

Supporting Information

**Direct Observation of Aryl Gold(I) Carbenes that Undergo
Cyclopropanation, C–H Insertion, and Dimerization Reactions**

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1. General Methods

Unless otherwise stated, the reactions were carried out under argon using standard Schlenk techniques and solvents dried by passing through an activated alumina column on a PureSolv™ solvent purification system. Deuterated solvents were dried over activated MS 3Å for at least three days and deoxygenated by bubbling argon for 30 minutes before storing them in the glovebox. All the glassware used was dried in the oven at 100 °C for at least 12 hours before use. Thin layer chromatography was carried out using TLC aluminium sheets coated with 0.2 mm of silica gel (Merck GF₂₃₄) using UV light as the visualizing agent and a solution of vanillin as stain. Reactions were followed using NMR techniques, GCMS apparatus or TLC. Chromatographic purifications were carried out using flash grade silica gel (SDS Chromatogel 60 ACC, 40-60 µm) or automated flash chromatographer CombiFlash Companion. Preparative TLC was performed on 20 cm × 20 cm silica gel plates (2.0 mm or 1.0 mm thick, Analtech).

NMR data were recorded in deuterated solvents on a Bruker Advance 400 Ultra Shield (400 MHz for ¹H, 100 MHz for ¹³C, 162 MHz for ³¹P and 376 MHz for ¹⁹F), Bruker 500 Ultrashield (500 MHz for ¹H, 125 MHz for ¹³C and 202 MHz for ³¹P) apparatus and Bruker 300 Ultrashield (300 MHz for ¹H and 75 MHz for ¹³C). Chemical shifts (δ) are reported in parts per million (ppm) and referenced to residual solvent or tetramethylsilane. Coupling constants (*J*) are reported in Hertz (Hz). Mass Spectra were recorded on a Waters LCT Premier Spectrometer (ESI) and Bruker Daltonics Autoflex (MALDI) spectrometers. Elemental analyses were performed on a LECO CHNS 932 micro-analyzer at the Universidad Complutense de Madrid. Melting points were determined using a Büchi melting point apparatus. Single crystal X-ray diffraction data were recorded on a Bruker Kappa APEX II DUO diffractometer equipped with an APPEX 2 4K CCD area detector, a Microsource with Mo_{Kα} radiation and an Oxford Cryostream 700 low temperature device (T = -173°C).

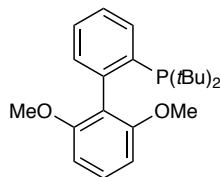
2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl,¹ 2'-bromo-2',6',4',6'-dimethoxybiphenyl,² 2'-bromo-2',4',6'-trimethoxybiphenyl,² and benzenesulfonic acid, 4-methyl-, 2-[(2',4',6'-trimethylphenyl)methylene]hydrazide³ were prepared following previously reported procedures. JohnPhosAuCl were purchased from commercial sources and used without further purification.

2. Ligand Synthesis

General procedure for the synthesis of ligands:

An oven-dried three-neck round-bottom flask equipped with a condenser was charged with magnesium turnings, the corresponding 2'-bromo-1,1'-biphenyl and dry THF under argon. Magnesium was activated by the addition of 1,2-dibromoethane (50 μ L) via syringe. The mixture was stirred at 70 $^{\circ}$ C for 2 h and then allowed to cool down to room temperature. It was filtered through a canula filter to a new oven-dried three-neck round-bottom flask charged with argon. Anhydrous CuCl was added in a single portion, followed by the slow addition of di-*tert*-butylchlorophosphine via syringe over a period of 30 minutes. The reaction mixture was stirred at 70 $^{\circ}$ C for 24 h. The mixture was allowed to cool down to room temperature and then washed with 30% aqueous NH₄OH and extracted with ethyl acetate. Brine was added as needed to help in the phase separation. This process was repeated at least six times until the aqueous phase was not blue colored. The organic phase was dried over Na₂SO₄, filtered and concentrated *in vacuo*. The crude was purified by flash column chromatography on silica gel under nitrogen.

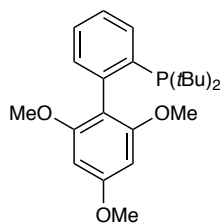
2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl (L1)



Ligand **L1** was synthesized according to the general procedure from 2'-bromo-2',6'-dimethoxy-1,1'-biphenyl (550 mg, 1.88 mmol), magnesium turnings (137 mg, 5.63 mmol), anhydrous CuCl (186 mg, 1.88 mmol) and di-*tert*-butylchlorophosphane (0.463 mL, 2.44 mmol). The crude was purified by silica gel flash column chromatography using a 95:5 to 9:1 mixture of cyclohexane:ethyl acetate as eluent to give the title ligand as a crystalline solid (300 mg, 0.84 mmol, 45% yield). The compound was stored in the glovebox.

mp 132.6 $^{\circ}$ C **¹H NMR** (400 MHz, CDCl₃) δ 7.84 (dt, $J = 7.6$ Hz, $J = 1.5$ Hz, 1H), 7.41 – 7.36 (m, 1H), 7.34 – 7.28 (m, 2H), 7.17 (ddd, $J = 7.6$ Hz, $J = 3.7$ Hz, $J = 1.5$ Hz, 1H), 6.58 (d, $J = 8.4$ Hz, 2H), 3.66 (s, 6H), 1.14 (d, $J(^1\text{H}-^{31}\text{P}) = 11.5$ Hz, 18H). **¹³C NMR** (126 MHz, CDCl₃) δ 157.45 (d, $J(^{13}\text{C}-^{31}\text{P}) = 1.1$ Hz), 143.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 35.1$ Hz), 137.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 25.8$ Hz), 135.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.4$ Hz), 131.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.8$ Hz), 128.7, 128.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 1.2$ Hz), 125.7, 120.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.2$ Hz), 103.3, 55.2, 32.2 (d, $J(^{13}\text{C}-^{31}\text{P}) = 24.5$ Hz). **³¹P NMR** (162 MHz, CDCl₃) δ 27.31. **HRMS** (APCI+) calculated for C₂₂H₃₂O₂P (M+H)⁺: 359.2134; found: 359.2120. **Elemental Analysis** calculated for C₂₂H₃₁O₂P: C, 73.72; H, 8.72; found: C, 73.64; H, 8.48.

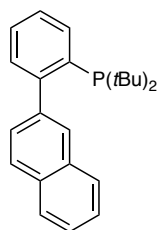
2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl (L2)



Ligand **L2** was synthesized according to the general procedure from 2'-bromo-2',4',6'-dimethoxy-1,1'-biphenyl (6.37 g, 19.7 mmol), magnesium turnings (1.44 g, 59.1 mmol), anhydrous CuCl (1.95 mg, 19.71 mmol) and di-*tert*-butylchlorophosphane (4.87 mL, 25.6 mmol). The crude was purified by silica gel column chromatography using a 95:5 to 9:1 mixture of cyclohexane: ethyl acetate as eluent to give the title ligand as a crystalline solid (5.03 mg, 12.95 mmol, 65.7 % yield). The compound was stored in the glovebox.

mp 115.4 °C **¹H NMR** (500 MHz, CDCl₃) δ 7.82 (dt, *J* = 7.6, 1.5 Hz, 1H), 7.40 – 7.34 (m, 1H), 7.29 (td, *J* = 7.6, 1.5 Hz, 1H), 7.15 (ddd, *J* = 7.6, 3.8, 1.5 Hz, 1H), 6.16 (s, 2H), 3.87 (s, 3H), 3.64 (s, 6H), 1.14 (d, *J* (¹H-³¹P) = 11.5 Hz, 18H). **¹³C NMR** (101 MHz, CDCl₃) δ 160.7, 158.0 (d, *J* (¹³C-³¹P) = 0.8 Hz), 143.6 (d, *J* (¹³C-³¹P) = 34.7 Hz), 138.2 (d, *J* (¹³C-³¹P) = 25.0 Hz), 135.4 (d, *J* (¹³C-³¹P) = 3.4 Hz), 132.2 (d, *J* (¹³C-³¹P) = 6.7 Hz), 128.4 (d, *J* (¹³C-³¹P) = 1.4 Hz), 125.6, 113.7 (d, *J* (¹³C-³¹P) = 7.5 Hz), 90.0, 55.3, 55.2, 32.2 (d, *J* (¹³C-³¹P) = 24.3 Hz), 30.8 (d, *J* (¹³C-³¹P) = 15.6 Hz). **³¹P NMR** (202 MHz, CDCl₃) δ 27.35. **HRMS** (ESI+) calculated for C₂₃H₃₄O₃P (M+H)⁺: 389.2240; found: 389.2245.

2-Di-*t*-butylphosphino-2-naphthyl (**L3**)



Ligand **L3** was synthesized according to the general procedure from 2-(2-bromophenyl)naphthalene (6.37 g, 19.7 mmol), magnesium turnings (0.463 g, 6.36 mmol), anhydrous CuCl (0.629 mg, 6.36 mmol) and di-*tert*-butylchlorophosphane (1.57 mL, 19.07 mmol). The crude was purified by silica gel column chromatography using a 95:5 to 9:1 mixture of cyclohexane: ethyl acetate as eluent to give the title ligand as a crystalline solid (1.13 g, 3.24 mmol, 51 % yield). The compound was stored in the glovebox.

mp 90.4 °C **¹H NMR** (400 MHz, CDCl₃) δ 7.97 – 7.92 (m, 1H), 7.89 – 7.84 (m, 1H), 7.83 – 7.78 (m, 2H), 7.68 – 7.64 (m, 1H), 7.50 – 7.44 (m, 3H), 7.44 – 7.36 (m, 1H), 7.36 – 7.30 (m, 1H), 1.15 (d, *J* (¹H-³¹P) = 11.6 Hz, 18H). **¹³C NMR** (101 MHz, CDCl₃) δ 151.2 (d, *J* (¹³C-³¹P) = 32.3 Hz), 141.7 (d, *J* (¹³C-³¹P) = 7.2 Hz), 135.8 (d, *J* (¹³C-³¹P) = 27.9 Hz), 135.4 (d, *J* (¹³C-³¹P) = 3.2 Hz), 133.0 (d, *J* (¹³C-³¹P) = 1.7 Hz), 132.2, 130.9 (d, *J* (¹³C-³¹P) = 6.4 Hz), 129.7 (d, *J* (¹³C-³¹P) = 4.9 Hz), 128.83 (d, *J* (¹³C-³¹P) = 2.2 Hz), 128.5, 128.0, 127.8, 126.2, 126.0, 125.8 (d, *J*

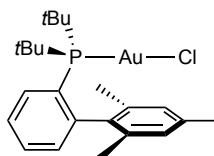
(^{13}C - ^{31}P) = 1.6 Hz), 125.5 (d, J (^{13}C - ^{31}P) = 1.7 Hz), 32.9 (d, J (^{13}C - ^{31}P) = 25.4 Hz), 30.8 (dd, J (^{13}C - ^{31}P) = 15.3, 1.8 Hz). ^{31}P NMR (162 MHz, CDCl_3) δ 21.32. HRMS (ESI+) calculated for $\text{C}_{24}\text{H}_{30}\text{P}$ (M+H) $^+$: 349.2080; found: 349.2085.

3. Synthesis of Gold(I) Chloride Complexes

General procedure for the synthesis of gold(I) chloride complexes:

In a Schlenk, (Me₂S)AuCl was added to a solution of the corresponding phosphine in dry CH₂Cl₂ under argon at 25 °C. The solution was stirred for 1 h, filtered through a pad of cotton/Celite/cotton and concentrated under vacuum. The crude was purified by flash column chromatography on silica gel.

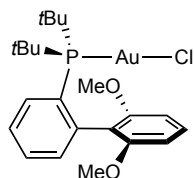
2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl gold(I) chloride (**6b**)



Gold(I) chloride complex **6b** was synthesized according to the general procedure from 2-di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl (90 mg, 0.264 mmol) and (Me₂S)AuCl (78 mg, 0.264 mmol). A white crystalline solid was obtained in 65% yield (98 mg, 0.172 mmol) after purification by flash column chromatography using a mixture of cyclohexane:ethyl acetate (8:2) as eluent.

¹H NMR (500 MHz, CDCl₃) δ 7.89 (td, J = 8.0, 1.5 Hz, 1H), 7.58 (tt, J = 7.5, 1.5 Hz, 1H), 7.49 (ddt, J = 8.0, 7.5, 1.5 Hz, 1H), 7.25 (ddd, J = 7.5, 4.5, 1.5 Hz, 1H), 7.02 (s, 2H), 2.47 (s, 3H), 1.95 (s, 6H), 1.44 (d, J (¹H-³¹P) = 15.5 Hz, 18H). **¹³C NMR** (126 MHz, CDCl₃) δ 149.4 (d, J (¹³C-³¹P) = 13.6 Hz), 138.9, 137.5 (d, J (¹³C-³¹P) = 5.9 Hz), 135.4, 134.5 (d, J (¹³C-³¹P) = 3.0 Hz), 133.9 (d, J (¹³C-³¹P) = 7.8 Hz), 131.5 (d, J (¹³C-³¹P) = 2.4 Hz), 129.4, 127.8 (d, J (¹³C-³¹P) = 43.6 Hz), 126.5 (d, J (¹³C-³¹P) = 6.9 Hz), 38.3 (d, J (¹³C-³¹P) = 26.4 Hz), 31.5 (d, J (¹³C-³¹P) = 6.5 Hz), 21.7, 21.5. **³¹P NMR** (202 MHz, CDCl₃) δ . 62.38. **HRMS** (ESI+) calculated for C₂₃H₃₃AuClP (M + Na)⁺: 595.1566; found: 595.1576. **Elemental Analysis** calculated for C₂₃H₃₃AuClP: C, 48.22; H, 5.81; found: C, 48.13; H, 5.56.

2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl gold(I) chloride (**6c**)

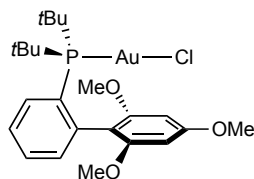


Gold(I) chloride complex **6c** was synthesized according to the general procedure from 2-di-*t*-butylphosphino-2',6'-dimethoxybiphenyl (100 mg, 0.279 mmol) and (Me₂S)AuCl (82 mg, 0.279 mmol). A white crystalline solid was obtained in 43% yield (70 mg, 0.120 mmol) after purification by flash column chromatography using a mixture of cyclohexane:ethyl acetate (8:2) as eluent.

¹H NMR (500 MHz, CDCl₃) δ 7.88 – 7.83 (m, 1H), 7.57 – 7.50 (m, 2H), 7.46 – 7.41 (m, 1H), 7.21 (ddd, J = 7.7, 4.3, 1.4 Hz, 1H), 6.64 (d, J = 8.4 Hz, 2H), 3.65 (s, 6H), 1.40 (d, J (¹H-³¹P) =

15.5 Hz, 18H). ^{13}C NMR (126 MHz, CDCl_3) δ 157.3, 143.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 13.3$ Hz), 134.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.8$ Hz), 133.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.0$ Hz), 131.2 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.4$ Hz), 130.3, 128.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 47.5$ Hz), 126.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.0$ Hz), 119.2 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.7$ Hz), 104.4, 55.3, 37.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 26.0$ Hz), 31.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.9$ Hz). ^{31}P NMR (202 MHz, CDCl_3) δ 64.26. HRMS (ESI+) calculated for $\text{C}_{22}\text{H}_{31}\text{AuClO}_2\text{P}$ ($\text{M} + \text{Na}$) $^+$: 613.1308; found: 613.1323. Elemental Analysis calculated for $\text{C}_{22}\text{H}_{31}\text{AuClO}_2\text{P}$: C, 44.72; H, 5.29; found: C, 45.47; H, 5.18.

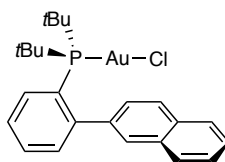
2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl gold(I) chloride (6d)



Gold chloride complex **6d** was synthesized according to the general procedure from 2-di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl (250 mg, 0.644 mmol) and $(\text{Me}_2\text{S})\text{AuCl}$ (190 mg, 0.644 mmol). A white crystalline solid was obtained in 92% yield (367 mg, 0.592 mmol) after purification by flash column chromatography using a mixture of cyclohexane:ethyl acetate (8:2) as eluent.

mp 251.4 °C ^1H NMR (500 MHz, CDCl_3) δ 7.86 (td, $J = 8.0, 1.5$ Hz, 1H), 7.55 (tt, $J = 7.6, 1.5$ Hz, 1H), 7.44 (ddt, $J = 8.0, 7.6, 1.5$ Hz, 1H), 7.24 (ddd, $J = 7.6, 4.3, 1.5$ Hz, 1H), 6.26 (s, 2H), 3.97 (s, 3H), 3.66 (s, 7H), 1.41 (d, $J(^1\text{H}-^{31}\text{P}) = 15.4$ Hz, 18H). ^{13}C NMR (126 MHz, CDCl_3) δ 162.9, 157.7, 143.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 13.3$ Hz), 134.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.6$ Hz), 133.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.2$ Hz), 131.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.3$ Hz), 128.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 48.3$ Hz), 126.3 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.2$ Hz), 111.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.9$ Hz), 91.7, 56.0, 55.2, 37.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 26.0$ Hz), 31.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.9$ Hz). ^{31}P NMR (202 MHz, CDCl_3) δ 64.16. HRMS (ESI+) calculated for $\text{C}_{23}\text{H}_{33}\text{AuClO}_3\text{NaP}$ ($\text{M} + \text{Na}$): 643.1414; found: 643.1436. Elemental Analysis calculated for $\text{C}_{23}\text{H}_{33}\text{AuClO}_3\text{P}$: C, 44.49; H, 5.36; found: C, 44.82; H, 5.25.

2-Di-*t*-butylphosphino-2-naphthyl gold(I) chloride (6e)



Gold chloride complex **6e** was synthesized according to the general procedure from 2-di-*t*-butylphosphino-2-naphthyl (559.2 mg, 1.605 mmol) and $(\text{Me}_2\text{S})\text{AuCl}$ (500 mg, 1.605 mmol). A white crystalline solid was obtained in 36.4% yield (338.9 mg, 0.58 mmol) after purification by flash column chromatography using a mixture of cyclohexane:ethyl acetate (4:1) as eluent.

mp 241.2 °C ^1H NMR (400 MHz, CDCl_3) δ 8.03 – 7.87 (m, 3H), 7.84 – 7.77 (m, 1H), 7.64 – 7.60 (m, 1H), 7.60 – 7.48 (m, 4H), 7.41 – 7.34 (m, 1H), 7.26 – 7.21 (m, 1H), 1.44 (d, $J = 4.1$

Hz, 11H), 1.40 (d, $J(^1\text{H}-^{31}\text{P}) = 4.1$ Hz, 11H). **^{13}C NMR** (101 MHz, CDCl_3) δ 150.3 (d, $J(^{13}\text{C}-^{31}\text{P}) = 13.7$ Hz), 139.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.5$ Hz), 133.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.8$ Hz), 133.6, 133.5, 133.3, 130.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.2$ Hz), 129.0, 128.4, 128.3, 128.0, 127.1, 127.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.3$ Hz), 126.4, 126.0, 38.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 22.2$ Hz), 37.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 22.1$ Hz), 31.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.1$ Hz), 31.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.0$ Hz). **^{31}P NMR** (162 MHz, CDCl_3) δ 63.02. **HRMS** (ESI+) calculated for $\text{C}_{24}\text{H}_{29}\text{AuClNaP}$ ($\text{M} + \text{Na}$) $^+$: 603.1254; found: 603.1254.

4. Synthesis of Chloromesityl(methyl) Gold(I) Carbenoids

Preparation of mesityldiazomethane in toluene solution

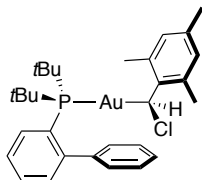
The used of protective shielding screens is highly recommended during the preparation of mesityldiazomethane solution due to the risk of explosion of aryl diazomethane compounds.

A 250 mL two-neck round-bottom flask with a findenser condenser was charged with an aqueous solution of NaOH (50 mL, 7 g, 24.5 mmol), benzyltriethylammonium chloride (0.968 g, 4.25 mmol and toluene (50 mL). Benzenesulfonic acid, 4-methyl-, 2-[(2,4,6-trimethylphenyl)methylene]hydrazide (0.538 g, 1.70 mmol) was sequentially added, *the addition must be done following the noted order*. The flask was covered with aluminum foil and protected by a three-walls shielding screen. The resulting mixture was stirred for 2 h at 70 °C. After being allowed to cool down to room temperature, the mixture was transferred to a separatory funnel. The orange organic phase was separated from the aqueous phase and transferred to a round-bottom flask charged with NaOH pellets and covered with aluminum foil under argon. The mesityldiazomethane solution was deoxygenated by bubbling argon through it for 30 minutes. The dry and deoxygenated solution was transferred to an oven-dried Schlenk under argon using a syringe connected to a Teflon filter. It was concentrated to 2 mL under vacuum in the Schlenk line and layered with 2 mL of dry pentane. After being cooled down to -70 °C for 30 minutes, white solid precipitated and the orange solution was filtered at -70 °C to a new oven-dried Schlenk using a cannula filter. The solution was concentrated to dryness in the Schlenk line (*be especially careful at that point!!!*). Followed by the addition of dry and deoxygenated toluene (5 mL). It was stored under argon and covered with aluminum foil in the freezer at -20 °C until it was used the very next day.

Synthesis of Chloroaryl(methyl) Gold(I) Carbenoids

The used of protective shielding screens is highly recommended during the synthesis of gold(I) carbenoids due to the risk of explosion of aryl diazomethane compounds.

2-Di-*t*-butylphosphinobiphenyl chloromesityl(methyl) gold(I) carbenoid (1a)

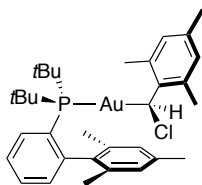


2-Di-*t*-butylphosphinobiphenyl gold(I) chloride (150 mg, 0.283 mmol) was added to a Schlenk charged with a freshly prepared solution of mesityldiazomethane (1.695 mmol of starting hydrazide, 5 mL) under argon and protected by a three-walls shielding screen. The Schlenk was located in an aluminum heating block with sand and heated up to 35 °C for 2 h. The solution was concentrated to 2 mL and stirred at 45 °C until full conversion was observed by ³¹P NMR. Once the starting material was consumed, the solution was allowed to cool down to room

temperature. At this point, toluene was evaporated to dryness leading to a red oil, **be especially careful!!** The orange oil was dissolved in 2 mL of pentane that were subsequently evaporated leading to an orange solid, the process was repeated twice. The orange solid was dissolved in dry toluene (0.5 mL) and dry pentane (2 mL). The resulting solution was cooled down to -30 °C and stirred until white solid precipitated. The solvent was filtered off using a cannula filter leading to a pinkish-white solid that was washed with dry pentane (1 mL x 3) at -30 °C. The resulting solid was dried for 24 h. 2-Di-*t*-butylphosphinobiphenyl chloromesityl(methyl) gold(I) carbenoid (**1a**) was obtained as a white solid in 48% yield, (90 mg, 0.136 mmol). The complex was stored in the glovebox at room temperature. X-ray quality crystals were obtained layering a toluene solution of the complex with pentane at -20 °C under argon.

¹H NMR (400 MHz, toluene-*d*₈) δ 7.54 – 7.48 (m, 1H), 7.43 – 7.38 (m, 1H), 7.17 – 7.08 (m, 2H), 7.03 – 6.92 (m, 5H), 6.82 (bs, 2H), 4.92 (d, *J* (¹H-³¹P) = 6.6 Hz, 1H), 2.70 (bs, 6H), 2.23 (s, 3H), 1.21 (d, *J* (¹H-³¹P) = 14.5 Hz, 9H), 1.04 (d, *J* (¹H-³¹P) = 14.5 Hz, 9H). ¹³C NMR (101 MHz, toluene-*d*₈) δ 150.9 (d, *J* (¹³C-³¹P) = 16.5 Hz), 144.4 (d, *J* (¹³C-³¹P) = 0.9 Hz), 143.1 (d, *J* (¹³C-³¹P) = 5.7 Hz), 134.8, 133.5, 133.1 (d, *J* (¹³C-³¹P) = 7.7 Hz), 130.1 (d, *J* (¹³C-³¹P) = 2.2 Hz), 129.6, 129.2, 129.2, 128.9, 128.5, 127.8, 126.3 (d, *J* (¹³C-³¹P) = 5.0 Hz), 69.7 (d, *J* (¹³C-³¹P) = 107.7 Hz), 37.1 (d, *J* (¹³C-³¹P) = 19.2 Hz), 36.9 (d, *J* (¹³C-³¹P) = 19.0 Hz), 30.8 (d, *J* (¹³C-³¹P) = 6.9 Hz), 30.6 (d, *J* (¹³C-³¹P) = 7.0 Hz), 22.3, 21.0. ³¹P NMR (162 MHz, toluene-*d*₈) δ 66.42. HRMS (ESI+) calculated for C₃₀H₃₉AuP (M-Cl)⁺: 627.2450; found: 627.2436.

2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid (1b)

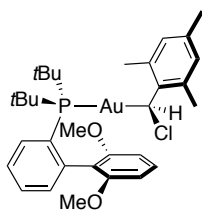


2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl gold(I) chloride (200 mg, 0.349 mmol) was added to a Schlenk charged with a freshly prepared solution of mesityldiazomethane (3.490 mmol of starting hydrazide, 5 mL) under argon and protected by a three-walls shielding screen. The Schlenk was located in an aluminum heating block with sand and heated up to 55 °C for 2 h. The solution was concentrated to 2 mL and stirred at 55 °C until full conversion was observed by ³¹P NMR. Once the starting material was consumed, the solution was allowed to cool down to room temperature. At this point, toluene was evaporated to dryness leading to an orange oil, **be especially careful!!** The orange oil was dissolved in 2 mL of pentane that was subsequently evaporated giving an oily orange solid, the process was repeated twice. The oily solid was dissolved in dry pentane (2 mL) and stirred until a white solid precipitated. The solvent was filtered off using a cannula filter leading to a pinkish-white solid that was washed with dry pentane (1 mL x 3). The resulting solid was dried for 24 h. 2-Di-*t*-butylphosphino-2',4',6'-

trimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid (**1b**) was obtained as a white solid in 41% yield, (100 mg, 0.143 mmol). The complex was stored in the glovebox at room temperature. X-ray quality crystals were obtained layering a toluene solution of the complex with pentane at -20 °C under argon.

^1H NMR (400 MHz, toluene- d_8) δ 7.55 – 7.48 (m, 1H), 7.18 (s, 1H), 7.12 – 7.08 (m, 1H), 7.07 – 7.01 (m, 2H), 6.86 – 6.78 (m, 3H), 4.90 (d, $J(^1\text{H}-^{31}\text{P}) = 6.9$ Hz, 1H), 2.75 (bs, 6H), 2.49 (s, 3H), 2.20 (s, 3H), 2.06 (s, 3H), 1.88 (s, 3H), 1.22 (d, $J(^1\text{H}-^{31}\text{P}) = 14.4$ Hz, 9H), 0.98 (d, $J(^1\text{H}-^{31}\text{P}) = 14.4$ Hz, 9H). $^{13}\text{C}\{^1\text{H}\}$ NMR (101 MHz, toluene- d_8) δ 150.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 16.9$ Hz), 144.3, 139.2 (d, $J(^{13}\text{C}-^{31}\text{P}) = 4.5$ Hz), 137.4, 136.0, 135.7, 135.4, 133.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 8.2$ Hz), 133.3, 131.0, 130.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.3$ Hz), 130.7, 129.9, 125.9 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.1$ Hz), 70.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 108.4$ Hz), 37.5 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.5$ Hz), 37.3 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.9$ Hz), 31.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.8$ Hz), 31.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.7$ Hz), 22.2, 21.9, 21.5, 21.0. $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CD_2Cl_2 , -90 °C) C1 71.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 107.2$ Hz). ^{13}C NMR (126 MHz, CD_2Cl_2 , -90 °C) C1 71.8 (d, $J(^{13}\text{C}-^1\text{H}) = 143.9$ Hz, $J(^{13}\text{C}-^{31}\text{P}) = 107.2$ Hz). ^{31}P NMR (162 MHz, toluene- d_8) δ 67.16. HRMS (ESI+) calculated for $\text{C}_{33}\text{H}_{45}\text{AuP}$ (M-Cl) $^+$: 669.2919; found: 669.2916. Elemental Analysis calculated for $\text{C}_{33}\text{H}_{45}\text{AuClP}$: C, 56.21; H, 6.43; found: C, 54.41; H, 6.51.

2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (1c)

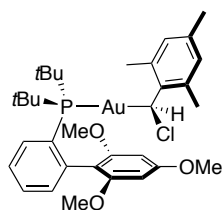


2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl gold(I) chloride (200 mg, 0.338 mmol) was added to a Schlenk charged with a freshly prepared solution of mesityldiazomethane (4.06 mmol of starting hydrazide, 20 mL) under argon and protected by a three-walls shielding screen. The Schlenk was located in an aluminum heating block with sand and heated up to 65 °C for 1 h. The solution was concentrated to 5 mL and stirred for 2 h. The solution was further concentrated to 2 mL and stirred until full conversion was observed by ^{31}P NMR. Once the starting material was consumed, the solution was allowed to cool down to room temperature. At this point, toluene was evaporated to dryness leading to an orange solid, *be especially careful!!* The orange solid was washed with 2 mL of pentane that were subsequently evaporated. The orange solid was dissolved in dry toluene (0.5 mL) and dry pentane (2 mL). Instantaneously, solid precipitated and the solvent was filtered off using a cannula filter leading to a pale rose solid that was washed with dry pentane (1 mL x 3). The resulting solid was dried for 24 h. 2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (**1c**) was obtained as a pinkish-white solid in 57% yield, (140 mg, 0.192 mmol). The complex was stored

in the glovebox at room temperature. X-ray quality crystals were obtained layering a toluene solution of the complex with pentane at -20 °C under argon.

¹H NMR (400 MHz, toluene-*d*₈) δ 7.59 (t, *J* = 7.0 Hz, 1H), 7.23 (t, *J* = 8.4 Hz, 1H), 7.09 – 7.02 (m, 1H), 6.84 (s, 2H), 6.65 (d, *J* = 8.4 Hz, 1H), 6.26 (d, *J* = 8.3 Hz, 1H), 4.84 (d, *J* (¹H-³¹P) = 6.7 Hz, 1H), 3.50 (s, 3H), 3.16 (s, 3H), 2.76 (bs, 6H), 2.22 (s, 3H), 1.33 (d, *J* (¹H-³¹P) = 14.3 Hz, 10H), 1.10 (d, *J* (¹H-³¹P) = 14.3 Hz, 9H). **¹³C{¹H} NMR** (126 MHz, CD₂Cl₂, -90 °C) δ 156.8 (d, *J* (¹³C-³¹P) = 3.4 Hz), 142.9, 142.6 (d, *J* (¹³C-³¹P) = 16.0 Hz), 137.5, 135.2, 134.0, 133.8 (d, *J* (¹³C-³¹P) = 3.6 Hz), 132.7 (d, *J* (¹³C-³¹P) = 8.2 Hz), 130.7, 130.4, 128.9 (d, *J* (¹³C-³¹P) = 50.1 Hz), 128.7, 127.9, 127.7, 126.4 (d, *J* (¹³C-³¹P) = 4.8 Hz), 124.9, 119.5 (d, *J* (¹³C-³¹P) = 5.6 Hz), 102.9 (d, *J* (¹³C-³¹P) = 165.8 Hz), 73.7 (C1, d, *J* (¹³C-³¹P) = 107.4 Hz), 55.3, 54.9, 36.3 (d, *J* (¹³C-³¹P) = 10.5 Hz), 36.1 (d, *J* (¹³C-³¹P) = 10.5 Hz), 30.7, 29.6, 21.8, 21.6, 20.4. **¹³C NMR** (126 MHz, CD₂Cl₂, -90 °C) C1 73.7 (d, *J* (¹³C-¹H) = 144.3 Hz, *J* (¹³C-³¹P) = 107.4 Hz). **³¹P NMR** (162 MHz, toluene-*d*₈) δ 67.76. **HRMS** (ESI+) calculated for C₃₂H₄₃AuO₂P (M-Cl)⁺: 687.2661; found: 687.2652.

