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Electronic Supplementary Information

Pd-promoted cross coupling of iodobenzene with vinylgold via an unprecedented phenyl transmetalation from Pd to Au

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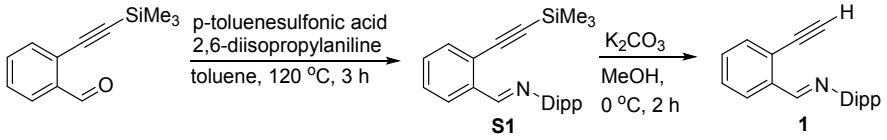
General Methods

Unless otherwise stated, all reactions and manipulations were performed using standard Schlenk techniques. All solvents were purified by distillation using standard methods. Commercially available reagents were used without further purification. NMR spectra were recorded by using a Bruker 400 MHz spectrometer. Chemical shifts are reported in ppm from tetramethylsilane with the solvent resonance as the internal standar (^{1}H NMR $CDCl_3$: 7.26 ppm; ^{13}C NMR $CDCl_3$: 77.0 ppm; ^{13}C NMR DMSO: 39.43 ppm). Mass spectra were recorded on the HP-5989 instrument by EI/ESI methods. X-ray diffraction analysis was performed by using a Bruker Smart-1000X-ray diffractometer.

Trimethylsilyl acetylene, 2,6-diisopropylaniline and 2-bromoisophthalaldehyde are commercially available and were used as received without further purification. 2-(trimethylsilyl)ethynyl)benzaldehyde,[1] 2-(phenylethynyl) isophthalaldehyde,[2] IPrAuCl,[3] $Pd(CH_3CN)_4(BF_4)_2$[4] and [PCP]PdCl[5] was synthesized by the procedures previously reported.

Preparation and characterization

Synthesis of complex 1

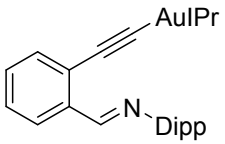


Scheme S1. The synthetic route for the preparation of terminal alkynyl **1**.

A mixture of 2-((trimethylsilyl)ethynyl)benzaldehyde (500 mg, 2.47 mmol), *p*-toluenesulfonic acid (43 mg, 0.25 mmol) and 2,6-diisopropylaniline (525 mg, 2.96 mmol) was refluxed in the toluene (15 mL) at 120 °C for 3 h. The mixture was then filtered and all volatiles were removed under reduced pressure. The residue was washed with methanol and filtered to afford **S1** as a yellow solid (829 mg, 93%).

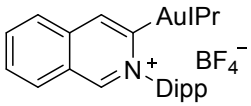
S1 (500 mg, 1.38 mmol) was dissolved in methanol (20 mL), potassium carbonate (478 mg, 3.46 mmol) was added, and then the mixture was stirred at 0 °C for 2 h. All volatiles were removed under reduced pressure and dissolved in DCM. The mixture was filtered through Celite and the filtrate was concentrated to afford **1** as a pale yellow solid (367 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.84 (s,1H), 8.39 (d, J = 7.2 Hz, 1H), 7.67 (d, J = 7.2 Hz, 1H), 7.59-7.47 (m, 2H), 7.29-7.27 (m, 1H), 7.25-7.17 (m, 2H), 3.36 (s, 1H), 3.15-3.03 (m, 2H), 1.28 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.76, 149.16, 137.65, 137.36, 133.14, 130.80, 129.21, 126.24, 124.26, 123.69, 123.04, 83.19, 80.35, 27.90, 23.55. HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{21}H_{24}N^+$: 290.1909; found: 290.1906.

Synthesis of complex 2



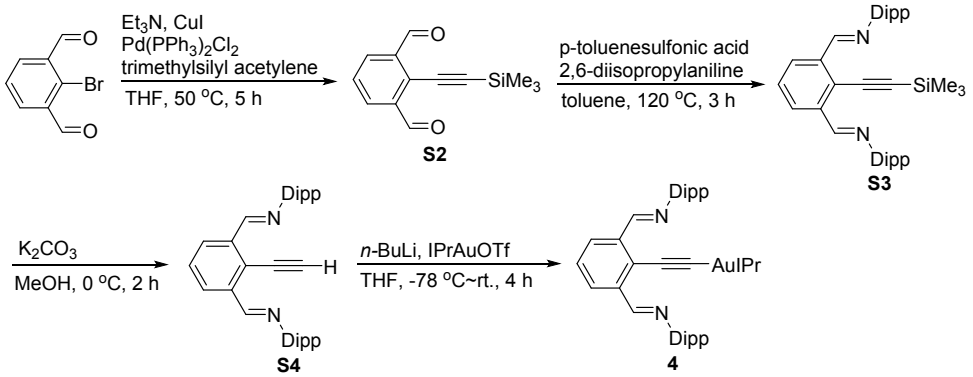
In a nitrogen-filled round-bottom flask, a solution of **1** (200 mg, 0.69 mmol) in THF (6 mL) was cooled to -78 °C, and *n*-butyllithium (1.6 M in THF, 0.52 mL, 0.83 mmol) was added dropwise. After stirring 10 min, IPrAuCl (428 mg, 0.69 mmol) was added. The solution was then warmed to room temperature. After 4 h at room temperature, the mixture was filtered and all volatiles were removed under reduced pressure, the crude product was purified by column chromatography using neutral aluminum oxide (v/v, PE/ EtOAc = 80:1) to afford pure **2** as a yellow solid (314 mg, 52%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.72 (s, 1H), 8.10 (d, J = 7.2 Hz, 1H), 7.43 (t, J = 7.6 Hz, 2H), 7.37 (d, J = 7.2 Hz, 1H), 7.24-7.20 (m, 5H), 7.19-7.12 (m, 4H), 7.10 (s, 2H), 2.99-2.85 (m, 2H), 2.60-2.45 (m, 4H), 1.24 (d, J = 6.8 Hz, 12H), 1.19 (d, J = 6.8 Hz, 12H), 1.10 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 190.59, 162.94, 149.77, 145.46, 137.75, 137.08, 136.64, 134.03, 132.76, 130.29, 128.28, 125.92, 125.38, 124.00, 123.43, 123.07, 122.60, 99.88, 28.64, 27.64, 24.37, 23.87, 23.62. Anal. calcd. for $C_{48}H_{58}AuN_3$ (1.25 CH_2Cl_2): C, 60.35; H, 6.22; N, 4.29; found: C, 60.68; H, 6.60; N, 4.32.

Synthesis of complex 3



Complex **1** (100 mg, 0.11 mmol) and $Pd(CH_3CN)_4(BF_4)_2$ (62 mg, 0.14 mmol) was dissolved in the DCM (2 mL). After stirring at 25 °C for 10 min, the mixture was filtered, and all volatiles were removed under reduced pressure to give the crude product, which was washed with Et_2O and dried to afford pure **3** as a yellow solid (72 mg, 68%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.05 (s, 1H), 8.18 (d, J = 8.4 Hz, 1H), 8.01 (t, J = 8.4 Hz, 1H), 7.84 (d, J = 8.4 Hz, 1H), 7.77 (s, 1H), 7.74 (t, J = 7.2 Hz, 1H), 7.41 (t, J = 7.8 Hz, 2H), 7.31 (t, J = 7.8 Hz, 1H), 7.23 (d, J = 11.0 Hz, 4H), 7.20 (s, 2H), 7.02 (d, J = 7.8 Hz, 2H), 2.55-2.41 (m, 4H), 1.72-1.60 (m, 2H), 1.15 (dd, J = 10.6, 6.8 Hz, 24H), 0.90 (d, J = 6.8 Hz, 6H), 0.50 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 187.29, 147.77, 145.18, 143.94, 142.31, 136.43, 135.92, 135.64, 133.81, 130.41, 130.13, 129.89, 129.25, 125.98, 125.41, 124.16, 124.03, 28.57, 28.02, 24.26, 23.97, 23.37. HRMS (MALDI): m/z $[M\text{-}BF_4]^+$ calcd. for $C_{48}H_{59}AuN_3^+$: 874.4369; found: 874.4188.

Synthesis of complex 4



Scheme S2. The synthetic route for the preparation of gold acetylide **4**.

2-Bromoisophthalaldehyde (2.00 g, 9.44 mmol), CuI (179 mg, 0.94mmol), $Pd(PPh_3)_2Cl_2$ (330 mg, 0.47 mmol) under a nitrogen atmosphere was added into anhydrous THF (40 mL), and then Et_3N (20 mL) and trimethylsilyl acetylene (1.39 g, 14.15mmol) was added. The mixture was stirred at 50 °C for 5 h. All volatiles were removed under reduced pressure, and the residue was purified by column chromatography using silica gel (v/v, PE/ EtOAc = 150:1) to afford pure **S2** as a white solid (1.7 g, 78 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 10.63 (s, 2H), 8.15 (d, J = 7.8 Hz, 2H), 7.57 (t, J = 7.8 Hz, 1H), 0.31 (s, 9H).

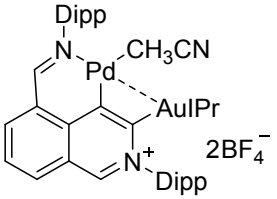
S2 (500 mg, 2.17 mmol), *p*-toluenesulfonic acid (38 mg, 0.22 mmol) and 2,6-diisopropylaniline (847 mg, 4.78 mmol) was added into toluene (15 mL), and the mixture was refluxed in at 120 °C for 3 h. The mixture was filtered and all volatiles were removed under reduced pressure to afford **S3** as a yellow solid (1.11 g, 93%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.79 (s, 2H), 8.45 (d, J = 8.0 Hz, 2H), 7.61 (t, J = 7.8 Hz, 1H), 7.22-7.17 (m, 4H), 7.15 (s, 2H), 3.07-2.92 (m, 4H), 1.21 (d, J = 6.8 Hz, 24H), 0.10 (s, 9H).

S3 (500 mg, 0.91 mmol) was dissolved in methanol (20 mL), and potassium carbonate (629 mg, 4.55 mmol) was added, then the mixture was stirred at 0 °C for 2 h. All volatiles were removed under reduced pressure and dissolved in DCM. The mixture was filtered through Celite and the filtrate was concentrated to afford **S4** as a pale yellow solid (400 mg, 92%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.82 (s, 2H), 8.46 (d, J = 7.8 Hz, 2H), 7.66 (t, J = 7.8 Hz, 1H), 7.21-7.14 (m, 6H), 3.55 (s, 1H), 3.05-2.95 (m, 4H), 1.21 (d, J = 6.8 Hz, 24H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.21, 148.71, 137.81, 137.42, 129.09, 128.73, 124.23, 122.89, 27.73, 23.33. HRMS (ESI): m/z $[M+H]^+$ calcd. for $C_{34}H_{41}N_2^+$: 477.3270; found: 477.3271.

In a nitrogen-filled round-bottom flask, a solution of **S4** (200 mg, 0.42 mmol) in THF (6 mL) was

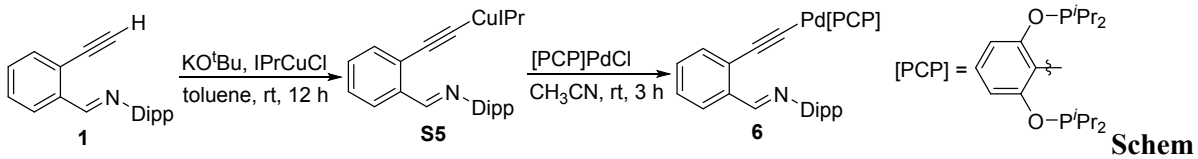
cooled to -78 °C, and *n*-butyllithium (1.6 M in THF, 0.31 mL, 0.50 mmol) was added dropwise. The solution was stirred in 10 min, and then IPrAuOTf (308 mg, 0.42 mmol) was added.The solution was warmed to room temperature, and stirred for 4 h at room temperature. The mixture was filtered and all volatiles were removed under reduced pressure. The residue was washed with methanol and dried in vacuum to afford pure **4** as a gray solid (326 mg, 73%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.78 (s, 2H), 8.23 (d, J = 7.6 Hz, 2H), 7.40 (t, J = 7.8 Hz, 2H), 7.31 (t, J = 7.8 Hz, 1H), 7.18-7.10 (m, 10H), 7.08 (s, 2H), 2.98-2.86 (m, 4H), 2.50-2.38 (m, 4H), 1.14 (dd, J = 10.2, 6.8 Hz, 24H), 1.08 (d, J = 6.8 Hz, 24H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 190.46, 162.55, 149.35, 145.79, 145.43, 137.82, 137.29, 133.89, 130.44, 130.19, 128.28, 125.68, 123.98, 123.65, 123.02, 122.72, 95.89, 28.62, 27.67, 24.30, 23.75. HRMS (MALDI): m/z $[M+H]^+$ calcd. for $C_{61}H_{76}AuN_4^+$: 1061.5736; found: 1061.5538.

Synthesis of complex 5



The mixture of **4** (400 mg, 0.38 mmol) and $Pd(CH_3CN)_4(BF_4)_2$ (253 mg, 0.57 mmol) was dissolved in the acetonitrile (8 mL). The solution was stirred at 25 °C for 30 min. The mixture was then filtered and all volatiles were removed under reduced pressure. The residue was washed with Et_2O and dried in vacuum to afford pure **5** as a yellow solid (463 mg, 94%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.65 (s, 1H), 9.14 (d, J = 8.0 Hz, 1H), 8.75 (d, J = 7.2 Hz, 1H), 8.59 (s, 1H), 8.15 (d, J = 7.8 Hz, 1H), 7.52-7.46 (m, 2H), 7.46-7.37 (m, 6H), 7.29 (d, J = 7.8 Hz, 2H), 7.17 (s, 2H), 7.13 (d, J = 7.8 Hz, 2H), 3.25-3.13 (m, 4H), 2.59-2.50 (m, 2H), 1.89 (s, 3H), 1.72-1.70 (m, 2H), 1.46 (d, J = 6.4 Hz, 6H), 1.34 (d, J = 6.8 Hz, 6H), 1.22 (d, J = 7.2 Hz, 9H), 1.12 (d, J = 6.4 Hz, 12H), 1.00 (d, J = 6.8 Hz, 9H), 0.37 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 193.08, 164.32, 159.56, 149.14, 147.96, 147.39, 145.38, 144.26, 142.18, 141.27, 140.83, 132.96, 131.30, 130.10, 129.67, 126.73, 126.15, 125.09, 124.73, 124.52, 124.30, 121.49, 120.13, 28.40, 25.71, 23.48. Anal. calcd. for $C_{63}H_{78}AuB_2F_8N_5Pd$ (0.5 CH_2Cl_2): C, 53.53; H, 5.59; N, 4.92; found: C, 53.11; H, 5.94; N, 4.44.

Synthesis of complex 6



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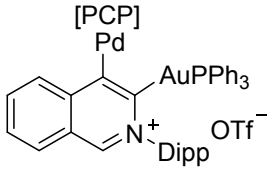
e S3. The synthetic route of **6** through alkynyl transformation from Cu to Pd.

