SUPPORTING INFORMATION

for

Synthesis and reactivity of [Au(NHC)(Bpin)] complexes

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General Information

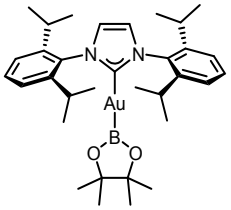
Degassed anhydrous solvents were used when experiments were conducted under inert atmosphere or in the glovebox. ^{1}H, $^{13}C\{^{1}H\}$ and ^{11}B Nuclear Magnetic Resonance (NMR) spectra were recorded on Bruker-400 and 500 MHz spectrometers at ambient temperature. Chemical shifts (ppm) are referenced to the residual solvent peak. Coupling constants, J, are given in Hertz. Abbreviations used in the designation of the signals: s = singlet, d = doublet, t = triplet, sept = septuplet, m = multiplet. Elemental analyses were performed at London Metropolitan University.

Synthesis of [Au(NHC)(BPin)] complexes

General procedure

A vial was charged with the corresponding [Au(NHC)(OH)] complex and dissolved in anhydrous methanol (0.16 M). The solvent was evaporated off under reduced pressure at 50 °C. This was repeated 5 times. The vial was taken into the glovebox, where the vial was charged with a stirring bar, bis(pinacolato)diboron (B_2pin_2) (1.1 equiv.) and benzene (0.16 M). The reaction mixture was stirred for 20 h at room temperature. Work up: In the glovebox the solvent was removed under reduced pressure. The solid was washed with cold hexane. [Au(NHC)(Bpin)] was obtained as a white solid.

[Au(IPr)(Bpin)]



Following the general procedure [Au(IPr)(OH)] (300.0 mg, 0.49 mmol) and anhydrous methanol (3.00 mL) were used. In the glovebox, B_2pin_2 (138.8 mg, 0.55 mmol) and benzene (3.00 mL) were charged into the vial. [Au(IPr)(Bpin)] was obtained as a white crystalline solid in 84% yield (302.0 mg).

^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.12 (m, 2H, CH_{Ar}), 7.04 (m, 4H, CH_{Ar}), 6.27 (s, 2H, CH_{Imid}), 2.70-2.63 (sept, *J* = 6.8 Hz, 4H, CH_{IPr}), 1.53 (d, *J* = 7.5 Hz, 12H, $CH_{3(IPr)}$), 1.08 (d, *J* = 6.1 Hz, 12H, $CH_{3(IPr)}$), 0.98 (s, 12H, $CH_{3(Bpin)}$).

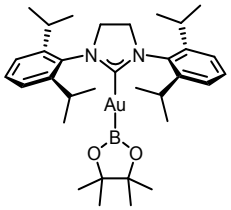
$^{13}C\{^{1}H\}$ NMR (100 MHz, benzene-d_6): δ (ppm) = δ 216.7 ($C_{carbene}$), 145.8 (C_{Ar}), 135.0 (C_{Ar}), 130.4 (CH_{Ar}), 124.1 (CH_{Ar}), 122.6 ($CH_{Imid.}$), 79.8 (CO_{Bpin}), 29.0 (CH_{IPr}), 25.8 ($CH_{3(BPin)}$), 25.1 ($CH_{3(Bpin)}$), 24.8 ($CH_{3(IPr)}$), 23.9 ($CH_{3(IPr)}$).

^{11}B NMR (400 MHz, benzene-d_6): δ (ppm) 49.5.

Anal. Calcd. for $C_{33}H_{48}AuBN_2O_2$ C 55.55, H 6.92, N 3.93. Found: C 55.62, H 6.85, N 3.82.

ν_{max} (thin film) = 2960 (C-H stretching), 1458 (C=$C_{aromatic}$ stretching), 1363 (C-H_{alkane} bending), 1128 (C-O stretching).

[Au(SIPr)(Bpin)]



Following the general procedure [Au(SIPr)(OH)] (100.0 mg, 0.16 mmol) and anhydrous methanol (1.00 mL) were used. In the glovebox, B_2pin_2 (46.1 mg, 0.18 mmol) and benzene (3.00 mL) were charged into the vial. [Au(SIPr)(Bpin)] was obtained as a white crystalline solid in 65% yield (77.0 mg).

^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.10 – 7.01 (m, 6H, CH_{Ar}), 3.11 (s, 4H, $CH_{2(Imid)}$), 3.06-3.01 (sept, *J* = 6.8 Hz, 4H, $CH_{(SIPr)}$), 1.65 (d, *J* = 7.2 Hz, 12H, $CH_{3(SIPr)}$), 1.20 (d, *J* = 8.1 Hz, 12H, $CH_{3(SIPr)}$), 0.95 (s, 12H, $CH_{3(Bpin)}$).

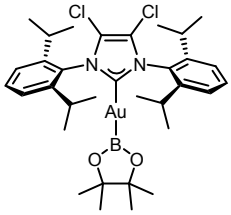
^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 146.8 (C_{Ar}), 135.1 (C_{Ar}), 129.7 (CH_{Ar}), 124.4 (CH_{Ar}), 79.7 (CO_{Bpin}), 53.9 ($CH_{2(Imid)}$), 29.2 (CH_{SIPr}), 25.7 ($CH_{3(Bpin)}$), 25.7 ($CH_{3(SIPr)}$), 24.1 ($CH_{3(SIPr)}$).

^{11}B NMR (400 MHz, benzene-d_6): δ (ppm): 49.3.

Anal. Calcd. for $C_{33}H_{50}AuBN_2O_2$ C 55.47, H 7.05, N 3.92. Found: C 55.80, H 7.05, N 4.06.

ν_{max} (thin film) = 2962 (C-H_{alkane} stretching), 1483 (C=$C_{aromatic}$ stretching), 1456 (C=$C_{aromatic}$ stretching), 1363 (C-H_{alkane} bending), 1126 (C-O stretching).

[Au(IPr^{Cl})(Bpin)]



Following the general procedure [Au(IPr^{Cl})(OH)] (100.0 mg, 0.15 mmol) and anhydrous methanol (1 mL) were used. In the glovebox, B_2pin_2 (41.6 mg, 0.16 mmol) and benzene (2 mL) were charged into the vial. Au(IPr^{Cl})(Bpin)] was obtained as a white crystalline solid in 56% yield (65.0 mg).

^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.10 – 7.08 (m, 2H, CH_{Ar}), 7.02 – 7.00 (m, 4H, CH_{Ar}), 2.67 (sept, *J* = 7.3 Hz, 4H, CH_{IPrCl}), 1.53 (d, *J* = 7.5 Hz, 12H, ($CH_{3(IPrCl)}$), 1.10 (d, *J* = 7.5 Hz, 12H, $CH_{3(IPrCl)}$), 0.96 (s, 12H, $CH_{3(BPin)}$).

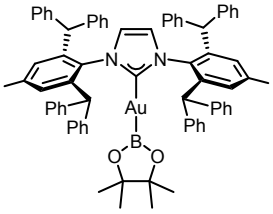
^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 216.9 ($C_{carbene}$), 146.3 (C_{Ar}), 131.7 (C_{Ar}), 131.3 (CH_{Ar}), 124.4 (CH_{Ar}), 119.2 (C_{Imid}), 80.0 (CO_{Bpin}), 29.5 ($CH_{3(IPrCl)}$), 25.7 ($CH_{3(Bpin)}$), 25.0 ($CH_{3(IPrCl)}$), 23.4 ($CH_{3(IPrCl)}$).

^{11}B NMR (400 MHz, benzene-d_6): δ (ppm): 49.5.

Anal. Calcd. for $C_{33}H_{48}AuBCl_2N_2O_2$ C 50.72, H 5.93, N 3.59. Found: C 50.81, H 5.86, N 3.59.

ν_{max} (thin film) = 2960 (C-H_{alkane} stretching), 1463 (C=$C_{aromatic}$ stretching), 1373 (C-H_{alkane} bending), 1128 (C-O stretching).

[Au(IPr*)(Bpin)]



Following the general procedure [Au(IPr*)(OH)] (100.0 mg, 0.09 mmol) and anhydrous methanol (2 mL) were used. In the glovebox, B_2pin_2 (24.6 mg, 0.097 mmol) and benzene (5 mL) were charged into the vial. The complex was recrystallized using CH_2Cl_2 (3 mL)/ pentane (10 mL). [Au(IPr*)(Bpin)] was obtained as a white crystalline solid in 70% yield (76.0 mg).

^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.82 (m, 8H, CH_{Ar}), 7.41 (m, 8H, CH_{Ar}), 6.99 (m, 28H, CH_{Ar}), 5.84 (s, 4H, CH_{IPr*}), 5.58 (s, 2H, CH_{Imid}), 1.54 (s, 6H, $CH_{3(IPr*)}$), 1.15 (s, 12H, $CH_{3(Bpin)}$).

^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 215.0 ($C_{carbene}$), 143.9 (C_{Ar}), 143.2 (C_{Ar}), 141.3 (C_{Ar}), 140.1 (C_{Ar}), 134.6 (C_{Ar}), 130.7 (CH_{Ar}), 130.3 (CH_{Ar}), 129.7 (CH_{Ar}), 128.7 (CH_{Ar}), 127.6 (CH_{Ar}), 126.6 (CH_{Ar}), 126.4 (CH_{Ar}), 123.2 (CH_{Imid}), 79.9 (CO_{Bpin}), 51.3 (CH_{IPr*}), 25.9 ($CH_{3(Bpin)}$), 20.9 ($CH_{3(IPr*)}$).

^{11}B NMR (400 MHz, benzene-d_6): δ (ppm): 46.2.

Anal. Calcd. for $C_{75}H_{69}AuBN_2O_2$ CH_2Cl_2: C 68.99, H 5.42, N 2.21. Found: C 69.84, H 5.94, N 2.32.

ν_{max} (thin film) = 3059 (C-H_{alkane} stretching), 1598 (C=$C_{aromatic}$ stretching), 1492 (C=$C_{aromatic}$ stretching), 1444 (C=$C_{aromatic}$ stretching), 1105 (C-O stretching).

Preliminary experiments

[Au(IPr)(Bpin)] (0.11 mmol, 8.0 mg) was transferred to a NMR tube inside the glovebox, benzene-d_6 was added followed by R (0.11 mmol). The NMR tube was stirred for 5 min, and then a ^{1}H NMR spectrum was recorded. The NMR tube was heated to 60 °C for 16 h, and then a ^{1}H NMR was recorded.

R = *p*-tolylaldehyde (0.011 mmol, 1.4 mg)
R = diphenylacetylene (0.11 mmol, 2.0 mg)
R = phenylacetylene (0.11 mmol, 1.9 mg)
R = styrene (0.11 mmol, 1.00 mg)

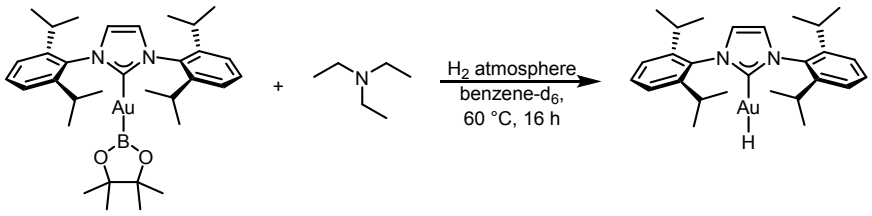
In situ experiment with *p*-tolylaldehyde

[Au(IPr)(OH)] (0.11 mmol, 7.0 mg) was transferred to a vial and dissolved in anhydrous methanol (0.5 mL). The solvent was removed under reduced pressure at 50 °C. This was repeated 4 times. The vial was transferred to the glovebox where benzene-d_6 (0.4 mL) was added followed by B_2pin_2 (0.01 mmol, 3.1 mg) and *p*-tolylaldehyde (0.11 mmol, 1.3 mg). The mixture was transferred to a NMR tube and the tube was shaken for 5 min. The first ^{1}H NMR spectrum was taken. Next the tube was heated to 50 °C for 1.30

h. A second ^{1}H NMR was taken. Next the NMR tube was heated to 60 °C for 16 h. The third NMR spectrum was taken. The solution changed colour from colourless to reddish/brown.

No change in ^{1}H NMR spectra observed

Reactivity with NEt_3 and activation of H_2



In the glovebox, [Au(IPr)(Bpin)] (7.0 mg, 0.01 mmol) and triethylamine were added to a J-Young NMR tube followed by benzene-d_6. A ^{1}H NMR spectrum was recorded and no change was observed. The J-Young tube was exposed to H_2 *via* freeze-pump-thaw method a total of 3 times on the Schlenk line. Again, no change was observed *via* ^{1}H NMR spectroscopy. Then the tube was heated to 60 °C for 16 h. No change was observed for reactions a), b) and c). A new complex was observed for reaction d) and it was identified as [Au(IPr)H]. The reaction mixture was concentrated and washed with pentane. [Au(IPr)H] was isolated in 97% yield (5.0 mg).

Table S-1: Activation of H_2

Entry		Mr	Mass	Moles	Equiv.
	[Au(IPr)(Bpin)]	713.54 mg/mol	7.0 mg	0.01 mmol	1.00
a)	NEt_3	101.19 mg/mol	0.5 mg	0.004 mmol	0.50
b)	NEt_3	101.19 mg/mol	1.0 mg	0.01 mmol	1.00
c)	NEt_3	101.19 mg/mol	2.0 mg	0.02 mmol	2.00
d)	NEt_3	101.19 mg/mol	2.7 mg	0.03 mmol	3.00

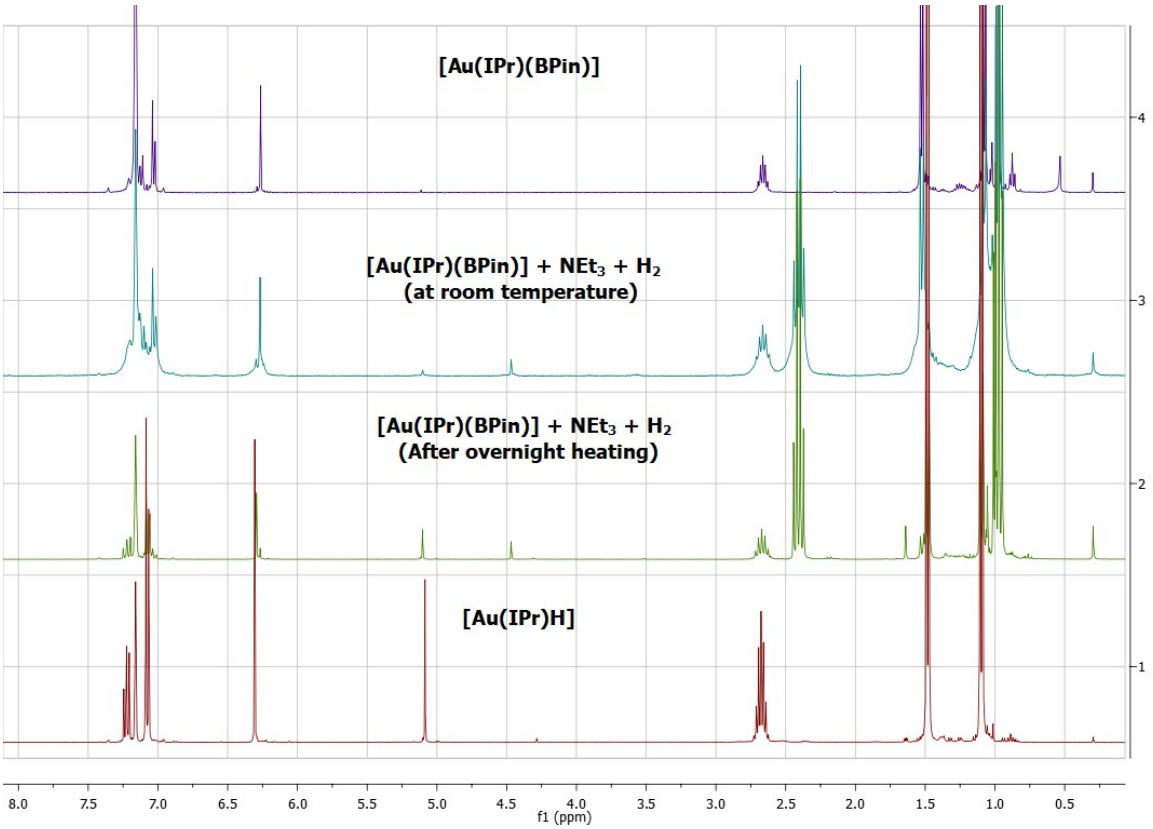
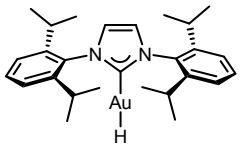


Figure S-1: ^{1}H NMR spectra of the activation of H_2

[Au(IPr)H]

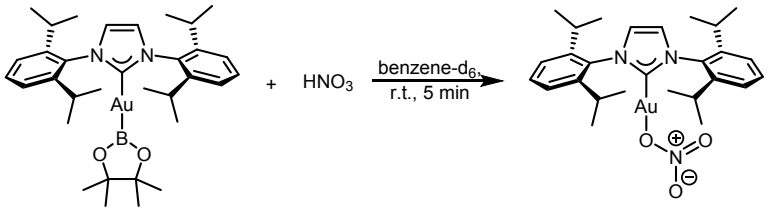


^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.24 (t, *J* = 7.9 Hz, 2H, CH_{Ar}), 7.09 (d, *J*= 7.9 Hz, 4H, CH_{Ar}), 6.31 (s, 2H, CH_{Imid}), 5.09 (s, 1H, Au-H), 2.73-2.62 (sept., *J* = 6.4 Hz, 4H, CH_{IPr}), 1.49 (d, *J* = 6.8 Hz, 12H, $CH_{3(IPr)}$), 1.11 (d, *J* = 6.4 Hz, 12H, $CH_{3(IPr)}$).

^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 204.5 ($C_{carbene}$), 145.9 (C_{Ar}), 135.1 (C_{Ar}), 130.5 (CH_{Ar}), 124.1 (CH_{Ar}), 122.4 (CH_{Imid}), 29.1 (CH_{IPr}), 25.0 ($CH_{3(IPr)}$), 23.9 ($CH_{3(IPr)}$).
Analytical data obtained were in agreement with literature.[1]

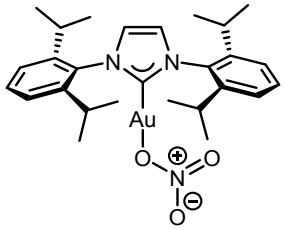
Reactivity with Brønsted acids

Reaction with HNO_3



In the glovebox, [Au(IPr)(Bpin)] (10.0 mg, 0.01 mmol) and HNO_3 (0.9 mg, 0.01 mmol) were added to a J-Young NMR tube followed by benzene-d_6. The tube was shaken for 5 min at room temperature. ^{1}H NMR spectrum was recorded and a new complex was detected. The crude mixture was concentrated and washed with hexane. The solid was identified as [Au(IPr)(ONO_2)], which is in agreement with the literature.[2] The complex was isolated in 98% yield (9.0 mg). The hexane filtrate was concentrated and identified as HBpin when compared to a commercially available sample.

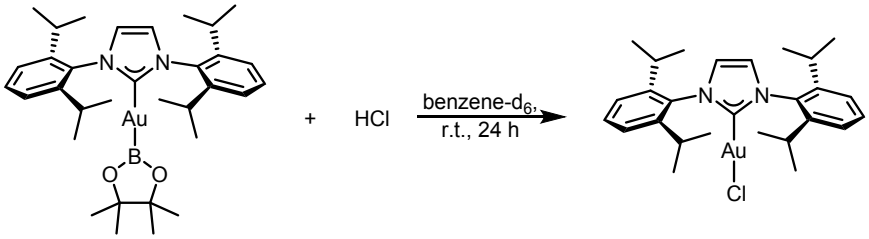
[Au(IPr)(ONO_2)]



^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.16-7.10 (m, 2H, CH_{Ar}), 7.03 (d, *J* = 12.4 Hz, 4H, CH_{Ar}), 6.27 (s, 2H, CH_{Imid}), 2.48-2.41 (sept, *J* = 8.7 Hz, 4H, CH_{IPr}), 1.36 (d, *J* = 7.8 Hz, 12H, $CH_{3(IPr)}$), 1.04 (d, *J* = 7.8 Hz, 12H, $CH_{3(IPr)}$).

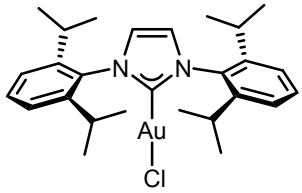
^{13}C {^{1}H} NMR (100 MHz, $CDCl_3$): δ (ppm) = δ 164.9 ($C_{carbene}$), 145.7 (C_{Ar}), 133.8 (C_{Ar}), 131.1 (CH_{Ar}), 124.4 (CH_{Ar}), 123.7 (CH_{Imid}), 29.0 (CH_{IPr}), 24.5 ($CH_{3(IPr)}$), 24.2 ($CH_{3(IPr)}$).
Analytical data obtained were in agreement with literature.[2]

Reaction with HCl



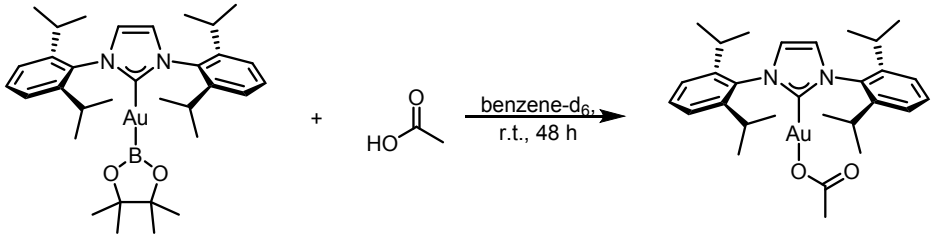
In the glovebox, [Au(IPr)(Bpin)] (10 mg, 0.014 mmol) and 4 M HCl in dioxane (7 μL, 0.028 mmol) were added to a J-Young tube followed by benzene-d_6. The reaction was monitored over time, after 24 h the full conversion of [Au(IPr)(Bpin)] into [Au(IPr)Cl] was observed. The solvent was removed under reduced pressure and the solid washed with hexane resulting in 99% yield (8.5 mg).