2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (1d)

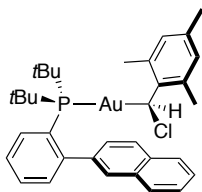


2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl gold(I) chloride (150 mg, 0.242 mmol) was added to a Schlenk charged with a freshly prepared solution of mesityldiazomethane (2.416 mmol of starting hydrazide, 5 mL) under argon and protected by a three-walls shielding screen. The Schlenk was located in an aluminum heating block with sand and heated up to 65 °C until full conversion was observed by ³¹P NMR. Once the starting material was consumed, the solution was allowed to cool down to room temperature. At this point, toluene was evaporated to dryness leading to an orange oil, ***be especially careful!!*** The orange oil was dissolved in 2 mL of pentane that was subsequently evaporated giving an oily solid, the process was repeated twice. The oily solid was dissolved in dry diethyl ether (2 mL) and stirred at -20 °C until white solid precipitated. The solvent was filtered off using a cannula filter leading to a pinkish-white solid that was washed with dry pentane (1 mL x 3). The resulting solid was dried for 24 h. 2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (**1d**) was obtained as a white solid in 33% yield, (60 mg, 0.080 mmol). The complex was stored in the glovebox at room temperature.

¹H NMR (500 MHz, toluene-*d*₈) δ 7.59 (ddd, *J* = 7.8, 6.4, 1.6 Hz, 1H), 7.17 (ddd, *J* = 7.8, 4.1, 1.6 Hz, 1H), 7.14 – 7.10 (m, 1H), 7.04 – 6.99 (m, 1H), 6.82 (s, 2H), 6.45 (d, *J* = 2.2 Hz, 1H),

6.29 (d, $J = 2.1$ Hz, 1H), 4.88 (d, $J(^1\text{H}-^{31}\text{P}) = 6.7$ Hz, 1H), 3.81 (s, 3H), 3.59 (s, 3H), 3.17 (s, 3H), 2.81 (bs, 6H), 2.19 (s, 3H), 1.34 (d, $J(^1\text{H}-^{31}\text{P}) = 14.3$ Hz, 9H), 1.03 (d, $J(^1\text{H}-^{31}\text{P}) = 14.3$ Hz, 9H). ^{13}C NMR (126 MHz, toluene- d_8) δ 161.8, 158.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 33.8$ Hz), 144.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 16.4$ Hz), 143.9 (d, $J(^{13}\text{C}-^{31}\text{P}) = 1.3$ Hz), 134.7, 134.5, 133.0, 131.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 35.9$ Hz), 130.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.2$ Hz), 125.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.5$ Hz), 125.0, 113.2 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.7$ Hz), 91.8, 89.8, e (d, $J(^{13}\text{C}-^{31}\text{P}) = 109.6$ Hz), 54.7, 54.5, 54.2, 36.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 14.4$ Hz), 36.5 (d, $J(^{13}\text{C}-^{31}\text{P}) = 14.4$ Hz), 31.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.1$ Hz), 30.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.0$ Hz), 21.8, 20.6. ^{31}P NMR (202 MHz, toluene- d_8) δ 67.53. HRMS (ESI+) calculated for $\text{C}_{33}\text{H}_{45}\text{AuO}_3\text{P}$ (M-Cl) $^+$: 717.2767; found: 717.2771.

2-Di-*t*-butylphosphino-2-naphthyl chloromesityl(methyl) gold(I) carbenoid (**1e**)



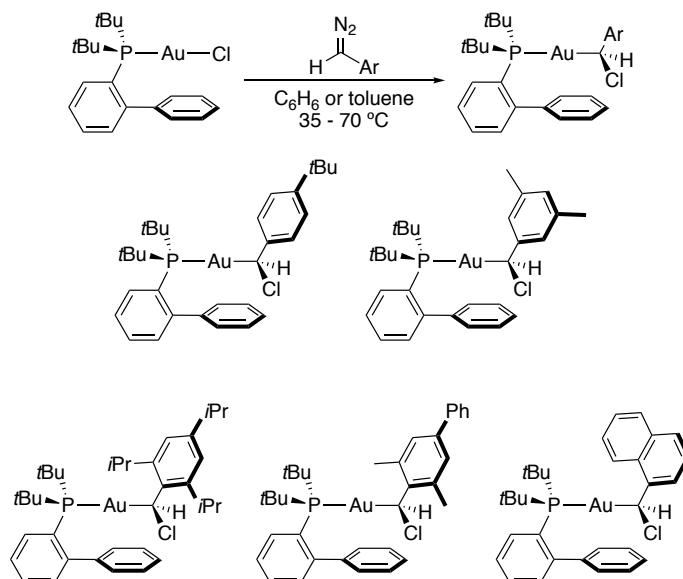
2-Di-*t*-butylphosphinobiphenyl gold(I) chloride (338.9 mg, 0.583 mmol) was added to a Schlenk charged with a freshly prepared solution of mesityldiazomethane (3.56 mmol of starting hydrazide, 10 mL) under argon and protected by a three-walls shielding screen. The Schlenk was located in an aluminum heating block with sand and heated up to 35 °C for 1 h. The solution was concentrated to 2 mL and stirred at 45 °C until full conversion was observed by ^{31}P NMR. Once the starting material was consumed, the solution was allowed to cool down to room temperature. At this point, toluene was evaporated to dryness leading to a red oil, **be especially careful!!** The orange oil was dissolved in 2 mL of pentane that were subsequently evaporated leading to an orange solid, the process was repeated twice. The orange solid was dissolved in dry toluene (0.5 mL) and dry pentane (2 mL). The resulting solution was cooled down to -30 °C and stirred until white solid precipitated. The solvent was filtered off using a cannula filter leading to a pinkish-white solid that was washed with dry pentane (1 mL x 3) at -30 °C. The resulting solid was dried for 24 h. 2-Di-*t*-butylphosphino-2-naphthyl chloromesityl(methyl) gold(I) carbenoid (**1e**) was obtained as a white solid in 29% yield, (120 mg, 0.168 mmol). The complex was stored in the glovebox at room temperature. X-ray quality crystals were obtained layering a toluene solution of the complex with pentane at -20 °C under argon. The complex was a 3:1 (A:B) mixture of two regioisomers in solution.

^1H NMR (500 MHz, CD_2Cl_2 , -90 °C) δ 8.08 – 8.03 (A, m, 1H), 8.01 (A, d, $J = 8.3$ Hz, 1H), 7.91 (B, q, $J = 4.7$ Hz, 0.66H), 7.89 – 7.85 (B, m, 1H), 7.81 – 7.77 (B, m, 0.66H), 7.72 (B, d, $J = 1.7$ Hz, 0.33H), 7.61 – 7.45 (A, m, 7H), 7.37 (A, dd, $J = 8.3, 1.7$ Hz, 1H), 7.25 – 7.19 (B, m, 0.66H), 7.16 (B, dd, $J = 8.3, 1.7$ Hz, 0.33H), 6.62 (B, d, $J = 9.3$ Hz, 0.66H), 6.56 (A, d, $J = 2.0$ Hz, 1H), 6.44 (A, d, $J = 2.0$ Hz, 1H), 3.25 (A, d, $J(^1\text{H}-^{31}\text{P}) = 6.0$ Hz, 1H), 3.22 (B, d, $J(^1\text{H}-^{31}\text{P}) = 6.0$ Hz, 0.33H), 2.50 (A, s, 3H), 2.48 (B, s, 1H), 2.10 (B, s, 1H), 2.03 (A, s, 3H), 1.93 (B, s,

1H), 1.46 (A, d, $J(^1\text{H}-^{31}\text{P}) = 14.7$ Hz, 9H), 1.39 (B, d, $J(^1\text{H}-^{31}\text{P}) = 14.8$ Hz, 3H), 1.27 – 1.18 (B, m, 3H), 1.17 – 1.08 (A, m, 9H), 1.07 (A, s, 3H). ^{13}C NMR (126 MHz, CD_2Cl_2 , -90 °C) δ 149.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 16.1$ Hz), 142.3, 140.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.4$ Hz), 137.1, 134.6, 133.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 2.8$ Hz), 132.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.5$ Hz), 132.5, 131.9, 129.8, 128.9, 127.8, 127.5, 127.5, 127.3 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.0$ Hz), 127.2 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.3$ Hz), 126.6, 126.4, 126.0, 99.5, 70.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 107.0$ Hz), 36.5 (d, $J(^{13}\text{C}-^{31}\text{P}) = 20.4$ Hz), 36.4 – 36.1 (m), 30.6, 29.9 (d, $J(^{13}\text{C}-^{31}\text{P}) = 59.0$ Hz), 21.5 (A), 20.3, 19.5. ^{31}P NMR (162 MHz, CD_2Cl_2 , -90 °C) δ 66.47, 66.37. HRMS (ESI+) calculated for $\text{C}_{34}\text{H}_{41}\text{AuP}$ (M-Cl) $^+$: 677.2590; found: 677.2606.

Alternative aryl gold(I) carbenoids

The following gold(I) carbenoids were prepared in small amounts. As they were not suitable precursors to generate gold(I) carbenes in solution, their synthesis was not scaled up and they were not fully characterized.



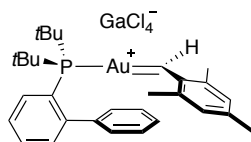
Scheme S1. Alternative gold(I) carbenoids prepared and tested as gold(I) carbenes precursors.

5. Generation of Mesityl(methyl) Gold(I) Carbenes in Solution

General procedure for the generation of gold(I) carbenes in solution

In a glovebox, the corresponding chloromesityl(methyl) gold(I) carbenoid was weighed in an oven-dried standard NMR tube and capped with a rubber septum. Separately, GaCl₃ (1.2 equiv) was dissolved in CD₂Cl₂ (0.5 mL) in a HPLC vial and taken in a syringe with a long needle protected from air. Besides that, CD₂Cl₂ (0.5 mL) was taken in a syringe protected from air. Outside the glovebox, the capped NMR tube was cooled down to -90 °C in an acetone/liquid nitrogen bath and cold CD₂Cl₂ (0.5 mL) was injected into the NMR tube. The NMR tube was shaken until the solution was homogeneous. Afterwards, the cold GaCl₃ solution was added over the mixture in the NMR tube at -90 °C. The solution turned deep red instantaneously. The sample was transferred to the NMR instrument set at -90 °C as fast as possible. The mesityl(methyl) gold(I) carbenes generated were characterized by ¹H NMR, ¹³C NMR, ³¹P NMR, ¹H-¹³C HSQC and ¹H-³¹P HMBC.

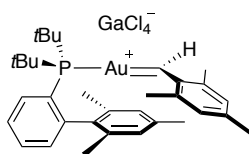
2-Di-*t*-butylphosphinobiphenyl mesityl(methyl) gold(I) carbene (**5a**)



2-Di-*t*-butylphosphinobiphenyl mesityl(methyl) gold(I) carbene (**5a**) was generated according to the general procedure from 2-di-*t*-butylphosphinobiphenyl chloromesityl(methyl) gold(I) carbenoid (**1a**) (5 mg, 7.5 μmol) and GaCl₃ (1.52 mg, 8.8 μmol). Deep red solution.

¹H NMR (400 MHz, CD₂Cl₂, -90 °C) δ 12.35 (bs, 1H, *carbenic proton*), 7.90 – 7.83 (m, 1H), 7.58 – 7.49 (m, 3H), 7.27 – 7.16 (m, 5H), 7.02 – 6.94 (m, 1H), 2.87 (s, 3H), 2.54 (bs, 3H), 2.53 (bs, 3H), 1.35 (d, *J* (¹H-³¹P) = 15.3 Hz, 18H). ¹³C NMR (101 MHz, CD₂Cl₂, -80 °C) δ 290.0 (d, *J* (¹³C-³¹P) = 98.3 Hz, *carbenic carbon*), 172.4, 159.8, 156.6 (d, *J* (¹³C-³¹P) = 5.4 Hz), 151.4, 148.7 (d, *J* (¹³C-³¹P) = 14.4 Hz), 143.7 (d, *J* (¹³C-³¹P) = 5.8 Hz), 134.9, 134.1, 130.1, 128.9, 38.1 (d, *J* (¹³C-³¹P) = 26.3 Hz), 30.6, 25.2, 25.2, 22.7. *The complete assignment of carbon signals was not possible due to decomposition of the compound over time.* ³¹P NMR (162 MHz, CD₂Cl₂, -90 °C) δ 64.96. Important correlations: ¹H-¹³C HSQC (CD₂Cl₂, -90 °C), correlation between carbonylic proton (12.35 ppm) and carbenic carbon (290.0 ppm). ¹H-³¹P HMBC (CD₂Cl₂, -90 °C), correlation between carbonylic proton (12.35 ppm) and ³¹P signal (64.96 ppm). [(2-Di-*t*-butylphosphinobiphenylAu)₂Cl]GaCl₄ (**10a**), *E*-1,2-dimesitylethene (**E-3b**), *Z*-1,2-dimesitylethene (**Z-2b**) and 2,4,6-trimethylbenzaldehyde (**8**) were detected by NMR as minor products at -90 °C (see section 6 for further details).

2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl mesityl(methyl) gold(I) carbene (**5b**)

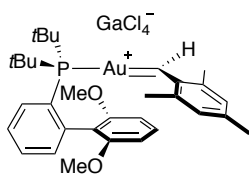


2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl mesityl(methyl) gold(I) carbene (**5b**) was generated according to the general procedure from 2-di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid (**1b**) (5 mg, 7.09 μmol) and GaCl_3 (1.5 mg, 8.5 μmol). Deep red solution.

^1H NMR (500 MHz, CD_2Cl_2 , -90°C) δ 12.67 (s, 1H), 7.87 (t, $J = 7.6$ Hz, 1H), 7.58 – 7.47 (m, 2H), 7.28 (s, 2H), 7.08 – 7.03 (m, 1H), 6.68 (s, 2H), 2.83 (s, 3H), 2.58 (s, 3H), 2.57 (s, 3H), 1.91 (s, 6H), 1.45 (s, 3H), 1.37 (d, $J(^1\text{H}-^{31}\text{P}) = 15.3$ Hz, 18H). $^{13}\text{C}\{^1\text{H}\}$ NMR (126 MHz, CD_2Cl_2 , -90°C) 288.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 99.4$ Hz), 171.6, 159.4, 156.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.3$ Hz), 150.4, 147.3 (d, $J(^{13}\text{C}-^{31}\text{P}) = 14.9$ Hz), 138.3 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.3$ Hz), 136.9, 136.5, 135.3, 133.7, 132.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.7$ Hz), 131.4, 128.1, 127.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.1$ Hz), 38.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 27.0$ Hz), 37.82 (d, $J(^{13}\text{C}-^{31}\text{P}) = 27.2$ Hz), 30.6, 30.6, 25.0, 24.7, 22.1, 21.3, 19.8. ^{13}C NMR (126 MHz, CD_2Cl_2 , -90°C) selected signals 288.4 (dd, $^1J(^{13}\text{C}-^1\text{H}) = 129.1$ Hz, $^2J(^{13}\text{C}-^{31}\text{P}) = 99.4$ Hz) ^{31}P NMR (202 MHz, CD_2Cl_2 , -90°C) δ 65.69. Important correlations: ^1H - ^{13}C HSQC (CD_2Cl_2 , -90°C), correlation between carbonic proton (12.67 ppm) and carbenic carbon (288.4 ppm). ^1H - ^{31}P HMBC (CD_2Cl_2 , -90°C), correlation between carbonic proton (12.67 ppm) and ^{31}P signal (65.69 ppm).

[(2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenylAu) $_2$ Cl] GaCl_4 (**10b**), *E*-1,2-dimesitylethene (**E-2b**) and 2,4,6-trimethylbenzaldehyde (**8**) were detected by NMR as minor products at -90°C (see section 6 for further details).

2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl mesityl(methyl) gold(I) carbene (**5c**)



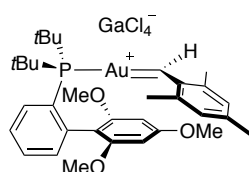
2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl mesityl(methyl) gold(I) carbene (**5c**) was generated according to the general procedure from 2-di-*t*-butylphosphino-2',6'-dimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid (**1c**) (5 mg, 6.9 μmol) and GaCl_3 (1.5 mg, 8.3 μmol). Deep red solution.

^1H NMR (500 MHz, CD_2Cl_2 , -90°C) δ 12.32 (s, 1H), 7.87 (t, $J = 7.7$ Hz, 1H), 7.57 (t, $J = 7.7$ Hz, 1H), 7.50 (t, $J = 7.7$ Hz, 1H), 7.27 (d, $J = 12.9$ Hz, 2H), 7.12 – 7.08 (m, 1H), 7.03 (t, $J = 8.3$ Hz, 1H), 6.44 (d, $J = 8.4$ Hz, 2H), 3.62 (s, 6H), 2.91 (s, 3H), 2.59 (s, 3H), 2.55 (s, 3H), 1.33 (d, $J(^1\text{H}-^{31}\text{P}) = 15.1$ Hz, 18H). ^{13}C NMR (126 MHz, CD_2Cl_2 , -90°C) 290.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 99.8$ Hz), 172.4, 159.6, 158.0, 156.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.2$ Hz), 151.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.3$ Hz), 142.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 14.8$ Hz), 135.6, 134.1, 133.2 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.8$ Hz), 129.9, 129.4, 129.2,

128.4, 103.4, 55.8, 38.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 26.9$ Hz), 37.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 27.1$ Hz), 30.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.1$ Hz), 25.3, 25.1, 22.8. ^{31}P NMR (202 MHz, CD_2Cl_2 , -90 °C) δ 66.31. Important correlations: $^1\text{H}-^{13}\text{C}$ HSQC (CD_2Cl_2 , -90 °C), correlation between carbonic proton (12.32 ppm) and carbenic carbon (290.0 ppm). $^1\text{H}-^{31}\text{P}$ HMBC (CD_2Cl_2 , -90 °C), correlation between carbonic proton (12.32 ppm) and ^{31}P signal (66.32 ppm).

$[(2\text{-Di-}t\text{-butylphosphino-2',6'-dimethoxybiphenylAu})_2\text{Cl}]\text{GaCl}_4$ (**10c**), *E*-1,2-dimesitylethene (*E*-**2b**), *Z*-1,2-dimesitylethene (*Z*-**2b**) and 2,4,6-trimethylbenzaldehyde (**8**) were detected by NMR as minor products at -90 °C (see section 6 for further details).

2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl mesityl(methyl) gold(I) carbene (**5d**)

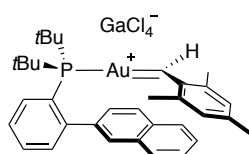


2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl mesityl(methyl) gold(I) carbene (**5d**) was generated according to the general procedure from 2-di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid (**1d**) (5 mg, 6.6 μmol) and GaCl_3 (1.4 mg, 8.0 μmol). Deep red solution.

^1H NMR (500 MHz, CD_2Cl_2 , -90 °C) δ 12.57 (s, 1H), 7.88 – 7.82 (m, 1H), 7.56 – 7.51 (m, 1H), 7.51 – 7.44 (m, 1H), 7.29 (d, $J = 13.1$ Hz, 2H), 7.07 – 7.01 (m, 1H), 5.92 (s, 2H), 3.64 (bs, 6H), 3.13 (bs, 3H), 2.93 (bs, 3H), 2.61 (bs, 3H), 2.57 (bs, 3H), 1.33 (d, $J(^1\text{H}-^{31}\text{P}) = 15.5$ Hz, 18H). ^{13}C NMR (126 MHz, CD_2Cl_2 , -90 °C) 289.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 96.8$ Hz), 172.2, 161.0, 158.7, 157.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 5.1$ Hz), 150.9 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.5$ Hz), 142.4 (d, $J(^{13}\text{C}-^{31}\text{P}) = 17.12$ Hz), 135.4, 134.1, 133.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.6$ Hz), 132.36, 129.7, 127.5 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.6$ Hz), 111.5, 89.6, 55.9, 55.1, 37.8 (m), 30.6 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.7$ Hz), 25.2, 22.4. ^{31}P NMR (202 MHz, CD_2Cl_2 , -90 °C) δ 66.47. Important correlations: $^1\text{H}-^{13}\text{C}$ HSQC (CD_2Cl_2 , -90 °C), correlation between carbonic proton (12.57 ppm) and carbenic carbon (289.0 ppm). $^1\text{H}-^{31}\text{P}$ HMBC (CD_2Cl_2 , -90 °C), correlation between carbonic proton (12.57 ppm) and ^{31}P signal (66.47 ppm).

$[(2\text{-Di-}t\text{-butylphosphino-2',4',6'-trimethoxybiphenylAu})_2\text{Cl}]\text{GaCl}_4$ (**10d**), *E*-1,2-dimesitylethene (*E*-**2b**) and 2,4,6-trimethylbenzaldehyde (**8**) were detected by NMR as minor products at -90 °C (see section 6 for further details).

2-Di-*t*-butylphosphinonaphthylphenyl mesityl(methyl) gold(I) carbene (**5e**)



Gold(I) carbene (**5e**) was generated according to the general procedure from gold(I) carbenoid **1e** (4.99 mg, 7 μ mol) and GaCl₃ (1.2 mg, 7.0 μ mol). Deep red solution.

¹H NMR (500 MHz, CD₂Cl₂, -90 °C) δ 11.74 (s, 1H), 7.91 (td, J = 6.9, 3.2 Hz, 1H), 7.78 (d, J = 8.4 Hz, 1H), 7.66 (s, 1H), 7.65 – 7.61 (m, 1H), 7.59 – 7.54 (m, 2H), 7.46 (d, J = 7.9 Hz, 1H), 7.34 – 7.26 (m, 2H), 7.11 – 7.04 (m, 3H), 6.99 (ddd, J = 8.1, 6.9, 1.3 Hz, 1H), 2.67 (s, 3H), 2.52 (s, 3H), 2.17 (s, 3H), 1.37 (t, J (¹H-³¹P) = 16.4 Hz, 18H). ¹³C NMR (126 MHz, CD₂Cl₂, -90 °C) 284.6 (d, J (¹³C-³¹P) = 97.8 Hz), 171.2, 158.9, 155.8 (d, J (¹³C-³¹P) = 5.1 Hz), 149.9 (d, J (¹³C-³¹P) = 3.5 Hz), 148.1 (d, J (¹³C-³¹P) = 14.7 Hz), 140.2 (d, J (¹³C-³¹P) = 6.1 Hz), 134.3, 133.2, 132.2, 132.1 (d, J (¹³C-³¹P) = 7.4 Hz), 131.8, 130.9, 130.4, 127.9, 127.8 (d, J (¹³C-³¹P) = 3.1 Hz), 127.4 (d, J (¹³C-³¹P) = 6.5 Hz), 126.9, 126.5 (d, J (¹³C-³¹P) = 12.2 Hz), 126.2, 125.6, 36.7 (d, J (¹³C-³¹P) = 22.1 Hz), 36.5 (d, J (¹³C-³¹P) = 22.3 Hz), 30.2, 29.9, 24.6, 24.5, 21.7. ³¹P NMR (202 MHz, CD₂Cl₂, -90 °C) δ 65.38. Important correlations: ¹H-³¹P HMBC (CD₂Cl₂, -90 °C), correlation between carbonyl proton (11.74 ppm) and ³¹P signal (65.38 ppm).

[(2-Di-*t*-butylphosphinonaphthylphenylAu)₂Cl]GaCl₄ (**10e**) and 2,4,6-trimethylbenzaldehyde (**8**) were detected by NMR as minor products at -90 °C (see section 6 for further details).

Table S1. Selected NMR data for the gold(I) carbenes **5a-e**.

Entry	Complex	¹ H (ppm) ^a	¹³ C (ppm) ^a	² J (¹³ C- ³¹ P) (Hz) ^b	¹ J (¹³ C- ¹ H) (Hz) ^c
1	5a	12.35	290.0 (d) ^d	98.3	-
2	5b	12.67	288.4 (d)	99.4	129.1
3	5c	12.32	290.0 (d)	99.8	127.8
4	5d	12.57	289.0 (d)	96.8	-
5	5e	11.74	284.6 (d)	97.8	-

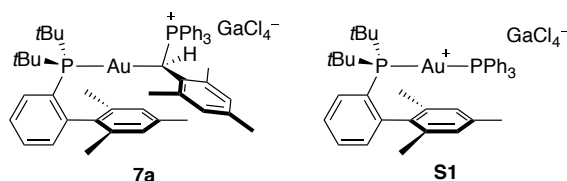
^a Chemical shifts corresponding to the carbonyl ¹H and ¹³C measured in CD₂Cl₂ solution at -90 °C. ^b Coupling constant for the carbonyl ¹³C with the ³¹P signal. ^c Coupling constant for the carbonyl ¹³C with the carbonyl ¹H signal. ^d -80 °C.

6. Trapping of Gold(I) Carbenes 5b-c with PPh₃

General procedure for the synthesis of phosphonium ylid complexes 7

In a glovebox, gold(I) carbenoid was weighed in a Schlenk. Separately, GaCl₃ (1 equiv) was dissolved in dry CD₂Cl₂ (1 mL) in a HPLC vial and taken out in a syringe protected from air. A solution of PPh₃ (1 equiv) in dry CD₂Cl₂ (1 mL) was prepared and taken in a syringe protected from air. Besides that, dry CD₂Cl₂ (2 mL) was also taken in a syringe protected from air. The Schlenk was cooled down to -90 °C and CD₂Cl₂ (2 mL) was added. Followed by the addition of GaCl₃ solution at the same temperature leading to a dark red solution. Afterwards, the PPh₃ solution was added over the mixture at -90 °C. The color faded away immediately after the addition of PPh₃ generating a colorless solution. The sample was allowed to warm up to room temperature. A white solid was obtained after evaporation of the solvent under vacuum in the line. The white solid was washed with dry pentane (1 mL x 3) and dried in the line. A mixture of two inseparable gold(I) complexes **7** and **S1/S2** was obtained. The complexes were stored in the glovebox at room temperature.

Synthesis of phosphonium ylid complex 7a

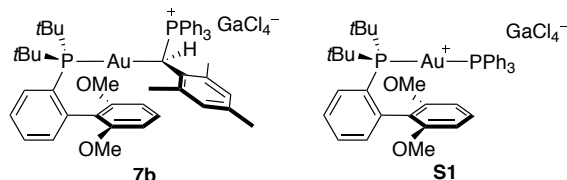


Phosphonium ylid complex **7a** was synthesized following the general procedure from 2-di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid **5b** (30.0 mg, 0.043 mmol), GaCl₃ (7.5 mg, 0.043 mmol) and PPh₃ (11.16 mg, 0.043 mmol). Complex **7a** was obtained as a mixture with complex **S1** (29.2 mg, **7a**:**S1** = 7:1). The complexes were stored in the glovebox at room temperature. X-ray quality crystals were obtained layering a CD₂Cl₂ solution of the complex with dry toluene under argon at -20 °C.

¹H NMR (500 MHz, CD₂Cl₂) δ 7.93 (td, *J* = 7.4, 1.8 Hz, 1H), 7.74 – 7.68 (m, 2H), 7.53 – 7.43 (m, 8H), 7.34 – 7.28 (m, 7H), 6.86 (ddd, *J* = 7.4, 4.4, 1.8 Hz, 1H), 6.78 (d, *J* = 3.9 Hz, 2H), 6.77 (s, 1H), 6.27 (s, 1H), 3.67 (dd, *J* (¹H-³¹P) = 18.9, 9.1 Hz, 1H), 2.31 (d, *J* (¹H-³¹P) = 3.1 Hz, 3H), 2.03 (d, *J* (¹H-³¹P) = 1.9 Hz, 3H), 1.96 (s, 3H), 1.92 (s, 3H), 1.72 (s, 3H), 1.66 (d, *J* (¹H-³¹P) = 1.5 Hz, 3H), 1.47 (d, *J* (¹H-³¹P) = 15.0 Hz, 9H), 1.07 (d, *J* (¹H-³¹P) = 15.0 Hz, 9H). ¹³C NMR (126 MHz, CD₂Cl₂) δ 149.2 (d, *J* (¹³C-³¹P) = 14.6 Hz), 139.9 (dd, *J* (¹³C-³¹P) = 7.6, 3.5 Hz), 139.3 (d, *J* (¹³C-³¹P) = 4.41 Hz), 138.0, 137.6 (dd, *J* (¹³C-³¹P) = 6.0, 2.9 Hz), 136.7, 136.4, 136.1, 134.5 (d, *J* (¹³C-³¹P) = 9.1 Hz), 134.4 (d, *J* (¹³C-³¹P) = 2.7 Hz), 132.1 (d, *J* (¹³C-³¹P) = 2.5 Hz), 131.1 (d, *J* (¹³C-³¹P) = 4.4 Hz), 130.9 (d, *J* (¹³C-³¹P) = 3.9 Hz), 129.9, 129.0 (d, *J* (¹³C-³¹P) = 8.2 Hz), 127.1 (d, *J* (¹³C-³¹P) = 6.1 Hz), 123.8, 123.1, 38.4 (d, *J* (¹³C-³¹P) = 21.3 Hz), 35.2 (dd, *J* (¹³C-³¹P) = 80.2, 28.5 Hz), 31.8 (d, *J* (¹³C-³¹P) = 5.9 Hz), 31.25 (d, *J* (¹³C-³¹P) = 6.4 Hz), 23.9, 22.5, 22.3, 21.5, 21.0. ³¹P NMR (202 MHz, CD₂Cl₂) δ 69.50 (d, *J* (³¹P-³¹P) = 4.3 Hz), 27.21 (d, *J* (³¹P-³¹P))

= 4.9 Hz). ^1H - ^{13}C HSQC (CD_2Cl_2 , 25 °C), correlation between H1 (3.67 ppm) and C1 (35.2 ppm) signals. ^1H - ^{31}P HMBC (CD_2Cl_2 , 25 °C), correlation between H1 (3.67 ppm) and ^{31}P signals (69.50 and 27.21 ppm). HRMS (ESI+) calculated for $\text{C}_{51}\text{H}_{60}\text{AuP}_2$ (M-GaCl_4) $^+$: 931.3830; found: 931.3811.

Synthesis of phosphonium ylid complex **7b**



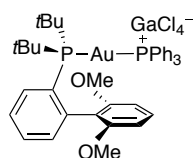
Phosphonium ylid complex **7b** was synthesized following the general procedure from 2-di-*t*-butylphosphino-2',6'-dimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid **5c** (30.0 mg, 0.041 mmol), GaCl_3 (7.3 mg, 0.041 mmol) and PPh_3 (10.9 mg, 0.041 mmol). Complex **7b** was obtained as a mixture with complex **S2** (41.5 mg, **7b**:**S2** = 6:1). The complexes were stored in the glovebox at room temperature. X-ray quality crystals were obtained layering a CD_2Cl_2 solution of the complex with dry pentane under argon at -20 °C.

Data listed as a mixture of gold(I) complexes **7b**:**S2** (6:1).