In a nitrogen-filled round-bottom flask, the mixture of **1** (200 mg, 0.69 mmol), KOBu^t (232 mg, 2.07 mmol) and IPrCuCl (336 mg, 0.69 mmol) was mixed in the anhydrous toluene (10 mL). After stirring at 25 °C for 12 h, the mixture was filtered and all volatiles were removed under reduced pressure. The residue was washed with hexane and dried in vacuum to afford pure **S5** as a yellow solid (454 mg, 89%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.66 (s, 1H), 8.09 (d, J = 7.2 Hz, 1H), 7.38-7.30 (m, 4H), 7.19-7.13 (m, 8H), 7.05 (s, 2H), 2.93-2.83 (m, 2H), 2.53-2.44 (m, 4H), 1.16 (d, J = 6.8 Hz, 24H), 1.09 (d, J = 6.8 Hz, 12H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 182.20, 163.01, 150.04, 145.87, 145.45, 137.60, 136.06, 134.33, 132.60, 130.21, 129.32, 125.35, 123.98, 123.39, 122.91, 122.53, 101.18, 28.57, 27.62, 24.81, 24.71, 23.66, 23.49. Anal. calcd. for $C_{48}H_{58}CuN_3$ (0.5 CH_2Cl_2): C, 74.40; H, 7.60; N, 5.37; found: C, 74.00; H, 7.78; N, 5.18.

S5 (400 mg, 0.54 mmol) and [PCP]PdCl (261 mg, 0.54 mmol) was dissolved in the anhydrous acetonitrile (8 mL). After stirring at 25 °C for 3 h, the solution was filtered and all volatiles were removed under reduced pressure. The residue was purified by column chromatography using basic alumina (v/v, PE/ EtOAc = 25:1) to afford pure **6** as a yellow solid (286 mg, 72%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.95 (s, 1H), 8.21 (d, J = 7.6 Hz, 1H), 7.40-7.30 (m, 2H), 7.24 (t, J = 7.6 Hz, 1H), 7.15-7.02 (m, 3H), 6.95 (t, J = 8.0 Hz, 1H), 6.54 (d, J = 8.0 Hz, 2H), 3.05-2.89 (m, 2H), 2.37-2.20 (m, 4H), 1.20-1.11 (m, 36H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 166.17, 163.30, 150.59, 137.49, 137.16, 135.02, 131.92, 130.87, 130.63, 128.15, 125.28, 123.56, 122.54, 114.34, 105.04, 28.98, 27.77, 23.35, 17.41, 16.70. ^{31}P NMR (162 MHz, $CDCl_3$) δ = 193.04. HRMS (MALDI): m/z $[M+H]^+$ calcd. For $C_{39}H_{54}NO_2P_2Pd^+$: 736.2665; found: 736.3112.

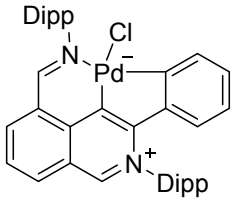
Synthesis of complex 7



6 (200 mg, 0.27 mmol) and PPh_3AuOTf (164 mg, 0.27 mmol) was dissolved in the DCE (4 mL). After stirring at 25 °C for 3 h, the mixture was filtered and all volatiles were removed under reduced pressure. The residue was washed with Et_2O and dried in vaccum to afford pure **7** as a yellow solid (352 mg, 97%). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.83 (s, 1H), 8.15 (d, J = 8.4 Hz, 1H), 8.05 (d, J = 8.4 Hz, 1H), 7.97 (t, J =7.6 Hz, 1H), 7.77 (t, J = 7.2 Hz, 1H), 7.50 (t, J = 7.8 Hz, 1H), 7.41 (t, J = 7.4 Hz, 3H), 7.31 (d, J = 8.0 Hz, 2H), 7.20-7.12 (m, 7H), 7.12-7.05 (m, 6H), 6.72 (d, J = 8.0 Hz, 2H), 2.34-2.14 (m, 6H), 1.27-1.21 (m, 6H), 1.15-1.01 (m, 24H), 0.74 (dd, J = 16.4, 8.2 Hz, 6H). ^{13}C NMR (100

MHz, $CDCl_3$) δ = 193.56 (d, $J_{P\text{-}C}$ =133.3 Hz), 177.46, 165.14, 144.35, 143.98, 143.28, 141.34, 138.13, 133.60 (d, $J_{P\text{-}C}$ = 13.0 Hz), 133.20, 132.77, 131.49, 130.27, 129.62, 129.15, 128.86 (d, $J_{P\text{-}C}$ = 10.6 Hz), 128.28, 124.09, 105.46, 29.94, 28.54, 28.40 (d, $J_{P\text{-}C}$ = 24.2 Hz), 25.36, 23.14, 18.06, 17.27, 16.60, 15.87. ^{31}P NMR (162 MHz, $CDCl_3$) δ = 180.74, 39.08. Anal. calcd. for $C_{58}H_{68}AuF_3NO_5P_3PdS$ (0.5 CH_2Cl_2): C, 50.66; H, 5.01; N, 1.01; found: C, 50.78; H, 5.01; N, 1.01. HRMS (MALDI): m/z $[M\text{-}OTf]^+$ calcd. For $C_{57}H_{68}AuNO_2P_3Pd^+$: 1194.3163; found: 1194.2997.

Synthesis of complex 8



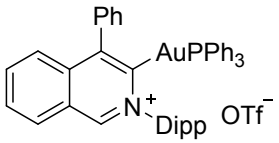
From the coupling reaction of 5 with PhI:

In a nitrogen-filled round-bottom flask, **5** (200 mg, 0.15 mmol) and PhI (306 mg, 1.5 mmol) was dissolved in the anhydrous acetonitrile (6 mL), and the solution was refluxed at 110 °C. After 24 h, the mixture was filtered and all volatiles were removed under reduced pressure. Then the residue was purified by column chromatography using neutral alumina (v/v, DCM/ EtOH = 100:1) to afford pure **8** as an orange red solid (52 mg, 50 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 8.44 (d, J = 7.6 Hz, 1H), 8.21 (s, 1H), 8.17 (s, 1H), 7.84 (d, J = 7.6 Hz, 1H), 7.78 (d, J = 6.8 Hz, 1H), 7.67 (t, J = 7.6 Hz, 1H), 7.55-7.50 (m, 1H), 7.45 (d, J = 7.9 Hz, 2H), 7.25-7.19 (m, 3H), 6.79 (t, J = 7.6 Hz, 1H), 6.38 (t, J = 7.6 Hz, 1H), 5.48 (d, J = 7.2 Hz, 1H), 3.48-3.40 (m, 2H), 2.44-2.36 (m, 2H), 1.42 (d, J = 6.8 Hz, 5H), 1.18-1.10 (m, 12H), 1.06 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, DMSO) δ = 167.98, 166.96, 166.32, 160.35, 149.54, 147.29, 145.74, 142.87, 139.37, 138.88, 137.09, 136.80, 134.18, 131.74, 129.31, 128.31, 125.53, 124.81, 124.12, 122.76, 122.25, 28.16, 27.88, 24.43, 24.11, 22.67. HRMS (MALDI): m/z $[M\text{-}Cl]^+$ calcd. For $C_{40}H_{43}N_2Pd^+$: 657.2461; found: 657.2396.

From $Pd(CH_3CN)_4(BF_4)_2$ promoted cyclization reaction of 10:

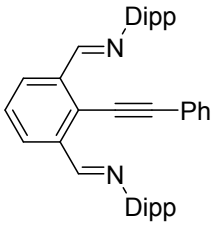
10 (200 mg, 0.36 mmol) and $Pd(CH_3CN)_4(BF_4)_2$ (191 mg, 0.43 mmol) was dissolved in the acetonitrile (4 mL). After stirring at 25 °C for 30 min, the mixture was filtered and all volatiles were removed under reduced pressure. The residue was purified by column chromatography using neutral alumina (v/v, DCM/ EtOH = 100:1) to afford pure **8** as a orange red solid (115 mg, 46 %).

Synthesis of complex 9



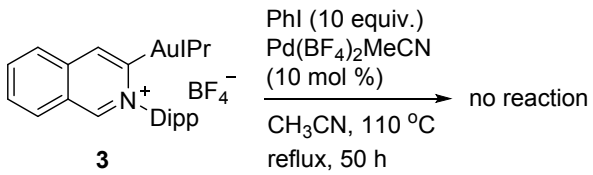
In a nitrogen-filled round-bottom flask, **7** (200 mg, 0.15 mmol) and PhI (304 mg, 1.5 mmol) was dissolved in anhydrous acetonitrile (6 mL), and the solution was refluxed at 110 °C. After 48 h, the mixture was filtered and all volatiles were removed under reduced pressure. The residue was purified by column chromatography using neutral alumina (v/v, DCM/ EtOH = 100:1) to afford pure **9** as offwhite solid (121 mg, 83 %). ^{1}H NMR (400 MHz, $CDCl_3$) δ = 9.69 (s, 1H), 8.67 (d, J = 8.4 Hz, 1H), 8.04 (t, J = 8.0 Hz, 1H), 7.93-7.86 (m, 3H), 7.77 (td, J = 8.4, 4.0 Hz, 2H), 7.64-7.59 (m, 4H), 7.50-7.45 (m, 5H), 7.39-7.35 (m, 5H), 6.97 (dd, J = 12.8, 6.8 Hz, 6H), 2.27-2.16 (m, 2H), 1.18 (d, J = 6.8 Hz, 6H), 1.05 (d, J = 6.8 Hz, 6H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 188.60 (d, $J_{P\text{-}C}$ = 116.9 Hz), 147.99, 146.87, 143.90, 143.50, 138.19, 136.95, 135.67, 134.26 (d, $J_{P\text{-}C}$ = 10.4 Hz), 133.64 (d, $J_{P\text{-}C}$ = 13.8 Hz), 131.74, 130.73, 130.60, 129.07 (d, $J_{P\text{-}C}$ = 11.3 Hz), 128.55, 126.33, 125.52, 124.54, 117.79, 116.90, 28.55, 24.37, 23.73, 18.00. ^{31}P NMR (162 MHz, $CDCl_3$) δ = 40.010. HRMS (MALDI): m/z [M-OTf]$^+$ calcd. For $C_{45}H_{42}AuNP^+$: 824.2715; found: 824.2318.

Synthesis of compound 10



2-(Phenylethynyl) isophthalaldehyde (800 mg, 3.42 mmol), *p*-toluenesulfonic acid (59 mg, 0.34 mmol) and 2,6-diisopropylaniline (1.33 g, 7.52 mmol) was mixed in the toluene (20 mL). After refluxed at 120 °C for 10 min, the mixture was filtered and all volatiles were removed under reduced pressure. The residue was washed with methanol and dried in vaccum to afford **10** as a yellow solid (1.3 g, 69%). 1H NMR (400 MHz, $CDCl_3$) δ = 8.90 (s, 2H), 8.49 (d, J = 7.8 Hz, 2H), 7.65 (t, J = 7.8 Hz, 1H), 7.39-7.33 (m, 2H), 7.32-7.27 (m, 3H), 7.22-7.17 (m, 4H), 7.16-7.10 (m, 2H), 3.09-2.97 (m, 4H), 1.21 (d, J = 6.9 Hz, 24H). ^{13}C NMR (100 MHz, $CDCl_3$) δ = 160.36, 149.02, 137.51, 131.44, 129.13, 128.83, 128.37, 125.84, 124.34, 123.08, 121.79, 101.21, 82.46, 28.00, 23.60. HRMS (ESI): m/z [M+H]$^+$ calcd. for $C_{40}H_{45}N_2^+$: 553.3583; found: 553.3582.

Reaction of complex 3 with PhI in the presence of $Pd(CH_3CN)_4(BF_4)_2$:



Scheme S4. Reaction of complex **3** with PhI in the presence of $Pd(CH_3CN)_4(BF_4)_2$

In a nitrogen-filled round-bottom flask, **3** (100 mg, 0.10 mmol), $Pd(CH_3CN)_4(BF_4)_2$ (5 mg, 0.01 mmol) and PhI (212 mg, 1.04 mmol) was dissolved in anhydrous acetonitrile (4 mL). After refluxed at 110 °C for 50 h, all volatiles were removed under vacuum. The reaction residue was characterized by ^{1}H NMR analysis, and no expected coupling product was observed.

Testing the stability of 5 in acetonitrile at 110 °C:

In a nitrogen-filled round-bottom flask, the complex **5** (50 mg, 0.04 mmol) was dissolved in the anhydrous acetonitrile (2 mL). After refluxed at 110 °C for 20 h, all volatiles were removed under vacuum. The residue was characterized by ^{1}H NMR analysis, and no decomposition was observed.

References

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2. Y. Sota, M. Yamamoto, M. Murai, J. Uenishi and M. Uemura, *Chem. - Eur. J.,* 2015, **21**, 4398.

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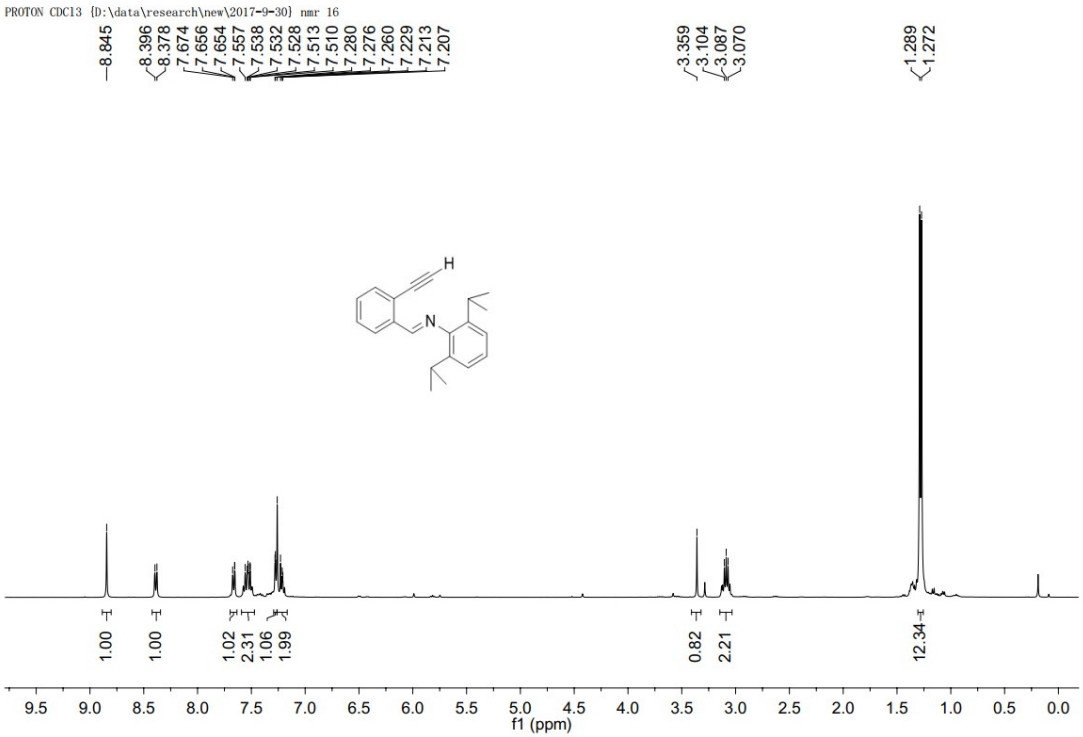
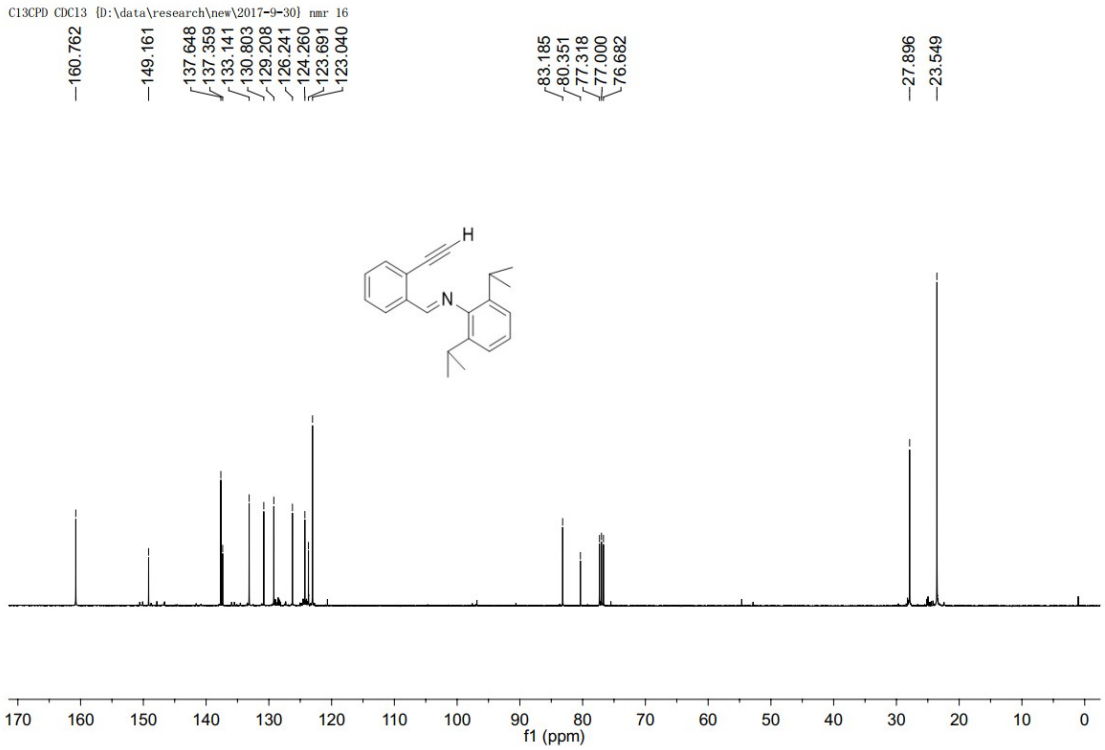
5. A. Adhikary, J. R. Schwartz, L. M. Meadows, J. A. Krause and H. Guan, *Inorg. Chem. Front.,* 2014, **1**, 71.

