*-Bu (0.014 g; 0.025 mmol). Collected 13.4 mg; 12%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.22 (t, *J* = 7.5 Hz, 1H), 7.05 (d, *J* = 7.5 Hz, 1H), 6.78 (t, *J* = 7.5 Hz, 1H), 6.61 (d, *J* = 8.5 Hz, 1H), 3.38 (bs, 1H), 3.19 (d, *J* = 7.0 Hz, 1H), 2.01 (bs, 1H), 1.91 (s, 3H), 1.71-1.69 (m, 2H), 1.44 (d, *J* = 10.0 Hz, 1H), 1.36-1.33 (m, 2H), 1.06 (d, *J* = 9.5 Hz, 2H), 0.87 (d, *J* = 10.0 Hz, 1H), 0.81 (d, *J* = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (C_6D_6, 126 MHz): δ 146.6, 130.3, 127.6, 121.3, 116.8, 110.4, 59.3, 44.0, 43.3, 42.3, 33.0, 29.4, 27.1, 17.4, 14.4. HRMS (EI^+) m/z calc'd for $C_{16}H_{21}N$ for [M+]: 215.1674, found 215.1673.

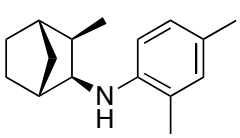
Preparation of anti-exo-3-methyl-endo-2-(3-trifluoromethylanilino)norbornane



A 4 ml vial was charged with 3-methylbicyclo[2.2.1]heptan-2-amine (0.069 g; 0.55 mmol), 3-bromobenzotrifluoride (0.113 g; 0.050 mmol), $Pd(OAc)_2$ (0.0056 g; 0.025 mmol), Josiphos - CyPF-*t*-Bu (0.014 g; 0.025 mmol), and NaO*t*Bu (0.067 g; 0.70 mmol). Collected 0.022 g; 16 %. ^{1}H NMR (C_6D_6, 500 MHz): δ 6.95-6.90 (m, 2H), 6.67 (s, 1H), 6.28 (d, *J* = 7.5 Hz, 1H), 3.30 (d, *J* = 6.0 Hz, 1H), 2.92 (d, *J* = 7.0 Hz, 1H), 1.76 (s, 1H), 1.63 (s, 1H), 1.56 (p, *J* = 7.5 Hz, 1H), 1.35-1.21 (m, 3H), 0.99-0.91 (m, 2H), 0.80 (dt, *J* = 10 Hz, 1.5 Hz, 1H), 0.64 (d, *J* = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (C_6D_6, 126 MHz): δ 148.9, 131.7 (q, *J* = 31.4 Hz), 129.9, 127.5 (q, *J* = 273 Hz), 115.3, 113.0, 109.2,

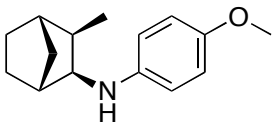
59.3, 43.9, 43.3, 42.5, 33.0, 29.1, 27.1, 14.6. ^{19}F NMR (C_6D_6, 470 MHz): δ -62.8. Anal. Calc'd. for $C_{15}H_{18}F_3N$: C, 66.90; H, 6.74; N, 5.20; found, C, 67.14; H, 7.06; N, 4.95.

Preparation of anti-exo-3-methyl-endo-2-(2,4-dimethylanilino)norbornane



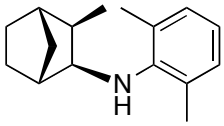
Prepared according to procedure 2 using 3-methylbicyclo[2.2.1]heptan-2-amine (0.069 g; 0.55 mmol), 1-bromo-2,4-dimethylbenzene (0.0925 g; 0.050 mmol), NaO*t*Bu (0.067 g; 0.70 mmol),Chloro[2-(dicyclohexylphosphino)-3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl][2-(2-aminoethyl)phenyl]palladium(II) (0.0200 g; 0.025 mmol) and 2-(Dicyclohexylphosphino)3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl (0.0134 g; 0.025 mmol). Collected 0.033 g; 29%. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.04 (d, *J* = 8.5, Hz, 1H), 6.87 (s, 1H), 6.58 (d, *J* = 8.5 Hz, 1H), 3.29 (s, 1H), 3.22, (t, *J* = 6.5 Hz, 1H), 2.26 (s, 3H), 2.04 (s, 1H), 1.95 (s, 3H), 1.74-1.71 (m, 2H), 1.47 (dt, *J* = 10.0, 2.0 Hz, 1H), 1.36-1.33 (m, 2H), 1.09-1.06 (m, 2H), 0.88 (dt, *J* = 10.0, 1.5 Hz, 1H), 0.84 (d, *J* = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR ($CDCl_3$, 126 MHz): δ 144.0, 130.8, 127.3, 125.1, 121.3, 109.9, 59.3, 43.7, 42.9, 42.0, 32.8, 29.1, 26.9, 20.3, 17.4, 14.4. HRMS (EI$^+$) m/z calc'd for $C_{16}H_{23}N$ for [M+]: 229.1831, found 229.1839.

Preparation of anti-exo-3-methyl-endo-2-(4-methoxyanilino)norbornane



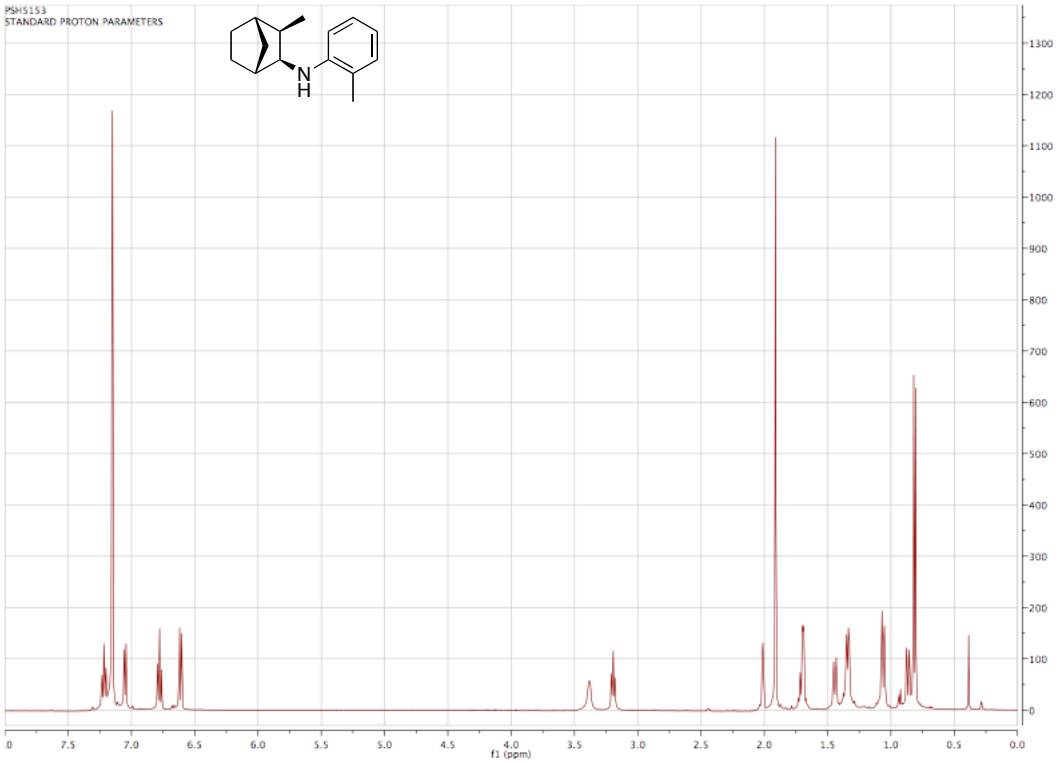
Prepared according to procedure 2 using 3-methylbicyclo[2.2.1]heptan-2-amine (0.150 g; 1.20 mmol), 4-bromoanisole (0.187 g; 1.00 mmol), NaO*t*Bu (0.135 g; 1.40 mmol), Chloro[2-(dicyclohexylphosphino)-3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl][2-(2-aminoethyl)phenyl]palladium(II) (0.0399 g; 0.050 mmol) and 2-(Dicyclohexylphosphino)3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl (0.0268 g; 0.050 mmol). Collected 0.034 g; 16%. ^{1}H NMR (C_6D_6, 500 MHz): δ 6.84 (d, *J* = 9.0 Hz, 2H), 6.42 (d, *J* = 9.0 Hz, 2H), 3.43 (s, 3H), 3.15 (bs, 1H), 3.10 (d, *J* = 7.5 Hz, 1H), 1.95 (s, 1H), 1.71-1.68 (m, 2H), 1.40-1.33 (m, 3H), 1.07-1.04 (m, 2H), 0.86 (d, *J* = 9.5 Hz, 1H), 0.82 (d, *J* = 7.5 Hz, 3H). ^{13}C{^{1}H} NMR (C_6D_6, 126 MHz): δ 152.3, 143.3, 115.2, 114.0, 60.3, 55.4, 44.1, 43.3, 42.6, 33.0, 29.3, 27.3,14.8. HRMS (EI$^+$) m/z calc'd for $C_{16}H_{21}NO$ for [M+]: 231.1623, found 231.1617.

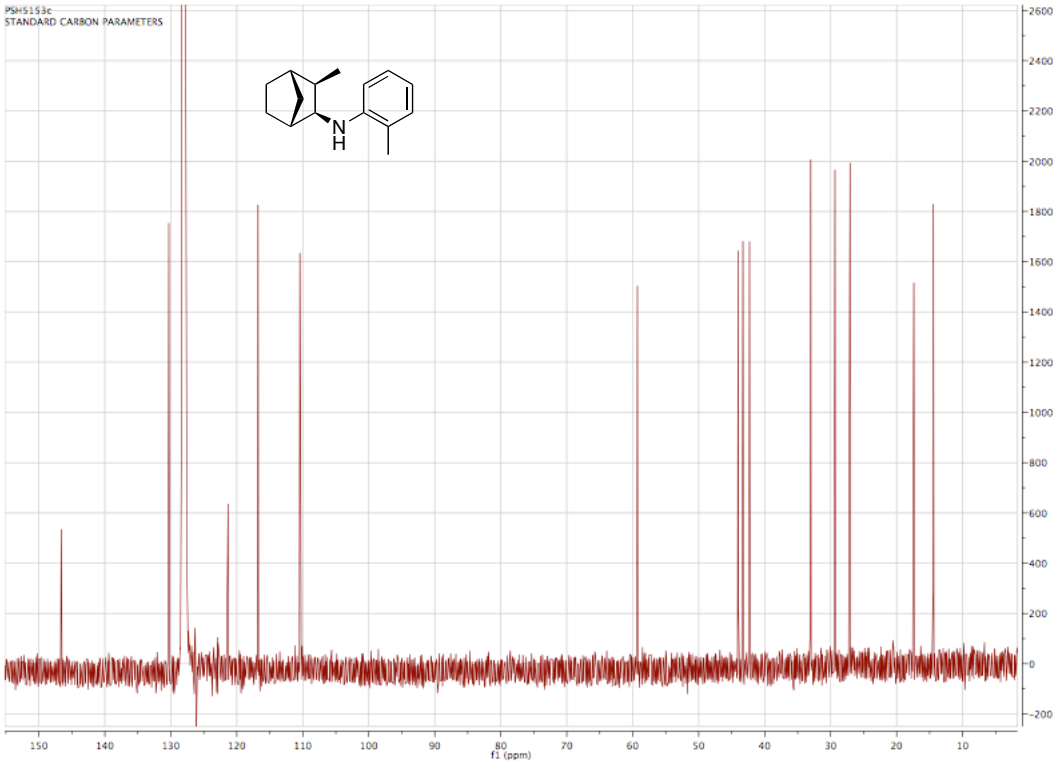
Preparation of anti-exo-3-methyl-endo-2-(2,6-dimethylanilino)norbornane

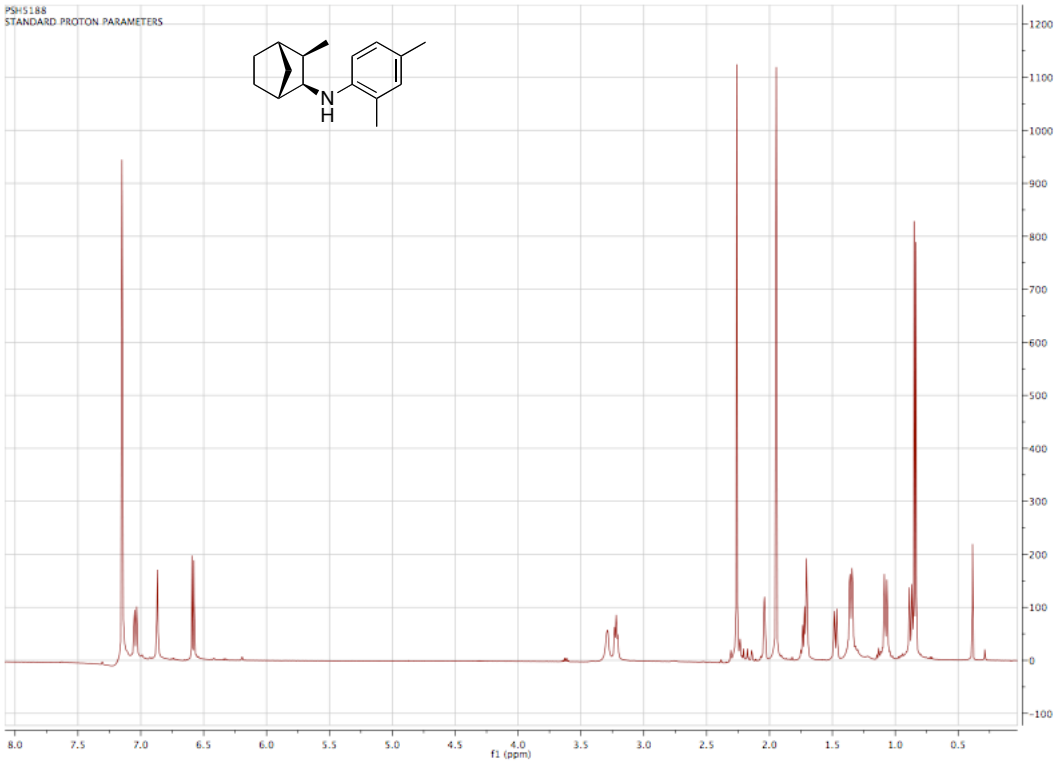


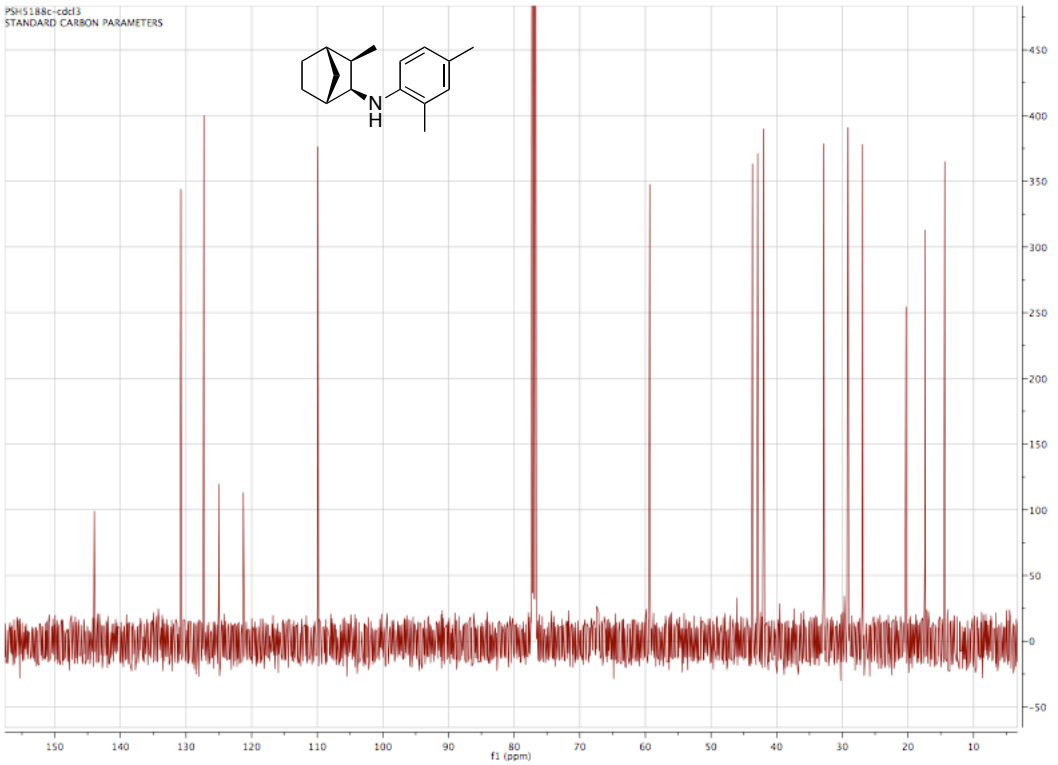
Prepared according to procedure 2 using 3-methylbicyclo[2.2.1]heptan-2-amine (0.150 g; 1.20 mmol), 1-bromo-2,6-dimethylbenzene (0.185 g; 1.00 mmol), NaO*t*Bu (0.135 g; 1.40 mmol), Chloro[2-(dicyclohexylphosphino)-3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl][2-(2-aminoethyl)phenyl]palladium(II) (0.0399 g; 0.050 mmol) and 2-(Dicyclohexylphosphino)3,6-dimethoxy-2′,4′,6′-triisopropyl-1,1′-biphenyl (0.0268 g; 0.050 mmol). This compound could not be cleanly isolated; GCMS indicated the major product of this reaction has an M/Z of 229. The aryl resonances and methyl groups in ^{1}H NMR spectrum of the crude product in benzene-d_6 matched those of the product formed from the reductive elimination of **2e**. ^{1}H NMR (C_6D_6, 500 MHz): δ 7.01 (d, J = 7.5 Hz, 2H), 6.87 (d, J = 7.5 Hz, 1H), 2.18 (s, 6H), 1.04 (d, J = 6.0 Hz, 3H). 1H and ^{13}C NMR spectrum of the same material was collected in $CDCl_3$ and included below. ^{13}C NMR (101 MHz, $CDCl_3$) δ 146.33, 128.94, 127.99, 120.48, 63.33, 43.64, 42.51, 41.66, 32.32, 29.21, 26.91, 19.17, 15.05.

NMR Spectra for Norbornylamine Products






PSH5188
STANDARD PROTON PARAMETERS
N
H
f1 (ppm)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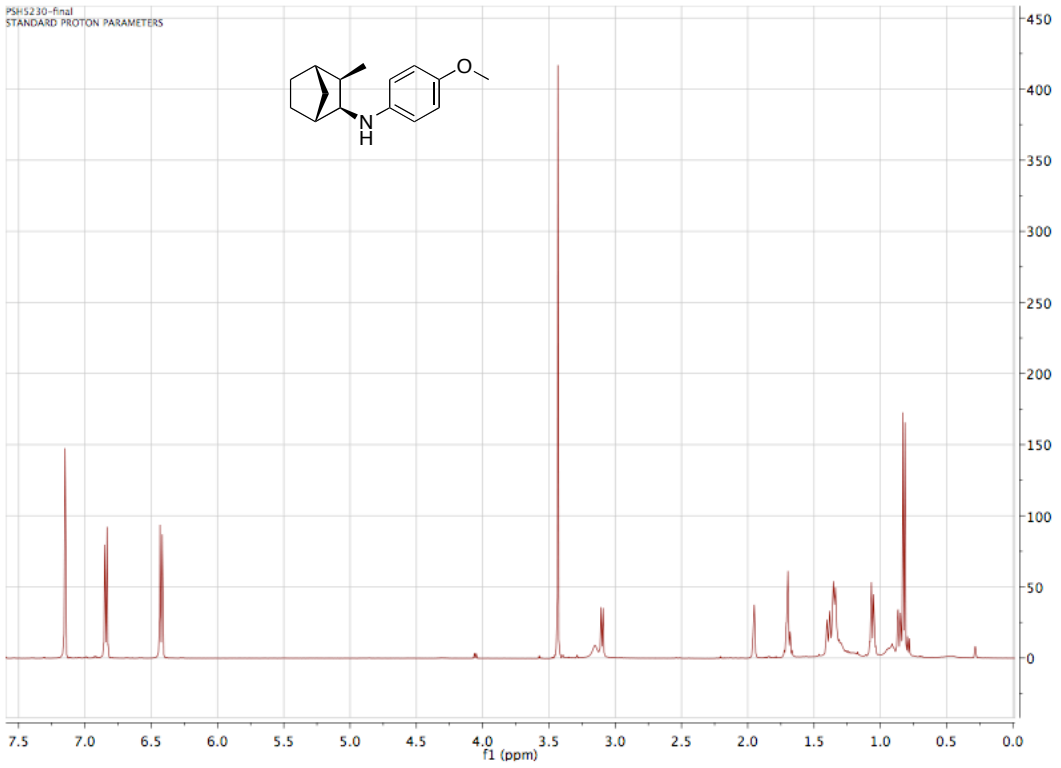
N
H
f1 (ppm)


PSH5230-final
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7.0
6.5
6.0
5.5
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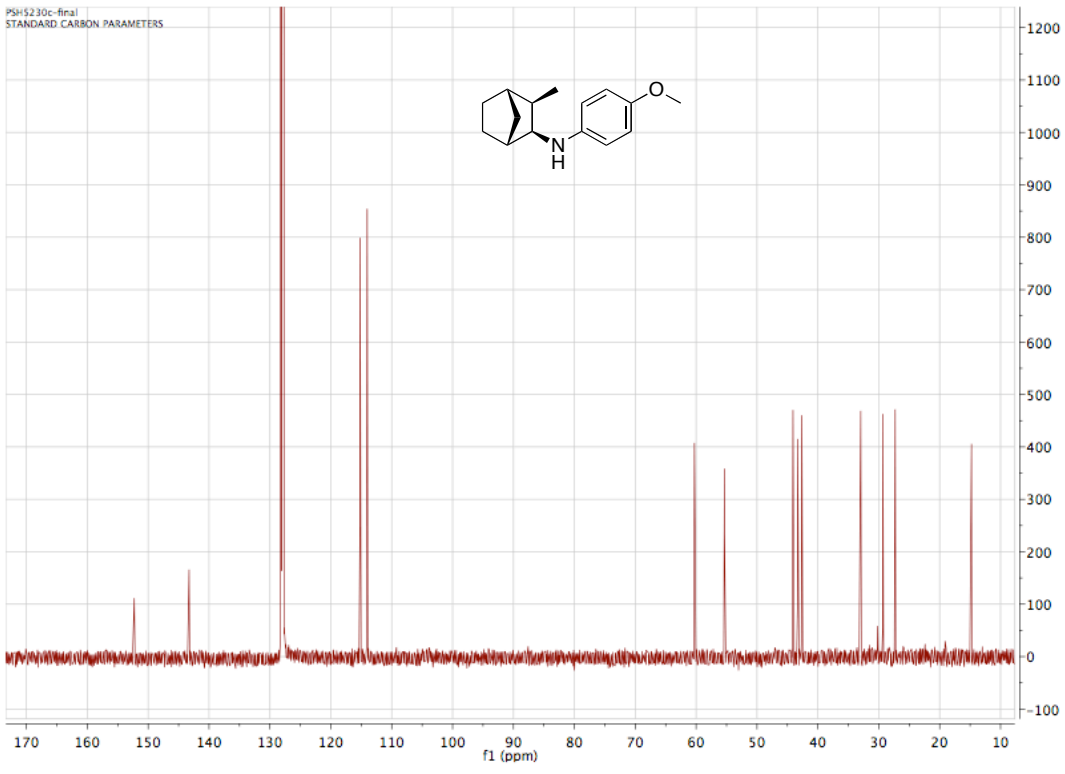
0.0
f1 (ppm)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H
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700
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200
100
0
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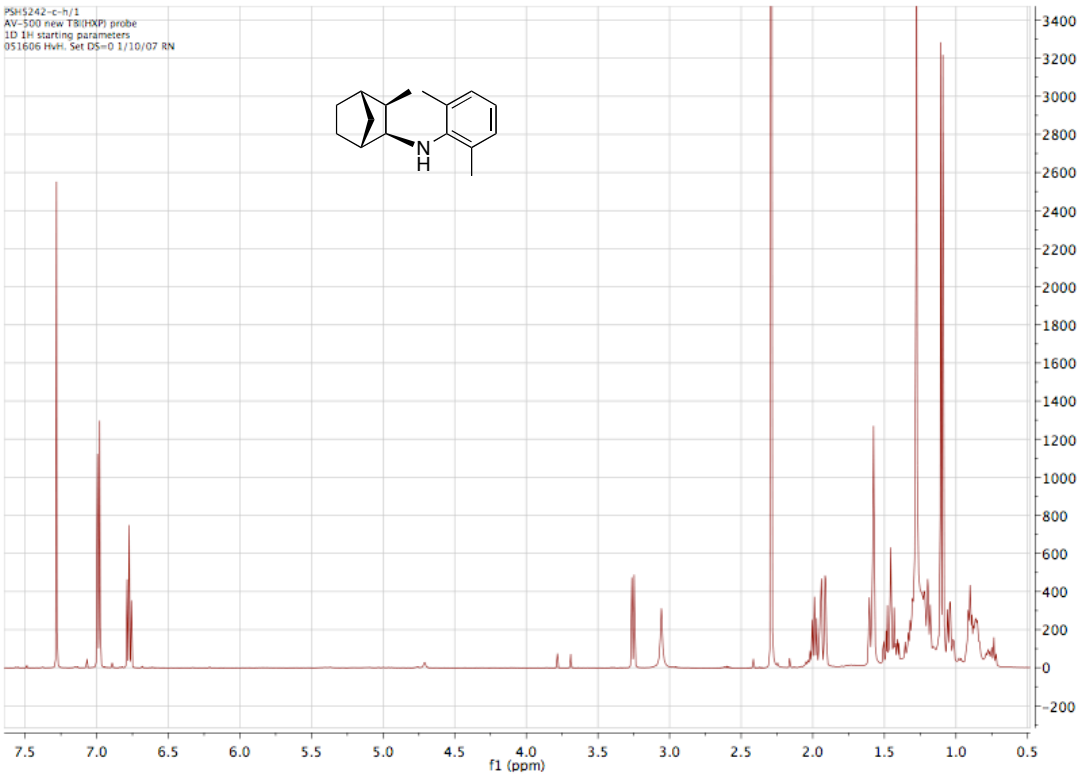
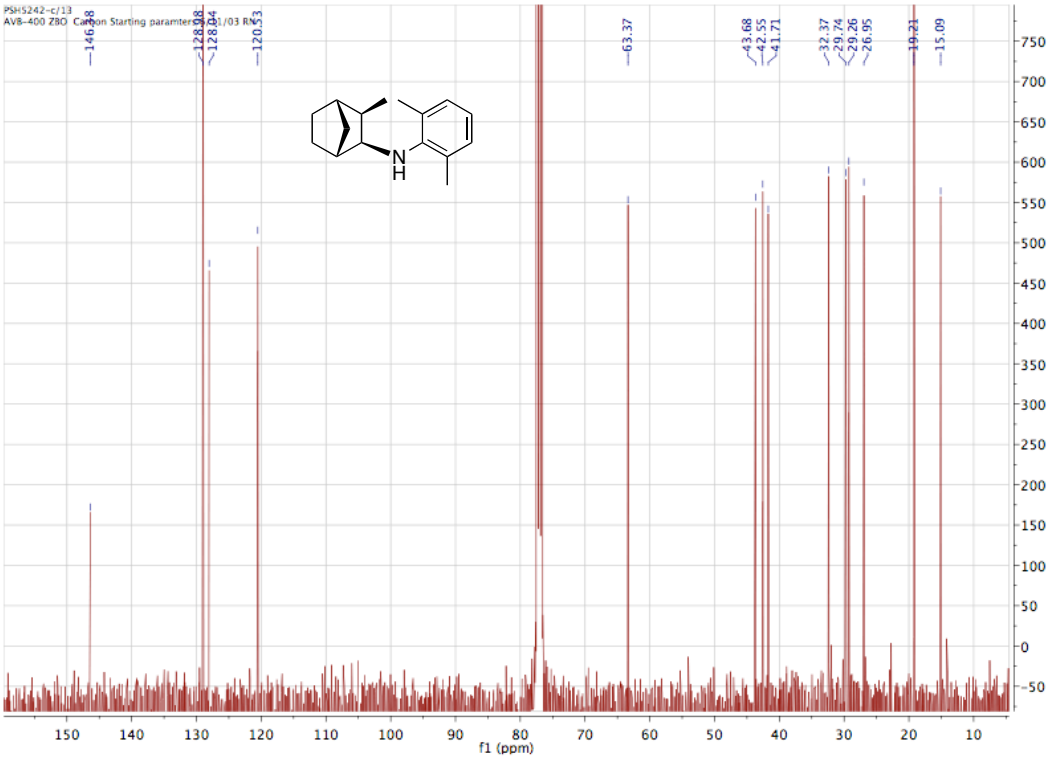
140
130
120
110
100
90
80
70
60
50
40
30
20
10
f1 (ppm)

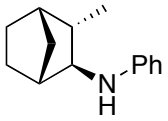

PSH5242-c-h/1
AV-500 new TBI(HXP) probe
1D 1H starting parameters
051606 HvH. Set DS=0 1/10/07 RN
N
H
f1 (ppm)


PSH5242-c/13
AV8-400 ZBO Carbon Starting paramters 02/03 RN
146.88
128.88
128.64
120.53
63.37
43.68
42.55
41.71
32.37
29.74
29.26
26.95
19.21
15.09
N
H
f1 (ppm)

Computational Details

Computations of the relative ground state free energies of the norbornylamine products were conducted with density functional theory with the Gaussian 09 package.[5] The B3LYP functional with polarized triple- basis sets was used.