^1H NMR (400 MHz, CD_2Cl_2) δ 7.88 (**S2**, td, J = 7.6, 1.5 Hz, 1H), 7.76 – 7.69 (**7b**, m, 3H), 7.66 (**S2**, td, J = 7.3, 1.8 Hz, 0.5H), 7.62 – 7.52 (**S2**, m, 1.5H), 7.51 – 7.44 (**7b**, m, 8H), 7.42 (**S2**, t, J = 1.5 Hz, 0.5H), 7.41 (**S2**, t, J = 1.5 Hz, 0.35H), 7.40 – 7.31 (**7b**, m, 7H), 7.11 – 7.05 (**S2**, m, 0.17H), 6.94 (**7b**, ddd, J = 7.5, 4.2, 1.7 Hz, 1H), 6.82 (**7b**, d, J = 7.5 Hz, 1H), 6.75 (**7b**, t, J = 8.3 Hz, 1H), 6.60 (**7b**, dd, J = 8.4, 0.9 Hz, 1H), 6.45 (**S2**, t, J = 8.4 Hz, 0.17H), 6.11 (**S2**, d, J = 8.4 Hz, 0.35H), 5.58 (**7b**, d, J = 8.5 Hz, 1H), 3.71 (**7b**, s, 3H), 3.61 (**S2**, s, 1H), 3.40 (**7b**, dd, J (^1H - ^{31}P) = 18.8, 9.1 Hz, 1H), 3.22 (**7b**, s, 3H), 2.33 (**7b**, d, J (^1H - ^{31}P) = 3.1 Hz, 3H), 2.12 (**S2**, s, 0.5H), 2.09 (**7b**, d, J (^1H - ^{31}P) = 1.9 Hz, 3H), 1.67 (**7b**, s, 3H), 1.48 (**S2**, d, J (^1H - ^{31}P) = 15.7 Hz, 3H), 1.47 (**7b**, d, J (^1H - ^{31}P) = 15.0 Hz, 9H), 1.04 (**7b**, d, J (^1H - ^{31}P) = 15.1 Hz, 9H). ^{13}C NMR (101 MHz, CD_2Cl_2) δ 157.8 (**7b**, d, J (^{13}C - ^{31}P) = 39.4 Hz), 143.5 (**7b**, d, J (^{13}C - ^{31}P) = 14.9 Hz), 140.9 (**7b**, dd, J (^{13}C - ^{31}P) = 7.4, 3.4 Hz), 137.7 (**7b**, d, J (^{13}C - ^{31}P) = 4.4), 136.7 (**7b**, d, J (^{13}C - ^{31}P) = 4.4 Hz), 135.2 (**7b**, d, J (^{13}C - ^{31}P) = 1.7 Hz), 134.7 (**S2**, d, J (^{13}C - ^{31}P) = 13.0 Hz), 134.5 (**7b**, d, J (^{13}C - ^{31}P) = 8.7 Hz), 134.1 (**7b**, d, J (^{13}C - ^{31}P) = 8.2 Hz), 133.1 (**S2**, d, J (^{13}C - ^{31}P) = 2.6 Hz), 131.5 (**7b**, d, J (^{13}C - ^{31}P) = 2.2 Hz), 131.4 (**7b**), 131.2 (**S2**, d, J (^{13}C - ^{31}P) = 2.2 Hz), 131.1 (**S2**, d, J (^{13}C - ^{31}P) = 2.3 Hz), 131.0 (**7b**, d, J (^{13}C - ^{31}P) = 4.2 Hz), 130.7 (**S2**), 130.4 (**7b**, d, J (^{13}C - ^{31}P) = 4.0 Hz), 130.1 (**S2**, d, J (^{13}C - ^{31}P) = 11.3 Hz), 129.9 (**7b**, d, J (^{13}C - ^{31}P) = 11.5 Hz), 127.0 (**7b**, d, J (^{13}C - ^{31}P) = 6.4 Hz), 123.9 (**7b**), 123.1 (**7b**), 119.8 (**S2**, d, J (^{13}C - ^{31}P) = 5.9 Hz), 104.9 (**S2**), 103.7 (**7b**), 102.9 (**7b**), 55.9 (Y), 55.9 (**7b**), 55.0 (**7b**), 38.9 (Y, d, J (^{13}C - ^{31}P) = 22 Hz), 38.1 (**7b**, d, J (^{13}C - ^{31}P) = 19.4 Hz), 37.9 (**7b**, d, J (^{13}C - ^{31}P) = 18.9 Hz), 35.5 (**7b**, dd, J (^{13}C - ^{31}P) = 81.4, 28.8 Hz), 34.7 (**S2**), 31.56 (**S2**, d, J (^{13}C - ^{31}P) = 5.6 Hz), 31.5 (**7b**, d, J (^{13}C - ^{31}P) = 6.5 Hz), 30.7 (**7b**, d, J (^{13}C - ^{31}P) = 6.5 Hz), 24.1 (**7b**, d, J (^{13}C - ^{31}P) = 1.9 Hz), 22.9 (**S2**), 22.8 (**7b**, d, J

(^{13}C - ^{31}P) = 1.3 Hz), 21.1 (**7b**, d, J (^{13}C - ^{31}P) = 1.7 Hz), 14.38 (**S2**). ^{31}P NMR (162 MHz, CD_2Cl_2) δ 73.22 (**S2**, d, J (^{31}P - ^{31}P) = 300.4 Hz), 69.68 (**7b**, d, J (^{31}P - ^{31}P) = 5.0 Hz), 47.27 (**S2**, d, J (^{31}P - ^{31}P) = 300.3 Hz), 26.82 (**7b**, d, J (^{31}P - ^{31}P) = 4.9 Hz). ^1H - ^{31}P HMBC (CD_2Cl_2 , 25 °C), correlation between carbonic proton (3.40 ppm) and ^{31}P signals (69.68 and 26.82 ppm). Some signals coming from **S2** are missing due to the low amount of complex present in the analysed mixture. HRMS (ESI+) calculated for $\text{C}_{50}\text{H}_{58}\text{AuO}_2\text{P}_2$ (M-GaCl $_4$) $^+$: 949.3572; found: 949.3527.

Synthesis of [oMeOJPAuPPh $_3$][GaCl $_4$] (**S2**)



Inside the glovebox, 2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl gold(I) chloride (10.0 mg, 0.017 mmol) was dissolved in dry CD_2Cl_2 (0.4 mL) in an oven-dried standard NMR tube and capped with a rubber septum. Separately, GaCl $_3$ (3.0 mg, 0.017 mmol) was dissolved in CD_2Cl_2 (0.3 mL) in a HPLC vial and taken in a syringe protected from air. Besides that, a solution of PPh $_3$ (4.4 mg, 0.017 mmol) in dry CD_2Cl_2 (0.3 mL) was also taken in a syringe protected from air. Outside the glovebox, the PPh $_3$ solution was injected into the NMR tube. Followed by the addition of the GaCl $_3$ solution. The solution was analyzed by NMR. X-ray quality crystals were obtained layering a CD_2Cl_2 solution of the complex with dry pentane under argon at -20 °C.

^1H NMR (500 MHz, CD_2Cl_2) δ 7.94 (td, J = 7.7, 1.4 Hz, 1H), 7.74 – 7.66 (m, 2H), 7.64 – 7.58 (m, 8H), 7.42 – 7.36 (m, 7H), 7.12 (ddd, J = 7.7, 4.5, 1.6 Hz, 1H), 6.49 (t, J = 8.3 Hz, 1H), 6.15 (d, J = 8.4 Hz, 2H), 3.65 (s, 6H), 1.52 (d, J (^1H - ^{31}P) = 15.8 Hz, 18H). ^{13}C NMR (126 MHz, CD_2Cl_2) δ 157.9, 135.2 (dd, J (^{13}C - ^{31}P) = 4.6, 2.3 Hz), 134.7 (d, J (^{13}C - ^{31}P) = 13.4 Hz), 134.4, 134.2 (d, J (^{13}C - ^{31}P) = 8.4 Hz), 133.0 (d, J (^{13}C - ^{31}P) = 2.7 Hz), 132.4 (d, J (^{13}C - ^{31}P) = 2.4 Hz), 130.7, 130.1 (d, J (^{13}C - ^{31}P) = 11.4 Hz), 129.8 (d, J (^{13}C - ^{31}P) = 24.3 Hz), 128.6 (d, J (^{13}C - ^{31}P) = 1.7 Hz), 128.1 (d, J (^{13}C - ^{31}P) = 1.8 Hz), 127.8 (d, J (^{13}C - ^{31}P) = 6.6 Hz), 104.9, 55.9, 38.9 (d, J (^{13}C - ^{31}P) = 21.9 Hz), 31.6 (d, J (^{13}C - ^{31}P) = 6.3 Hz). ^{31}P NMR (203 MHz, CD_2Cl_2) δ 73.18 (d, J (^{31}P - ^{31}P) = 300.4 Hz), 47.25 (d, J (^{31}P - ^{31}P) = 300.3 Hz).

General procedure for the thermal stability test of complexes **7a-b**

In a glovebox, phosphonium ylide gold(I) complexes **7a-b** (5 mg) were weighed in an oven-dried NMR tube and dissolved in dry 1,1,2,2-tetrachloroethane- d_4 (0.5 mL). ^1H NMR and ^{31}P NMR spectra were taken every 10 °C from 25 to 125 °C. No decomposition was observed through any experiment.

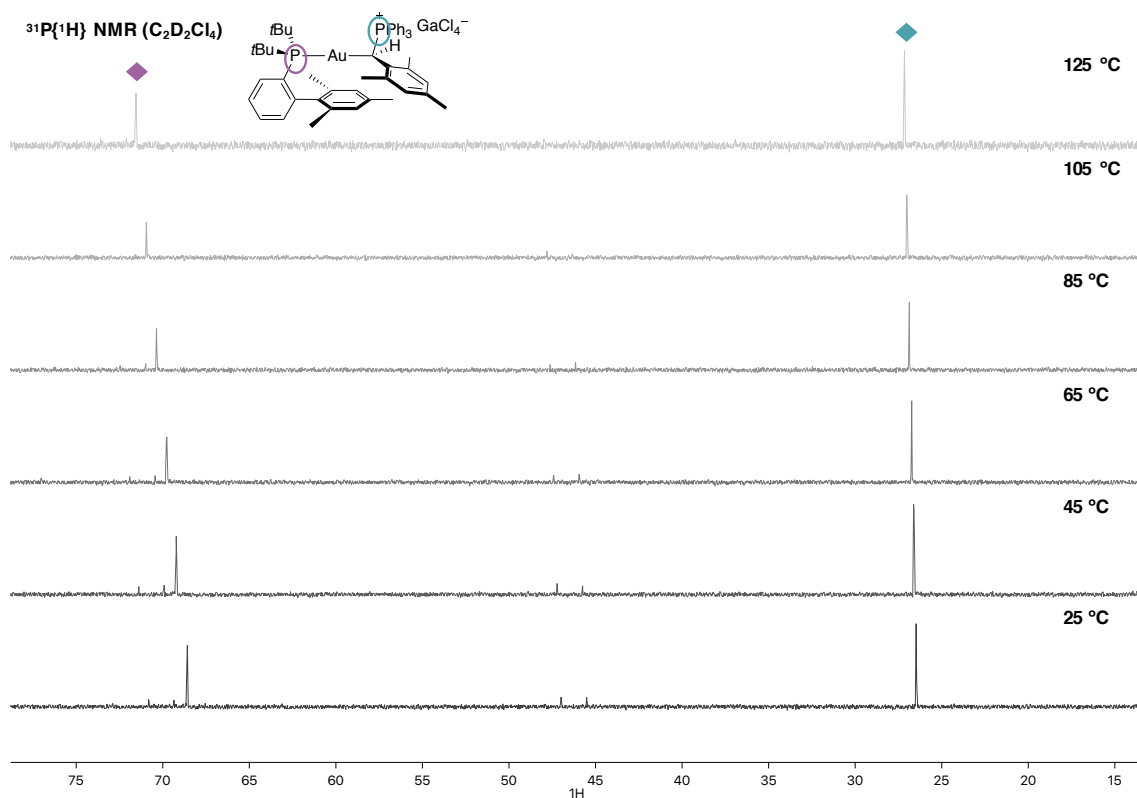


Figure S1. Thermal stability of phosphonium ylid complex **7a**

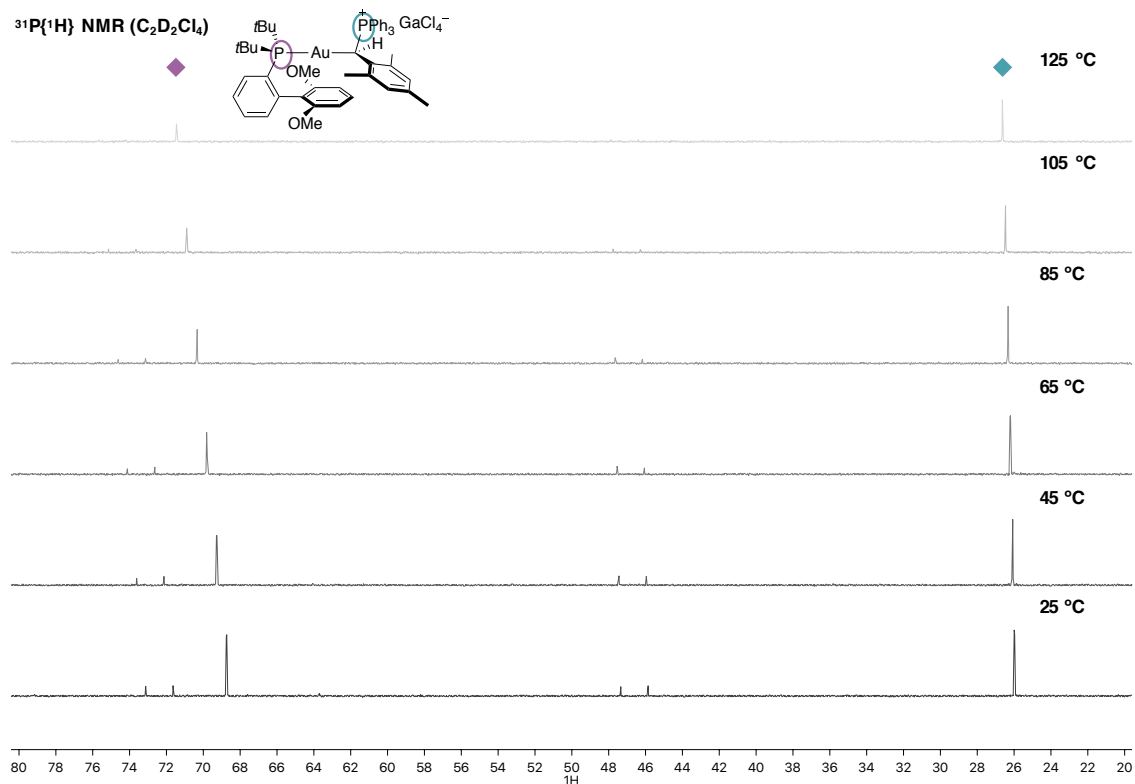
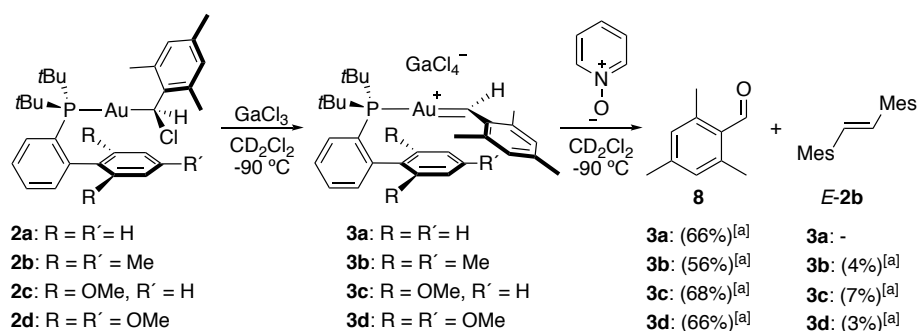


Figure S2. Thermal stability of phosphonium ylid complex **7b**

7. Gold(I) Promoted Oxidation

Method A: Generation of mesityl(methyl) gold(I) carbenes in the presence of pyridine N-oxide.

In a glovebox, the corresponding chloromesityl(methyl) gold(I) carbenoid (0.007 mmol) was weighed in an oven-dried microwave vial and capped. Separately, GaCl₃ (1 equiv) was dissolved in dry CD₂Cl₂ (0.3 mL) in a HPLC vial and taken in a syringe protected from air. A solution of pyridine N-oxide (10 equiv) in dry CD₂Cl₂ (0.2 mL) was prepared and taken in a syringe protected from air. Besides that, dry CD₂Cl₂ (0.5 mL) was also taken in a syringe protected from air. The microwave vial was cooled down to -90 °C and CD₂Cl₂ (0.5 mL) was added. Afterwards, the GaCl₃ solution was added over the solution in the microwave vial at -90 °C. Followed by the addition of the pyridine N-oxide solution. The sample was kept at -90 °C for two minutes and allowed to warm up to room temperature. Followed by the addition of a CD₂Cl₂ solution of diphenylmethane (0.05 mmol, 0.1 mL, 0.5 M). The reaction was opened to air and transferred to a NMR tube. The yield was calculated by integration of the ¹H NMR of the product and the internal standard.



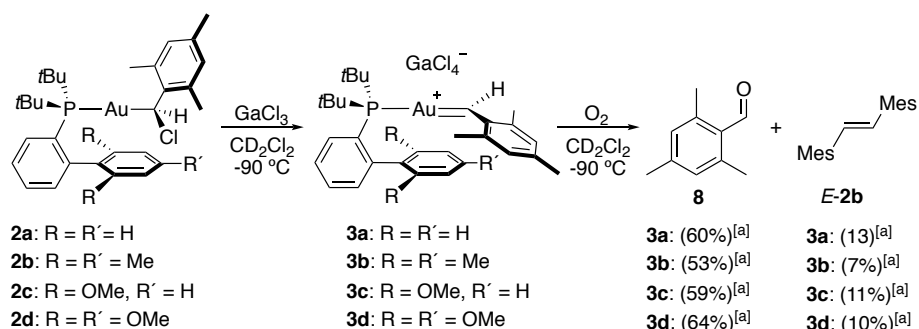
Scheme S2. Oxidation of gold(I) carbenes with pyridine N-oxide. ^[a]Yield determined by ¹H NMR using diphenylmethane as internal standard.

2,4,6-trimethylbenzaldehyde **8** was detected by ¹H NMR and GCMS from the crude reactions of the oxidation. The ¹H NMR data of 2,4,6-trimethylbenzaldehyde **8** was identical to the data of an original sample.

Method B: Generation of mesityl(methyl) gold(I) carbenes in the presence of oxygen.

In a glovebox, the corresponding chloromesityl(methyl) gold(I) carbenoid **1a-e** (0.007 mmol) was weighed in an oven-dried microwave vial and capped. Separately, GaCl₃ (1 equiv) was dissolved in dry CD₂Cl₂ (0.5 mL) in a HPLC vial and taken in a syringe protected from air. Besides that, dry CD₂Cl₂ (0.5 mL) was also taken in a syringe protected from air. The microwave vial was cooled down to -90 °C and CD₂Cl₂ (0.5 mL) was added. Afterwards, the GaCl₃ solution was added over the mixture in the microwave vial at -90 °C. Oxygen was bubble through the mixture until the dark red color of the solution faded away, approximately 1 minute. The sample was allowed to warm up to room temperature. Followed by the addition of a CD₂Cl₂ solution of diphenylmethane (0.05 mmol, 0.1 mL, 0.5 M). The reaction was opened to air and

transferred to a NMR tube. The yield was calculated by integration of the ^1H NMR of the product and the internal standard.



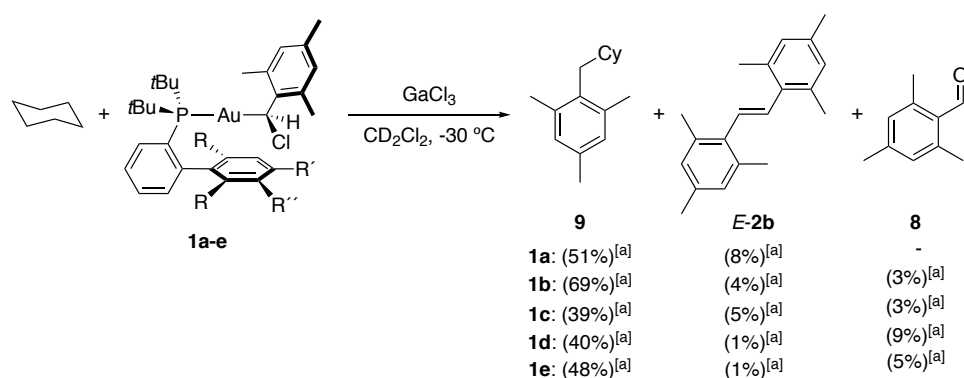
Scheme S3. Oxidation of gold(I) carbenes with oxygen.

2,4,6-trimethylbenzaldehyde **8** was detected by ^1H NMR and GCMS from the crude reactions of the oxidation. The ^1H NMR data of 2,4,6-trimethylbenzaldehyde **8** was identical to the data of an original sample.

8. Gold(I) Promoted C–H Insertion

Method A: Generation of mesityl(methyl) gold(I) carbenes in the presence of cyclohexane

In a glovebox, the corresponding chloromesityl(methyl) gold(I) carbenoid (0.007 mmol) and cyclohexane (50 equiv) were weighed in an oven-dried microwave vial and capped. Separately, GaCl₃ (1.0 equiv) was dissolved in dry CD₂Cl₂ (0.5 mL) in a HPLC vial and taken in a syringe protected from air. Besides that, dry CD₂Cl₂ (0.5 mL) were also taken in a syringe protected from air. Outside the glovebox, both syringes containing GaCl₃ solution and CD₂Cl₂ were cooled down with dry ice. The microwave vial was cooled down to -30 °C and dissolved in cold CD₂Cl₂ (0.5 mL). Afterwards, the cold GaCl₃ solution was added over the mixture in the microwave vial at -30 °C. The sample was kept at -30 °C for 15 minutes and allowed to warm up to room temperature. Followed by the addition of a CD₂Cl₂ solution of diphenylmethane (0.05 mmol, 0.1 mL, 0.5 M). The reaction was opened to air and transferred to a NMR tube. The yield was calculated by integration of the ¹H NMR of the product and the internal standard. Generation of mesityl(methyl) gold(I) carbene followed by addition of cyclohexane at -90 °C also generated 2-(cyclohexylmethyl)-1,3,5-trimethylbenzene **9** together with *E*-1,2-dimesitylethene (*E*-**2b**), *Z*-1,2-dimesitylethene (*Z*-**2b**), 2,4,6-trimethylbenzaldehyde (**8**) and 1,2,3-trimesitylcyclopropane (**3b**). To avoid competitive transformations, gold(I) carbenes **5a-b** were generated in the presence of an excess of cyclohexane at -30 °C.



Scheme S4. CH insertion of cyclohexane by *in situ* generation of gold(I) carbenes. ^[a]Yield determined by ¹H NMR using diphenylmethane as internal standard.

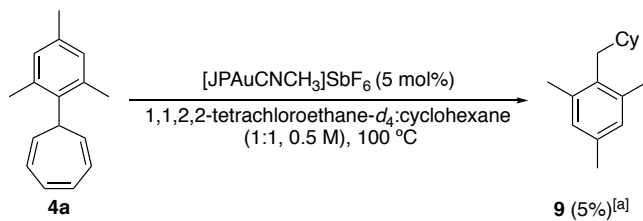
2-(Cyclohexylmethyl)-1,3,5-trimethylbenzene **9** was detected by ¹H NMR and GCMS from the crude reactions of the C–H insertion of cyclohexane. The ¹H NMR data of 2-(cyclohexylmethyl)-1,3,5-trimethylbenzene **9** was identical to the previously reported.⁴

Method B: Gold(I)-promoted CH insertion by retro-Buchner reaction

A microwave vial was charged with 7-mesitylcyclohepta-1,3,5-triene (**4a**) (0.3 mmol) and [JonhPhosAu(NCCH₃)]SbF₆ (5 mol %). 1,1,2,2-Tetrachloroethane-*d*₄ (0.3 mL, 0.5 M) and cyclohexane (0.3 mL, 0.5M) was added via syringe. The vial was capped with a microwave cap with septum and the reaction was heated to 100 °C until 7-mesitylcyclohepta-1,3,5-triene (**4a**) was consumed (12 h). The mixture was allowed to cool down to room temperature, internal

standard was added and it was transferred to a NMR tube. ^1H NMR yield was calculated by integration of the ^1H NMR of the product and the internal standard.

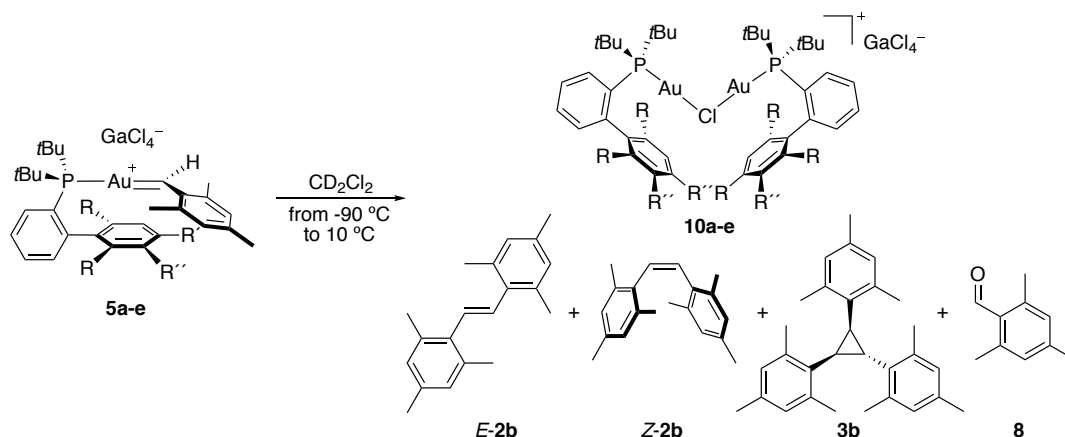
These reactions are carried out in a microwave vial at a temperature higher of the boiling point of cyclohexane.



Scheme S5. C–H insertion of cyclohexane by gold(I)-promoted retro-Buchner reaction. ^[a]Yield determined by ^1H NMR using diphenylmethane as internal standard.

9. Stability and Decomposition Pathways

Mesityl gold(I) carbenes decompose through a bimolecular process generating *E*-1,2-dimesitylethene (**E-2b**) and *Z*-1,2-dimesitylethene (**Z-2b**), cyclopropane (*r*)-1,2,3-trimesitylcyclopropane (**3b**) was also formed *via* cyclopropanation of the previously formed olefins and small amounts of 2,4,6-trimethylbenzaldehyde (**8**) were generated through oxidation by oxygen (Scheme S1). All these organic products were obtained together with the corresponding chloride bridge gold(I) dimer (**10a-e**).



Scheme S6. Decomposition pathways of gold(I) carbenes **5a-e**.

General procedures for the quantification of the decay of gold(I) carbenes in solution

Method A

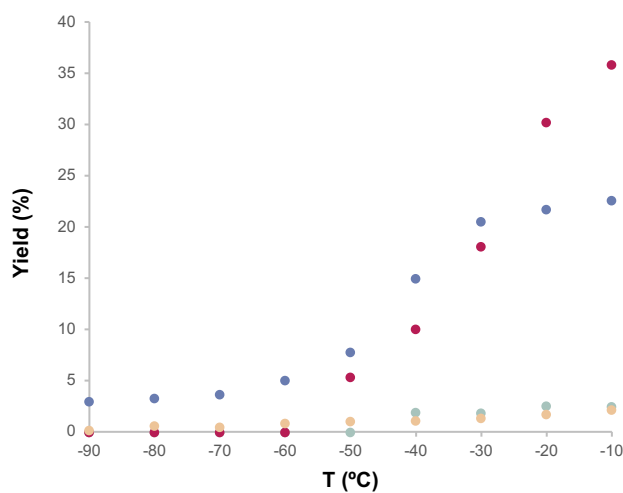
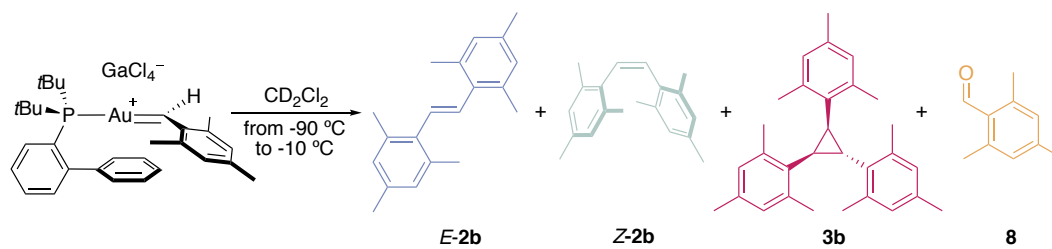
In a glovebox, the corresponding chloromesityl(methyl) gold(I) carbenoid **1a-e** (0.007 mmol) was weighed in an oven-dried standard NMR tube and capped with a rubber septum. Separately, GaCl_3 (1.0 equiv) was dissolved in CD_2Cl_2 (0.4 mL) in a HPLC vial and taken in a syringe with a long needle protected from air. Besides that, CD_2Cl_2 (0.5 mL) and a solution of 1,3,5-trifluoromethylbenzene used as internal standard (0.1 mL, 0.007 mmol, 0.07 M) was taken in a syringe protected from air. Outside the glovebox, the capped NMR tube was cooled down to $-90\text{ }^\circ\text{C}$ in an acetone/liquid nitrogen cooling bath and CD_2Cl_2 (0.5 mL) was injected into the NMR tube. The NMR tube was shaken until the solution was homogeneous. Afterwards, a solution of the internal standard (0.1 mL) was added to the previous solution at $-90\text{ }^\circ\text{C}$. A ^1H NMR was taken at $-90\text{ }^\circ\text{C}$ to calculate the exact amount of chloromesityl(methyl) gold(I) carbenoid in every case. The NMR tube was ejected and cooled down to $-90\text{ }^\circ\text{C}$ in the acetone/liquid nitrogen cooling bath again. Ultimately, the GaCl_3 solution was added over the mixture in the NMR tube at $-90\text{ }^\circ\text{C}$. The solution turned deep red instantaneously. The sample was transferred to the NMR instrument set at $-90\text{ }^\circ\text{C}$ as fast as possible. ^1H and ^{31}P NMR experiments were taken every ten degrees, from $-90\text{ }^\circ\text{C}$ to the mesityl gold(I) carbene decomposition temperature.

Method B

In a glovebox, the corresponding chloromethyl(methyl) gold(I) carbenoid (0.007 mmol) was weighed in an oven-dried standard NMR tube and capped with a rubber septum. Separately, GaCl₃ (1.0 equiv) was dissolved in CD₂Cl₂ (0.4 mL) in a HPLC vial and taken in a syringe with a long needle protected from air. Besides that, CD₂Cl₂ (0.5 mL) and a solution of 1,3,5-trifluoromethylbenzene used as internal standard (0.1 mL, 0.007 mmol, 0.07 M) was taken in a syringe protected from air. Outside the glovebox, the capped NMR tube was cooled down to 0 °C and CD₂Cl₂ (0.5 mL) was injected into the NMR tube. The NMR tube was shaken until the solution was homogeneous. Afterwards, a solution of the internal standard (0.1 mL) was added to the previous solution at 0 °C. Ultimately, the GaCl₃ solution was added over the mixture in the NMR tube at 0 °C. The mixture turned deep red and the color faded away instantaneously. After 10 minutes at 0 °C, the solution was warmed up to room temperature and the yield was calculated by ¹H NMR.

2-Di-*t*-butylphosphinobiphenyl mesityl(methyl) gold(I) carbene (**5a**)

Method A

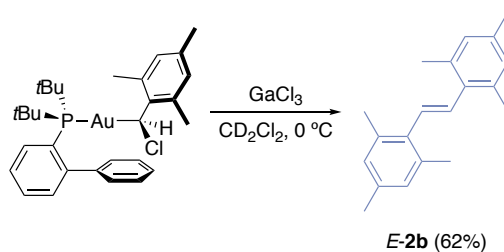


Entry	T ($^\circ\text{C}$)	E-2b yield (%) ^a	Z-2b yield (%) ^a	3b yield (%) ^a	8 yield (%) ^a	Overall Yield (%) ^a
1	-90	3.0	0.0	0.0	> 1.0 (0.2)	3.2
2	-80	3.3	0.0	0.0	> 1.0 (0.6)	3.9
3	-70	3.6	0.0	0.0	> 1.0 (0.5)	4.1
4	-60	5.0	0.0	0.0	> 1.0 (0.8)	5.8
5	-50	7.8	0.0	5.4	1.0	14.2
6	-40	14.9	1.9	10.1	1.1	28.0
7	-30	20.5	1.8	18.1	1.3	41.7
8	-20	21.7	2.5	30.2	1.7	56.1
9	-10	22.6	2.5	35.9	2.2	63.2

^a ^1H NMR yield calculated using 1,3,5-trifluoromethylbenzene as internal standard.

Figure S3. Decay of carbene **5a**.

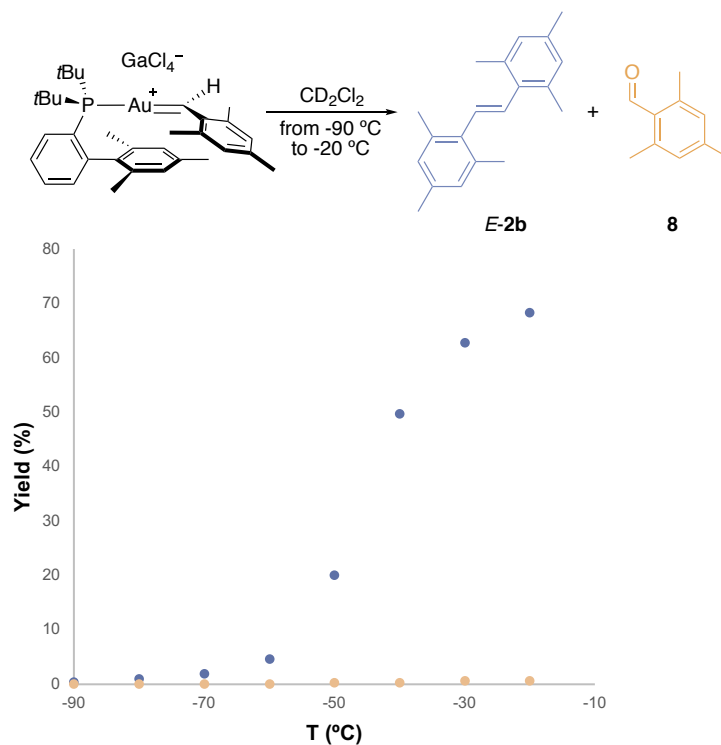
Method B



Scheme S7. Formation of olefin **E-2b** through a bimolecular process.