NMR Spectra

Compound 1

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130.803
129.208
126.241
124.260
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80.351
77.318
77.000
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27.896
23.549
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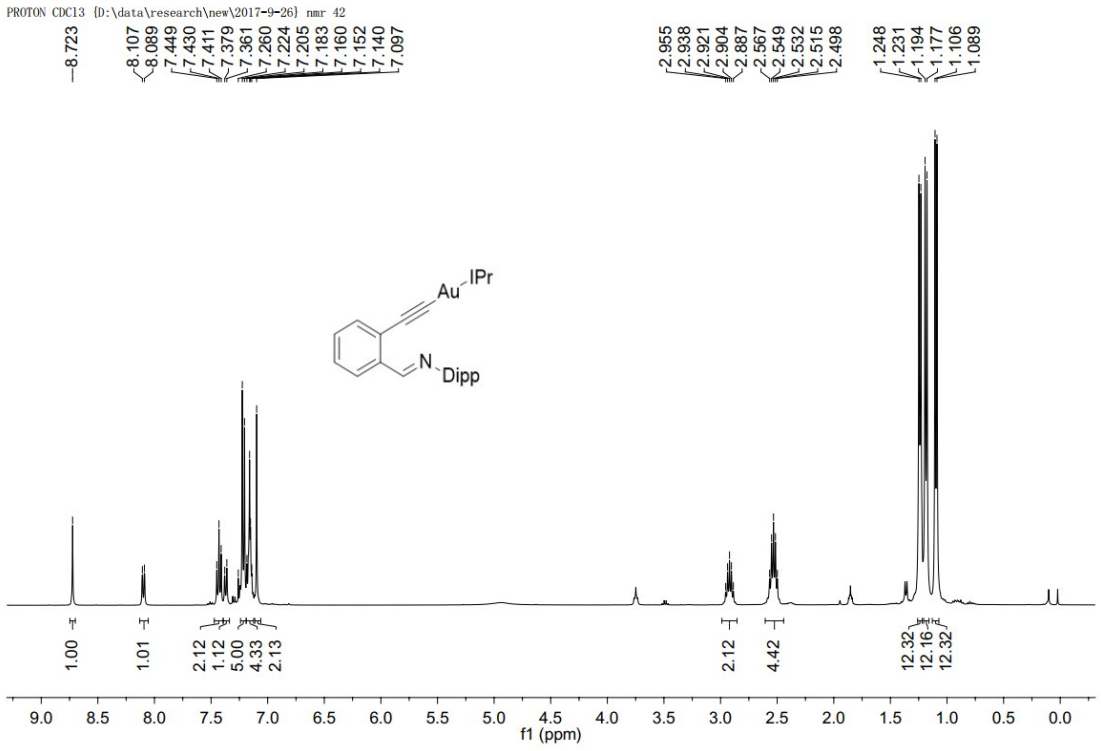
N
f1 (ppm)

Complex 2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7.361
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7.224
7.205
7.183
7.160
7.152
7.140
7.097
2.955
2.938
2.921
2.904
2.887
2.567
2.549
2.532
2.515
2.498
1.248
1.231
1.194
1.177
1.106
1.089
Au
IPr
N
Dipp
1.00
1.01
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5.00
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2.13
2.12
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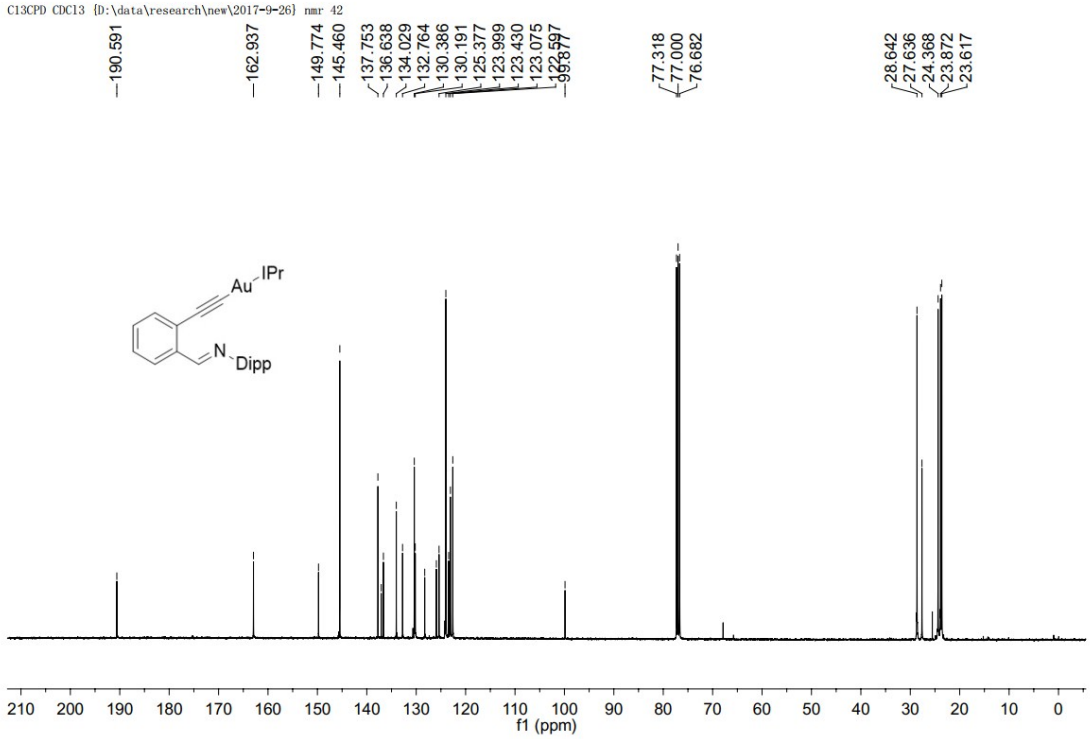
12.32
f1 (ppm)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123.999
123.430
123.075
122.597
93.877
77.318
77.000
76.682
28.642
27.636
24.368
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IPr
N
Dipp
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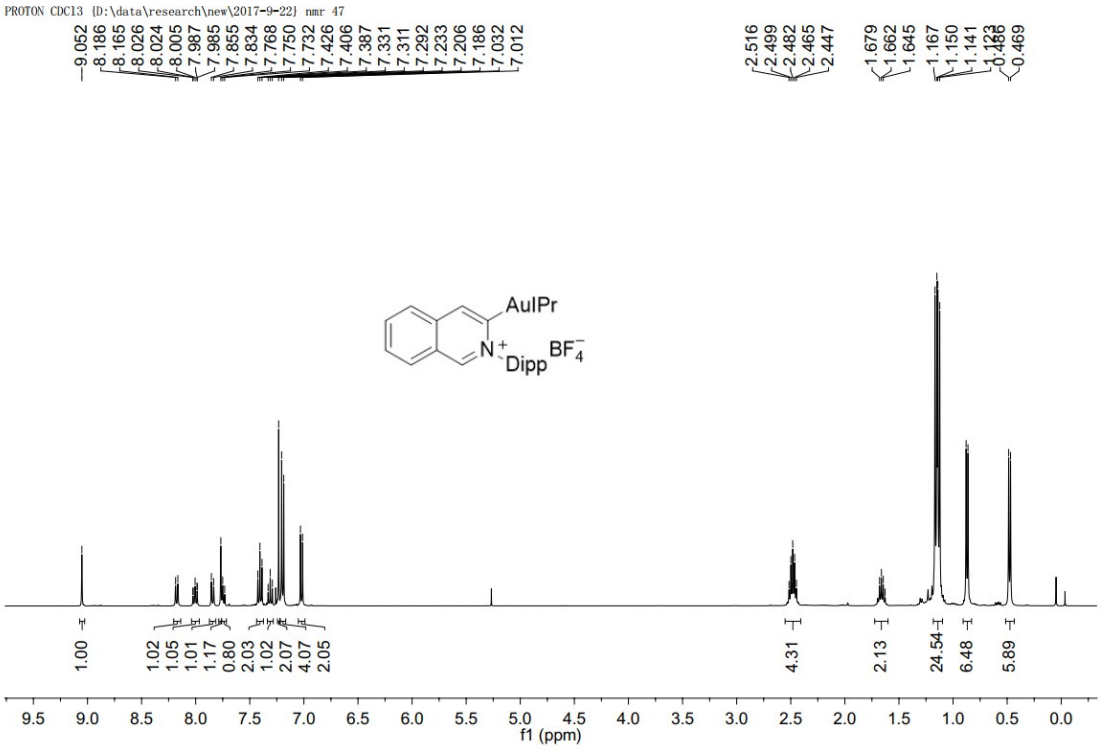
f1 (ppm)

Complex 3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7.985
7.855
7.834
7.768
7.750
7.732
7.426
7.406
7.387
7.331
7.311
7.292
7.233
7.206
7.186
7.032
7.012
2.516
2.499
2.482
2.465
2.447
1.679
1.662
1.645
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1.141
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0.469
AuIPr
N
Dipp
BF4
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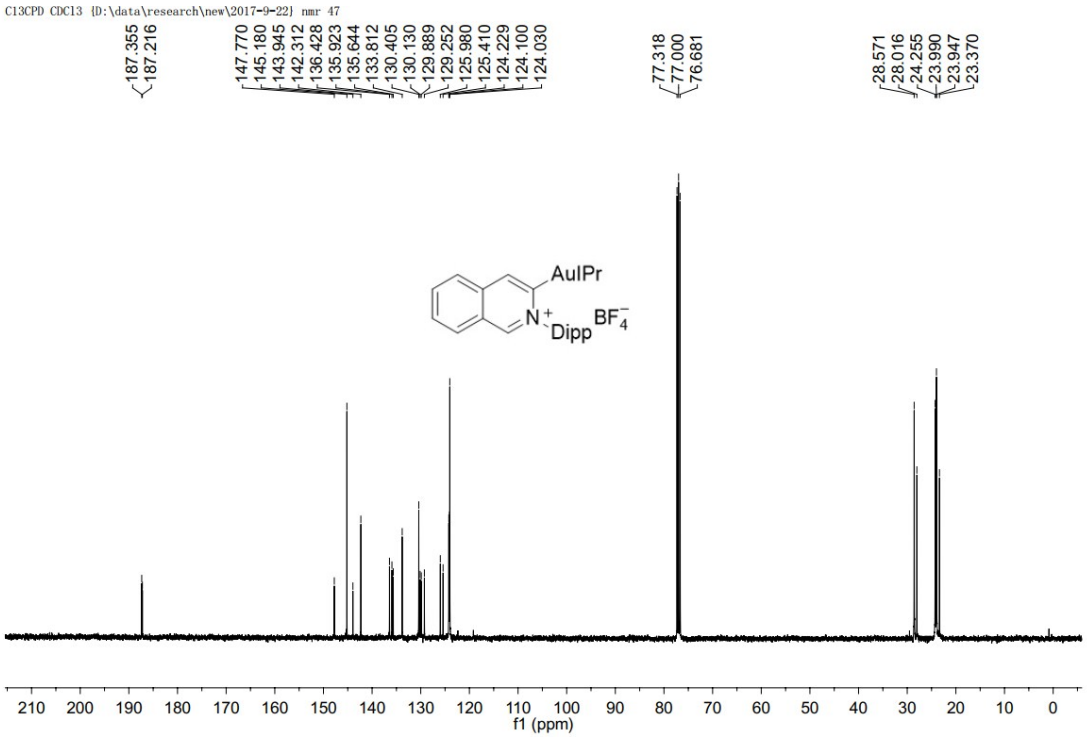
1.02
1.05
1.01
1.17
0.80
2.03
1.02
2.07
4.07
2.05
4.31
2.13
24.54
6.48
5.89
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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133.812
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130.130
129.889
129.252
125.980
125.410
124.229
124.100
124.030
77.318
77.000
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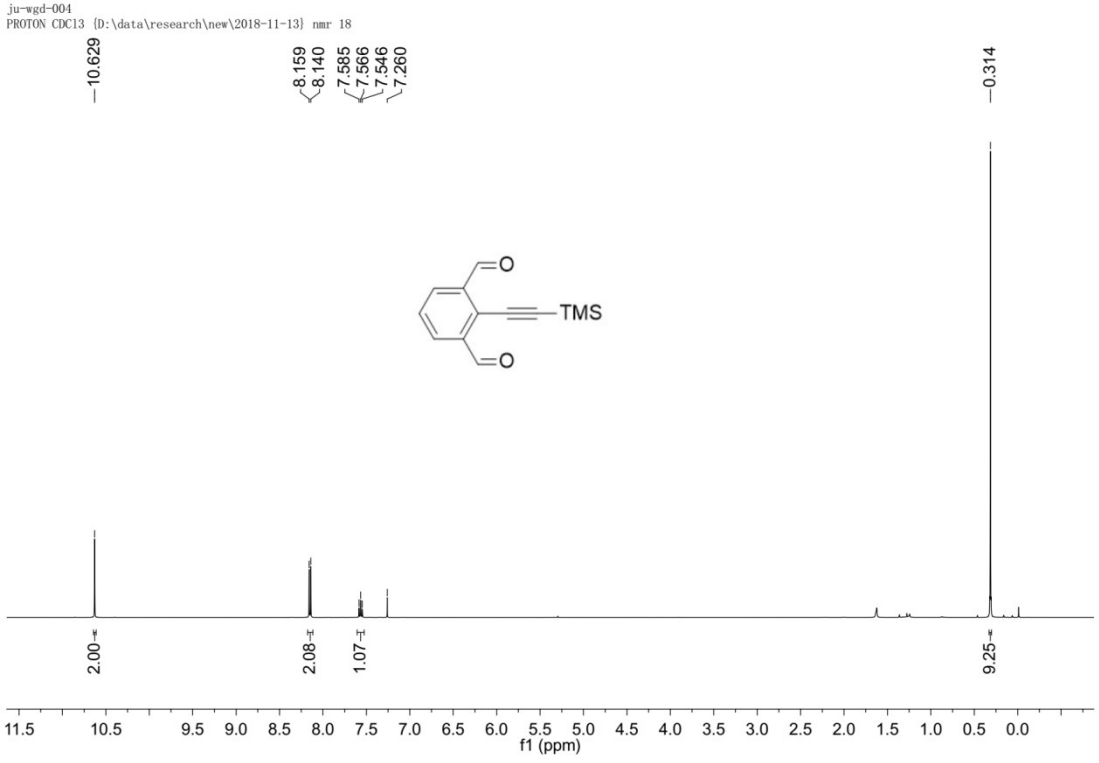
24.255
23.990
23.947
23.370
AuIPr
Dipp
BF4
f1 (ppm)