[Au(IPr)Cl]



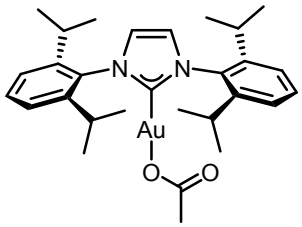
^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = δ 7.51 (t, *J* = 7.8 Hz, 2H), 7.29 (d, *J* = 7.8 Hz, 4H), 7.17 (s, 2H), 2.58 (sept, *J* = 6.8 Hz, 4H), 1.35 (d, *J* = 6.9 Hz, 12H), 1.22 (d, *J* = 6.9 Hz, 12H). **^{13}C {^{1}H} NMR (100 MHz, d-benzene):** δ (ppm) = δ 175.4 ($C_{carbene}$), 145.7 (C_{Ar}), 134.1 (C_{Ar}), 130.8 (CH_{Ar}), 124.4 (CH_{Ar}), 123.2 (CH_{Imid}), 28.9 (CH_{IPr}), 24.6 ($CH_{3(IPr)}$), 24.1 ($CH_{3(IPr)}$).
This is in agreement with the literature.[3b]

Reaction with $HCOOCH_3$



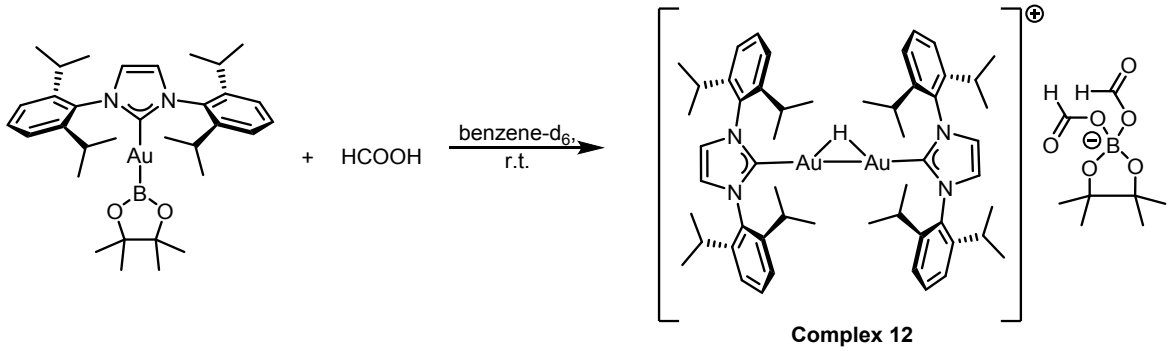
In the glovebox, [Au(IPr)(Bpin)] (20 mg, 0.028 mmol) and acetic acid (1.8 mg, 0.03 mmol)) were added to a J-Young tube followed by benzene-d_6. The reaction was monitored over time, after 48 h the full conversion of [Au(IPr)(Bpin)] into [Au(IPr)(OCOMe)] was observed. The solvent was removed under reduced pressure and the solid washed with hexane resulting in 98% yield (17.7 mg).

[Au(IPr)(OCOMe)]



^{1}H NMR (400 MHz,$CDCl_3$): δ (ppm) = δ 7.52 (t, *J* = 7.9 Hz, 2H), 7.30 (d, *J* = 8.0 Hz, 4H), 7.18 (s, 2H), 2.57 (sept, *J* = 6.9 Hz, 4H), 1.77 (s, 3H), 1.38 (d, *J* = 6.9 Hz, 12H), 1.22 (d, *J* = 6.8 Hz, 12H). **^{13}C {^{1}H} NMR (100 MHz, d-benzene):** δ (ppm) = δ 176.5 ($C_{carbene}$), 145.8 (C_{Ar}), 134.2 (C_{Ar}), 130.9 (CH_{Ar}), 124.2 (CH_{Ar}), 123.3 (CH_{Imid}), 29.0 (CH_{IPr}) 24.6 ($CH_{3(IPr)}$), 24.5 ($CH_{3(Ac)}$), 24.2 ($CH_{3(IPr)}$).
Analytical data obtained were in agreement with literature.[3a]

Reaction with HCOOH



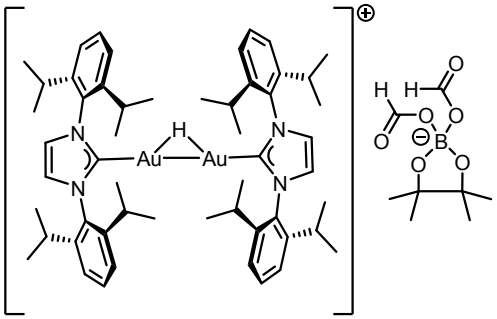
Complex 12

In the glovebox, [Au(IPr)(Bpin)] (10.0 mg, 0.01 mmol) and HCOOH (1.9 mg, 0.04 mmol) were added to a J-Young NMR tube followed by benzene-d_6. The reaction was monitored for 3 h. ^{1}H NMR were recorded after 5 min, 1 h, 2 h and 3 h. The solvent was removed under reduced pressure, the solid was washed with hexane resulting in 83% yield (11.5 mg,). Crystals were grown by vapor diffusion of pentane into a solution of the compound in benzene.

Larger scale synthesis:

In the glovebox, [Au(IPr)(Bpin)] (50.0 mg, 0.07 mmol) and HCOOH (5.5 mg, 0.12 mmol) were added to a J-Young NMR tube followed by benzene-d_6. The reaction was stirred for 6 h. The solvent was removed under reduced pressure, the solid was washed with hexane resulting in 88% yield (85.7 mg).

$[Au(IPr)_2(\mu\text{-}H)][(HOCO)_2Bpin]$



^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 13.33 (s, $2H_{formato}$), 8.62 (s, $4H_{imid}$), 7.31 (t, *J* = 8.4 Hz, $4H_{aryl}$), 7.06 (d, *J* = 7.4 Hz, $8H_{aryl}$), 2.44 (m, $8H_{IPr(CH)}$), 1.25 – 1.01 (m, $60H_{CH3,\ IPr\ and\ Bpin}$).

^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 186.5 ($C_{carbene}$), 164.8 ($COH_{formato}$), 145.7 (C_{Ar}), 133.6 (C_{Ar}), 131.1 (CH_{Ar}), 124.7 (CH_{Ar}), 122.7 (CH_{Imid}), 82.8 (CO_{Bpin}), 28.9 (CH_{IPr}), 25.0 ($CH_{3(IPr)}$), 24.5 ($CH_{3(Bpin)}$), 23.9 ($CH_{3(IPr)}$), 23.7 ($CH_{3(Bpin)}$).

^{11}B NMR (400 MHz, benzene-d_6): δ (ppm) = 7.35.

Anal. Calcd. for $C_{33}H_{48}AuBN_2O_2\ 2CH_2Cl_2$: C 49.24, H 6.00 N 3.59. Found C 49.55 H 6.04 N 3.60.

ν_{max} (thin film) =2962 (C-H stretching), 1610 (C=O stretching), 1458 (C=$C_{aromatic}$ stretching), 1384 (CH_3 bending), 1263 (C-O stretching).

X-ray structure of 12

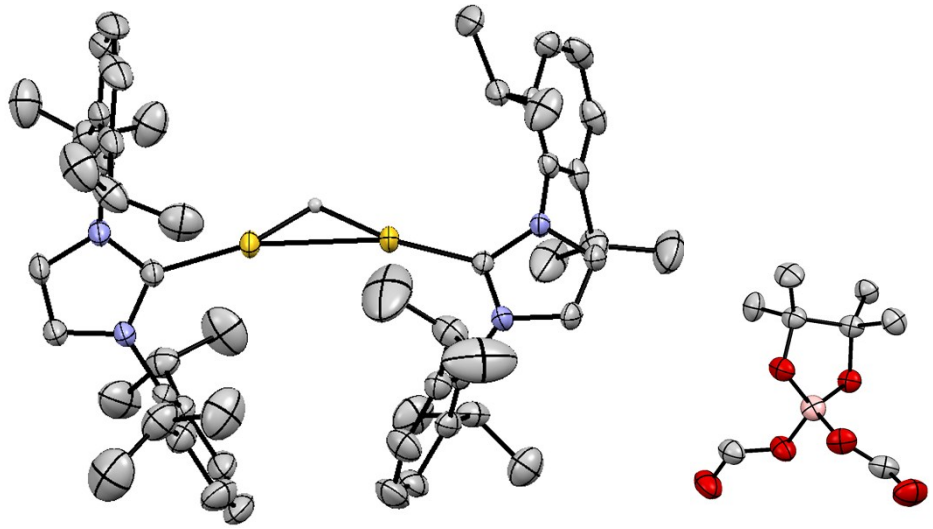
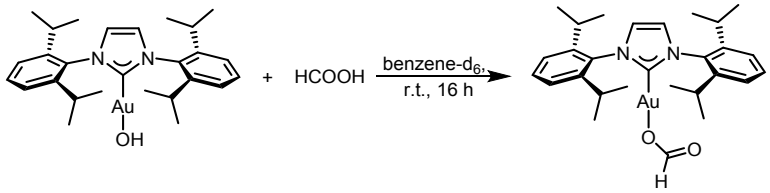


Figure S-2: Crystal structure of **12**. Hydrogen atoms (except for the hydride) are omitted for clarity. Thermal displacement ellipsoids are shown at the 50% probability level.

Mechanistic studies for the formation of complex 12

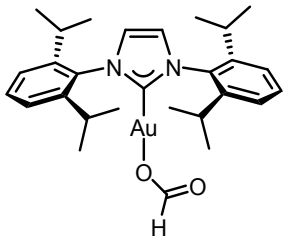
Mechanistic studies were carried out to investigate the formation of the diformato gold hydride dimer, $[Au_2(IPr)_2(\mu\text{-}H][(HOCO)_2Bpin]$ (**12**). Firstly, [Au(IPr)(OCOH)] was synthesized independently from [Au(IPr)(OH)] and HCOOH (1.1 equiv.) in toluene. The desired compound was isolated in 92% yield.

Synthesis of [Au(OCOH)(IPr)] from [Au(OH)(IPr)]



Outside the glovebox [Au(IPr)(OH)] (200.0 mg, 0.33 mmol) was added to a round bottom flask, followed by formic acid (12.5 µL, 0.33 mmol). The mixture was dissolved in anhydrous toluene (50 mL) and left to stir for 16 h at room temperature. The crude product was concentrated and recrystallized with CH_2Cl_2 and pentane. [Au(IPr)(OCOH)] was obtained as a white powder in 92% isolated yield (192.0 mg).

[Au(IPr)(OCOH)]



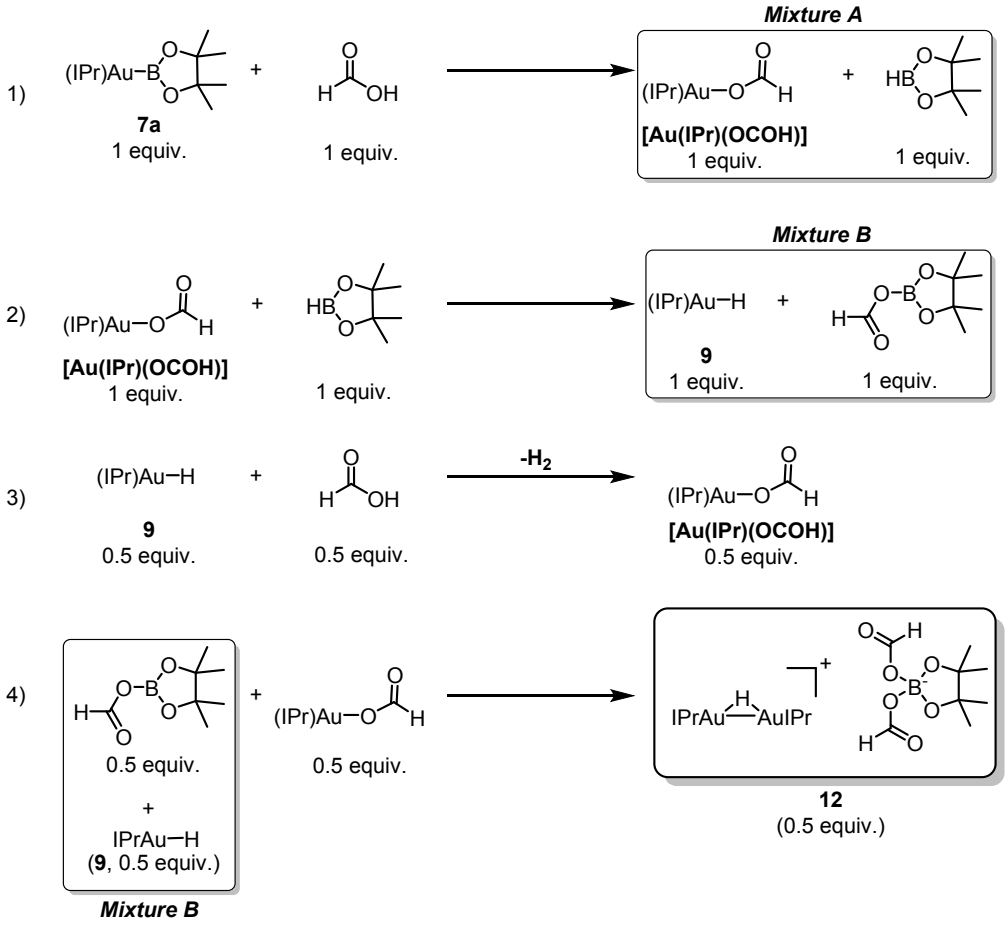
^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 9.26 (s, 1H, $CH_{formato}$), 7.21 (m, 2H, CH_{Ar}), 7.04 (d, *J* = 8.2 Hz, 4H, CH_{Ar}), 6.25 (s, 2H, CH_{Imid}), 2.59-2.52 (sept, *J* = 8.7 Hz, 4H, CH_{IPr}), 1.48 (d, *J* = 7.5 Hz, 12H, $CH_{3(IPr)}$), 1.06 (d, *J* = 8.2 Hz, 12H, $CH_{3(IPr)}$).

^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 175.6 ($C_{carbene}$), 166.7 (COH), 145.7 (C_{Ar}), 134.1 (C_{Ar}), 130.9 (CH_{Ar}), 124.4 (CH_{Ar}), 123.2 (CH_{Imid}), 28.9 (CH_{IPr}), 24.6 ($CH_{3(IPr)}$),24.2 ($CH_{3(IPr)}$).

ν_{max} (thin film) 2960 (C-H stretching), 1641 (C=O stretching), 1469 (C=$C_{aromatic}$ stretching).

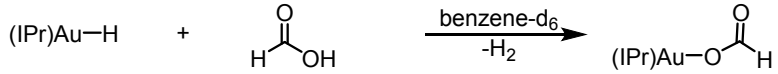
Discussion and results

The postulated mechanism involves the initial formation of [Au(IPr)(OCOH)] and HBpin (Mixture A, Scheme S-1) starting from **7a** and formic acid, similarly to the reactions of **7a** with acetic acid and HCl. However, in this case, [Au(IPr)(OCOH)] can react with HBpin to afford [Au(IPr)H] (**9**) and Bpin-formate species (Mixture B, Scheme S-1). Next, in the presence of additional formic acid, [Au(IPr)H] can further react to reform [Au(IPr)(OCOH)] (eq. 3, Scheme S-1). As it forms, [Au(IPr)(OCOH)] can directly react with Mixture B to form the final complex **12** (eq. 4, Scheme S-1).



Scheme S-1: Proposed reaction mechanism for the formation of **12**.

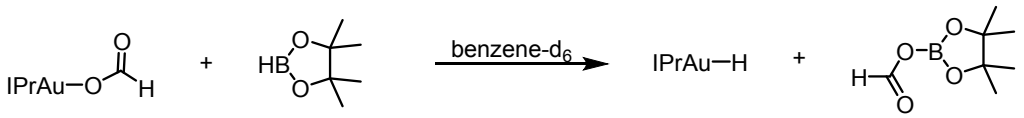
To investigate the feasibility of this mechanism, several key reactions in the mechanism were explored. First of all, the reaction of complex **9** with formic acid was investigated. Upon mixing [Au(IPr)H] (**9**) with formic acid, the formation of [Au(IPr)(OCOH)] was immediately observed.



Procedure: In the glovebox, [Au(IPr)H] (15 mg, 0.025 mmol) was transferred into a J-Young NMR tube, followed by HCOOH (1.2 mg, 0.025) in benzene-d_6 (0.5 mL). The NMR tube was shaken for 5 min and a ^{1}H NMR spectrum was taken, confirming the formation of [Au(IPr)(OCOH)].

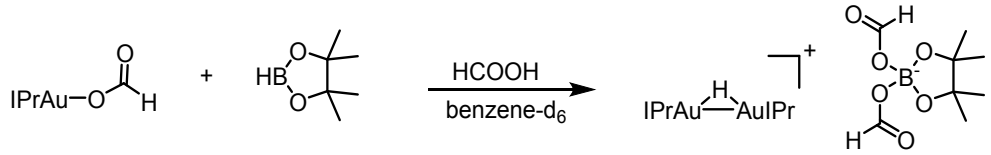
^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 9.23 (s, 1H, $CH_{formato}$), 7.18 (m, 2H, CH_{Ar}), 7.00 (d, *J* = 7.6 Hz, 4H, CH_{Ar}), 6.22 (s, 2H, CH_{Imid}), 2.57 (sept, *J* = 6.5 Hz, 4H, CH_{IPr}), 1.45 (d, *J* = 7.6 Hz, 12H, $CH_{3(IPr)}$), 1.03 (d, *J* = 8.1 Hz, 12H, $CH_{3(IPr)}$).

Then, [Au(IPr)(OCOH)] and HBpin were reacted together in a 1:1 ratio. The reaction quickly afforded the expected complex, [Au(IPr)H] (**9**). This reaction was done to allow us to mimic the formation of Mixture B from eq. 2 of the proposed mechanism in a controlled manner (the absence of any formic acid should allow the reaction to stop at this stage).



Procedure: In the glovebox, [Au(IPr)(OCOH)] (10 mg, 0.015 mmol) was transferred into a J-Young NMR tube, followed by 4,4,5,5-tetramethyl-1,3,2-dioxaborolane (HBpin) (2 mg, 0.015 mmol) in benzene-d_6 (0.5 mL). The NMR tube was shaken and a ^{1}H NMR was taken, confirming the formation of [Au(IPr)H]. **^{1}H NMR (400 MHz, benzene-d_6):** δ (ppm) = δ 7.24 (t, *J* = 7.9 Hz, 2H, CH_{Ar}), 7.09 (d, *J*= 7.9 Hz, 4H, CH_{Ar}), 6.31 (s, 2H, CH_{Imid}), 5.09 (s, 1H, Au-H), 2.73-2.62 (sept., *J* = 6.4 Hz, 4H, CH_{IPr}), 1.49 (d, *J* = 6.8 Hz, 12H, $CH_{3(IPr)}$), 1.11 (d, *J* = 6.4 Hz, 12H, $CH_{3(IPr)}$).

Making use of this mixture, we reacted [Au(IPr)(OCOH)] and HBpin, followed by HCOOH in a 1:1:1 ratio. Since we know from the above reaction that we are forming Mixture B (from the reaction of [Au(IPr)(OCOH)] and HBpin), the formic acid present in the reaction mixture should theoretically afford the final hydride dimer **12**. Under these conditions, the final product **12** is indeed obtained.

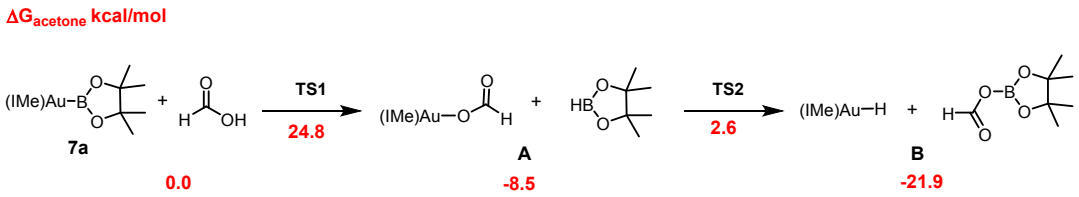


Procedure: In the glovebox, [Au(IPr)(OCOH)] (20 mg, 0.032 mmol) was transferred into a J-Young NMR tube, followed by HBpin (4 mg, 0.032 mmol) and benzene-d_6 (0.5 mL). Afterwards, HCOOH (2.9 mg, 0.032 mmol) was added. The NMR tube was shaken and a ^{1}H NMR was taken after 16 h, confirming the formation of $[Au_2(IPr)_2(\mu\text{-H})][(OCOH)_2Bpin]$. **^{1}H NMR (400 MHz, benzene-d_6):** δ (ppm) = δ 13.33 (s, $2H_{formato}$), 8.62 (s, $4H_{imid}$), 7.31(t, *J* = 8.4 Hz, $4H_{aryl}$), 7.06 (d, *J* = 7.4 Hz, $8H_{aryl}$), 2.44 (m, $8H_{IPr(CH)}$), 1.25 - 1.01 (m, $60H_{IPr\ and\ Bpin}$).