2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl mesityl(methyl) gold(I) carbene (**5b**)

Method A

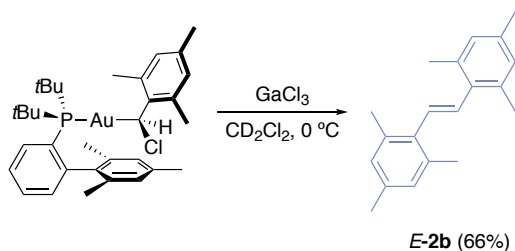


Entry	T (°C)	<i>E</i> - 2b yield (%) ^a	8 yield (%) ^a	Overall Yield (%) ^a
1	-90	< 1.0 (0.3)	0.0	0.3
2	-80	1.0	0.0	1.0
3	-70	1.9	0.0	1.9
4	-60	4.6	0.0	4.6
5	-50	20.0	< 1.0 (0.2)	20.2
6	-40	59.7	< 1.0 (0.2)	59.9
7	-30	62.7	< 1.0 (0.6)	63.3
8	-20	68.3	< 1.0 (0.6)	68.8

^a¹H NMR yield calculated using 1,3,5-trifluoromethylbenzene as internal standard.

Figure S4. Decay of Carbene **5b**.

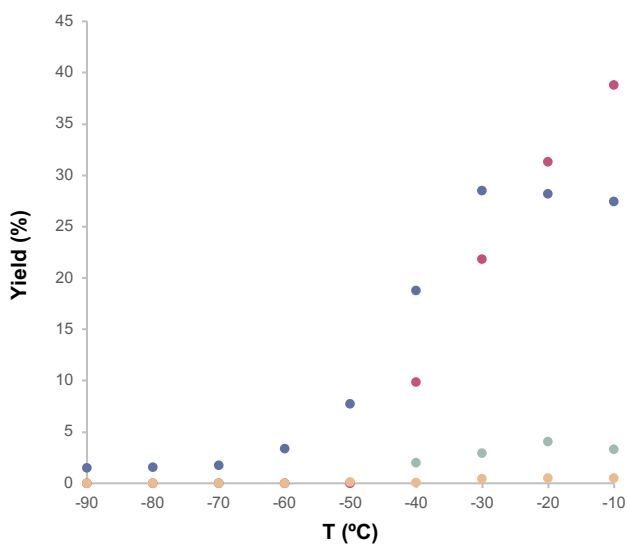
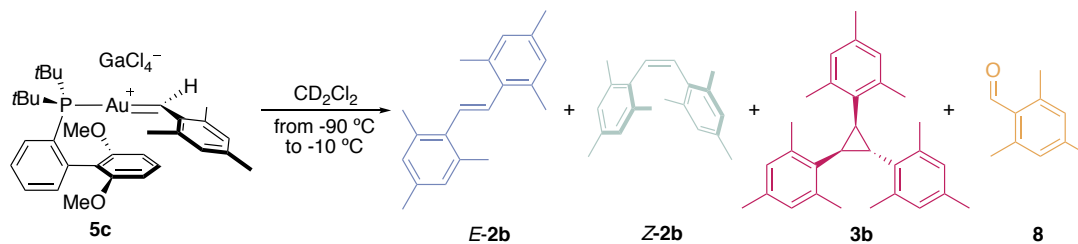
Method B



Scheme S8. Formation of olefin *E*-**2b** through a bimolecular process.

2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl mesityl(methyl) gold(I) carbene (**5c**)

Method A

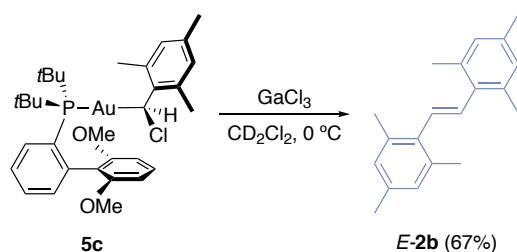


Entry	T (°C)	<i>E</i> - 2b yield (%) ^a	<i>Z</i> - 2b yield (%) ^a	3b yield (%) ^a	8 yield (%) ^a	Overall Yield (%) ^a
1	-90	1.5	0.0	0.0	0.0	1.5
2	-80	1.6	0.0	0.0	0.0	1.6
3	-70	1.7	0.0	0.0	0.0	1.7
4	-60	3.4	0.0	0.0	0.0	3.4
5	-50	7.7	0.0	0.0	< 1.0 (0.2)	7.9
6	-40	18.8	2.0	9.9	< 1.0 (0.1)	30.8
7	-30	28.5	2.9	21.8	< 1.0 (0.4)	53.6
8	-20	28.2	4.1	31.3	< 1.0 (0.5)	64.1
9	-10	27.5	3.3	38.8	< 1.0 (0.5)	70.1

^a¹H NMR yield calculated using 1,3,5-trifluoromethylbenzene as internal standard.

Figure S5. Decay of Carbene **5c**.

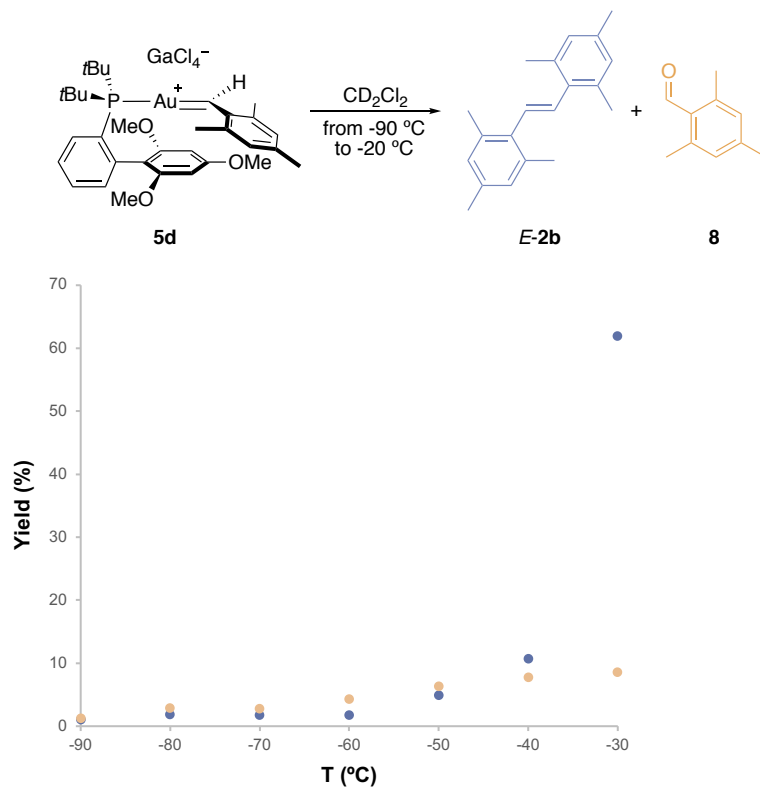
Method B



Scheme S9. Formation of olefin **E-2b** through a bimolecular process.

2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl mesityl(methyl) gold(I) carbene (**5d**)

Method A

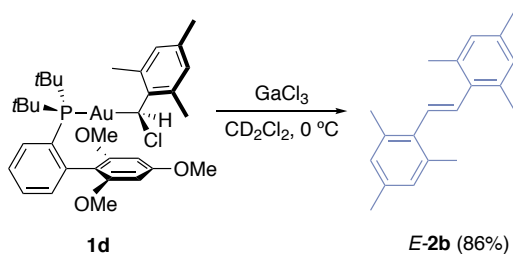


Entry	T ($^\circ\text{C}$)	E-2b yield (%) ^a	8 yield (%) ^a	Overall Yield (%) ^a
1	-90	1.0	1.2	2.2
2	-80	1.9	3.0	4.9
3	-70	1.8	2.8	4.6
4	-60	1.8	4.3	6.1
5	-50	5.0	6.3	11.3
6	-40	10.7	7.8	18.5
7	-30	62.0	8.7	70.6

^a ^1H NMR yield calculated using 1,3,5-trifluoromethylbenzene as internal standard.

Figure S6. Decay of Carbene **5d**.

Method B



Scheme S10. Formation of olefin **E-2b** through a bimolecular process.

2-Di-*t*-butylphosphinonaphthylphenyl mesityl(methyl) gold(I) carbene (**5e**)

Method A

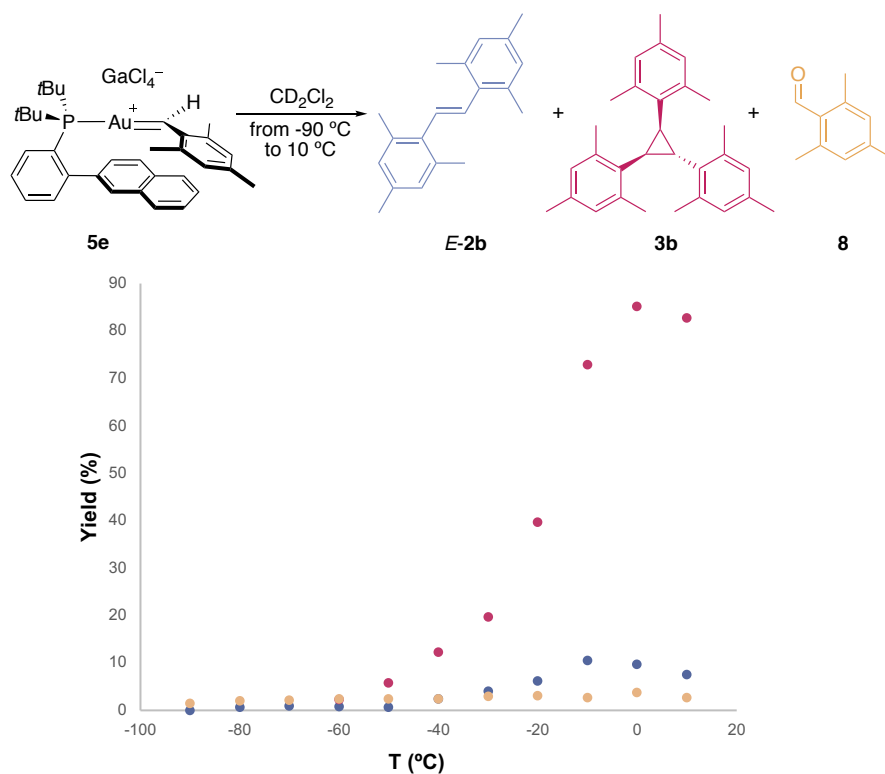


Figure S7. Decay of Carbene **5e**.

Kinetics Measurements

In a glovebox, gold(I) carbenoid **1b** (0.007 mmol) was weighed in an oven-dried standard NMR tube and capped with a rubber septum. Separately, GaCl₃ solution in CD₂Cl₂ (0.4 mL, 0.007 mmol, 0.11 M) was taken out with a Hamilton syringe connected to a long protected from air. Besides that, CD₂Cl₂ (0.5 mL) and a solution of 1,3,5-trifluoromethylbenzene used as internal standard (0.1 mL, 0.007 mmol, 0.07 M) were taken in Hamilton syringes protected from air. Outside the glovebox, the capped NMR tube was cooled down to -90 °C in an acetone/liquid nitrogen cooling bath and CD₂Cl₂ (0.5 mL) was injected into the NMR tube. The NMR tube was shaken until the solution was homogeneous. Afterwards, the internal standard (0.1 mL) was added to the previous solution at -90 °C. Ultimately, the GaCl₃ solution was added over the mixture in the NMR tube at -90 °C. The solution turned deep red instantaneously. The sample was transferred to the NMR instrument set at -40 °C or -35 °C as fast as possible. ¹H experiments were taken every two minutes until full consumption of gold(I) carbene **3b**.

Kinetics at -40 °C

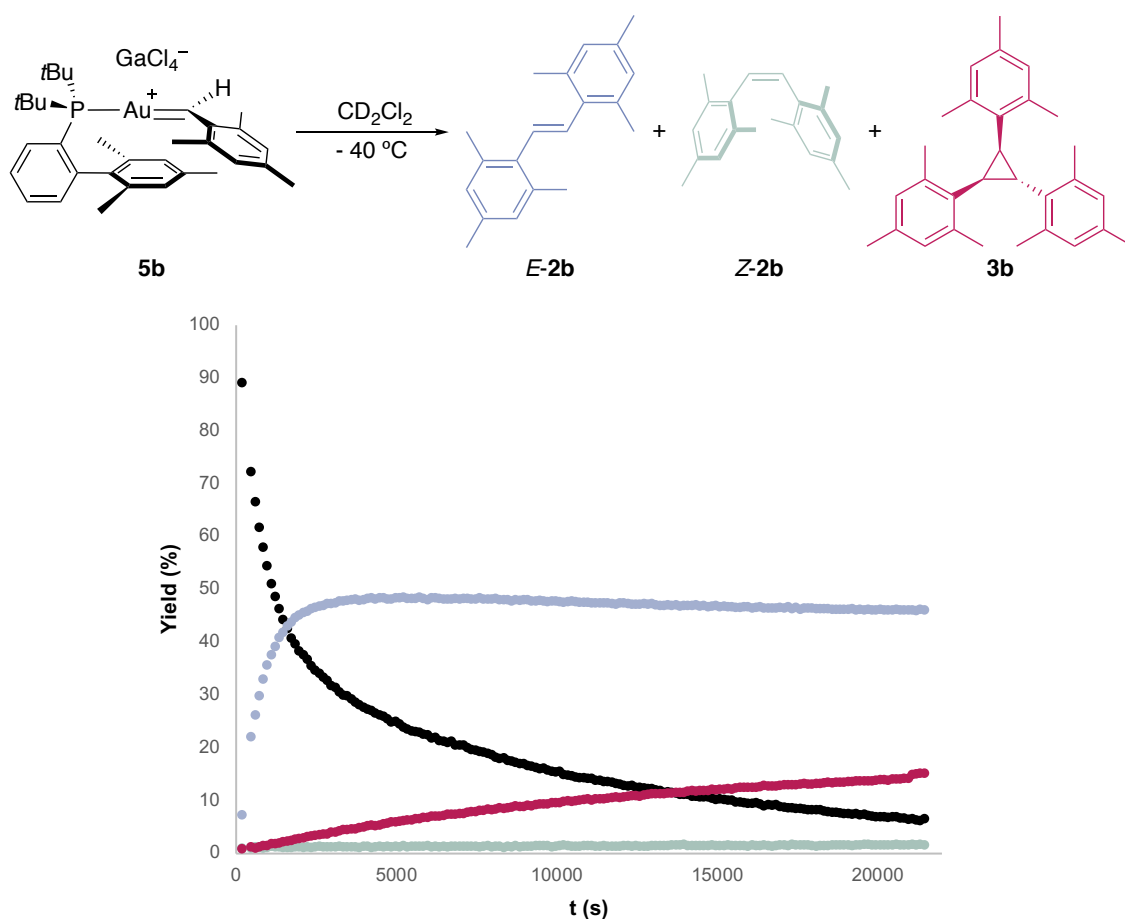


Figure S8. ¹H NMR monitoring of gold(I) carbene **5b** decomposition at -40 °C to generate *E*-**2b**, *Z*-**2b** and **3b**.

Considering $\Delta\Delta G^{\ddagger}_{trans-cis\text{cyclopropanation}} = 8.5$ kcal/mol between the cyclopropanation of *E*-**2b** and *Z*-

2b by gold(I) carbene **5b** to give cyclopropane **3b** (see DFTs section, Figures SX and SX), we could assume that cyclopropane **3b** is only being formed *via* cyclopropanation of *E-2b* at -40 °C. Based on this assumption, the moles of **5b** related to the formation of *E-2b* at any time were calculated using equation S1.

$$\text{mmol } \mathbf{5b} = \text{mmol } \mathbf{5b}_{\text{remaining}} + (2 * \text{mmol } Z - \mathbf{2b}) + \text{mmol } \mathbf{3b}$$

Equation 1. Where $\text{mmol } \mathbf{5b} = \text{mmol } \mathbf{5b}_{\text{initial}} (0.007) - \text{mmol } \mathbf{5b} \text{ consumed to form } E\text{-}\mathbf{2b} \text{ at time } t$, $\text{mmol } \mathbf{5b}_{\text{remaining}} = \text{mmol } \mathbf{5b} \text{ remaining at time } t$, $\text{mmol } Z\text{-}\mathbf{2b} = \text{mmol of } Z\text{-}\mathbf{5a} \text{ formed at time } t$ and $\text{mmol } \mathbf{3b} = \text{mmol of cyclopropane } \mathbf{3b} \text{ at time } t$.

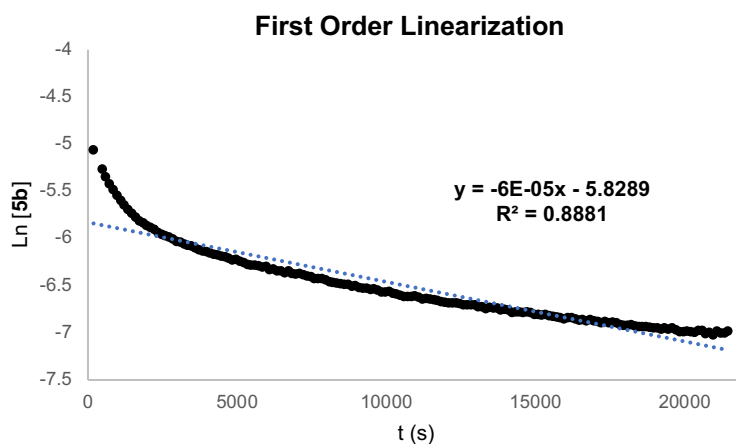


Figure S9. First order linearization plot for the consumption of gold(I) carbene **5b** in the formation of *E-2b* at -40 °C.

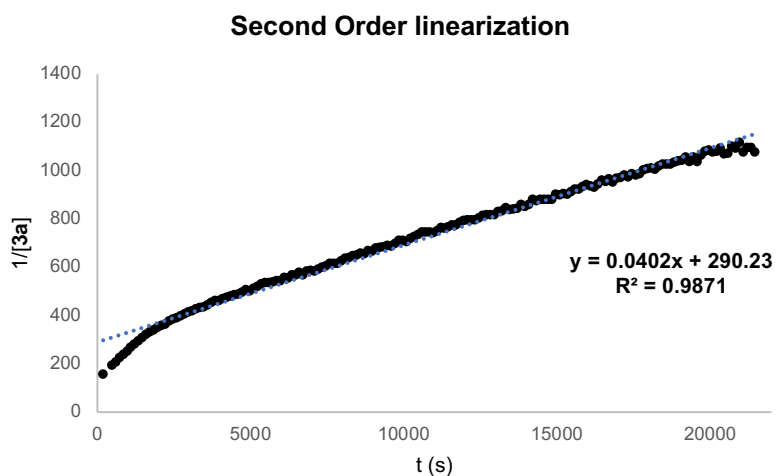


Figure S10. Second order linearization plot for the consumption of gold(I) carbene **5b** in the formation of *E-2b* at -40 °C.

Kinetics at -35 °C

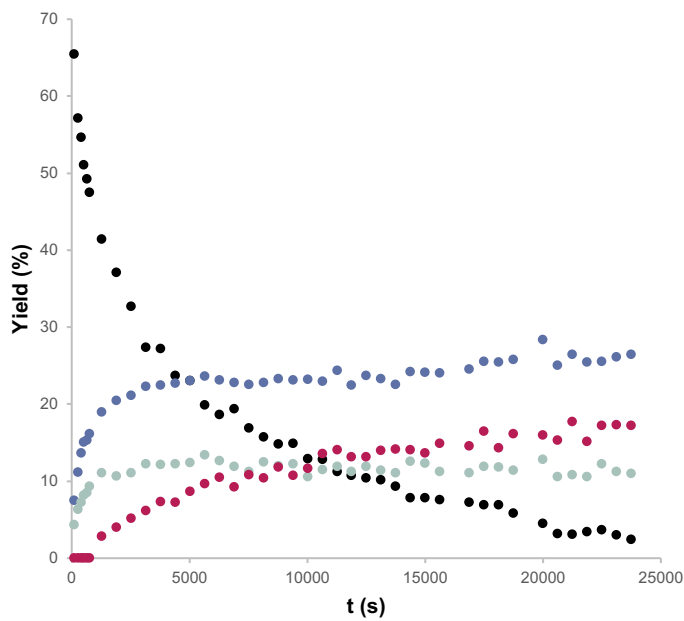
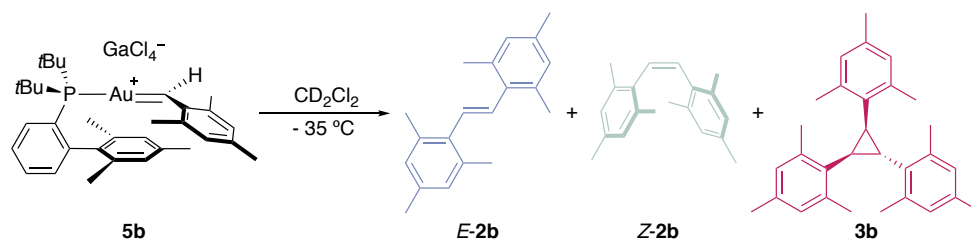


Figure S11. ^1H NMR monitoring of gold(I) carbene **5b** decomposition at $-35\text{ }^\circ\text{C}$ to generate *E*-**2b**, *Z*-**2b** and **3b**.

Considering $\Delta\Delta G^\ddagger_{\text{trans-cis-cyclopropanation}} = 8.5\text{ kcal/mol}$ between the cyclopropanation of *E*-**2b** and *Z*-**2b** by gold(I) carbene **5b** (see DFTs section, Figures SX and SX), we could assume that cyclopropane **3b** is only being formed *via* cyclopropanation of *E*-**2b** at $-35\text{ }^\circ\text{C}$. Based on this assumption, the moles of **5b** related to the formation of *Z*-**2b** at any time were calculated using equation S1.

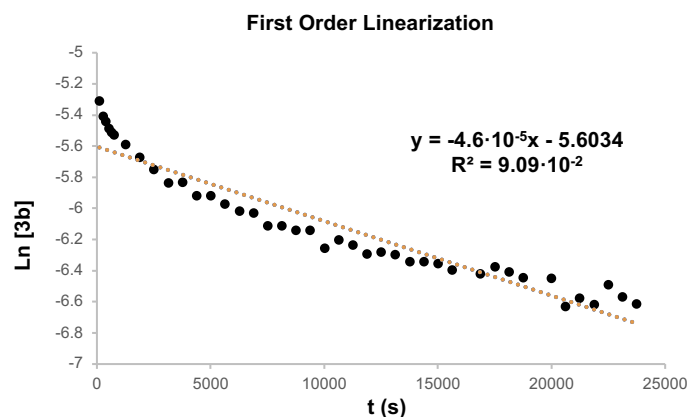


Figure S12. First order linearization plot for the change of gold(I) carbene **3b** in the formation of *trans*-**5a**.

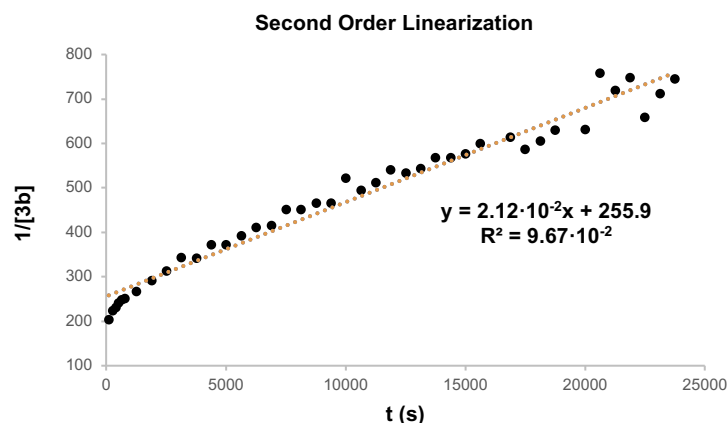


Figure S13. Second order linearization plot for the change of gold(I) carbene **3b** in the formation of *trans*-**5a**.

Eyring Plot

Table S2. Calculated k_{obs} at different temperatures.

T (K)	k_{obs} ($\text{M}^{-1}\text{s}^{-1}$)	1/T	$\text{Ln}(k_{\text{obs}}/T)$
233	0.0402	0.004291845	-8.664926737
235	0.0287	0.004255319	-9.01044367
238	0.0159	0.004201681	-9.613706843
240	0.010	0.004166667	-10.08580911

Measured Activation parameters:

$$\Delta H^\ddagger = -22.5 \text{ Kcal/mol}$$

$$\Delta S^\ddagger = -156.4 \text{ cal/Kmol} \cdot \text{k}$$

$$\Delta G^\ddagger = 24.1 \text{ Kcal/mol}$$

A negative ΔH^\ddagger is related to a decreased in the reaction rate when temperature increases. This fact can be explained considering that when temperature increases cyclopropanation together with *cis*-dimerization takes place. Therefore, those activation parameters cannot be compared to

the ones calculated by DFTs because they have been measured under conditions in which carbene *trans*-dimerization is not the only carbene consumption pathway.

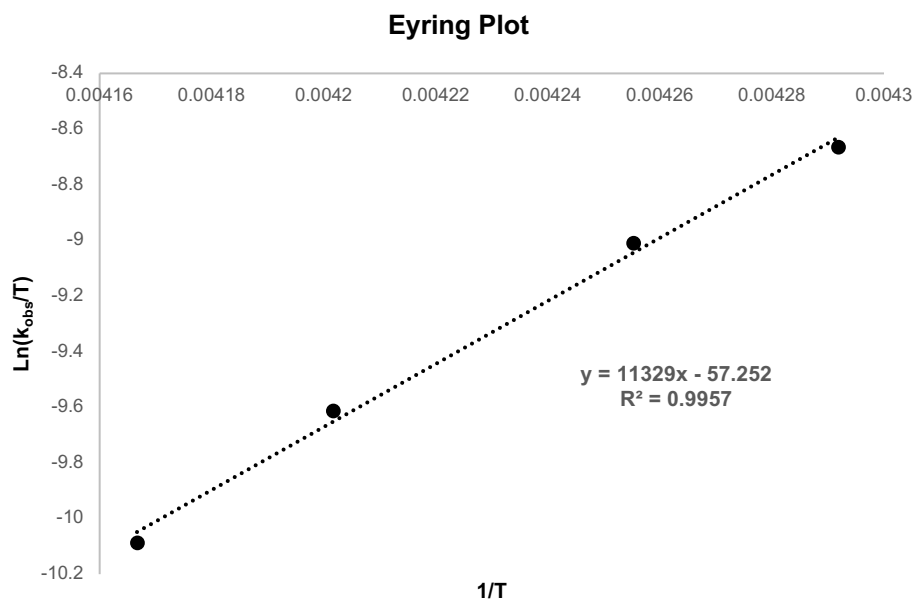


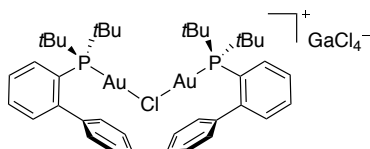
Figure S14. Eyring plot.

Characterization of Chloride Bridge Digold(I) Complexes

General procedure for the synthesis of chloride bridge digold(I) complexes:

In a Schlenk in the glovebox, the corresponding gold(I) chloride complex was dissolved in dry CH_2Cl_2 . Followed by the one pot addition of a dichloromethane solution of GaCl_3 at 25 °C. The Schlenk was taken out from the glovebox and stirred under argon. After 15 minutes, the solution was concentrated to dryness in the Schlenk line giving a solid that was washed with pentane (x3). The complexes were stored in the glovebox.

[(2-Di-*t*-butylphosphinobiphenylAu)₂Cl]GaCl₄ (**10a**)



Complex **10a** was synthesized according to the general procedure from 2-di-*t*-butylphosphinobiphenyl gold(I) chloride (**6a**) (50 mg, 0.094 mmol) and GaCl_3 (8.3 mg, 0.047 mmol). A white solid was obtained in 52% yield (60 mg, 0.048 mmol). X-ray quality crystals were obtained layering a CD_2Cl_2 solution of the complex with dry pentane under argon at -20 °C.

¹H NMR (400 MHz, CD_2Cl_2) δ 7.93 – 7.84 (m, 2H), 7.64 – 7.56 (m, 4H), 7.55 – 7.48 (m, 2H), 7.43 – 7.35 (m, 4H), 7.34 – 7.28 (m, 2H), 7.17 – 7.11 (m, 4H), 1.40 (d, $J(^1\text{H}-^{31}\text{P}) = 16.1$ Hz, 36H). **¹³C NMR** (101 MHz, CD_2Cl_2) δ 149.8 (d, $J(^{13}\text{C}-^{31}\text{P}) = 12.4$ Hz), 143.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.7$ Hz), 133.9 (d, $J(^{13}\text{C}-^{31}\text{P}) = 3.3$ Hz), 133.8, 131.9, 130.0, 129.3, 128.8, 128.1 (d, $J(^{13}\text{C}-^{31}\text{P}) = 7.3$ Hz), 125.0 (d, $J(^{13}\text{C}-^{31}\text{P}) = 49.5$ Hz), 38.7 (d, $J(^{13}\text{C}-^{31}\text{P}) = 26.0$ Hz), 31.3 (d, $J(^{13}\text{C}-^{31}\text{P}) = 6.4$ Hz). **³¹P NMR** (162 MHz, CD_2Cl_2) δ 64.68. **HRMS** (ESI+) calculated for $\text{C}_{40}\text{H}_{54}\text{Au}_2\text{ClP}_2$ (M-GaCl₄)⁺: 1025.2715; found: 1025.2667.

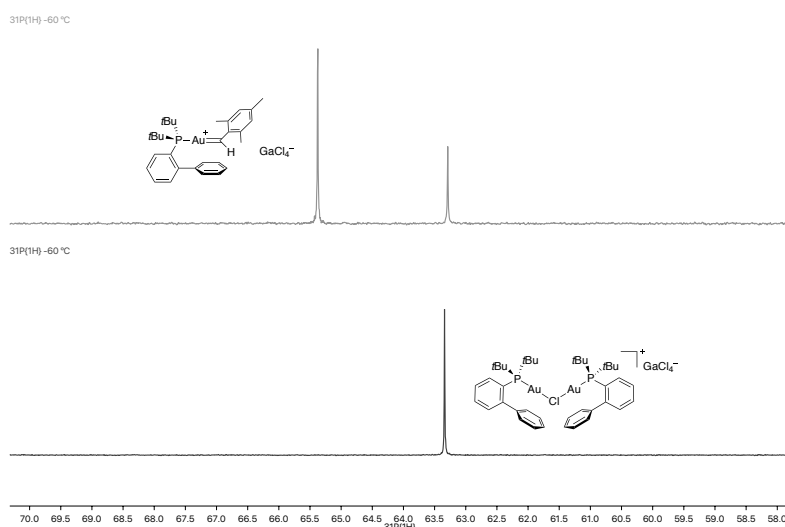
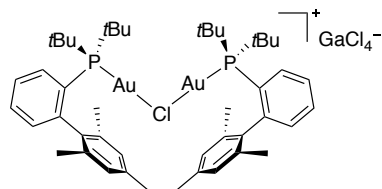


Figure S15. Top: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of the generation of 2-di-*t*-butylphosphinobiphenyl mesityl(methyl) gold(I) carbene (**5a**) at $-60\text{ }^\circ\text{C}$. Bottom: $^{31}\text{P}\{^1\text{H}\}$ NMR spectrum of an authentic sample of [(2-di-*t*-butylphosphinobiphenylAu)₂Cl]GaCl₄ (**10a**) at $-60\text{ }^\circ\text{C}$.

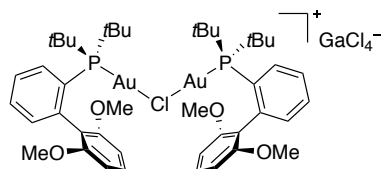
[(2-Di-*t*-butyl-2',4',6'-trimethylphosphinobiphenylAu)₂Cl]GaCl₄ (10b**)**



Complex X was synthesized according to the general procedure from 2-di-*t*-butyl-2',4',6'-trimethylphosphinobiphenyl gold(I) chloride (**6b**) (30 mg, 0.052 mmol) and GaCl₃ (4.62 mg, 0.026 mmol). A white solid was obtained in 43% yield (30 mg, 0.023 mmol).