Compound S2


ju-wgd-004
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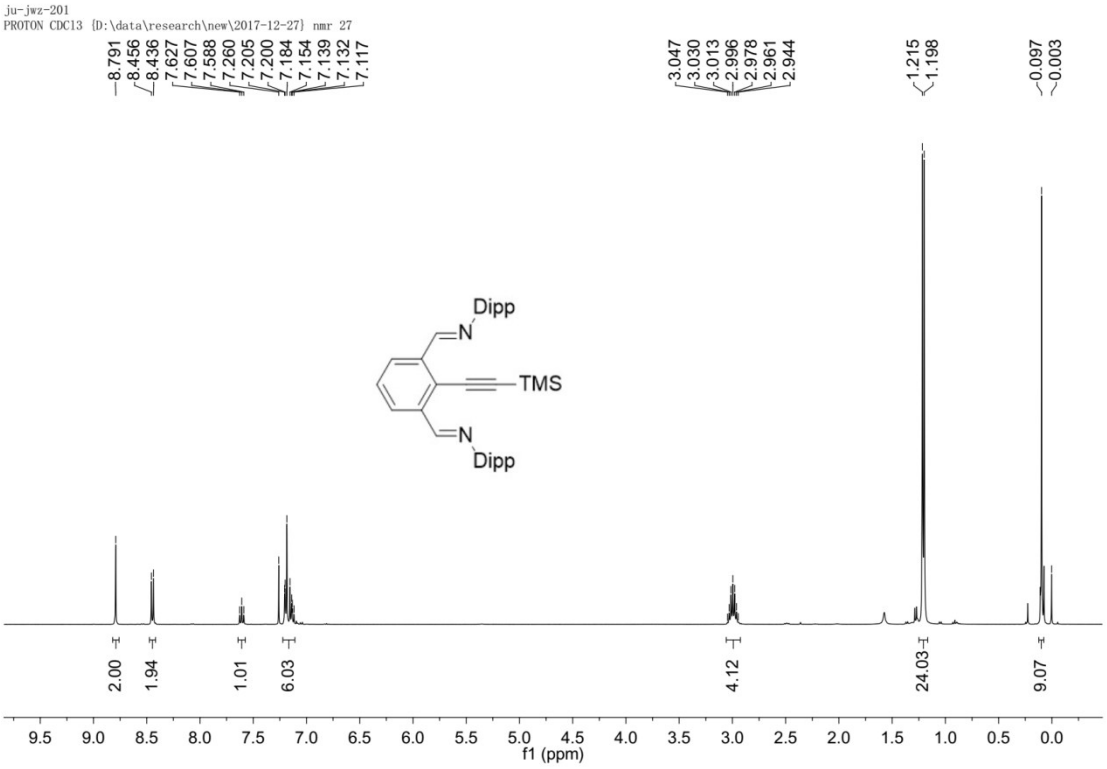
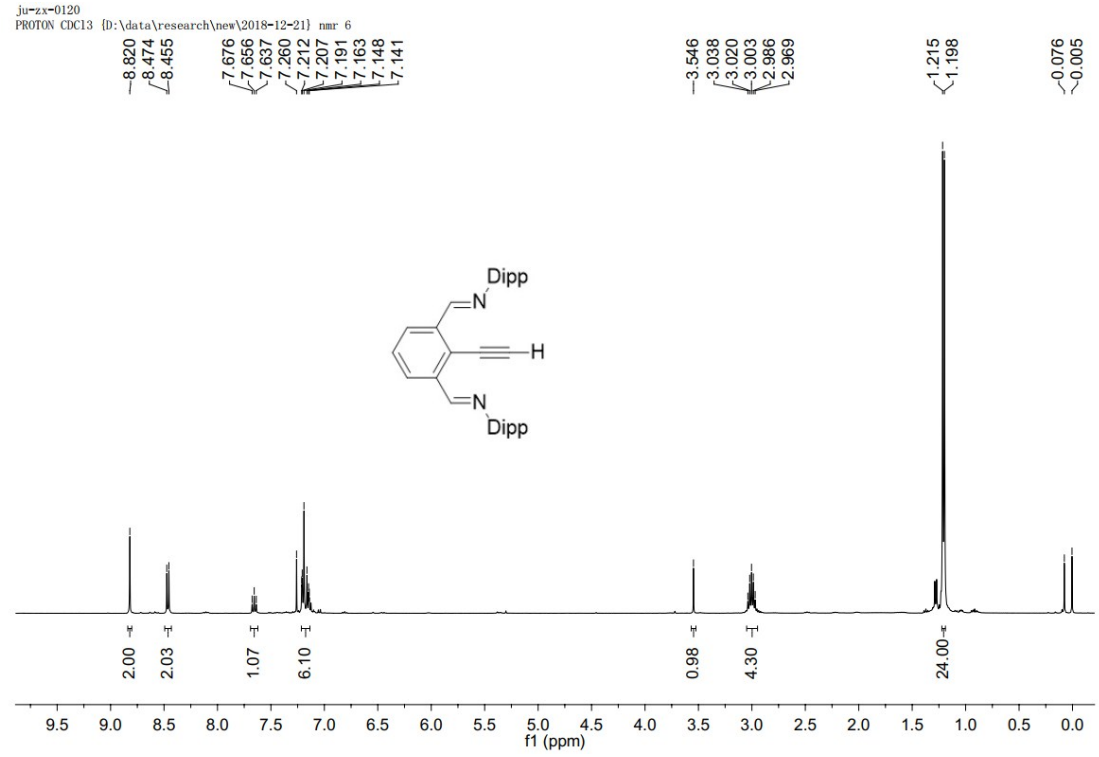
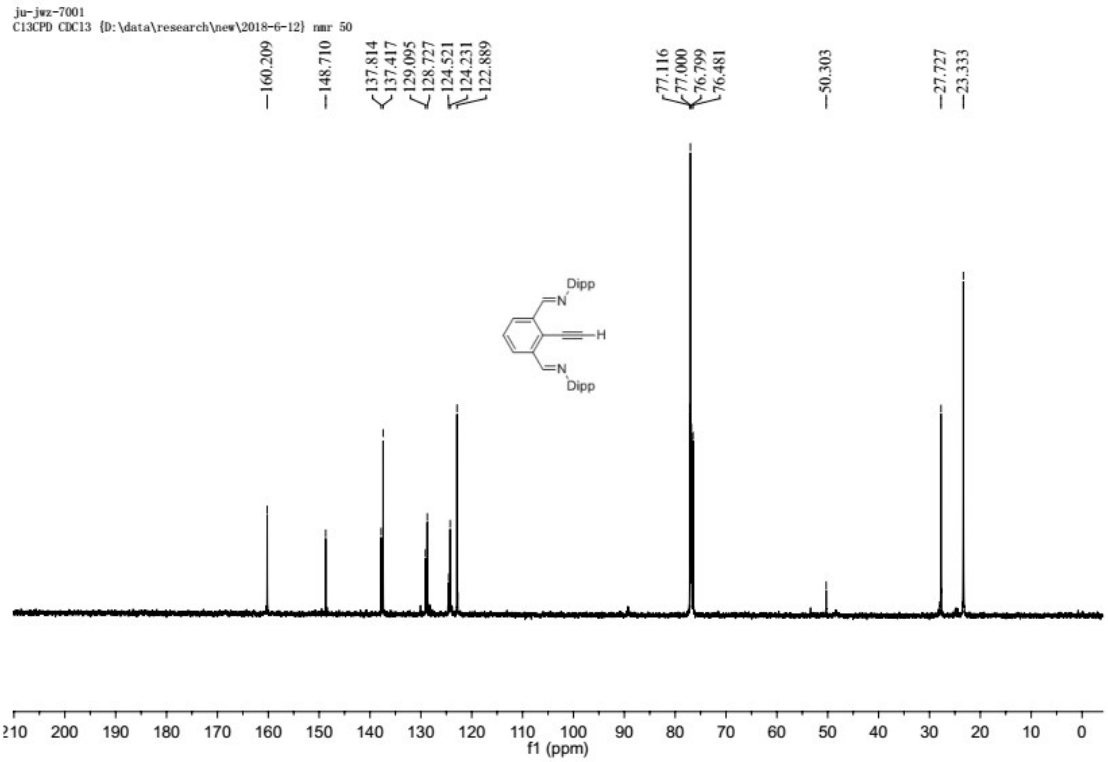
1.07
9.25
f1 (ppm)

Compound S3



Compound S4




ju-jwz-7001
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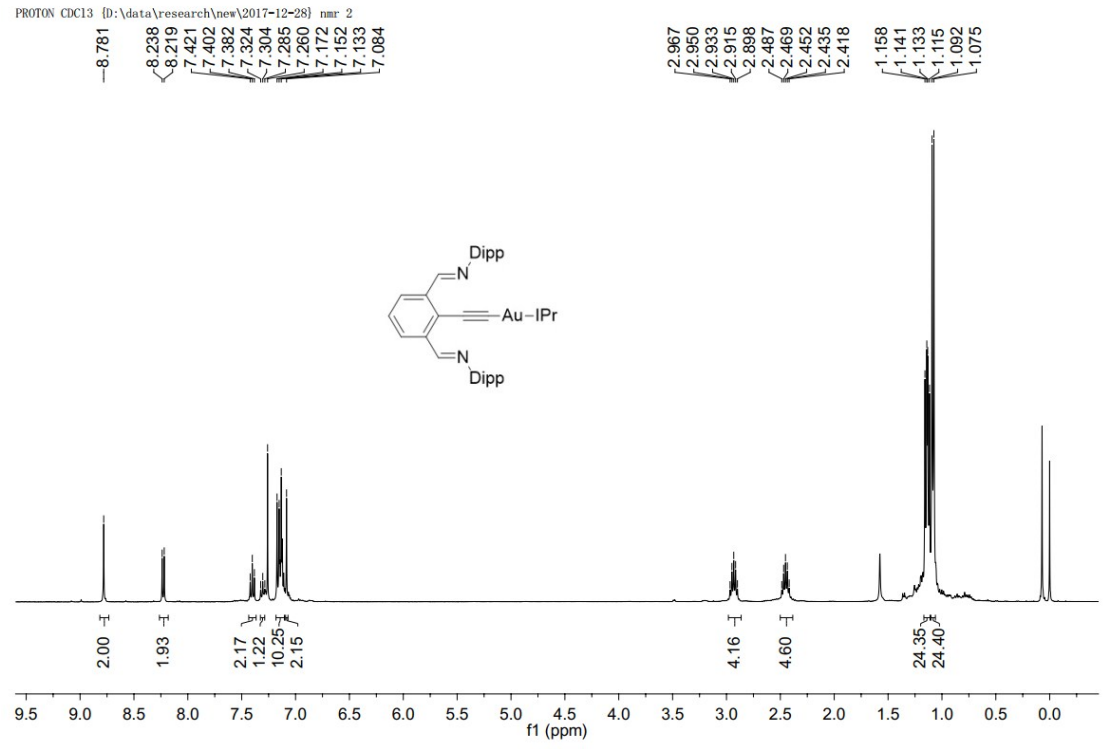
H
Dipp
f1 (ppm)

Complex 4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7.133
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2.933
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2.898
2.487
2.469
2.452
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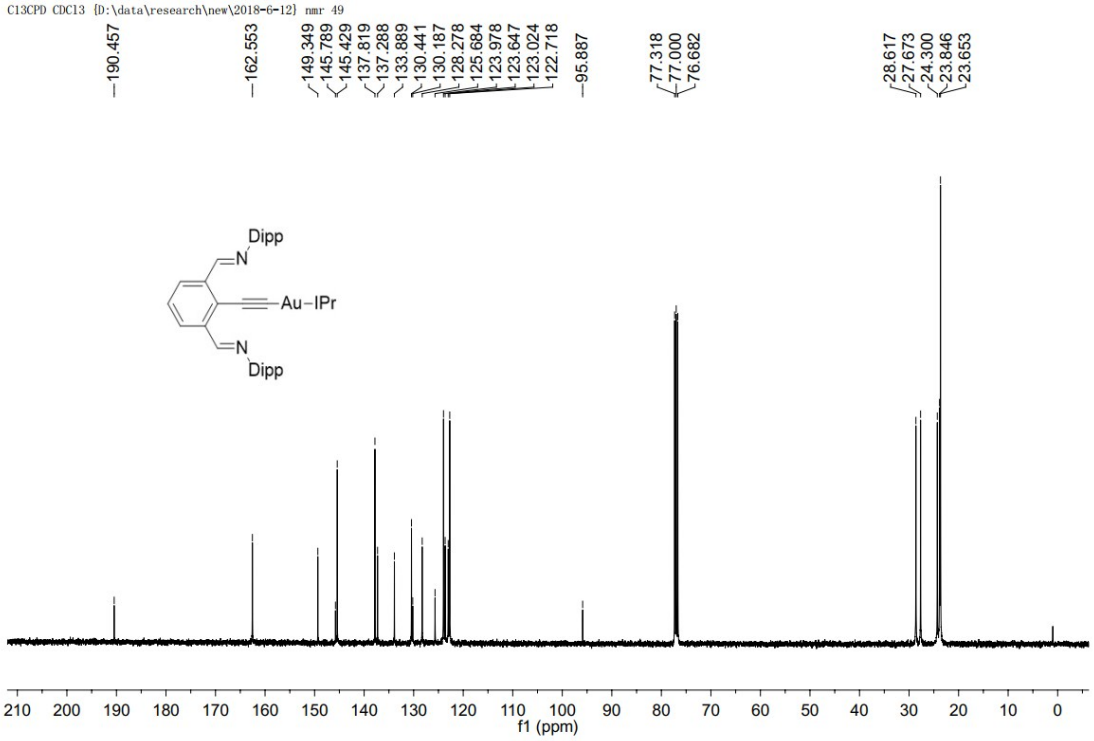
f1 (ppm)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122.718
95.887
77.318
77.000
76.682
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Au–IPr
N
Dipp
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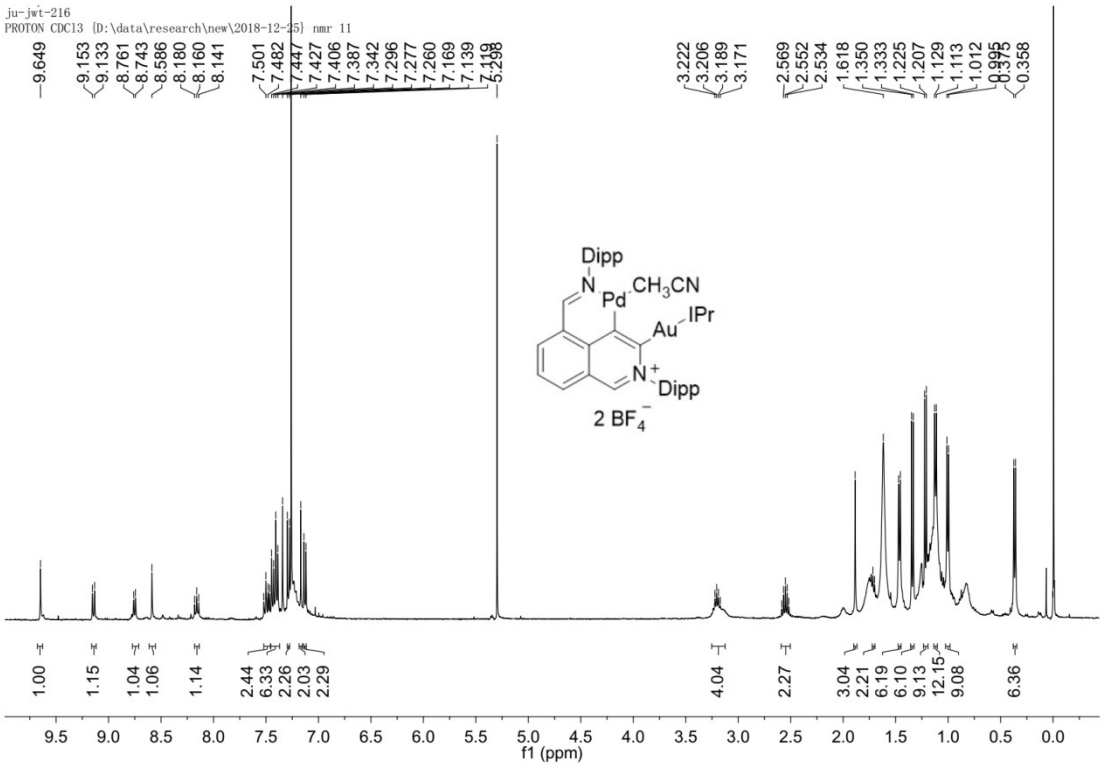
f1 (ppm)