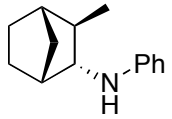
6



C	-2.200749	1.811536	-0.270478
C	-1.175489	1.024110	0.576922
C	-0.728934	-0.216805	-0.256311
C	-1.971149	-1.166495	-0.163267
C	-3.005536	-0.308267	0.613388
C	-3.467948	0.896927	-0.237243
C	-2.086712	0.381496	1.643371
H	-1.839049	1.992389	-1.286924
H	-2.405321	2.787430	0.176734
H	-0.339160	1.621691	0.940079
H	-0.561178	0.075075	-1.297694
H	-3.827830	-0.900579	1.020266
H	-4.304501	1.402937	0.251659
H	-3.810400	0.609385	-1.232908
H	-1.564222	-0.322666	2.297628
H	-2.603485	1.115334	2.267992
H	-1.698454	-2.000996	0.495775
C	-2.415093	-1.768112	-1.495549
H	-1.610585	-2.370855	-1.926076
H	-2.678055	-0.999688	-2.227285
H	-3.285996	-2.417822	-1.365767
N	0.470076	-0.895450	0.203918
H	0.339502	-1.528231	0.978211
C	1.756462	-0.390419	0.074265

C	2.062691	0.717429	-0.736222
C	3.380506	1.147161	-0.874942
C	4.422269	0.506059	-0.211790
C	4.123869	-0.587581	0.602861
C	2.817466	-1.030772	0.745386
H	1.275631	1.246657	-1.257516
H	3.588213	2.002675	-1.509027
H	5.443554	0.850003	-0.322401
H	4.918154	-1.102813	1.132561
H	2.602723	-1.889381	1.374914

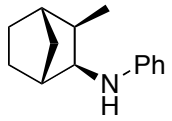
7



C	-3.151942	-0.892169	-1.001991
C	-2.904007	0.568874	-0.561939
C	-1.389182	0.878352	-0.697909
C	-0.770467	0.091264	0.528031
C	-2.001066	-0.634168	1.132767
C	-2.525619	-1.721168	0.165733
C	-3.079144	0.455751	0.969619
C	-1.068690	2.375689	-0.699817
H	-2.693509	-1.111149	-1.969943
H	-4.222035	-1.094733	-1.096726
H	-3.544175	1.294543	-1.067929
H	-1.000481	0.443131	-1.624546
H	-1.816963	-0.996429	2.145068
H	-3.282760	-2.327731	0.668866
H	-1.753522	-2.419403	-0.167435
H	-2.848724	1.377815	1.509402

H	-4.077258	0.120921	1.264782
H	-1.536799	2.874100	-1.554285
H	0.008465	2.548631	-0.763904
H	-1.432772	2.867027	0.208361
N	0.337438	-0.800247	0.246115
H	0.096016	-1.614460	-0.297487
H	-0.423264	0.812012	1.272287
C	1.668349	-0.420875	0.124825
C	2.164747	0.818856	0.566261
C	3.522466	1.113323	0.466987
C	4.422203	0.201174	-0.076130
C	3.936769	-1.028872	-0.522022
C	2.587876	-1.337182	-0.425010
H	1.496111	1.556657	0.989081
H	3.875180	2.077499	0.817868
H	5.475779	0.441018	-0.153039
H	4.616204	-1.757965	-0.950665
H	2.228684	-2.302846	-0.768997

8



C	3.644953	0.323905	0.841331
C	2.896864	0.665812	-0.466016
C	1.454103	1.125491	-0.114011
C	0.758246	-0.233789	0.328954
C	1.910921	-1.259171	0.188270
C	2.944279	-0.992154	1.307424
C	2.657339	-0.738882	-1.058408
C	0.764361	1.853988	-1.268937

N	-0.388817	-0.627678	-0.477981
H	3.570466	1.126918	1.578850
H	4.707991	0.156206	0.648745
H	3.427185	1.373024	-1.106659
H	1.487062	1.804353	0.745148
H	0.438760	-0.171054	1.374393
H	1.556083	-2.291959	0.160558
H	3.656300	-1.818606	1.370989
H	2.470172	-0.897125	2.287445
H	2.048838	-0.733424	-1.965871
H	3.583210	-1.283698	-1.263328
H	1.296661	2.783440	-1.492566
H	-0.269343	2.107998	-1.026067
H	0.743243	1.248791	-2.177841
H	-0.263408	-1.463486	-1.027596
C	-1.703465	-0.342070	-0.146997
C	-2.047535	0.659465	0.779272
C	-3.384420	0.924227	1.068140
C	-4.409771	0.216194	0.448866
C	-4.075167	-0.774784	-0.475794
C	-2.748673	-1.053033	-0.770428
H	-1.273787	1.239714	1.265701
H	-3.621172	1.701822	1.786728
H	-5.446732	0.430365	0.677729
H	-4.856925	-1.340885	-0.971087
H	-2.505094	-1.829848	-1.489400

Computations of the alkylpalladium amido complex **2f** were conducted at the Department of Chemistry and Center for Advanced Scientific Computing and Modeling, University of North Texas, Denton, TX, 76203. The Dipp substituents of SIPr and the methyl groups of the anilido ligand were modeled with the UFF force field,[6] while the remainder of the complex was modeled with the M06 functional in conjunction with the 6-311++G(d,p) basis set for main group atoms and the Stevens pseudopotentials and valence basis sets[7] for palladium. QM/MM calculations employed the ONION formalism.[8] Initial conformational searches were performed at a lower level of theory to identify the lowest energy conformations of the various stationary points.

Ground State **2f**

Pd	-0.117956000	-0.717837000	-0.061356000
C	0.612173000	1.152437000	0.403411000
N	1.780641000	1.508566000	0.977118000
N	-0.143898000	2.263132000	0.387900000
N	-1.110248000	-2.518259000	-0.306032000
H	-0.796102000	-3.203971000	0.373901000
C	0.517184000	3.460334000	0.913511000
H	-0.113030000	3.991500000	1.631370000
H	0.778400000	4.154641000	0.106903000
C	1.758946000	2.856985000	1.564210000
H	2.661931000	3.425485000	1.333955000
H	1.659329000	2.804568000	2.655477000
C	-1.445239000	2.286507000	-0.154595000
C	-2.560345000	2.020482000	0.683627000
C	-1.644546000	2.632723000	-1.518059000
C	-3.852915000	2.060063000	0.131009000
C	-2.957843000	2.691877000	-2.019275000
C	-4.046541000	2.400084000	-1.203863000
H	-4.721315000	1.839559000	0.737791000
H	-3.145308000	2.968867000	-3.048148000
H	-5.049498000	2.439408000	-1.609171000

C	2.760906000	0.560153000	1.343246000
C	2.538234000	-0.323270000	2.438267000
C	4.007033000	0.541109000	0.657270000
C	3.531469000	-1.265732000	2.762425000
C	4.977133000	-0.405169000	1.034034000
C	4.730112000	-1.311256000	2.059302000
H	3.387793000	-1.962171000	3.577944000
H	5.940008000	-0.437523000	0.542397000
H	5.486590000	-2.036058000	2.331309000
C	1.287561000	-0.236296000	3.311761000
C	1.650393000	0.104017000	4.762855000
C	0.457018000	-1.522870000	3.243047000
H	0.625188000	0.579658000	2.970366000
H	2.266075000	1.028446000	4.793783000
H	0.726453000	0.284571000	5.353083000
H	2.216023000	-0.722251000	5.242584000
H	0.126307000	-1.702895000	2.200865000
H	1.037253000	-2.400432000	3.597086000
H	-0.451839000	-1.424820000	3.874092000
C	-2.389761000	1.724002000	2.170737000
C	-2.811429000	0.289715000	2.499013000
C	-3.152526000	2.736108000	3.034998000
H	-1.326651000	1.813516000	2.468224000
H	-2.186640000	-0.420011000	1.919994000
H	-2.653986000	0.081453000	3.578678000
H	-3.881190000	0.117795000	2.256236000
H	-2.854133000	3.770698000	2.760874000
H	-4.250476000	2.631090000	2.908420000
H	-2.908630000	2.578567000	4.107452000
C	-0.476419000	2.982310000	-2.435825000
C	-0.500474000	4.471214000	-2.799795000

C	-0.468705000	2.115006000	-3.700383000
H	0.490867000	2.790504000	-1.927391000
H	-0.494858000	5.089834000	-1.877283000
H	0.398708000	4.731528000	-3.398118000
H	-1.405736000	4.723138000	-3.392202000
H	-0.553756000	1.047140000	-3.424838000
H	-1.308476000	2.375290000	-4.378248000
H	0.484297000	2.257767000	-4.253399000
C	4.346044000	1.571256000	-0.419395000
C	4.807225000	0.919699000	-1.730481000
C	5.410845000	2.548247000	0.093946000
H	3.450520000	2.174145000	-0.677014000
H	4.047031000	0.204756000	-2.093400000
H	4.940491000	1.697829000	-2.512142000
H	5.772119000	0.385868000	-1.606660000
H	5.075988000	3.017915000	1.042943000
H	6.374505000	2.026711000	0.276973000
H	5.579936000	3.354722000	-0.651218000
C	-2.457614000	-2.242534000	-0.218767000
C	-2.990395000	-1.352859000	-1.182566000
C	-3.372662000	-2.762976000	0.737105000
C	-4.322231000	-0.998192000	-1.209792000
H	-2.309849000	-0.969011000	-1.939601000
C	-4.713569000	-2.387574000	0.689034000
C	-5.212823000	-1.502656000	-0.263264000
H	-4.659932000	-0.324977000	-1.994771000
H	-5.402874000	-2.787833000	1.431800000
C	-2.899589000	-3.696120000	1.823082000
H	-2.475326000	-4.616215000	1.369242000
H	-2.122411000	-3.193724000	2.436381000
H	-3.727979000	-3.997043000	2.499060000

C	-6.660159000	-1.106877000	-0.252784000
H	-6.889465000	-0.393087000	-1.072504000
H	-7.295181000	-2.008615000	-0.380202000
H	-6.905829000	-0.621536000	0.715254000
C	1.351511000	-1.172442000	-1.478015000
C	0.740283000	-1.572165000	-2.824956000
C	2.357849000	-2.308406000	-1.168331000
H	1.839555000	-0.197507000	-1.545362000
C	0.827807000	-3.096367000	-2.815824000
C	1.803623000	-1.223198000	-3.884330000
H	-0.249099000	-1.163787000	-3.029853000
C	2.320311000	-3.120208000	-2.480729000
H	3.356036000	-1.869666000	-1.022971000
H	0.609661000	-3.533048000	-3.797881000
H	0.169918000	-3.538785000	-2.064606000
H	1.379785000	-1.333740000	-4.889506000
H	2.162989000	-0.192043000	-3.795441000
C	2.906293000	-2.281567000	-3.622394000
H	2.780541000	-4.108323000	-2.371922000
H	3.071302000	-2.903049000	-4.509378000
H	3.874086000	-1.841517000	-3.356978000
C	2.080685000	-3.214569000	0.021049000
H	2.932692000	-3.884470000	0.185900000
H	1.195804000	-3.834762000	-0.147277000
H	1.912756000	-2.643831000	0.935508000

Transition State **2f**

Pd	-0.355200000	0.239651000	-0.336865000
C	1.432038000	0.639396000	0.621613000
N	2.288925000	-0.045013000	1.408738000
N	1.727907000	1.940214000	0.828407000

N	-2.283108000	0.199326000	-1.046902000
C	2.889022000	2.182884000	1.688333000
C	3.115049000	0.793519000	2.284797000
C	1.100371000	2.959094000	0.082959000
C	1.539800000	3.255249000	-1.236138000
C	0.026052000	3.688334000	0.655962000
C	0.882677000	4.266404000	-1.960814000
C	-0.584504000	4.707860000	-0.096584000
C	-0.163403000	4.986405000	-1.392776000
C	2.410279000	-1.448608000	1.368231000
C	3.373460000	-2.047546000	0.511698000
C	1.598991000	-2.261382000	2.205087000
C	3.469766000	-3.450157000	0.470584000
C	1.758878000	-3.658691000	2.158503000
C	2.671254000	-4.243762000	1.286996000
C	4.325547000	-1.208362000	-0.336738000
C	4.103997000	-1.450283000	-1.832716000
C	5.786575000	-1.467015000	0.051861000
C	2.702559000	2.508407000	-1.883285000
C	3.836134000	3.465465000	-2.271982000
C	2.229012000	1.692071000	-3.089936000
C	-0.484001000	3.386202000	2.061339000
C	-1.970851000	3.010567000	2.043114000
C	-0.227663000	4.567992000	3.003099000
C	0.570127000	-1.658135000	3.154804000
C	1.015360000	-1.829193000	4.610923000
C	-0.824167000	-2.263667000	2.936341000
C	-3.454548000	0.007008000	-0.342503000
C	-3.340116000	-0.296897000	1.025200000
C	-4.759304000	0.072176000	-0.889575000
C	-4.438444000	-0.535719000	1.822881000

C	-5.857784000	-0.146951000	-0.058322000
C	-5.724688000	-0.460717000	1.290910000
C	-4.986343000	0.393923000	-2.345748000
C	-6.941457000	-0.700812000	2.136594000
C	-1.478432000	-1.668345000	-1.350467000
C	-0.240316000	-2.560400000	-1.080528000
C	-1.737795000	-1.861676000	-2.861716000
C	0.469386000	-2.616722000	-2.427725000
C	-0.808302000	-3.988324000	-0.986146000
C	-0.787961000	-3.029352000	-3.196568000
C	-1.233990000	-4.286732000	-2.442590000
C	-1.441110000	-0.666857000	-3.770747000
H	-2.401292000	0.493053000	-2.005315000
H	2.678843000	2.931495000	2.456593000
H	3.753611000	2.525903000	1.105390000
H	4.168272000	0.500595000	2.271859000
H	2.758146000	0.735252000	3.320384000
H	1.184478000	4.507585000	-2.971556000
H	-1.399024000	5.287912000	0.316925000
H	-0.651434000	5.767339000	-1.961736000
H	4.182148000	-3.936634000	-0.182568000
H	1.169107000	-4.305075000	2.794571000
H	2.769527000	-5.321189000	1.253475000
H	4.151400000	-0.127690000	-0.169997000
H	4.779554000	-0.799839000	-2.428426000
H	4.298616000	-2.508366000	-2.106693000
H	3.060787000	-1.191522000	-2.100141000
H	6.093031000	-2.504789000	-0.197074000
H	6.454273000	-0.764588000	-0.491452000
H	5.924766000	-1.302060000	1.141897000
H	3.146775000	1.784028000	-1.174772000

H	4.715448000	2.886685000	-2.627474000
H	3.522575000	4.157125000	-3.081803000
H	4.148910000	4.061897000	-1.388257000
H	1.448710000	0.971848000	-2.768009000
H	1.812810000	2.347735000	-3.883466000
H	3.076318000	1.114447000	-3.517030000
H	0.050023000	2.514337000	2.493592000
H	-2.150542000	2.224623000	1.282168000
H	-2.276250000	2.614854000	3.035296000
H	-2.607916000	3.887894000	1.803845000
H	-0.533224000	4.302824000	4.037793000
H	0.855041000	4.816752000	3.013786000
H	-0.798589000	5.466029000	2.685182000
H	0.467752000	-0.567456000	2.976668000
H	0.293492000	-1.328902000	5.291294000
H	1.076998000	-2.903730000	4.885932000
H	2.013094000	-1.363911000	4.760214000
H	-0.874087000	-3.311720000	3.298737000
H	-1.584602000	-1.671507000	3.488892000
H	-1.083653000	-2.251859000	1.857656000
H	-2.336331000	-0.292930000	1.442315000
H	-4.274515000	-0.762874000	2.873586000
H	-6.860815000	-0.082387000	-0.477412000
H	-4.536703000	1.379212000	-2.589901000
H	-4.528676000	-0.392948000	-2.978403000
H	-6.067868000	0.442014000	-2.594167000
H	-7.520283000	-1.553804000	1.723984000
H	-6.664398000	-0.937202000	3.186015000
H	-7.581224000	0.206707000	2.136460000
H	-2.303229000	-1.997685000	-0.718203000
H	0.355058000	-2.277341000	-0.219838000

H	-2.783603000	-2.165109000	-3.011456000
H	0.874438000	-1.653445000	-2.745834000
H	1.264038000	-3.371210000	-2.457271000
H	-0.017088000	-4.671379000	-0.653314000
H	-1.629139000	-4.064959000	-0.266403000
H	-0.673191000	-3.175258000	-4.274993000
H	-0.727287000	-5.176007000	-2.832275000
H	-2.311948000	-4.457400000	-2.542818000
H	-0.583560000	-0.087710000	-3.417188000
H	-1.222831000	-1.013175000	-4.786469000
H	-2.288555000	0.020001000	-3.858062000

Crystallographic Data for 1

Table S1. Crystal data and structure refinement for **1**.

Identification code	**1**	
Empirical formula	$C_{40}H_{63}ClN_2Pd$	
Formula weight	713.77	
Temperature	193(2) K	
Wavelength	1.54178 Å	
Crystal system	Orthorhombic	
Space group	P 21 21 21	
Unit cell dimensions	a = 9.7615(3) Å	a= 90°.
	b = 13.4772(5) Å	b= 90°.
	c = 29.0572(13) Å	g = 90°.
Volume	3822.7(3) $Å^3$	
Z	4	
Density (calculated)	1.240 Mg/m^3	
Absorption coefficient	4.753 mm^{-1}	
F(000)	1520	
Crystal size	0.42 x 0.134 x 0.045 mm^3	
Theta range for data collection	4.47 to 67.54°.	
Index ranges	-11<=h<=11, -16<=k<=15, -20<=l<=34	
Reflections collected	30073	
Independent reflections	6751 [R(int) = 0.1238]	
Completeness to theta = 67.54°	99.1 %	
Absorption correction	Integration	
Max. and min. transmission	0.8439 and 0.3790	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6751 / 364 / 457	
Goodness-of-fit on F^2	1.058	
Final R indices [I>2sigma(I)]	R1 = 0.0586, wR2 = 0.1453	
R indices (all data)	R1 = 0.0694, wR2 = 0.1540	

Absolute structure parameter	0.444(9)
Largest diff. peak and hole	0.709 and -1.677 e.Å^{-3}

Table S2. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **1**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	9133(1)	7726(1)	8314(1)	47(1)
Cl(1)	11371(1)	7484(1)	8052(1)	71(1)
N(1)	6269(3)	7114(2)	8256(2)	54(1)
N(2)	6368(3)	8692(2)	8426(1)	50(1)
C(1)	9213(5)	8010(3)	8994(2)	57(1)
C(2)	9890(5)	7122(4)	9244(2)	70(1)
C(3)	9462(6)	7227(5)	9759(2)	86(2)
C(4)	10282(6)	8122(5)	9925(2)	83(2)
C(5)	11089(5)	8436(4)	9492(2)	75(1)
C(6)	10096(5)	8928(4)	9139(2)	60(1)
C(7)	11369(5)	7433(4)	9265(2)	70(1)
C(8)	10837(6)	9498(4)	8785(2)	70(2)
C(1B)	9198(10)	7643(6)	9007(2)	64(2)
C(2B)	9990(9)	8482(7)	9256(3)	67(2)
C(3B)	9586(13)	8412(9)	9774(3)	79(2)
C(4B)	10337(15)	7489(9)	9946(3)	79(2)
C(5B)	11027(10)	7091(6)	9504(3)	72(2)
C(6B)	9925(10)	6671(6)	9169(4)	68(2)
C(7B)	11421(9)	8063(8)	9266(5)	71(2)
C(8B)	10500(20)	5970(10)	8832(5)	72(5)
C(9)	7120(3)	7869(3)	8354(2)	43(1)
C(10)	4829(4)	7454(3)	8233(2)	69(2)
C(11)	4929(4)	8540(3)	8336(2)	61(1)
C(12)	6643(4)	6129(3)	8128(2)	54(1)
C(13)	6569(5)	5364(3)	8442(2)	61(2)
C(14)	6876(5)	4414(3)	8305(2)	72(2)

C(15)	7263(5)	4219(4)	7861(2)	69(2)
C(16)	7326(5)	4963(4)	7555(2)	66(2)
C(17)	6993(5)	5952(3)	7663(2)	59(1)
C(18)	6104(6)	5552(4)	8937(2)	70(2)
C(19)	7052(7)	5051(5)	9284(3)	95(2)
C(20)	4614(6)	5182(6)	9001(3)	88(2)
C(21)	7010(3)	6759(4)	7304(2)	66(2)
C(22)	5660(8)	6850(30)	7030(4)	91(5)
C(23)	8241(8)	7098(18)	7010(5)	70(5)
C(22B)	6062(6)	6526(6)	6892(2)	85(2)
C(23B)	8494(5)	6912(6)	7137(3)	78(2)
C(24)	6911(4)	9683(3)	8450(2)	50(1)
C(25)	7529(4)	10107(3)	8058(2)	53(1)
C(26)	7986(5)	11085(3)	8091(2)	63(1)
C(27)	7838(5)	11628(4)	8486(2)	69(2)
C(28)	7210(5)	11209(4)	8862(2)	68(2)
C(29)	6702(5)	10220(3)	8857(2)	59(1)
C(30)	7690(5)	9555(3)	7590(2)	61(1)
C(31)	9138(5)	9641(4)	7406(2)	68(1)
C(32)	6662(5)	9956(5)	7247(2)	77(2)
C(33)	5987(5)	9795(4)	9271(2)	64(1)
C(34)	6753(7)	9970(5)	9722(2)	86(2)
C(35)	4603(6)	10251(5)	9318(2)	87(2)

Table S3. Bond lengths [Å] and angles [°] for **1**.