^1H NMR (400 MHz, CD₂Cl₂) δ 7.93 – 7.85 (m, 2H), 7.68 – 7.60 (m, 2H), 7.60 – 7.52 (m, 2H), 7.21 (ddd, J = 7.8, 4.7, 1.6 Hz, 2H), 6.92 (s, 4H), 2.40 (s, 6H), 1.90 (s, 12H), 1.42 (d, J (^1H - ^{31}P) = 16.1 Hz, 36H). ^{13}C NMR (101 MHz, CD₂Cl₂) δ 148.9 (d, J (^{13}C - ^{31}P) = 12.8 Hz), 138.9, 138.3 (d, J (^{13}C - ^{31}P) = 6.2 Hz), 136.6, 134.8 (d, J (^{13}C - ^{31}P) = 3.9 Hz), 134.4 (d, J (^{13}C - ^{31}P) = 8.0 Hz), 132.8, 129.7, 127.8 (d, J (^{13}C - ^{31}P) = 7.4 Hz), 126.4 (d, J (^{13}C - ^{31}P) = 47.9 Hz), 39.1 (d, J (^{13}C - ^{31}P) = 26.8 Hz), 31.8 (d, J (^{13}C - ^{31}P) = 6.2 Hz), 22.0, 21.7. ^{31}P NMR (162 MHz, CD₂Cl₂) δ 63.78. HRMS (ESI+) calculated for C₄₆H₆₆Au₂ClP₂ (M-GaCl₄)⁺: 1109.3654; found: 1109.3687.

[(2-Di-*t*-butyl-2',6'-dimethoxyphosphinobiphenylAu)₂Cl]GaCl₄ (10c**)**



Complex X was synthesized according to the general procedure from 2-di-*t*-butyl-2',6'-dimethoxyphosphinobiphenyl gold(I) chloride (**6c**) (20 mg, 0.034 mmol) and GaCl₃ (2.98 mg, 0.017 mmol). A white solid was obtained in 28.3% yield (13 mg, 0.010 mmol). X-ray quality crystals were from the decomposition of gold(I) carbene **5c** at $-90\text{ }^\circ\text{C}$ in toluene.

^1H NMR (400 MHz, CD₂Cl₂) δ 7.91 – 7.82 (m, 1H), 7.63 – 7.56 (m, 1H), 7.55 – 7.45 (m, 2H), 7.18 (ddd, J = 7.7, 4.4, 1.6 Hz, 1H), 6.61 (d, J = 8.4 Hz, 2H), 3.64 (s, 6H), 1.38 (d, J (^1H - ^{31}P) = 16.0 Hz, 18H). ^{13}C NMR (126 MHz, CD₂Cl₂) δ 158.1, 143.6 (d, J (^{13}C - ^{31}P) = 12.0 Hz), 134.5 (d, J (^{13}C - ^{31}P) = 7.8 Hz), 134.1 (bs), 132.0 (bs), 130.8, 127.4 (d, J (^{13}C - ^{31}P) = 6.0 Hz), 119.9 (d, J (^{13}C - ^{31}P) = 7.0 Hz), 104.7, 55.8, 38.4 (d, J (^{13}C - ^{31}P) = 26.6 Hz), 31.3 (d, J (^{13}C - ^{31}P) = 6.7 Hz). ^{31}P NMR (203 MHz, CD₂Cl₂) δ 65.79 (bs). HRMS (ESI+) calculated for C₄₄H₆₂Au₂ClP₂ (M-GaCl₄)⁺: 1145.3138; found: 1145.3157.

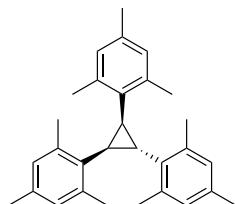
Characterization of Detected Organic Products

E-1,2-dimesitylene (**E-2b**), *Z*-1,2-dimesitylene (**Z-2b**), 2,4,6-trimethylbenzaldehyde (**8**) and (*r*)-1,2,3-trimesitylcyclopropane (**3b**) were detected by ^1H NMR and GCMS as organic

products from the decomposition of mesityl(methyl) gold(I) carbenes **5a-e** from the reaction crudes.

The ^1H NMR data of *E*-1,2-dimesitylethene (*E*-**2b**)⁵ and *Z*-1,2-dimesitylethene (*Z*-**2b**)⁵ were identical to the previously reported. The ^1H NMR data of 2,4,6-trimethylbenzaldehyde (**8**) was compared to an original sample purchased from commercial sources. However, 1,2,3-trimesitylcyclopropane (**3b**) was isolated from the reaction crude and characterized.

1,2,3-trimesitylcyclopropane (3b)



2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl mesityl(methyl) gold(I) carbene (**5c**) was generated according to the general procedure for the generation of gold(I) carbenes in solution from 2-di-*t*-butylphosphino-2',6'-dimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (**1c**) (20 mg, 0.028 mmol) and GaCl₃ (5.84 mg, 0.033 mmol) at -90 °C. The tube NMR was allowed to warm up to room temperature and the solution was filtered through a small pad of celite. Cyclopropane **3b** was obtained from the reaction crude as a yellowish oil after purification by preparative TLC with pentane as eluent.

^1H NMR (500 MHz, CD₂Cl₂) δ 6.83 (s, 2H), 6.70 (s, 4H), 3.79 (t, J = 7.1 Hz, 1H), 2.63 (d, J = 7.1 Hz, 2H), 2.36 (s, 6H), 2.24 (s, 3H), 2.22 (s, 12H), 2.18 (s, 6H). ^{13}C NMR (126 MHz, CD₂Cl₂) δ 137.8, 137.5, 136.1, 135.41, 135.0, 132.2, 129.8, 129.3, 31.9, 26.3, 21.4, 20.7, 20.4, 20.3. The configuration was assigned by COSY, ^1H - ^{13}C HSQC and NOESY. HRMS (APCI+) calculated for C₃₀H₃₇ (M+H)⁺: 397.2886; found: 397.2890.

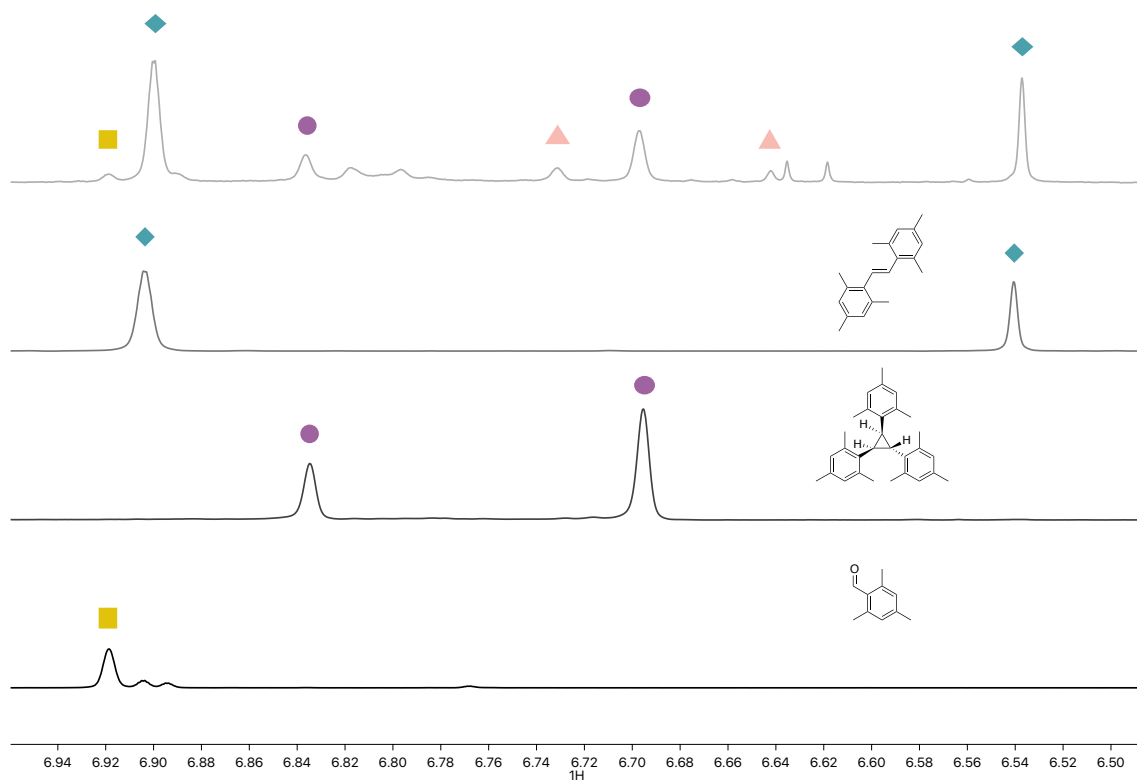
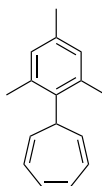


Figure S16. From top to bottom: a) ^1H NMR spectrum after a sample of **5c** was allowed to warm up to room temperature. Peaks labelled with salmon triangles correspond to **Z-2b**. b) ^1H NMR spectrum of an authentic sample of **E-2b**. c) ^1H NMR spectrum of an authentic sample of **3b**. d) ^1H NMR spectrum of an authentic sample of **8**.

10. Alkene Cyclopropanation

Synthesis of Cycloheptatriene

7-mesitylcyclohepta-1,3,5-triene (**4a**)



This compound was prepared following a reported procedure for the synthesis of cyclohepta-1,3,5-trienes.⁶ An oven-dried two-neck round-bottom flask equipped with a condenser was charged with magnesium turnings (243 mg, 10.0 mmol), dry THF (30 mL) and two drops of 1,2-dibromoethane. A solution of 2-bromo-1,3,5-trimethylbenzene (995 mg, 5 mmol) in dry THF (10 mL) was added slowly over a period of 30 minutes at room temperature. The mixture was heated up to 70 °C for 1 h and then allowed to cool down to room temperature. Then tropylium tetrafluoroborate (1.335 g, 7.5 mmol) was added in one portion and the reaction was stirred at room temperature for 14 h. Then, the mixture was washed with sat. NH₄Cl solution and extracted with ethyl acetate. The combined organic extracts were dried over MgSO₄, filtered and concentrated *in vacuo*. 7-Mesitylcyclohepta-1,3,5-triene (**4a**) was obtained as a white solid in 40% yield (420 mg, 2 mmol) after purification by flash column chromatography using cyclohexane as eluent.

¹H NMR (300 MHz, CDCl₃) δ 6.90 (s, 2H), 6.61 (t, *J* = 3.3 Hz, 2H), 6.21 – 6.12 (m, 2H), 5.38 – 5.27 (m, 2H), 3.50 – 3.41 (m, 1H), 2.28 (s, 9H). ¹³C NMR (126 MHz, CDCl₃) δ 137.3, 136.5, 135.9, 130.9, 130.0, 129.3, 124.7, 40.4, 27.1, 21.6, 20.9. HRMS (APCI+) calculated for C₁₆H₁₉ (M+H): 211.1481; found: 211.1480.

General procedure for the gold(I)-promoted alkene cyclopropanation

Method A: Generation of mesityl(methyl) gold(I) carbenes in the presence of alkenes

In a glovebox, the corresponding chloromesityl(methyl) gold(I) carbenoid (0.007 mmol) was weighed in an oven-dried microwave vial and capped. Separately, GaCl₃ (1 equiv) was dissolved in dry CD₂Cl₂ (0.3 mL) in a HPLC vial and taken in a syringe protected from air. A solution of the corresponding alkene (10 equiv) in dry CD₂Cl₂ (0.2 mL) was prepared and taken in a syringe protected from air. Besides that, dry CD₂Cl₂ (0.5 mL) was also taken in a syringe protected from air. Outside the glovebox, the microwave vial was cooled down to -90 °C and cold CD₂Cl₂ was added. The vial was shaken until the solution was homogenous. Afterwards, the cold GaCl₃ solution was injected into the microwave vial at -90 °C. Followed by the addition of the alkene solution at -90 °C. The deep red color corresponding to the carbene complexes faded away as soon as the alkene solution was added due to the fast cyclopropanation reaction in all cases. The sample was kept at -90 °C for 2 minutes and allowed to warm up to room temperature. Followed by the addition of a CD₂Cl₂ solution of diphenylmethane (0.05 mmol,

0.1 mL, 0.5 M). The reaction was opened to air and transferred to a NMR tube. The yield was calculated by integration of the ^1H NMR of the cyclopropanes and the internal standard.

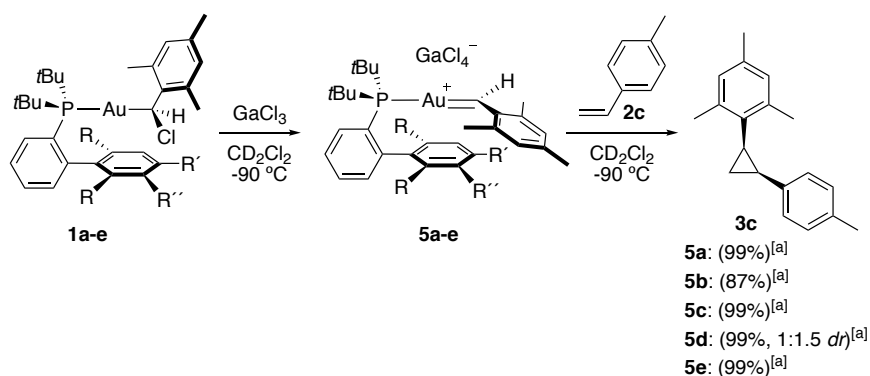
Method B: Gold(I)-catalyzed cyclopropanation by retro-Buchner reaction

A microwave vial was charged with 7-mesitylcyclohepta-1,3,5-triene (**4a**) (0.2 mmol), the corresponding alkene (0.4 mmol) and $[\text{JonhPhosAu}(\text{NCCH}_3)]\text{SbF}_6$ (5 mol %). 1,2-Dichloroethane (0.5 M) was added via syringe and the vial was capped with a microwave cap with septum. The reaction was heated to 100 °C until 7-mesitylcyclohepta-1,3,5-triene (**4a**) was consumed (6-24 h). The reaction was allowed to cool down to room temperature, filtered through a pad of celite and concentrated *in vacuo*. ^1H NMR yield was calculated by integration of the ^1H NMR of the cyclopropanes and the internal standard.

These reactions are carried out in a microwave vial at a temperature higher of the boiling point of 1,2-dichloroethane.

Cyclopropanation of tolylstyrene (2c)

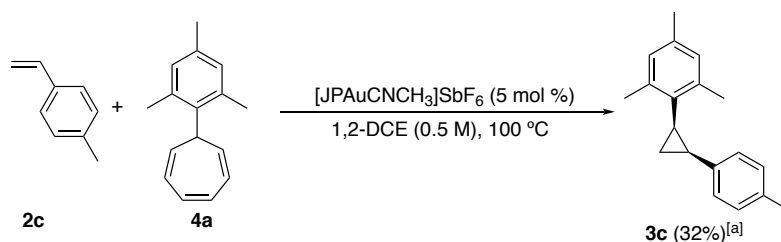
Method A



Scheme S11. Cyclopropanation of tolylstyrene (**2c**) by *in situ* generated gold(I) carbenes **5a-e**.

^[a]Yield determined by ^1H NMR using diphenylmethane as internal standard.

Method B

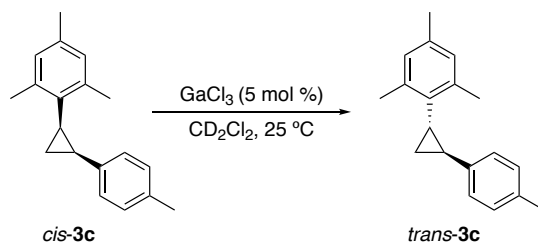


Scheme S12. Cyclopropanation of tolylstyrene by gold(I)-catalyzed retro-Buchner reaction.

^[a]Yield determined by ^1H NMR using diphenylmethane as internal standard.

GaCl₃ Catalyzed Isomerization

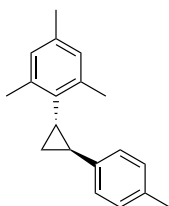
Table S3. ¹H NMR monitoring of the *cis* to *trans* isomerization of **3c**.



Entry	t (s)	<i>cis</i> - 3c (mmol) ^[a]	<i>trans</i> - 3c (mmol) ^[a]
1	0	0.020	0
2	352	0.016	0.004
3	906	0.014	0.006
4	1829	0.013	0.007
5	10529	0.004	0.016

^[a] mmol calculated by ¹H NMR using diphenylmethane as internal standard.

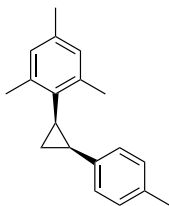
Cyclopropane *trans*-**3c**



Cyclopropane *trans*-**3c** was synthesized according to method A from 1-methyl-4-vinylbenzene (10 equiv), the corresponding chloromesityl(methyl) gold(I) carbenoid (5 mg) and GaCl₃ (1.2 equiv). ¹H NMR yield was calculated from the reaction crude. A colorless oil was obtained after purification by preparative TLC using pentane as eluent.

¹H NMR (500 MHz, CD₂Cl₂) δ 7.13 – 7.04 (m, 4H), 6.80 (s, 2H), 2.33 (s, 6H), 2.32 (s, 3H), 2.22 (s, 3H), 1.99 – 1.93 (m, 1H), 1.90 (dt, *J* = 8.8, 5.5 Hz, 1H), 1.39 (ddd, *J* = 8.8, 5.5, 4.8 Hz, 1H), 1.18 (ddd, *J* = 8.8, 6.6, 4.8 Hz, 1H). ¹³C NMR (126 MHz, CD₂Cl₂) δ 140.3, 138.4, 135.6, 135.4, 135.0, 128.9, 128.6, 125.2, 25.5, 24.7, 20.6, 20.5, 20.5, 19.3. The configuration was assigned by COSY, NOESY, ¹H-¹³C HSQC, ¹H-¹³C HMBC. HRMS (APCI+) calculated for C₁₉H₂₃ (M+H)⁺: 251.1794; found: 251.1793.

Cyclopropane *cis*-**3c**



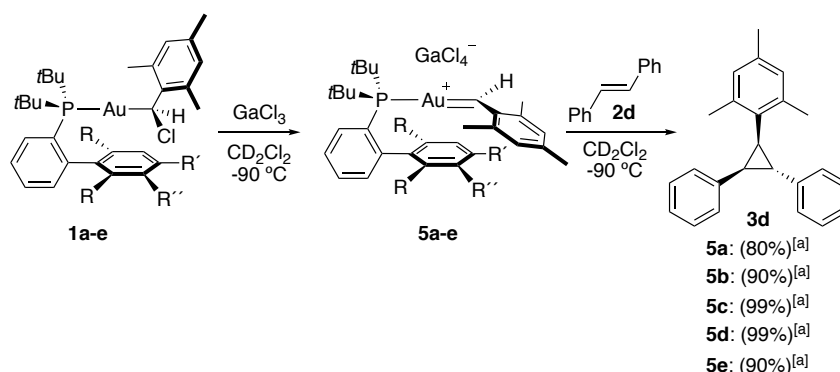
Cyclopropane *cis*-**3c** was synthesized according to method B from 1-methyl-4-vinylbenzene (47.3 mg, 0.4 mmol), 7-mesitylcyclohepta-1,3,5-triene (**4a**) (42.1 mg, 0.2 mmol) and

[JonhPhosAu(NCCH₃)]SbF₆ (7.7 mg, 0.01 mmol). 32% ¹H NMR yield was calculated from the crude. A colorless oil was obtained in 20% yield (10 mg, 0.04 mmol) after purification by preparative TLC using pentane as eluent.

¹H NMR (500 MHz, CDCl₃) δ 6.84 – 6.80 (m, 2H), 6.71 (s, 2H), 6.55 – 6.50 (m, 2H), 2.37 – 2.10 (m, 14H), 1.73 – 1.66 (m, 1H), 1.10 – 1.05 (m, 1H). ¹³C NMR (126 MHz, CDCl₃) δ 139.1, 138.1, 135.6, 134.4, 131.2, 128.8, 128.2, 126.3, 23.3, 22.9, 21.1, 21.0, 20.9, 17.8. The configuration was assigned by COSY, NOESY, ¹H-¹³C HSQC, ¹H-¹³C HMBC. HRMS (APCI+) calculated for C₁₉H₂₃ (M+H)⁺: 251.1794; found: 251.1795.

Cyclopropanation of *trans*-stilbene (**2d**)

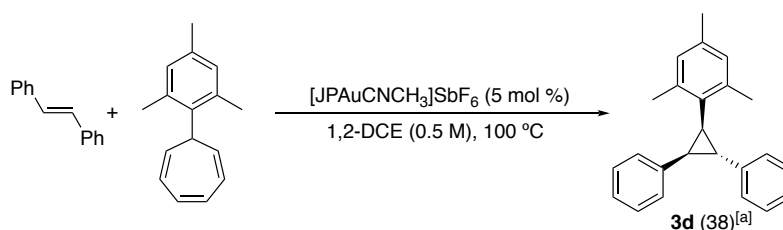
Method A



Scheme S13. Cyclopropanation of *trans*-stilbene **2c** by *in situ* generated gold(I) carbenes **5a-e**.

^[a]Yield determined by ¹H NMR using diphenylmethane as internal standard.

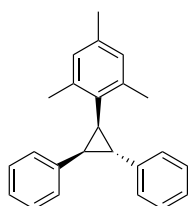
Method B



Scheme S14. Cyclopropanation of *trans*-stilbene by gold(I)-catalyzed retro-Buchner reaction.

^[a]Yield determined by ¹H NMR using diphenylmethane as internal standard.

Cyclopropane **3d**



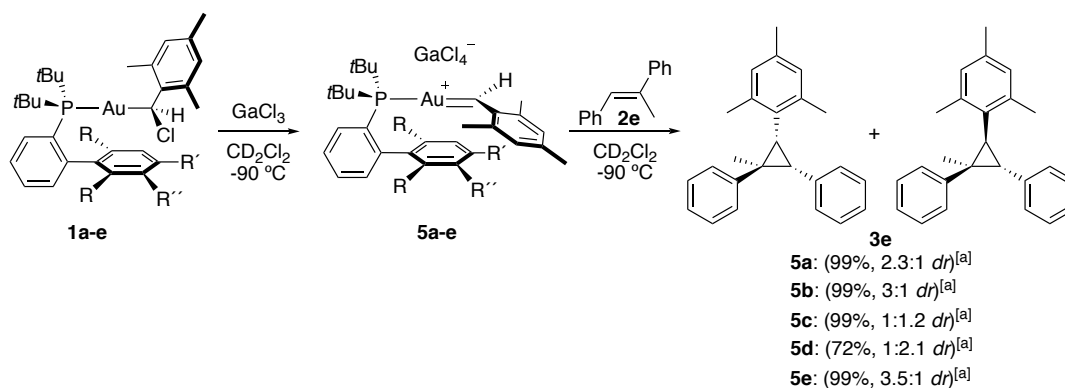
Cyclopropane **3d** was synthesized according to method B from *trans*-stilbene (72 mg, 0.4 mmol), 7-mesitylcyclohepta-1,3,5-triene (**4a**) (42.1 mg, 0.2 mmol) and

[JonhPhosAu(NCCH₃)]SbF₆ (7.7 mg, 0.01 mmol). 38% ¹H NMR yield was calculated from the crude. A yellowish oil was obtained in 25% yield (15.5 mg, 0.05 mmol) after purification by preparative TLC using pentane as eluent. Cyclopropane **3d** was also obtained by method A.

¹H NMR (400 MHz, CDCl₃) δ 7.39 – 7.33 (m, 2H), 7.32 – 7.28 (m, 2H), 7.26 – 7.21 (m, 1H), 7.09 – 7.03 (m, 3H), 6.76 (bs, 2H), 6.73 – 6.68 (m, 2H), 2.78 – 2.71 (m, 1H), 2.64 (dd, *J* = 9.0, 5.4 Hz, 1H), 2.54 (dd, *J* = 7.0, 5.4 Hz, 1H), 2.24 (s, 3H), 2.21 – 2.09 (m, 6H). ¹³C NMR (101 MHz, CDCl₃) δ 142.2, 140.1, 138.3, 135.9, 130.3, 128.9, 128.7, 128.5, 127.5, 126.5, 126.0, 125.4, 35.6, 35.5, 32.6, 21.0, 20.9, 20.6. The configuration was assigned by COSY, NOESY, ¹H-¹³C HSQC, ¹H-¹³C HMBC. HRMS (APCI+) calculated for C₂₄H₂₅ (M+H)⁺: 313.1951; found: 313.1948.

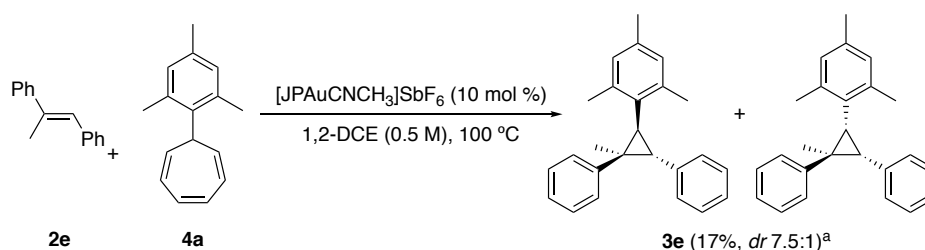
Cyclopropanation of (*E*)-prop-1-ene-1,2-diylidibenzene (**2e**)

Method A



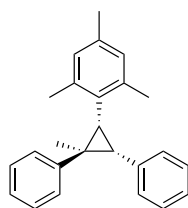
Scheme S15. Cyclopropanation of (*E*)-prop-1-ene-1,2-diylidibenzene (**2e**) by *in situ* generated gold(I) carbenes **5a-e**. ^[a]Yield determined by ¹H NMR using diphenylmethane as internal standard.

Method B



Scheme S16. Cyclopropanation of (*E*)-prop-1-ene-1,2-diylidibenzene (**2e**) by gold(I)-catalyzed retro-Buchner reaction. ^[a]Yield determined by ¹H NMR using diphenylmethane as internal standard.

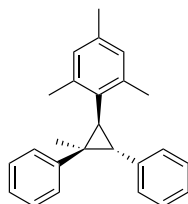
Cyclopropane 3e



Cyclopropane **3e** was synthesized according to method A from (*E*)-prop-1-ene-1,2-diyldibenzene (10 equiv), the corresponding chloromesityl(methyl) gold(I) carbenoid (5 mg) and GaCl₃ (1.2 equiv). ¹H NMR yield was calculated from the reaction crude. Both enantiomers could be separately after two TLC plates in a row with pentane as eluent. Yellowish oil.

¹H NMR (500 MHz, CD₂Cl₂) δ 7.52 – 7.47 (m, 2H), 7.39 – 7.34 (m, 2H), 7.26 – 7.21 (m, 1H), 7.13 – 7.09 (m, 3H), 6.85 (s, 2H), 6.81 – 6.75 (m, 2H), 3.00 (d, *J* = 9.7 Hz, 1H), 2.56 (d, *J* = 9.7 Hz, 1H), 2.29 (s, 3H), 2.21 (s, 6H), 1.25 (s, 3H). ¹³C NMR (126 MHz, CD₂Cl₂) δ 149.6, 139.5, 135.7, 129.9, 128.9, 128.8, 128.5, 127.4, 126.8, 125.8, 125.1, 36.2, 31.7, 31.3, 29.7, 20.6 (d, *J* = 1.7 Hz), 17.9. A quaternary carbon is missing. The configuration was assigned by COSY, NOESY, GOESY, ¹H-¹³C HSQC, ¹H-¹³C HMBC. HRMS (APCI+) calculated for C₂₅H₂₇ (M+H)⁺: 327.2107; found: 327.2108.

((1*S**,2*S**,3*R**)-3-mesityl-1-methylcyclopropane-1,2-diyl)dibenzene (**3e**)



Cyclopropane **3e** was synthesized according to the general procedure from (*E*)-prop-1-ene-1,2-diyldibenzene (78 mg, 0.4 mmol), 7-mesitylcyclohepta-1,3,5-triene (**4a**) (42.1 mg, 0.2 mmol) and [JonhPhosAu(NCCH₃)]SbF₆ (15 mg, 0.02 mmol). 17% (*dr* 7.5:1) ¹H NMR yield was calculated from the crude. Both enantiomers could be separately after two TLC plates in a row with pentane as eluent. Yellowish oil.

¹H NMR (500 MHz, CD₂Cl₂) δ 7.40 – 7.32 (m, 4H), 7.30 – 7.22 (m, 1H), 7.10 – 7.02 (m, 3H), 6.95 – 6.89 (m, 2H), 6.81 – 6.57 (m, 2H), 3.13 (d, *J* = 8.0 Hz, 1H), 2.66 (d, *J* = 8.0 Hz, 1H), 2.39 (s, 3H), 2.23 (s, 3H), 2.20 (s, 3H), 1.36 (s, 3H). ¹³C NMR (126 MHz, CD₂Cl₂) δ 143.5, 138.8, 138.1, 135.5, 135.5, 135.3, 131.3, 129.2, 128.2, 127.2, 126.3, 125.4, 40.2, 35.4, 31.4, 20.6, 20.5, 20.4, 19.7. The configuration was assigned by COSY, NOESY, ¹H-¹³C HSQC, ¹H-¹³C HMBC. HRMS (APCI+) calculated for C₂₅H₂₇ (M+H)⁺: 327.2107; found: 327.2103.

11. X-Ray Crystal Structure

2-Di-*t*-butylphosphinobiphenyl chloromesityl(methyl) gold(I) carbenoid (**1a**)

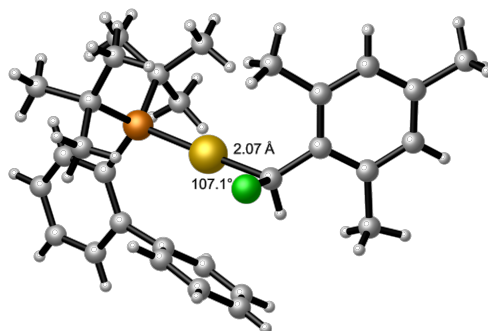


Table S4. Crystal data and structure refinement for **1a**.

Identification code	mo_CGJS020109_0m	
Empirical formula	C ₃₀ H ₃₉ Au Cl P	
Formula weight	663.00	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 8.7383(6)Å	a = 93.9248(17)°.
	b = 10.6161(6)Å	b = 105.5298(17)°.
	c = 16.2054(11)Å	g =
	107.0370(17)°.	
Volume	1367.15(15) Å ³	
Z	2	
Density (calculated)	1.611 Mg/m ³	
Absorption coefficient	5.553 mm ⁻¹	
F(000)	660	
Crystal size	0.05 x 0.05 x 0.05 mm ³	
Theta range for data collection	2.032 to 24.711°.	
Index ranges	-8 ≤ h ≤ 10, -12 ≤ k ≤ 9, -18 ≤ l ≤ 19	
Reflections collected	9039	
Independent reflections	4539[R(int) = 0.0157]	
Completeness to theta = 24.711°	97.399994%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.769 and 0.688	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	4539/ 0/ 307	
Goodness-of-fit on F ²	1.056	
Final R indices [I > 2σ(I)]	R1 = 0.0228, wR2 = 0.0527	
R indices (all data)	R1 = 0.0255, wR2 = 0.0537	
Largest diff. peak and hole	3.227 and -0.793 e.Å ⁻³	

2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid (1b)

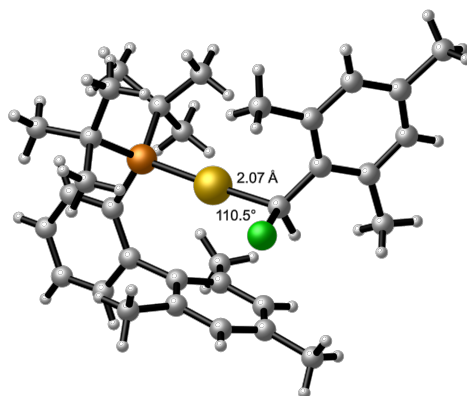


Table S5. Crystal data and structure refinement for **1b**

Identification code	CGS-02-316	
Empirical formula	C ₃₃ H ₄₅ Au Cl P	
Formula weight	705.07	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 12.16734(6)Å	α = 90°.
	b = 16.07131(6)Å	β = 101.6845(5)°.
	c = 15.75663(8)Å	γ = 90°.
Volume	3017.28(2) Å ³	
Z	4	
Density (calculated)	1.552 Mg/m ³	
Absorption coefficient	5.037 mm ⁻¹	
F(000)	1416	
Crystal size	0.1 x 0.1 x 0.05 mm ³	
Theta range for data collection	1.830 to 27.485°.	
Index ranges	-15 ≤ h ≤ 15, -20 ≤ k ≤ 20, -20 ≤ l ≤ 20	
Reflections collected	178839	
Independent reflections	6911 [R(int) = 0.0349]	
Completeness to theta = 27.485°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.787 and 0.605	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	6911/ 0/ 337	
Goodness-of-fit on F ²	1.559	
Final R indices [I > 2σ(I)]	R1 = 0.0168, wR2 = 0.0582	
R indices (all data)	R1 = 0.0182, wR2 = 0.0587	
Largest diff. peak and hole	2.417 and -1.043 e.Å ⁻³	

2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (1c)

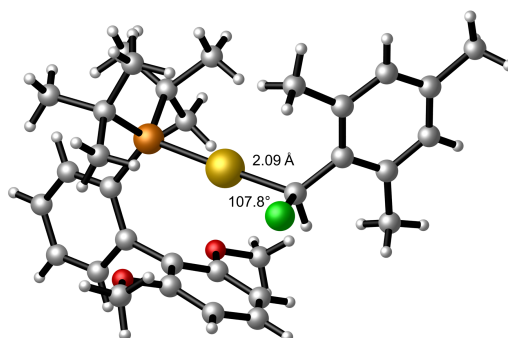


Table S6. Crystal data and structure refinement for **1c**.