DFT calculations

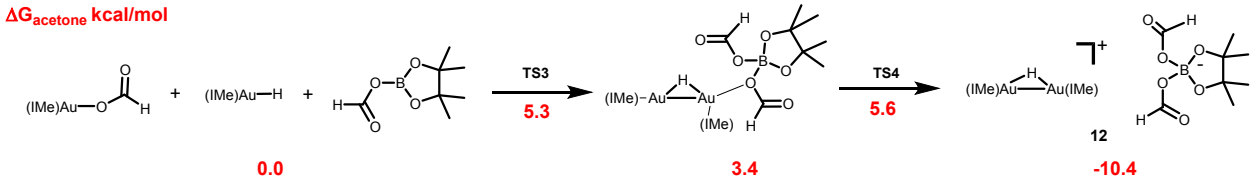
In order to support the mechanistic hypothesis reported above, DFT calculations on the reaction of **7a** with formic acid have been performed (for computational details see below). The small IMe NHC has been selected to reduce the computational cost and facilitate the modelling. The favored pathways with the corresponding energies are reported in Scheme S-2 and S-3.

The addition of the acid molecule to the (IMe)Au-Bpin system leads to the exothermic formation of **A** (at -8.5 kcal/mol) through a concerted transition state in which the carboxylic oxygen adds to the gold and the hydrogen transfers to the boron assisted by the gold with an accessible barrier of almost 25 kcal/mol, see Figure S-3a. In the following step, an easy ligand exchange process takes place with a barrier of only 10 kcal/mol. The lowest transition state located is reported in Figure S-3b and it consists of a six members TS involving the reactivity of both oxygen from the formiate moiety leading to the formation of the very stable intermediate **B** (at almost -22 kcal/mol).



Scheme S-2. Reaction mechanism for the formation of **A** and **B**.

In presence of a mixture of **A** and **B** the two gold species can react through a three molecules low energy transition state in which the Au-Au dimer forms in a concerted way with the transfer of the formiate moiety to the borane system, see **Figure S-3c**. The kinetic adduct formed easily evolves to **12** with an overall energy gain of 10 kcal/mol.



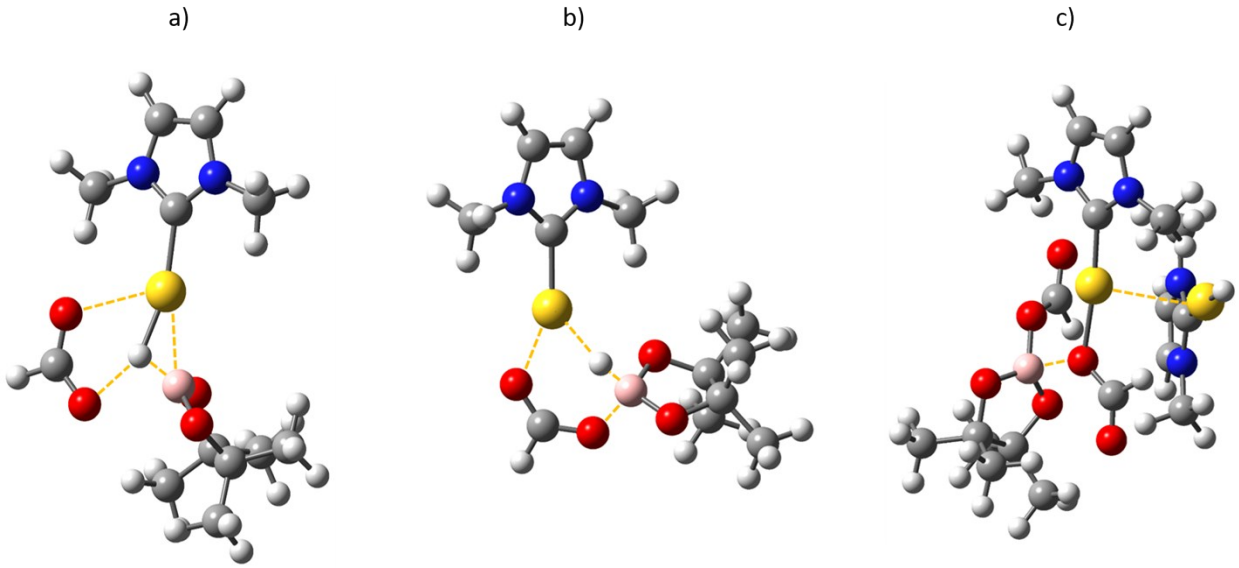
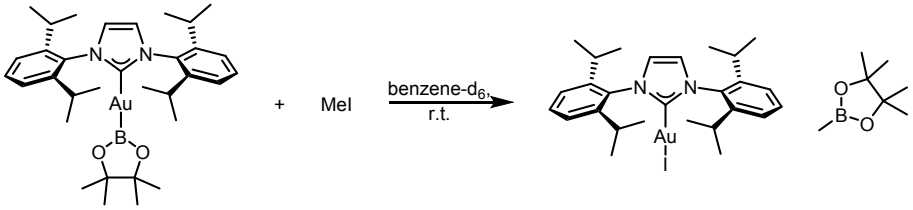


Figure S-3. Reaction mechanism for the formation **12** and Optimized geometries of a) TS1, b) TS2, c) TS3

Reactions with MeI



Time optimization

Inside the glovebox, [Au(IPr)(Bpin)] (50.0 mg, 0.07 mmol) was added to a J-Young NMR tube, followed by methyl iodide (10.0 mg, 0.07 mmol) and the mixture was dissolved in benzene-d_6 (0.6 mL). ^{1}H NMR spectra were taken over 16 h. See Figure S-4 for reaction optimization.

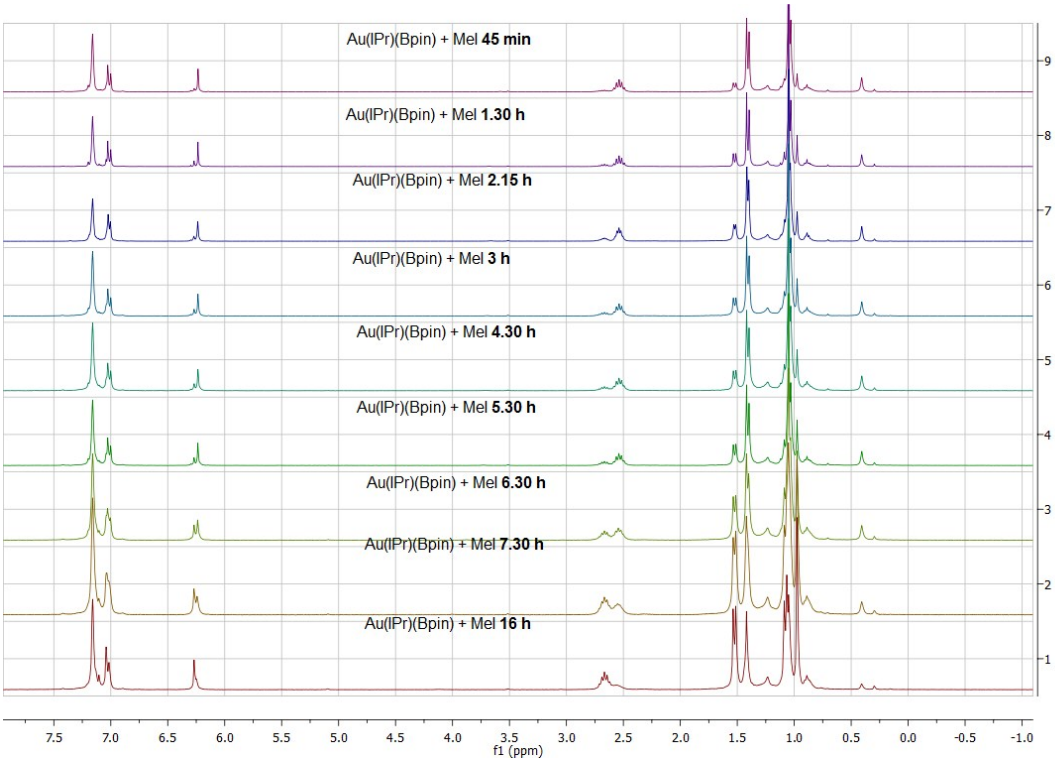
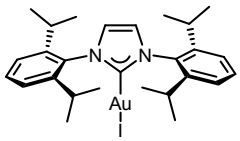


Figure S-4: Time optimization of [Au(IPr)I].

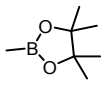
The crude mixture was concentrated and washed with pentane. ^{1}H NMR of the solid was recorded and identified as [Au(IPr)I] the pentane wash was concentrated and identified as 2,4,4,5,5-pentamethyl-1,3,2-dioxaborolane.

[Au(IPr)I]



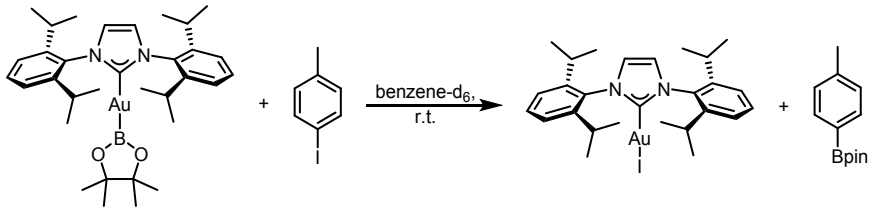
^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.20 (m, 2H, CH_{Ar}), 7.03 (t, *J* = 7.8 Hz, 4H, CH_{Ar}), 6.23 (s, 2H, CH_{Imid}), 2.58-2.49 (sept, *J* = 6.8 Hz, 4H, $CH_{(IPr)}$), 1.42 (d, *J* = 6.8 Hz, 12H, $CH_{3(IPr)}$), 1.05 (d, *J* = 7.5 Hz, 12H, $CH_{3(IPr)}$).
^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 187.3 ($C_{carbene}$), 145.7 (C_{Ar}), 134.3 (C_{Ar}), 131.0 (CH_{Ar}), 124.4 (CH_{Ar}), 122.4 (CH_{imid}), 29.0 (CH_{IPr}), 24.7 ($CH_{3(IPr)}$), 24.0 ($CH_{3(IPr)}$). This is in agreement with the literature.[3]

2,4,4,5,5-pentamethyl-1,3,2-dioxaborolane



^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 1.05 (s, 12H, CH_3), 0.39 (s, 3H, CH_3)
NMR analysis was in agreement with a commercially available sample.

Reaction with tolyl iodide

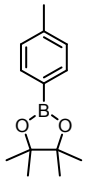


Outside the glovebox [Au(IPr)(Bpin)] (10.0 mg, 0.01 mmol) was added to a NMR tube, followed by 4-iodotoluene (6.1 mg, 0.03 mmol) and the mixture was dissolved in benzene-d_6 (0.6 mL). The reaction was left to stir for 48 h in air. The crude product was concentrated and washed with pentane. ^{1}H NMR spectrum of the solid was recorded and the compound identified as [Au(IPr)I].

[Au(IPr)I]

^{1}H NMR (400 MHz, benzene-d_6): δ (ppm) = δ 7.20 (m, 2H, CH_{Ar}), 7.03 (t, *J* = 7.8 Hz, 4H, CH_{Ar}), 6.23 (s, 2H, CH_{Imid}), 2.58-2.49 (sept, *J* = 6.8 Hz, 4H, $CH_{(IPr)}$), 1.42 (d, *J* = 6.8 Hz, 12H, $CH_{3(IPr)}$), 1.05 (d, *J* = 7.5 Hz, 12H, $CH_{3(IPr)}$).
This is in agreement with the literature.[3]

4,4,5,5-tetramethyl-2-(p-tolyl)-1,3,2-dioxaborolane



Chemical Formula: $C_{13}H_{19}BO_2$
Molecular Weight: 218.10

^{1}H NMR (400 MHz, $CDCl_3$): δ (ppm) = δ 7.75 (d, *J* = 7.6 Hz, 2H), 7.21 (d, *J* = 7.7 Hz, 2H), 2.39 (s, 3H), 1.37 (s, 12H).
^{13}C {^{1}H} NMR (100 MHz, benzene-d_6): δ (ppm) = δ 141.5 (C_{Ar}), 134.9 (CH_{Ar}), 128.6 (CH_{Ar}), 83.7 (CO_{Bpin}), 25.0 ($CH_{3(Bpin)}$), 21.8 ($CH_{3(tol)}$).
This is in agreement with the literature.[4]

Computational Analysis

Computational details. The dissociation free energies have been calculated using the Gaussian09 package.[5] The BP86 GGA functional of Becke and Perdew was used. Geometry optimizations were

performed with the standard split-valence basis set with a polarization function of Ahlrichs and coworkers for H, C, N, O, F and B atoms (SVP keyword in Gaussian)[6] while the quasi relativistic small-core Stuttgart effective core potential (ECP) was used for Gold (SDD keyword in Gaussian09).[7] The reported free energies have been obtained via single point energy calculations with the triple-ζ basis set of Ahlrichs for H, C, N, O, F and B atoms (TZVP keyword in Gaussian09). Solvent effects, CH_2Cl_2, were included using the PCM method.[8]

The dissociation free energies were computed as the free energy difference between the fully optimized IPr-Au-X complexes and the optimized fragments, i.e. IPr-Au^+ and X^-, for the anionic bond as well as IPr and Au-X for the [Au]-IPr bond.
The energy to dissociate the anionic X ligand increases in the order F (212 kJ/mol) < OH (263 kJ/mol) < Bpin (376 kJ/mol). Looking at the dissociation free energy of IPr, it decreases in the order F (272 kJ/mol) > OH (236 kJ/mol) > Bpin (105 kJ/mol). Significant weakening of the Au-IPr bond by the Bpin ligand is an unexpected feature, as the NHC-transition metal (TM) bond is usually the strongest bond in TM-NHC complexes.[9]

The energy decomposition analysis (EDA) has been performed using the Amsterdam Density Functional (ADF) program.[10] The electronic configuration of the molecular systems was described by a triple-ζ STO basis set with a polarization function (ADF basis set TZP).[11]
The relativistic effects have been inlcuded via ZORA approximation. The local exchange-correlation potential by Vosko *et al.*,[12] augmented in a self-consistent manner with Becke's exchange gradient correction and Perdew's correlation gradient correction was used in this analysis.[13]
The energy decomposition analysis (EDA) has been performed computing the bond snapping energy (BSE)[14] corresponding to the interaction of two rigid fragments that both possess the local equilibrium geometry of the final molecule and which both have an electronic structure suitable for bond formation. Although BSE does not always correlate with the bond dissociation enthalpies, since reorganization and relaxation of the fragments are not taken into account, BSE is closely related to bond enthalpy terms, which in turn provide a good approximation to bond strength values. In addition, BSE can be decomposed into two main components, namely steric interaction ΔE_0 and orbital interaction ΔE_{int} (eq. (1)):

$$BSE = -[\Delta E_0 + \Delta E_{int}] \quad (1)$$

The steric interaction term ΔE_0 can be split further into an electrostatic interaction term ΔE_{Elstat} and a Pauli repulsion term ΔE_{Pauli}, which is directly related to the two-orbital electron interactions between occupied orbitals on both interacting fragments (eq. (2)):

$$\Delta E_0 = \Delta E_{Elstat} + \Delta E_{Pauli} \quad (2)$$

where ΔE_{elstat} constitutes a stabilizing contribution to BSE, ΔE_{Pauli} constitutes a destabilizing contribution, and it is the relative size of electrostatic interaction and Pauli repulsion that determines the overall character of the steric interaction term.
The total orbital interaction energy ΔE_{int} can be broken down further into contributions from the orbital interactions within the various irreproducible representations τ of the overall symmetry group of the system (eq. (3)):

$$\Delta E_{int} = \sum_{\tau} \Delta E_{int}^{\tau} \quad (3)$$

All the molecules studied in the present work possess C_S symmetry; the NHC and the BPin ligands are located in the σ_{xy} mirror plane of the molecule. Therefore, A' contributions to the orbital interaction

energy are associated with σ-bonding and A" contributions represent π-bonding. The A' and A" contributions of the orbital interaction energy are further divided into both σ/π–donation and σ/π–backdonation.

In order to estimate these interactions, additional constrained space orbital variation (CSOV) calculations have been performed. In particular, to assess the contribution of σ/π-donation, the bond decomposition analysis was performed by again considering the interaction of the fragments, but now excluding the set of virtual a' and a" orbitals of the ligand from the variational space. This way, the A'/A" contribution of the orbital interaction energy can be associated only with the ligand to metal fragment donation. Similarly, the amount of σ/π-backdonation is determined explicitly excluding all virtual a' and a" orbitals on the [Au] fragment. Results are summarised in Table S-2.

Table S-2. Bond decomposition analysis (in kJ/mol) of the (IPr)Au-L and IPr-Au(L) bonds for L = BPin, F, OH.

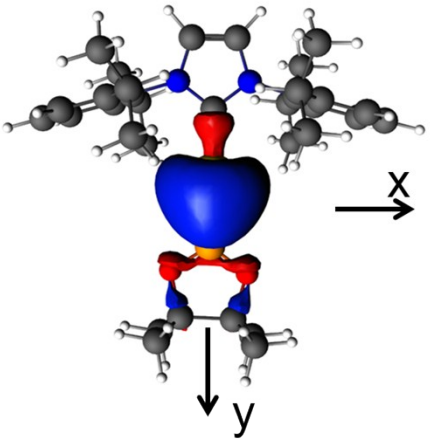
	(IPr)Au-BPin	(IPr)Au-F	(IPr)Au-OH	IPr-Au(BPin)	IPr-Au(F)	IPr-Au(OH)
ΔE_{elstat}	-1740	-800	-947	-619	-923	-882
ΔE_{Pauli}	1320	408	547	670	887	877
ΔE_0	-420	-392	-399	52	-36	-5
ΔE_{int} (σ)	-366	-243	-276	-188	-264	-249
ΔE_{int} (π)	-52	-62	-81	-34	-71	-71
ΔE_{int}	-418	-305	-357	-222	-335	-320
BSE	-838	-696	-756	-170	-371	-325

Studying the Au-X bonds, it was found that the orbital term is mainly σ-interaction, consisting of 77%, 86% and 83% ligand to metal σ-donation and the remaining 23%, 13% and 17% derived from metal to ligand σ-backdonation for Au-Bpin, Au-F and Au-OH bonds, respectively.

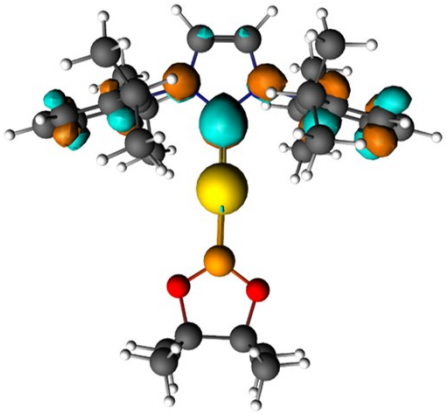
Moving to the steric term, ΔE_{elstat} is around twice higher for Au-Bpin system, indicating a higher polarization of this bond. These results are supported by the Hirshfeld charge analysis, showing values for F = -0.71e, OH = -0.38e and Bpin = -0.82e with the positive charge on Au for **8** = 0.75e, **2** = 0.52e and **7a** = 0.83e.

The Au-IPr bond, instead, is weaker in **7a** due to a greater unfavorable steric term (ΔE_0) together with a smaller stabilizing interaction term (ΔE_{int}).

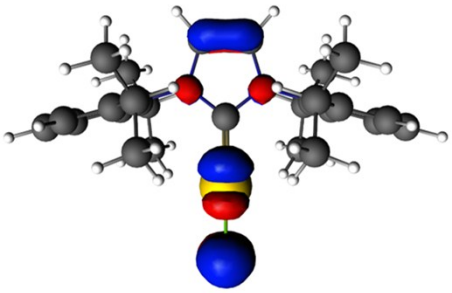
Figure S-5 shows the HOMO and LUMO analysis for all three complexes.



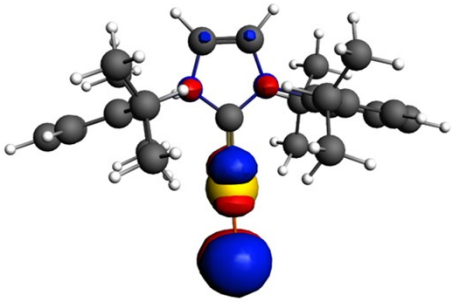
HOMO for [Au(IPr)(Bpin)]



LUMO for [Au(IPr)(Bpin)]



HOMO for [Au(IPr)(F)]



HOMO for [Au(IPr)(OH)]

Figure S-5. Images of HOMO and LUMO for [Au(IPr(Bpin)] and HOMO for [Au(IPr)F] and [Au(IPr)(OH)].

Cartesian Coordinates.