Pd(1)-C(9)	1.978(3)
Pd(1)-C(1)	2.014(4)
Pd(1)-C(1B)	2.016(7)
Pd(1)-Cl(1)	2.3364(11)
N(1)-C(9)	1.344(5)
N(1)-C(12)	1.426(6)
N(1)-C(10)	1.480(5)
N(2)-C(9)	1.346(5)
N(2)-C(24)	1.439(5)
N(2)-C(11)	1.443(5)
C(1)-C(2)	1.549(7)
C(1)-C(6)	1.565(6)
C(1)-H(1A)	1.0000
C(2)-C(7)	1.504(7)
C(2)-C(3)	1.560(7)
C(2)-H(2A)	1.0000
C(3)-C(4)	1.526(9)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.544(7)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(7)	1.530(7)
C(5)-C(6)	1.561(7)
C(5)-H(5A)	1.0000
C(6)-C(8)	1.472(8)
C(6)-H(6A)	1.0000
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900

C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(1B)-C(2B)	1.549(9)
C(1B)-C(6B)	1.564(9)
C(1B)-H(1B)	1.0000
C(2B)-C(7B)	1.506(10)
C(2B)-C(3B)	1.559(10)
C(2B)-H(2B)	1.0000
C(3B)-C(4B)	1.528(11)
C(3B)-H(3C)	0.9900
C(3B)-H(3D)	0.9900
C(4B)-C(5B)	1.544(10)
C(4B)-H(4C)	0.9900
C(4B)-H(4D)	0.9900
C(5B)-C(7B)	1.530(10)
C(5B)-C(6B)	1.557(10)
C(5B)-H(5B)	1.0000
C(6B)-C(8B)	1.474(11)
C(6B)-H(6B)	1.0000
C(7B)-H(7C)	0.9900
C(7B)-H(7D)	0.9900
C(8B)-H(8D)	0.9800
C(8B)-H(8E)	0.9800
C(8B)-H(8F)	0.9800
C(10)-C(11)	1.497(6)
C(10)-H(10A)	0.9900
C(10)-H(10B)	0.9900
C(11)-H(11A)	0.9900
C(11)-H(11B)	0.9900
C(12)-C(13)	1.379(7)

C(12)-C(17)	1.413(8)
C(13)-C(14)	1.373(7)
C(13)-C(18)	1.529(8)
C(14)-C(15)	1.371(9)
C(14)-H(14A)	0.9500
C(15)-C(16)	1.340(8)
C(15)-H(15A)	0.9500
C(16)-C(17)	1.407(7)
C(16)-H(16A)	0.9500
C(17)-C(21)	1.507(8)
C(18)-C(19)	1.526(9)
C(18)-C(20)	1.549(8)
C(18)-H(18A)	1.0000
C(19)-H(19A)	0.9800
C(19)-H(19B)	0.9800
C(19)-H(19C)	0.9800
C(20)-H(20A)	0.9800
C(20)-H(20B)	0.9800
C(20)-H(20C)	0.9800
C(21)-C(23B)	1.542(6)
C(21)-C(22)	1.543(8)
C(21)-C(23)	1.544(8)
C(21)-C(22B)	1.546(6)
C(21)-H(21A)	1.0000
C(21)-H(21B)	0.9602
C(22)-H(22A)	0.9800
C(22)-H(22B)	0.9800
C(22)-H(22C)	0.9800
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800

C(22B)-H(22D)	0.9800
C(22B)-H(22E)	0.9800
C(22B)-H(22F)	0.9800
C(23B)-H(23D)	0.9800
C(23B)-H(23E)	0.9800
C(23B)-H(23F)	0.9800
C(24)-C(29)	1.401(7)
C(24)-C(25)	1.411(7)
C(25)-C(26)	1.396(6)
C(25)-C(30)	1.556(8)
C(26)-C(27)	1.369(8)
C(26)-H(26A)	0.9500
C(27)-C(28)	1.374(8)
C(27)-H(27A)	0.9500
C(28)-C(29)	1.423(7)
C(28)-H(28A)	0.9500
C(29)-C(33)	1.503(8)
C(30)-C(32)	1.516(8)
C(30)-C(31)	1.516(7)
C(30)-H(30A)	1.0000
C(31)-H(31A)	0.9800
C(31)-H(31B)	0.9800
C(31)-H(31C)	0.9800
C(32)-H(32A)	0.9800
C(32)-H(32B)	0.9800
C(32)-H(32C)	0.9800
C(33)-C(35)	1.491(8)
C(33)-C(34)	1.526(8)
C(33)-H(33A)	1.0000
C(34)-H(34A)	0.9800
C(34)-H(34B)	0.9800

C(34)-H(34C)	0.9800
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800

C(9)-Pd(1)-C(1)	87.89(18)
C(9)-Pd(1)-C(1B)	88.8(3)
C(1)-Pd(1)-C(1B)	14.2(3)
C(9)-Pd(1)-Cl(1)	164.07(13)
C(1)-Pd(1)-Cl(1)	108.04(14)
C(1B)-Pd(1)-Cl(1)	106.7(3)
C(9)-N(1)-C(12)	127.0(3)
C(9)-N(1)-C(10)	111.2(3)
C(12)-N(1)-C(10)	121.3(3)
C(9)-N(2)-C(24)	124.9(3)
C(9)-N(2)-C(11)	112.7(3)
C(24)-N(2)-C(11)	119.9(3)
C(2)-C(1)-C(6)	104.5(4)
C(2)-C(1)-Pd(1)	109.3(3)
C(6)-C(1)-Pd(1)	115.8(3)
C(2)-C(1)-H(1A)	109.0
C(6)-C(1)-H(1A)	109.0
Pd(1)-C(1)-H(1A)	109.0
C(7)-C(2)-C(1)	102.3(4)
C(7)-C(2)-C(3)	101.2(4)
C(1)-C(2)-C(3)	105.4(4)
C(7)-C(2)-H(2A)	115.4
C(1)-C(2)-H(2A)	115.4
C(3)-C(2)-H(2A)	115.4
C(4)-C(3)-C(2)	103.6(5)
C(4)-C(3)-H(3A)	111.0

C(2)-C(3)-H(3A)	111.0
C(4)-C(3)-H(3B)	111.0
C(2)-C(3)-H(3B)	111.0
H(3A)-C(3)-H(3B)	109.0
C(3)-C(4)-C(5)	103.1(4)
C(3)-C(4)-H(4A)	111.2
C(5)-C(4)-H(4A)	111.2
C(3)-C(4)-H(4B)	111.2
C(5)-C(4)-H(4B)	111.2
H(4A)-C(4)-H(4B)	109.1
C(7)-C(5)-C(4)	101.6(5)
C(7)-C(5)-C(6)	101.6(4)
C(4)-C(5)-C(6)	109.6(4)
C(7)-C(5)-H(5A)	114.2
C(4)-C(5)-H(5A)	114.2
C(6)-C(5)-H(5A)	114.2
C(8)-C(6)-C(5)	112.0(4)
C(8)-C(6)-C(1)	119.7(4)
C(5)-C(6)-C(1)	100.6(4)
C(8)-C(6)-H(6A)	108.0
C(5)-C(6)-H(6A)	108.0
C(1)-C(6)-H(6A)	108.0
C(2)-C(7)-C(5)	95.3(4)
C(2)-C(7)-H(7A)	112.7
C(5)-C(7)-H(7A)	112.7
C(2)-C(7)-H(7B)	112.7
C(5)-C(7)-H(7B)	112.7
H(7A)-C(7)-H(7B)	110.2
C(2B)-C(1B)-C(6B)	104.1(6)
C(2B)-C(1B)-Pd(1)	116.2(6)
C(6B)-C(1B)-Pd(1)	111.3(6)

C(2B)-C(1B)-H(1B)	108.3
C(6B)-C(1B)-H(1B)	108.3
Pd(1)-C(1B)-H(1B)	108.3
C(7B)-C(2B)-C(1B)	101.4(7)
C(7B)-C(2B)-C(3B)	101.1(7)
C(1B)-C(2B)-C(3B)	106.3(7)
C(7B)-C(2B)-H(2B)	115.4
C(1B)-C(2B)-H(2B)	115.4
C(3B)-C(2B)-H(2B)	115.4
C(4B)-C(3B)-C(2B)	104.1(7)
C(4B)-C(3B)-H(3C)	110.9
C(2B)-C(3B)-H(3C)	110.9
C(4B)-C(3B)-H(3D)	110.9
C(2B)-C(3B)-H(3D)	110.9
H(3C)-C(3B)-H(3D)	109.0
C(3B)-C(4B)-C(5B)	102.7(7)
C(3B)-C(4B)-H(4C)	111.2
C(5B)-C(4B)-H(4C)	111.2
C(3B)-C(4B)-H(4D)	111.2
C(5B)-C(4B)-H(4D)	111.2
H(4C)-C(4B)-H(4D)	109.1
C(7B)-C(5B)-C(4B)	100.9(7)
C(7B)-C(5B)-C(6B)	101.6(7)
C(4B)-C(5B)-C(6B)	110.1(8)
C(7B)-C(5B)-H(5B)	114.2
C(4B)-C(5B)-H(5B)	114.2
C(6B)-C(5B)-H(5B)	114.2
C(8B)-C(6B)-C(5B)	112.7(9)
C(8B)-C(6B)-C(1B)	120.6(9)
C(5B)-C(6B)-C(1B)	101.4(6)
C(8B)-C(6B)-H(6B)	107.1

C(5B)-C(6B)-H(6B)	107.1
C(1B)-C(6B)-H(6B)	107.1
C(2B)-C(7B)-C(5B)	95.6(6)
C(2B)-C(7B)-H(7C)	112.6
C(5B)-C(7B)-H(7C)	112.6
C(2B)-C(7B)-H(7D)	112.6
C(5B)-C(7B)-H(7D)	112.6
H(7C)-C(7B)-H(7D)	110.1
C(6B)-C(8B)-H(8D)	109.5
C(6B)-C(8B)-H(8E)	109.5
H(8D)-C(8B)-H(8E)	109.5
C(6B)-C(8B)-H(8F)	109.5
H(8D)-C(8B)-H(8F)	109.5
H(8E)-C(8B)-H(8F)	109.5
N(1)-C(9)-N(2)	108.7(3)
N(1)-C(9)-Pd(1)	121.9(3)
N(2)-C(9)-Pd(1)	129.1(3)
N(1)-C(10)-C(11)	103.4(3)
N(1)-C(10)-H(10A)	111.1
C(11)-C(10)-H(10A)	111.1
N(1)-C(10)-H(10B)	111.1
C(11)-C(10)-H(10B)	111.1
H(10A)-C(10)-H(10B)	109.1
N(2)-C(11)-C(10)	103.8(3)
N(2)-C(11)-H(11A)	111.0
C(10)-C(11)-H(11A)	111.0
N(2)-C(11)-H(11B)	111.0
C(10)-C(11)-H(11B)	111.0
H(11A)-C(11)-H(11B)	109.0
C(13)-C(12)-C(17)	121.2(4)
C(13)-C(12)-N(1)	120.7(5)

C(17)-C(12)-N(1)	117.9(4)
C(14)-C(13)-C(12)	119.7(6)
C(14)-C(13)-C(18)	119.4(5)
C(12)-C(13)-C(18)	120.9(4)
C(15)-C(14)-C(13)	120.7(6)
C(15)-C(14)-H(14A)	119.7
C(13)-C(14)-H(14A)	119.7
C(16)-C(15)-C(14)	119.5(5)
C(16)-C(15)-H(15A)	120.2
C(14)-C(15)-H(15A)	120.2
C(15)-C(16)-C(17)	123.4(6)
C(15)-C(16)-H(16A)	118.3
C(17)-C(16)-H(16A)	118.3
C(16)-C(17)-C(12)	115.4(5)
C(16)-C(17)-C(21)	121.8(5)
C(12)-C(17)-C(21)	122.8(4)
C(19)-C(18)-C(13)	111.6(5)
C(19)-C(18)-C(20)	110.3(5)
C(13)-C(18)-C(20)	109.8(5)
C(19)-C(18)-H(18A)	108.3
C(13)-C(18)-H(18A)	108.3
C(20)-C(18)-H(18A)	108.3
C(18)-C(19)-H(19A)	109.5
C(18)-C(19)-H(19B)	109.5
H(19A)-C(19)-H(19B)	109.5
C(18)-C(19)-H(19C)	109.5
H(19A)-C(19)-H(19C)	109.5
H(19B)-C(19)-H(19C)	109.5
C(18)-C(20)-H(20A)	109.5
C(18)-C(20)-H(20B)	109.5
H(20A)-C(20)-H(20B)	109.5

C(18)-C(20)-H(20C)	109.5
H(20A)-C(20)-H(20C)	109.5
H(20B)-C(20)-H(20C)	109.5
C(17)-C(21)-C(23B)	109.0(4)
C(17)-C(21)-C(22)	113.8(11)
C(23B)-C(21)-C(22)	129.0(7)
C(17)-C(21)-C(23)	127.2(7)
C(22)-C(21)-C(23)	110.9(8)
C(17)-C(21)-C(22B)	112.5(4)
C(23B)-C(21)-C(22B)	110.2(5)
C(23)-C(21)-C(22B)	95.6(7)
C(17)-C(21)-H(21A)	99.5
C(23B)-C(21)-H(21A)	99.7
C(22)-C(21)-H(21A)	99.5
C(23)-C(21)-H(21A)	99.5
C(22B)-C(21)-H(21A)	124.5
C(17)-C(21)-H(21B)	107.8
C(23B)-C(21)-H(21B)	111.7
C(22)-C(21)-H(21B)	80.4
C(23)-C(21)-H(21B)	106.0
C(22B)-C(21)-H(21B)	105.6
C(21)-C(22)-H(22A)	109.5
C(21)-C(22)-H(22B)	109.5
C(21)-C(22)-H(22C)	109.5
C(21)-C(23)-H(23A)	109.5
C(21)-C(23)-H(23B)	109.5
C(21)-C(23)-H(23C)	109.5
C(21)-C(22B)-H(22D)	109.5
C(21)-C(22B)-H(22E)	109.5
H(22D)-C(22B)-H(22E)	109.5
C(21)-C(22B)-H(22F)	109.5

H(22D)-C(22B)-H(22F)	109.5
H(22E)-C(22B)-H(22F)	109.5
C(21)-C(23B)-H(23D)	109.5
C(21)-C(23B)-H(23E)	109.5
H(23D)-C(23B)-H(23E)	109.5
C(21)-C(23B)-H(23F)	109.5
H(23D)-C(23B)-H(23F)	109.5
H(23E)-C(23B)-H(23F)	109.5
C(29)-C(24)-C(25)	122.4(4)
C(29)-C(24)-N(2)	117.9(4)
C(25)-C(24)-N(2)	119.5(4)
C(26)-C(25)-C(24)	117.6(5)
C(26)-C(25)-C(30)	118.6(5)
C(24)-C(25)-C(30)	123.7(4)
C(27)-C(26)-C(25)	121.9(5)
C(27)-C(26)-H(26A)	119.0
C(25)-C(26)-H(26A)	119.0
C(26)-C(27)-C(28)	119.6(5)
C(26)-C(27)-H(27A)	120.2
C(28)-C(27)-H(27A)	120.2
C(27)-C(28)-C(29)	122.2(6)
C(27)-C(28)-H(28A)	118.9
C(29)-C(28)-H(28A)	118.9
C(24)-C(29)-C(28)	116.1(5)
C(24)-C(29)-C(33)	123.1(4)
C(28)-C(29)-C(33)	120.8(5)
C(32)-C(30)-C(31)	110.9(5)
C(32)-C(30)-C(25)	109.7(4)
C(31)-C(30)-C(25)	111.5(4)
C(32)-C(30)-H(30A)	108.2
C(31)-C(30)-H(30A)	108.2

C(25)-C(30)-H(30A)	108.2
C(30)-C(31)-H(31A)	109.5
C(30)-C(31)-H(31B)	109.5
H(31A)-C(31)-H(31B)	109.5
C(30)-C(31)-H(31C)	109.5
H(31A)-C(31)-H(31C)	109.5
H(31B)-C(31)-H(31C)	109.5
C(30)-C(32)-H(32A)	109.5
C(30)-C(32)-H(32B)	109.5
H(32A)-C(32)-H(32B)	109.5
C(30)-C(32)-H(32C)	109.5
H(32A)-C(32)-H(32C)	109.5
H(32B)-C(32)-H(32C)	109.5
C(35)-C(33)-C(29)	109.7(5)
C(35)-C(33)-C(34)	107.5(5)
C(29)-C(33)-C(34)	113.6(5)
C(35)-C(33)-H(33A)	108.6
C(29)-C(33)-H(33A)	108.6
C(34)-C(33)-H(33A)	108.6
C(33)-C(34)-H(34A)	109.5
C(33)-C(34)-H(34B)	109.5
H(34A)-C(34)-H(34B)	109.5
C(33)-C(34)-H(34C)	109.5
H(34A)-C(34)-H(34C)	109.5
H(34B)-C(34)-H(34C)	109.5
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5

Table S4. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **1**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	35(1)	50(1)	57(1)	-2(1)	-1(1)	2(1)
Cl(1)	40(1)	100(1)	72(1)	-13(1)	4(1)	6(1)
N(1)	35(1)	48(2)	78(3)	-2(2)	-5(2)	-4(1)
N(2)	34(1)	47(2)	68(3)	0(2)	1(2)	2(1)
C(1)	41(2)	72(2)	59(2)	2(2)	1(2)	2(2)
C(2)	62(2)	81(2)	65(2)	5(2)	-2(2)	4(2)
C(3)	77(3)	106(3)	74(3)	13(3)	0(2)	0(3)
C(4)	75(2)	106(3)	70(3)	-1(3)	-6(2)	-2(2)
C(5)	61(2)	93(2)	70(2)	-3(2)	-6(2)	-2(2)
C(6)	54(2)	69(2)	57(3)	-14(2)	-8(2)	-2(2)
C(7)	60(2)	88(3)	62(2)	13(2)	-10(2)	6(2)
C(8)	71(3)	66(3)	75(4)	-10(3)	-19(3)	-8(3)
C(1B)	55(3)	74(3)	63(3)	0(3)	-1(3)	3(3)
C(2B)	58(3)	79(3)	64(3)	-2(3)	-4(3)	0(3)
C(3B)	72(3)	94(3)	72(3)	2(3)	-3(3)	-1(3)
C(4B)	73(3)	92(3)	71(3)	4(3)	-4(3)	-1(3)
C(5B)	66(3)	83(3)	68(3)	4(3)	-5(3)	2(3)
C(6B)	63(4)	76(4)	66(4)	1(4)	-4(3)	3(4)
C(7B)	63(3)	82(3)	67(3)	0(3)	-7(3)	0(3)
C(8B)	70(7)	72(7)	75(8)	-2(6)	4(6)	4(6)
C(9)	38(2)	47(2)	45(2)	-9(2)	-3(2)	0(1)
C(10)	39(2)	61(3)	106(5)	-21(3)	-2(2)	6(2)
C(11)	40(2)	56(2)	86(4)	1(3)	-2(3)	4(2)
C(12)	32(2)	54(2)	77(3)	-17(2)	-2(2)	-5(2)
C(13)	51(2)	52(2)	79(4)	-3(2)	-6(2)	0(2)
C(14)	74(3)	47(2)	93(4)	-7(3)	-11(3)	0(2)

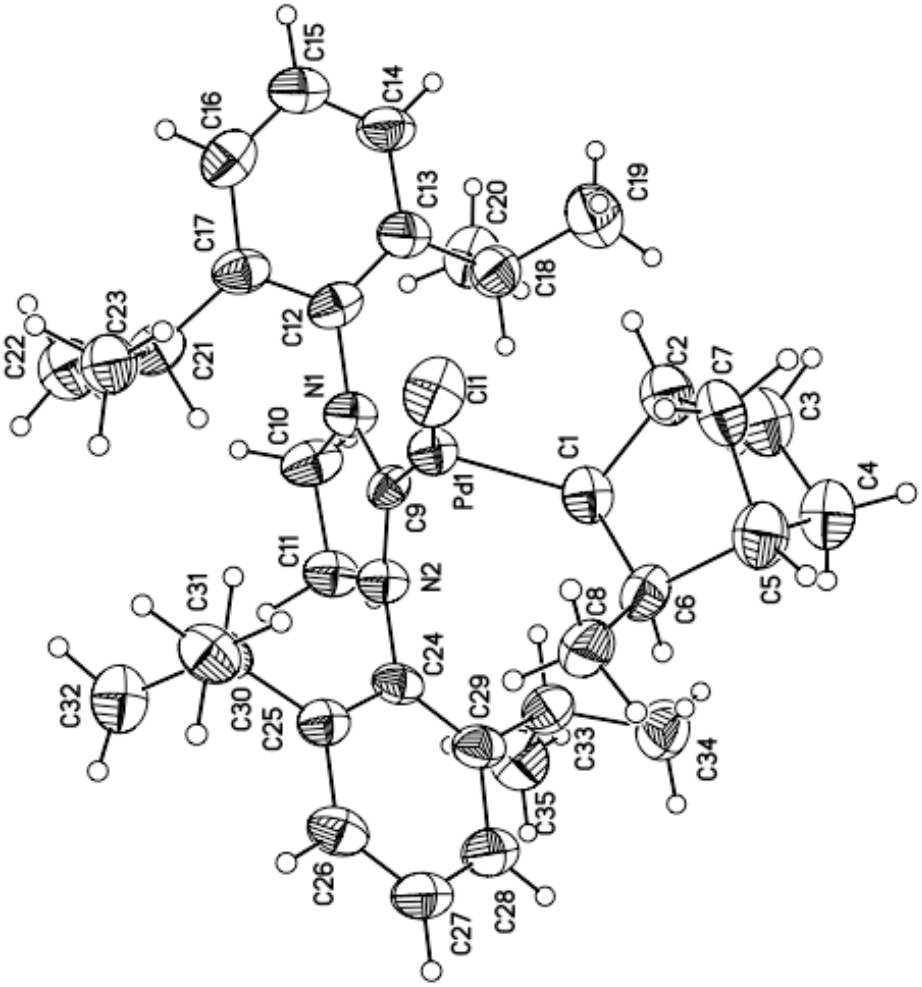
C(15)	65(3)	52(2)	90(4)	-6(3)	1(3)	6(2)
C(16)	49(2)	79(3)	71(4)	-17(3)	1(2)	-8(2)
C(17)	45(2)	50(2)	83(4)	-12(2)	-4(2)	3(2)
C(18)	78(3)	67(3)	65(3)	1(3)	1(3)	-4(3)
C(19)	90(4)	99(4)	96(5)	18(4)	-15(4)	-9(4)
C(20)	71(3)	109(5)	85(4)	-4(4)	11(3)	-5(3)
C(21)	59(2)	63(3)	74(4)	-14(3)	3(3)	-5(2)
C(22)	91(8)	90(8)	91(8)	1(6)	-3(6)	2(6)
C(23)	67(7)	74(7)	68(8)	2(6)	-3(6)	1(6)
C(22B)	82(4)	91(4)	82(4)	-2(3)	-12(3)	-9(3)
C(23B)	67(3)	85(4)	82(4)	11(3)	-2(3)	-5(3)
C(24)	42(2)	40(2)	67(3)	3(2)	-2(2)	8(2)
C(25)	43(2)	49(2)	66(3)	-2(2)	-3(2)	2(2)
C(26)	55(2)	52(2)	83(4)	11(3)	3(3)	-3(2)
C(27)	68(3)	47(2)	93(4)	-2(3)	-6(3)	-1(2)
C(28)	71(3)	54(2)	80(4)	-6(3)	-3(3)	1(2)
C(29)	52(2)	46(2)	78(4)	0(2)	-7(2)	6(2)
C(30)	51(2)	54(2)	77(4)	13(2)	11(2)	4(2)
C(31)	57(2)	71(3)	76(4)	13(3)	8(3)	9(3)
C(32)	53(3)	105(4)	73(4)	-1(3)	-1(3)	8(3)
C(33)	62(3)	64(3)	66(3)	-10(2)	6(3)	0(2)
C(34)	97(4)	93(4)	68(4)	-9(4)	0(4)	9(3)
C(35)	76(3)	99(4)	84(5)	5(4)	18(3)	1(3)

Table S5. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for 1.

	x	y	z	U(eq)
H(1A)	8260	8098	9113	69
H(2A)	9717	6457	9103	83
H(3A)	8465	7348	9788	103
H(3B)	9704	6624	9936	103
H(4A)	10908	7937	10179	100
H(4B)	9668	8661	10031	100
H(5A)	11931	8834	9559	90
H(6A)	9489	9398	9310	72
H(7A)	11789	7500	8956	84
H(7B)	11931	6989	9460	84
H(8A)	11343	10040	8932	106
H(8B)	10181	9772	8564	106
H(8C)	11481	9060	8625	106
H(1B)	8236	7636	9125	77
H(2B)	9902	9156	9115	80
H(3C)	9886	9010	9944	95
H(3D)	8582	8337	9809	95
H(4C)	9689	6998	10075	94
H(4D)	11026	7662	10182	94
H(5B)	11814	6633	9562	87
H(6B)	9250	6293	9360	82
H(7C)	12057	8470	9452	85
H(7D)	11802	7956	8954	85
H(8D)	10438	5293	8953	109
H(8E)	11463	6135	8774	109

H(8F)	9984	6015	8543	109
H(10A)	4257	7109	8465	82
H(10B)	4436	7338	7923	82
H(11A)	4623	8941	8069	73
H(11B)	4370	8717	8608	73
H(14A)	6819	3886	8521	86
H(15A)	7485	3562	7770	83
H(16A)	7611	4816	7250	80
H(18A)	6123	6283	8994	84
H(19A)	8001	5099	9176	142
H(19B)	6797	4351	9315	142
H(19C)	6967	5381	9583	142
H(20A)	4041	5438	8751	132
H(20B)	4259	5418	9297	132
H(20C)	4600	4455	8996	132
H(21A)	6914	7352	7509	79
H(21B)	6644	7350	7442	79
H(22A)	4891	6917	7245	136
H(22B)	5531	6250	6843	136
H(22C)	5702	7431	6830	136
H(23A)	9094	6880	7156	104
H(23B)	8238	7823	6985	104
H(23C)	8172	6805	6702	104
H(22D)	6458	5985	6710	127
H(22E)	5968	7118	6699	127
H(22F)	5158	6326	7006	127
H(23D)	9089	7042	7401	117
H(23E)	8527	7478	6925	117
H(23F)	8808	6313	6977	117
H(26A)	8413	11383	7831	76
H(27A)	8167	12291	8500	83

H(28A)	7112	11594	9134	82
H(30A)	7487	8836	7642	73
H(31A)	9783	9369	7632	102
H(31B)	9354	10340	7349	102
H(31C)	9213	9268	7117	102
H(32A)	5755	9991	7391	116
H(32B)	6622	9515	6979	116
H(32C)	6942	10621	7148	116
H(33A)	5876	9064	9225	77
H(34A)	7721	9797	9682	129
H(34B)	6353	9555	9964	129
H(34C)	6677	10670	9809	129
H(35A)	4066	10118	9040	130
H(35B)	4698	10969	9360	130
H(35C)	4136	9966	9586	130


C15
C16
C14
C13
C20
C19
C17
C18
C23
C12
C22
C21
N1
Cl1
C2
C7
C10
C1
C3
C9
Pd1
C4
C11
N2
C31
C8
C6
C5
C24
C32
C30
C29
C25
C33
C34
C35
C26
C28
C27

Crystallographic Data for 2b

Table S6. Crystal data and structure refinement for **2b**.

Identification code	**2b**	
Empirical formula	$C_{42}H_{59}N_3OPd$	
Formula weight	728.32	
Temperature	193(2) K	
Wavelength	1.54178 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.8298(3) Å	a= 90°.
	b = 15.9470(3) Å	b= 108.1840(10)°.
	c = 19.8577(4) Å	g = 90°.
Volume	3859.92(14) $Å^3$	
Z	4	
Density (calculated)	1.253 Mg/m^3	
Absorption coefficient	4.128 mm^{-1}	
F(000)	1544	
Crystal size	0.378 x 0.198 x 0.064 mm^3	
Theta range for data collection	3.63 to 67.96°.	
Index ranges	-15<=h<=15, -18<=k<=17, -23<=l<=23	
Reflections collected	33291	
Independent reflections	6914 [R(int) = 0.0387]	
Completeness to theta = 67.96°	98.2 %	
Absorption correction	Integration	
Max. and min. transmission	0.8404 and 0.3866	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	6914 / 385 / 530	
Goodness-of-fit on F^2	1.071	
Final R indices [I>2sigma(I)]	R1 = 0.0390, wR2 = 0.1023	
R indices (all data)	R1 = 0.0437, wR2 = 0.1056	

Largest diff. peak and hole	1.499 and -0.491 e.Å^{-3}

Table S7. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3)for **2b**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	2136(1)	1951(1)	4083(1)	35(1)
N(2)	3586(2)	2927(1)	5331(1)	33(1)
N(3)	1868(2)	3287(2)	5019(1)	33(1)
C(1)	2988(3)	2591(2)	3532(2)	42(1)
C(2)	2159(3)	2904(2)	2826(2)	54(1)
C(3)	2774(3)	3595(2)	2544(2)	64(1)
C(4)	3604(4)	3078(3)	2300(2)	68(1)
C(5)	3385(3)	2185(2)	2476(2)	57(1)
C(6)	3810(3)	2056(2)	3291(2)	51(1)
C(7)	2134(3)	2192(3)	2324(2)	62(1)
C(8)	3931(3)	1146(3)	3506(2)	67(1)
N(1)	1347(2)	964(2)	3489(2)	54(1)
C(9)	212(4)	945(7)	3117(4)	49(2)
C(10)	-330(6)	1711(6)	3000(5)	40(1)
C(11)	-1464(6)	1737(5)	2696(6)	44(2)
C(12)	-2054(3)	996(6)	2510(4)	54(2)
C(13)	-1512(6)	229(5)	2628(7)	58(2)
C(14)	-378(6)	204(6)	2931(7)	58(2)
O(1)	-3212(5)	1024(8)	2194(6)	62(2)
C(15)	-3740(10)	1387(11)	2678(8)	82(3)
C(9B)	238(5)	993(11)	3089(6)	50(2)
C(10B)	-395(11)	1690(9)	3122(9)	51(2)
C(11B)	-1529(10)	1658(11)	2823(9)	52(2)
C(12B)	-2030(5)	929(12)	2492(7)	59(2)
C(13B)	-1396(10)	233(9)	2459(8)	57(2)
C(14B)	-263(10)	265(9)	2758(8)	52(2)

O(1B)	-3182(8)	820(11)	2293(11)	72(3)
C(15B)	-3746(15)	1554(14)	2449(15)	88(5)
C(16)	2602(2)	2792(2)	4848(1)	30(1)
C(17)	3521(2)	3465(2)	5922(2)	41(1)
C(18)	2357(2)	3797(2)	5654(2)	42(1)
C(19)	4540(2)	2430(2)	5386(2)	36(1)
C(20)	4570(2)	1592(2)	5614(2)	42(1)
C(21)	5511(3)	1128(2)	5648(2)	52(1)
C(22)	6373(3)	1479(2)	5476(2)	59(1)
C(23)	6334(3)	2301(3)	5276(2)	57(1)
C(24)	5419(2)	2801(2)	5230(2)	44(1)
C(25)	3678(3)	1211(2)	5861(2)	48(1)
C(26)	4085(4)	1096(3)	6673(2)	72(1)
C(27)	3256(4)	387(2)	5492(2)	68(1)
C(28)	5440(3)	3728(2)	5054(2)	52(1)
C(29)	6150(3)	4200(2)	5704(2)	64(1)
C(30)	5826(4)	3907(3)	4415(3)	74(1)
C(31)	714(2)	3330(2)	4621(2)	34(1)
C(32)	12(2)	2710(2)	4734(2)	42(1)
C(33)	-1103(3)	2784(2)	4348(2)	52(1)
C(34)	-1487(3)	3428(2)	3878(2)	52(1)
C(35)	-779(2)	4035(2)	3780(2)	46(1)
C(36)	343(2)	3999(2)	4153(2)	38(1)
C(37)	405(3)	2003(2)	5254(2)	57(1)
C(38)	-205(12)	2042(9)	5814(6)	63(4)
C(39)	333(13)	1134(5)	4941(8)	71(4)
C(38B)	190(20)	2180(9)	5956(6)	68(5)
C(39B)	-65(19)	1152(6)	4959(8)	65(5)
C(38C)	620(30)	2232(12)	6023(5)	60(5)
C(39C)	-330(20)	1229(10)	5042(12)	63(5)
C(40)	1081(2)	4694(2)	4051(2)	38(1)
C(41)	821(3)	5513(2)	4363(2)	54(1)

C(42)	984(3)	4839(2)	3277(2)	59(1)

Table S8. Bond lengths [Å] and angles [°] for **2b**.