Complex 5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Au
IPr
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Dipp
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1.06
1.14
2.44
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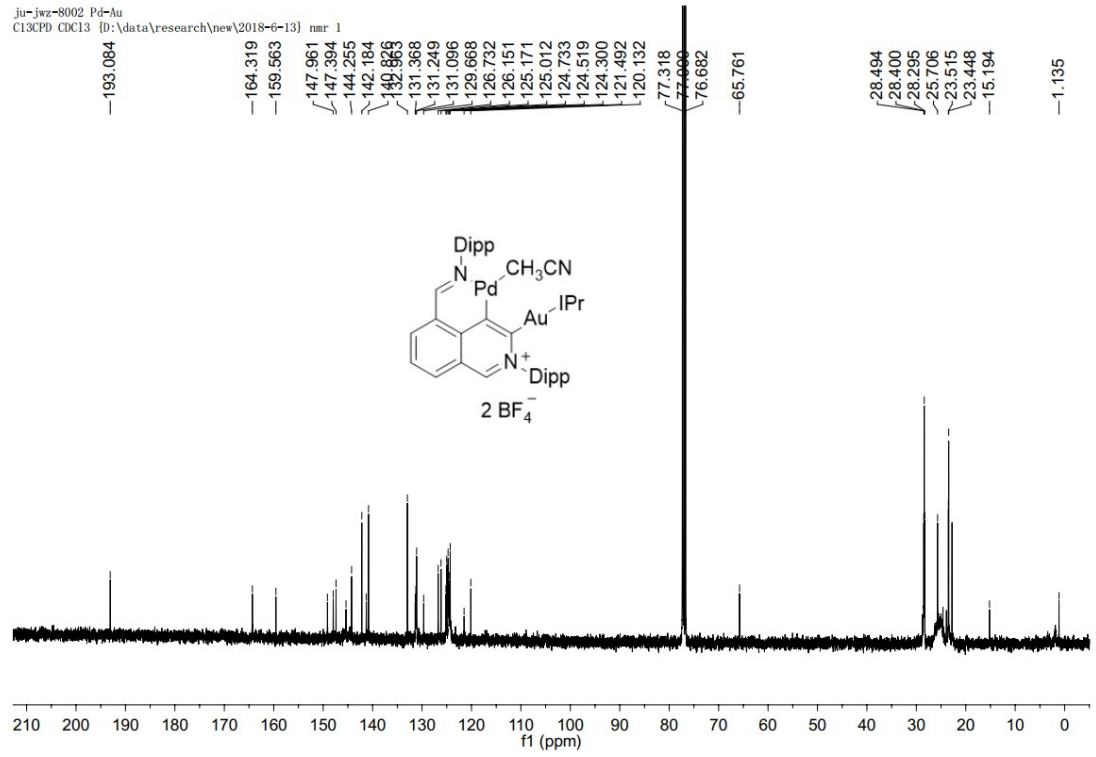
2.26
2.03
2.29
4.04
2.27
3.04
2.21
6.19
6.10
9.13
12.15
9.08
6.36
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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129.668
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125.171
125.012
124.733
124.519
124.300
121.492
120.132
77.318
76.682
65.761
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28.295
25.706
23.515
23.448
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CH3CN
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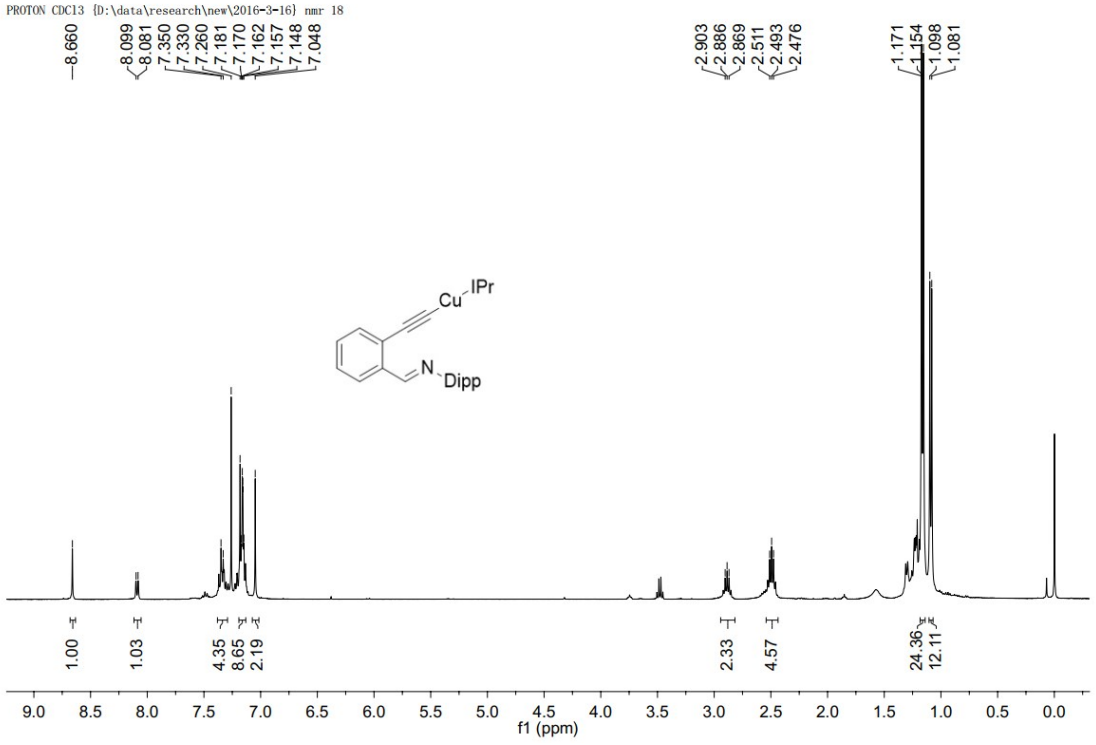
IPr
N+
Dipp
2 BF4−
f1 (ppm)

Complex S5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7.048
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2.886
2.869
2.511
2.493
2.476
1.171
1.154
1.098
1.081
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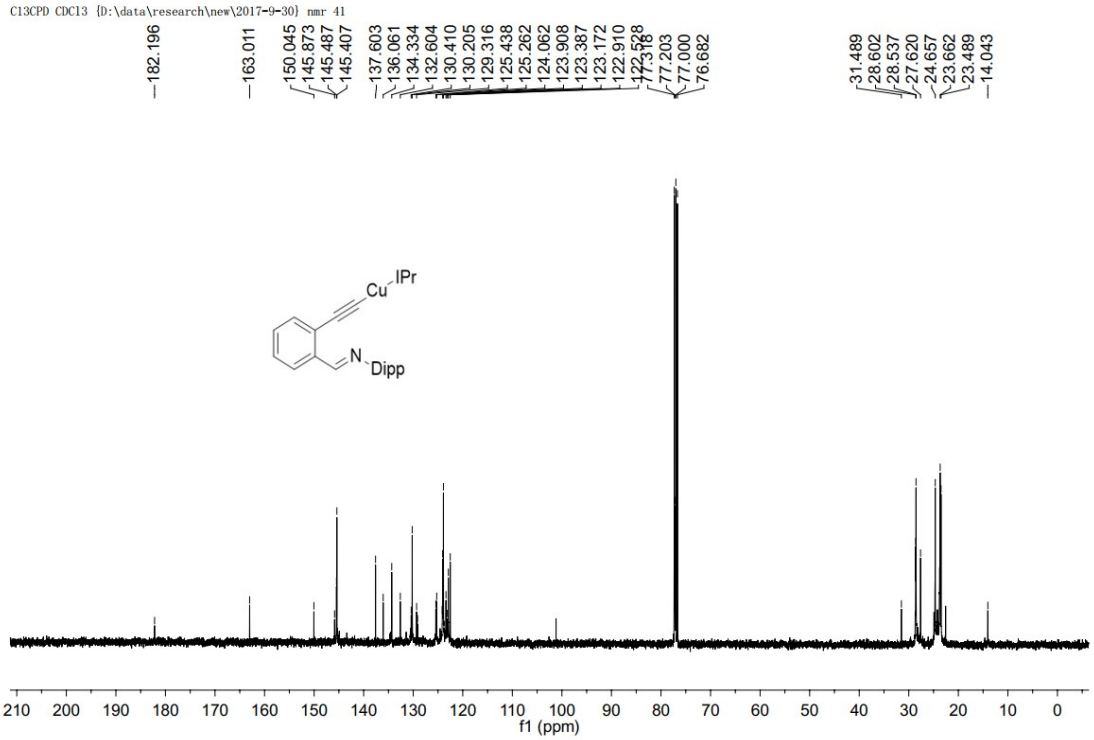
f1 (ppm)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130.205
129.316
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124.062
123.908
123.387
123.172
122.910
122.528
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77.203
77.000
76.682
31.489
28.602
28.537
27.620
24.657
23.662
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IPr
N
Dipp
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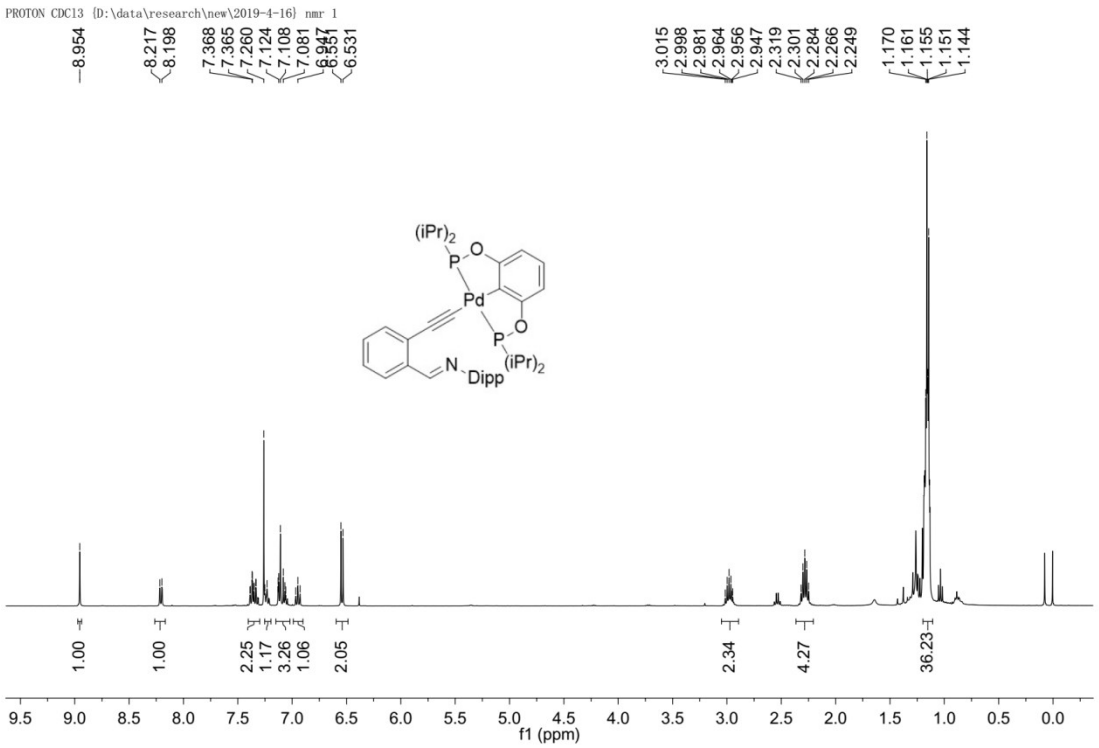
f1 (ppm)