IPr-Au-BPin

C	3.122570	-1.712413	1.245628
C	2.469391	-1.904341	0.000000
C	3.122570	-1.712413	-1.245628
C	4.476755	-1.320712	-1.214655
C	5.149346	-1.128549	0.000000
C	4.476755	-1.320712	1.214655
N	1.084677	-2.332025	0.000000
C	0.001265	-1.485729	0.000000
N	-1.080248	-2.334470	0.000000
C	-0.681809	-3.672045	0.000000
C	0.689262	-3.670489	0.000000
C	-2.465962	-1.910028	0.000000
C	-3.119616	-1.719674	1.245625
C	-4.474772	-1.331325	1.214648
C	-5.147844	-1.140834	0.000000
C	-4.474772	-1.331325	-1.214648
C	-3.119616	-1.719674	-1.245625
C	-2.394477	-1.865594	2.583454
C	-3.136269	-2.802319	3.558731
C	-2.394477	-1.865594	-2.583454
C	-3.136269	-2.802319	-3.558731
Au	-0.000881	0.637840	0.000000
B	-0.002444	2.723170	0.000000
O	-1.150762	3.511994	0.000000
C	-0.808770	4.924031	0.000000
C	-1.444870	5.547778	-1.253326
C	2.397895	-1.860459	-2.583474
C	2.137822	-0.472040	-3.209391
C	2.397895	-1.860459	2.583474
C	2.137822	-0.472040	3.209391
C	3.141464	-2.796825	-3.557759
C	3.141464	-2.796825	3.557759
O	1.144616	3.513811	0.000000
C	0.800356	4.925326	0.000000
C	1.435480	5.550069	-1.253324
C	1.435480	5.550069	1.253324
C	-2.136477	-0.476196	-3.208105
C	-2.136477	-0.476196	3.208105
C	-1.444870	5.547778	1.253326
H	6.206652	-0.819050	0.000000
H	-6.205908	-0.833939	0.000000
H	1.407185	-2.318627	2.380863
H	5.011397	-1.155572	2.163258
H	5.011397	-1.155572	-2.163258
H	1.407185	-2.318627	-2.380863
H	1.412867	-4.491741	0.000000
H	-1.403564	-4.494927	0.000000
H	-1.403065	-2.322326	-2.381023
H	-1.403065	-2.322326	2.381023
H	-5.009797	-1.167500	-2.163252
H	-5.009797	-1.167500	2.163252
H	2.553209	-2.930007	-4.489861
H	4.130863	-2.387189	-3.851996
H	3.312021	-3.800155	-3.114639
H	1.555009	-0.570103	-4.149593
H	1.568754	0.178183	-2.510724
H	3.091225	0.043245	-3.453306
H	-2.547415	-2.933945	-4.490673
H	-3.305551	-3.806226	-3.116429

H	-4.126127	-2.393920	-3.853138
H	-1.553326	-0.572474	-4.148283
H	-3.090667	0.037789	-3.451715
H	-1.568580	0.174312	-2.508733
H	2.553209	-2.930007	4.489861
H	3.312021	-3.800155	3.114639
H	4.130863	-2.387189	3.851996
H	1.555009	-0.570103	4.149593
H	3.091225	0.043245	3.453306
H	1.568754	0.178183	2.510724
H	-1.553326	-0.572474	4.148283
H	-1.568580	0.174312	2.508733
H	-3.090667	0.037789	3.451715
H	-2.547415	-2.933945	4.490673
H	-4.126127	-2.393920	3.853138
H	-3.305551	-3.806226	3.116429
H	1.225232	6.637235	-1.324592
H	2.535269	5.414386	-1.208049
H	1.076703	5.060979	-2.179177
H	-1.236327	6.635271	-1.324605
H	-1.085318	5.059238	-2.179170
H	-2.544444	5.410366	-1.208060
H	1.225232	6.637235	1.324592
H	1.076703	5.060979	2.179177
H	2.535269	5.414386	1.208049
H	-2.544444	5.410366	1.208060
H	-1.085318	5.059238	2.179170
H	-1.236327	6.635271	1.324605

IPr-Au-OH

C	3.117252	-1.245583	-0.646461
C	2.462798	0.000004	-0.836967
C	3.117258	1.245587	-0.646458
C	4.474078	1.214517	-0.264020
C	5.148323	-0.000003	-0.076956
C	4.474073	-1.214520	-0.264022
N	1.077112	0.000007	-1.257097
C	-0.007044	0.000002	-0.403807
N	-1.099562	0.000007	-1.245498
C	-0.702681	0.000014	-2.584138
C	0.667135	0.000014	-2.591138
C	-2.482280	0.000004	-0.817327
C	-3.137168	1.245496	-0.627388
C	-4.493995	1.214609	-0.244471
C	-5.168376	-0.000001	-0.057423
C	-4.493991	-1.214608	-0.244473
C	-3.137164	-1.245490	-0.627391
C	-2.416629	2.584978	-0.779559
C	-3.116426	3.512584	-1.794666
C	-2.416620	-2.584969	-0.779563
C	-3.116414	-3.512578	-1.794669
Au	0.019887	-0.000019	1.570360
O	0.154193	0.000100	3.566911
C	2.397508	2.585595	-0.797915
C	2.238319	3.278305	0.573694
C	2.397497	-2.585587	-0.797918
C	2.238304	-3.278297	0.573690
C	3.090797	3.506159	-1.824066
C	3.090782	-3.506155	-1.824070
C	-2.243666	-3.269514	0.594458
C	-2.243678	3.269523	0.594461

H	-6.228374	-0.000003	0.242816
H	6.207583	-0.000005	0.225668
H	-1.398833	2.376856	-1.170409
H	-5.029716	2.163615	-0.084190
H	-5.029708	-2.163616	-0.084194
H	-1.398825	-2.376843	-1.170413
H	-1.429317	0.000018	-3.402300
H	1.385191	0.000018	-3.416904
H	1.375898	-2.377601	-1.179117
H	1.375909	2.377613	-1.179113
H	5.009211	-2.163414	-0.101377
H	5.009221	2.163408	-0.101373
H	-2.538678	-4.451876	-1.923193
H	-4.135860	-3.797368	-1.458468
H	-3.214133	-3.032509	-2.790603
H	-1.664759	-4.211353	0.490481
H	-1.703273	-2.607848	1.303447
H	-3.226278	-3.526194	1.044772
H	2.515456	-4.447158	-1.951398
H	3.177807	-3.021308	-2.818717
H	4.114310	-3.788289	-1.498246
H	1.661020	-4.221127	0.468605
H	3.225153	-3.535481	1.013971
H	1.704626	-2.622867	1.293322
H	-2.538694	4.451885	-1.923189
H	-3.214144	3.032515	-2.790600
H	-4.135874	3.797371	-1.458465
H	-1.664775	4.211365	0.490484
H	-3.226291	3.526199	1.044776
H	-1.703282	2.607860	1.303450
H	1.661040	4.221138	0.468610
H	1.704638	2.622878	1.293326
H	3.225171	3.535484	1.013975
H	2.515475	4.447165	-1.951394
H	4.114327	3.788289	-1.498244
H	3.177819	3.021313	-2.818714
H	-0.754492	-0.000055	3.928738

IPr-Au-F

C	-0.631335	-3.126420	1.245964
C	-0.822636	-2.473283	0.000000
C	-0.631335	-3.126420	-1.245964
C	-0.247641	-4.482882	-1.214662
C	-0.060637	-5.156937	0.000000
C	-0.247641	-4.482882	1.214662
N	-1.249305	-1.088774	0.000000
C	-0.405783	0.000000	0.000000
N	-1.249303	1.088776	0.000000
C	-2.584747	0.685214	0.000000
C	-2.584750	-0.685208	0.000000
C	-0.822631	2.473285	0.000000
C	-0.631322	3.126422	-1.245964
C	-0.247632	4.482883	-1.214662
C	-0.060631	5.156940	0.000000
C	-0.247632	4.482883	1.214662
C	-0.631322	3.126422	1.245964
C	-0.778568	2.404926	-2.585527
C	-1.789250	3.104793	-3.517930
C	-0.778568	2.404926	2.585527
C	-1.789250	3.104793	3.517930
Au	1.552156	-0.000006	0.000000

F	3.536108	-0.000027	0.000000
C	-0.778574	-2.404917	-2.585524
C	0.598317	-2.231404	-3.264566
C	-0.778574	-2.404917	2.585524
C	0.598317	-2.231404	3.264566
C	-1.789280	-3.104754	-3.517926
C	-1.789280	-3.104754	3.517926
C	0.598324	2.231387	3.264560
C	0.598324	2.231387	-3.264560
H	0.242158	6.216115	0.000000
H	0.242157	-6.216110	0.000000
H	-1.171494	1.387350	-2.379193
H	-0.084362	5.017957	-2.163414
H	-0.084362	5.017957	2.163414
H	-1.171494	1.387350	2.379193
H	-3.406576	1.407697	0.000000
H	-3.406580	-1.407689	0.000000
H	-1.171477	-1.387335	2.379180
H	-1.171477	-1.387335	-2.379180
H	-0.084367	-5.017954	2.163414
H	-0.084367	-5.017954	-2.163414
H	-1.914179	2.526552	4.457376
H	-2.787154	-3.204144	-3.042234
H	-1.450489	4.123499	3.802022
H	-2.787130	3.204186	3.042262
H	0.497847	1.650997	4.205861
H	1.308070	1.695054	2.600492
H	1.048857	3.213695	3.521200
H	-1.914217	-2.526491	4.457358
H	-2.787154	-3.204144	3.042244
H	-1.450536	-4.123456	3.802047
H	0.497851	-1.650983	4.205849
H	1.048815	-3.213718	3.521238
H	1.308089	-1.695115	2.600489
H	-1.914179	2.526552	-4.457376
H	-2.787130	3.204186	-3.042262
H	-1.450489	4.123499	-3.802022
H	0.497847	1.650997	-4.205861
H	1.048857	3.213695	-3.521200
H	1.308070	1.695054	-2.600492
H	0.497851	-1.650983	-4.205849
H	1.308089	-1.695115	-2.600489
H	1.048815	-3.213718	-3.521238
H	-1.914217	-2.526491	-4.457358
H	-1.450536	-4.123456	-3.802047

HCOH

C	-0.132830	0.400710	-0.000008
O	-1.145065	-0.262610	0.000001
O	1.126231	-0.093612	-0.000003
H	1.033997	-1.075018	0.000031
H	-0.086343	1.520536	0.000035

IMe-Au-Bpin

C	-3.132597	-2.452297	-0.274952
N	-3.591252	-1.074909	-0.119453
C	-2.748074	0.000038	0.000029
N	-3.591116	1.075032	0.120132
C	-4.924762	0.682316	0.077112
C	-4.924851	-0.682111	-0.075349
C	-3.132303	2.452429	0.275096
Au	-0.618282	-0.000053	-0.000464
B	1.465517	-0.000088	-0.000141
O	2.260638	1.145434	-0.091296
C	3.647716	0.741545	-0.279383
C	3.937285	0.819135	-1.789702
O	2.260700	-1.145538	0.091346
C	3.647685	-0.741517	0.279951
C	4.551718	-1.720822	-0.476000
C	3.936730	-0.819073	1.790389
C	4.551401	1.720928	0.476891
H	-5.754944	-1.392111	-0.154590
H	-5.754762	1.392340	0.157145
H	5.616135	-1.409930	-0.417343
H	4.466656	-2.731194	-0.026033
H	4.265825	-1.802386	-1.541870
H	4.998525	0.594467	-2.023255
H	3.293239	0.116749	-2.355912
H	3.712189	1.845131	-2.145012
H	4.997866	-0.594245	2.024303
H	3.292390	-0.116782	2.356375
H	3.711660	-1.845102	2.145615
H	4.466407	2.731296	0.026903
H	4.265154	1.802454	1.542660
H	5.615869	1.410142	0.418584
H	-3.479321	2.871727	1.241276
H	-2.025402	2.442549	0.255757
H	-3.509492	3.082943	-0.555320
H	-3.509774	-3.083053	0.555277
H	-3.479695	-2.871226	-1.241229
H	-2.025674	-2.442566	-0.255630

H-Bpin

C	1.482451	-0.498570	-1.295848
C	0.795436	-0.189957	0.044607
O	1.096059	1.209094	0.356001
B	0.000006	1.954969	-0.000065
O	-1.096052	1.209067	-0.356004
C	-0.795441	-0.189940	-0.044588
C	-1.482499	-0.498575	1.295856
C	1.380551	-1.069226	1.152858
C	-1.380507	-1.069233	-1.152858
H	-0.000046	3.164230	0.000203
H	1.123473	-2.136306	0.989817
H	2.485791	-0.980885	1.154038
H	1.016856	-0.767439	2.153241
H	-1.369973	-1.564319	1.580036
H	-1.075513	0.128430	2.114385

H	-2.564465	-0.275158	1.204538
H	1.369944	-1.564326	-1.580012
H	1.075422	0.128402	-2.114378
H	2.564413	-0.275124	-1.204564
H	-2.485748	-0.980886	-1.154100
H	-1.016752	-0.767443	-2.153222
H	-1.123431	-2.136304	-0.989792

HOCO-Bpin

C	-0.743086	1.777619	1.019241
C	-0.923015	0.840430	-0.185658
O	0.404229	0.661822	-0.780018
B	0.897977	-0.508166	-0.268649
O	-0.003167	-1.277669	0.417110
C	-1.314537	-0.650069	0.227295
C	-2.017082	-1.428866	-0.895802
C	-1.839893	1.480963	-1.229123
C	-2.100205	-0.770417	1.534239
O	2.211964	-0.955675	-0.491771
C	3.288269	-0.223977	-0.103041
H	4.219072	-0.671815	-0.536350
O	3.256969	0.742382	0.621523
H	-2.876292	1.567825	-0.842646
H	-1.478144	2.501443	-1.467547
H	-1.861012	0.900536	-2.170829
H	-3.053931	-1.071224	-1.057037
H	-1.465133	-1.347425	-1.853958
H	-2.058776	-2.501183	-0.617982
H	-1.713659	2.024410	1.494852
H	-0.075097	1.333220	1.783968
H	-0.273037	2.719682	0.673293
H	-2.307540	-1.838222	1.748980
H	-1.536176	-0.355733	2.390744
H	-3.072824	-0.241652	1.460096

IMe-Au-H

C	3.072071	0.686141	-0.000182
C	3.072071	-0.686141	-0.000178
N	1.738964	-1.082731	0.000059
C	0.895580	0.000006	0.000155
N	1.738967	1.082736	-0.000023
C	1.285982	-2.470571	0.000186
Au	-1.189539	-0.000001	-0.000024
H	-2.806415	-0.000023	-0.000309
C	1.285959	2.470577	0.000211
H	3.901524	-1.401111	-0.000300
H	3.901523	1.401113	-0.000385
H	0.178984	2.464502	0.000592
H	1.651160	2.997937	0.904675
H	1.650944	-2.998093	-0.904274
H	1.650791	-2.997897	0.904825
H	0.179004	-2.464520	0.000089
H	1.650557	2.998094	-0.904421

IMe-Au-OCOH

C	-3.649979	-0.437672	0.130110
C	-3.530921	0.928227	0.089182
N	-2.171664	1.210947	0.019807
C	-1.431758	0.054701	0.017845
N	-2.360261	-0.954522	0.086953
C	-1.609247	2.557621	-0.041373
Au	0.542850	-0.123098	-0.070164
O	2.551504	-0.406020	-0.229096

C	-2.039584	-2.379667	0.104388
H	-4.293846	1.713273	0.102742
H	-4.537200	-1.076761	0.185026
H	-0.938307	-2.484418	0.101896
H	-2.451033	-2.854759	1.017281
H	-2.016815	3.104050	-0.915212
H	-1.842815	3.117915	0.886294
H	-0.511719	2.465814	-0.146153
H	-2.455671	-2.880998	-0.792501
C	3.456888	0.407460	0.303591
O	4.660788	0.250208	0.212219
H	3.014985	1.288149	0.868844

TS1

C	-2.206672	3.332836	-0.336799
C	-2.741560	2.916596	0.856739
N	-2.340020	1.598963	1.044728
C	-1.560569	1.180464	0.000841
N	-1.478796	2.259874	-0.842449
C	-2.672492	0.766581	2.203430
Au	-0.764110	-0.659142	-0.292482
B	1.447985	-0.761054	-0.114612
O	2.067906	-0.826100	1.118201
C	3.225551	0.066555	1.070354
C	4.353839	-0.563170	1.891138
C	-0.772586	2.249836	-2.120118
O	-3.062486	-2.099751	1.019253
C	-2.903581	-2.689683	-0.067699
O	-2.036433	-2.439555	-0.984853
O	2.195244	-0.097585	-1.075346
C	3.512975	0.169664	-0.491576
C	4.454780	-0.928180	-1.012987
C	3.988384	1.544396	-0.968052
C	2.790453	1.399937	1.702042
H	0.655107	-1.779763	-0.441724
H	-2.286787	4.289159	-0.863532
H	-3.369666	3.444339	1.581653
H	-2.795940	-0.286778	1.861271
H	-1.865303	0.823797	2.962126
H	-3.617827	1.133005	2.646678
H	0.082528	1.550088	-2.048135
H	-1.441393	1.917207	-2.940375
H	-0.399850	3.268291	-2.343193
H	4.056448	-0.613655	2.957992
H	4.580995	-1.592361	1.555448
H	5.279265	0.045440	1.822315
H	3.633375	2.117199	1.769827
H	1.967496	1.871645	1.128579
H	2.418854	1.204969	2.727998
H	5.500839	-0.763103	-0.684337
H	4.133332	-1.933441	-0.674487
H	4.434573	-0.921739	-2.121345
H	4.953899	1.813383	-0.491914
H	4.143627	1.527839	-2.065867
H	3.251485	2.337277	-0.738975
H	-3.583590	-3.558266	-0.318782

TS2

N	-2.356651	1.880149	-0.536649
C	-3.537615	2.591453	-0.353309
C	-4.408897	1.757570	0.299933
N	-3.742337	0.550806	0.492174

C	-2.470100	0.611627	-0.022302
C	-4.304272	-0.614109	1.165560
Au	-1.030484	-0.748118	0.009779
O	-0.144977	-2.696170	-0.769007
C	1.083604	-2.933456	-0.719568
O	2.032152	-2.162180	-0.314569
B	1.819418	-0.754686	0.321515
O	1.811923	0.313003	-0.660072
C	3.098469	0.967396	-0.576197
C	2.938871	2.432111	-1.000799
C	-1.165665	2.394125	-1.212060
O	2.901375	-0.536348	1.230958
C	3.473859	0.751422	0.951751
C	2.808104	1.792120	1.876752
C	4.979362	0.689341	1.240721
C	4.078175	0.254747	-1.531127
H	-3.659792	3.623159	-0.698624
H	-5.435550	1.922352	0.642534
H	-3.622804	-1.468679	0.992740
H	-4.391833	-0.435761	2.256969
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H	-0.310659	1.718046	-1.003253
H	-1.330602	2.441571	-2.308111
H	-0.932120	3.408657	-0.833482
H	5.144084	0.523777	2.325366
H	5.459720	-0.146781	0.697854
H	5.484691	1.637210	0.958722
H	3.273444	2.796322	1.791066
H	1.725176	1.882015	1.655654
H	2.912155	1.449571	2.926358
H	5.062616	0.765305	-1.581128
H	4.239465	-0.796976	-1.222300
H	3.640723	0.246934	-2.550670
H	3.890132	2.990845	-0.873961
H	2.657378	2.486100	-2.073306
H	2.153111	2.945224	-0.413144
H	0.663633	-0.854071	0.937570
H	1.438256	-3.940040	-1.060070

TS3

C	0.366669	2.695346	0.556449
N	-0.884545	3.222483	0.365721
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C	-0.431937	3.552980	2.509479
C	-1.628062	3.162256	-0.892504
C	1.830639	2.452541	2.575882
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H	-0.420498	3.810481	3.573398
Au	1.613746	1.823915	-0.867478
B	-2.501412	-0.949668	0.526373
O	-3.301852	0.186036	0.442739
O	-3.164857	-2.125835	0.236633
C	-4.663679	-0.249869	0.149877
C	-4.485056	-1.793088	-0.271708
C	-5.470094	-0.058977	1.446499
C	-5.230345	0.641833	-0.959752
C	-5.486500	-2.747086	0.395646
C	-4.493120	-2.028172	-1.790887
H	-6.539801	-0.317762	1.310191
H	-5.065216	-0.673727	2.275135

H	-5.410429	1.005368	1.753156
H	-6.237328	0.296966	-1.272955
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H	-5.269605	-3.786046	0.074327
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H	-6.527837	-2.508856	0.095520
H	-5.507424	-1.885156	-2.216746
H	-3.790528	-1.349709	-2.309967
H	-4.184085	-3.075197	-1.987125
H	2.543242	2.088480	1.811813
H	2.288964	3.285711	3.145438
H	1.559899	1.619217	3.254668
H	-2.370070	2.339457	-0.859843
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H	-0.911949	2.965302	-1.711547
Au	0.849261	-1.290096	-0.377569
C	4.764784	-2.597546	0.397510
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H	5.800138	-2.710280	0.060834
H	4.574196	-3.404186	2.486052
N	3.783513	-2.020573	-0.398514
N	2.831918	-2.557698	1.485397
C	2.584199	-1.991606	0.262055
C	1.816198	-2.775800	2.519413
H	1.150475	-3.613183	2.229598
H	2.327006	-3.026026	3.468234
H	1.200124	-1.863869	2.660124
C	3.985660	-1.535343	-1.763888
H	3.591785	-2.268232	-2.496444
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C	-0.772331	3.425411	2.513266
C	-1.882162	3.018362	-0.915022
C	1.547735	2.456062	2.609580
H	-2.739178	3.986600	1.581442
H	-0.796747	3.662196	3.581688
Au	1.422165	1.872379	-0.856642
B	-2.226616	-1.008667	0.184455
O	-3.123780	0.096278	0.194341
O	-2.931019	-2.218509	0.003017
C	-4.481644	-0.407787	0.210111
C	-4.322110	-1.939990	-0.249947
C	-5.012053	-0.257227	1.649365
C	-5.327018	0.448651	-0.741889
C	-5.160328	-2.932620	0.572584