Pd(1)-C(16)	1.974(3)
Pd(1)-N(1)	2.037(3)
Pd(1)-C(1)	2.044(3)
N(2)-C(16)	1.343(3)
N(2)-C(19)	1.435(4)
N(2)-C(17)	1.476(4)
N(3)-C(16)	1.350(4)
N(3)-C(31)	1.447(3)
N(3)-C(18)	1.468(4)
C(1)-C(6)	1.545(4)
C(1)-C(2)	1.555(5)
C(1)-H(1)	1.0000
C(2)-C(7)	1.505(5)
C(2)-C(3)	1.556(5)
C(2)-H(2)	1.0000
C(3)-C(4)	1.541(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.513(5)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(7)	1.537(6)
C(5)-C(6)	1.550(5)
C(5)-H(5)	1.0000
C(6)-C(8)	1.508(5)
C(6)-H(6)	1.0000
C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9800

C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
N(1)-C(9B)	1.397(7)
N(1)-C(9)	1.412(5)
N(1)-H(1A)	0.8799(10)
C(9)-C(10)	1.3900
C(9)-C(14)	1.3900
C(10)-C(11)	1.3900
C(10)-H(10A)	0.9500
C(11)-C(12)	1.3900
C(11)-H(11A)	0.9500
C(12)-C(13)	1.3900
C(12)-O(1)	1.421(5)
C(13)-C(14)	1.3900
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500
O(1)-C(15)	1.458(9)
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(9B)-C(10B)	1.3900
C(9B)-C(14B)	1.3900
C(10B)-C(11B)	1.3900
C(10B)-H(10B)	0.9500
C(11B)-C(12B)	1.3900
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.3900
C(12B)-O(1B)	1.417(7)
C(13B)-C(14B)	1.3900
C(13B)-H(13B)	0.9500
C(14B)-H(14B)	0.9500

O(1B)-C(15B)	1.459(11)
C(15B)-H(15D)	0.9800
C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800
C(17)-C(18)	1.517(4)
C(17)-H(17A)	0.9900
C(17)-H(17B)	0.9900
C(18)-H(18A)	0.9900
C(18)-H(18B)	0.9900
C(19)-C(24)	1.391(4)
C(19)-C(20)	1.407(4)
C(20)-C(21)	1.399(5)
C(20)-C(25)	1.507(5)
C(21)-C(22)	1.376(6)
C(21)-H(21)	0.9500
C(22)-C(23)	1.367(6)
C(22)-H(22)	0.9500
C(23)-C(24)	1.399(5)
C(23)-H(23)	0.9500
C(24)-C(28)	1.521(5)
C(25)-C(27)	1.521(5)
C(25)-C(26)	1.542(5)
C(25)-H(25)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(30)	1.524(6)
C(28)-C(29)	1.527(5)

C(28)-H(28)	1.0000
C(29)-H(29A)	0.9800
C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(31)-C(36)	1.398(4)
C(31)-C(32)	1.401(4)
C(32)-C(33)	1.401(5)
C(32)-C(37)	1.506(5)
C(33)-C(34)	1.371(6)
C(33)-H(33)	0.9500
C(34)-C(35)	1.383(5)
C(34)-H(34)	0.9500
C(35)-C(36)	1.399(4)
C(35)-H(35)	0.9500
C(36)-C(40)	1.513(4)
C(37)-C(39)	1.510(7)
C(37)-C(38C)	1.511(8)
C(37)-C(39B)	1.526(7)
C(37)-C(38B)	1.529(8)
C(37)-C(39C)	1.533(8)
C(37)-C(38)	1.548(7)
C(37)-H(37A)	1.0000
C(37)-H(37B)	1.0000
C(37)-H(37C)	0.9999
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800

C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(38B)-H(38D)	0.9800
C(38B)-H(38E)	0.9800
C(38B)-H(38F)	0.9800
C(39B)-H(39D)	0.9800
C(39B)-H(39E)	0.9800
C(39B)-H(39F)	0.9800
C(38C)-H(38G)	0.9800
C(38C)-H(38H)	0.9800
C(38C)-H(38I)	0.9800
C(39C)-H(39G)	0.9800
C(39C)-H(39H)	0.9800
C(39C)-H(39I)	0.9800
C(40)-C(42)	1.520(5)
C(40)-C(41)	1.527(4)
C(40)-H(40)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800

C(16)-Pd(1)-N(1)	161.28(12)
C(16)-Pd(1)-C(1)	89.35(12)
N(1)-Pd(1)-C(1)	109.15(13)
C(16)-N(2)-C(19)	123.7(2)
C(16)-N(2)-C(17)	112.8(2)
C(19)-N(2)-C(17)	121.3(2)
C(16)-N(3)-C(31)	124.4(2)

C(16)-N(3)-C(18)	113.3(2)
C(31)-N(3)-C(18)	122.3(2)
C(6)-C(1)-C(2)	103.8(3)
C(6)-C(1)-Pd(1)	114.9(2)
C(2)-C(1)-Pd(1)	108.3(2)
C(6)-C(1)-H(1)	109.9
C(2)-C(1)-H(1)	109.9
Pd(1)-C(1)-H(1)	109.9
C(7)-C(2)-C(1)	102.9(3)
C(7)-C(2)-C(3)	101.8(3)
C(1)-C(2)-C(3)	105.7(3)
C(7)-C(2)-H(2)	114.9
C(1)-C(2)-H(2)	114.9
C(3)-C(2)-H(2)	114.9
C(4)-C(3)-C(2)	102.2(3)
C(4)-C(3)-H(3A)	111.3
C(2)-C(3)-H(3A)	111.3
C(4)-C(3)-H(3B)	111.3
C(2)-C(3)-H(3B)	111.3
H(3A)-C(3)-H(3B)	109.2
C(5)-C(4)-C(3)	103.6(3)
C(5)-C(4)-H(4A)	111.0
C(3)-C(4)-H(4A)	111.0
C(5)-C(4)-H(4B)	111.0
C(3)-C(4)-H(4B)	111.0
H(4A)-C(4)-H(4B)	109.0
C(4)-C(5)-C(7)	101.8(3)
C(4)-C(5)-C(6)	109.6(3)
C(7)-C(5)-C(6)	102.3(3)
C(4)-C(5)-H(5)	114.0
C(7)-C(5)-H(5)	114.0

C(6)-C(5)-H(5)	114.0
C(8)-C(6)-C(1)	117.6(3)
C(8)-C(6)-C(5)	113.3(3)
C(1)-C(6)-C(5)	101.5(3)
C(8)-C(6)-H(6)	108.0
C(1)-C(6)-H(6)	108.0
C(5)-C(6)-H(6)	108.0
C(2)-C(7)-C(5)	94.0(3)
C(2)-C(7)-H(7A)	112.9
C(5)-C(7)-H(7A)	112.9
C(2)-C(7)-H(7B)	112.9
C(5)-C(7)-H(7B)	112.9
H(7A)-C(7)-H(7B)	110.3
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
C(9B)-N(1)-Pd(1)	122.5(7)
C(9)-N(1)-Pd(1)	124.4(5)
C(9B)-N(1)-H(1A)	126(3)
C(9)-N(1)-H(1A)	124(3)
Pd(1)-N(1)-H(1A)	110(3)
C(10)-C(9)-C(14)	120.0
C(10)-C(9)-N(1)	116.7(7)
C(14)-C(9)-N(1)	123.0(7)
C(9)-C(10)-C(11)	120.0
C(9)-C(10)-H(10A)	120.0
C(11)-C(10)-H(10A)	120.0
C(10)-C(11)-C(12)	120.0

C(10)-C(11)-H(11A)	120.0
C(12)-C(11)-H(11A)	120.0
C(13)-C(12)-C(11)	120.0
C(13)-C(12)-O(1)	120.1(7)
C(11)-C(12)-O(1)	119.9(7)
C(12)-C(13)-C(14)	120.0
C(12)-C(13)-H(13A)	120.0
C(14)-C(13)-H(13A)	120.0
C(13)-C(14)-C(9)	120.0
C(13)-C(14)-H(14A)	120.0
C(9)-C(14)-H(14A)	120.0
C(12)-O(1)-C(15)	111.0(8)
C(10B)-C(9B)-C(14B)	120.0
C(10B)-C(9B)-N(1)	120.5(11)
C(14B)-C(9B)-N(1)	118.6(11)
C(11B)-C(10B)-C(9B)	120.0
C(11B)-C(10B)-H(10B)	120.0
C(9B)-C(10B)-H(10B)	120.0
C(10B)-C(11B)-C(12B)	120.0
C(10B)-C(11B)-H(11B)	120.0
C(12B)-C(11B)-H(11B)	120.0
C(13B)-C(12B)-C(11B)	120.0
C(13B)-C(12B)-O(1B)	117.6(11)
C(11B)-C(12B)-O(1B)	121.5(11)
C(14B)-C(13B)-C(12B)	120.0
C(14B)-C(13B)-H(13B)	120.0
C(12B)-C(13B)-H(13B)	120.0
C(13B)-C(14B)-C(9B)	120.0
C(13B)-C(14B)-H(14B)	120.0
C(9B)-C(14B)-H(14B)	120.0
C(12B)-O(1B)-C(15B)	112.6(10)

O(1B)-C(15B)-H(15D)	109.5
O(1B)-C(15B)-H(15E)	109.5
H(15D)-C(15B)-H(15E)	109.5
O(1B)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5
N(2)-C(16)-N(3)	107.5(2)
N(2)-C(16)-Pd(1)	130.5(2)
N(3)-C(16)-Pd(1)	121.54(19)
N(2)-C(17)-C(18)	102.6(2)
N(2)-C(17)-H(17A)	111.2
C(18)-C(17)-H(17A)	111.2
N(2)-C(17)-H(17B)	111.2
C(18)-C(17)-H(17B)	111.2
H(17A)-C(17)-H(17B)	109.2
N(3)-C(18)-C(17)	102.5(2)
N(3)-C(18)-H(18A)	111.3
C(17)-C(18)-H(18A)	111.3
N(3)-C(18)-H(18B)	111.3
C(17)-C(18)-H(18B)	111.3
H(18A)-C(18)-H(18B)	109.2
C(24)-C(19)-C(20)	122.3(3)
C(24)-C(19)-N(2)	118.6(3)
C(20)-C(19)-N(2)	119.1(3)
C(21)-C(20)-C(19)	117.0(3)
C(21)-C(20)-C(25)	120.2(3)
C(19)-C(20)-C(25)	122.7(3)
C(22)-C(21)-C(20)	121.5(3)
C(22)-C(21)-H(21)	119.3
C(20)-C(21)-H(21)	119.3
C(23)-C(22)-C(21)	120.2(3)

C(23)-C(22)-H(22)	119.9
C(21)-C(22)-H(22)	119.9
C(22)-C(23)-C(24)	121.3(3)
C(22)-C(23)-H(23)	119.4
C(24)-C(23)-H(23)	119.4
C(19)-C(24)-C(23)	117.7(3)
C(19)-C(24)-C(28)	122.7(3)
C(23)-C(24)-C(28)	119.5(3)
C(20)-C(25)-C(27)	112.5(3)
C(20)-C(25)-C(26)	110.2(3)
C(27)-C(25)-C(26)	110.8(3)
C(20)-C(25)-H(25)	107.7
C(27)-C(25)-H(25)	107.7
C(26)-C(25)-H(25)	107.7
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-C(28)-C(30)	114.1(3)
C(24)-C(28)-C(29)	109.4(3)
C(30)-C(28)-C(29)	110.4(3)
C(24)-C(28)-H(28)	107.6
C(30)-C(28)-H(28)	107.6

C(29)-C(28)-H(28)	107.6
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
H(29A)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
H(29A)-C(29)-H(29C)	109.5
H(29B)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
H(30A)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
H(30A)-C(30)-H(30C)	109.5
H(30B)-C(30)-H(30C)	109.5
C(36)-C(31)-C(32)	122.8(3)
C(36)-C(31)-N(3)	118.5(3)
C(32)-C(31)-N(3)	118.6(3)
C(31)-C(32)-C(33)	116.8(3)
C(31)-C(32)-C(37)	122.9(3)
C(33)-C(32)-C(37)	120.3(3)
C(34)-C(33)-C(32)	121.6(3)
C(34)-C(33)-H(33)	119.2
C(32)-C(33)-H(33)	119.2
C(33)-C(34)-C(35)	120.5(3)
C(33)-C(34)-H(34)	119.7
C(35)-C(34)-H(34)	119.7
C(34)-C(35)-C(36)	120.6(3)
C(34)-C(35)-H(35)	119.7
C(36)-C(35)-H(35)	119.7
C(31)-C(36)-C(35)	117.7(3)
C(31)-C(36)-C(40)	123.5(2)
C(35)-C(36)-C(40)	118.8(3)

C(32)-C(37)-C(39)	116.1(7)
C(32)-C(37)-C(38C)	115.3(7)
C(39)-C(37)-C(38C)	127.4(10)
C(32)-C(37)-C(39B)	113.2(6)
C(38C)-C(37)-C(39B)	121.9(10)
C(32)-C(37)-C(38B)	111.7(6)
C(39)-C(37)-C(38B)	122.6(9)
C(39B)-C(37)-C(38B)	110.6(8)
C(32)-C(37)-C(39C)	111.6(8)
C(38C)-C(37)-C(39C)	111.9(9)
C(38B)-C(37)-C(39C)	97.3(11)
C(32)-C(37)-C(38)	109.0(5)
C(39)-C(37)-C(38)	110.7(8)
C(39B)-C(37)-C(38)	94.8(11)
C(39C)-C(37)-C(38)	79.7(15)
C(32)-C(37)-H(37A)	106.8
C(39)-C(37)-H(37A)	106.8
C(38C)-C(37)-H(37A)	67.1
C(39B)-C(37)-H(37A)	124.5
C(38B)-C(37)-H(37A)	87.0
C(39C)-C(37)-H(37A)	136.2
C(38)-C(37)-H(37A)	106.8
C(32)-C(37)-H(37B)	106.9
C(39)-C(37)-H(37B)	87.7
C(38C)-C(37)-H(37B)	87.5
C(39B)-C(37)-H(37B)	106.9
C(38B)-C(37)-H(37B)	107.0
C(39C)-C(37)-H(37B)	121.8
C(38)-C(37)-H(37B)	125.5
C(32)-C(37)-H(37C)	105.7
C(39)-C(37)-H(37C)	69.8

C(38C)-C(37)-H(37C)	105.7
C(39B)-C(37)-H(37C)	89.6
C(38B)-C(37)-H(37C)	124.2
C(39C)-C(37)-H(37C)	105.7
C(38)-C(37)-H(37C)	139.7
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
C(37)-C(38B)-H(38D)	109.5
C(37)-C(38B)-H(38E)	109.5
H(38D)-C(38B)-H(38E)	109.5
C(37)-C(38B)-H(38F)	109.5
H(38D)-C(38B)-H(38F)	109.5
H(38E)-C(38B)-H(38F)	109.5
C(37)-C(39B)-H(39D)	109.5
C(37)-C(39B)-H(39E)	109.5
H(39D)-C(39B)-H(39E)	109.5
C(37)-C(39B)-H(39F)	109.5
H(39D)-C(39B)-H(39F)	109.5
H(39E)-C(39B)-H(39F)	109.5
C(37)-C(38C)-H(38G)	109.5
C(37)-C(38C)-H(38H)	109.5
C(37)-C(38C)-H(38I)	109.5
C(37)-C(39C)-H(39G)	109.5
C(37)-C(39C)-H(39H)	109.5
C(37)-C(39C)-H(39I)	109.5
C(36)-C(40)-C(42)	112.9(3)
C(36)-C(40)-C(41)	110.3(3)

C(42)-C(40)-C(41)	108.8(3)
C(36)-C(40)-H(40)	108.2
C(42)-C(40)-H(40)	108.2
C(41)-C(40)-H(40)	108.2
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S9. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **2b**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	35(1)	31(1)	37(1)	-6(1)	8(1)	0(1)
N(2)	31(1)	32(1)	32(1)	-3(1)	6(1)	3(1)
N(3)	31(1)	31(1)	37(1)	-6(1)	9(1)	1(1)
C(1)	46(2)	39(2)	43(2)	-5(1)	16(1)	-5(1)
C(2)	61(2)	44(2)	55(2)	7(2)	18(2)	8(2)
C(3)	77(3)	52(2)	62(2)	11(2)	24(2)	7(2)
C(4)	75(3)	75(3)	62(2)	11(2)	30(2)	4(2)
C(5)	72(2)	58(2)	45(2)	-4(2)	26(2)	11(2)
C(6)	47(2)	55(2)	54(2)	-2(2)	21(2)	6(2)
C(7)	70(2)	64(2)	44(2)	-1(2)	6(2)	-2(2)
C(8)	68(2)	67(3)	73(3)	12(2)	34(2)	31(2)
N(1)	50(2)	42(2)	62(2)	-15(1)	6(1)	0(1)
C(9)	55(3)	46(3)	43(3)	-6(3)	11(3)	-7(2)
C(10)	42(2)	45(3)	35(3)	-10(2)	13(2)	-13(2)
C(11)	43(2)	56(3)	35(3)	-4(2)	16(2)	-9(2)
C(12)	48(2)	66(3)	45(3)	-13(2)	11(2)	-18(2)
C(13)	56(3)	61(3)	55(4)	-18(3)	13(3)	-23(2)
C(14)	65(3)	49(3)	58(4)	-5(3)	17(3)	-12(3)
O(1)	47(2)	76(4)	58(3)	-5(3)	9(2)	-19(2)
C(15)	50(4)	111(7)	92(7)	-3(6)	32(5)	-16(4)
C(9B)	51(3)	47(4)	50(4)	-14(4)	12(4)	-16(3)
C(10B)	47(3)	53(4)	51(4)	-13(3)	14(3)	-13(3)
C(11B)	48(3)	61(4)	45(4)	-6(3)	13(3)	-13(3)
C(12B)	53(3)	68(4)	50(3)	-7(3)	7(3)	-24(3)
C(13B)	63(3)	61(3)	44(4)	-8(3)	11(3)	-30(3)
C(14B)	66(4)	45(4)	44(4)	-5(3)	15(3)	-14(3)
O(1B)	56(3)	79(5)	68(5)	-4(4)	2(3)	-29(3)
C(15B)	52(6)	119(9)	90(10)	-12(8)	20(7)	-14(6)
C(16)	31(1)	26(1)	32(1)	3(1)	7(1)	1(1)
C(17)	40(2)	41(2)	37(2)	-9(1)	5(1)	4(1)
C(18)	38(2)	43(2)	43(2)	-13(1)	9(1)	3(1)

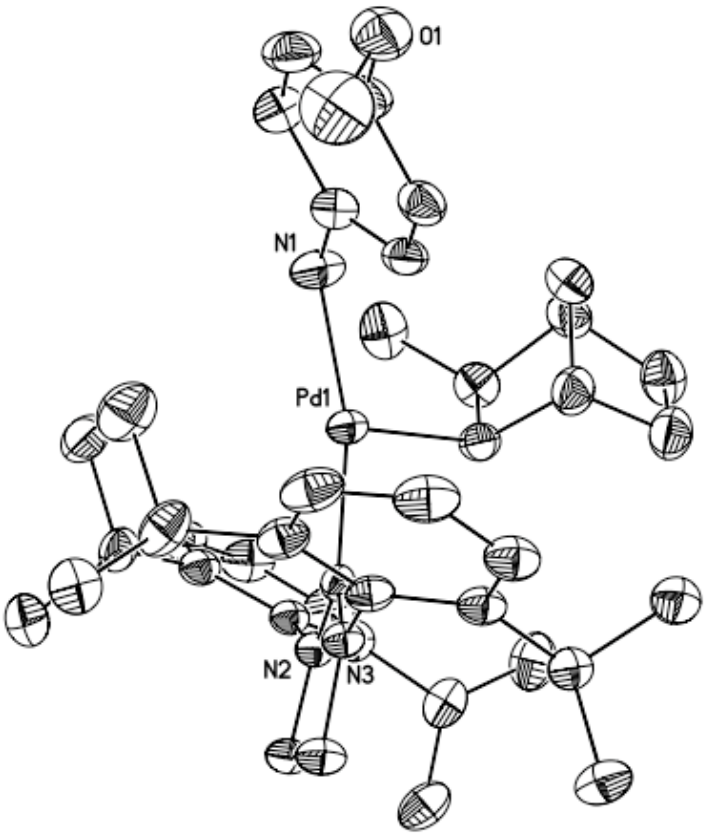
C(19)	33(1)	35(2)	34(1)	-3(1)	2(1)	4(1)
C(20)	42(2)	38(2)	36(2)	-2(1)	-1(1)	6(1)
C(21)	55(2)	38(2)	52(2)	-3(1)	1(2)	14(2)
C(22)	42(2)	58(2)	69(2)	-11(2)	6(2)	18(2)
C(23)	36(2)	61(2)	72(2)	-7(2)	14(2)	7(2)
C(24)	35(2)	47(2)	48(2)	1(1)	8(1)	6(1)
C(25)	55(2)	35(2)	48(2)	10(1)	5(1)	4(1)
C(26)	90(3)	71(3)	53(2)	11(2)	18(2)	-4(2)
C(27)	76(3)	46(2)	70(3)	5(2)	5(2)	-10(2)
C(28)	36(2)	48(2)	73(2)	8(2)	17(2)	2(1)
C(29)	47(2)	47(2)	96(3)	-3(2)	18(2)	-7(2)
C(30)	63(2)	75(3)	90(3)	16(2)	34(2)	-4(2)
C(31)	28(1)	33(2)	42(2)	-11(1)	11(1)	1(1)
C(32)	39(2)	38(2)	53(2)	-11(1)	19(1)	-1(1)
C(33)	40(2)	47(2)	74(2)	-21(2)	24(2)	-13(2)
C(34)	30(2)	58(2)	63(2)	-18(2)	6(1)	-1(1)
C(35)	35(2)	50(2)	47(2)	-10(1)	4(1)	4(1)
C(36)	34(1)	38(2)	39(2)	-9(1)	8(1)	4(1)
C(37)	50(2)	43(2)	84(3)	4(2)	31(2)	-4(2)
C(38)	69(7)	62(6)	58(6)	1(5)	22(5)	-3(5)
C(39)	75(7)	50(6)	93(7)	-1(5)	34(6)	13(5)
C(38B)	79(9)	52(6)	55(6)	-7(5)	-5(5)	-19(6)
C(39B)	85(9)	41(5)	84(6)	-10(4)	48(6)	6(5)
C(38C)	55(9)	55(7)	61(7)	5(6)	5(6)	-12(6)
C(39C)	73(8)	45(7)	81(8)	-9(6)	40(6)	-3(6)
C(40)	31(1)	39(2)	42(2)	-2(1)	6(1)	4(1)
C(41)	56(2)	40(2)	68(2)	-14(2)	26(2)	-4(2)
C(42)	77(2)	51(2)	52(2)	-4(2)	25(2)	-3(2)

Table S10. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^{2}x 10^3) for **2b**.

	x	y	z	U(eq)
H(1)	3375	3080	3818	50
H(2)	1427	3075	2858	64
H(3A)	2266	3907	2145	76
H(3B)	3149	3995	2924	76
H(4A)	3477	3146	1785	82
H(4B)	4367	3246	2560	82
H(5)	3648	1751	2203	68
H(6)	4548	2326	3475	61
H(7A)	1729	2332	1825	75
H(7B)	1851	1664	2464	75
H(8A)	4144	1104	4024	100
H(8B)	4497	885	3339	100
H(8C)	3231	856	3296	100
H(1A)	1760(30)	514(17)	3590(20)	81
H(10A)	73	2218	3127	49
H(11A)	-1835	2261	2616	53
H(13A)	-1915	-277	2500	70
H(14A)	-7	-320	3011	70
H(15A)	-4536	1309	2485	123
H(15B)	-3573	1987	2735	123
H(15C)	-3467	1109	3140	123
H(10B)	-53	2188	3348	61
H(11B)	-1962	2134	2845	62
H(13B)	-1738	-265	2233	69
H(14B)	170	-212	2736	62
H(15D)	-4541	1473	2253	131
H(15E)	-3530	2052	2236	131
H(15F)	-3545	1629	2964	131
H(17A)	4063	3927	6010	49
H(17B)	3645	3137	6363	49
H(18A)	1969	3714	6009	51

H(18B)	2346	4401	5535	51
H(21)	5555	559	5795	63
H(22)	6998	1148	5495	71
H(23)	6941	2538	5165	68
H(25)	3050	1615	5745	58
H(26A)	4326	1638	6901	108
H(26B)	4702	701	6802	108
H(26C)	3488	875	6831	108
H(27A)	2982	477	4978	102
H(27B)	2660	176	5656	102
H(27C)	3854	-24	5602	102
H(28)	4674	3946	4942	63
H(29A)	5876	4094	6105	97
H(29B)	6118	4802	5602	97
H(29C)	6911	4006	5823	97
H(30A)	5345	3619	3998	111
H(30B)	6580	3705	4511	111
H(30C)	5801	4513	4327	111
H(33)	-1605	2378	4413	62
H(34)	-2246	3457	3618	63
H(35)	-1056	4481	3457	55
H(37A)	1198	2111	5510	68
H(37B)	1219	1967	5360	68
H(37C)	1133	1832	5214	68
H(38A)	-969	1870	5596	94
H(38B)	-183	2617	5992	94
H(38C)	152	1664	6208	94
H(39A)	810	1099	4640	106
H(39B)	-426	1018	4655	106
H(39C)	569	721	5324	106
H(38D)	483	2734	6132	102
H(38E)	555	1751	6304	102
H(38F)	-600	2168	5883	102
H(39D)	28	1069	4492	98
H(39E)	-848	1133	4914	98
H(39F)	322	707	5281	98

H(38G)	996	2773	6120	90
H(38H)	1072	1800	6326	90
H(38I)	-85	2273	6122	90
H(39G)	-402	1073	4552	94
H(39H)	-1061	1357	5078	94
H(39I)	-10	762	5359	94
H(40)	1857	4538	4310	46
H(41A)	897	5430	4866	80
H(41B)	68	5684	4108	80
H(41C)	1331	5950	4317	80
H(42A)	1112	4310	3064	88
H(42B)	1530	5253	3245	88
H(42C)	246	5046	3023	88



Crystallographic Data for 3

Table S11. Crystal data and structure refinement for **3**.