Identification code	mo_CGJS02264_0m	
Empirical formula	C ₃₂ H ₄₃ Au Cl O ₂ P	
Formula weight	723.05	
Temperature	100(2) K	
Wavelength	null Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 15.3944(10)Å	a = 90°.
	b = 9.3499(6)Å	b = 100.6183(16)°.
	c = 21.2741(14)Å	g = 90°.
Volume	3009.7(3) Å ³	
Z	4	
Density (calculated)	1.596 Mg/m ³	
Absorption coefficient	5.057 mm ⁻¹	
F(000)	1448	
Crystal size	0.10 x 0.10 x 0.02 mm ³	
Theta range for data collection	2.386 to 24.712°.	
Index ranges	-18 ≤ h ≤ 18, -10 ≤ k ≤ 8, -25 ≤ l ≤ 24	
Reflections collected	21583	
Independent reflections	5109[R(int) = 0.0326]	
Completeness to theta = 24.712°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	_exptl_absorpt_correction_T_max 0.7467 and	
_exptl_absorpt_correction_T_min	0.6322	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	5109/ 0/ 345	
Goodness-of-fit on F ²	1.009	
Final R indices [I > 2σ(I)]	R1 = 0.0215, wR2 = 0.0517	
R indices (all data)	R1 = 0.0242, wR2 = 0.0528	
Largest diff. peak and hole	2.848 and -0.668 e.Å ⁻³	

2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (1d)

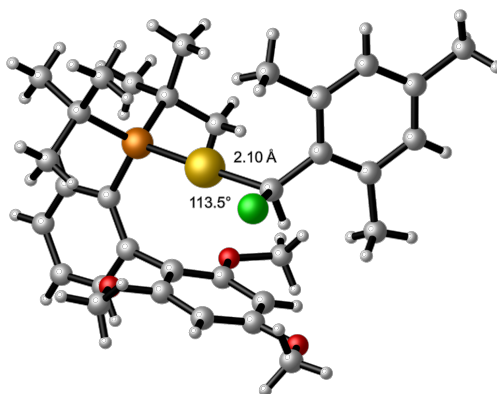
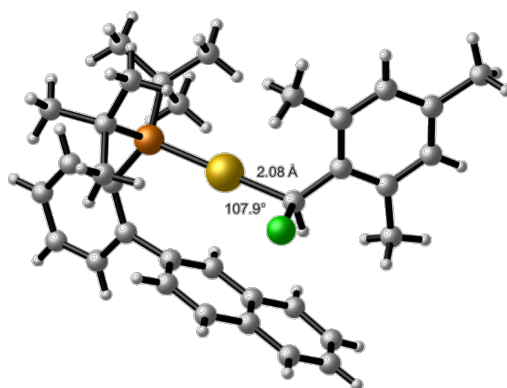


Table S7. Crystal data and structure refinement for **1d**.

Identification code	CGJS02-332	
Empirical formula	C33 H45 Au Cl O3 P	
Formula weight	753.07	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	I2/a	
Unit cell dimensions	a = 22.3984(10)Å b = 9.8047(3)Å c = 30.7411(10)Å	a = 90° b = 104.245(4)° g = 90°.
Volume	6543.5(4) Å ³	
Z	8	
Density (calculated)	1.529 Mg/m ³	
Absorption coefficient	4.657 mm ⁻¹	
F(000)	3024	
Crystal size	? x ? x ? mm ³	
Theta range for data collection	2.187 to 31.912°.	
Index ranges	-31 ≤ h ≤ 31, -13 ≤ k ≤ 14, -44 ≤ l ≤ 22	
Reflections collected	27147	
Independent reflections	10192 [R(int) = 0.0417]	
Completeness to theta = 31.912°	90.3%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.955 and 0.735	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	10192 / 0 / 364	
Goodness-of-fit on F ²	0.940	
Final R indices [I > 2σ(I)]	R1 = 0.0307, wR2 = 0.0701	
R indices (all data)	R1 = 0.0514, wR2 = 0.0774	
Largest diff. peak and hole	2.604 and -0.691 e.Å ⁻³	

2-Di-*t*-butylphosphino-2-naphthyl chloromesityl(methyl) gold(I) carbenoid (1e)**Table S8.** Crystal data and structure refinement for **1e**.

Identification code	mo_CGJS02560_0m	
Empirical formula	C ₃₄ H ₄₁ Au Cl P	
Formula weight	713.05	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)	
Unit cell dimensions	a = 11.1431(5) Å b = 16.2846(7) Å c = 16.7392(7) Å	a = 90°. b = 100.0600(10)°. g = 90°.
Volume	2990.8(2) Å ³	
Z	4	
Density (calculated)	1.584 Mg/m ³	
Absorption coefficient	5.083 mm ⁻¹	
F(000)	1424	
Crystal size	0.15 x 0.15 x 0.06 mm ³	
Theta range for data collection	1.235 to 32.714°	
Index ranges	-16 ≤ h ≤ 16, -24 ≤ k ≤ 24, -25 ≤ l ≤ 25	
Reflections collected	80205	
Independent reflections	20682 [R(int) = 0.0265]	
Completeness to theta = 32.714°	96.100006%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.750 and 0.515	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	20682 / 585 / 789	
Goodness-of-fit on F ²	1.215	
Final R indices [I > 2σ(I)]	R1 = 0.0222, wR2 = 0.0483	
R indices (all data)	R1 = 0.0252, wR2 = 0.0491	
Flack parameter	x = 0.361(6)	
Largest diff. peak and hole	1.432 and -0.747 e.Å ⁻³	

Phosponium ylid complex 7a

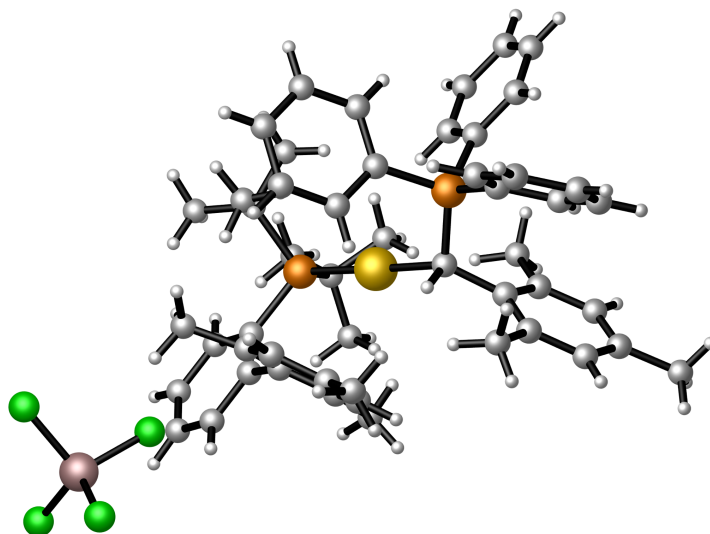


Table S9. Crystal data and structure refinement for **7a**.

Identification code	mo_CGJS02512_0m	
Empirical formula	C ₅₁ H ₆₀ Au Cl ₄ Ga P ₂	
Formula weight	1143.41	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 15.1297(5)Å	a = 90°.
	b = 15.1006(5)Å	b = 101.4222(18)°.
	c = 22.1469(8)Å	g = 90°.
Volume	4959.6(3) Å ³	
Z	4	
Density (calculated)	1.531 Mg/m ³	
Absorption coefficient	3.811 mm ⁻¹	
F(000)	2296	
Crystal size	0.20 x 0.20 x 0.20 mm ³	
Theta range for data collection	1.643 to 33.344°.	
Index ranges	-22 ≤ h ≤ 12, -18 ≤ k ≤ 22, -32 ≤ l ≤ 31	
Reflections collected	42998	
Independent reflections	16383[R(int) = 0.0393]	
Completeness to theta = 33.344°	85.299995%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.516 and 0.397	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	16383/ 48/ 580	
Goodness-of-fit on F ²	1.019	
Final R indices [I > 2σ(I)]	R1 = 0.0318, wR2 = 0.0563	
R indices (all data)	R1 = 0.0503, wR2 = 0.0611	
Largest diff. peak and hole	0.926 and -1.018 e.Å ⁻³	

Phosponium ylid complex 7b

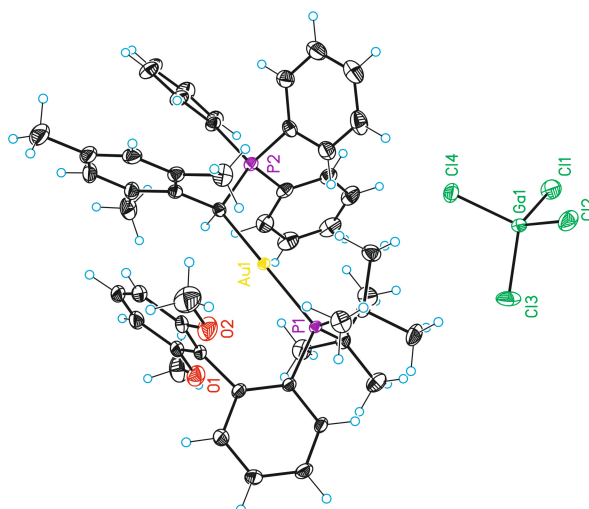
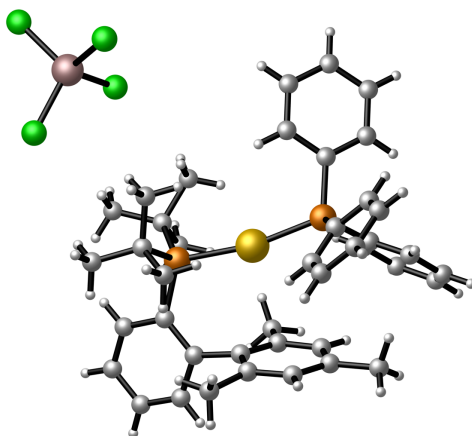
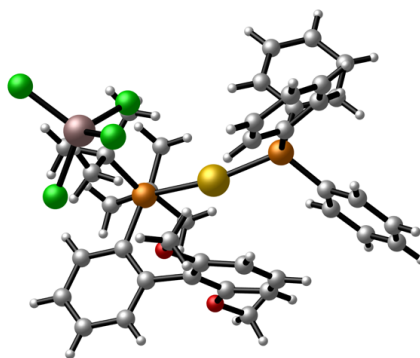


Table S10. Crystal data and structure refinement for **7b**.

Identification code	mo_CGJS460_0m	
Empirical formula	C ₅₇ H ₆₆ Au Cl ₄ Ga O ₂ P ₂	
Formula weight	1253.52	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.5933(5)Å	a = 80.4789(11)°.
	b = 15.5453(7)Å	b = 76.1721(10)°.
	c = 16.4650(7)Å	g = 75.7588(11)°.
Volume	2774.8(2) Å ³	
Z	2	
Density (calculated)	1.500 Mg/m ³	
Absorption coefficient	3.416 mm ⁻¹	
F(000)	1264	
Crystal size	0.20 x 0.20 x 0.10 mm ³	
Theta range for data collection	1.760 to 33.881°.	
Index ranges	-15 ≤ h ≤ 18, -23 ≤ k ≤ 24, -25 ≤ l ≤ 24	
Reflections collected	45728	
Independent reflections	21068 [R(int) = 0.0366]	
Completeness to theta = 33.881°	93.8%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.726 and 0.601	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	21068 / 804 / 1013	
Goodness-of-fit on F ²	1.038	
Final R indices [I > 2σ(I)]	R1 = 0.0376, wR2 = 0.0749	
R indices (all data)	R1 = 0.0531, wR2 = 0.0796	
Largest diff. peak and hole	1.204 and -1.114 e.Å ⁻³	

[MeJPAuPPh₃][GaCl₄] (S1)**Table S11.** Crystal data and structure refinement for S1.

Identification code	mo_CGJS02512_b_0m	
Empirical formula	C41 H48 Au Cl4 Ga P2	
Formula weight	1011.22	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 9.8240(3)Å	$\alpha = 90.8386(11)^\circ$.
	b = 13.8807(5)Å	$\beta = 102.3072(10)^\circ$.
	c = 15.8756(6)Å	$\gamma = 99.3037(10)^\circ$.
Volume	2084.58(13) Å ³	
Z	2	
Density (calculated)	1.611 Mg/m ³	
Absorption coefficient	4.522 mm ⁻¹	
F(000)	1004	
Crystal size	0.20 x 0.10 x 0.10 mm ³	
Theta range for data collection	1.935 to 30.561°.	
Index ranges	-9 ≤ h ≤ 13, -14 ≤ k ≤ 19, -22 ≤ l ≤ 21	
Reflections collected	22182	
Independent reflections	11705 [R(int) = 0.0296]	
Completeness to theta = 30.561°	91.7%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.661 and 0.462	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11705 / 56 / 452	
Goodness-of-fit on F ²	1.028	
Final R indices [I > 2σ(I)]	R1 = 0.0304, wR2 = 0.0555	
R indices (all data)	R1 = 0.0386, wR2 = 0.0581	
Largest diff. peak and hole	0.890 and -1.068 e.Å ⁻³	

[oMeOJPAuPPh₃][GaCl₄] (S2)**Table S12.** Crystal data and structure refinement for S2.

Identification code	mo_CGJS02489B_0m	
Empirical formula	C60 H69 Au1.50 Cl6 Ga1.50 O3 P3	
Formula weight	1543.79	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/n	
Unit cell dimensions	a = 14.858(5)Å	a = 90°.
	b = 25.357(8)Å	b = 92.193(12)°.
	c = 33.572(7)Å	g = 90°.
Volume	12640(6) Å ³	
Z	8	
Density (calculated)	1.623 Mg/m ³	
Absorption coefficient	4.480 mm ⁻¹	
F(000)	6120	
Crystal size	? x ? x ? mm ³	
Theta range for data collection	1.521 to 25.505°.	
Index ranges	-17<=h<=14,-30<=k<=30,-40<=l<=38	
Reflections collected	70460	
Independent reflections	22417[R(int) = 0.0987]	
Completeness to theta =25.505°	95.3%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.916 and 0.752	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	22417/ 3/ 1375	
Goodness-of-fit on F ²	0.929	
Final R indices [I>2sigma(I)]	R1 = 0.0511, wR2 = 0.0892	
R indices (all data)	R1 = 0.1221, wR2 = 0.1124	
Largest diff. peak and hole	1.021 and -0.772 e.Å ⁻³	

[(2-Di-*t*-butylphosphinobiphenylAu)₂Cl]GaCl₄ (10a)

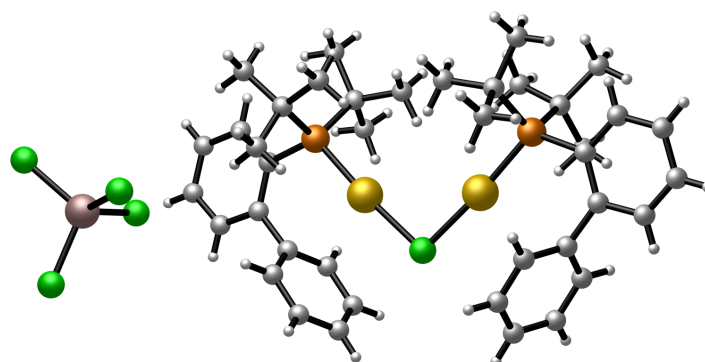


Table S13. Crystal data and structure refinement for **10a**.

Identification code	cgs-02-340	
Empirical formula	C ₄₀ H ₅₄ Au ₂ Cl ₅ Ga P ₂	
Formula weight	1237.67	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 11.34310(10)Å b = 15.01070(10)Å c = 15.71570(10)Å	a = 66.0970(10)° b = 69.0110(10)° g = 71.1750(10)°
Volume	2234.10(4) Å ³	
Z	2	
Density (calculated)	1.840 Mg/m ³	
Absorption coefficient	7.547 mm ⁻¹	
F(000)	1196	
Crystal size	? x ? x ? mm ³	
Theta range for data collection	2.026 to 26.372°	
Index ranges	-14 ≤ h ≤ 14, -18 ≤ k ≤ 18, -19 ≤ l ≤ 19	
Reflections collected	125845	
Independent reflections	9134[R(int) = 0.0381]	
Completeness to theta = 26.372°	99.9%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.805 and 0.619	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	9134/ 0/ 463	
Goodness-of-fit on F ²	1.070	
Final R indices [I > 2σ(I)]	R1 = 0.0224, wR2 = 0.0615	
R indices (all data)	R1 = 0.0238, wR2 = 0.0624	
Largest diff. peak and hole	2.278 and -1.947 e.Å ⁻³	

[(2-Di-*t*-butyl-2',6'-dimethoxyphosphinobiphenylAu)₂Cl]GaCl₄ (10c)

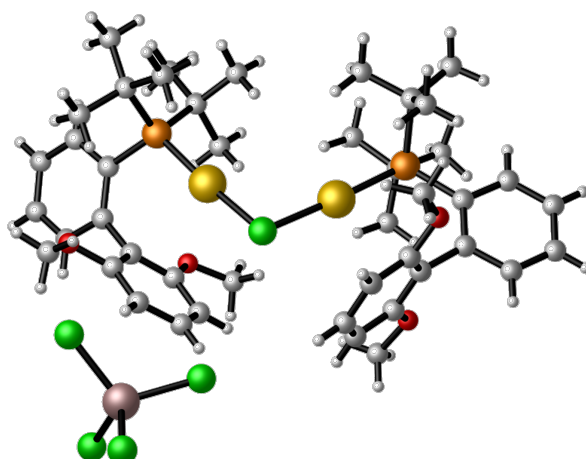


Table S14. Crystal data and structure refinement for **10c**.

Identification code	CGJS-02-0409	
Empirical formula	C ₅₁ H ₇₀ Au ₂ Cl ₅ Ga O ₄ P ₂	
Formula weight	1449.91	
Temperature	100(2) K	
Wavelength	0.71073 Å	
Crystal system	Triclinic	
Space group	P-1	
Unit cell dimensions	a = 13.3973(3)Å	α = 78.113(2)°.
	b = 14.6629(4)Å	β = 68.581(2)°.
	c = 16.4950(3)Å	γ = 69.576(2)°.
Volume	2815.43(12) Å ³	
Z	2	
Density (calculated)	1.710 Mg/m ³	
Absorption coefficient	6.008 mm ⁻¹	
F(000)	1424	
Crystal size	0.05 x 0.01 x 0.01 mm ³	
Theta range for data collection	1.802 to 26.371°.	
Index ranges	-15 ≤ h ≤ 16, -15 ≤ k ≤ 18, -20 ≤ l ≤ 20	
Reflections collected	39526	
Independent reflections	11520 [R(int) = 0.0432]	
Completeness to theta = 26.371°	100.0%	
Absorption correction	Multi-scan	
Max. and min. transmission	0.942 and 0.725	
Refinement method	Full-matrix least-squares on F ²	
Data / restraints / parameters	11520 / 99 / 655	
Goodness-of-fit on F ²	1.073	
Final R indices [I > 2σ(I)]	R1 = 0.0318, wR2 = 0.0787	
R indices (all data)	R1 = 0.0436, wR2 = 0.0828	
Largest diff. peak and hole	2.480 and -1.860 e.Å ⁻³	

12. DFT Calculations

All density functional calculations were performed using the Gaussian09 suite.⁷ The functional B3LYP⁸ was used in conjunction with Grimme's D3 dispersion correction. The basis set for Au and Ga used was SDD,⁹ and a 6-31G(d,p)¹⁰ for all other atoms. All structures were fully optimized and frequency calculations were undertaken. No imaginary frequencies for minima and a single imaginary frequency corresponding to the reaction coordinate in the case of the transition states were found. Additionally, single point of the optimized structures using the Polarizable Continuum Model (PCM)¹¹ to simulate dichloromethane ($\epsilon = 8.93$) as solvent were performed throughout all calculations. All the energies presented are potential (E) and free energies (G) in solution at 298.15 K and 1 atm in kcal/mol. Optimized geometries were visualized using CYLview.¹²

NMR data was calculated at B3LYP/6-311+G(2d,p) level of theory in dichloromethane (PCM) and previously calculated scaling factor were employed.¹³

Non covalent interaction analysis was performed with NCIPLOT.¹⁴

The bonding situation was analyzed using Natural Bond Orbital analysis (NBO 6.0).¹⁵ Charge transfer between the carbene moiety and gold atom has been calculated using Natural Population Analysis (NPA).¹⁶ The Natural Localized Molecular Orbitals (NLMO) associated to the Au-C1 and C1-C2 interactions have been determined.¹⁷ The NLMOs isosurface were visualized using ChemCraft, with the surface contour set at 0.4.¹⁸

Gold(I) Carbenes 5a'-e' Structures Optimization

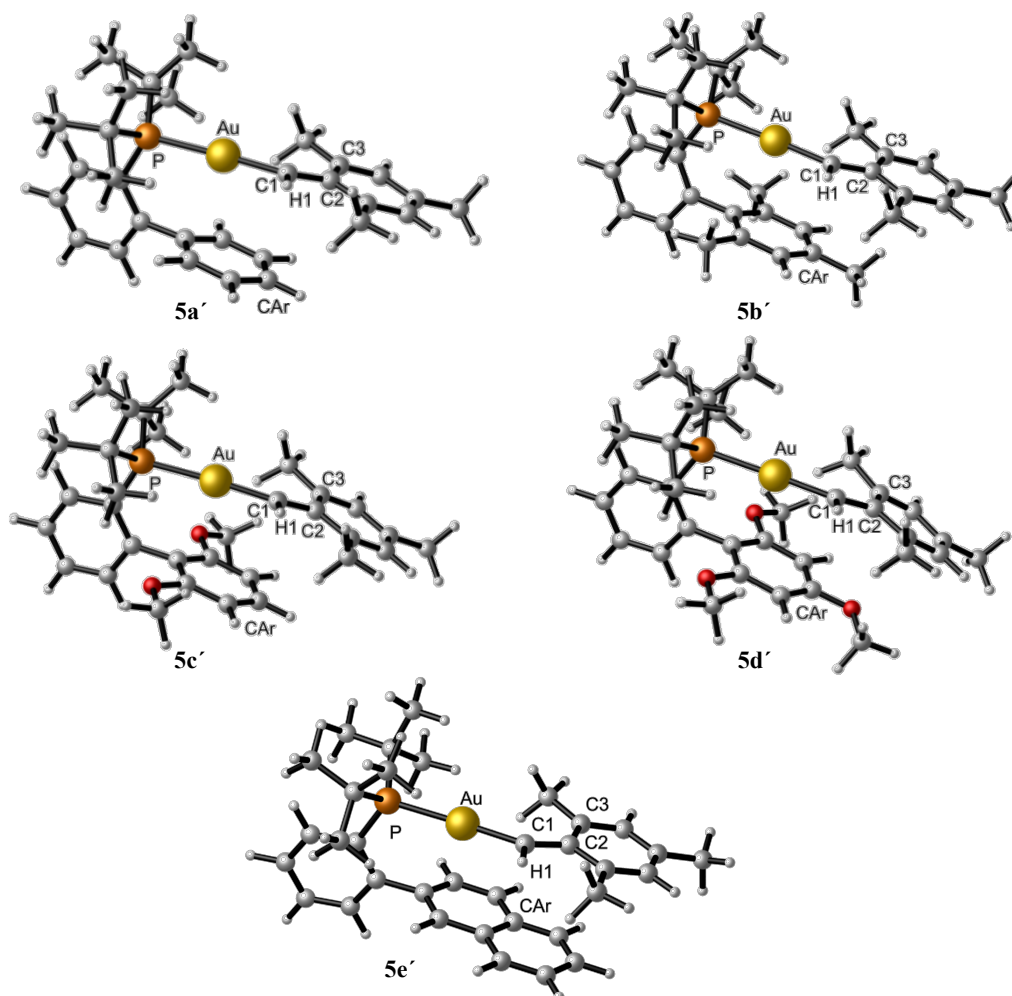


Figure S17. Optimized structures for gold(I) carbenes **5a'-e'**.

Table S15. Selected computed structural data for structure **5a'-e'**.

Computed Structural Data	5a'	5b'	5c'	5d'	5e'
P-Au (Å)	2.38	2.38	2.38	2.38	2.39
Au-C1 (Å)	2.03	2.03	2.03	2.03	2.03
C1-H1 (Å)	1.09	1.09	1.09	1.09	1.09
C1-C2 (Å)	1.40	1.40	1.40	1.40	1.40
P-Au-C1 (°)	176.6	175.9	176.5	176.2	174.5
CAr-C1-H1 (°)	97.5	100.2	100.2	108.0	110.7
CAr-C1-C2 (°)	81.2	80.3	73.8	72.2	78.8
CAr-C1-C2-C3 (°)	88.7	84.8	90.8	81.0	105.0

NMR Predictions

Previously calculated scaling factor¹³ were employed to achieve high-accuracy chemical shifts from the computed isotropic shielding constants of the optimized gold(I) complexes using equation S2.

$$\delta = \frac{\text{intercept} - \sigma}{-\text{slope}}$$

Equation S2. Where δ = chemical shift in ppm, σ = isotropic value, intercept = 31.9351 for ¹H and 181.2747 for ¹³C, slope = 1.0463 for ¹H and 1.0272 for ¹³C.

The calculated NMR data correlates with the experimental results as exposed below.

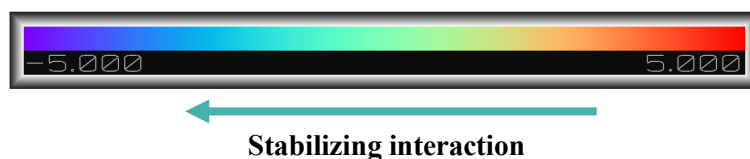
Table S16. Selected computed and experimental NMR data for structures **1a-e** and **5a-e**.

Complex	¹ H NMR (ppm, H1)		¹³ C NMR (ppm, C1) ^a		¹ J (¹³ C1- ¹ H1) ^a (Hz)	
	<i>DFT</i>	<i>Exp.</i>	<i>DFT</i>	<i>Exp.</i>	<i>DFT</i>	<i>Exp.</i>
1a'	4.22	4.92	72.2	69.7 ^c	144.2	-
5a'	12.12	12.35	280.8	290.0	125.2	-
1b'	4.24	4.28	71.2	71.8	143.4	143.9
5b'	12.17	12.67	280.2	287.9	124.4	129.8
1c'	4.30	4.17	75.4	73.7	144.6	144.3
5c'	12.09	12.32	278.9	290.0	126.1	127.8
1d'	4.69	4.24	74.0	71.4 ^c	144.4	-
5d'	12.03	12.57	274.6	289.0	125.6	-
1e'	-	3.26	-	70.7	-	-
5e'	11.06	11.74	272.4	284.6	125.4	-

^aNMR data computed at 25 °C in CH₂Cl₂. ^bNMR data measured at -90 °C in CD₂Cl₂.

^cNMR data measured at 25 °C in toluene-*d*₈.

Non-Covalent Interaction Analysis



Positive non-covalent interactions can be seen for carbenes **5a'-e'** between *ortho*-CH₃ in the mesitylidene unit and gold atom, (violet arrows), also between a *t*Bu group and gold atom (yellow arrows). There are also stabilizing interactions between the lower ring of the biaryl moiety and the mesitylidene fragment for all the carbenes. However, these interactions are more important for carbenes bearing substituted biaryl moieties **5b'-e'** (green arrows). Furthermore, gold(I) carbenes **5b'-d'** display positive interactions between substituted biaryl rings and *t*Bu substituents on P (red arrows). These results suggest that non-covalent interactions play a role in the higher stability of gold(I) carbenes **5b'-e'** vs **5a'**.

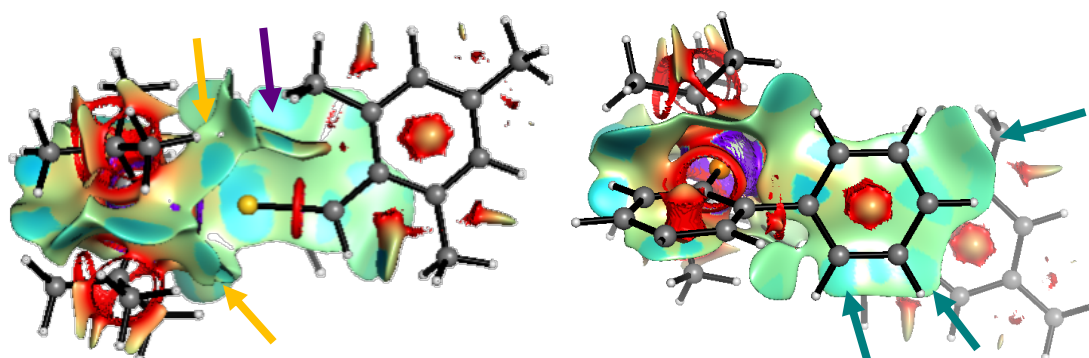


Figure S18. Non-Covalent interaction plot for structure **5a'**. Left: the mesitylidene moiety is showed in front. Right: the biaryl moiety is showed in front.

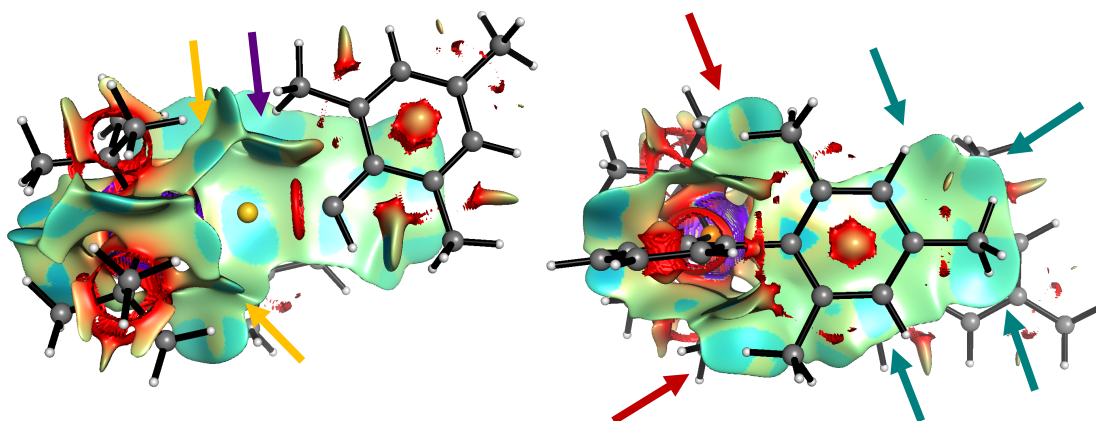


Figure S19. Non-Covalent interaction plot for structure **5b'**. Left: the biaryl moiety is showed in front. Right: the mesitylidene moiety is showed in front.

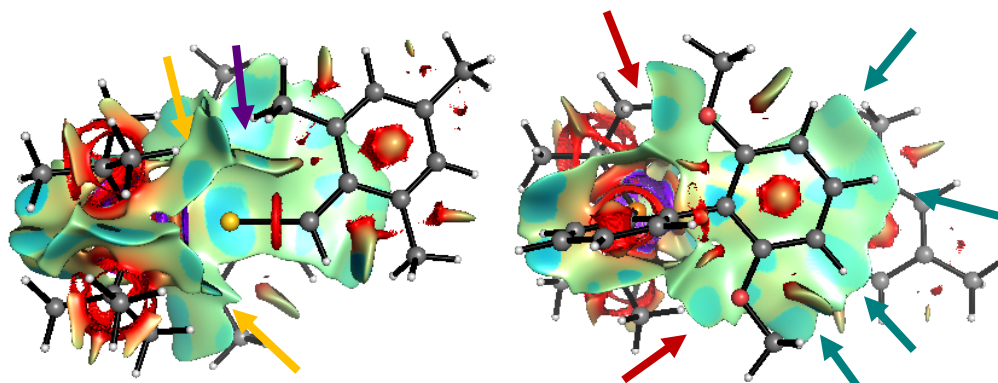


Figure S20. Non-Covalent interaction plot for structure **5c'**. Left: the biaryl moiety is showed in front. Right: the mesitylidene moiety is showed in front.