Complex 6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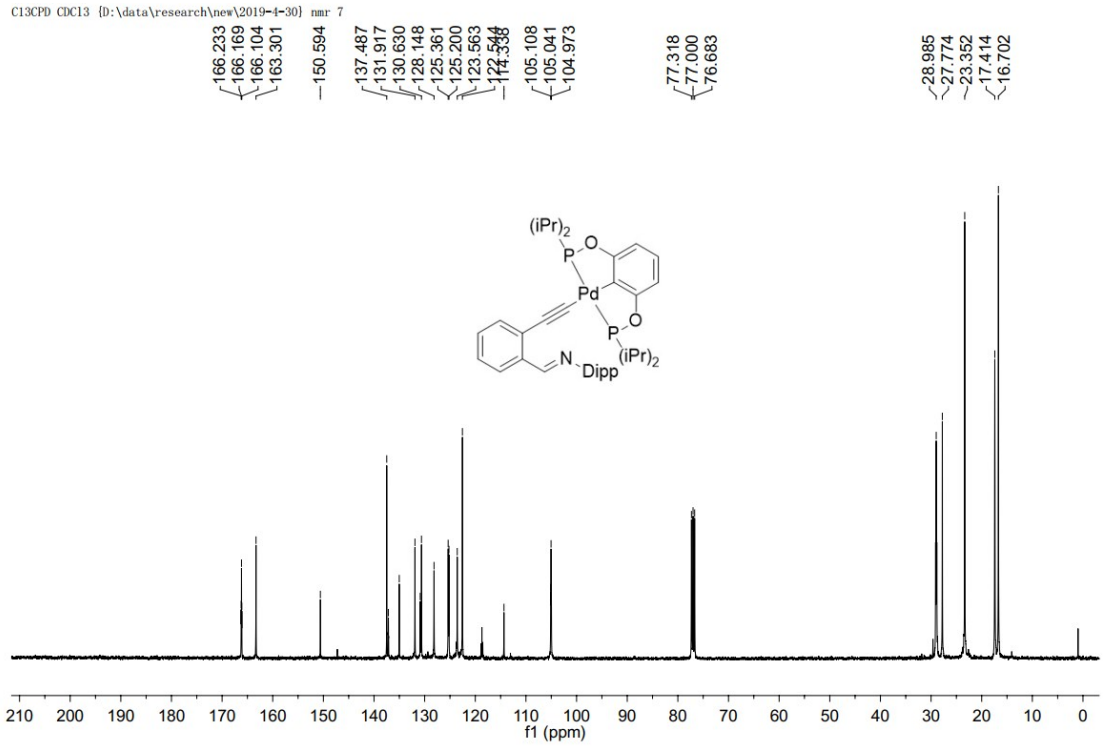
2.284
2.266
2.249
1.170
1.161
1.155
1.151
1.144
(iPr)2
P
O
Pd
P
O
N
Dipp
(iPr)2
1.00
1.00
2.25
1.17
3.26
1.06
2.05
2.34
4.27
36.23
9.5 9.0 8.5 8.0 7.5 7.0 6.5 6.0 5.5 5.0 4.5 4.0 3.5 3.0 2.5 2.0 1.5 1.0 0.5 0.0
f1 (ppm)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125.200
123.563
105.108
105.041
104.973
77.318
77.000
76.683
28.985
27.774
23.352
17.414
16.702
(iPr)2
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O
Pd
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N
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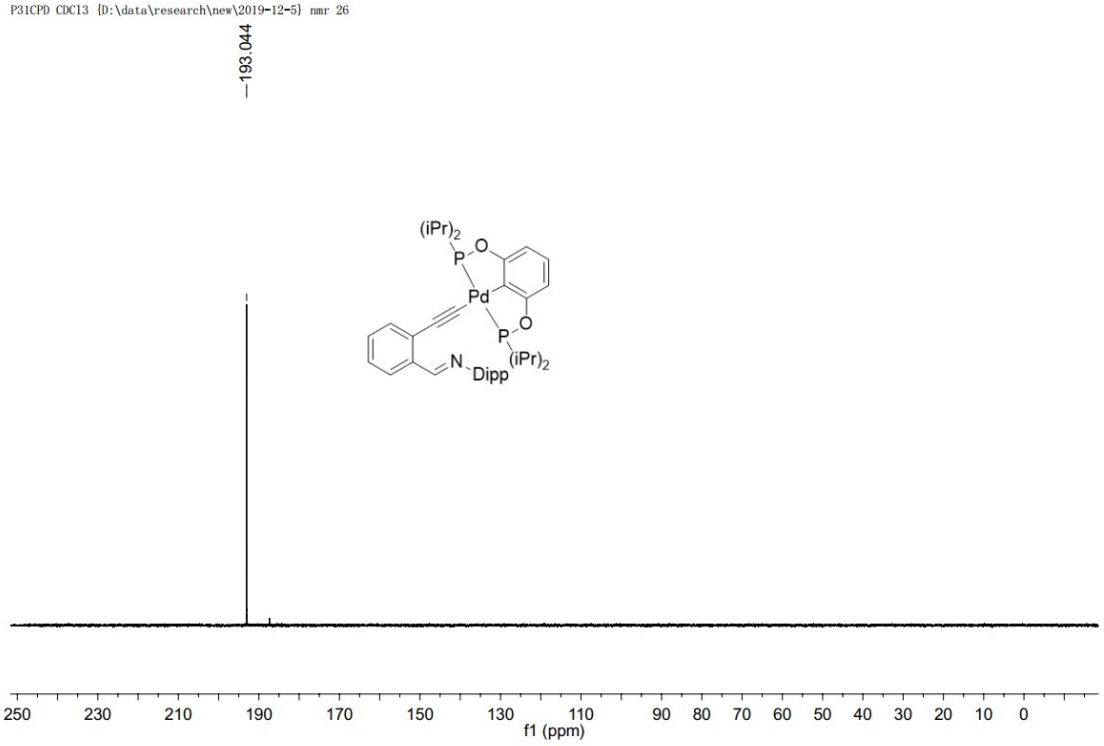
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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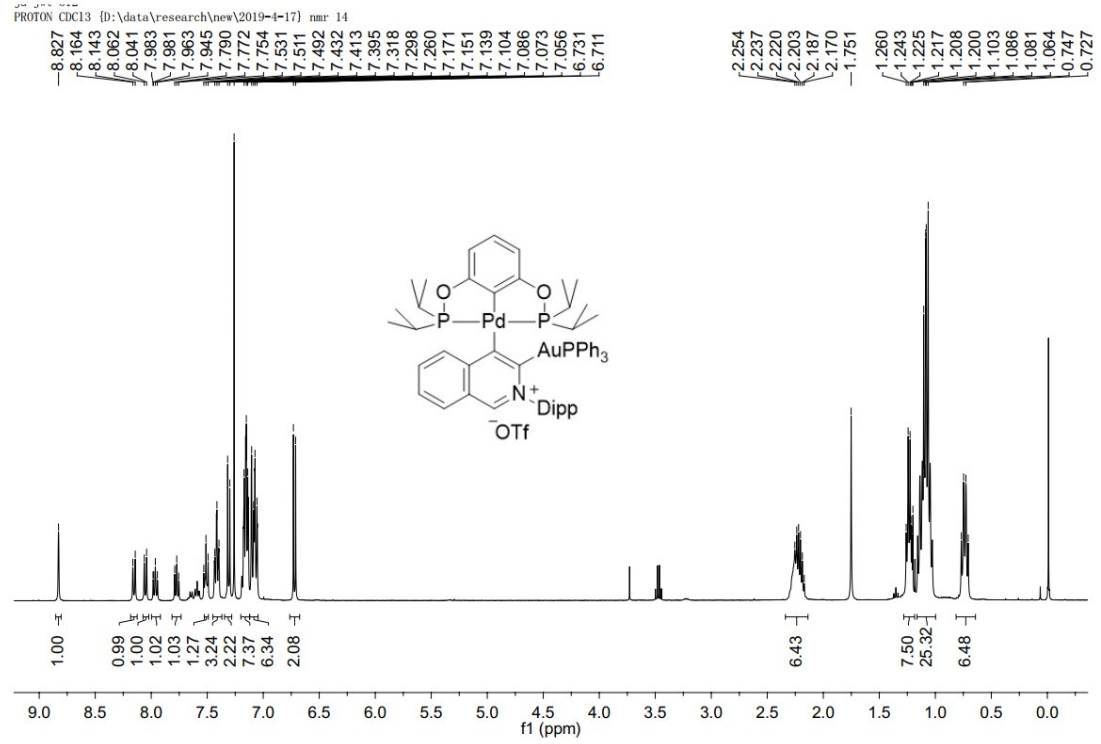
193.044
(iPr)2
P
O
Pd
P
O
(iPr)2
N
Dipp
250 230 210 190 170 150 130 110 90 80 70 60 50 40 30 20 10 0
f1 (ppm)

Complex 7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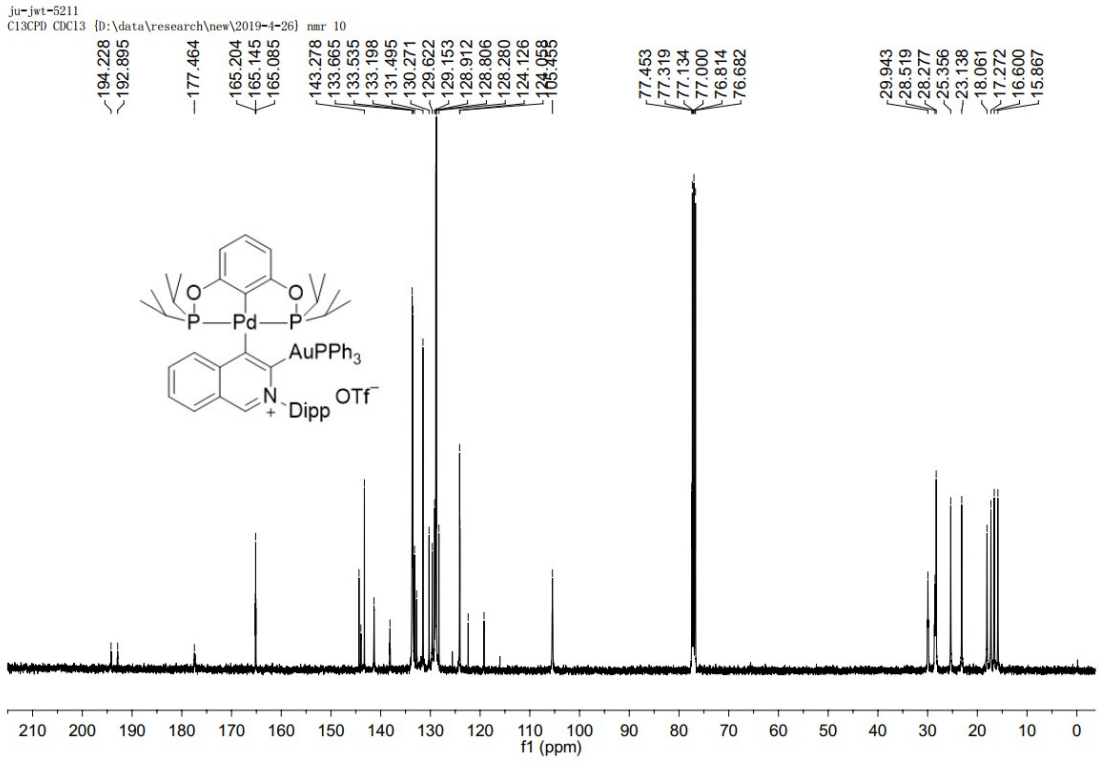
AuPPh3
Dipp
OTf
f1 (ppm)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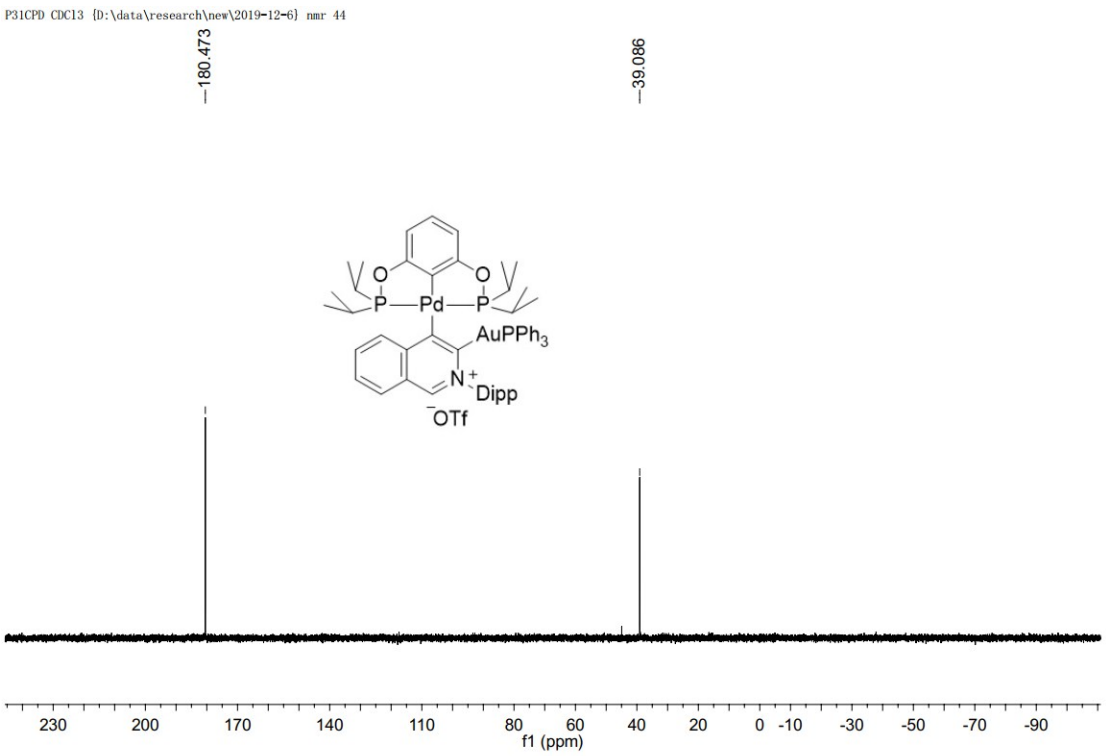
AuPPh3
Dipp
OTf
f1 (ppm)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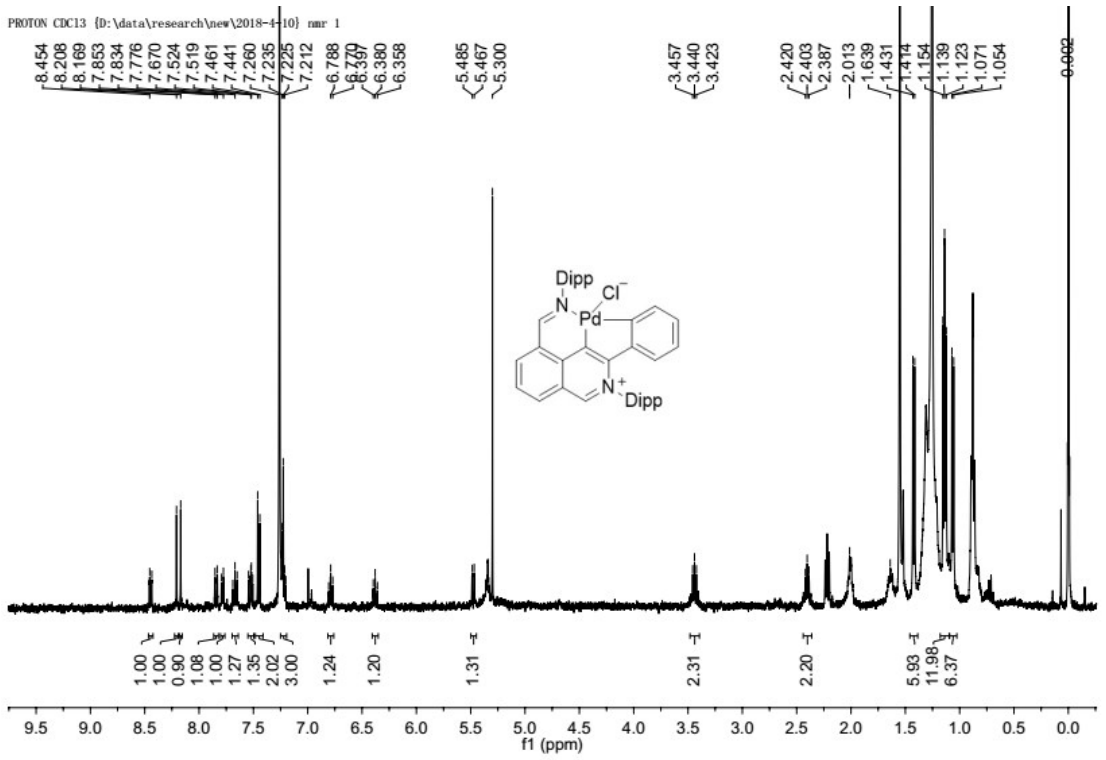
39.086
O
O
P
Pd
P
AuPPh3
N+
Dipp
OTf
230
200
170
140
110
80
60
40
20
0
-10
-30
-50
-70
-90
f1 (ppm)