Empirical formula	$C_{85}H_{116}Cl_2N_4Pd_2$	
Formula weight	1477.52	
Temperature	193(1) K	
Wavelength	1.54178 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.7161(5) Å	a= 102.478(3)°.
	b = 14.8135(6) Å	b= 92.417(3)°.
	c = 23.0484(13) Å	g = 109.701(2)°.
Volume	3648.2(3) $Å^3$	
Z	2	
Density (calculated)	1.345 Mg/m^3	
Absorption coefficient	5.005 mm^{-1}	
F(000)	1560	
Crystal size	0.315 x 0.131 x 0.045 mm^3	
Theta range for data collection	1.98 to 67.93°.	
Index ranges	-10<=h<=13, -17<=k<=17, -26<=l<=27	
Reflections collected	12743	
Independent reflections	12743 [R(int) = 0.0684]	
Completeness to theta = 67.93°	95.9 %	
Absorption correction	Integration	
Max. and min. transmission	0.8232 and 0.3926	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	12743 / 43 / 742	
Goodness-of-fit on F^2	1.031	
Final R indices [I>2sigma(I)]	R1 = 0.0399, wR2 = 0.1041	
R indices (all data)	R1 = 0.0679, wR2 = 0.1205	
Largest diff. peak and hole	0.947 and -1.044 $e.Å^{-3}$	

Table S12. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **3**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	3632(1)	7410(1)	3338(1)	24(1)
Pd(2)	5057(1)	9159(1)	2443(1)	25(1)
Cl(1)	3292(1)	7560(1)	2285(1)	31(1)
Cl(2)	5237(1)	8959(1)	3431(1)	40(1)
N(1)	1151(3)	5748(2)	2940(1)	27(1)
N(2)	2627(3)	5202(2)	3011(1)	26(1)
N(3)	4007(3)	9880(2)	1520(1)	29(1)
N(4)	4463(3)	8627(2)	1083(1)	31(1)
C(1)	2373(3)	6055(3)	3137(2)	25(1)
C(2)	685(4)	4742(3)	2689(2)	35(1)
C(3)	1606(4)	4402(3)	2727(2)	33(1)
C(4)	388(3)	6348(3)	3036(2)	30(1)
C(5)	-91(3)	6574(3)	2546(2)	35(1)
C(6)	-819(4)	7153(3)	2659(2)	43(1)
C(7)	-1071(4)	7474(3)	3222(2)	48(1)
C(8)	-638(4)	7195(3)	3697(2)	43(1)
C(9)	88(3)	6617(3)	3619(2)	34(1)
C(10)	70(4)	6166(3)	1906(2)	42(1)
C(11)	-1083(5)	5253(4)	1610(2)	62(1)
C(12)	318(4)	6915(4)	1520(2)	53(1)
C(13)	461(4)	6238(3)	4130(2)	38(1)
C(14)	-333(4)	5145(3)	4055(2)	49(1)
C(15)	380(4)	6823(4)	4750(2)	48(1)
C(16)	3744(3)	5111(3)	3230(2)	27(1)
C(17)	3730(3)	4727(3)	3736(2)	29(1)
C(18)	4795(4)	4631(3)	3948(2)	35(1)

C(19)	5841(4)	4925(3)	3675(2)	41(1)
C(20)	5828(4)	5297(3)	3174(2)	40(1)
C(21)	4781(3)	5391(3)	2932(2)	31(1)
C(22)	2578(4)	4384(3)	4033(2)	32(1)
C(23)	2020(4)	3252(3)	3890(2)	44(1)
C(24)	2797(4)	4799(3)	4715(2)	46(1)
C(25)	4755(4)	5714(3)	2355(2)	36(1)
C(26)	5800(4)	6660(3)	2365(2)	49(1)
C(27)	4751(5)	4875(4)	1828(2)	54(1)
C(28)	4059(3)	7321(3)	4200(2)	27(1)
C(29)	5453(4)	7691(3)	4402(2)	34(1)
C(30)	5628(4)	7179(3)	4898(2)	44(1)
C(31)	5061(5)	7650(3)	5423(2)	47(1)
C(32)	4725(4)	8442(3)	5178(2)	42(1)
C(33)	3577(4)	7912(3)	4706(2)	35(1)
C(34)	5742(4)	8747(3)	4785(2)	41(1)
C(35)	3064(4)	8649(3)	4532(2)	39(1)
C(36)	6484(3)	10505(3)	2622(2)	31(1)
C(37)	6522(4)	11223(3)	3236(2)	40(1)
C(38)	7210(5)	12274(3)	3171(2)	51(1)
C(39)	8535(4)	12279(3)	3120(2)	55(1)
C(40)	8458(4)	11267(3)	3227(2)	48(1)
C(41)	7794(4)	10453(3)	2656(2)	41(1)
C(42)	7493(4)	11104(3)	3652(2)	47(1)
C(43)	7884(4)	9454(3)	2691(2)	48(1)
C(44)	4601(3)	9265(3)	1625(2)	26(1)
C(45)	3474(4)	9594(3)	925(2)	37(1)
C(46)	3761(4)	8825(3)	653(2)	37(1)
C(47)	4020(3)	10771(3)	1936(2)	31(1)
C(48)	3286(4)	10698(3)	2397(2)	35(1)
C(49)	3346(4)	11580(3)	2785(2)	44(1)

C(50)	4087(4)	12479(3)	2714(2)	46(1)
C(51)	4789(4)	12530(3)	2251(2)	44(1)
C(52)	4769(4)	11675(3)	1845(2)	37(1)
C(53)	2355(4)	9720(3)	2450(2)	41(1)
C(54)	2460(20)	9660(15)	3110(4)	54(3)
C(55)	1064(8)	9671(14)	2247(12)	53(3)
C(54B)	2110(30)	9490(30)	3062(9)	53(6)
C(55B)	1145(15)	9524(19)	2066(13)	39(5)
C(56)	5509(4)	11775(3)	1319(2)	44(1)
C(57)	4983(6)	12248(4)	894(2)	64(1)
C(58)	6865(5)	12365(4)	1512(3)	70(2)
C(59)	5044(4)	7907(3)	927(2)	31(1)
C(60)	6321(4)	8256(3)	917(2)	38(1)
C(61)	6849(5)	7548(4)	741(2)	54(1)
C(62)	6179(5)	6566(4)	560(3)	63(1)
C(63)	4925(5)	6233(3)	553(2)	50(1)
C(64)	4320(4)	6897(3)	736(2)	40(1)
C(65)	7072(4)	9351(3)	1051(2)	44(1)
C(66)	8451(5)	9582(4)	1195(2)	63(1)
C(67)	6881(5)	9775(4)	520(2)	57(1)
C(68)	2950(4)	6503(3)	706(2)	41(1)
C(69)	2343(5)	6196(4)	51(2)	55(1)
C(70)	2467(5)	5616(3)	983(2)	49(1)

Table S13. Bond lengths [Å] and angles [°] for **3**.

Pd(1)-C(1)	1.991(4)
Pd(1)-C(28)	2.071(3)
Pd(1)-Cl(2)	2.3858(10)
Pd(1)-Cl(1)	2.5125(8)
Pd(2)-C(44)	1.991(3)
Pd(2)-C(36)	2.068(4)
Pd(2)-Cl(2)	2.3682(9)
Pd(2)-Cl(1)	2.5058(9)
N(1)-C(1)	1.371(5)
N(1)-C(2)	1.381(5)
N(1)-C(4)	1.451(4)
N(2)-C(1)	1.368(4)
N(2)-C(3)	1.381(5)
N(2)-C(16)	1.441(4)
N(3)-C(44)	1.372(5)
N(3)-C(45)	1.396(5)
N(3)-C(47)	1.449(5)
N(4)-C(44)	1.360(5)
N(4)-C(46)	1.401(5)
N(4)-C(59)	1.441(5)
C(2)-C(3)	1.342(5)
C(2)-H(2A)	0.9500
C(3)-H(3A)	0.9500
C(4)-C(5)	1.392(5)
C(4)-C(9)	1.410(6)
C(5)-C(6)	1.395(6)
C(5)-C(10)	1.514(6)
C(6)-C(7)	1.364(7)
C(6)-H(6A)	0.9500

C(7)-C(8)	1.385(6)
C(7)-H(7A)	0.9500
C(8)-C(9)	1.388(5)
C(8)-H(8A)	0.9500
C(9)-C(13)	1.516(5)
C(10)-C(12)	1.529(6)
C(10)-C(11)	1.552(7)
C(10)-H(10A)	1.0000
C(11)-H(11A)	0.9800
C(11)-H(11B)	0.9800
C(11)-H(11C)	0.9800
C(12)-H(12A)	0.9800
C(12)-H(12B)	0.9800
C(12)-H(12C)	0.9800
C(13)-C(15)	1.528(6)
C(13)-C(14)	1.538(6)
C(13)-H(13A)	1.0000
C(14)-H(14A)	0.9800
C(14)-H(14B)	0.9800
C(14)-H(14C)	0.9800
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(16)-C(17)	1.402(5)
C(16)-C(21)	1.404(5)
C(17)-C(18)	1.385(5)
C(17)-C(22)	1.522(5)
C(18)-C(19)	1.381(6)
C(18)-H(18A)	0.9500
C(19)-C(20)	1.384(6)
C(19)-H(19A)	0.9500

C(20)-C(21)	1.387(5)
C(20)-H(20A)	0.9500
C(21)-C(25)	1.512(5)
C(22)-C(23)	1.533(6)
C(22)-C(24)	1.535(5)
C(22)-H(22A)	1.0000
C(23)-H(23A)	0.9800
C(23)-H(23B)	0.9800
C(23)-H(23C)	0.9800
C(24)-H(24A)	0.9800
C(24)-H(24B)	0.9800
C(24)-H(24C)	0.9800
C(25)-C(26)	1.513(6)
C(25)-C(27)	1.537(6)
C(25)-H(25A)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(33)	1.547(5)
C(28)-C(29)	1.552(5)
C(28)-H(28A)	1.0000
C(29)-C(34)	1.536(5)
C(29)-C(30)	1.542(5)
C(29)-H(29A)	1.0000
C(30)-C(31)	1.552(6)
C(30)-H(30A)	0.9900
C(30)-H(30B)	0.9900
C(31)-C(32)	1.558(6)

C(31)-H(31A)	0.9900
C(31)-H(31B)	0.9900
C(32)-C(34)	1.533(6)
C(32)-C(33)	1.552(6)
C(32)-H(32A)	1.0000
C(33)-C(35)	1.523(5)
C(33)-H(33A)	1.0000
C(34)-H(34A)	0.9900
C(34)-H(34B)	0.9900
C(35)-H(35A)	0.9800
C(35)-H(35B)	0.9800
C(35)-H(35C)	0.9800
C(36)-C(41)	1.562(5)
C(36)-C(37)	1.564(5)
C(36)-H(36A)	1.0000
C(37)-C(42)	1.537(6)
C(37)-C(38)	1.537(6)
C(37)-H(37A)	1.0000
C(38)-C(39)	1.559(7)
C(38)-H(38A)	0.9900
C(38)-H(38B)	0.9900
C(39)-C(40)	1.544(6)
C(39)-H(39A)	0.9900
C(39)-H(39B)	0.9900
C(40)-C(42)	1.519(6)
C(40)-C(41)	1.546(6)
C(40)-H(40A)	1.0000
C(41)-C(43)	1.537(6)
C(41)-H(41A)	1.0000
C(42)-H(42A)	0.9900
C(42)-H(42B)	0.9900

C(43)-H(43A)	0.9800
C(43)-H(43B)	0.9800
C(43)-H(43C)	0.9800
C(45)-C(46)	1.331(6)
C(45)-H(45A)	0.9500
C(46)-H(46A)	0.9500
C(47)-C(48)	1.395(5)
C(47)-C(52)	1.397(6)
C(48)-C(49)	1.392(6)
C(48)-C(53)	1.525(6)
C(49)-C(50)	1.372(6)
C(49)-H(49A)	0.9500
C(50)-C(51)	1.373(6)
C(50)-H(50A)	0.9500
C(51)-C(52)	1.395(6)
C(51)-H(51A)	0.9500
C(52)-C(56)	1.525(6)
C(53)-C(55)	1.537(7)
C(53)-C(55B)	1.543(8)
C(53)-C(54)	1.545(7)
C(53)-C(54B)	1.538(8)
C(53)-H(53A)	1.0000
C(53)-H(53B)	0.9601
C(54)-H(54A)	0.9800
C(54)-H(54B)	0.9800
C(54)-H(54C)	0.9800
C(55)-H(55A)	0.9800
C(55)-H(55B)	0.9800
C(55)-H(55C)	0.9800
C(54B)-H(54D)	0.9800
C(54B)-H(54E)	0.9800

C(54B)-H(54F)	0.9800
C(55B)-H(55D)	0.9800
C(55B)-H(55E)	0.9800
C(55B)-H(55F)	0.9800
C(56)-C(58)	1.524(7)
C(56)-C(57)	1.538(7)
C(56)-H(56A)	1.0000
C(57)-H(57A)	0.9800
C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(58)-H(58A)	0.9800
C(58)-H(58B)	0.9800
C(58)-H(58C)	0.9800
C(59)-C(64)	1.406(6)
C(59)-C(60)	1.412(6)
C(60)-C(61)	1.387(6)
C(60)-C(65)	1.516(6)
C(61)-C(62)	1.358(7)
C(61)-H(61A)	0.9500
C(62)-C(63)	1.382(7)
C(62)-H(62A)	0.9500
C(63)-C(64)	1.403(6)
C(63)-H(63A)	0.9500
C(64)-C(68)	1.504(6)
C(65)-C(67)	1.531(6)
C(65)-C(66)	1.540(6)
C(65)-H(65A)	1.0000
C(66)-H(66A)	0.9800
C(66)-H(66B)	0.9800
C(66)-H(66C)	0.9800
C(67)-H(67A)	0.9800

C(67)-H(67B)	0.9800
C(67)-H(67C)	0.9800
C(68)-C(70)	1.533(6)
C(68)-C(69)	1.544(6)
C(68)-H(68A)	1.0000
C(69)-H(69A)	0.9800
C(69)-H(69D)	0.9800
C(69)-H(69B)	0.9800
C(70)-H(70D)	0.9800
C(70)-H(70A)	0.9800
C(70)-H(70B)	0.9800

C(1)-Pd(1)-C(28)	91.96(14)
C(1)-Pd(1)-Cl(2)	171.15(10)
C(28)-Pd(1)-Cl(2)	94.40(11)
C(1)-Pd(1)-Cl(1)	90.93(9)
C(28)-Pd(1)-Cl(1)	175.50(11)
Cl(2)-Pd(1)-Cl(1)	82.36(3)
C(44)-Pd(2)-C(36)	92.06(15)
C(44)-Pd(2)-Cl(2)	170.20(10)
C(36)-Pd(2)-Cl(2)	94.58(11)
C(44)-Pd(2)-Cl(1)	90.23(10)
C(36)-Pd(2)-Cl(1)	176.69(11)
Cl(2)-Pd(2)-Cl(1)	82.85(3)
Pd(2)-Cl(1)-Pd(1)	93.84(3)
Pd(2)-Cl(2)-Pd(1)	100.89(3)
C(1)-N(1)-C(2)	110.8(3)
C(1)-N(1)-C(4)	126.1(3)
C(2)-N(1)-C(4)	122.8(3)
C(1)-N(2)-C(3)	111.1(3)
C(1)-N(2)-C(16)	124.8(3)

C(3)-N(2)-C(16)	123.4(3)
C(44)-N(3)-C(45)	110.6(3)
C(44)-N(3)-C(47)	126.2(3)
C(45)-N(3)-C(47)	122.9(3)
C(44)-N(4)-C(46)	110.8(3)
C(44)-N(4)-C(59)	127.0(3)
C(46)-N(4)-C(59)	121.9(3)
N(2)-C(1)-N(1)	103.8(3)
N(2)-C(1)-Pd(1)	124.4(2)
N(1)-C(1)-Pd(1)	129.7(2)
C(3)-C(2)-N(1)	107.4(3)
C(3)-C(2)-H(2A)	126.3
N(1)-C(2)-H(2A)	126.3
C(2)-C(3)-N(2)	106.9(3)
C(2)-C(3)-H(3A)	126.6
N(2)-C(3)-H(3A)	126.6
C(5)-C(4)-C(9)	122.6(3)
C(5)-C(4)-N(1)	119.0(3)
C(9)-C(4)-N(1)	118.2(3)
C(4)-C(5)-C(6)	117.2(4)
C(4)-C(5)-C(10)	123.3(4)
C(6)-C(5)-C(10)	119.4(4)
C(7)-C(6)-C(5)	121.7(4)
C(7)-C(6)-H(6A)	119.1
C(5)-C(6)-H(6A)	119.1
C(6)-C(7)-C(8)	120.0(4)
C(6)-C(7)-H(7A)	120.0
C(8)-C(7)-H(7A)	120.0
C(7)-C(8)-C(9)	121.4(4)
C(7)-C(8)-H(8A)	119.3
C(9)-C(8)-H(8A)	119.3

C(8)-C(9)-C(4)	116.9(4)
C(8)-C(9)-C(13)	120.9(4)
C(4)-C(9)-C(13)	122.0(3)
C(5)-C(10)-C(12)	114.1(4)
C(5)-C(10)-C(11)	109.4(4)
C(12)-C(10)-C(11)	109.4(4)
C(5)-C(10)-H(10A)	107.9
C(12)-C(10)-H(10A)	107.9
C(11)-C(10)-H(10A)	107.9
C(10)-C(11)-H(11A)	109.5
C(10)-C(11)-H(11B)	109.5
H(11A)-C(11)-H(11B)	109.5
C(10)-C(11)-H(11C)	109.5
H(11A)-C(11)-H(11C)	109.5
H(11B)-C(11)-H(11C)	109.5
C(10)-C(12)-H(12A)	109.5
C(10)-C(12)-H(12B)	109.5
H(12A)-C(12)-H(12B)	109.5
C(10)-C(12)-H(12C)	109.5
H(12A)-C(12)-H(12C)	109.5
H(12B)-C(12)-H(12C)	109.5
C(9)-C(13)-C(15)	114.0(3)
C(9)-C(13)-C(14)	110.1(3)
C(15)-C(13)-C(14)	108.7(4)
C(9)-C(13)-H(13A)	108.0
C(15)-C(13)-H(13A)	108.0
C(14)-C(13)-H(13A)	108.0
C(13)-C(14)-H(14A)	109.5
C(13)-C(14)-H(14B)	109.5
H(14A)-C(14)-H(14B)	109.5
C(13)-C(14)-H(14C)	109.5

H(14A)-C(14)-H(14C)	109.5
H(14B)-C(14)-H(14C)	109.5
C(13)-C(15)-H(15A)	109.5
C(13)-C(15)-H(15B)	109.5
H(15A)-C(15)-H(15B)	109.5
C(13)-C(15)-H(15C)	109.5
H(15A)-C(15)-H(15C)	109.5
H(15B)-C(15)-H(15C)	109.5
C(17)-C(16)-C(21)	122.8(3)
C(17)-C(16)-N(2)	117.2(3)
C(21)-C(16)-N(2)	119.9(3)
C(18)-C(17)-C(16)	117.8(4)
C(18)-C(17)-C(22)	120.2(3)
C(16)-C(17)-C(22)	122.0(3)
C(19)-C(18)-C(17)	120.8(4)
C(19)-C(18)-H(18A)	119.6
C(17)-C(18)-H(18A)	119.6
C(18)-C(19)-C(20)	120.3(4)
C(18)-C(19)-H(19A)	119.9
C(20)-C(19)-H(19A)	119.9
C(19)-C(20)-C(21)	121.7(4)
C(19)-C(20)-H(20A)	119.2
C(21)-C(20)-H(20A)	119.2
C(20)-C(21)-C(16)	116.7(4)
C(20)-C(21)-C(25)	120.8(4)
C(16)-C(21)-C(25)	122.4(3)
C(17)-C(22)-C(23)	111.3(3)
C(17)-C(22)-C(24)	112.8(3)
C(23)-C(22)-C(24)	109.2(3)
C(17)-C(22)-H(22A)	107.8
C(23)-C(22)-H(22A)	107.8

C(24)-C(22)-H(22A)	107.8
C(22)-C(23)-H(23A)	109.5
C(22)-C(23)-H(23B)	109.5
H(23A)-C(23)-H(23B)	109.5
C(22)-C(23)-H(23C)	109.5
H(23A)-C(23)-H(23C)	109.5
H(23B)-C(23)-H(23C)	109.5
C(22)-C(24)-H(24A)	109.5
C(22)-C(24)-H(24B)	109.5
H(24A)-C(24)-H(24B)	109.5
C(22)-C(24)-H(24C)	109.5
H(24A)-C(24)-H(24C)	109.5
H(24B)-C(24)-H(24C)	109.5
C(21)-C(25)-C(26)	112.9(4)
C(21)-C(25)-C(27)	109.5(3)
C(26)-C(25)-C(27)	110.7(4)
C(21)-C(25)-H(25A)	107.8
C(26)-C(25)-H(25A)	107.8
C(27)-C(25)-H(25A)	107.8
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5
C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5

C(33)-C(28)-C(29)	103.8(3)
C(33)-C(28)-Pd(1)	116.5(2)
C(29)-C(28)-Pd(1)	113.5(2)
C(33)-C(28)-H(28A)	107.5
C(29)-C(28)-H(28A)	107.5
Pd(1)-C(28)-H(28A)	107.5
C(34)-C(29)-C(30)	99.6(3)
C(34)-C(29)-C(28)	103.7(3)
C(30)-C(29)-C(28)	106.7(3)
C(34)-C(29)-H(29A)	115.0
C(30)-C(29)-H(29A)	115.0
C(28)-C(29)-H(29A)	115.0
C(29)-C(30)-C(31)	103.3(3)
C(29)-C(30)-H(30A)	111.1
C(31)-C(30)-H(30A)	111.1
C(29)-C(30)-H(30B)	111.1
C(31)-C(30)-H(30B)	111.1
H(30A)-C(30)-H(30B)	109.1
C(30)-C(31)-C(32)	102.7(3)
C(30)-C(31)-H(31A)	111.2
C(32)-C(31)-H(31A)	111.2
C(30)-C(31)-H(31B)	111.2
C(32)-C(31)-H(31B)	111.2
H(31A)-C(31)-H(31B)	109.1
C(34)-C(32)-C(33)	102.0(3)
C(34)-C(32)-C(31)	101.1(4)
C(33)-C(32)-C(31)	108.9(3)
C(34)-C(32)-H(32A)	114.4
C(33)-C(32)-H(32A)	114.5
C(31)-C(32)-H(32A)	114.4
C(35)-C(33)-C(28)	116.0(3)

C(35)-C(33)-C(32)	111.4(3)
C(28)-C(33)-C(32)	102.1(3)
C(35)-C(33)-H(33A)	109.0
C(28)-C(33)-H(33A)	109.0
C(32)-C(33)-H(33A)	109.0
C(32)-C(34)-C(29)	94.4(3)
C(32)-C(34)-H(34A)	112.8
C(29)-C(34)-H(34A)	112.8
C(32)-C(34)-H(34B)	112.8
C(29)-C(34)-H(34B)	112.8
H(34A)-C(34)-H(34B)	110.3
C(33)-C(35)-H(35A)	109.5
C(33)-C(35)-H(35B)	109.5
H(35A)-C(35)-H(35B)	109.5
C(33)-C(35)-H(35C)	109.5
H(35A)-C(35)-H(35C)	109.5
H(35B)-C(35)-H(35C)	109.5
C(41)-C(36)-C(37)	102.8(3)
C(41)-C(36)-Pd(2)	115.6(3)
C(37)-C(36)-Pd(2)	114.5(3)
C(41)-C(36)-H(36A)	107.8
C(37)-C(36)-H(36A)	107.8
Pd(2)-C(36)-H(36A)	107.8
C(42)-C(37)-C(38)	99.8(4)
C(42)-C(37)-C(36)	103.9(3)
C(38)-C(37)-C(36)	106.4(4)
C(42)-C(37)-H(37A)	115.0
C(38)-C(37)-H(37A)	115.0
C(36)-C(37)-H(37A)	115.0
C(37)-C(38)-C(39)	102.5(4)
C(37)-C(38)-H(38A)	111.3

C(39)-C(38)-H(38A)	111.3
C(37)-C(38)-H(38B)	111.3
C(39)-C(38)-H(38B)	111.3
H(38A)-C(38)-H(38B)	109.2
C(40)-C(39)-C(38)	103.2(4)
C(40)-C(39)-H(39A)	111.1
C(38)-C(39)-H(39A)	111.1
C(40)-C(39)-H(39B)	111.1
C(38)-C(39)-H(39B)	111.1
H(39A)-C(39)-H(39B)	109.1
C(42)-C(40)-C(39)	101.6(4)
C(42)-C(40)-C(41)	101.9(3)
C(39)-C(40)-C(41)	108.7(4)
C(42)-C(40)-H(40A)	114.4
C(39)-C(40)-H(40A)	114.4
C(41)-C(40)-H(40A)	114.4
C(43)-C(41)-C(40)	111.2(4)
C(43)-C(41)-C(36)	116.5(3)
C(40)-C(41)-C(36)	102.3(3)
C(43)-C(41)-H(41A)	108.8
C(40)-C(41)-H(41A)	108.8
C(36)-C(41)-H(41A)	108.8
C(40)-C(42)-C(37)	94.7(3)
C(40)-C(42)-H(42A)	112.8
C(37)-C(42)-H(42A)	112.8
C(40)-C(42)-H(42B)	112.8
C(37)-C(42)-H(42B)	112.8
H(42A)-C(42)-H(42B)	110.2
C(41)-C(43)-H(43A)	109.5
C(41)-C(43)-H(43B)	109.5
H(43A)-C(43)-H(43B)	109.5