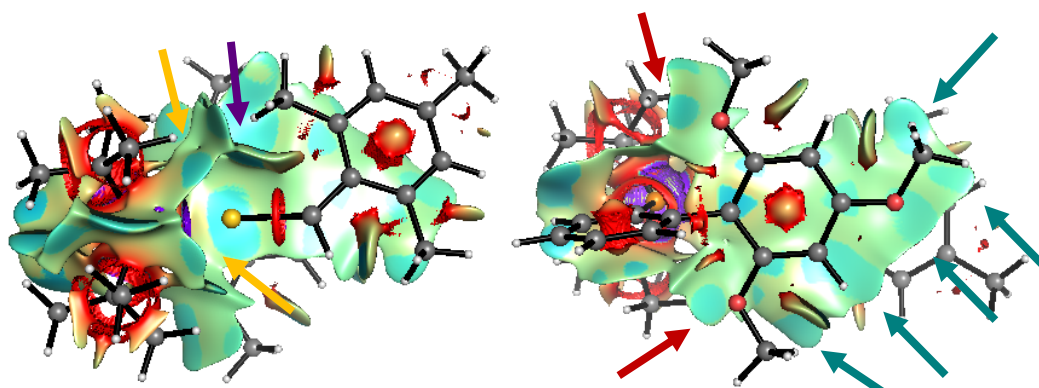


Figure S21. Non-Covalent interaction plot for structure **5d'**. Left: the biaryl moiety is showed in front. Right: the mesitylidene moiety is showed in front.

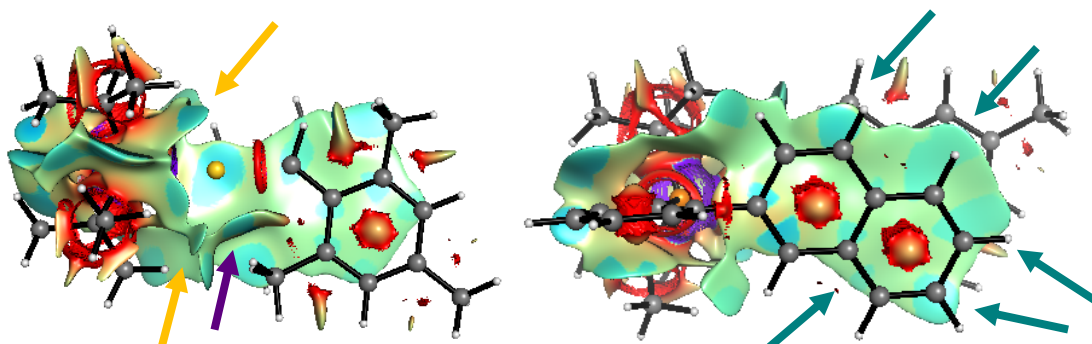


Figure S22. Non-Covalent interaction plot for structure **5e'**. Left: the biaryl moiety is showed in front. Right: the mesitylidene moiety is showed in front.

Gold(I) Carbenes **5c'**-CF₃ and **5c'**-MeO

To study the influence of the aryl group in the gold(I) carbene stabilization, the structure of two non-experimentally synthesized gold(I) carbenes were optimized. These complexes bear the same ligand as **5c'** and highly electron deficient (CF₃, **5c'**-CF₃) or electron donating (MeO, **5c'**-MeO) substituents in the aryl group.

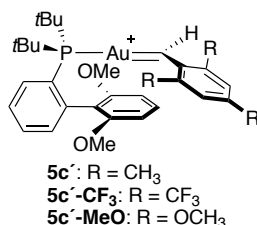


Figure S23. Gold(I) carbenes varying the substituents in the aryl.

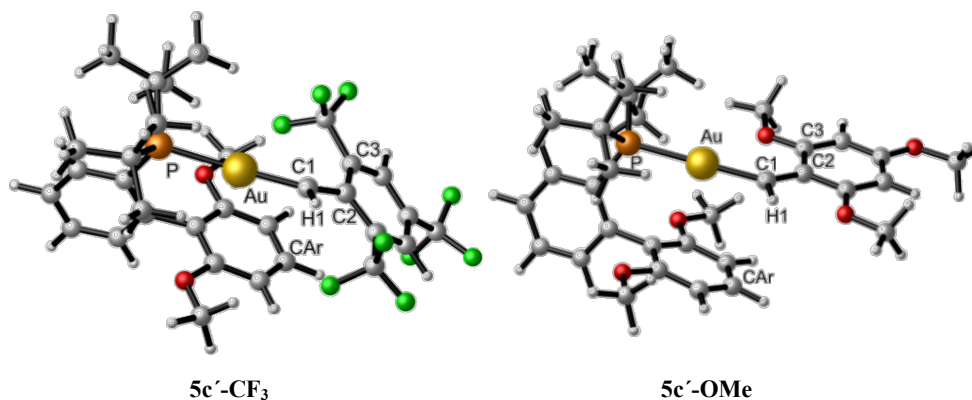


Figure S24. Optimized structures for gold(I) carbenes **5c'**-CF₃ and **5c'**-MeO.

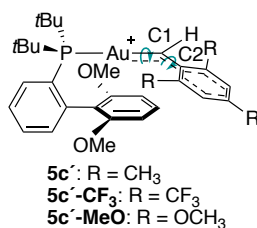
Table S17. Selected computed structural data for structure **5c'**, **5c'**-CF₃ and **5c'**-OMe.

Computed Structural Data	5c' -CF ₃	5c'	5c' -OMe
P-Au (Å)	2.38	2.38	2.38
Au-C1 (Å)	2.00	2.03	2.03
C1-H1 (Å)	1.08	1.09	1.09
C1-C2 (Å)	1.44	1.40	1.38
P-Au-C1 (°)	172.4	176.5	178.5
CAr-C1-H1 (°)	121.8	100.2	73.4
CAr-C1-C2 (°)	63.3	73.8	106.7
CAr-C1-C2-C3 (°)	86.4	90.8	101.5

Barrier to bond rotation

The strength of π -bonds on the carbenes was evaluated by calculating the rotational barrier of Au-C1 and C1-C2 bonds for **5c'** and their substituted analogues.

Table S18. Calculated rotational barriers for Au-C1 and C1-C2 bonds.



Gold(I) Carbene	$\Delta G^\ddagger_{\text{Au-C1}}$ (Kcal/mol) ^a	$\Delta G^\ddagger_{\text{C1-C2}}$ (Kcal/mol) ^a
$5c'$ -CF ₃	3.5	2.5
$5c'$	1.3	18.6
$5c'$ -MeO	2.5	32.1

^aFree energies in solution referred to the lowest energy isomer of gold(I) carbenes.

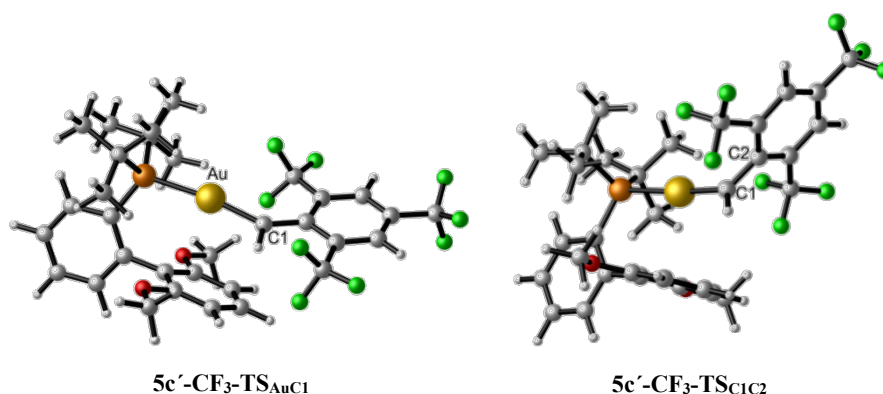


Figure S25. Optimized transition states TS_{AuC1} and TS_{C1C2} for gold(I) carbene $5c'$ -CF₃.

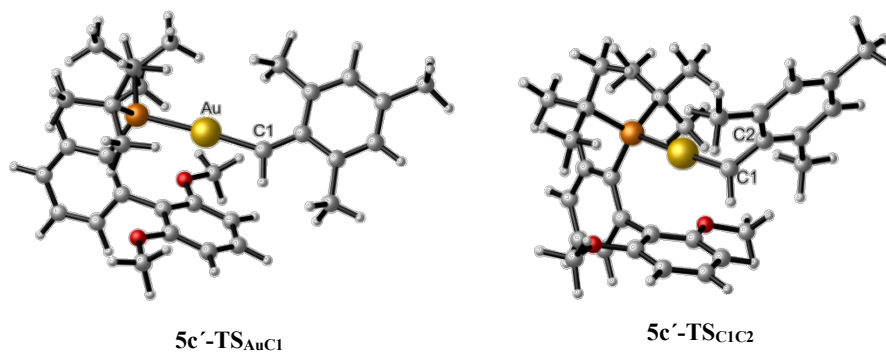


Figure S26. Optimized transition states TS_{AuC1} and TS_{C1C2} for gold(I) carbene $5c'$.

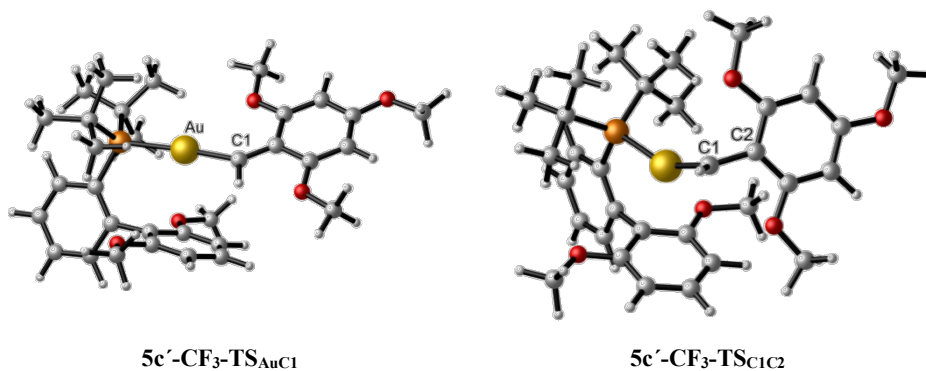


Figure S27. Optimized transition states TS_{AuC1} and TS_{C1C2} for gold(I) carbene $5c'$ -MeO.

Frontier orbitals

Table S19. Energy of the HOMO and LUMO orbitals.

Structure	HOMO (eV)	LUMO (eV)	Gap (eV)
5c'-CF₃	-6.20	-4.41	1.79
5c'	-6.06	-3.50	2.56
5c'-MeO	-5.98	-2.98	3.00

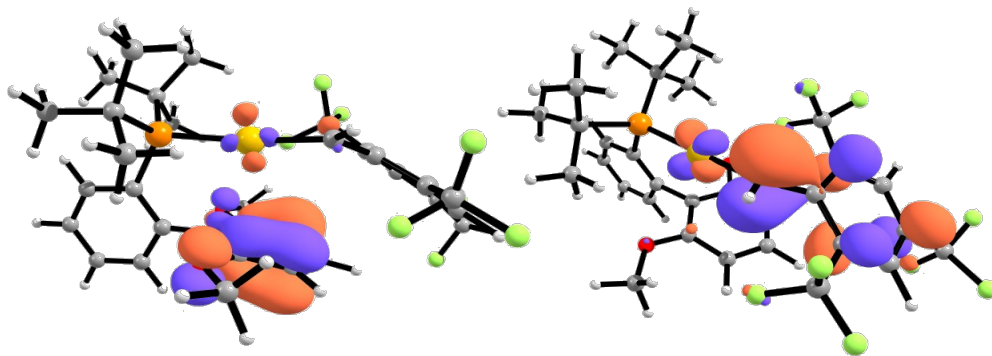


Figure S28. HOMO (left) and LUMO (right) for structure **5c'-CF₃**.

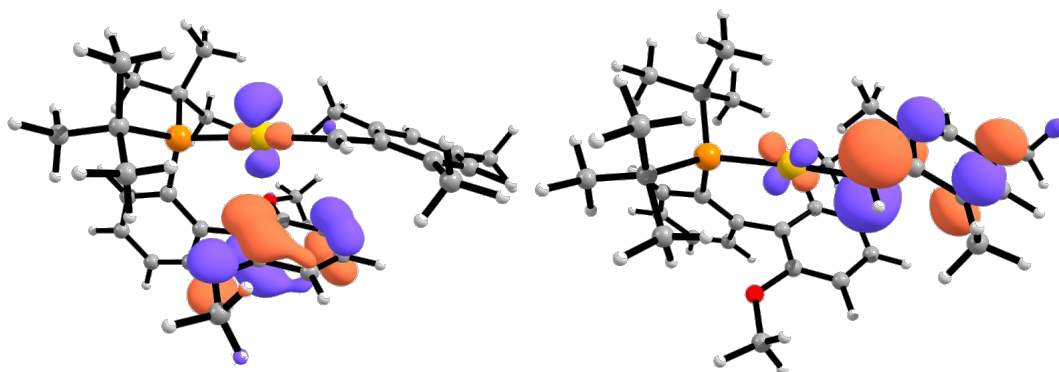


Figure S29. HOMO (left) and LUMO (right) of structure **5c'**.

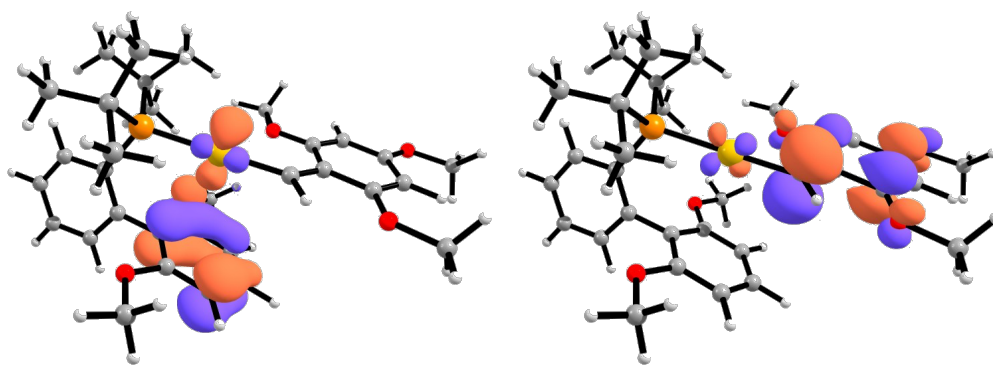


Figure S30. HOMO (left) and LUMO (right) of structure **5c'-MeO**.

Bond Orbital Analysis

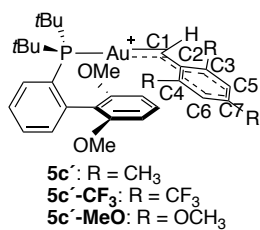


Table S20. Charge transfer from carbene to gold based on natural population analysis.

Natural Charge	$5c'$ -CF ₃	$5c'$	$5c'$ -MeO
Au	0.46	0.37	0.36
C1	-0.25	-0.31	-0.35
C2	-0.11	-0.18	-0.25
C3	-0.07	0.11	0.45
C4	-0.07	0.10	0.45
C5	-0.18	-0.27	-0.41
C6	-0.19	-0.27	-0.44
C7	-0.09	0.10	0.45
Natural Charge Carbene	0.13	0.28	0.33
CT (Carbene to Au)	-0.33	-0.09	-0.02

Table S21. Natural localized molecular orbitals associated to C1 stabilization for **5c'-CF₃**, **5c'** and **5c'-MeO**. Contribution of main atoms in percent and NBOs donor-acceptor related to the analyzed NLMO.

Interaction	Analysis	5c'-CF₃	5c'	5c'-MeO	
π -backdonation	NLMO	$d_{xz}(\text{Au})$	$d_{xy}(\text{Au})$	$d_{xz}(\text{Au})$	
	Au	88.8%	93.8%	94.8	
	C1	10.0%	3.7%	2.8	
	C _{Aryl} -system	0.5%	1.5%	1.2%	
	NBO donor	n_{Au}	n_{Au}	n_{Au}	
	NBO acceptor	n_{C1}^* (31.6 Kcal/mol)	n_{C1}^* (24.4 Kcal/mol)	$\Omega_{\text{C1-C2}}^*$ (10.1 Kcal/mol)	
	Interaction	$d_{xz}(\text{Au})$ to $2p_z(\text{C1})$	$d_{xy}(\text{Au})$ to $2p_y(\text{C1})$	$d_{xz}(\text{Au})$ to $2p_z(\text{C1})$	
$\pi_{\text{C1-C2}}$ bond	NLMO		$2p_y(\text{C2})$	$\pi_{\text{C1-C2}}$	
	C1		23.5	27.3	
	C2		51.1	54.9	
	C3		8.5	5.36	
	C4		8.6	6.0	
	C5		0.8	0.8	
	C6		0.8	0.8	
	C7	No NLMO	6.2	3.0	
	NBO donor		n_{C2}	$\Omega_{\text{C1-C2}}$	
	NBO acceptor			$\Omega_{\text{C3-C5}}^*$ (82.3 Kcal/mol)	$\Omega_{\text{C1-C2}}^*$ (6.0 Kcal/mol)
				$\Omega_{\text{C4-C6}}^*$ (81.8 Kcal/mol)	$\Omega_{\text{C3-C5}}^*$ (27.4 Kcal/mol)
				$\Omega_{\text{C4-C6}}^*$ (29.9 Kcal/mol)	
Interaction		$2p^\pi(\text{C2})$ to $2p^\pi(\text{C1})$	$\Omega_{\text{C1-C2}}$ to $\Omega_{\text{C=C}^{\text{aryl}}}^*$		

NBO types: n_{A} = nonbonded lone pair (1 center, valence), n_{A}^* = unfilled nonbonded (1 center, valence), $\Omega_{\text{A-B}}$ = bond (2 centers, valence), $\Omega_{\text{A-B}}^*$ = antibond (2 centers, valence).

NLMO Plots for Main Electronic Contributions in the π -Orbital Stabilization of C1.

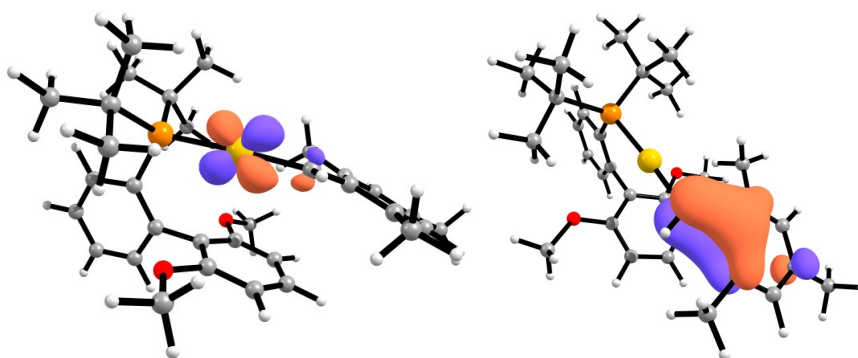


Figure S31. Plot for NLMO associated to π -backdonation from Au to C1 (left) and lone pair at C2 (right) for **5c'**. Cutoff: 0.05.

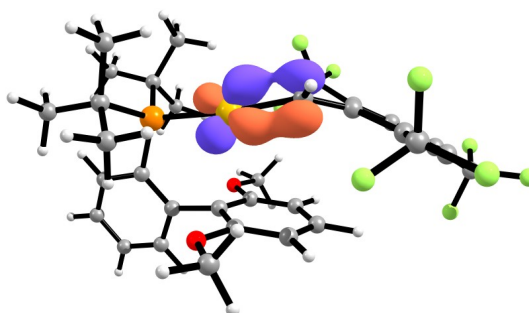


Figure S32. Plot for NLMO associated to π -backdonation from Au to C1 for **5c'-CF₃**.

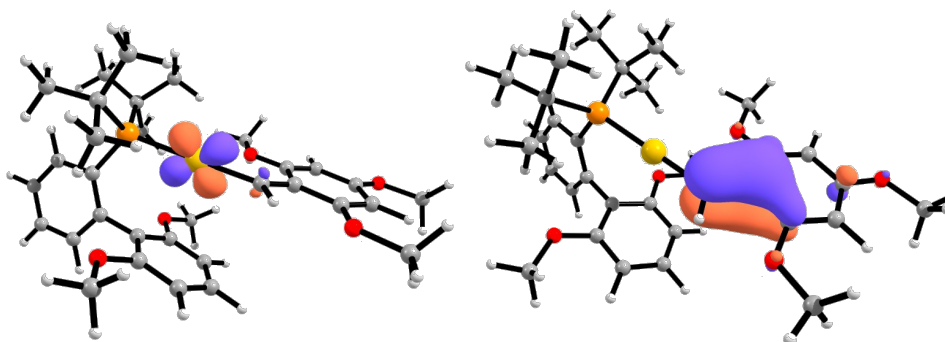
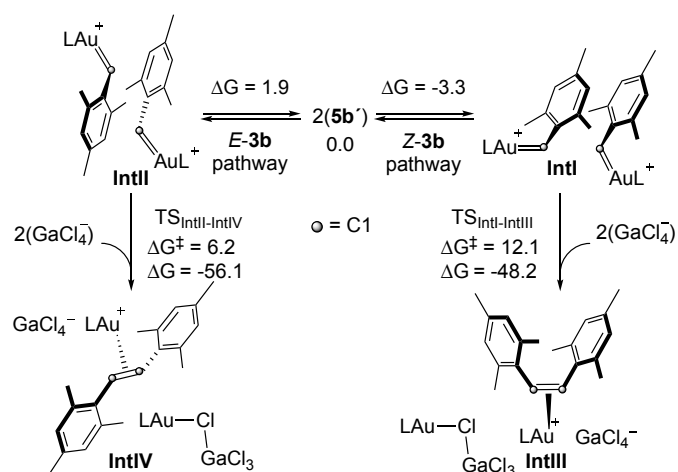


Figure S33. Plot for NLMO associated to π -backdonation from Au to C1 (left) and C1-C2 π -bond (right) for **5c'-OMe**. Cutoff: 0.05.

Dimerization of 5b to form E-2b and Z-2b.



Scheme 17. Calculated free energy profile for dimerization of gold(I) carbene **5b'** forming *E*-**2b'** and *Z*-**2b'**. PCM(CH₂Cl₂)-B3LYP-D3, SDD(Au, Ga), 6-31G(d,p) (C, H, O, P, Cl, F). L = 2-di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl.

T (K)	2b (<i>E/Z</i> ratio)
183	5.7
193	5.2
203	4.8
213	4.5
223	4.2
233	3.9
243	3.7
253	3.5
263	3.4
273	3.2
283	3.1
293	3.0
298	2.9

Table S21. Calculated *E*-**2b**/*Z*-**2b** ratio based on $\Delta\Delta G^\ddagger_{\text{trans-cis}} = 0.6$ kcal/mol.

Non-Covalent Interaction Analysis of IntI and IntII



Stabilizing interaction

Both intermediates **IntI** and **IntII** display face-to-face π - π stacking interactions between the two mesitylidenes units.

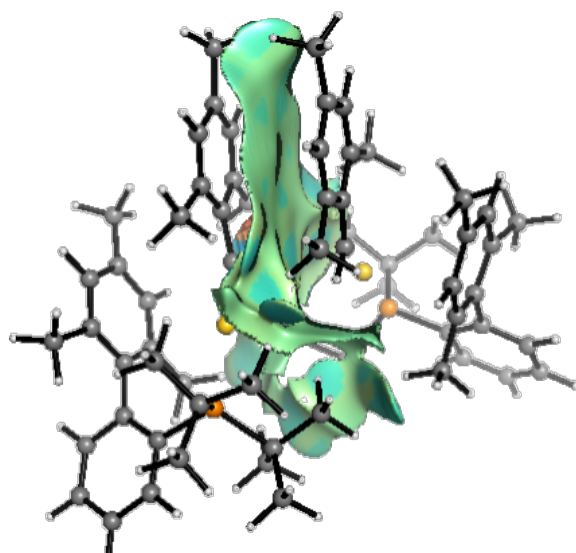


Figure S34. Non-covalent interactions plot for **IntI**.

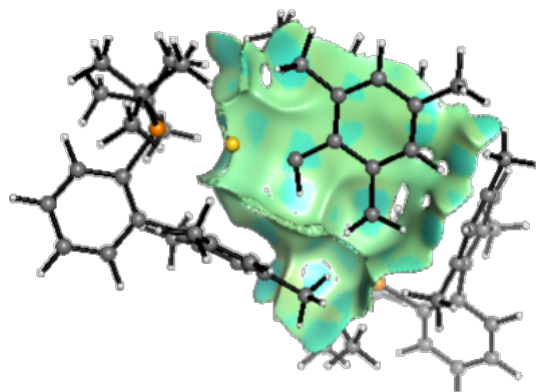


Figure S35. Non-covalent interactions plot for **IntII**.

Cyclopropanation of *E*-2b by gold(I) carbene **5b'**

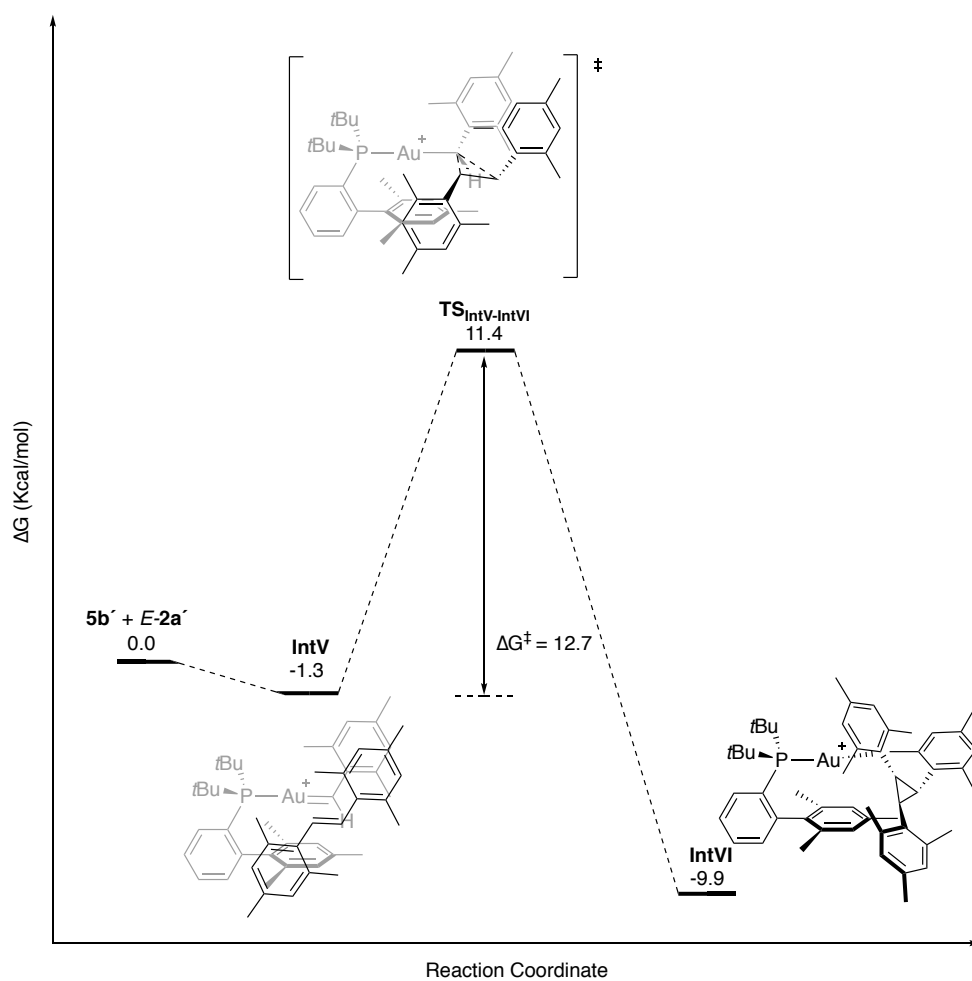


Figure S36. Calculated free energy profile for the cyclopropanation of *E*-2b' with gold(I) carbene **5b'**. PCM(CH₂Cl₂)-B3LYP-D3, SDD(Au), 6-31G(d,p) (C, H, O, P, Cl, F).

Cyclopropanation of Z-2b' by gold(I) carbene 5b'

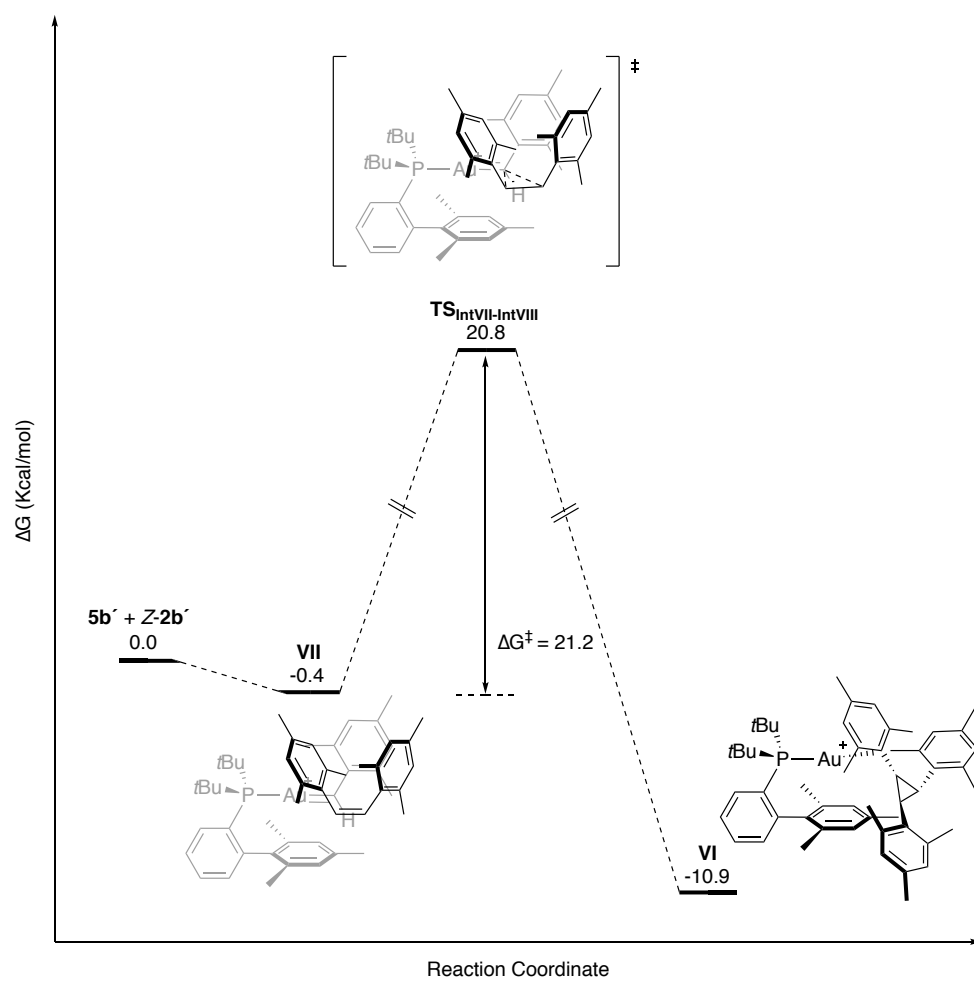
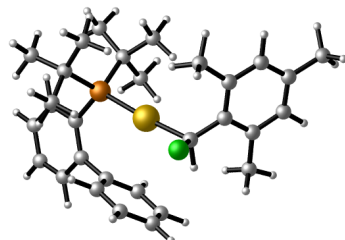


Figure S37. Calculated free energy profile for cyclopropanation of Z-2b' with gold(I) carbene 5b'. PCM(CH₂Cl₂)-B3LYP-D3, SDD(Au), 6-31G(d,p) (C, H, O, P, Cl, F).

Cartesian coordinates (Å) and absolute energies (a. u.) for all stationary points

In some structures hydrogens have been omitted for clarity.