Complex 8


PROTON CDCl3 {D:\data\research\new\2018-4-10} nmr 1
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8.208
8.169
7.853
7.834
7.776
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7.524
7.519
7.461
7.441
7.260
7.235
7.225
7.212
6.788
6.777
6.397
6.380
6.358
5.485
5.467
5.300
3.457
3.440
3.423
2.420
2.403
2.387
2.013
1.639
1.431
1.414
1.154
1.139
1.123
1.071
1.054
0.002
Dipp
Cl−
N
Pd
N+
Dipp
1.00
1.00
0.90
1.08
1.00
1.27
1.35
2.02
3.00
1.24
1.20
1.31
2.31
2.20
5.93
11.98
6.37
9.5
9.0
8.5
8.0
7.5
7.0
6.5
6.0
5.5
5.0
4.5
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3.5
3.0
2.5
2.0
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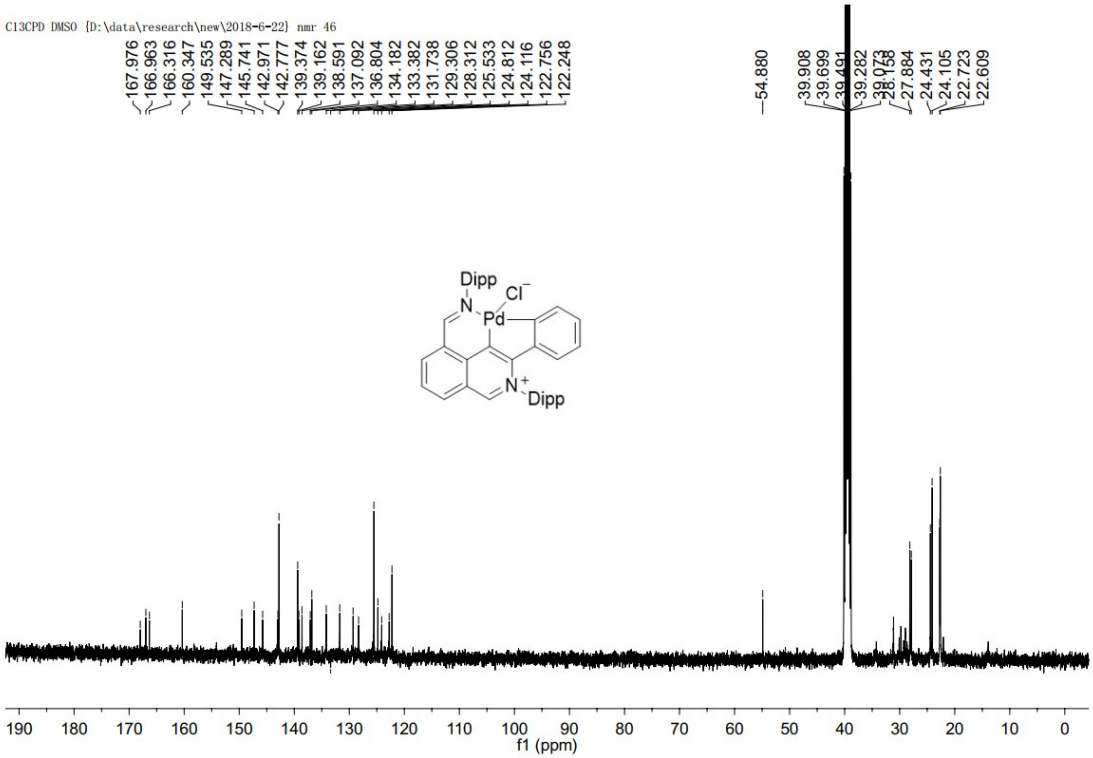
1.0
0.5
0.0
f1 (ppm)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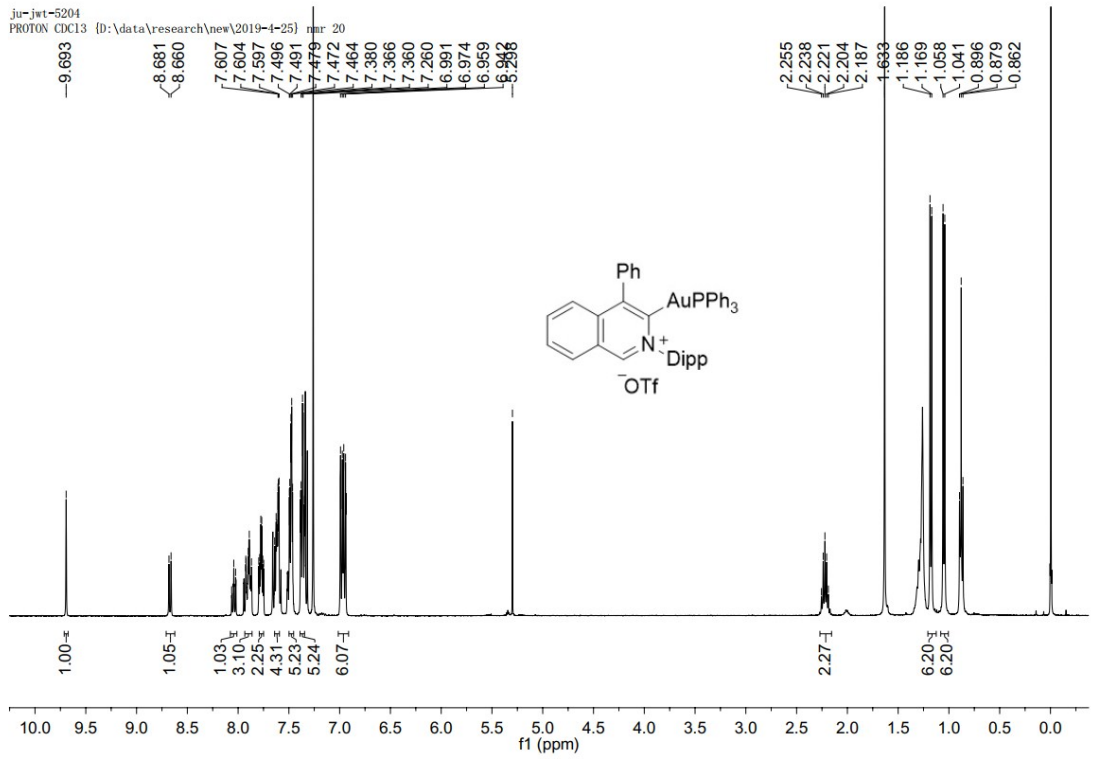
Dipp
Cl⁻
N
Pd
N⁺
Dipp
f1 (ppm)

Complex 9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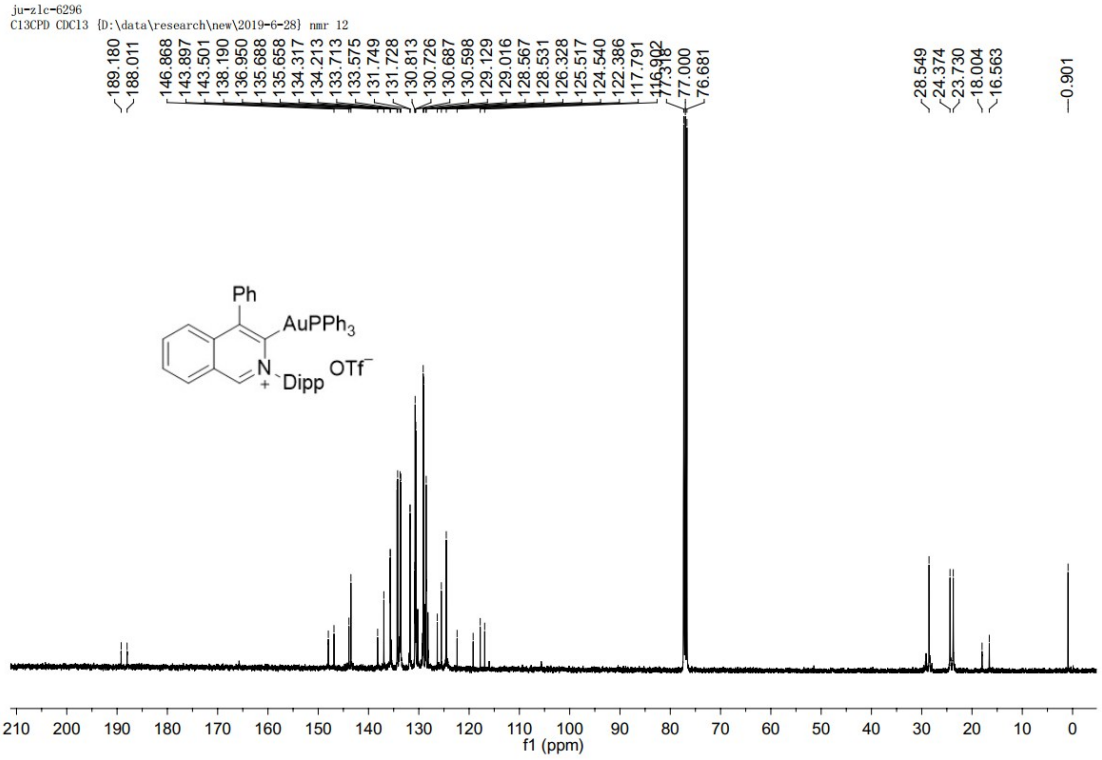
PROTON CDCl3 {D:\data\research\new\2019-4-25} nmr 20
Ph
AuPPh3
N⁺
Dipp
⁻OTf
f1 (ppm)


ju-z1c-6296
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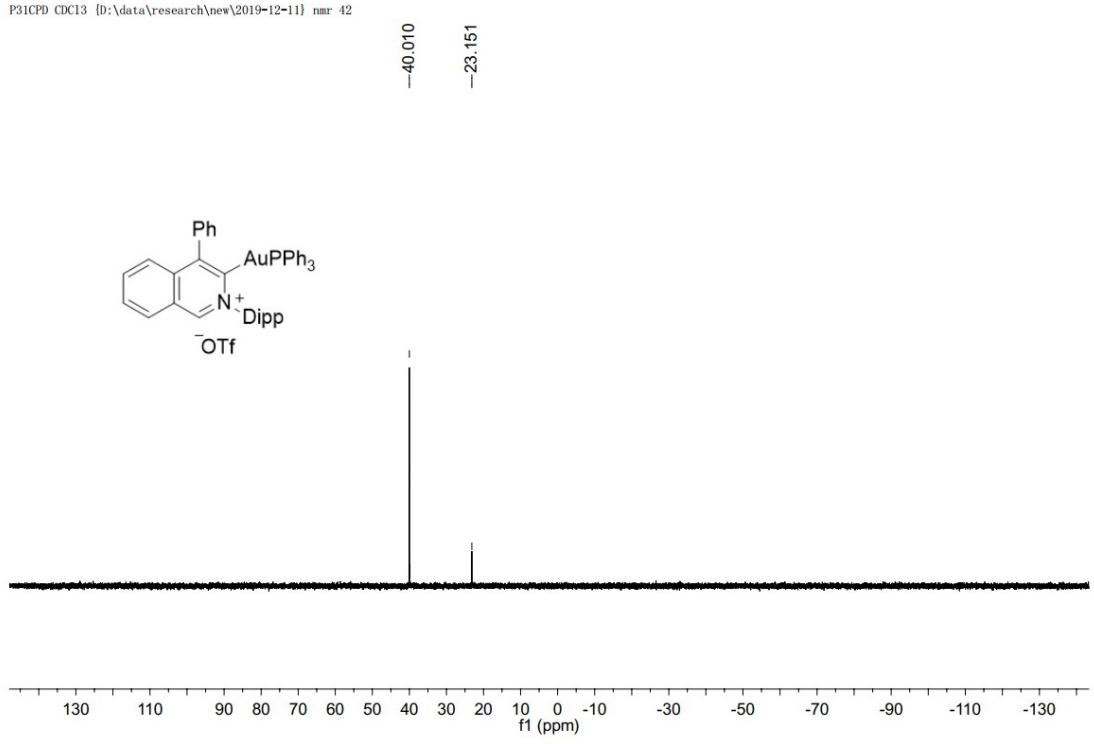
188.011
146.868
143.897
143.501
138.190
136.950
135.688
135.658
134.317
134.213
133.713
133.575
131.749
131.728
130.813
130.726
130.687
130.598
129.129
129.016
128.567
128.531
126.328
125.517
124.540
122.386
117.791
77.000
76.681
28.549
24.374
23.730
18.004
16.563
0.901
Ph
AuPPh3
N+
Dipp
OTf−
210 200 190 180 170 160 150 140 130 120 110 100 90 80 70 60 50 40 30 20 10 0
f1 (ppm)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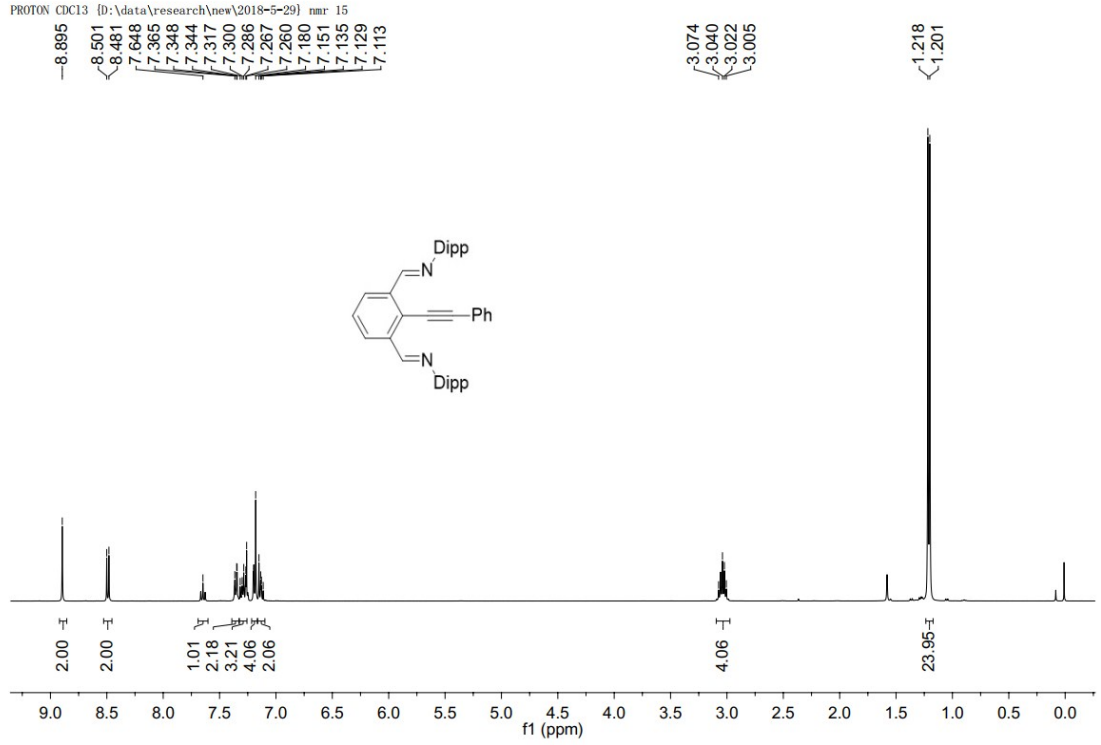
40.010
23.151
Ph
AuPPh3
N+
Dipp
−OTf
130 110 90 80 70 60 50 40 30 20 10 0 -10 -30 -50 -70 -90 -110 -130
f1 (ppm)