C	-4.605928	-2.170465	-1.746321
H	-6.074979	-0.561773	1.739583
H	-4.418064	-0.855357	2.369084
H	-4.936346	0.808648	1.949049
H	-6.360859	0.054772	-0.828714
H	-5.395992	1.486201	-0.352568
H	-4.870553	0.487718	-1.748072
H	-4.967308	-3.961920	0.207026
H	-4.898253	-2.905457	1.647333
H	-6.246839	-2.732417	0.463995
H	-5.682966	-2.054113	-1.986871
H	-4.018575	-1.477855	-2.377200
H	-4.309997	-3.208690	-2.002338
H	2.306563	2.173271	1.855836
H	1.929227	3.297826	3.221470
H	1.316983	1.581568	3.251244
H	-2.563483	2.143005	-0.893997
H	-2.453185	3.951662	-1.087836
H	-1.140058	2.887503	-1.724672
Au	0.966307	-1.221042	-0.377313
C	4.958733	-2.244907	0.423602
C	4.368623	-2.626757	1.603785
H	6.004423	-2.278718	0.102045
H	4.799955	-3.060980	2.511286
N	3.947900	-1.746854	-0.388640
N	3.012704	-2.352804	1.484418
C	2.742079	-1.810581	0.255764
C	2.001002	-2.646707	2.505279
H	1.404212	-3.530705	2.204060
H	2.517458	-2.861261	3.459680
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C	4.131829	-1.249138	-1.752119
H	3.808837	-2.012431	-2.488216
H	3.530160	-0.325956	-1.889919
H	5.202541	-1.019358	-1.907319
O	-1.262626	-1.109104	1.337778
C	-1.143738	-0.193717	2.283343
H	-1.925413	0.610769	2.240643
O	-0.260666	-0.215752	3.136413
O	-1.068610	-0.777521	-0.987903
C	-1.273255	-0.303244	-2.237876
H	-0.292812	-0.190184	-2.773655
O	-2.345734	-0.021322	-2.727585
H	2.455475	1.369284	-2.004278

TS4

C	-0.948341	2.907290	0.367122
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C	-2.987325	3.526608	1.149388
C	-2.063621	3.813657	2.125843
C	-2.905033	2.408315	-1.114821
C	0.417307	3.433949	2.396250
H	-4.071959	3.672873	1.125309
H	-2.186129	4.256978	3.119265
Au	0.517241	2.013894	-0.794004
B	-1.663721	-1.478226	0.125621
O	-2.889478	-0.733485	0.108898
O	-1.949413	-2.870029	0.106488
C	-3.985153	-1.645044	0.346255
C	-3.365792	-3.077509	-0.028891

C	-4.382798	-1.531650	1.832223
C	-5.167904	-1.221325	-0.534716
C	-3.776820	-4.208972	0.928177
C	-3.667618	-3.512476	-1.476273
H	-5.266657	-2.155606	2.078021
H	-3.550833	-1.830720	2.500832
H	-4.637622	-0.475084	2.057124
H	-6.006002	-1.945065	-0.459056
H	-5.548598	-0.231585	-0.204884
H	-4.861293	-1.137250	-1.593833
H	-3.290992	-5.153066	0.606741
H	-3.457306	-4.006198	1.968175
H	-4.875143	-4.372036	0.917135
H	-4.738282	-3.768523	-1.618330
H	-3.383634	-2.722224	-2.196490
H	-3.066887	-4.417742	-1.702008
H	1.266916	3.456908	1.688569
H	0.450312	4.328038	3.048561
H	0.473225	2.502715	2.998034
H	-3.109981	1.328670	-0.950558
H	-3.843326	2.952390	-1.335269
H	-2.207936	2.520387	-1.965796
Au	1.536359	-0.692219	-0.457075
C	5.443204	-1.739926	0.750656
C	4.733832	-2.144534	1.854529
H	6.517373	-1.763151	0.541353
H	5.071944	-2.586144	2.797510
N	4.515646	-1.241104	-0.157243
N	3.394280	-1.888609	1.593326
C	3.243719	-1.331878	0.350446
C	2.282264	-2.190470	2.501181
H	1.619179	-2.948921	2.041876
H	2.699957	-2.582673	3.447305
H	1.673445	-1.283386	2.700319
C	4.841914	-0.719412	-1.480132
H	5.059703	-1.546614	-2.186636
H	3.970296	-0.145627	-1.848488
H	5.722758	-0.050953	-1.414353
O	-0.729474	-1.158060	1.284452
C	-0.889435	-0.122308	2.084274
H	-1.846072	0.439808	1.914084
O	-0.076887	0.201329	2.950014
O	-0.696786	-1.027743	-1.068066
C	-1.060727	-0.810279	-2.343033
H	-0.169123	-0.483039	-2.943529
O	-2.173333	-0.926635	-2.816927
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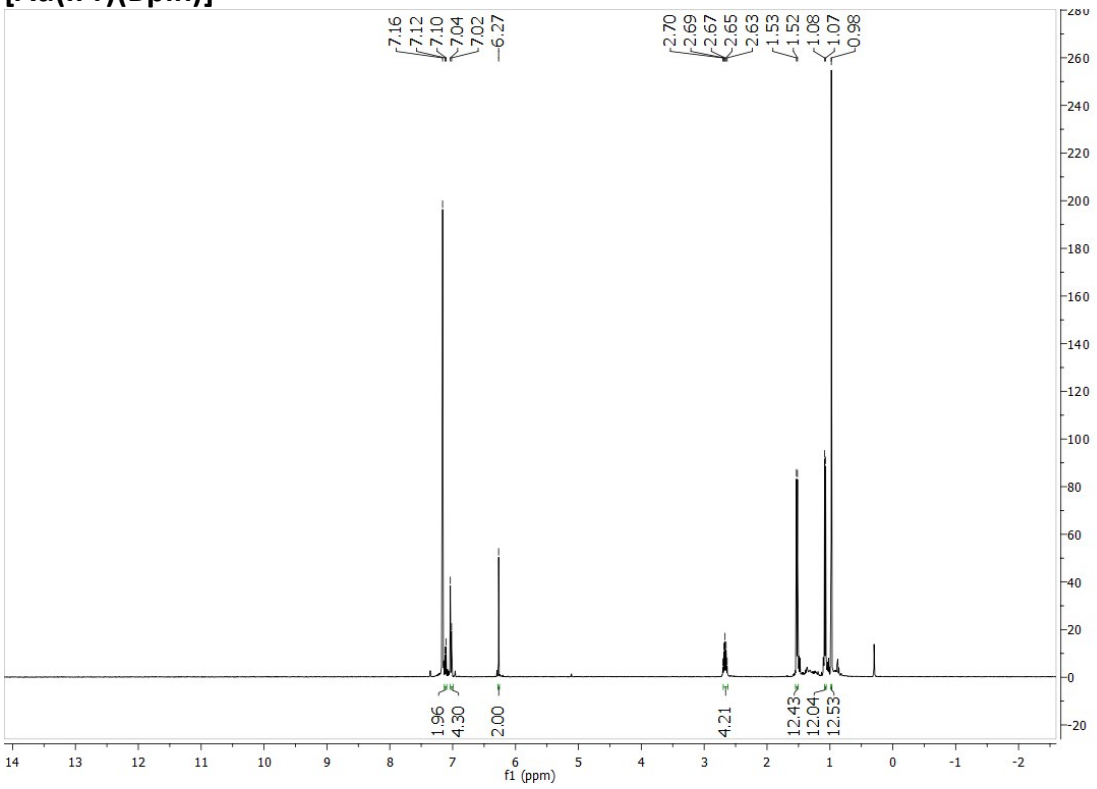
12

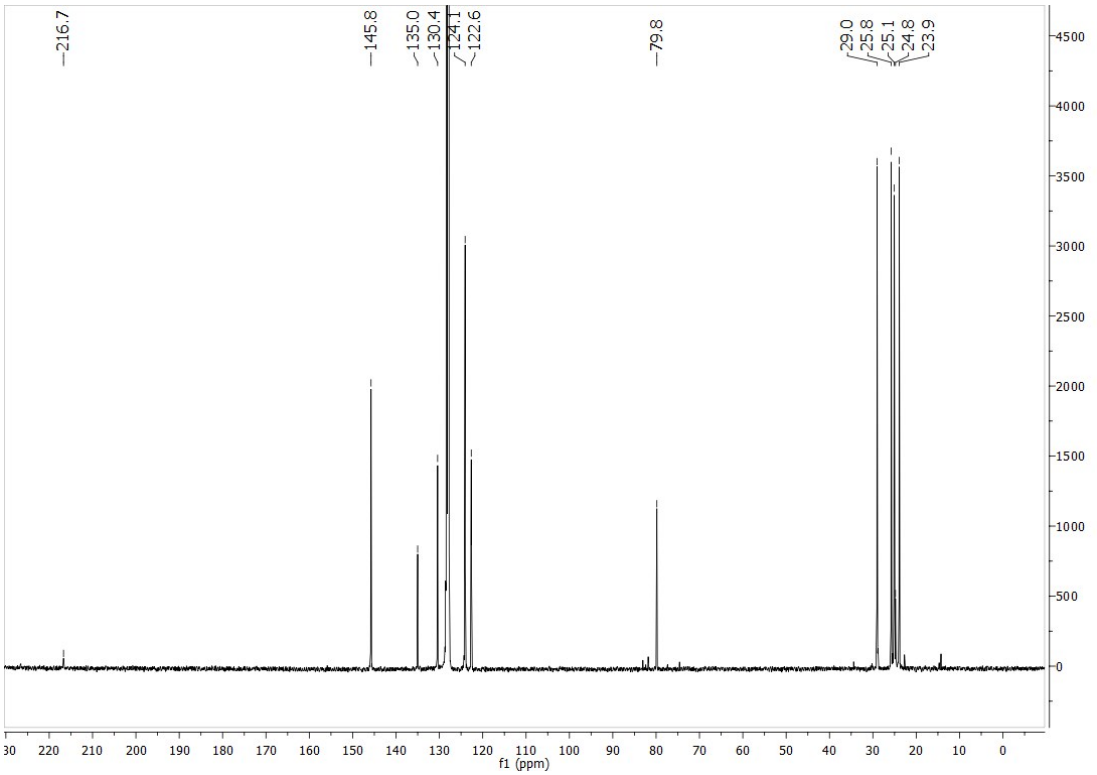
C	0.110714	2.650201	0.563582
N	-1.163514	3.109245	0.355822
N	0.337666	2.860457	1.899651
C	-1.723066	3.582112	1.534866
C	-0.772331	3.425411	2.513266
C	-1.882162	3.018362	-0.915022
C	1.547735	2.456062	2.609580
H	-2.739178	3.986600	1.581442
H	-0.796747	3.662196	3.581688
Au	1.422165	1.872379	-0.856642
B	-2.226616	-1.008667	0.184455
O	-3.123780	0.096278	0.194341

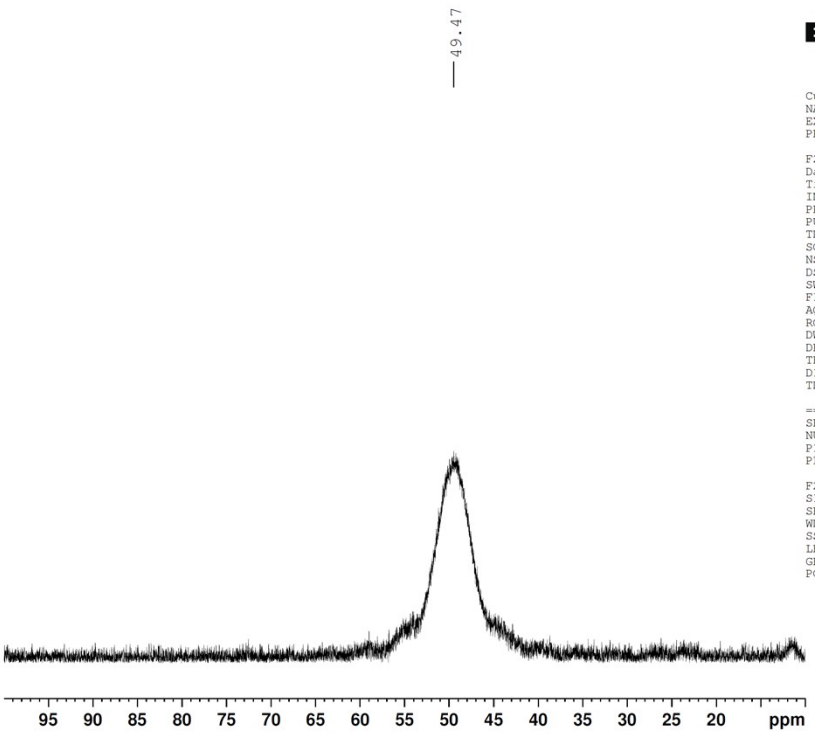
O	-2.931019	-2.218509	0.003017
C	-4.481644	-0.407787	0.210111
C	-4.322110	-1.939990	-0.249947
C	-5.012053	-0.257227	1.649365
C	-5.327018	0.448651	-0.741889
C	-5.160328	-2.932620	0.572584
C	-4.605928	-2.170465	-1.746321
H	-6.074979	-0.561773	1.739583
H	-4.418064	-0.855357	2.369084
H	-4.936346	0.808648	1.949049
H	-6.360859	0.054772	-0.828714
H	-5.395992	1.486201	-0.352568
H	-4.870553	0.487718	-1.748072
H	-4.967308	-3.961920	0.207026
H	-4.898253	-2.905457	1.647333
H	-6.246839	-2.732417	0.463995
H	-5.682966	-2.054113	-1.986871
H	-4.018575	-1.477855	-2.377200
H	-4.309997	-3.208690	-2.002338
H	2.306563	2.173271	1.855836
H	1.929227	3.297826	3.221470
H	1.316983	1.581568	3.251244
H	-2.563483	2.143005	-0.893997
H	-2.453185	3.951662	-1.087836
H	-1.140058	2.887503	-1.724672
Au	0.966307	-1.221042	-0.377313
C	4.958733	-2.244907	0.423602
C	4.368623	-2.626757	1.603785
H	6.004423	-2.278718	0.102045
H	4.799955	-3.060980	2.511286
N	3.947900	-1.746854	-0.388640
N	3.012704	-2.352804	1.484418
C	2.742079	-1.810581	0.255764
C	2.001002	-2.646707	2.505279
H	1.404212	-3.530705	2.204060
H	2.517458	-2.861261	3.459680
H	1.313235	-1.785004	2.641372
C	4.131829	-1.249138	-1.752119
H	3.808837	-2.012431	-2.488216
H	3.530160	-0.325956	-1.889919
H	5.202541	-1.019358	-1.907319
O	-1.262626	-1.109104	1.337778
C	-1.143738	-0.193717	2.283343
H	-1.925413	0.610769	2.240643
O	-0.260666	-0.215752	3.136413
O	-1.068610	-0.777521	-0.987903
C	-1.273255	-0.303244	-2.237876
H	-0.292812	-0.190184	-2.773655
O	-2.345734	-0.021322	-2.727585
H	2.455475	1.369284	-2.004278

NMR Spectra

[Au(IPr)(Bpin)]







Current Data Parameters
NAME Au(IPr)(Bpin)
EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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PULPROG zg30
TD 65536
SOLVENT C6D6
NS 500
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 192.66
DW 7.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1

======== CHANNEL f1 ========
SFO1 160.3974112 MHz
NUC1 11B
P1 14.50 usec
PLW1 90.00000000 W

F2 - Processing parameters
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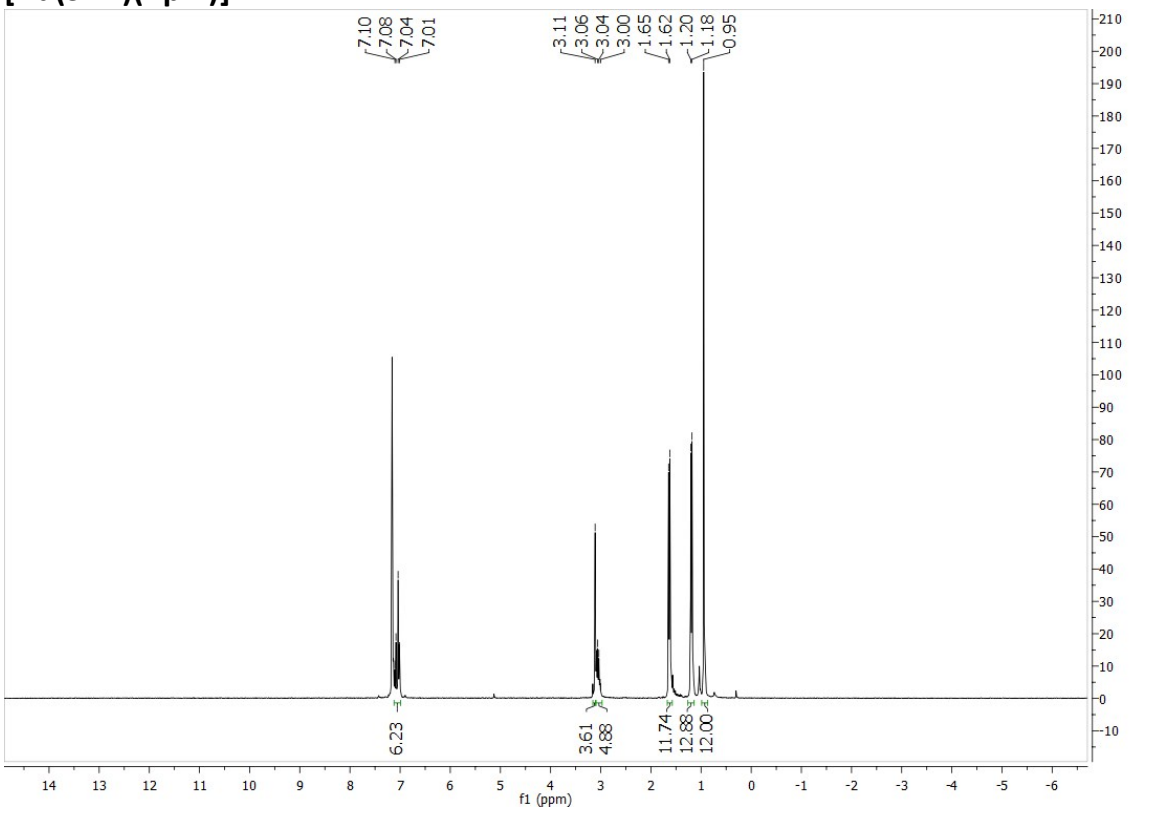
SF 160.3974112 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

[Au(SIPr)(Bpin)]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7.08
7.04
7.01
3.11
3.06
3.04
3.00
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1.62
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1.18
0.95
6.23
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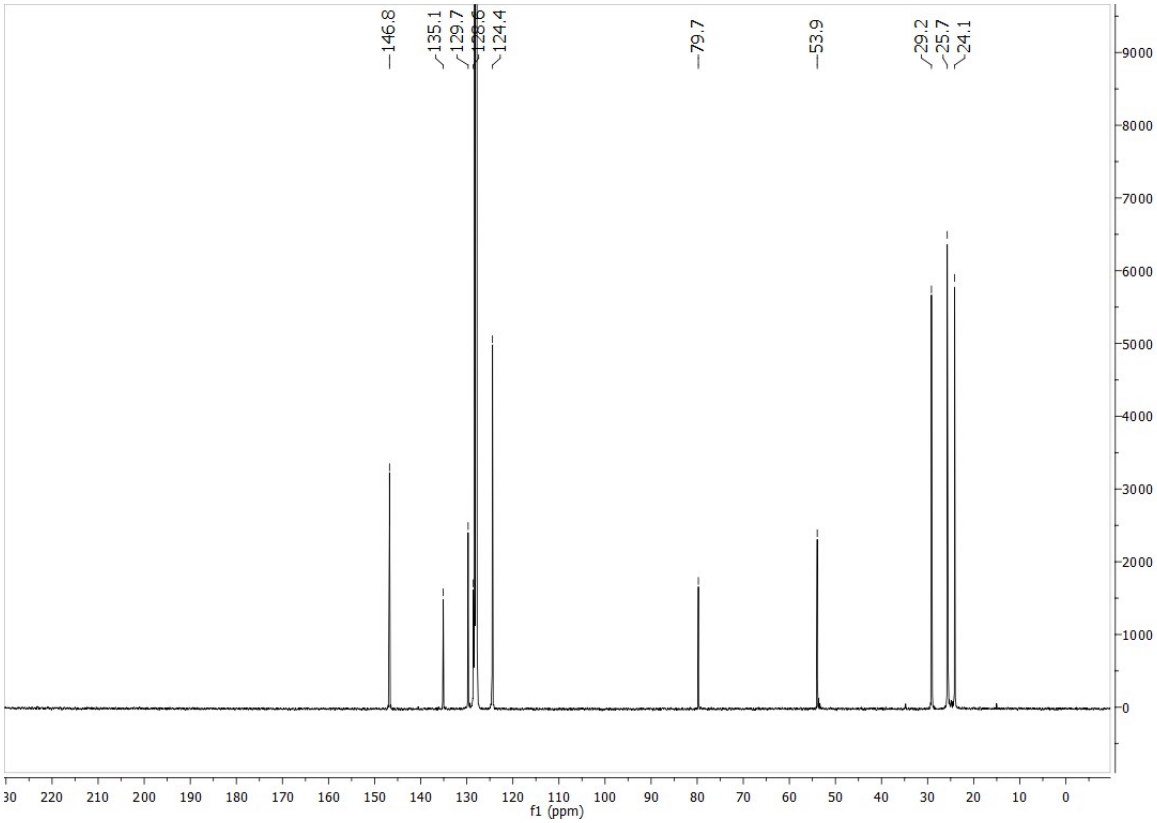
4.88
11.74
12.88
12.00
f1 (ppm)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135.1
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53.9
29.2
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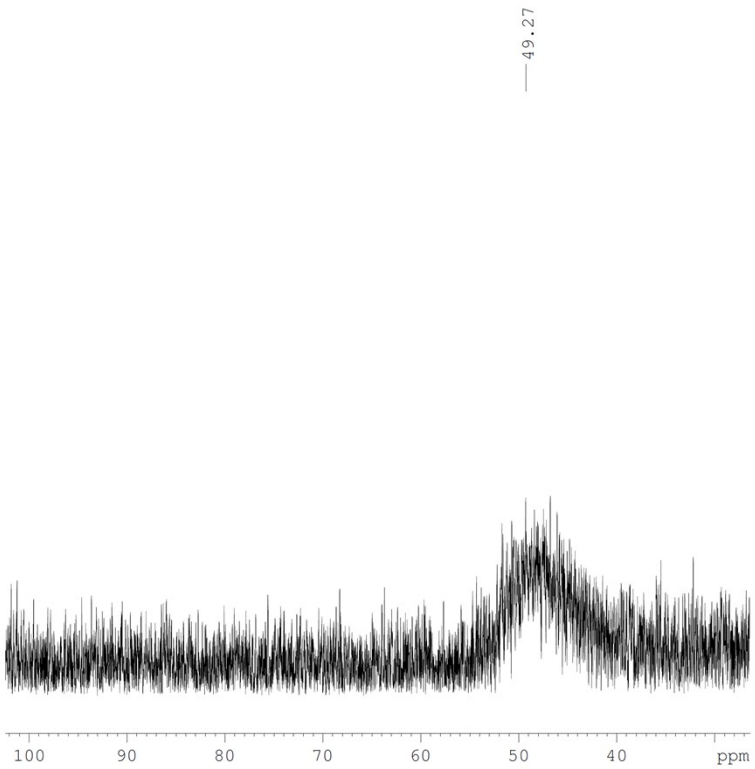
24.1
f1 (ppm)