C(41)-C(43)-H(43C)	109.5
H(43A)-C(43)-H(43C)	109.5
H(43B)-C(43)-H(43C)	109.5
N(4)-C(44)-N(3)	104.2(3)
N(4)-C(44)-Pd(2)	130.3(3)
N(3)-C(44)-Pd(2)	123.1(3)
C(46)-C(45)-N(3)	107.1(3)
C(46)-C(45)-H(45A)	126.4
N(3)-C(45)-H(45A)	126.4
C(45)-C(46)-N(4)	107.1(3)
C(45)-C(46)-H(46A)	126.4
N(4)-C(46)-H(46A)	126.4
C(48)-C(47)-C(52)	122.9(4)
C(48)-C(47)-N(3)	119.7(4)
C(52)-C(47)-N(3)	117.4(3)
C(49)-C(48)-C(47)	117.0(4)
C(49)-C(48)-C(53)	120.0(4)
C(47)-C(48)-C(53)	122.8(4)
C(50)-C(49)-C(48)	121.5(4)
C(50)-C(49)-H(49A)	119.3
C(48)-C(49)-H(49A)	119.3
C(49)-C(50)-C(51)	120.4(4)
C(49)-C(50)-H(50A)	119.8
C(51)-C(50)-H(50A)	119.8
C(50)-C(51)-C(52)	121.1(4)
C(50)-C(51)-H(51A)	119.5
C(52)-C(51)-H(51A)	119.5
C(51)-C(52)-C(47)	117.1(4)
C(51)-C(52)-C(56)	118.9(4)
C(47)-C(52)-C(56)	123.9(4)
C(48)-C(53)-C(55)	109.3(6)

C(48)-C(53)-C(55B)	108.7(10)
C(48)-C(53)-C(54)	108.7(9)
C(55)-C(53)-C(54)	110.0(6)
C(55B)-C(53)-C(54)	124.4(10)
C(48)-C(53)-C(54B)	121.6(16)
C(55)-C(53)-C(54B)	97.3(12)
C(55B)-C(53)-C(54B)	110.5(10)
C(48)-C(53)-H(53A)	109.6
C(55)-C(53)-H(53A)	109.6
C(55B)-C(53)-H(53A)	94.5
C(54)-C(53)-H(53A)	109.6
C(54B)-C(53)-H(53A)	108.5
C(48)-C(53)-H(53B)	105.9
C(55)-C(53)-H(53B)	118.1
C(55B)-C(53)-H(53B)	103.1
C(54)-C(53)-H(53B)	104.3
C(54B)-C(53)-H(53B)	105.3
C(53)-C(54)-H(54A)	109.5
C(53)-C(54)-H(54B)	109.5
C(53)-C(54)-H(54C)	109.5
C(53)-C(55)-H(55A)	109.5
C(53)-C(55)-H(55B)	109.5
C(53)-C(55)-H(55C)	109.5
C(53)-C(54B)-H(54D)	109.5
C(53)-C(54B)-H(54E)	109.5
H(54D)-C(54B)-H(54E)	109.5
C(53)-C(54B)-H(54F)	109.5
H(54D)-C(54B)-H(54F)	109.5
H(54E)-C(54B)-H(54F)	109.5
C(53)-C(55B)-H(55D)	109.5
C(53)-C(55B)-H(55E)	109.5

H(55D)-C(55B)-H(55E)	109.5
C(53)-C(55B)-H(55F)	109.5
H(55D)-C(55B)-H(55F)	109.5
H(55E)-C(55B)-H(55F)	109.5
C(58)-C(56)-C(52)	113.0(4)
C(58)-C(56)-C(57)	110.0(4)
C(52)-C(56)-C(57)	110.0(4)
C(58)-C(56)-H(56A)	107.9
C(52)-C(56)-H(56A)	107.9
C(57)-C(56)-H(56A)	107.9
C(56)-C(57)-H(57A)	109.5
C(56)-C(57)-H(57B)	109.5
H(57A)-C(57)-H(57B)	109.5
C(56)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
C(56)-C(58)-H(58A)	109.5
C(56)-C(58)-H(58B)	109.5
H(58A)-C(58)-H(58B)	109.5
C(56)-C(58)-H(58C)	109.5
H(58A)-C(58)-H(58C)	109.5
H(58B)-C(58)-H(58C)	109.5
C(64)-C(59)-C(60)	122.3(4)
C(64)-C(59)-N(4)	119.5(3)
C(60)-C(59)-N(4)	117.9(4)
C(61)-C(60)-C(59)	116.7(4)
C(61)-C(60)-C(65)	121.3(4)
C(59)-C(60)-C(65)	121.9(4)
C(62)-C(61)-C(60)	122.4(5)
C(62)-C(61)-H(61A)	118.8
C(60)-C(61)-H(61A)	118.8

C(61)-C(62)-C(63)	120.5(4)
C(61)-C(62)-H(62A)	119.8
C(63)-C(62)-H(62A)	119.8
C(62)-C(63)-C(64)	120.8(5)
C(62)-C(63)-H(63A)	119.6
C(64)-C(63)-H(63A)	119.6
C(63)-C(64)-C(59)	117.1(4)
C(63)-C(64)-C(68)	119.0(4)
C(59)-C(64)-C(68)	123.9(4)
C(60)-C(65)-C(67)	110.5(4)
C(60)-C(65)-C(66)	113.2(4)
C(67)-C(65)-C(66)	108.2(4)
C(60)-C(65)-H(65A)	108.3
C(67)-C(65)-H(65A)	108.3
C(66)-C(65)-H(65A)	108.3
C(65)-C(66)-H(66A)	109.5
C(65)-C(66)-H(66B)	109.5
H(66A)-C(66)-H(66B)	109.5
C(65)-C(66)-H(66C)	109.5
H(66A)-C(66)-H(66C)	109.5
H(66B)-C(66)-H(66C)	109.5
C(65)-C(67)-H(67A)	109.5
C(65)-C(67)-H(67B)	109.5
H(67A)-C(67)-H(67B)	109.5
C(65)-C(67)-H(67C)	109.5
H(67A)-C(67)-H(67C)	109.5
H(67B)-C(67)-H(67C)	109.5
C(64)-C(68)-C(70)	113.3(4)
C(64)-C(68)-C(69)	110.8(4)
C(70)-C(68)-C(69)	108.4(4)
C(64)-C(68)-H(68A)	108.1

C(70)-C(68)-H(68A)	108.1
C(69)-C(68)-H(68A)	108.1
C(68)-C(69)-H(69A)	109.5
C(68)-C(69)-H(69D)	109.5
H(69A)-C(69)-H(69D)	109.5
C(68)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
H(69D)-C(69)-H(69B)	109.5
C(68)-C(70)-H(70D)	109.5
C(68)-C(70)-H(70A)	109.5
H(70D)-C(70)-H(70A)	109.5
C(68)-C(70)-H(70B)	109.5
H(70D)-C(70)-H(70B)	109.5
H(70A)-C(70)-H(70B)	109.5

Table S14. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **3**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	25(1)	19(1)	26(1)	6(1)	0(1)	5(1)
Pd(2)	26(1)	20(1)	27(1)	7(1)	1(1)	5(1)
Cl(1)	32(1)	25(1)	30(1)	8(1)	-2(1)	3(1)
Cl(2)	45(1)	29(1)	31(1)	10(1)	-6(1)	-6(1)
N(1)	23(2)	23(2)	34(2)	8(1)	1(1)	6(1)
N(2)	26(2)	21(2)	29(2)	6(1)	-1(1)	4(1)
N(3)	32(2)	24(2)	31(2)	4(1)	3(1)	10(1)
N(4)	34(2)	26(2)	31(2)	6(1)	2(1)	10(2)
C(1)	28(2)	28(2)	24(2)	10(1)	3(1)	13(2)
C(2)	29(2)	29(2)	40(2)	4(2)	-6(2)	5(2)
C(3)	37(2)	16(2)	38(2)	3(2)	-3(2)	3(2)
C(4)	20(2)	24(2)	41(2)	7(2)	-2(2)	5(2)
C(5)	23(2)	34(2)	45(2)	14(2)	-2(2)	4(2)
C(6)	29(2)	50(3)	56(3)	26(2)	1(2)	14(2)
C(7)	36(2)	48(3)	72(3)	26(2)	12(2)	24(2)
C(8)	35(2)	43(3)	55(3)	11(2)	10(2)	18(2)
C(9)	26(2)	25(2)	45(2)	8(2)	3(2)	3(2)
C(10)	35(2)	48(3)	41(2)	17(2)	-3(2)	10(2)
C(11)	59(3)	62(3)	51(3)	13(2)	-16(2)	6(3)
C(12)	43(3)	69(3)	52(3)	32(2)	2(2)	17(3)
C(13)	33(2)	42(2)	40(2)	10(2)	8(2)	15(2)
C(14)	54(3)	40(3)	53(3)	18(2)	12(2)	13(2)
C(15)	43(3)	51(3)	46(2)	9(2)	15(2)	12(2)
C(16)	26(2)	18(2)	34(2)	0(1)	0(1)	6(2)
C(17)	32(2)	23(2)	30(2)	4(1)	1(2)	10(2)
C(18)	37(2)	34(2)	36(2)	9(2)	0(2)	15(2)

C(19)	32(2)	41(3)	49(2)	9(2)	-7(2)	16(2)
C(20)	30(2)	37(2)	51(2)	11(2)	5(2)	10(2)
C(21)	28(2)	25(2)	40(2)	7(2)	0(2)	9(2)
C(22)	34(2)	29(2)	36(2)	10(2)	3(2)	12(2)
C(23)	46(3)	37(2)	46(2)	12(2)	7(2)	8(2)
C(24)	53(3)	41(3)	38(2)	8(2)	11(2)	12(2)
C(25)	34(2)	35(2)	43(2)	15(2)	9(2)	14(2)
C(26)	42(3)	45(3)	63(3)	25(2)	12(2)	13(2)
C(27)	81(4)	51(3)	39(2)	15(2)	15(2)	32(3)
C(28)	32(2)	21(2)	23(2)	5(1)	-6(1)	5(2)
C(29)	35(2)	34(2)	32(2)	6(2)	-3(2)	12(2)
C(30)	47(3)	40(3)	43(2)	8(2)	-10(2)	15(2)
C(31)	62(3)	37(2)	34(2)	10(2)	-9(2)	10(2)
C(32)	59(3)	25(2)	34(2)	4(2)	-4(2)	8(2)
C(33)	41(2)	23(2)	37(2)	4(2)	3(2)	8(2)
C(34)	46(3)	33(2)	36(2)	8(2)	-8(2)	7(2)
C(35)	42(2)	31(2)	43(2)	6(2)	10(2)	12(2)
C(36)	33(2)	20(2)	36(2)	9(2)	0(2)	4(2)
C(37)	39(2)	22(2)	45(2)	-1(2)	-3(2)	0(2)
C(38)	58(3)	30(2)	56(3)	1(2)	2(2)	12(2)
C(39)	44(3)	34(3)	70(3)	14(2)	-9(2)	-7(2)
C(40)	34(2)	34(3)	59(3)	10(2)	-8(2)	-4(2)
C(41)	34(2)	38(2)	50(2)	16(2)	4(2)	7(2)
C(42)	49(3)	34(2)	38(2)	2(2)	-13(2)	-5(2)
C(43)	32(2)	44(3)	70(3)	14(2)	6(2)	16(2)
C(44)	20(2)	19(2)	32(2)	3(1)	1(1)	0(2)
C(45)	45(2)	34(2)	36(2)	9(2)	-5(2)	18(2)
C(46)	42(2)	38(2)	30(2)	7(2)	-3(2)	15(2)
C(47)	34(2)	29(2)	32(2)	6(2)	3(2)	14(2)
C(48)	33(2)	35(2)	40(2)	10(2)	4(2)	15(2)
C(49)	53(3)	42(3)	45(2)	9(2)	15(2)	24(2)

C(50)	57(3)	31(2)	50(3)	1(2)	9(2)	21(2)
C(51)	53(3)	26(2)	52(3)	11(2)	6(2)	12(2)
C(52)	41(2)	31(2)	44(2)	12(2)	7(2)	17(2)
C(53)	39(2)	35(2)	54(2)	16(2)	17(2)	17(2)
C(54)	53(7)	47(6)	64(5)	26(4)	23(4)	10(6)
C(55)	40(4)	51(6)	73(7)	14(5)	19(4)	23(4)
C(54B)	50(9)	52(9)	56(7)	18(6)	12(6)	14(7)
C(55B)	27(6)	34(7)	56(8)	2(6)	16(5)	15(5)
C(56)	51(3)	26(2)	55(3)	11(2)	19(2)	11(2)
C(57)	86(4)	62(4)	51(3)	21(3)	16(3)	30(3)
C(58)	61(4)	69(4)	79(4)	29(3)	29(3)	14(3)
C(59)	39(2)	33(2)	26(2)	9(2)	7(2)	17(2)
C(60)	41(2)	45(3)	33(2)	7(2)	8(2)	21(2)
C(61)	52(3)	54(3)	62(3)	10(2)	19(2)	28(3)
C(62)	70(4)	51(3)	76(4)	5(3)	22(3)	37(3)
C(63)	63(3)	35(3)	46(2)	-1(2)	8(2)	19(2)
C(64)	52(3)	35(2)	34(2)	5(2)	5(2)	17(2)
C(65)	38(2)	44(3)	44(2)	7(2)	10(2)	9(2)
C(66)	45(3)	74(4)	66(3)	10(3)	18(2)	20(3)
C(67)	62(3)	55(3)	53(3)	21(2)	13(2)	14(3)
C(68)	49(3)	32(2)	35(2)	2(2)	1(2)	8(2)
C(69)	61(3)	55(3)	37(2)	7(2)	-2(2)	10(3)
C(70)	63(3)	34(2)	43(2)	4(2)	3(2)	10(2)

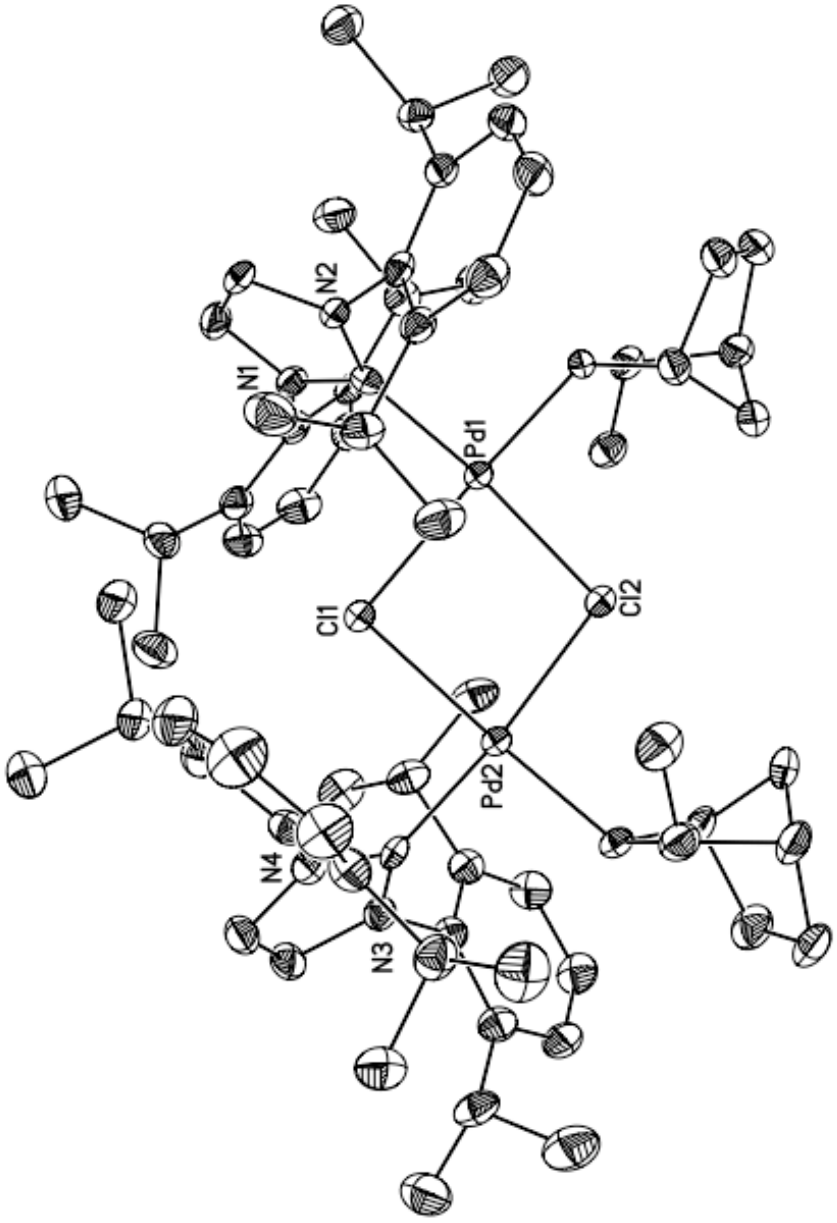
Table S15. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **3**.

	x	y	z	U(eq)
H(2A)	-136	4360	2521	42
H(3A)	1564	3739	2585	39
H(6A)	-1147	7329	2334	52
H(7A)	-1543	7888	3289	57
H(8A)	-842	7404	4086	52
H(10A)	781	5938	1916	50
H(11A)	-1261	4783	1865	94
H(11B)	-937	4934	1216	94
H(11C)	-1781	5467	1563	94
H(12A)	1031	7500	1713	79
H(12B)	-396	7110	1477	79
H(12C)	478	6616	1124	79
H(13A)	1328	6281	4111	45
H(14A)	-251	4756	3667	73
H(14B)	-1190	5083	4071	73
H(14C)	-64	4900	4378	73
H(15A)	779	7532	4780	72
H(15B)	790	6632	5057	72
H(15C)	-480	6681	4810	72
H(18A)	4808	4359	4285	42
H(19A)	6572	4872	3832	49
H(20A)	6554	5492	2991	48
H(22A)	1966	4626	3867	39
H(23A)	1266	3052	4075	66
H(23B)	2603	2994	4049	66

H(23C)	1836	2986	3455	66
H(24A)	3191	5520	4809	68
H(24B)	3327	4515	4895	68
H(24C)	2014	4625	4878	68
H(25A)	3974	5836	2295	44
H(26A)	5835	7167	2724	73
H(26B)	5672	6890	2008	73
H(26C)	6571	6536	2369	73
H(27A)	4050	4277	1820	80
H(27B)	5509	4742	1876	80
H(27C)	4690	5072	1452	80
H(28A)	3710	6609	4209	32
H(29A)	5967	7633	4070	41
H(30A)	6504	7316	5013	53
H(30B)	5193	6455	4766	53
H(31A)	5659	7960	5789	56
H(31B)	4326	7153	5513	56
H(32A)	4671	9000	5495	50
H(33A)	2936	7438	4876	42
H(34A)	6568	9031	5014	49
H(34B)	5624	9200	4549	49
H(35A)	2412	8305	4196	59
H(35B)	3716	9168	4415	59
H(35C)	2732	8947	4875	59
H(36A)	6400	10839	2298	37
H(37A)	5713	11124	3388	48
H(38A)	7187	12779	3525	62
H(38B)	6866	12393	2807	62
H(39A)	8771	12337	2719	66
H(39B)	9132	12829	3428	66
H(40A)	9254	11243	3383	57

H(41A)	8181	10649	2302	49
H(42A)	7739	11617	4035	56
H(42B)	7243	10436	3729	56
H(43A)	8740	9503	2702	72
H(43B)	7402	8942	2338	72
H(43C)	7567	9280	3054	72
H(45A)	2996	9892	747	45
H(46A)	3534	8475	244	44
H(49A)	2863	11558	3106	53
H(50A)	4116	13070	2986	55
H(51A)	5296	13158	2206	53
H(53A)	2529	9159	2191	49
H(53B)	2634	9215	2241	49
H(54A)	3308	9772	3249	82
H(54B)	1933	9005	3142	82
H(54C)	2202	10167	3357	82
H(55A)	980	9639	1818	79
H(55B)	930	10262	2471	79
H(55C)	459	9080	2325	79
H(54D)	1550	8807	3003	79
H(54E)	1735	9941	3283	79
H(54F)	2879	9583	3291	79
H(55D)	1295	9524	1651	59
H(55E)	819	10044	2224	59
H(55F)	554	8880	2079	59
H(56A)	5426	11095	1091	53
H(57A)	4098	11898	799	96
H(57B)	5366	12204	524	96
H(57C)	5149	12945	1089	96
H(58A)	7291	12413	1157	105
H(58B)	7206	12030	1758	105

H(58C)	6970	13030	1747	105
H(61A)	7712	7757	747	64
H(62A)	6576	6106	437	75
H(63A)	4467	5545	423	59
H(65A)	6787	9697	1406	53
H(66A)	8584	9234	1493	94
H(66B)	8866	10296	1355	94
H(66C)	8780	9363	828	94
H(67A)	6019	9697	448	85
H(67B)	7115	9420	163	85
H(67C)	7387	10478	611	85
H(68A)	2692	7045	931	50
H(69A)	2620	6762	-129	82
H(69D)	1453	5974	43	82
H(69B)	2570	5655	-176	82
H(70D)	2867	5791	1395	74
H(70A)	2643	5055	747	74
H(70B)	1582	5434	986	74


N2
N1
Pd1
Cl1
Cl2
Pd2
N4
N3

Crystallographic Data for 4

Table S16. Crystal data and structure refinement for **4**.

Identification code	**4**	
Empirical formula	$C_{173}\ H_{240}\ N_{12}\ Pd_4$	
Formula weight	2913.37	
Temperature	183(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 10.517(5) Å	a= 90°.
	b = 22.963(11) Å	b= 97.774(7)°.
	c = 32.741(16) Å	g = 90°.
Volume	7835(7) $Å^3$	
Z	2	
Density (calculated)	1.235 Mg/m^3	
Absorption coefficient	0.506 mm^{-1}	
F(000)	3092	
Crystal size	0.56 x 0.23 x 0.099 mm^3	
Theta range for data collection	1.09 to 25.37°.	
Index ranges	-12<=h<=12, -27<=k<=27, -39<=l<=39	
Reflections collected	74015	
Independent reflections	14240 [R(int) = 0.0886]	
Completeness to theta = 25.37°	99.1 %	
Absorption correction	Integration	
Max. and min. transmission	0.9688 and 0.8744	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	14240 / 477 / 949	
Goodness-of-fit on F^2	1.061	
Final R indices [I>2sigma(I)]	R1 = 0.0468, wR2 = 0.0979	
R indices (all data)	R1 = 0.0791, wR2 = 0.1081	

Largest diff. peak and hole	0.882 and -0.523 e.Å^{-3}

Table S17. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for **4**. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Pd(1)	3060(1)	1814(1)	549(1)	36(1)
N(1)	4578(3)	2172(2)	331(1)	49(1)
N(2)	262(3)	1670(1)	357(1)	31(1)
N(3)	729(3)	1507(1)	1008(1)	33(1)
C(1)	3723(3)	1040(2)	810(1)	40(1)
C(2)	4417(4)	680(2)	504(1)	50(1)
C(3)	4428(4)	52(2)	649(1)	61(1)
C(4)	5382(4)	71(2)	1062(2)	68(1)
C(5)	5817(4)	698(2)	1090(1)	62(1)
C(6)	4730(4)	1088(2)	1203(1)	52(1)
C(7)	5839(4)	854(2)	637(1)	64(1)
C(8)	5211(5)	1692(2)	1334(1)	73(2)
C(9)	5086(12)	2031(8)	-24(3)	43(2)
C(10)	6328(11)	2187(6)	-80(3)	48(2)
C(11)	6815(10)	2023(5)	-437(3)	51(2)
C(12)	6059(11)	1702(5)	-738(2)	41(2)
C(13)	4817(11)	1546(5)	-682(3)	42(2)
C(14)	4331(11)	1710(7)	-325(3)	43(2)
C(15)	6577(14)	1504(6)	-1130(3)	58(3)
C(9B)	4970(20)	1995(14)	-54(5)	46(2)
C(10B)	6190(20)	2112(11)	-145(5)	46(2)
C(11B)	6563(16)	1918(9)	-514(5)	47(2)
C(12B)	5703(19)	1608(8)	-792(4)	45(3)
C(13B)	4475(18)	1492(9)	-701(5)	44(2)
C(14B)	4106(18)	1685(13)	-332(6)	45(2)
C(15B)	6120(30)	1401(10)	-1205(5)	65(4)

C(16)	1291(3)	1636(2)	662(1)	33(1)
C(17)	-893(3)	1566(2)	508(1)	40(1)
C(18)	-603(3)	1469(2)	912(1)	38(1)
C(19)	374(3)	1870(2)	-60(1)	34(1)
C(20)	467(3)	1457(2)	-363(1)	40(1)
C(21)	541(4)	1668(2)	-762(1)	52(1)
C(22)	516(4)	2256(2)	-840(1)	62(1)
C(23)	440(4)	2651(2)	-531(1)	53(1)
C(24)	358(3)	2470(2)	-130(1)	42(1)
C(25)	456(4)	810(2)	-278(1)	48(1)
C(26)	-929(4)	577(2)	-382(1)	63(1)
C(27)	1388(5)	460(2)	-501(1)	66(1)
C(28)	249(3)	2913(2)	204(1)	48(1)
C(29)	-872(13)	3320(7)	29(8)	66(4)
C(30)	1476(12)	3265(8)	345(7)	50(4)
C(29B)	-929(14)	3323(8)	173(10)	51(5)
C(30B)	1501(15)	3271(10)	242(10)	56(5)
C(31)	1405(3)	1467(2)	1424(1)	36(1)
C(32)	1988(4)	1972(2)	1608(1)	42(1)
C(33)	2616(4)	1915(2)	2007(1)	53(1)
C(34)	2622(4)	1396(2)	2222(1)	58(1)
C(35)	2010(4)	917(2)	2039(1)	53(1)
C(36)	1400(4)	936(2)	1631(1)	40(1)
C(37)	1816(4)	2565(2)	1400(1)	50(1)
C(38)	432(7)	2797(6)	1376(5)	58(3)
C(39)	2791(10)	3024(5)	1588(6)	53(3)
C(38B)	572(14)	2822(8)	1528(8)	54(5)
C(39B)	2929(17)	3004(10)	1493(10)	81(7)
C(40)	756(4)	389(2)	1447(1)	40(1)
C(41)	-470(4)	253(2)	1640(1)	56(1)
C(42)	1656(4)	-135(2)	1502(1)	50(1)

Pd(2)	6928(1)	526(1)	3472(1)	35(1)
N(4)	5427(3)	922(1)	3680(1)	43(1)
N(5)	9531(3)	765(1)	3306(1)	29(1)
N(6)	9412(3)	-166(1)	3316(1)	32(1)
C(43)	6086(3)	-43(2)	3043(1)	41(1)
C(44)	4969(4)	246(2)	2757(1)	46(1)
C(45)	4762(4)	-123(2)	2361(1)	56(1)
C(46)	4194(4)	-707(2)	2508(1)	67(1)
C(47)	4093(4)	-579(2)	2967(1)	57(1)
C(48)	5427(4)	-589(2)	3218(1)	52(1)
C(49)	3783(3)	77(2)	2949(1)	48(1)
C(50)	5349(4)	-585(2)	3682(1)	68(1)
C(51)	4719(3)	1383(2)	3503(1)	35(1)
C(52)	3499(3)	1528(2)	3601(1)	42(1)
C(53)	2812(4)	2000(2)	3421(1)	42(1)
C(54)	3290(4)	2356(2)	3135(1)	37(1)
C(55)	4503(4)	2217(2)	3038(1)	40(1)
C(56)	5203(3)	1745(2)	3214(1)	37(1)
C(57)	2527(4)	2865(2)	2941(1)	53(1)
C(58)	8684(3)	320(2)	3349(1)	29(1)
C(59)	10735(3)	561(2)	3259(1)	34(1)
C(60)	10663(3)	-20(2)	3266(1)	36(1)
C(61)	9199(3)	1374(2)	3347(1)	30(1)
C(62)	9152(4)	1593(2)	3744(1)	38(1)
C(63)	8841(4)	2180(2)	3774(1)	50(1)
C(64)	8610(4)	2525(2)	3430(1)	50(1)
C(65)	8649(4)	2290(2)	3043(1)	46(1)
C(66)	8940(3)	1710(2)	2990(1)	33(1)
C(67)	9453(4)	1232(2)	4133(1)	47(1)
C(68)	10784(4)	1370(2)	4351(1)	75(2)
C(69)	8463(5)	1314(3)	4429(1)	86(2)

C(70)	8924(4)	1448(2)	2561(1)	42(1)
C(71)	9238(5)	1872(2)	2242(1)	71(2)
C(72)	7582(4)	1169(2)	2421(1)	72(2)
C(73)	8979(3)	-757(2)	3359(1)	37(1)
C(74)	8695(4)	-1098(2)	3006(1)	44(1)
C(75)	8271(4)	-1667(2)	3060(2)	60(1)
C(76)	8146(4)	-1870(2)	3447(2)	66(1)
C(77)	8445(4)	-1539(2)	3787(2)	58(1)
C(78)	8906(4)	-969(2)	3759(1)	46(1)
C(79)	8873(4)	-879(2)	2580(1)	49(1)
C(80)	10188(4)	-1064(2)	2467(1)	63(1)
C(81)	7821(4)	-1085(2)	2237(1)	68(1)
C(82)	9381(4)	-628(2)	4141(1)	59(1)
C(83)	10491(8)	-980(5)	4390(2)	87(3)
C(84)	8409(7)	-452(5)	4427(3)	89(3)
C(83B)	10826(8)	-618(15)	4284(7)	94(7)
C(84B)	8580(20)	-786(14)	4485(6)	83(7)

Table S18. Bond lengths [Å] and angles [°] for **4**.