Compound 10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8.895
8.501
8.481
7.648
7.365
7.348
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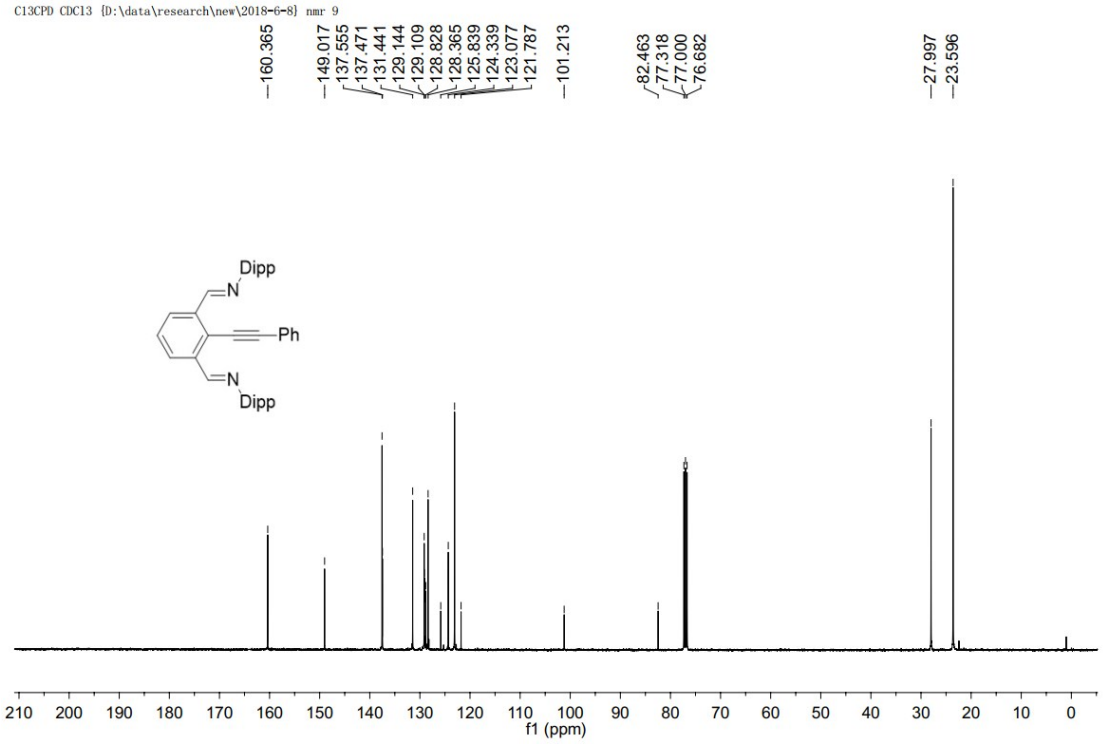
7.317
7.300
7.286
7.267
7.260
7.180
7.151
7.135
7.129
7.113
3.074
3.040
3.022
3.005
1.218
1.201
Dipp
N
Ph
N
Dipp
2.00
2.00
1.01
2.18
3.21
4.06
2.06
4.06
23.95
f1 (ppm)


C13CPD CDCl3 {D:\data\research\new\2018-6-8} nmr 9
160.365
149.017
137.555
137.471
131.441
129.144
129.109
128.828
128.365
125.839
124.339
123.077
121.787
101.213
82.463
77.318
77.000
76.682
27.997
23.596
Dipp
N
Ph
N
Dipp
f1 (ppm)

X-Ray Crystallography

Each crystal was mounted on a glass fiber. Crystallographic measurements were made on a Bruker Smart Apex 100 CCD area detector using graphite monochromated Mo-Kαradiation ($\lambda_{\text{Mo-K}\alpha}$ = 0.71073 Å). The structures were solved by directed methods (SHELXS-97) and refined on F^2 by full-matrix least squares (SHELX-97) using all unique data. All the calculations were carried out with the SHELXTL18 program.

Key details of the crystal and structure refinement data are summarized in Table S1-S2. Further crystallographic details may be found in the respective CIF files, which were deposited at the Cambridge Crystallographic Data Centre, Cambridge. CCDC 1936618 (**2**), CCDC 1936631 (**5**), CCDC 1936630 (**7**), CCDC 1936627 (**8**), and CCDC 1936626 (**9**) contain the supplementary crystallographic data for this paper. These data can be obtained free of charge from The Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

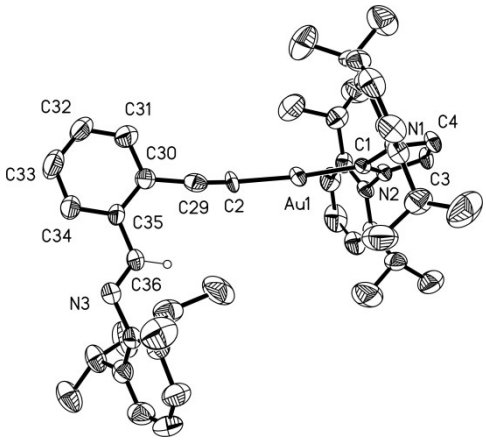


Figure S1. X-ray crystal structures of **2**. The hydrogen atoms have been omitted for clarity.

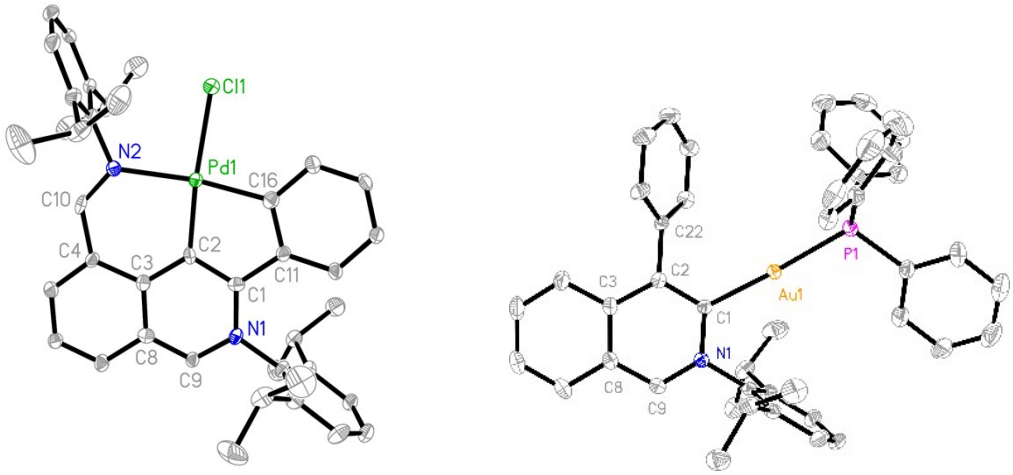


Figure S2 X-ray crystal structures of **8** (left) and **9** (right). The counter anions and hydrogen atoms have been omitted for clarity.

Table S1. Crystal Data, Data Collection, and Structure Refinement for **2**, **5** and **7**.

	2	**5**	**7**
Identification code	mo_d8v17144_0m	wmj18009_0m	mo_dd19079_0m
Formula	$C_{48}H_{58}AuN_3$	$C_{63}H_{78}AuB_2F_8N_5Pd$	$C_{59}H_{70}AuCl_2F_3NO_5P_3PdS$
Formula weight	873.94	1341.39	1429.39
T, K	301.47	170.0	193(2)
crystal system	Monoclinic	Monoclinic	Triclinic
space group	P 1 21/n 1	P 1 21/m 1	P -1
a, Å	10.7970(12)	15.3922(2)	13.9859(4)
b, Å	16.6498(18)	14.4465(2)	14.7350(4)
c, Å	24.697(3)	16.7191(2)	15.1208(3)
α, deg	90	90	84.5370(10)
β, deg	95.768(4)	115.7160(10)	82.4420(10)

γ, deg	90	90	89.5620(10)
Volume, Å ^{3}	4417.2(8)	3349.50(8)	3074.99(14)
Z	4	2	2
D_{calc}, Mg / m^3	1.314	1.371	1.544
absorption coefficient, mm^{-1}	3.364	4.657	2.929
F(000)	1784	1396	1436
crystal size, mm	0.12 x 0.03 x 0.02	0.05 x 0.03 x 0.02	0.160 x 0.140 x 0.120
2θ range, deg	2.447 to 25.998	2.839 to 52.980	2.938 to 26.000
reflections collected /unique	43661/8678 [R(int) = 0.1217]	36285/6170 [R(int) = 0.0494]	47284/12027 [R(int) = 0.0293]
data / restraints/ parameters	8678 / 12 / 482	6170 / 64 / 412	12027 / 0 / 698
goodness of fit on F^2	1.045	1.059	1.023
final R indices [I >2σ(I)]^a	R1 = 0.0555, wR2 = 0.0938	R1 = 0.0390, wR2 = 0.0901	R1 = 0.0209, wR2 = 0.0495
R indices (all data)	R1 = 0.1095, wR2 = 0.1146	R1 = 0.0442, wR2 = 0.0929	R1 = 0.0228, wR2 = 0.0507
largest diff peak and hole, e/Å^3	1.137 and -0.904	2.343 and -1.368	1.125 and -0.742

Table S2. Crystal Data, Data Collection, and Structure Refinement for **8** and **9**.

	8	**9**
Identification code	mo_dd18042_0 m	mo_d8v19375_0m
Formula	C_{41} $H_{45}Cl_3N_2Pd$	$C_{46}H_{42}AuF_3NO_3PS$
Formula weight	778.54	973.80
T, K	173(2)	193(2)
crystal system	Monoclinic	Monoclinic
space group	P 21/n	P 21/c
a, Å	8.822(2)	14.4529(3)
b, Å	20.173(5)	13.4595(3)
c, Å	21.011(6)	21.5529(6)
α, deg	90	90

β, deg	93.993(11)	93.9560(10)
γ, deg	90	90
Volume, Å^3	3730.0(17)	3730.0(17)
Z	4	4
D_{calc}, Mg / m^3	1.386	1.546
absorption coefficient, mm^{-1}	0.743	3.660
F(000)	1608	1944
crystal size, mm	0.140 x 0.100 x 0.050	0.120 x 0.100 x 0.070
2θ range, deg	2.190 to 25.497	2.317 to 26.000
reflections collected /unique	6544/6544 [R(int) = ?]	20534/8206 [R(int) = 0.0275]
data / restraints/ parameters	6544 / 0 / 433	8206 / 110 / 546
goodness of fit on F^2	1.033	1.028
final R indices [I >2σ(I)][a]	R1 = 0.0746, wR2 = 0.1728	R1 = 0.0271, wR2 = 0.0551
R indices (all data)	R1 = 0.0968, wR2 = 0.1921	R1 = 0.0373, wR2 = 0.0593
largest diff peak and hole, e/Å^3	1.766 and -1.704	1.063 and -0.664

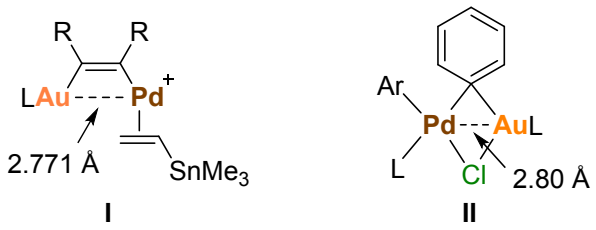


Figure S3 Related Pd/Au intermediates **I** and **II**.

Computational Details

The geometries of compounds have been optimized at wB97XD/6-31G(d)/LANL2DZ level. The subsequent frequency calculations on the stationary points were carried out at the same level of theory to ascertain the nature of the stationary points as minima on the respective potential energy surfaces. The conformational space of flexible systems has first been searched manually. Thermochemical corrections to 298.15 K have been calculated for all minima from unscaled vibrational frequencies obtained at this same level. All quantum mechanical calculations have been performed with Gaussian 09.

Table S3. The total energies, enthalpies and free energies of all species in gas phase shown in Scheme 7

	E_{tot}	H_{298}	G_{298}
Int1	-2982.523813	-2981.158668	-2981.342231
PhI	-242.9473684	-242.84916	-242.887609
TS1	-3225.471182	-3224.007828	-3224.229840
Int2	-3225.450089	-3223.982486	-3224.201633
TS2	-3225.460457	-3223.991230	-3224.213267
TS2'	-3225.431501	-3223.968147	-3224.197012
Int3	-3225.458751	-3223.995398	-3224.190159
TS3	-3225.440266	-3223.976912	-3224.217410
Int4+IAuL	-3225.485046	-3224.021692	-3224.198924

Archive Entries

Int1

1\1\GINC-OM103\FOpt\RwB97XD\GenECP\C63H78Au1N5Pd1(2+)\WEIY\02-Mar-2020
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PhI

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d/genecp opt freq\\Title Card Required\\0,1\C,-2.6088041057,0.90548932

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\C,-2.6086821402,3.3137541911,0.0103130029\C,-3.3067753145,2.109641771
1,0.0108230049\H,-3.1462133736,-0.0380855848,0.0122609935\H,-0.6744833
48,-0.0422719402,0.0131517422\H,-0.6742714545,4.2613228873,0.010389873
\H,-3.1460401607,4.2573579101,0.0095186253\H,-4.392322555,2.1097093897
,0.0104289727\I,1.5973877472,2.1094620254,0.012586519\\Version=ES64L-G
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252925,-0.0000224,0.003091,-0.004545\PG=C01 [X(C6H5I1)]\\@

TS1

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,-0.8075219402,-2.961347631\C,0.752006612,0.1338132499,1.9762185669\C,
2.0754542975,0.313251394,2.2395268947\C,2.5971318184,0.6542867995,3.49
4099582\C,3.9725748227,0.8823169089,3.7699866449\C,4.3587694206,1.2453
067649,5.0469587555\C,3.4234389095,1.380297314,6.0964887406\C,2.096365
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7\C,0.3170514225,0.501004791,4.2859925421\C,5.0019267725,0.672307204,2
.7693689032\C,-0.5520870842,0.1040127704,-1.9646253054\C,-1.0436431295
,-0.1791411401,-4.1449144357\C,-0.691348141,-2.2466811816,-2.821260324
\C,-1.739543542,-2.836427748,-2.0842119891\C,-1.7031864192,-4.22211569
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41347231\H,-3.3210529376,-1.0332978919,-3.521975618\H,-4.6994104708,-1
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Int2

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\C,1.5410584291,-0.7258401564,4.600471058\C,0.2609294105,-0.3925806183
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.5349494611\H,-3.2666990117,0.1058612887,-0.0920900601\H,7.7839264229,
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TS2

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,-3.2118617389\C,1.9515730487,-1.6571743262,-4.1823469411\C,1.70731325
27,-2.1269088793,-5.627498317\C,3.4637662029,-1.6467965341,-3.90371726
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TS2'

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\C,-2.895740272,-3.6845111189,0.648200602\C,-2.7413772351,-2.057359665
4,2.4794233193\C,-4.0837236345,-1.810924404,2.8203396932\C,-4.37081024
66,-1.5717366762,4.1638276351\C,-3.368068002,-1.5717483641,5.124957616
\C,-2.0490622026,-1.783282518,4.7513818719\C,-1.7064952892,-2.03236304
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Int3

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Int4

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IAuL

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p opt wb97xd/genecp\\Title Card Required\\0,1\Au,-1.8350304872,0.19504
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