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Current Data Parameters
NAME      Boron NMRs CZ
EXPNO                10
PROCNO                1

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Time              11.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG         zgpg30
TD               65536
SOLVENT            C6D6
NS                   256
DS                     4
SWH           64102.563 Hz
FIDRES         0.978127 Hz
AQ            0.5111808 sec
RG               192.66
DW                7.800 usec
DE                6.50 usec
TE                293.0 K
D1           1.50000000 sec
D11          0.03000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1        160.3974110 MHz
NUC1                11B
P1                14.50 usec
PLW1        90.00000000 W

======== CHANNEL f2 ========
SFO2        499.9330873 MHz
NUC2                1H
CPDPRG[2         waltz65
PCPD2             80.00 usec
PLW2        16.00000000 W
PLW12        0.27563000 W
PLW13        0.13864000 W

F2 - Processing parameters
SI                65536
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WDW                  EM
SSB       0
LB                2.00 Hz
GB        0
PC                1.40
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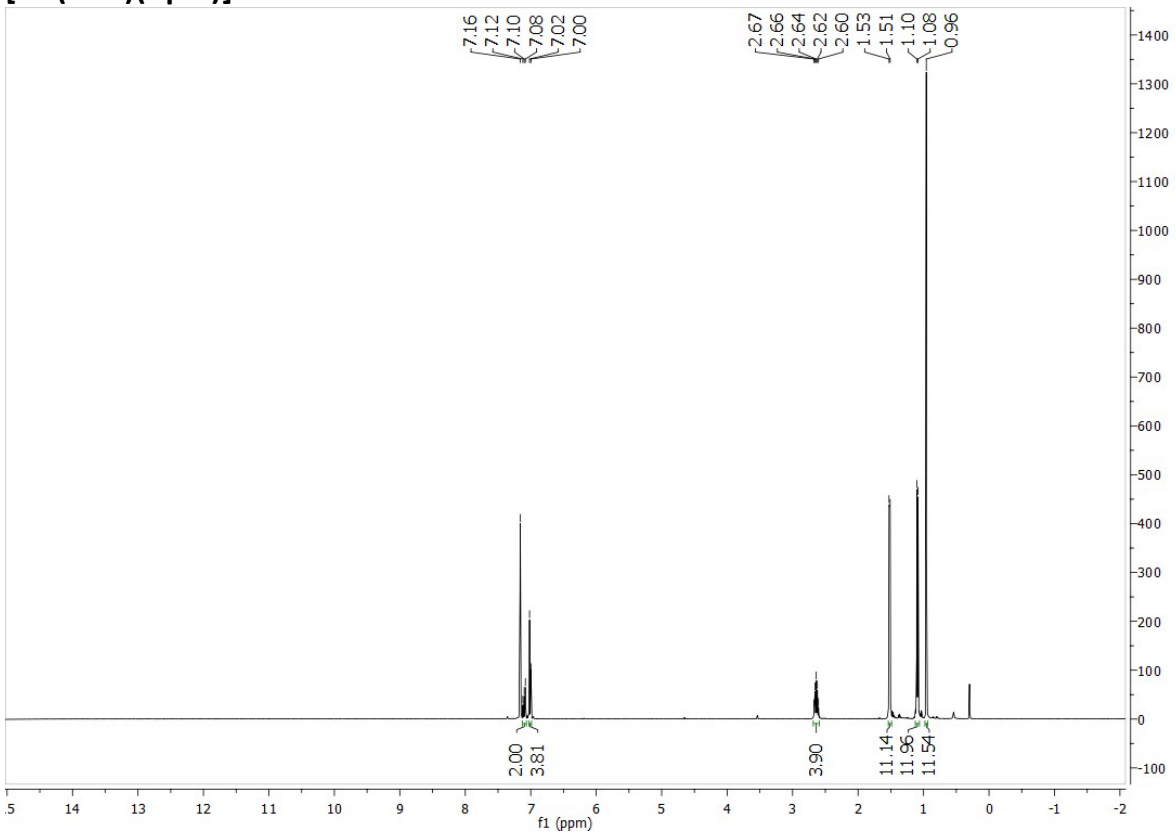
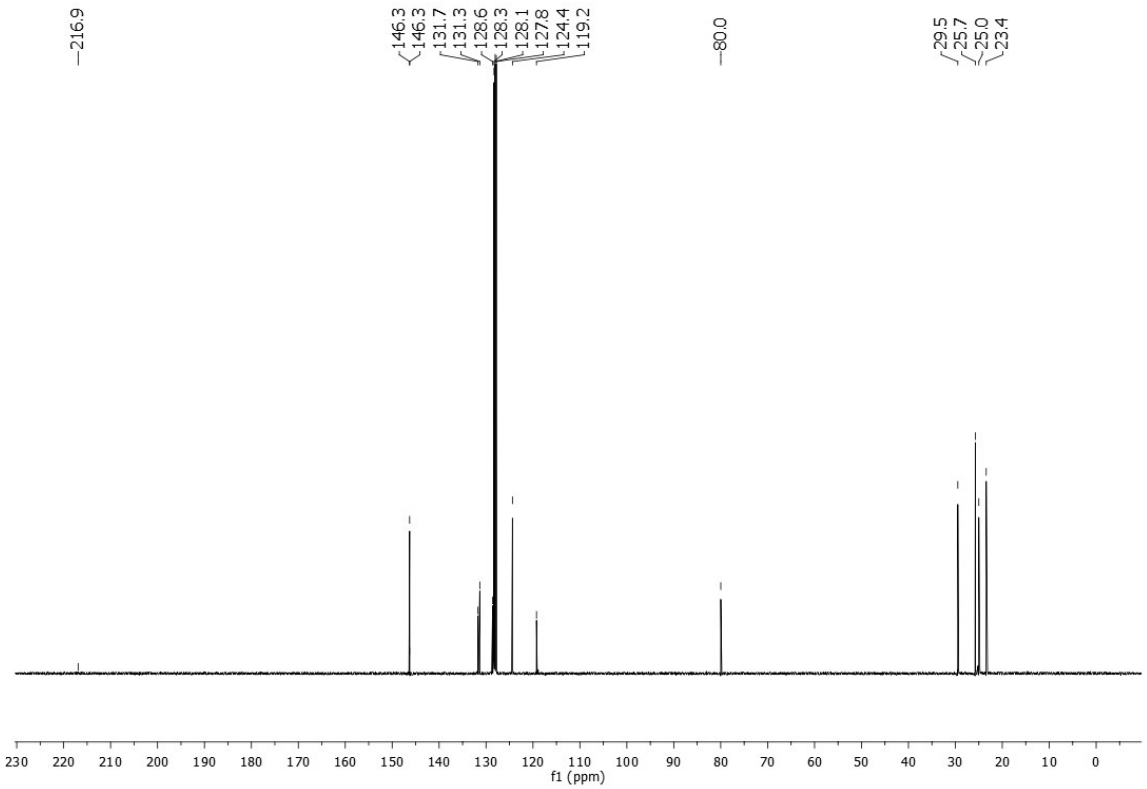
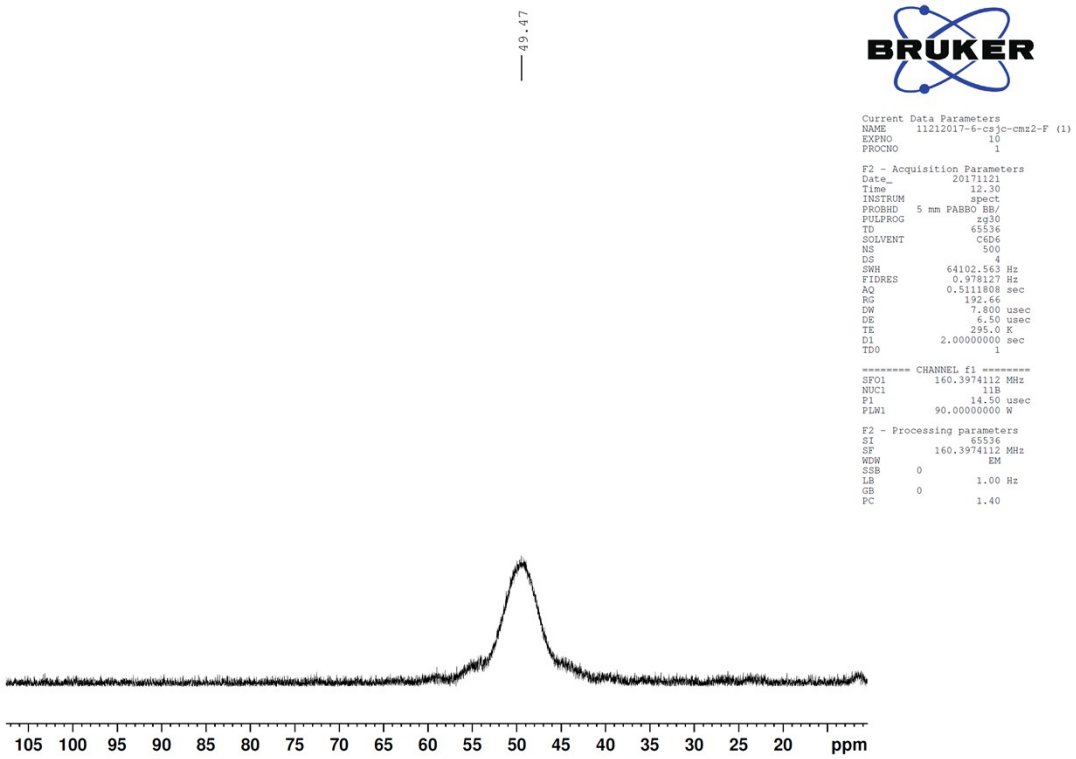
[Au(IPr^{Cl})(Bpin)]







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EXPNO 10
PROCNO 1

F2 - Acquisition Parameters
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Time 12.30
INSTRUM spect
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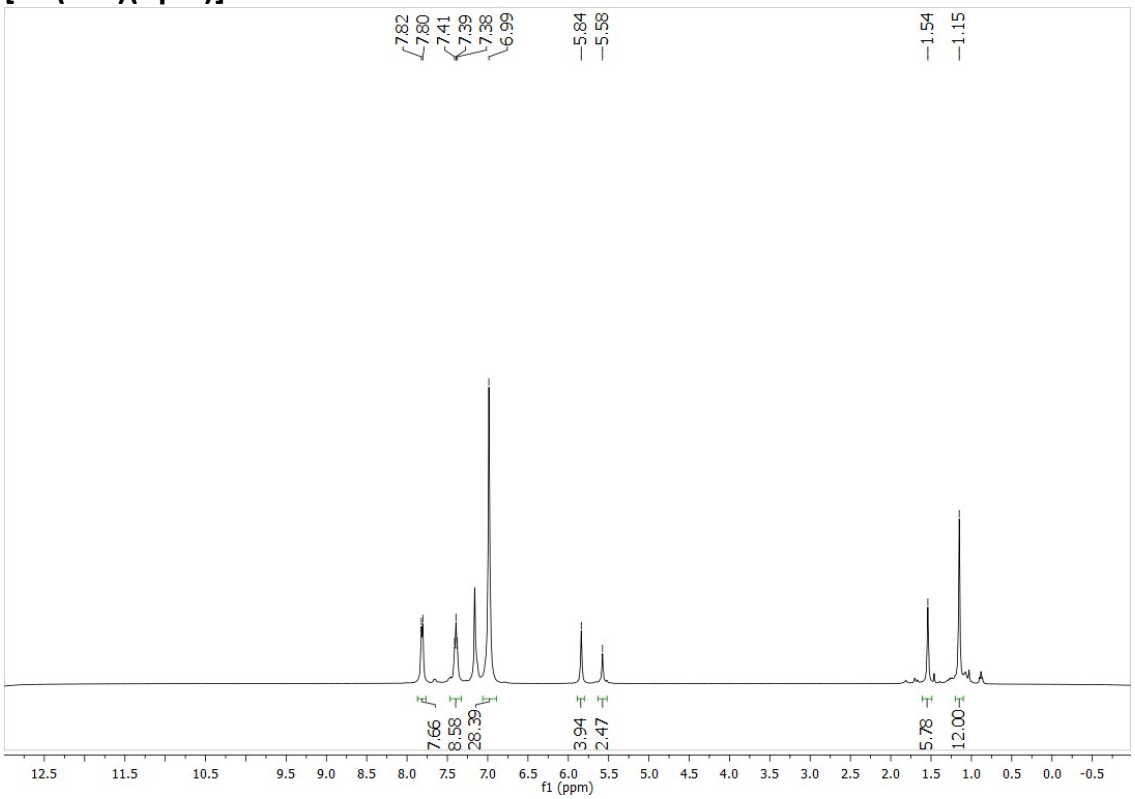
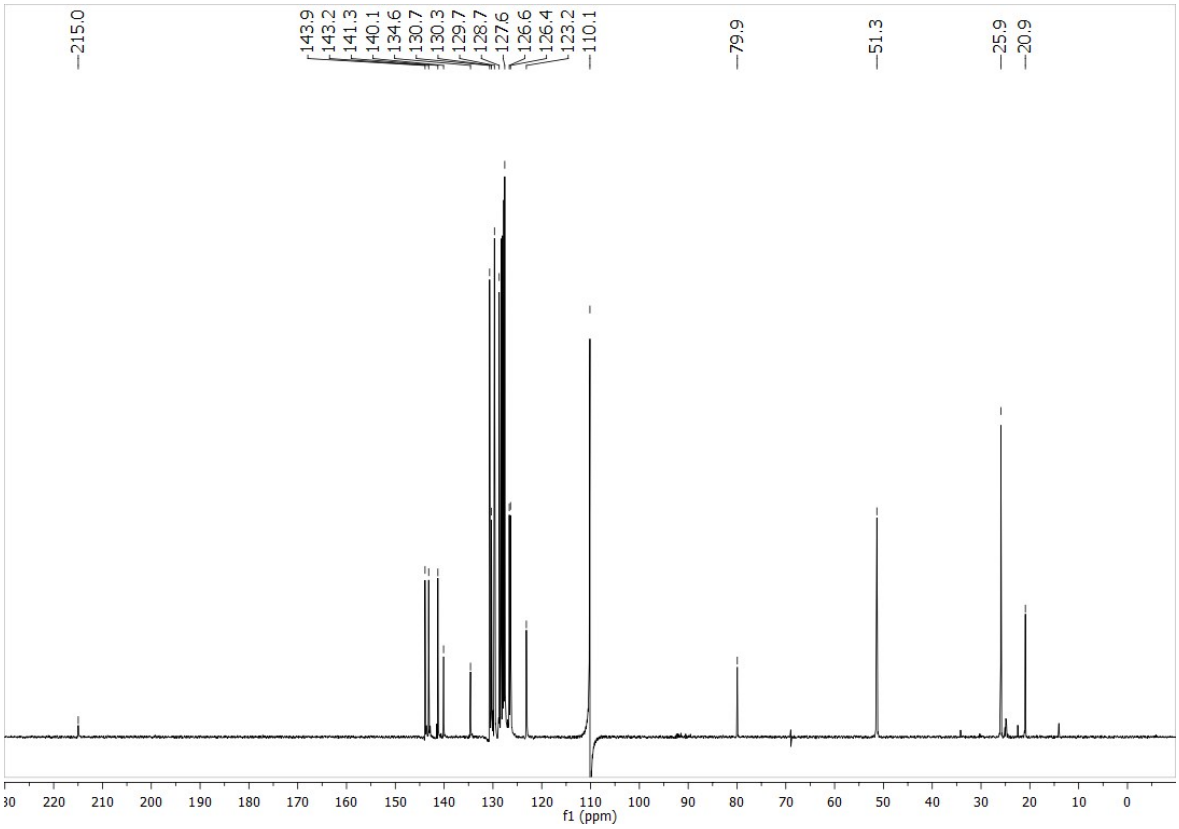
PULPROG zg30
TD 65536
SOLVENT C6D6
NS 500
DS 4
SWH 64102.563 Hz
FIDRES 0.978127 Hz
AQ 0.5111808 sec
RG 192.66
DW 7.800 usec
DE 6.50 usec
TE 295.0 K
D1 2.00000000 sec
TD0 1

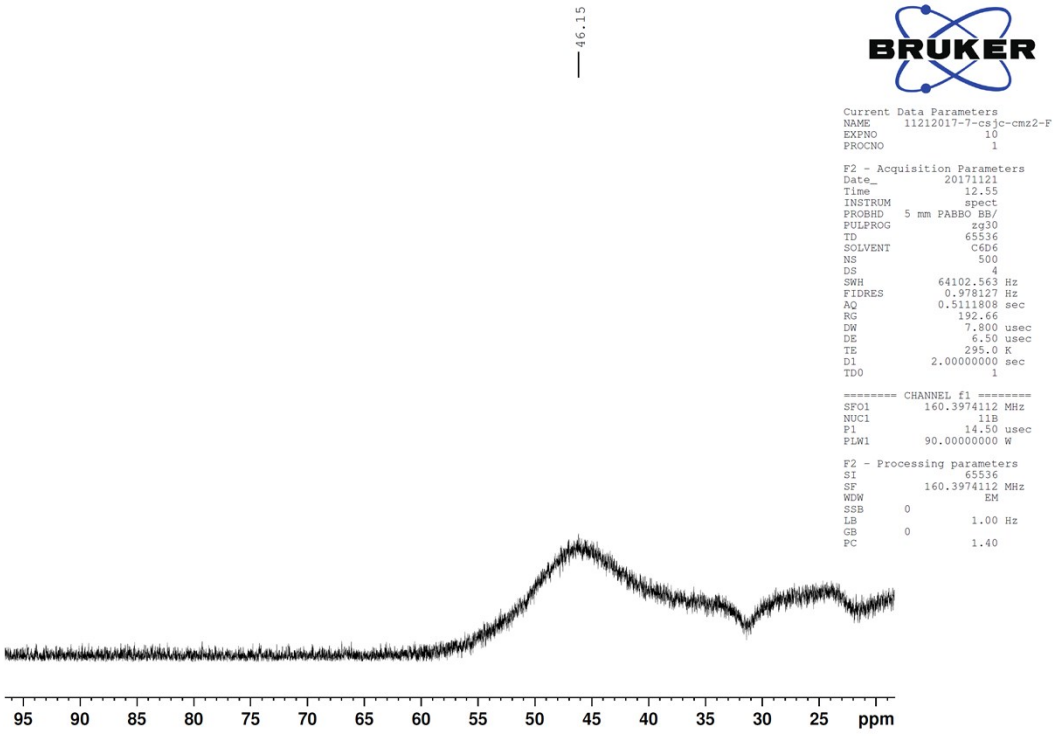
======== CHANNEL f1 ========
SFO1 160.3974112 MHz
NUC1 11B
P1 14.50 usec
PLW1 90.00000000 W

F2 - Processing parameters
SI 65536
SF 160.3974112 MHz
WDW EM
SSB 0
LB 1.00 Hz
GB 0
PC 1.40

[Au(IPr*)(Bpin)]