Pd(1)-C(16)	1.988(4)
Pd(1)-N(1)	2.011(3)
Pd(1)-C(1)	2.053(4)
N(1)-C(9)	1.382(5)
N(1)-C(9B)	1.436(7)
N(1)-H(1A)	0.8800
N(2)-C(16)	1.371(4)
N(2)-C(17)	1.394(4)
N(2)-C(19)	1.459(4)
N(3)-C(16)	1.379(4)
N(3)-C(18)	1.397(4)
N(3)-C(31)	1.450(4)
C(1)-C(2)	1.555(5)
C(1)-C(6)	1.558(5)
C(1)-H(1B)	1.0000
C(2)-C(3)	1.520(6)
C(2)-C(7)	1.553(6)
C(2)-H(2A)	1.0000
C(3)-C(4)	1.570(6)
C(3)-H(3A)	0.9900
C(3)-H(3B)	0.9900
C(4)-C(5)	1.509(6)
C(4)-H(4A)	0.9900
C(4)-H(4B)	0.9900
C(5)-C(7)	1.527(6)
C(5)-C(6)	1.538(6)
C(5)-H(5A)	1.0000
C(6)-C(8)	1.517(6)
C(6)-H(6A)	1.0000

C(7)-H(7A)	0.9900
C(7)-H(7B)	0.9900
C(8)-H(8A)	0.9800
C(8)-H(8B)	0.9800
C(8)-H(8C)	0.9800
C(9)-C(10)	1.3900
C(9)-C(14)	1.3900
C(10)-C(11)	1.3900
C(10)-H(10A)	0.9500
C(11)-C(12)	1.3900
C(11)-H(11A)	0.9500
C(12)-C(13)	1.3900
C(12)-C(15)	1.531(6)
C(13)-C(14)	1.3900
C(13)-H(13A)	0.9500
C(14)-H(14A)	0.9500
C(15)-H(15A)	0.9800
C(15)-H(15B)	0.9800
C(15)-H(15C)	0.9800
C(9B)-C(10B)	1.3900
C(9B)-C(14B)	1.3900
C(10B)-C(11B)	1.3900
C(10B)-H(10B)	0.9500
C(11B)-C(12B)	1.3900
C(11B)-H(11B)	0.9500
C(12B)-C(13B)	1.3900
C(12B)-C(15B)	1.552(8)
C(13B)-C(14B)	1.3900
C(13B)-H(13B)	0.9500
C(14B)-H(14B)	0.9500
C(15B)-H(15D)	0.9800

C(15B)-H(15E)	0.9800
C(15B)-H(15F)	0.9800
C(17)-C(18)	1.335(5)
C(17)-H(17A)	0.9500
C(18)-H(18A)	0.9500
C(19)-C(20)	1.388(5)
C(19)-C(24)	1.397(5)
C(20)-C(21)	1.405(5)
C(20)-C(25)	1.512(5)
C(21)-C(22)	1.374(6)
C(21)-H(21A)	0.9500
C(22)-C(23)	1.367(6)
C(22)-H(22A)	0.9500
C(23)-C(24)	1.390(5)
C(23)-H(23A)	0.9500
C(24)-C(28)	1.511(5)
C(25)-C(27)	1.529(6)
C(25)-C(26)	1.546(6)
C(25)-H(25A)	1.0000
C(26)-H(26A)	0.9800
C(26)-H(26B)	0.9800
C(26)-H(26C)	0.9800
C(27)-H(27A)	0.9800
C(27)-H(27B)	0.9800
C(27)-H(27C)	0.9800
C(28)-C(30)	1.540(6)
C(28)-C(30B)	1.544(7)
C(28)-C(29B)	1.548(7)
C(28)-C(29)	1.552(6)
C(28)-H(28A)	1.0000
C(29)-H(29A)	0.9800

C(29)-H(29B)	0.9800
C(29)-H(29C)	0.9800
C(30)-H(30A)	0.9800
C(30)-H(30B)	0.9800
C(30)-H(30C)	0.9800
C(29B)-H(29D)	0.9800
C(29B)-H(29E)	0.9800
C(29B)-H(29F)	0.9800
C(30B)-H(30D)	0.9800
C(30B)-H(30E)	0.9800
C(30B)-H(30F)	0.9800
C(31)-C(36)	1.395(5)
C(31)-C(32)	1.409(5)
C(32)-C(33)	1.388(5)
C(32)-C(37)	1.523(5)
C(33)-C(34)	1.382(6)
C(33)-H(33A)	0.9500
C(34)-C(35)	1.371(6)
C(34)-H(34A)	0.9500
C(35)-C(36)	1.403(5)
C(35)-H(35A)	0.9500
C(36)-C(40)	1.512(5)
C(37)-C(39)	1.539(6)
C(37)-C(38)	1.541(6)
C(37)-C(39B)	1.543(7)
C(37)-C(38B)	1.543(7)
C(37)-H(37A)	1.0000
C(38)-H(38A)	0.9800
C(38)-H(38B)	0.9800
C(38)-H(38C)	0.9800
C(39)-H(39A)	0.9800

C(39)-H(39B)	0.9800
C(39)-H(39C)	0.9800
C(38B)-H(38D)	0.9800
C(38B)-H(38E)	0.9800
C(38B)-H(38F)	0.9800
C(39B)-H(39D)	0.9800
C(39B)-H(39E)	0.9800
C(39B)-H(39F)	0.9800
C(40)-C(42)	1.527(5)
C(40)-C(41)	1.543(5)
C(40)-H(40A)	1.0000
C(41)-H(41A)	0.9800
C(41)-H(41B)	0.9800
C(41)-H(41C)	0.9800
C(42)-H(42A)	0.9800
C(42)-H(42B)	0.9800
C(42)-H(42C)	0.9800
Pd(2)-C(58)	2.001(3)
Pd(2)-N(4)	2.018(3)
Pd(2)-C(43)	2.032(4)
N(4)-C(51)	1.376(5)
N(4)-H(4C)	0.8800
N(5)-C(58)	1.375(4)
N(5)-C(59)	1.378(4)
N(5)-C(61)	1.451(4)
N(6)-C(58)	1.367(4)
N(6)-C(60)	1.389(4)
N(6)-C(73)	1.443(5)
C(43)-C(44)	1.549(5)
C(43)-C(48)	1.577(5)
C(43)-H(43A)	1.0000

C(44)-C(49)	1.520(5)
C(44)-C(45)	1.539(5)
C(44)-H(44A)	1.0000
C(45)-C(46)	1.570(6)
C(45)-H(45A)	0.9900
C(45)-H(45B)	0.9900
C(46)-C(47)	1.546(6)
C(46)-H(46A)	0.9900
C(46)-H(46B)	0.9900
C(47)-C(48)	1.527(5)
C(47)-C(49)	1.541(6)
C(47)-H(47A)	1.0000
C(48)-C(50)	1.534(6)
C(48)-H(48A)	1.0000
C(49)-H(49A)	0.9900
C(49)-H(49B)	0.9900
C(50)-H(50A)	0.9800
C(50)-H(50B)	0.9800
C(50)-H(50C)	0.9800
C(51)-C(52)	1.404(5)
C(51)-C(56)	1.406(5)
C(52)-C(53)	1.388(5)
C(52)-H(52A)	0.9500
C(53)-C(54)	1.389(5)
C(53)-H(53A)	0.9500
C(54)-C(55)	1.393(5)
C(54)-C(57)	1.508(5)
C(55)-C(56)	1.391(5)
C(55)-H(55A)	0.9500
C(56)-H(56A)	0.9500
C(57)-H(57A)	0.9800

C(57)-H(57B)	0.9800
C(57)-H(57C)	0.9800
C(59)-C(60)	1.336(5)
C(59)-H(59A)	0.9500
C(60)-H(60A)	0.9500
C(61)-C(66)	1.398(5)
C(61)-C(62)	1.402(5)
C(62)-C(63)	1.392(5)
C(62)-C(67)	1.516(5)
C(63)-C(64)	1.372(5)
C(63)-H(63A)	0.9500
C(64)-C(65)	1.384(5)
C(64)-H(64A)	0.9500
C(65)-C(66)	1.385(5)
C(65)-H(65A)	0.9500
C(66)-C(70)	1.524(5)
C(67)-C(68)	1.516(6)
C(67)-C(69)	1.526(6)
C(67)-H(67A)	1.0000
C(68)-H(68A)	0.9800
C(68)-H(68B)	0.9800
C(68)-H(68C)	0.9800
C(69)-H(69A)	0.9800
C(69)-H(69B)	0.9800
C(69)-H(69C)	0.9800
C(70)-C(71)	1.498(5)
C(70)-C(72)	1.561(5)
C(70)-H(70A)	1.0000
C(71)-H(71A)	0.9800
C(71)-H(71B)	0.9800
C(71)-H(71C)	0.9800

C(72)-H(72A)	0.9800
C(72)-H(72B)	0.9800
C(72)-H(72C)	0.9800
C(73)-C(74)	1.395(5)
C(73)-C(78)	1.408(5)
C(74)-C(75)	1.399(6)
C(74)-C(79)	1.518(6)
C(75)-C(76)	1.372(6)
C(75)-H(75A)	0.9500
C(76)-C(77)	1.351(6)
C(76)-H(76A)	0.9500
C(77)-C(78)	1.404(6)
C(77)-H(77A)	0.9500
C(78)-C(82)	1.503(6)
C(79)-C(80)	1.539(5)
C(79)-C(81)	1.540(5)
C(79)-H(79A)	1.0000
C(80)-H(80A)	0.9800
C(80)-H(80B)	0.9800
C(80)-H(80C)	0.9800
C(81)-H(81A)	0.9800
C(81)-H(81B)	0.9800
C(81)-H(81C)	0.9800
C(82)-C(83B)	1.528(7)
C(82)-C(84)	1.530(6)
C(82)-C(84B)	1.536(7)
C(82)-C(83)	1.556(6)
C(82)-H(82A)	1.0000
C(82)-H(82B)	0.9602
C(83)-H(83A)	0.9800
C(83)-H(83B)	0.9800

C(83)-H(83C)	0.9800
C(84)-H(84A)	0.9800
C(84)-H(84B)	0.9800
C(84)-H(84C)	0.9800
C(83B)-H(83D)	0.9800
C(83B)-H(83E)	0.9800
C(83B)-H(83F)	0.9800
C(84B)-H(84D)	0.9800
C(84B)-H(84E)	0.9800
C(84B)-H(84F)	0.9800

C(16)-Pd(1)-N(1)	163.42(13)
C(16)-Pd(1)-C(1)	91.05(15)
N(1)-Pd(1)-C(1)	105.06(14)
C(9)-N(1)-Pd(1)	128.2(6)
C(9B)-N(1)-Pd(1)	122.0(10)
C(9)-N(1)-H(1A)	115.9
C(9B)-N(1)-H(1A)	122.1
Pd(1)-N(1)-H(1A)	115.9
C(16)-N(2)-C(17)	111.7(3)
C(16)-N(2)-C(19)	122.9(3)
C(17)-N(2)-C(19)	124.9(3)
C(16)-N(3)-C(18)	110.9(3)
C(16)-N(3)-C(31)	125.1(3)
C(18)-N(3)-C(31)	123.8(3)
C(2)-C(1)-C(6)	104.2(3)
C(2)-C(1)-Pd(1)	110.8(3)
C(6)-C(1)-Pd(1)	115.9(3)
C(2)-C(1)-H(1B)	108.6
C(6)-C(1)-H(1B)	108.6
Pd(1)-C(1)-H(1B)	108.6

C(3)-C(2)-C(7)	100.9(3)
C(3)-C(2)-C(1)	106.6(3)
C(7)-C(2)-C(1)	101.6(3)
C(3)-C(2)-H(2A)	115.3
C(7)-C(2)-H(2A)	115.3
C(1)-C(2)-H(2A)	115.3
C(2)-C(3)-C(4)	102.8(4)
C(2)-C(3)-H(3A)	111.2
C(4)-C(3)-H(3A)	111.2
C(2)-C(3)-H(3B)	111.2
C(4)-C(3)-H(3B)	111.2
H(3A)-C(3)-H(3B)	109.1
C(5)-C(4)-C(3)	103.4(4)
C(5)-C(4)-H(4A)	111.1
C(3)-C(4)-H(4A)	111.1
C(5)-C(4)-H(4B)	111.1
C(3)-C(4)-H(4B)	111.1
H(4A)-C(4)-H(4B)	109.0
C(4)-C(5)-C(7)	102.1(4)
C(4)-C(5)-C(6)	110.0(4)
C(7)-C(5)-C(6)	101.9(3)
C(4)-C(5)-H(5A)	113.9
C(7)-C(5)-H(5A)	113.9
C(6)-C(5)-H(5A)	113.9
C(8)-C(6)-C(5)	111.8(4)
C(8)-C(6)-C(1)	117.5(3)
C(5)-C(6)-C(1)	101.7(3)
C(8)-C(6)-H(6A)	108.5
C(5)-C(6)-H(6A)	108.5
C(1)-C(6)-H(6A)	108.5
C(5)-C(7)-C(2)	94.2(3)

C(5)-C(7)-H(7A)	112.9
C(2)-C(7)-H(7A)	112.9
C(5)-C(7)-H(7B)	112.9
C(2)-C(7)-H(7B)	112.9
H(7A)-C(7)-H(7B)	110.3
C(6)-C(8)-H(8A)	109.5
C(6)-C(8)-H(8B)	109.5
H(8A)-C(8)-H(8B)	109.5
C(6)-C(8)-H(8C)	109.5
H(8A)-C(8)-H(8C)	109.5
H(8B)-C(8)-H(8C)	109.5
N(1)-C(9)-C(10)	121.8(8)
N(1)-C(9)-C(14)	118.2(8)
C(10)-C(9)-C(14)	120.0
C(11)-C(10)-C(9)	120.0
C(11)-C(10)-H(10A)	120.0
C(9)-C(10)-H(10A)	120.0
C(10)-C(11)-C(12)	120.0
C(10)-C(11)-H(11A)	120.0
C(12)-C(11)-H(11A)	120.0
C(11)-C(12)-C(13)	120.0
C(11)-C(12)-C(15)	121.3(5)
C(13)-C(12)-C(15)	118.7(5)
C(14)-C(13)-C(12)	120.0
C(14)-C(13)-H(13A)	120.0
C(12)-C(13)-H(13A)	120.0
C(13)-C(14)-C(9)	120.0
C(13)-C(14)-H(14A)	120.0
C(9)-C(14)-H(14A)	120.0
C(10B)-C(9B)-C(14B)	120.0
C(10B)-C(9B)-N(1)	121.0(13)

C(14B)-C(9B)-N(1)	118.9(14)
C(11B)-C(10B)-C(9B)	120.0
C(11B)-C(10B)-H(10B)	120.0
C(9B)-C(10B)-H(10B)	120.0
C(10B)-C(11B)-C(12B)	120.0
C(10B)-C(11B)-H(11B)	120.0
C(12B)-C(11B)-H(11B)	120.0
C(11B)-C(12B)-C(13B)	120.0
C(11B)-C(12B)-C(15B)	119.6(10)
C(13B)-C(12B)-C(15B)	120.4(9)
C(14B)-C(13B)-C(12B)	120.0
C(14B)-C(13B)-H(13B)	120.0
C(12B)-C(13B)-H(13B)	120.0
C(13B)-C(14B)-C(9B)	120.0
C(13B)-C(14B)-H(14B)	120.0
C(9B)-C(14B)-H(14B)	120.0
C(12B)-C(15B)-H(15D)	109.5
C(12B)-C(15B)-H(15E)	109.5
H(15D)-C(15B)-H(15E)	109.5
C(12B)-C(15B)-H(15F)	109.5
H(15D)-C(15B)-H(15F)	109.5
H(15E)-C(15B)-H(15F)	109.5
N(2)-C(16)-N(3)	103.2(3)
N(2)-C(16)-Pd(1)	121.2(2)
N(3)-C(16)-Pd(1)	135.4(2)
C(18)-C(17)-N(2)	106.7(3)
C(18)-C(17)-H(17A)	126.6
N(2)-C(17)-H(17A)	126.6
C(17)-C(18)-N(3)	107.5(3)
C(17)-C(18)-H(18A)	126.3
N(3)-C(18)-H(18A)	126.3

C(20)-C(19)-C(24)	123.7(3)
C(20)-C(19)-N(2)	118.5(3)
C(24)-C(19)-N(2)	117.7(3)
C(19)-C(20)-C(21)	116.7(4)
C(19)-C(20)-C(25)	122.4(3)
C(21)-C(20)-C(25)	120.9(4)
C(22)-C(21)-C(20)	120.6(4)
C(22)-C(21)-H(21A)	119.7
C(20)-C(21)-H(21A)	119.7
C(23)-C(22)-C(21)	121.1(4)
C(23)-C(22)-H(22A)	119.4
C(21)-C(22)-H(22A)	119.4
C(22)-C(23)-C(24)	121.1(4)
C(22)-C(23)-H(23A)	119.4
C(24)-C(23)-H(23A)	119.4
C(23)-C(24)-C(19)	116.8(4)
C(23)-C(24)-C(28)	120.3(4)
C(19)-C(24)-C(28)	122.9(3)
C(20)-C(25)-C(27)	114.1(4)
C(20)-C(25)-C(26)	109.2(3)
C(27)-C(25)-C(26)	110.9(4)
C(20)-C(25)-H(25A)	107.4
C(27)-C(25)-H(25A)	107.4
C(26)-C(25)-H(25A)	107.4
C(25)-C(26)-H(26A)	109.5
C(25)-C(26)-H(26B)	109.5
H(26A)-C(26)-H(26B)	109.5
C(25)-C(26)-H(26C)	109.5
H(26A)-C(26)-H(26C)	109.5
H(26B)-C(26)-H(26C)	109.5
C(25)-C(27)-H(27A)	109.5

C(25)-C(27)-H(27B)	109.5
H(27A)-C(27)-H(27B)	109.5
C(25)-C(27)-H(27C)	109.5
H(27A)-C(27)-H(27C)	109.5
H(27B)-C(27)-H(27C)	109.5
C(24)-C(28)-C(30)	115.3(10)
C(24)-C(28)-C(30B)	105.6(11)
C(24)-C(28)-C(29B)	120.0(11)
C(30)-C(28)-C(29B)	109.4(14)
C(30B)-C(28)-C(29B)	110.3(9)
C(24)-C(28)-C(29)	105.3(10)
C(30)-C(28)-C(29)	111.1(7)
C(30B)-C(28)-C(29)	107.8(15)
C(24)-C(28)-H(28A)	108.3
C(30)-C(28)-H(28A)	108.3
C(30B)-C(28)-H(28A)	120.5
C(29B)-C(28)-H(28A)	92.7
C(29)-C(28)-H(28A)	108.3
C(28)-C(29)-H(29A)	109.5
C(28)-C(29)-H(29B)	109.5
C(28)-C(29)-H(29C)	109.5
C(28)-C(30)-H(30A)	109.5
C(28)-C(30)-H(30B)	109.5
C(28)-C(30)-H(30C)	109.5
C(28)-C(29B)-H(29D)	109.5
C(28)-C(29B)-H(29E)	109.5
H(29D)-C(29B)-H(29E)	109.5
C(28)-C(29B)-H(29F)	109.5
H(29D)-C(29B)-H(29F)	109.5
H(29E)-C(29B)-H(29F)	109.5
C(28)-C(30B)-H(30D)	109.5

C(28)-C(30B)-H(30E)	109.5
H(30D)-C(30B)-H(30E)	109.5
C(28)-C(30B)-H(30F)	109.5
H(30D)-C(30B)-H(30F)	109.5
H(30E)-C(30B)-H(30F)	109.5
C(36)-C(31)-C(32)	122.8(3)
C(36)-C(31)-N(3)	118.6(3)
C(32)-C(31)-N(3)	118.6(3)
C(33)-C(32)-C(31)	116.7(4)
C(33)-C(32)-C(37)	121.2(4)
C(31)-C(32)-C(37)	121.8(3)
C(34)-C(33)-C(32)	122.0(4)
C(34)-C(33)-H(33A)	119.0
C(32)-C(33)-H(33A)	119.0
C(35)-C(34)-C(33)	120.0(4)
C(35)-C(34)-H(34A)	120.0
C(33)-C(34)-H(34A)	120.0
C(34)-C(35)-C(36)	121.2(4)
C(34)-C(35)-H(35A)	119.4
C(36)-C(35)-H(35A)	119.4
C(31)-C(36)-C(35)	117.3(4)
C(31)-C(36)-C(40)	124.3(3)
C(35)-C(36)-C(40)	118.4(4)
C(32)-C(37)-C(39)	113.6(7)
C(32)-C(37)-C(38)	112.7(6)
C(39)-C(37)-C(38)	110.9(6)
C(32)-C(37)-C(39B)	117.0(12)
C(38)-C(37)-C(39B)	118.1(13)
C(32)-C(37)-C(38B)	106.0(7)
C(39)-C(37)-C(38B)	100.0(10)
C(39B)-C(37)-C(38B)	110.2(9)

C(32)-C(37)-H(37A)	106.3
C(39)-C(37)-H(37A)	106.3
C(38)-C(37)-H(37A)	106.3
C(39B)-C(37)-H(37A)	93.0
C(38B)-C(37)-H(37A)	124.8
C(37)-C(38)-H(38A)	109.5
C(37)-C(38)-H(38B)	109.5
H(38A)-C(38)-H(38B)	109.5
C(37)-C(38)-H(38C)	109.5
H(38A)-C(38)-H(38C)	109.5
H(38B)-C(38)-H(38C)	109.5
C(37)-C(39)-H(39A)	109.5
C(37)-C(39)-H(39B)	109.5
C(37)-C(39)-H(39C)	109.5
C(37)-C(38B)-H(38D)	109.5
C(37)-C(38B)-H(38E)	109.5
H(38D)-C(38B)-H(38E)	109.5
C(37)-C(38B)-H(38F)	109.5
H(38D)-C(38B)-H(38F)	109.5
H(38E)-C(38B)-H(38F)	109.5
C(37)-C(39B)-H(39D)	109.5
C(37)-C(39B)-H(39E)	109.5
H(39D)-C(39B)-H(39E)	109.5
C(37)-C(39B)-H(39F)	109.5
H(39D)-C(39B)-H(39F)	109.5
H(39E)-C(39B)-H(39F)	109.5
C(36)-C(40)-C(42)	111.8(3)
C(36)-C(40)-C(41)	111.1(3)
C(42)-C(40)-C(41)	109.3(3)
C(36)-C(40)-H(40A)	108.2
C(42)-C(40)-H(40A)	108.2

C(41)-C(40)-H(40A)	108.2
C(40)-C(41)-H(41A)	109.5
C(40)-C(41)-H(41B)	109.5
H(41A)-C(41)-H(41B)	109.5
C(40)-C(41)-H(41C)	109.5
H(41A)-C(41)-H(41C)	109.5
H(41B)-C(41)-H(41C)	109.5
C(40)-C(42)-H(42A)	109.5
C(40)-C(42)-H(42B)	109.5
H(42A)-C(42)-H(42B)	109.5
C(40)-C(42)-H(42C)	109.5
H(42A)-C(42)-H(42C)	109.5
H(42B)-C(42)-H(42C)	109.5
C(58)-Pd(2)-N(4)	163.83(13)
C(58)-Pd(2)-C(43)	92.04(15)
N(4)-Pd(2)-C(43)	103.67(14)
C(51)-N(4)-Pd(2)	127.4(2)
C(51)-N(4)-H(4C)	116.3
Pd(2)-N(4)-H(4C)	116.3
C(58)-N(5)-C(59)	112.0(3)
C(58)-N(5)-C(61)	122.6(3)
C(59)-N(5)-C(61)	125.1(3)
C(58)-N(6)-C(60)	111.1(3)
C(58)-N(6)-C(73)	124.9(3)
C(60)-N(6)-C(73)	123.7(3)
C(44)-C(43)-C(48)	103.0(3)
C(44)-C(43)-Pd(2)	111.5(3)
C(48)-C(43)-Pd(2)	115.6(3)
C(44)-C(43)-H(43A)	108.8
C(48)-C(43)-H(43A)	108.8
Pd(2)-C(43)-H(43A)	108.8

C(49)-C(44)-C(45)	100.2(3)
C(49)-C(44)-C(43)	103.8(3)
C(45)-C(44)-C(43)	106.5(3)
C(49)-C(44)-H(44A)	114.9
C(45)-C(44)-H(44A)	114.9
C(43)-C(44)-H(44A)	114.9
C(44)-C(45)-C(46)	103.2(3)
C(44)-C(45)-H(45A)	111.1
C(46)-C(45)-H(45A)	111.1
C(44)-C(45)-H(45B)	111.1
C(46)-C(45)-H(45B)	111.1
H(45A)-C(45)-H(45B)	109.1
C(47)-C(46)-C(45)	102.4(3)
C(47)-C(46)-H(46A)	111.3
C(45)-C(46)-H(46A)	111.3
C(47)-C(46)-H(46B)	111.3
C(45)-C(46)-H(46B)	111.3
H(46A)-C(46)-H(46B)	109.2
C(48)-C(47)-C(49)	102.0(3)
C(48)-C(47)-C(46)	109.9(4)
C(49)-C(47)-C(46)	101.0(4)
C(48)-C(47)-H(47A)	114.2
C(49)-C(47)-H(47A)	114.2
C(46)-C(47)-H(47A)	114.2
C(47)-C(48)-C(50)	111.4(4)
C(47)-C(48)-C(43)	102.1(3)
C(50)-C(48)-C(43)	116.1(3)
C(47)-C(48)-H(48A)	109.0
C(50)-C(48)-H(48A)	109.0
C(43)-C(48)-H(48A)	109.0
C(44)-C(49)-C(47)	94.8(3)