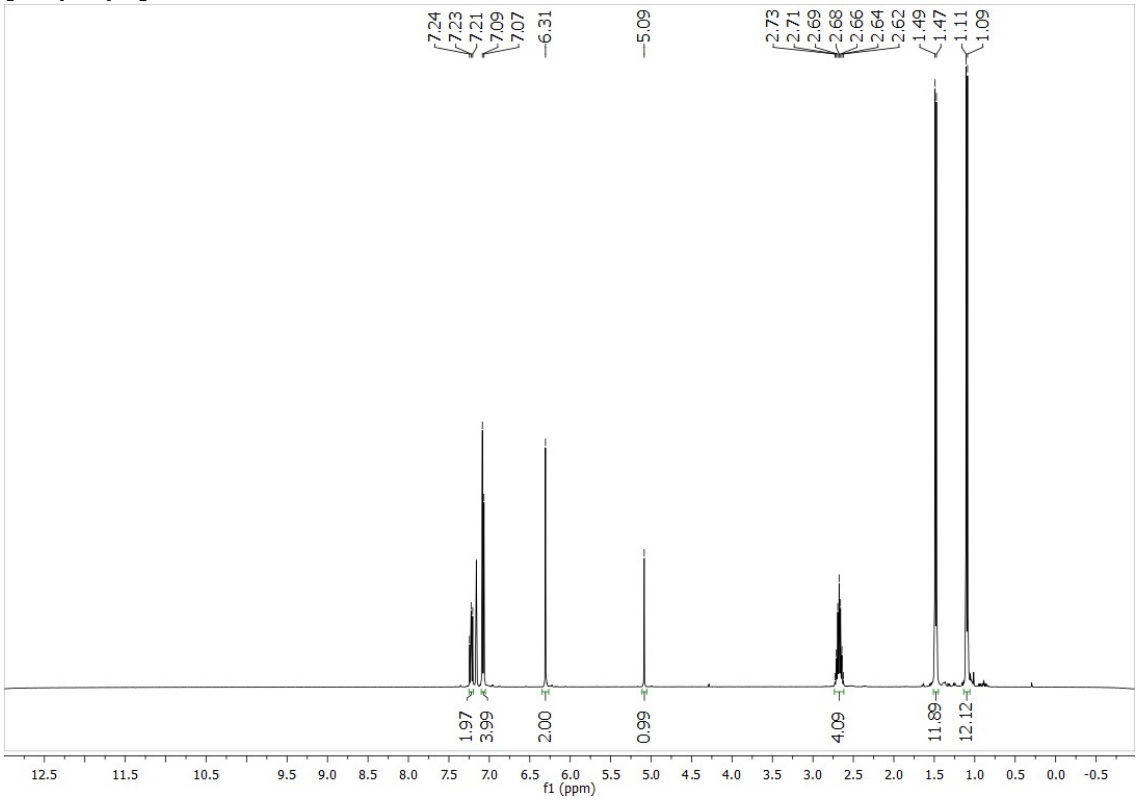

7.82
7.80
7.41
7.39
7.38
6.99
5.84
5.58
1.54
1.15
7.66
8.58
28.39
3.94
2.47
5.78
12.00
f1 (ppm)

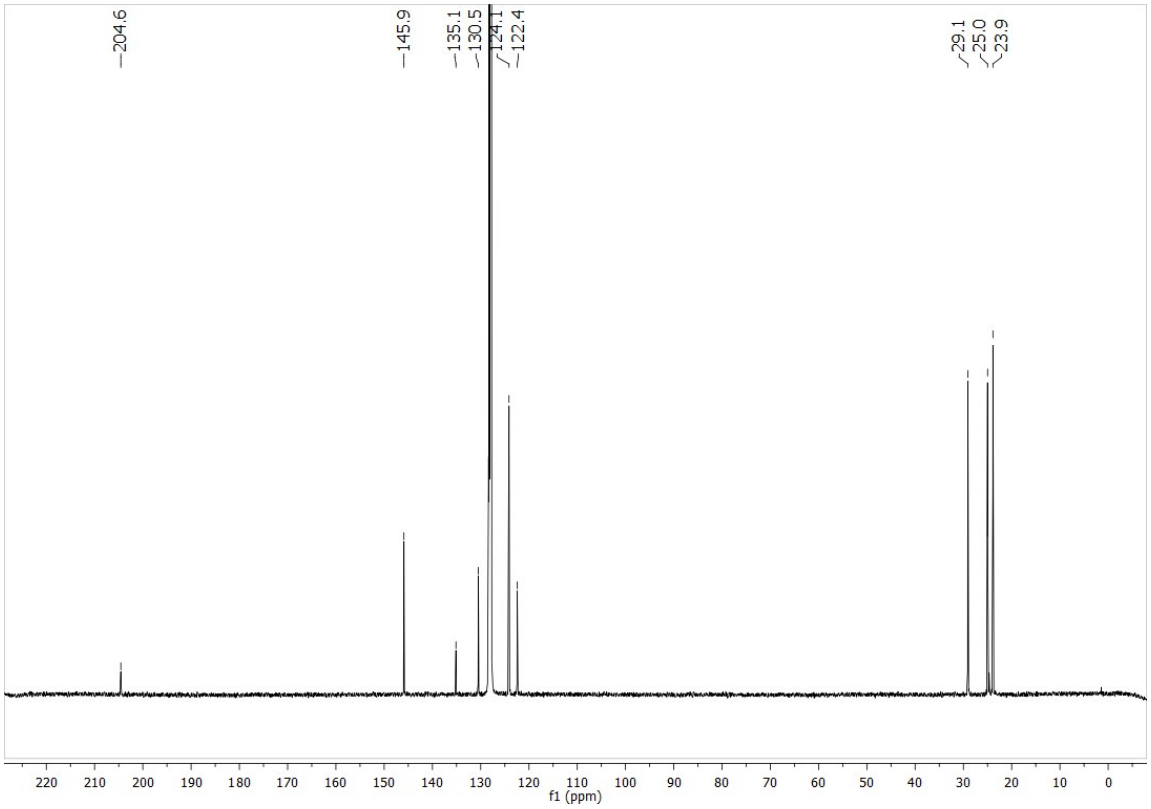

215.0
143.9
143.2
141.3
140.1
134.6
130.7
130.3
129.7
128.7
127.6
126.6
126.4
123.2
110.1
79.9
51.3
25.9
20.9
f1 (ppm)



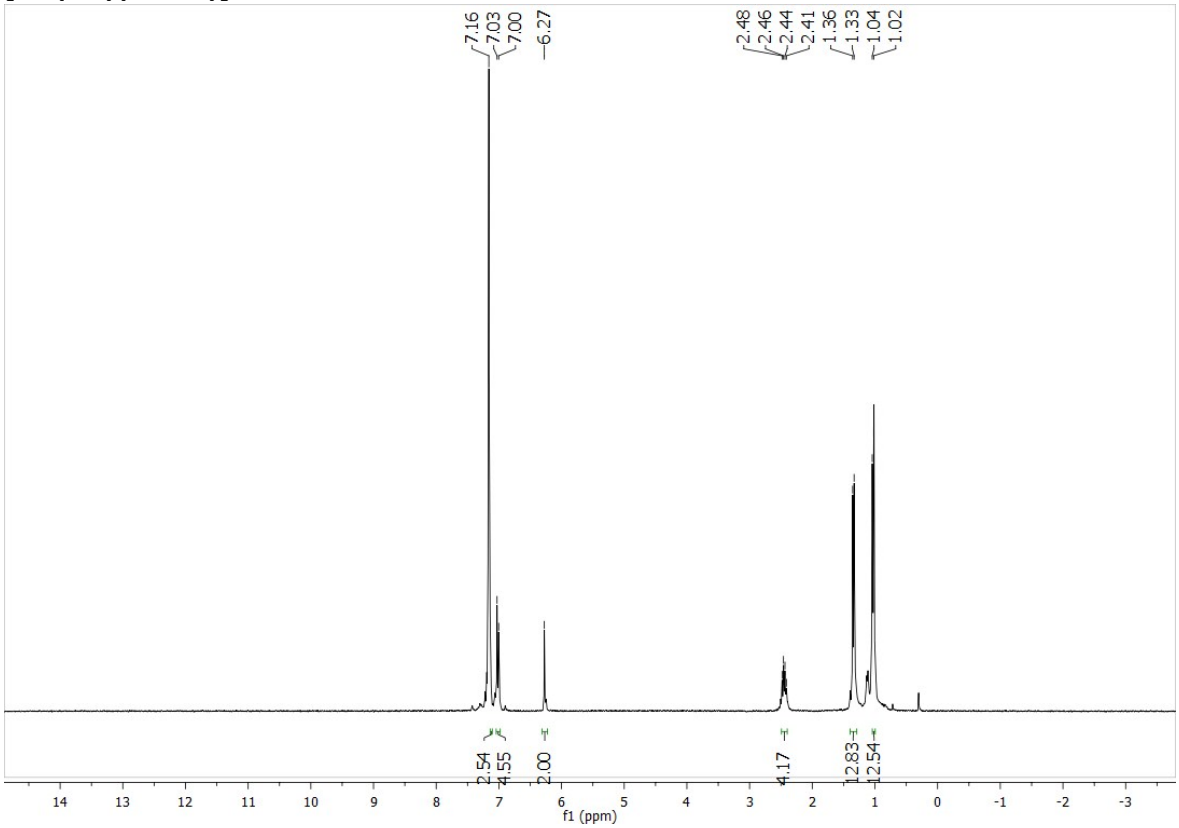

```
Current Data Parameters
NAME      11212017-7-csjc-cmz2-F
EXPNO                 10
PROCNO                 1

F2 - Acquisition Parameters
Date_           20171121
Time              12.55
INSTRUM           spect
PROBHD   5 mm PABBO BB/
PULPROG           zg30
TD               65536
SOLVENT           C6D6
NS                  500
DS                    4
SWH           64102.563 Hz
FIDRES         0.978127 Hz
AQ            0.5111808 sec
RG               192.66
DW                7.800 usec
DE                6.50 usec
TE                295.0 K
D1           2.00000000 sec
TD0                   1

======== CHANNEL f1 ========
SFO1         160.3974112 MHz
NUC1               11B
P1                14.50 usec
PLW1         90.00000000 W

F2 - Processing parameters
SI                65536
SF           160.3974112 MHz
WDW                 EM
SSB       0
LB                1.00 Hz
GB        0
PC                1.40
```

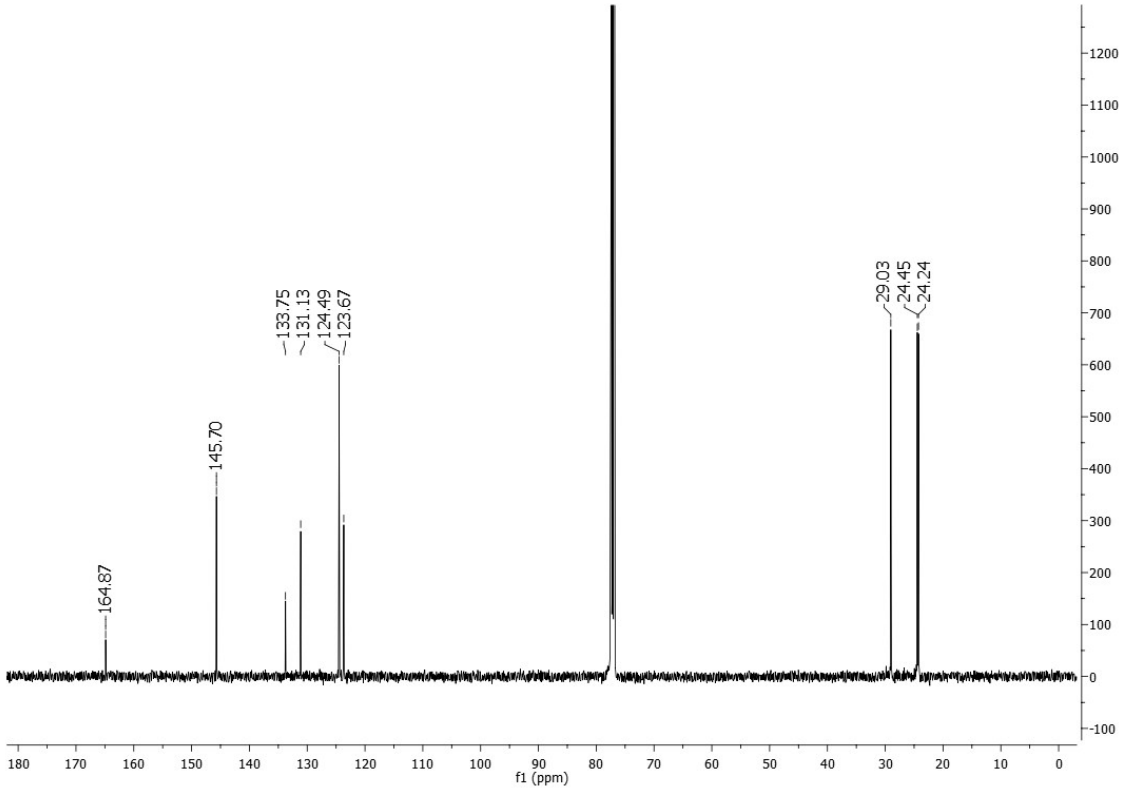
[Au(IPr)H]


7.24
7.23
7.21
7.09
7.07
6.31
5.09
2.73
2.71
2.69
2.68
2.66
2.64
2.62
1.49
1.47
1.11
1.09
1.97
3.99
2.00
0.99
4.09
11.89
12.12
f1 (ppm)

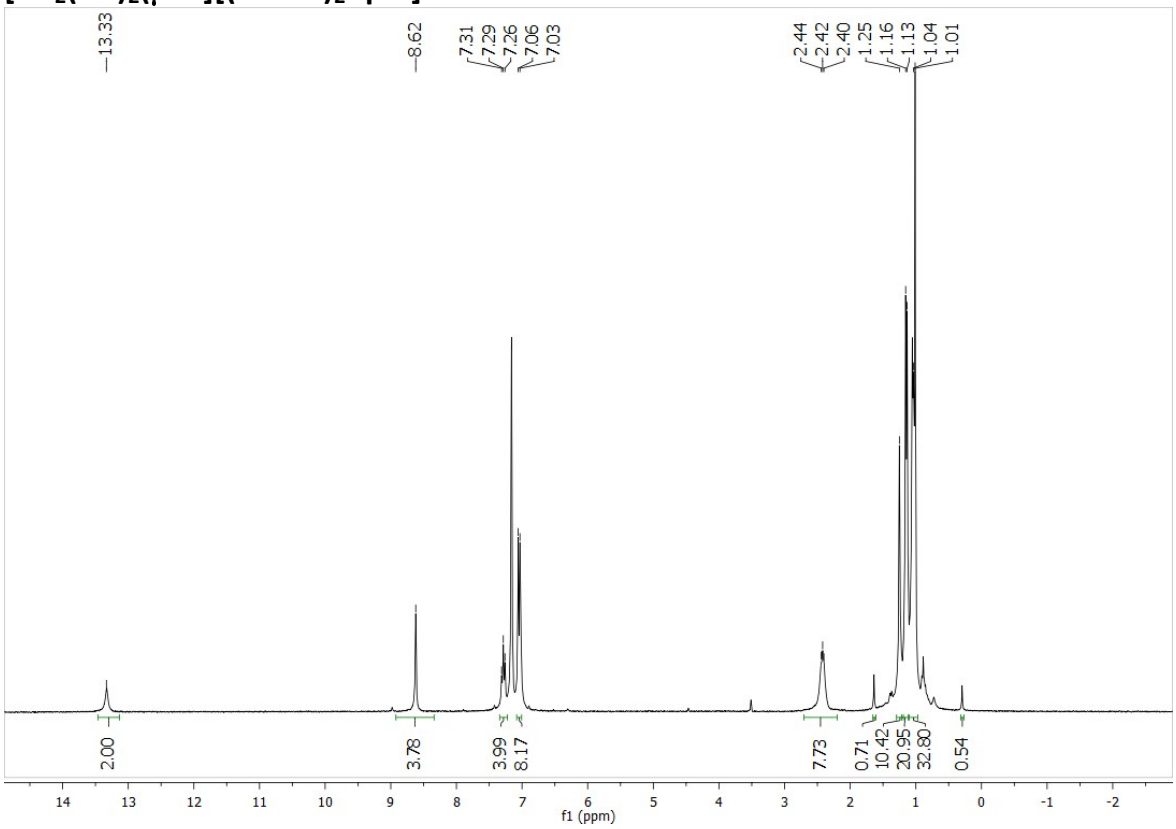

204.6
145.9
135.1
130.5
124.1
122.4
29.1
25.0
23.9
f1 (ppm)

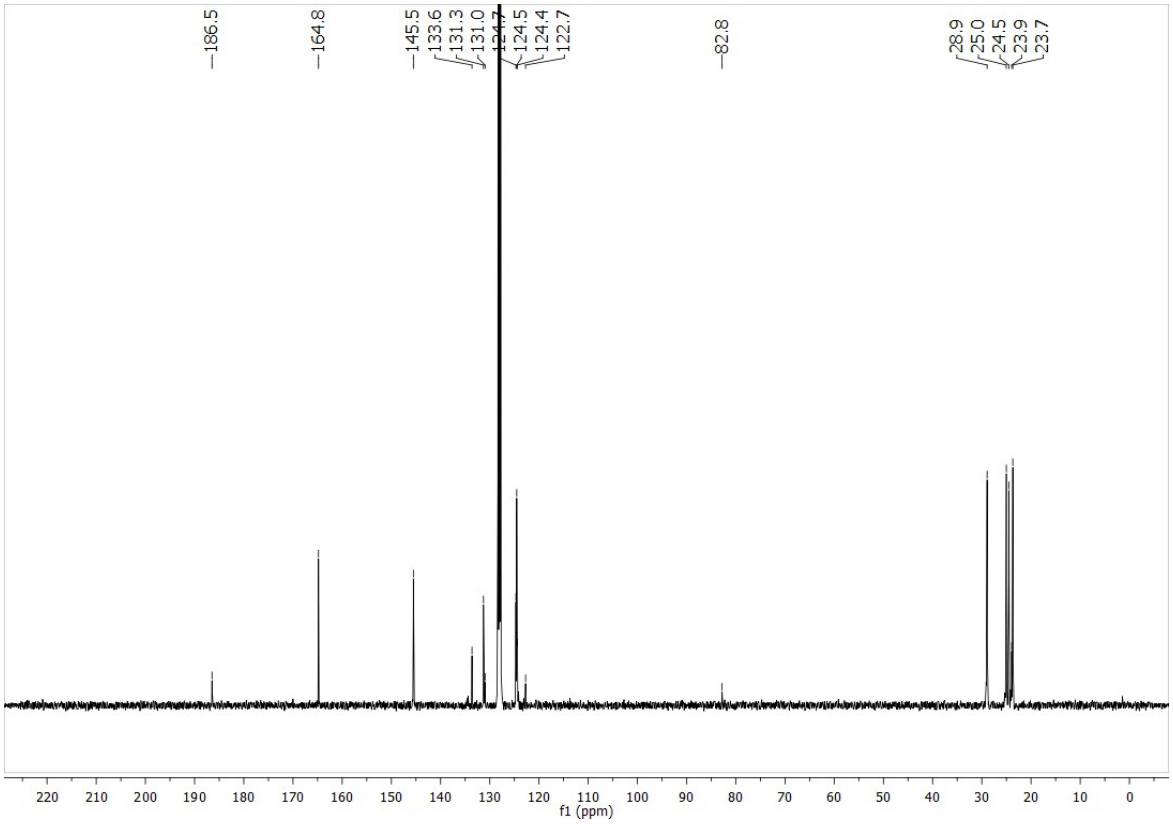
[Au(IPr)(ONO$_2$)]

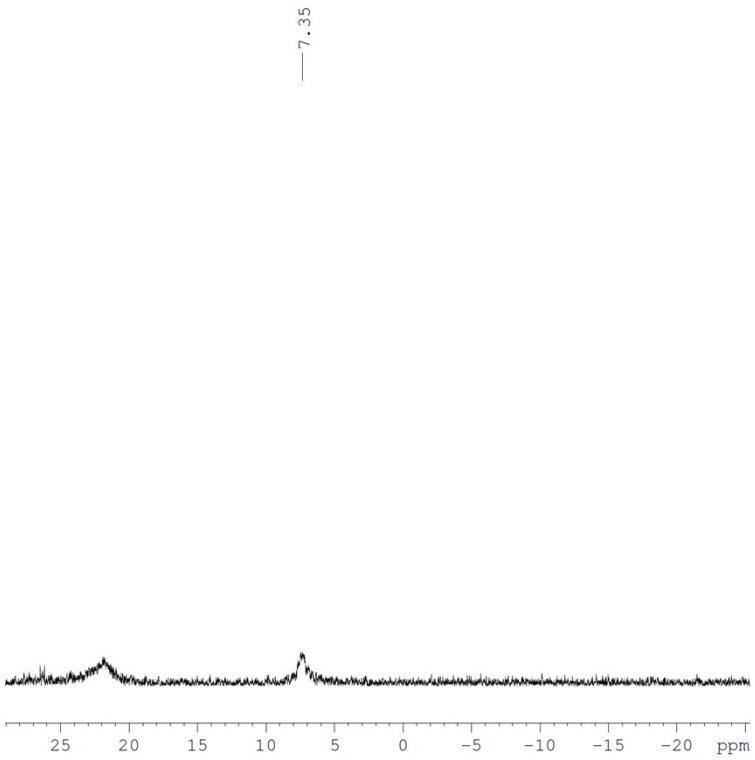

7.16
7.03
7.00
6.27
2.48
2.46
2.44
2.41
1.36
1.33
1.04
1.02
2.54
4.55
2.00
4.17
12.83
12.54
f1 (ppm)


164.87
145.70
133.75
131.13
124.49
123.67
29.03
24.45
24.24
f1 (ppm)