C(44)-C(49)-H(49A)	112.8
C(47)-C(49)-H(49A)	112.8
C(44)-C(49)-H(49B)	112.8
C(47)-C(49)-H(49B)	112.8
H(49A)-C(49)-H(49B)	110.2
C(48)-C(50)-H(50A)	109.5
C(48)-C(50)-H(50B)	109.5
H(50A)-C(50)-H(50B)	109.5
C(48)-C(50)-H(50C)	109.5
H(50A)-C(50)-H(50C)	109.5
H(50B)-C(50)-H(50C)	109.5
N(4)-C(51)-C(52)	123.0(3)
N(4)-C(51)-C(56)	120.9(3)
C(52)-C(51)-C(56)	116.0(3)
C(53)-C(52)-C(51)	121.8(4)
C(53)-C(52)-H(52A)	119.1
C(51)-C(52)-H(52A)	119.1
C(52)-C(53)-C(54)	122.2(4)
C(52)-C(53)-H(53A)	118.9
C(54)-C(53)-H(53A)	118.9
C(53)-C(54)-C(55)	116.3(4)
C(53)-C(54)-C(57)	121.4(3)
C(55)-C(54)-C(57)	122.3(4)
C(56)-C(55)-C(54)	122.4(4)
C(56)-C(55)-H(55A)	118.8
C(54)-C(55)-H(55A)	118.8
C(55)-C(56)-C(51)	121.3(3)
C(55)-C(56)-H(56A)	119.3
C(51)-C(56)-H(56A)	119.3
C(54)-C(57)-H(57A)	109.5
C(54)-C(57)-H(57B)	109.5

H(57A)-C(57)-H(57B)	109.5
C(54)-C(57)-H(57C)	109.5
H(57A)-C(57)-H(57C)	109.5
H(57B)-C(57)-H(57C)	109.5
N(6)-C(58)-N(5)	102.9(3)
N(6)-C(58)-Pd(2)	138.7(3)
N(5)-C(58)-Pd(2)	118.2(3)
C(60)-C(59)-N(5)	106.5(3)
C(60)-C(59)-H(59A)	126.8
N(5)-C(59)-H(59A)	126.8
C(59)-C(60)-N(6)	107.5(3)
C(59)-C(60)-H(60A)	126.3
N(6)-C(60)-H(60A)	126.3
C(66)-C(61)-C(62)	123.4(3)
C(66)-C(61)-N(5)	118.4(3)
C(62)-C(61)-N(5)	118.2(3)
C(63)-C(62)-C(61)	116.8(3)
C(63)-C(62)-C(67)	119.7(3)
C(61)-C(62)-C(67)	123.5(4)
C(64)-C(63)-C(62)	121.3(4)
C(64)-C(63)-H(63A)	119.3
C(62)-C(63)-H(63A)	119.3
C(63)-C(64)-C(65)	120.2(4)
C(63)-C(64)-H(64A)	119.9
C(65)-C(64)-H(64A)	119.9
C(64)-C(65)-C(66)	121.6(4)
C(64)-C(65)-H(65A)	119.2
C(66)-C(65)-H(65A)	119.2
C(65)-C(66)-C(61)	116.6(3)
C(65)-C(66)-C(70)	121.3(3)
C(61)-C(66)-C(70)	122.0(3)

C(62)-C(67)-C(68)	110.8(3)
C(62)-C(67)-C(69)	112.5(4)
C(68)-C(67)-C(69)	109.9(3)
C(62)-C(67)-H(67A)	107.8
C(68)-C(67)-H(67A)	107.8
C(69)-C(67)-H(67A)	107.8
C(67)-C(68)-H(68A)	109.5
C(67)-C(68)-H(68B)	109.5
H(68A)-C(68)-H(68B)	109.5
C(67)-C(68)-H(68C)	109.5
H(68A)-C(68)-H(68C)	109.5
H(68B)-C(68)-H(68C)	109.5
C(67)-C(69)-H(69A)	109.5
C(67)-C(69)-H(69B)	109.5
H(69A)-C(69)-H(69B)	109.5
C(67)-C(69)-H(69C)	109.5
H(69A)-C(69)-H(69C)	109.5
H(69B)-C(69)-H(69C)	109.5
C(71)-C(70)-C(66)	114.2(3)
C(71)-C(70)-C(72)	109.8(4)
C(66)-C(70)-C(72)	109.2(3)
C(71)-C(70)-H(70A)	107.8
C(66)-C(70)-H(70A)	107.8
C(72)-C(70)-H(70A)	107.8
C(70)-C(71)-H(71A)	109.5
C(70)-C(71)-H(71B)	109.5
H(71A)-C(71)-H(71B)	109.5
C(70)-C(71)-H(71C)	109.5
H(71A)-C(71)-H(71C)	109.5
H(71B)-C(71)-H(71C)	109.5
C(70)-C(72)-H(72A)	109.5

C(70)-C(72)-H(72B)	109.5
H(72A)-C(72)-H(72B)	109.5
C(70)-C(72)-H(72C)	109.5
H(72A)-C(72)-H(72C)	109.5
H(72B)-C(72)-H(72C)	109.5
C(74)-C(73)-C(78)	122.9(4)
C(74)-C(73)-N(6)	118.7(3)
C(78)-C(73)-N(6)	118.3(3)
C(73)-C(74)-C(75)	117.2(4)
C(73)-C(74)-C(79)	122.4(4)
C(75)-C(74)-C(79)	120.4(4)
C(76)-C(75)-C(74)	120.3(4)
C(76)-C(75)-H(75A)	119.8
C(74)-C(75)-H(75A)	119.8
C(77)-C(76)-C(75)	122.0(5)
C(77)-C(76)-H(76A)	119.0
C(75)-C(76)-H(76A)	119.0
C(76)-C(77)-C(78)	120.9(4)
C(76)-C(77)-H(77A)	119.5
C(78)-C(77)-H(77A)	119.5
C(77)-C(78)-C(73)	116.5(4)
C(77)-C(78)-C(82)	120.6(4)
C(73)-C(78)-C(82)	122.7(4)
C(74)-C(79)-C(80)	110.9(3)
C(74)-C(79)-C(81)	113.7(4)
C(80)-C(79)-C(81)	108.7(4)
C(74)-C(79)-H(79A)	107.8
C(80)-C(79)-H(79A)	107.8
C(81)-C(79)-H(79A)	107.8
C(79)-C(80)-H(80A)	109.5
C(79)-C(80)-H(80B)	109.5

H(80A)-C(80)-H(80B)	109.5
C(79)-C(80)-H(80C)	109.5
H(80A)-C(80)-H(80C)	109.5
H(80B)-C(80)-H(80C)	109.5
C(79)-C(81)-H(81A)	109.5
C(79)-C(81)-H(81B)	109.5
H(81A)-C(81)-H(81B)	109.5
C(79)-C(81)-H(81C)	109.5
H(81A)-C(81)-H(81C)	109.5
H(81B)-C(81)-H(81C)	109.5
C(78)-C(82)-C(83B)	117.9(10)
C(78)-C(82)-C(84)	118.1(5)
C(83B)-C(82)-C(84)	121.9(10)
C(78)-C(82)-C(84B)	109.5(10)
C(83B)-C(82)-C(84B)	113.4(10)
C(78)-C(82)-C(83)	107.8(4)
C(84)-C(82)-C(83)	109.4(5)
C(84B)-C(82)-C(83)	86.5(10)
C(78)-C(82)-H(82A)	107.0
C(83B)-C(82)-H(82A)	69.8
C(84)-C(82)-H(82A)	107.0
C(84B)-C(82)-H(82A)	134.7
C(83)-C(82)-H(82A)	107.0
C(78)-C(82)-H(82B)	105.1
C(83B)-C(82)-H(82B)	104.3
C(84)-C(82)-H(82B)	74.9
C(84B)-C(82)-H(82B)	105.4
C(83)-C(82)-H(82B)	138.7
C(82)-C(83)-H(83A)	109.5
C(82)-C(83)-H(83B)	109.5
C(82)-C(83)-H(83C)	109.5

C(82)-C(84)-H(84A)	109.5
H(82B)-C(84)-H(84A)	83.8
C(82)-C(84)-H(84B)	109.5
H(82B)-C(84)-H(84B)	96.2
C(82)-C(84)-H(84C)	109.5
H(82B)-C(84)-H(84C)	144.0
C(82)-C(83B)-H(83D)	109.5
C(82)-C(83B)-H(83E)	109.5
H(83D)-C(83B)-H(83E)	109.5
C(82)-C(83B)-H(83F)	109.5
H(83D)-C(83B)-H(83F)	109.5
H(83E)-C(83B)-H(83F)	109.5
C(82)-C(84B)-H(84D)	109.5
C(82)-C(84B)-H(84E)	109.5
H(84D)-C(84B)-H(84E)	109.5
C(82)-C(84B)-H(84F)	109.5
H(84D)-C(84B)-H(84F)	109.5
H(84E)-C(84B)-H(84F)	109.5

Symmetry transformations used to generate equivalent atoms:

Table S19. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for **4**. The anisotropic displacement factor exponent takes the form: $-2p^2[\ h^2\ a^{*2}U^{11} + ...\ + 2\ h\ k\ a^*\ b^*\ U^{12}\ ]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Pd(1)	30(1)	38(1)	40(1)	1(1)	4(1)	1(1)
N(1)	41(2)	40(2)	66(2)	0(2)	8(2)	-7(2)
N(2)	30(2)	33(2)	31(2)	2(1)	0(1)	1(1)
N(3)	30(2)	39(2)	30(2)	2(1)	4(1)	4(1)
C(1)	31(2)	43(3)	45(2)	1(2)	1(2)	5(2)
C(2)	54(3)	44(3)	52(2)	4(2)	12(2)	12(2)
C(3)	61(3)	49(3)	74(3)	-2(2)	15(2)	10(2)
C(4)	51(3)	63(4)	89(4)	16(3)	11(3)	22(3)
C(5)	41(2)	60(4)	80(3)	13(3)	-6(2)	8(2)
C(6)	45(2)	58(3)	49(2)	7(2)	-4(2)	10(2)
C(7)	43(3)	60(3)	95(4)	14(3)	29(2)	14(2)
C(8)	70(3)	68(4)	74(3)	-14(3)	-23(3)	1(3)
C(9)	32(3)	40(3)	56(3)	14(3)	4(3)	5(3)
C(10)	35(3)	47(4)	63(3)	12(3)	6(3)	-5(3)
C(11)	34(4)	51(4)	68(4)	16(3)	6(3)	-1(3)
C(12)	27(4)	46(4)	54(3)	23(3)	17(3)	5(3)
C(13)	31(4)	45(3)	51(3)	18(3)	10(3)	-6(3)
C(14)	30(4)	47(3)	56(3)	17(3)	16(3)	-4(3)
C(15)	48(5)	64(5)	66(5)	22(4)	20(4)	3(5)
C(9B)	34(4)	44(4)	62(4)	15(4)	14(4)	-1(4)
C(10B)	31(4)	46(4)	61(4)	13(4)	2(4)	-6(4)
C(11B)	28(4)	48(4)	65(4)	18(4)	2(4)	-3(4)
C(12B)	37(5)	46(4)	53(4)	22(4)	9(4)	1(4)
C(13B)	34(5)	47(4)	54(4)	20(4)	17(4)	-1(4)
C(14B)	35(4)	47(4)	55(4)	13(4)	14(4)	4(4)
C(15B)	52(7)	72(7)	78(7)	26(6)	33(6)	5(6)

C(16)	30(2)	34(2)	35(2)	-2(2)	1(2)	4(2)
C(17)	27(2)	45(3)	46(2)	11(2)	4(2)	1(2)
C(18)	29(2)	47(3)	40(2)	10(2)	11(2)	4(2)
C(19)	31(2)	39(3)	30(2)	6(2)	1(2)	-3(2)
C(20)	41(2)	42(3)	33(2)	8(2)	-3(2)	-1(2)
C(21)	65(3)	57(3)	31(2)	6(2)	0(2)	-7(2)
C(22)	67(3)	76(4)	40(2)	24(3)	-6(2)	-16(3)
C(23)	57(3)	46(3)	54(3)	19(2)	-2(2)	-11(2)
C(24)	36(2)	40(3)	50(2)	9(2)	-1(2)	-8(2)
C(25)	68(3)	42(3)	33(2)	1(2)	5(2)	4(2)
C(26)	79(3)	46(3)	64(3)	2(2)	8(2)	-12(3)
C(27)	80(3)	55(3)	63(3)	-11(2)	15(3)	8(3)
C(28)	45(2)	36(3)	64(3)	6(2)	9(2)	-6(2)
C(29)	61(6)	57(6)	79(8)	1(6)	10(5)	0(5)
C(30)	47(5)	49(6)	54(8)	2(5)	10(4)	-3(4)
C(29B)	43(6)	53(7)	58(8)	-3(6)	11(5)	7(5)
C(30B)	61(7)	55(8)	52(9)	-18(6)	-1(5)	-4(6)
C(31)	36(2)	44(3)	28(2)	-1(2)	4(2)	8(2)
C(32)	49(2)	44(3)	34(2)	-7(2)	4(2)	8(2)
C(33)	58(3)	50(3)	48(2)	-18(2)	-3(2)	2(2)
C(34)	78(3)	52(3)	39(2)	-8(2)	-12(2)	9(3)
C(35)	73(3)	44(3)	39(2)	-1(2)	-4(2)	16(2)
C(36)	46(2)	40(3)	32(2)	-4(2)	2(2)	11(2)
C(37)	60(3)	46(3)	45(2)	-5(2)	13(2)	-2(2)
C(38)	72(5)	55(5)	47(6)	-11(5)	3(4)	12(4)
C(39)	60(5)	38(5)	65(7)	-18(4)	19(4)	-8(4)
C(38B)	69(7)	25(7)	67(9)	26(6)	3(6)	-2(5)
C(39B)	89(9)	87(9)	68(10)	-24(7)	18(7)	-10(7)
C(40)	51(2)	36(3)	34(2)	-1(2)	2(2)	5(2)
C(41)	55(3)	60(3)	54(3)	6(2)	6(2)	3(2)
C(42)	62(3)	40(3)	49(2)	-4(2)	3(2)	7(2)

Pd(2)	26(1)	33(1)	45(1)	2(1)	7(1)	2(1)
N(4)	41(2)	46(2)	45(2)	6(2)	16(2)	6(2)
N(5)	30(2)	27(2)	30(2)	-1(1)	4(1)	0(1)
N(6)	25(2)	28(2)	43(2)	1(1)	5(1)	-1(1)
C(43)	33(2)	41(3)	48(2)	1(2)	4(2)	1(2)
C(44)	39(2)	45(3)	54(2)	6(2)	4(2)	-1(2)
C(45)	45(2)	66(3)	53(3)	-13(2)	-6(2)	-1(2)
C(46)	43(3)	64(4)	89(4)	-18(3)	-6(2)	-12(2)
C(47)	35(2)	62(3)	74(3)	7(3)	7(2)	-12(2)
C(48)	47(2)	31(3)	75(3)	1(2)	4(2)	-4(2)
C(49)	27(2)	50(3)	66(3)	8(2)	0(2)	0(2)
C(50)	69(3)	56(3)	77(3)	27(3)	3(3)	-9(3)
C(51)	28(2)	35(3)	41(2)	-6(2)	6(2)	-4(2)
C(52)	37(2)	39(3)	52(2)	2(2)	15(2)	-4(2)
C(53)	32(2)	46(3)	49(2)	-6(2)	8(2)	2(2)
C(54)	44(2)	30(2)	38(2)	-8(2)	10(2)	-1(2)
C(55)	47(2)	37(3)	38(2)	-8(2)	14(2)	-6(2)
C(56)	30(2)	40(3)	43(2)	-11(2)	13(2)	-5(2)
C(57)	65(3)	47(3)	49(2)	0(2)	14(2)	12(2)
C(58)	28(2)	27(2)	32(2)	1(2)	1(2)	-1(2)
C(59)	25(2)	36(3)	42(2)	1(2)	9(2)	0(2)
C(60)	23(2)	36(3)	50(2)	0(2)	11(2)	2(2)
C(61)	31(2)	22(2)	37(2)	-2(2)	8(2)	-6(2)
C(62)	43(2)	32(2)	37(2)	-7(2)	5(2)	-5(2)
C(63)	65(3)	47(3)	38(2)	-16(2)	11(2)	-3(2)
C(64)	65(3)	27(3)	60(3)	-5(2)	9(2)	7(2)
C(65)	55(3)	38(3)	48(2)	9(2)	9(2)	3(2)
C(66)	32(2)	28(2)	40(2)	0(2)	9(2)	-2(2)
C(67)	69(3)	39(3)	31(2)	-4(2)	6(2)	-9(2)
C(68)	60(3)	99(4)	65(3)	25(3)	6(2)	12(3)
C(69)	67(3)	145(6)	48(3)	24(3)	13(2)	-8(3)

C(70)	50(2)	42(3)	35(2)	5(2)	14(2)	7(2)
C(71)	102(4)	62(4)	54(3)	11(2)	34(3)	14(3)
C(72)	67(3)	108(5)	41(2)	-16(3)	6(2)	-11(3)
C(73)	24(2)	27(2)	60(3)	5(2)	3(2)	0(2)
C(74)	41(2)	27(3)	61(3)	4(2)	-2(2)	4(2)
C(75)	59(3)	33(3)	84(3)	-5(2)	-4(2)	-5(2)
C(76)	62(3)	37(3)	98(4)	23(3)	6(3)	-7(2)
C(77)	53(3)	44(3)	76(3)	23(3)	12(2)	4(2)
C(78)	38(2)	39(3)	61(3)	13(2)	9(2)	6(2)
C(79)	47(2)	35(3)	63(3)	-10(2)	-1(2)	-1(2)
C(80)	67(3)	52(3)	70(3)	-6(2)	16(2)	10(2)
C(81)	65(3)	60(3)	74(3)	-17(3)	-9(2)	-4(3)
C(82)	69(3)	54(3)	56(3)	20(2)	8(2)	4(2)
C(83)	83(5)	90(6)	83(5)	3(4)	-10(4)	2(4)
C(84)	88(5)	93(7)	93(5)	-13(5)	34(4)	2(5)
C(83B)	88(10)	98(11)	96(10)	-9(8)	10(8)	-16(8)
C(84B)	81(9)	88(11)	78(9)	-3(8)	13(7)	9(8)

Table S20. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$x 10^3) for **4**.

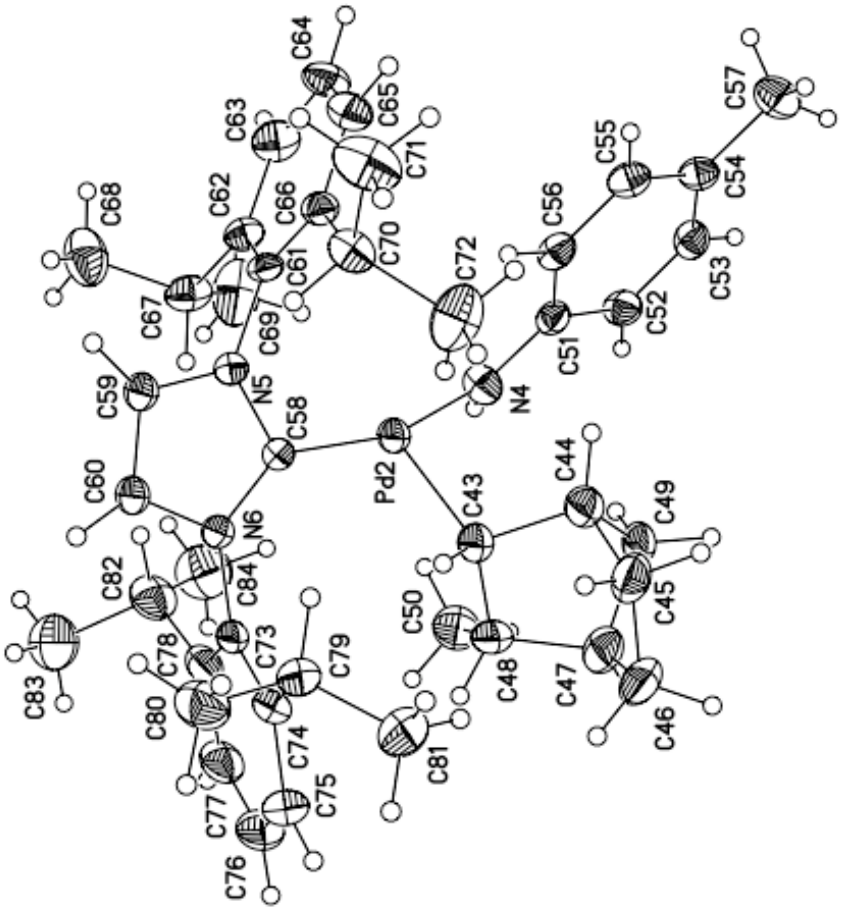
	x	y	z	U(eq)
H(1A)	4969	2454	481	58
H(1B)	2974	809	879	48
H(2A)	4092	741	205	60
H(3A)	4742	-213	447	73
H(3B)	3562	-75	699	73
H(4A)	4943	-36	1300	81
H(4B)	6116	-196	1050	81
H(5A)	6657	758	1268	74
H(6A)	4363	905	1439	62
H(7A)	6448	613	505	77
H(7B)	6002	1273	595	77
H(8A)	5713	1672	1608	110
H(8B)	4478	1953	1341	110
H(8C)	5753	1840	1136	110
H(10A)	6844	2406	126	58
H(11A)	7663	2129	-475	61
H(13A)	4301	1327	-888	50
H(14A)	3482	1604	-287	52
H(15A)	7496	1590	-1107	88
H(15B)	6123	1710	-1369	88
H(15C)	6442	1083	-1167	88
H(10B)	6782	2323	46	56
H(11B)	7402	1998	-575	57
H(13B)	3887	1280	-892	53
H(14B)	3267	1605	-271	54

H(15D)	5361	1371	-1414	98
H(15E)	6531	1019	-1166	98
H(15F)	6724	1681	-1296	98
H(17A)	-1726	1564	354	47
H(18A)	-1195	1389	1100	45
H(21A)	609	1402	-980	62
H(22A)	552	2391	-1112	75
H(23A)	444	3056	-592	64
H(25A)	717	755	25	58
H(26A)	-1490	777	-212	94
H(26B)	-939	158	-328	94
H(26C)	-1236	649	-674	94
H(27A)	2252	624	-439	98
H(27B)	1112	476	-799	98
H(27C)	1397	54	-408	98
H(28A)	-4	2705	449	58
H(29A)	-1647	3087	-51	98
H(29B)	-644	3525	-214	98
H(29C)	-1032	3603	239	98
H(30A)	2179	2997	442	75
H(30B)	1326	3527	570	75
H(30C)	1705	3493	113	75
H(29D)	-1718	3093	120	77
H(29E)	-893	3600	-53	77
H(29F)	-920	3537	432	77
H(30D)	2239	3010	302	85
H(30E)	1507	3556	465	85
H(30F)	1553	3476	-18	85
H(33A)	3054	2242	2136	63
H(34A)	3051	1372	2496	70
H(35A)	1997	566	2192	64

H(37A)	1979	2507	1109	59
H(38A)	-49	2696	1108	88
H(38B)	450	3221	1410	88
H(38C)	16	2620	1596	88
H(39A)	3663	2874	1588	80
H(39B)	2646	3109	1871	80
H(39C)	2684	3381	1423	80
H(38D)	-169	2606	1391	81
H(38E)	498	3233	1446	81
H(38F)	598	2791	1827	81
H(39D)	3642	2819	1670	121
H(39E)	2633	3344	1634	121
H(39F)	3218	3127	1234	121
H(40A)	506	455	1145	48
H(41A)	-1073	579	1589	85
H(41B)	-247	196	1937	85
H(41C)	-868	-102	1515	85
H(42A)	2430	-52	1376	76
H(42B)	1221	-476	1368	76
H(42C)	1895	-213	1796	76
H(4C)	5201	785	3911	52
H(43A)	6745	-181	2872	49
H(44A)	5071	673	2712	56
H(45A)	5582	-192	2252	67
H(45B)	4151	68	2146	67
H(46A)	3342	-791	2352	80
H(46B)	4776	-1039	2480	80
H(47A)	3443	-823	3085	68
H(48A)	5886	-949	3147	62
H(49A)	2974	167	2768	58
H(49B)	3772	250	3225	58

H(50A)	4447	-575	3727	102
H(50B)	5791	-240	3807	102
H(50C)	5758	-937	3808	102
H(52A)	3133	1297	3796	51
H(53A)	1990	2081	3496	50
H(55A)	4866	2454	2846	48
H(56A)	6025	1666	3137	45
H(57A)	2616	2886	2647	79
H(57B)	2847	3226	3077	79
H(57C)	1620	2814	2973	79
H(59A)	11470	788	3228	41
H(60A)	11343	-284	3241	43
H(63A)	8787	2344	4037	60
H(64A)	8424	2927	3458	60
H(65A)	8472	2534	2807	56
H(67A)	9440	813	4050	56
H(68A)	11418	1300	4163	112
H(68B)	10973	1119	4594	112
H(68C)	10821	1779	4437	112
H(69A)	7603	1238	4283	130
H(69B)	8507	1715	4533	130
H(69C)	8645	1043	4660	130
H(70A)	9578	1130	2581	50
H(71A)	10063	2059	2336	106
H(71B)	8565	2170	2198	106
H(71C)	9290	1666	1983	106
H(72A)	7595	967	2158	108
H(72B)	6927	1475	2387	108
H(72C)	7383	891	2630	108
H(75A)	8068	-1914	2827	72
H(76A)	7840	-2255	3476	79

H(77A)	8342	-1695	4050	69
H(79A)	8850	-444	2587	59
H(80A)	10870	-898	2666	94
H(80B)	10277	-921	2190	94
H(80C)	10253	-1489	2472	94
H(81A)	6975	-995	2316	102
H(81B)	7896	-1506	2199	102
H(81C)	7921	-884	1980	102
H(82A)	9765	-260	4049	71
H(82B)	9170	-230	4072	71
H(83A)	11166	-1051	4217	131
H(83B)	10159	-1354	4475	131
H(83C)	10845	-759	4635	131
H(84A)	7682	-254	4267	134
H(84B)	8820	-190	4641	134
H(84C)	8103	-801	4556	134
H(83D)	11246	-368	4101	141
H(83E)	11169	-1015	4277	141
H(83F)	10988	-467	4566	141
H(84D)	7669	-762	4379	124
H(84E)	8781	-513	4715	124
H(84F)	8793	-1183	4581	124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