$[Au_2(IPr)_2(\mu\text{-}H][(HOCO)_2Bpin]$

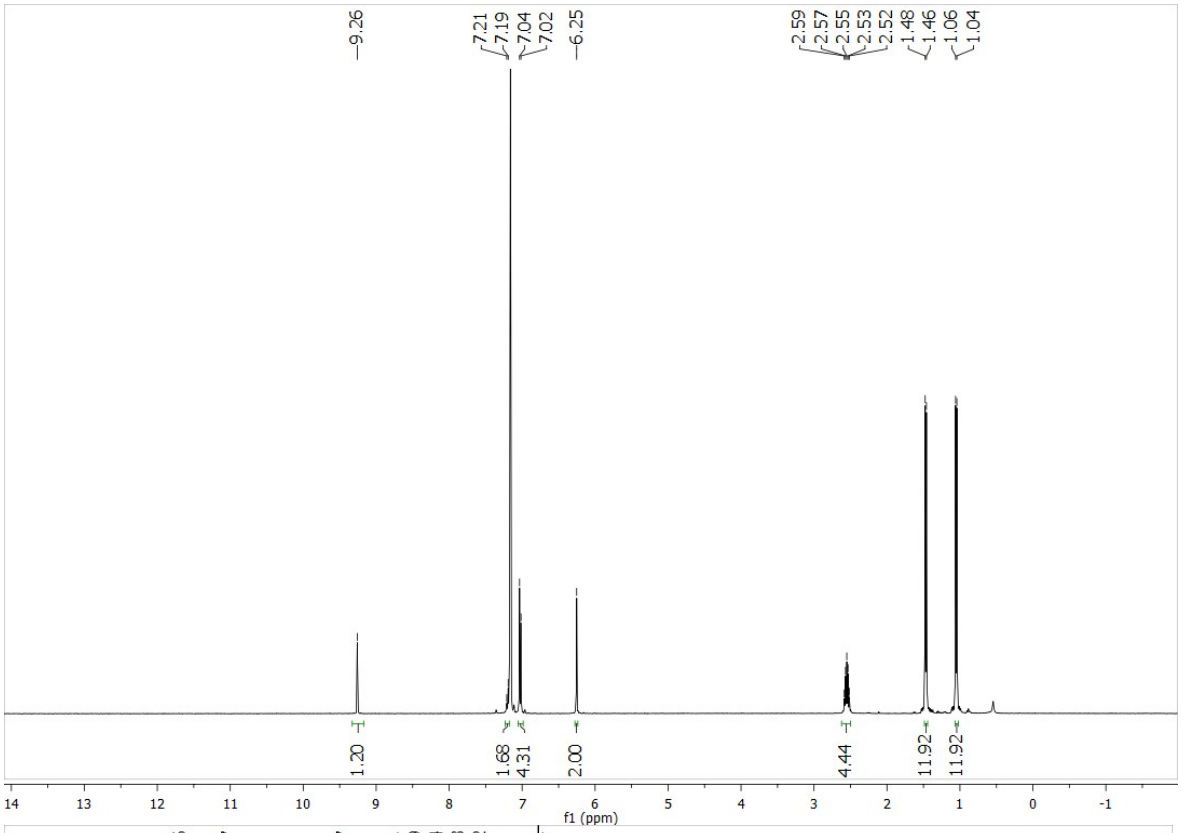


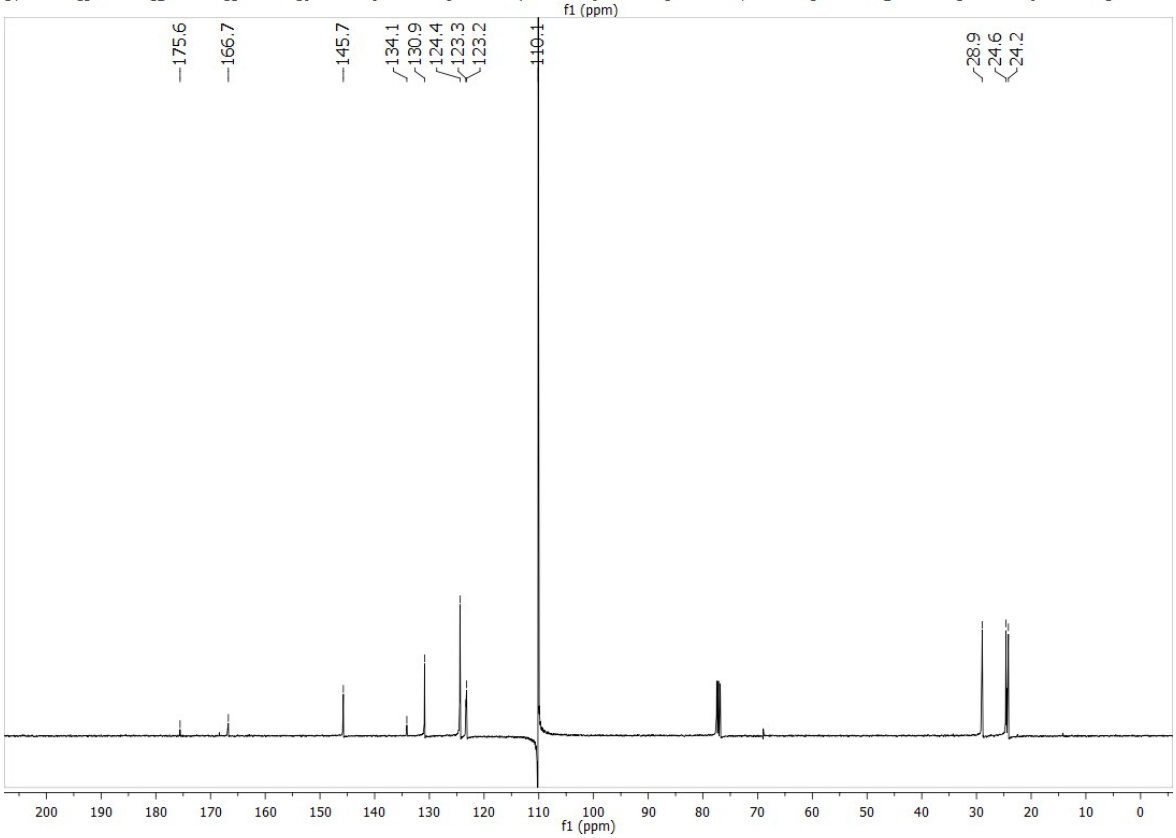




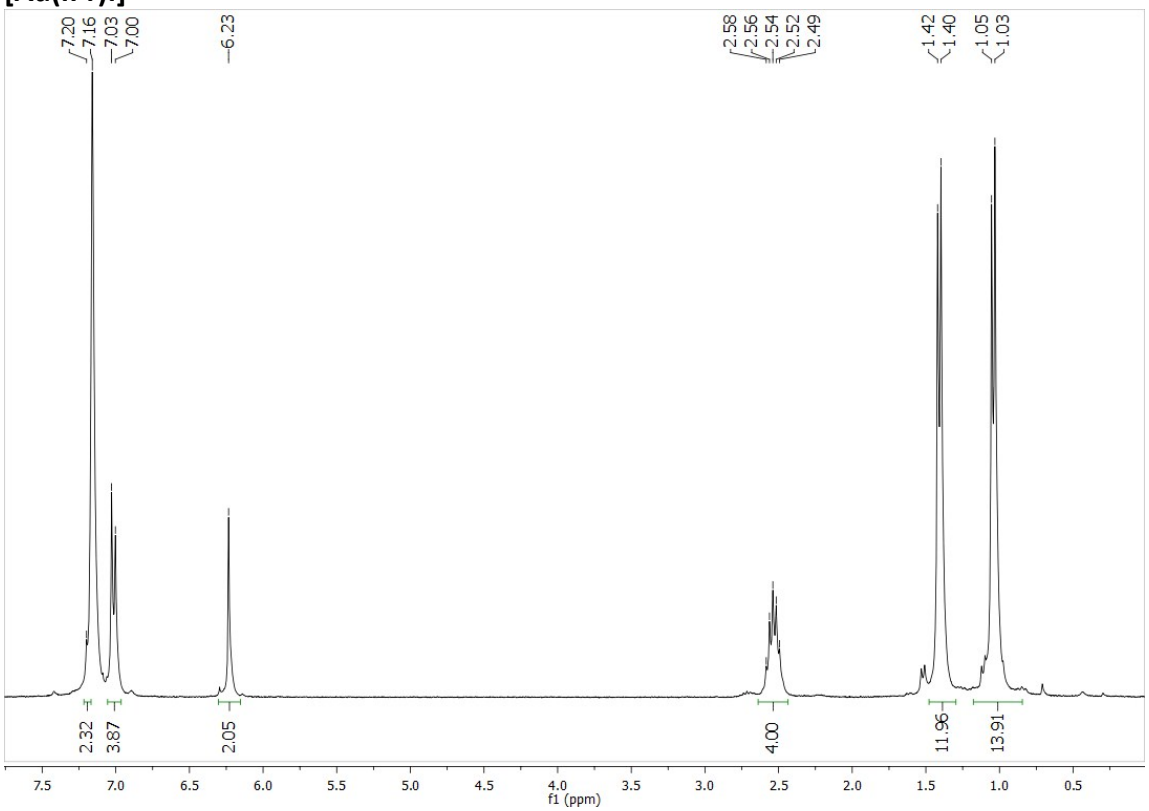

```
Current Data Parameters
NAME                  Au-9
EXPNO                 1001
PROCNO                   1

F2 - Acquisition Parameters
Date_              20160414
Time                 16.03
INSTRUM              av300
PROBHD    5 mm PABBO BB-
PULPROG               zg30
TD                   32650
SOLVENT               C6D6
NS                      64
DS                       2
SWH              24154.590 Hz
FIDRES               0.739804 Hz
AQ                0.6758550 sec
RG                    812.7
DW                   20.700 usec
DE                    6.50 usec
TE                   294.3 K
D1              1.50000000 sec
TD0                      1

======== CHANNEL f1 ========
NUC1                    11B
P1                   11.00 usec
PL1                   6.00 dB
SFO1            96.2687652 MHz

F2 - Processing parameters
SI                    32768
SF              96.2711786 MHz
WDW                     EM
SSB       0
LB                    1.00 Hz
GB        0
PC                    1.40
```

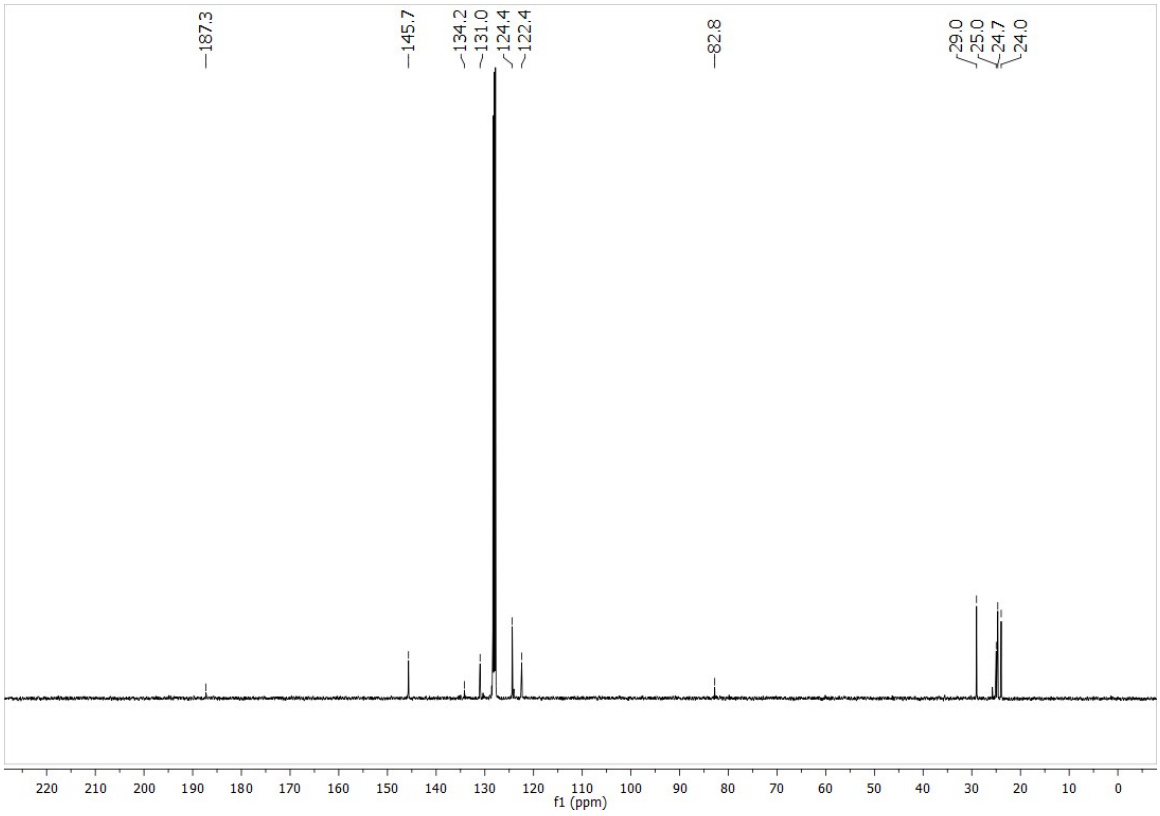
[Au(IPr)(OCOH)]


9.26
7.21
7.19
7.04
7.02
6.25
2.59
2.57
2.55
2.53
2.52
1.48
1.46
1.06
1.04
1.20
1.68
4.31
2.00
4.44
11.92
11.92
f1 (ppm)

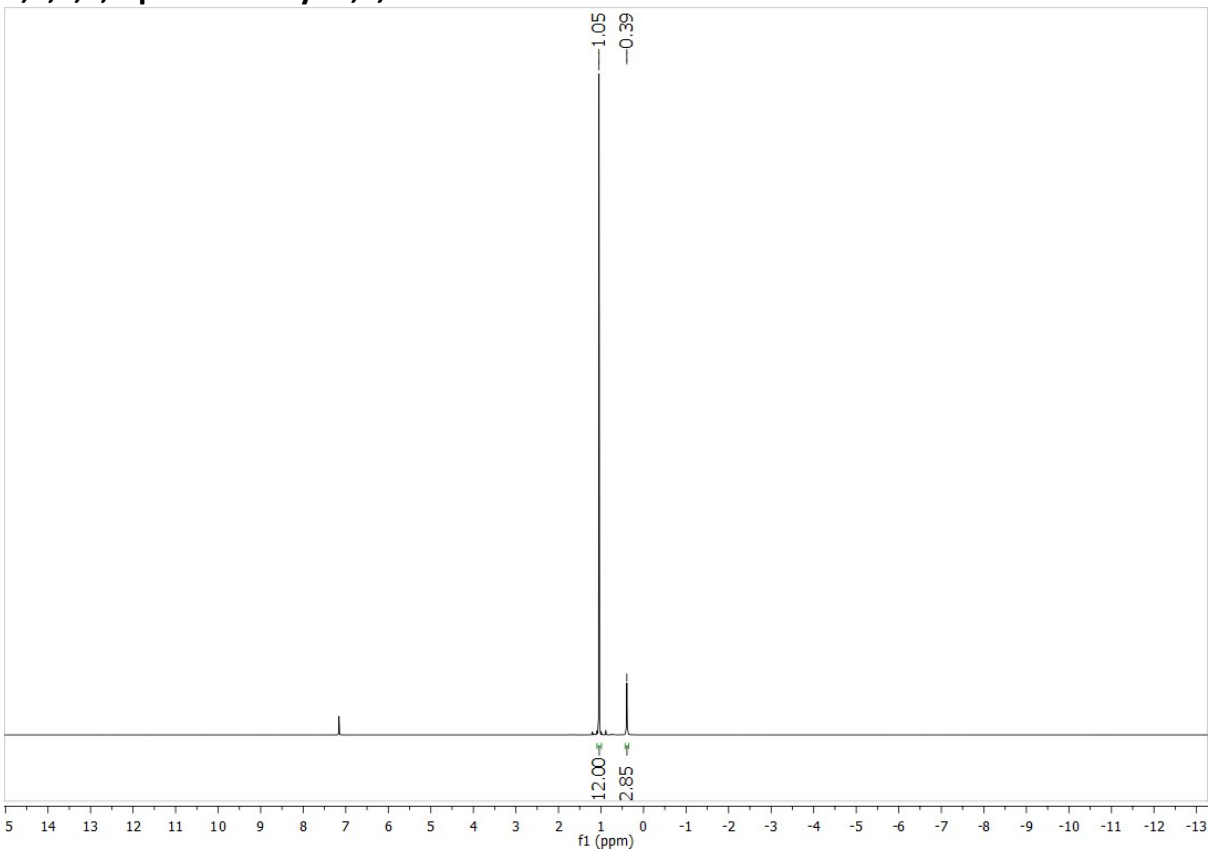

175.6
166.7
145.7
134.1
130.9
124.4
123.3
123.2
110.1
28.9
24.6
24.2
f1 (ppm)

[Au(IPr)I]

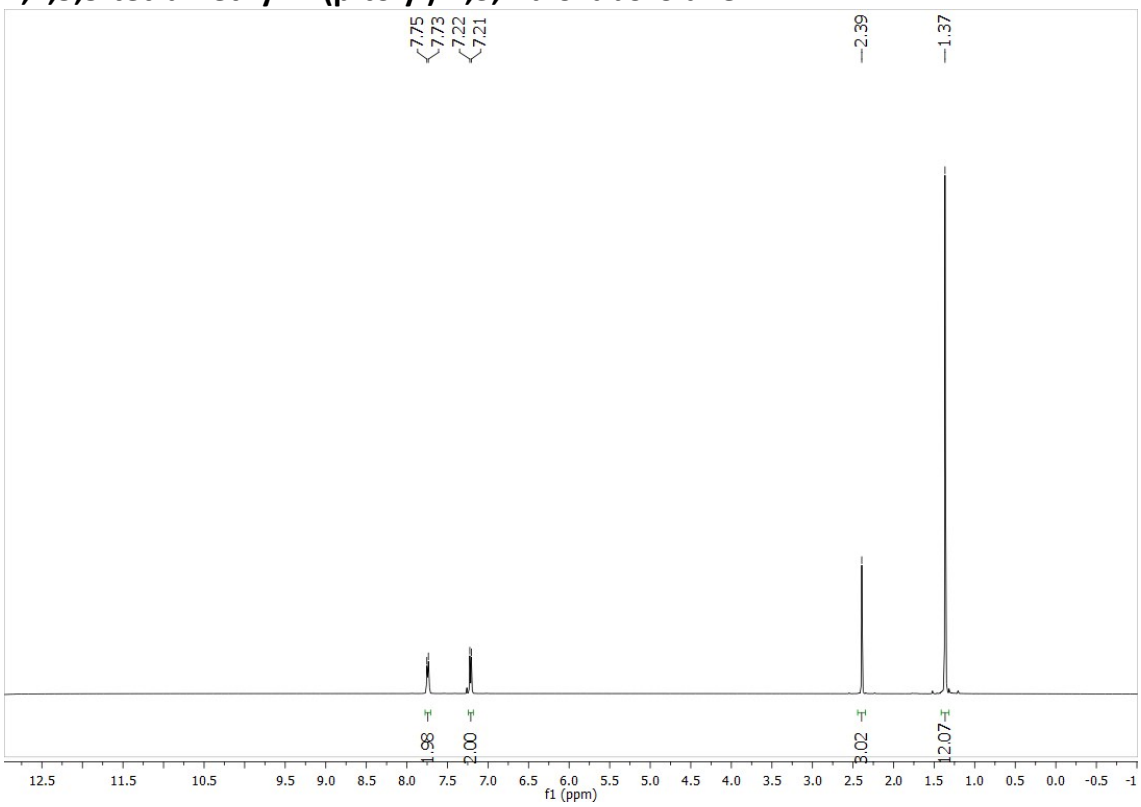

7.20
7.16
7.03
7.00
6.23
2.58
2.56
2.54
2.52
2.49
1.42
1.40
1.05
1.03
2.32
3.87
2.05
4.00
11.96
13.91
f1 (ppm)

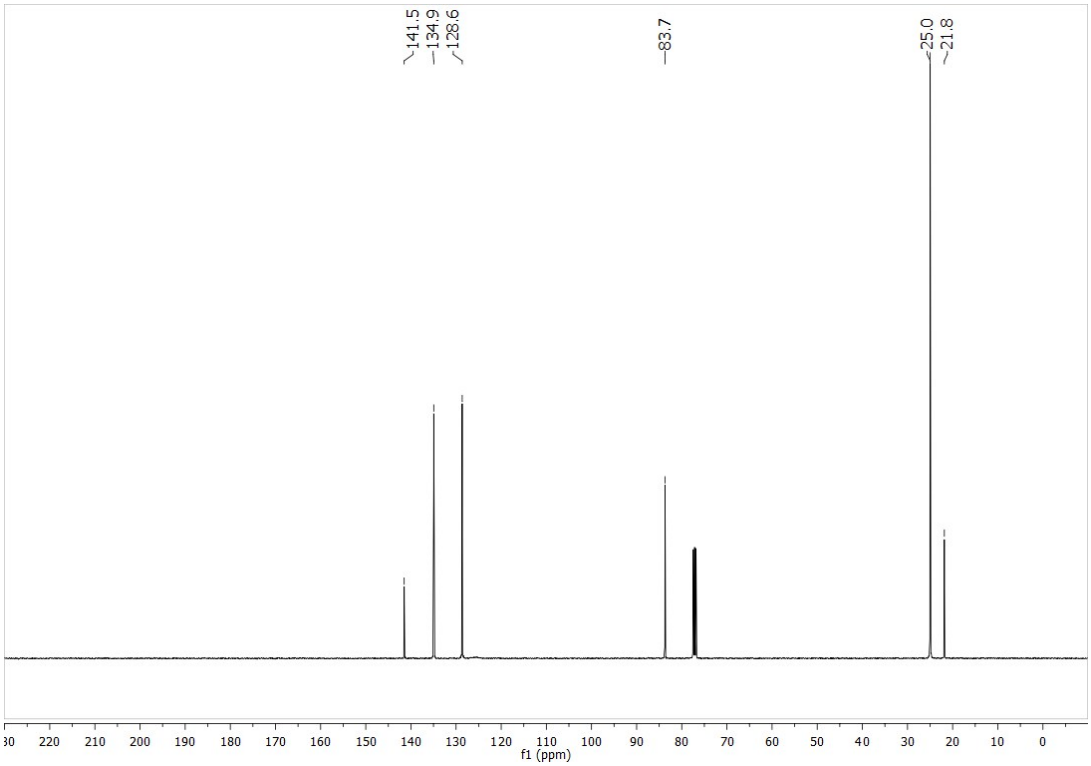

187.3
145.7
134.2
131.0
124.4
122.4
82.8
29.0
25.0
24.7
24.0
f1 (ppm)

2,4,4,5,5-pentamethyl-1,3,2-dioxaborolane



4,4,5,5-tetramethyl-2-(p-tolyl)-1,3,2-dioxaborolane





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