Gold(I) Carbenoid 1a'

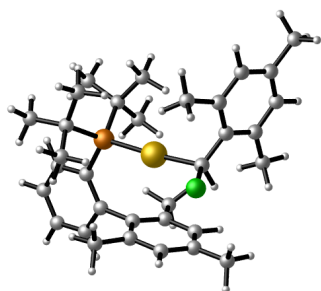


E = -2104.21100429

G = -2103.668056

Au	-0.28014600	0.10215200	0.44482800	H	4.15031500	3.12421500	-1.44918600
C	-2.14755800	1.00653800	0.73177300	C	3.11599300	1.37701900	-0.76374200
H	-2.05823900	2.01594900	0.34122800	C	1.94745600	2.24084600	-0.41250500
C	-3.27292500	0.27797900	0.06023000	C	1.14750900	2.77370200	-1.43357500
C	-3.84066500	0.84243200	-1.10898400	H	1.35097200	2.49956500	2.46487100
C	-4.82438900	0.14210300	-1.81454800	C	0.09198400	3.63531400	-1.13016900
H	-5.24530700	0.59090700	-2.71248200	H	-0.52630400	4.03190300	-1.92992200
C	-5.28532800	-1.10757800	-1.39805500	C	-0.17003400	3.98399500	0.19612200
C	-4.71196300	-1.65873100	-0.24939800	H	-0.99822900	4.64434100	0.43431700
H	-5.04321600	-2.63950700	0.08761400	C	0.63050300	3.47090900	1.21812300
C	-3.71860100	-1.00109400	0.48159900	H	0.42207300	3.72492000	2.25235000
C	-3.38287300	2.18222900	-1.64486900	C	1.68548200	2.60859300	0.91550700
H	-3.94261700	2.45104200	-2.54527800	H	2.30280900	2.20741000	1.71197300
H	-2.31711400	2.17255300	-1.90314200	C	1.39543700	-2.33325700	-1.33619300
H	-3.52515300	2.98610600	-0.91285100	C	1.35461200	-1.53423800	-2.65687000
C	-6.38321400	-1.82862000	-2.14352100	H	0.99811500	-2.18960300	-3.45997800
H	-6.24139900	-2.91419300	-2.11478300	H	2.33974500	-1.15473900	-2.94039900
H	-6.42632300	-1.52085700	-3.19315200	H	0.66368000	-0.68722000	-2.58426200
H	-7.36666000	-1.62016800	-1.70254400	C	-0.01264700	-2.92809700	-1.09270500
C	-3.13523200	-1.69429100	1.68913800	H	-0.23489800	-3.63448400	-1.90164300
H	-3.44997000	-2.74176500	1.72545200	H	-0.78889900	-2.15878000	-1.09304000
H	-3.43680000	-1.20786700	2.62052100	H	-0.08292300	-3.47382100	-0.14972400
H	-2.03908800	-1.65949300	1.66815700	C	2.39220600	-3.49933100	-1.45853600
C	3.18512100	-0.02848900	-0.59106900	H	2.41694900	-4.11264200	-0.55424000
C	4.37161600	-0.68476600	-0.97591900	H	3.40803200	-3.17343700	-1.68907000
H	4.45449700	-1.75549400	-0.85546500	H	2.07263700	-4.14908900	-2.28207200
C	5.45659600	-0.00227900	-1.51824200	C	2.36604900	-1.81353200	1.66942900
H	6.35127000	-0.54857800	-1.80179700	C	3.74293100	-2.50134100	1.63114200
C	5.37902000	1.37795000	-1.69629300	H	3.94410400	-2.93019600	2.62014000
H	6.21308300	1.92867000	-2.12121400	H	4.54506900	-1.79205600	1.41593200
C	4.21945100	2.04821800	-1.32060500	H	3.79459700	-3.31707400	0.90684500
				C	2.44206200	-0.64186200	2.67431500
				H	1.47505600	-0.14558500	2.79705900
				H	3.17949900	0.10434400	2.36125700
				H	2.75522900	-1.02858300	3.65138200
				C	1.30234600	-2.82037900	2.15133400
				H	1.28362700	-3.72239200	1.53331800
				H	0.30004400	-2.38205400	2.15875800
				H	1.54245600	-3.12993300	3.17525300
				Cl	-2.50117700	1.38060300	2.54161400
				P	1.75767900	-1.03814700	0.03421500

Gold(I) carbenoid 1b'



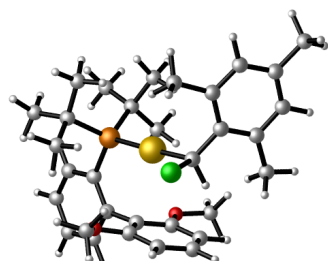
E = -2222.18169603

G = -2221.558599

Au	0.33461500	-0.06592300	0.40913200
C	2.15432700	0.95337700	0.60576300
H	2.03794500	1.86881500	0.03599200
C	3.31502700	0.16031700	0.08695200
C	3.84303800	0.50095300	-1.18376800
C	4.85249400	-0.28291500	-1.75066200
H	5.24282600	-0.00946600	-2.72931500
C	5.37699900	-1.39953500	-1.09730300
C	4.83920300	-1.73318700	0.14810100
H	5.21781100	-2.61135500	0.66838600
C	3.82038200	-0.98725600	0.74808700
C	3.30785400	1.67723300	-1.97264600
H	3.83090700	1.77299000	-2.92838300
H	3.42952800	2.62285200	-1.43115800
H	2.23667800	1.57019700	-2.18481400
C	6.50284200	-2.20460500	-1.70183700
H	6.43514100	-3.26148400	-1.42320400
H	7.48040700	-1.84212000	-1.35810100
H	6.50026200	-2.14207300	-2.79484500
C	3.26955100	-1.45286600	2.07443900
H	3.60218700	-2.47180100	2.29514500
H	2.17298700	-1.43509300	2.07108500
H	3.58144600	-0.80119400	2.89524400
C	-3.15100200	-0.33332600	-0.42515000
C	-4.34902100	-1.02646300	-0.69340800
H	-4.36782900	-2.10566300	-0.63495100
C	-5.52872400	-0.37111800	-1.03405900
H	-6.42870700	-0.94583000	-1.23165800
C	-5.53911300	1.01995800	-1.11603000
H	-6.44981400	1.55231900	-1.37466300
C	-4.36377800	1.72395700	-0.87418500
H	-4.35677000	2.80705200	-0.95291800
C	-3.15731300	1.08353200	-0.53850900
C	-1.96986500	1.99022300	-0.37561900
C	-1.22636600	2.37316500	-1.51250400

C	-0.13694900	3.23848500	-1.35658400
H	0.44477900	3.50911400	-2.23509300
C	0.22309300	3.75911900	-0.11324900
C	-0.56358000	3.41755300	0.98947800
H	-0.30627600	3.81587400	1.96779800
C	-1.65655300	2.55484400	0.88143700
C	-1.58578500	1.92242900	-2.91163100
H	-0.69419800	1.60391500	-3.46188700
H	-2.03276600	2.75022600	-3.47594500
H	-2.30194900	1.10174600	-2.91935700
C	1.43047800	4.64860100	0.05781400
H	1.15017900	5.62757200	0.46335400
H	1.94794200	4.81268300	-0.89174400
H	2.13813000	4.19656000	0.76214900
C	-2.45525500	2.25839800	2.12989000
H	-2.70962500	3.18787500	2.65005300
H	-1.86919100	1.64998300	2.82530100
H	-3.38583600	1.73017400	1.91473300
C	-2.07478900	-2.28143100	1.62360300
C	-3.41296800	-3.04319100	1.63398600
H	-3.49675600	-3.77716100	0.83068900
H	-4.26644800	-2.36412000	1.57775900
H	-3.49313900	-3.58763100	2.58249100
C	-2.12383100	-1.22848100	2.75059300
H	-1.17618200	-0.69127500	2.84916300
H	-2.33057600	-1.73323100	3.70196300
H	-2.91989400	-0.49948900	2.58101600
C	-0.92284600	-3.26456000	1.91493400
H	0.05428000	-2.77442700	1.86872700
H	-0.92106900	-4.11354700	1.22650100
H	-1.04938300	-3.66636400	2.92713700
C	-1.29708500	-2.49327000	-1.45221300
C	-2.24604800	-3.69722000	-1.58942000
H	-2.16748700	-4.38600200	-0.74474400
H	-1.97042500	-4.25986700	-2.48962200
H	-3.29108500	-3.40307400	-1.70672700
C	-1.38829600	-1.62285500	-2.72067700
H	-0.72542500	-0.75582800	-2.65332300
H	-2.40613700	-1.27024200	-2.90562900
H	-1.07403600	-2.21794600	-3.58607200
C	0.15347300	-3.02062400	-1.34635000
H	0.88355000	-2.20734400	-1.33187800
H	0.35908100	-3.64696100	-2.22295300
H	0.31863500	-3.63253500	-0.45877200
Cl	2.44852000	1.66623600	2.31878600
P	-1.63804300	-1.31469100	0.02778000

Gold(I) carbenoid 1c'



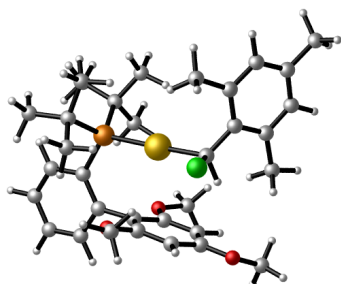
E = -2333.27610932

G = -2332.673481

Au	-0.42087500	0.14185700	0.38483200
C	-2.19235900	-0.88223600	0.83468900
H	-2.03864000	-1.90704200	0.51158100
C	-3.41623100	-0.30324200	0.19460600
C	-3.96619700	0.94614600	0.57681700
C	-5.05666500	1.46212700	-0.12922600
H	-5.46938000	2.42169400	0.17748300
C	-5.62619500	0.79676400	-1.21752400
C	-5.05908500	-0.41970700	-1.60108900
H	-5.47347400	-0.95230000	-2.45523300
C	-3.97636700	-0.98092400	-0.91718300
C	-3.39554800	1.75615300	1.71581100
H	-3.76839700	2.78460700	1.68548400
H	-2.30057700	1.77848400	1.66955400
H	-3.65045400	1.32418700	2.68763200
C	-6.82820500	1.36265900	-1.93581500
H	-6.81036000	2.45754500	-1.94700900
H	-7.76295200	1.06007000	-1.44611100
H	-6.87794600	1.01452900	-2.97256900
C	-3.40418800	-2.29072400	-1.41645800
H	-3.96260800	-2.64964900	-2.28581400
H	-3.44406300	-3.07369200	-0.64963600
H	-2.35169700	-2.19023200	-1.70875000
C	3.09512200	0.37604600	-0.39168700
C	4.29802600	1.04974700	-0.68261200
H	4.30405000	2.12633200	-0.77351400
C	5.50126800	0.37333500	-0.86155300
H	6.40617300	0.93136100	-1.08362200
C	5.53033900	-1.01552100	-0.75136400
H	6.46033500	-1.56139500	-0.88110100
C	4.34988100	-1.70125800	-0.48642800
H	4.35558100	-2.78488600	-0.42045800
C	3.12448900	-1.03677800	-0.31407400
C	1.93749500	-1.92513400	-0.12008200
C	1.48104100	-2.28004100	1.16187700

C	0.44139100	-3.20729600	1.32245800
H	0.06609600	-3.45909400	2.30473000
C	-0.15181900	-3.75992300	0.19200800
H	-0.96915200	-4.46439300	0.31402900
C	0.26239500	-3.41295100	-1.09374100
H	-0.22725300	-3.85020500	-1.95404400
C	1.31255600	-2.49920400	-1.24242300
C	1.48205100	-1.72116700	3.48402500
H	0.43270900	-1.40880700	3.43071000
H	2.04112200	-1.03389800	4.12045600
H	1.54632000	-2.73203600	3.90587200
C	1.13550000	-2.51897900	-3.62873400
H	1.20173000	-3.60732000	-3.75627800
H	1.64756600	-2.02919100	-4.45841400
H	0.07896400	-2.22037300	-3.62779300
C	1.23950000	2.25340200	-1.82363000
C	-0.20132000	2.81394100	-1.84482100
H	-0.35787200	3.60552800	-1.10991000
H	-0.94556700	2.03350200	-1.66398800
H	-0.39293700	3.24204900	-2.83639200
C	1.34004000	1.15242300	-2.90096100
H	1.07182500	1.58188700	-3.87375400
H	0.65185100	0.32848800	-2.69033700
H	2.34650100	0.73378500	-2.97405600
C	2.21729000	3.39382600	-2.15103300
H	1.95034800	3.81918200	-3.12603500
H	3.25153100	3.05227800	-2.22424400
H	2.16302100	4.20338300	-1.41872900
C	1.88452200	2.54768900	1.29938000
C	0.71572000	3.54904700	1.38987000
H	0.77769800	4.08107200	2.34659800
H	-0.25635200	3.04929000	1.34680900
H	0.75877000	4.29933000	0.59523200
C	1.88547000	1.65493100	2.56165200
H	2.61723600	0.84607100	2.48445500
H	0.90455100	1.20446700	2.73699700
H	2.13889400	2.27205200	3.43232700
C	3.21238100	3.32694000	1.26679300
H	3.33618300	3.92883000	0.36345800
H	4.07446600	2.66488900	1.36884000
H	3.22790800	4.01561500	2.12008100
Cl	-2.40309800	-1.16056800	2.69209000
O	2.10255000	-1.65181500	2.20041300
O	1.79957300	-2.08562000	-2.45152500
P	1.53995400	1.35505700	-0.15734800

Gold(I) carbenoid 1d'



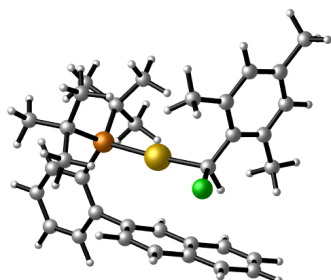
E = -2447.78290171

G = -2447.171876

Au	-0.31364300	-0.44365000	-0.37870500
C	-2.18889900	0.30904300	-0.93781700
H	-2.15984000	1.37987200	-0.76442600
C	-3.35179100	-0.30941400	-0.22386900
C	-3.74249600	-1.65855500	-0.41453900
C	-4.78180700	-2.18924100	0.35544100
H	-5.07072500	-3.22667300	0.19620800
C	-5.45390500	-1.43996800	1.32385200
C	-5.04789500	-0.11816100	1.51599400
H	-5.54728200	0.48606800	2.27141300
C	-4.02228400	0.45820800	0.76109400
C	-3.05841100	-2.55416300	-1.41832000
H	-3.31636300	-3.60310800	-1.24295500
H	-1.96933600	-2.44576900	-1.35973900
H	-3.33537200	-2.29509800	-2.44407100
C	-6.59820500	-2.02963000	2.11372600
H	-6.47952400	-3.10988800	2.24692100
H	-7.55734100	-1.86969800	1.60414200
H	-6.67919700	-1.57345800	3.10580300
C	-3.62970800	1.89171500	1.04477800
H	-4.27671900	2.32524600	1.81341000
H	-3.70247400	2.51950300	0.14983300
H	-2.59276300	1.96514900	1.39624600
C	3.21101900	-0.20456600	0.39909800
C	4.48543800	-0.71498100	0.71592800
H	4.61850100	-1.77673100	0.86358900
C	5.60095900	0.10668100	0.84859200
H	6.56565100	-0.32849000	1.09277600
C	5.46555400	1.48135700	0.66403400
H	6.32485300	2.13925400	0.75663300
C	4.21154900	2.00719300	0.37326200
H	4.08866700	3.07887900	0.25080600
C	3.07161300	1.19566600	0.24618200
C	1.78697700	1.92532000	0.02425500
C	1.26039300	2.14601600	-1.26414800
C	0.13035800	2.94197500	-1.45832500

H	-0.30623500	3.10159000	-2.43382200
C	-0.49697500	3.51630700	-0.34959200
C	-0.01654900	3.30469600	0.94659500
H	-0.51720700	3.73810500	1.79858900
C	1.12550400	2.50949600	1.11446300
C	1.28036100	1.45584600	-3.55114000
H	0.27527900	1.02837800	-3.46027500
H	1.90605000	0.80497500	-4.16328700
H	1.22226500	2.44488700	-4.02238100
C	0.98970800	2.67851600	3.50175200
H	0.94208100	3.77417700	3.55605100
H	1.56886900	2.30426900	4.34736400
H	-0.02839400	2.27041200	3.55149200
C	1.59670600	-2.21219600	1.94086700
C	0.22145000	-2.91542100	2.00943500
H	0.13573000	-3.74348000	1.30307000
H	-0.60211100	-2.22301200	1.81591000
H	0.09018300	-3.32654200	3.01789200
C	1.60063700	-1.05689200	2.96485100
H	1.36712700	-1.46042500	3.95747700
H	0.84841500	-0.30203400	2.71734200
H	2.56913200	-0.55363800	3.01631100
C	2.68740200	-3.23362900	2.30621500
H	2.48717800	-3.61853600	3.31365600
H	3.68656700	-2.79430100	2.32581800
H	2.69237500	-4.09159900	1.62844100
C	2.27461800	-2.59107900	-1.16326900
C	1.23550900	-3.72921700	-1.20316800
H	1.38118100	-4.30941900	-2.12197400
H	0.21020400	-3.34921300	-1.20747000
H	1.34982200	-4.41665200	-0.36047200
C	2.17821200	-1.77336200	-2.47171200
H	2.81534700	-0.88519400	-2.44258800
H	1.15420000	-1.44353100	-2.66661100
H	2.49972300	-2.40491100	-3.30894800
C	3.68519100	-3.20494500	-1.08951600
H	3.87474500	-3.73439800	-0.15323300
H	4.46326100	-2.45279100	-1.23224600
H	3.78542000	-3.93483700	-1.90182800
O	1.92342400	1.52379700	-2.27825200
O	1.67129500	2.23709400	2.33857400
P	1.78226500	-1.37091200	0.22924000
O	-1.60390900	4.26473200	-0.63153700
C	-2.15978500	5.06760900	0.40022500
H	-1.41267700	5.75502600	0.81862800
H	-2.96029500	5.64317600	-0.06717800
H	-2.58515100	4.46048200	1.20812700
Cl	-2.41230500	0.29997900	-2.81605500

Gold(I) Carbenoid 1e'



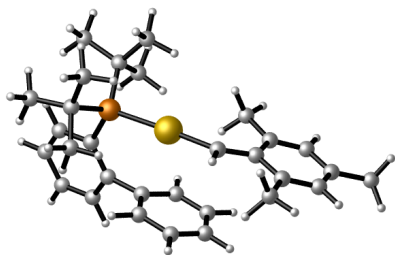
E = -2257.86566694

G = -2257.278242

C	3.38695500	0.04366100	-0.40663500
P	2.00047700	-1.14990000	-0.08264200
Cl	-2.43928400	0.83448300	2.51682500
Au	-0.15582900	-0.26039700	0.37953800
C	4.65380300	-0.45548800	-0.76972000
H	4.81944600	-1.52246800	-0.80921500
C	5.71913500	0.38220500	-1.08846400
H	6.67847100	-0.04619100	-1.36321000
C	5.54025200	1.76383500	-1.05604900
H	6.35822700	2.43352600	-1.30497100
C	4.29831500	2.28074500	-0.70040300
H	4.14599600	3.35534500	-0.67001600
C	3.21308700	1.45038500	-0.37110300
C	1.93893400	2.14681400	-0.02075300
C	1.54568700	2.30024400	1.33875400
H	2.16447100	1.87016600	2.11928900
C	0.38240000	2.95966500	1.66248700
H	0.06812300	3.03741000	2.69842600
C	-0.45201400	3.50560200	0.65167300
C	-1.68364300	4.14635600	0.95182200
H	-2.00116300	4.20509400	1.98843800
C	-2.47329000	4.65640600	-0.05466900
H	-3.41736000	5.13652300	0.18503900
C	-2.06526000	4.55063400	-1.40790700
H	-2.69869500	4.95471200	-2.19218100
C	-0.88166100	3.92577500	-1.73128100
H	-0.57292500	3.83120900	-2.76934100
C	-0.04878000	3.38158000	-0.71694700
C	1.16109400	2.70216400	-1.01767600
H	1.46195100	2.59674800	-2.05705400
C	2.55433200	-2.17381900	1.43408100

C	1.55625100	-3.33293300	1.62887100
H	1.73531100	-3.79542100	2.60672900
H	1.68326000	-4.11233800	0.87202700
H	0.51760000	-2.99178600	1.60533600
C	3.98586400	-2.73957700	1.40219700
H	4.14326300	-3.33337000	2.31060000
H	4.73727400	-1.94714500	1.39920500
H	4.16728000	-3.39796000	0.54975800
C	2.44881800	-1.20447400	2.63351300
H	2.73407400	-1.73534000	3.54948100
H	1.43252900	-0.82132000	2.76152700
H	3.12788900	-0.35331700	2.51794300
C	1.83493300	-2.18786300	-1.68823400
C	1.79093400	-1.15950500	-2.83997700
H	1.55661700	-1.68180200	-3.77487900
H	2.74644200	-0.64452800	-2.96985400
H	1.01169600	-0.40811800	-2.67243900
C	0.47970000	-2.93294300	-1.65821600
H	0.35591800	-3.46793100	-2.60752500
H	-0.36318100	-2.24707400	-1.54192300
H	0.42402600	-3.66983000	-0.85510600
C	2.94517700	-3.21979600	-1.95326300
H	2.73097900	-3.73054600	-2.89976000
H	2.98573700	-3.98644000	-1.17532200
H	3.93302100	-2.76700600	-2.05413400
C	-2.11527900	0.41399800	0.70829200
H	-2.18290100	1.40470200	0.26964700
C	-3.16630700	-0.48794900	0.13394000
C	-3.42531400	-1.78519600	0.64372900
C	-4.35463800	-2.60594000	-0.00225200
H	-4.54291100	-3.59920500	0.40176500
C	-5.04168700	-2.19911600	-1.14813200
C	-4.76620200	-0.92601100	-1.65005100
H	-5.28080100	-0.58734900	-2.54751900
C	-3.85332200	-0.06586800	-1.03192200
C	-2.71750400	-2.32262700	1.86412400
H	-2.84040900	-3.40768100	1.93784600
H	-3.09706100	-1.86762300	2.78343100
H	-1.64660000	-2.09190400	1.83166400
C	-6.06819300	-3.09367900	-1.80181100
H	-7.06091300	-2.95272100	-1.35473900
H	-5.81034700	-4.15173300	-1.68679900
H	-6.16215900	-2.88266200	-2.87197400
C	-3.60116700	1.29107400	-1.65231900
H	-4.23865000	1.44089900	-2.52851900
H	-2.56001000	1.40949500	-1.97472000
H	-3.80082100	2.10848900	-0.95101400

Gold(I) Carbene 5a'



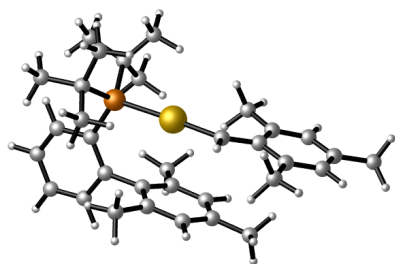
E = -1643.78502029

G = -1643.242214

Au	0.15748800	-0.76380000	-0.33699400
C	2.12474800	-0.89906200	-0.81734500
H	2.26402300	-1.13602900	-1.87332200
C	-2.80978500	1.13055000	0.25473100
C	-4.15183800	1.31424900	0.64484000
H	-4.78992700	0.45546500	0.79929200
C	-4.69591400	2.57845600	0.84955900
H	-5.73427500	2.67671200	1.14997800
C	-3.89724700	3.70657200	0.67051700
H	-4.30282400	4.70115100	0.82765100
C	-2.56958700	3.54852700	0.28551100
H	-1.94268400	4.42273400	0.13915300
C	-2.00292100	2.28041100	0.06720900
C	-0.56472300	2.29049500	-0.34597100
C	0.42797500	2.59824400	0.59836400
H	0.14339200	2.74367100	1.63670100
C	1.76313300	2.72795500	0.21163500
H	2.51926500	2.96404700	0.95454300
C	2.12396800	2.56888100	-1.12803600
H	3.16071100	2.68371400	-1.43006900
C	1.14400500	2.27496500	-2.07855500
H	1.41236200	2.16760900	-3.12555300
C	-0.19203100	2.13666700	-1.69126900
H	-0.95279600	1.92538100	-2.43497200
C	-2.52099900	-1.46934300	1.76536100
C	-2.09703400	-0.46830600	2.86135500
H	-2.12120300	-0.97543000	3.83217300
H	-2.76415800	0.39502400	2.91390000
H	-1.07600500	-0.10346900	2.70278500
C	-1.60953900	-2.71461800	1.86241800

H	-1.79795300	-3.21261700	2.82025400
H	-0.54945300	-2.44784700	1.82920300
H	-1.79977600	-3.44081400	1.06989700
C	-3.97370600	-1.91987200	2.00149000
H	-4.28823200	-2.68228800	1.28536000
H	-4.68863300	-1.09652100	1.97433800
H	-4.04086900	-2.36611900	3.00001600
C	-3.11869000	-1.36851900	-1.38508200
C	-4.65169300	-1.22501300	-1.34175200
H	-5.06874800	-1.72788100	-2.22140700
H	-4.96314400	-0.17930400	-1.38822600
H	-5.10241600	-1.68634000	-0.46166500
C	-2.60527700	-0.62521900	-2.63859600
H	-1.52620400	-0.74230600	-2.77634800
H	-2.83814400	0.44319700	-2.59363100
H	-3.10452900	-1.03561800	-3.52323900
C	-2.73621100	-2.85869800	-1.48096800
H	-3.17600500	-3.44869200	-0.67259300
H	-1.65129000	-3.00588400	-1.46936500
H	-3.11876800	-3.26367000	-2.42430100
P	-2.18301800	-0.60113000	0.08858000
C	3.33754600	-0.62532700	-0.17481400
C	3.41990700	-0.34927300	1.24861700
C	4.55752400	-0.55590100	-0.96560200
C	4.64415600	-0.00361000	1.79691700
C	5.74470400	-0.19222200	-0.35574600
C	5.81279000	0.08686500	1.02106500
H	4.71022200	0.20116000	2.86151800
H	6.65209400	-0.12216300	-0.94850500
C	4.56575300	-0.83455400	-2.44868000
H	4.19121500	-1.83792600	-2.67552300
H	3.94311300	-0.11827900	-2.99516600
H	5.57975200	-0.76254400	-2.84594200
C	7.12441300	0.43715400	1.65946800
H	7.64157600	-0.48359000	1.96070300
H	7.78336400	0.96532500	0.96535900
H	6.98968600	1.04421400	2.55814100
C	2.23145600	-0.43572100	2.16542800
H	1.48905000	0.32544400	1.90731300
H	1.73788900	-1.40816000	2.08948300
H	2.53475600	-0.28259300	3.20349500

Gold(I) Carbene 5b'



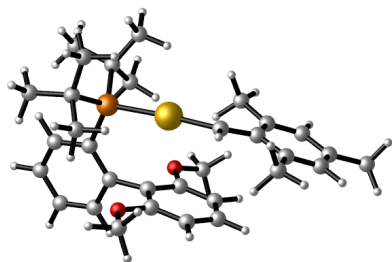
E = -1761.75758572

G = -1761.133641

Au	0.08441400	-0.81352400	-0.42270600
C	2.04050300	-0.82200600	-0.96938000
H	2.14291900	-0.79830900	-2.05537000
C	-2.91799200	0.92452200	0.29325300
C	-4.29125400	1.05456400	0.58655200
H	-4.90619500	0.17130200	0.68560000
C	-4.89971000	2.29451500	0.75512700
H	-5.96010200	2.34953500	0.98019500
C	-4.13704300	3.45394800	0.62906400
H	-4.59352100	4.43169000	0.74823600
C	-2.77531800	3.34785100	0.36382300
H	-2.17032200	4.24642700	0.28865400
C	-2.13473300	2.10632300	0.20358000
C	-0.64428300	2.18209100	0.01662900
C	0.18749800	2.27499900	1.15873700
C	1.56727600	2.42165800	0.98932800
H	2.19894300	2.48431400	1.87333200
C	2.15440800	2.52014500	-0.27554400
C	1.31432100	2.47728800	-1.38920600
H	1.74100600	2.58932300	-2.38406900
C	-0.07520700	2.32343100	-1.26878600
C	-2.55090000	-1.75003200	1.68421300
C	-2.11833500	-0.81305800	2.82877200
H	-2.16226300	-1.36358000	3.77503600
H	-2.77320500	0.05707000	2.91628500
H	-1.09097700	-0.46128700	2.69624600
C	-1.63619500	-2.99622700	1.70958500
H	-1.77635100	-3.51020000	2.66728100
H	-0.57931700	-2.72868000	1.62614000
H	-1.86716800	-3.70979000	0.91768500
C	-4.00246200	-2.20595900	1.91553700
H	-4.33406100	-2.92572400	1.16432600
H	-4.70930600	-1.37484800	1.94464400
H	-4.05895100	-2.70569800	2.88914000
C	-3.17458200	-1.54554500	-1.43785600

C	-4.71177100	-1.44670300	-1.40204000
H	-5.10710900	-1.97043100	-2.27953900
H	-5.05252400	-0.41127600	-1.46279500
H	-5.15627300	-1.91216500	-0.52125500
C	-2.68389100	-0.77788300	-2.68282400
H	-1.60473500	-0.88100700	-2.82858400
H	-2.92851400	0.28544600	-2.62334300
H	-3.18297400	-1.18503100	-3.56922400
C	-2.75398400	-3.02402300	-1.56042500
H	-3.19741500	-3.64572900	-0.77884700
H	-1.66635000	-3.14590100	-1.53064900
H	-3.10699400	-3.41178500	-2.52235300
P	-2.24749300	-0.78580700	0.05424100
C	3.28364900	-0.75734300	-0.32831500
C	3.41957800	-0.81730900	1.11541600
C	4.48636000	-0.59550200	-1.13076200
C	4.68231400	-0.71129600	1.67675500
C	5.71665500	-0.49920400	-0.50551300
C	5.83972800	-0.55723100	0.89375300
H	4.78815600	-0.75572600	2.75678200
H	6.61323900	-0.36950400	-1.10442400
C	3.64446800	2.71356300	-0.41659100
H	3.92955800	3.74581800	-0.18254700
H	4.19460000	2.06072900	0.26805000
H	3.98507200	2.50276600	-1.43423100
C	-0.90893600	2.33107400	-2.52893200
H	-0.79030700	1.39400700	-3.08264900
H	-1.97139700	2.46492500	-2.32074800
H	-0.59123100	3.14092300	-3.19287700
C	-0.36681300	2.28977200	2.56631800
H	0.23354500	1.66409100	3.23516400
H	-0.33794900	3.30818000	2.97118500
H	-1.40039400	1.95248100	2.61647300
C	4.43408000	-0.49456000	-2.63540700
H	5.43777000	-0.37293300	-3.04662600
H	3.99636600	-1.38946100	-3.08945500
H	3.83638500	0.36504100	-2.95690000
C	7.19214100	-0.48607500	1.53937400
H	7.62147700	-1.49490200	1.60099400
H	7.88594300	0.12522200	0.95632300
H	7.13664600	-0.09246500	2.55731800
C	2.24660600	-1.00220900	2.03741200
H	1.54283700	-0.17056300	1.94436800
H	1.69868100	-1.91867100	1.80118400
H	2.57940100	-1.05959700	3.07615300

Gold(I) Carbene 5c'



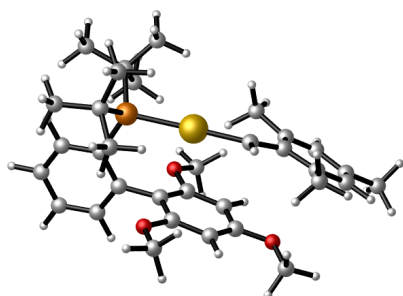
E = -1872.85105731

G = -1872.246067

Au	-0.09067100	-1.06360000	0.28559700
C	-2.02695800	-1.27752900	0.84043900
H	-2.13765600	-1.54843200	1.89138800
C	2.70598600	1.03937800	-0.25019900
C	4.03751700	1.35843000	-0.58409200
H	4.74490600	0.56924400	-0.79622300
C	4.48460300	2.67400600	-0.65409100
H	5.51819600	2.87982700	-0.91405800
C	3.59615600	3.71505200	-0.39038200
H	3.92592200	4.74824400	-0.43873900
C	2.27645900	3.41975600	-0.06635500
H	1.57747800	4.22544100	0.13573800
C	1.80508300	2.09826000	0.00761800
C	0.35350500	1.97230300	0.35665100
C	-0.63248000	2.19176600	-0.62495300
C	-1.98600400	2.30682900	-0.28007000
H	-2.74219600	2.47931000	-1.03428200
C	-2.35447200	2.18785400	1.05808100
H	-3.40267300	2.27455700	1.32797800
C	-1.41199800	1.94718200	2.05545600
H	-1.72462700	1.87283100	3.08906200
C	-0.05424100	1.85961200	1.70321900
C	2.50958100	-1.37462100	-2.02541600
C	1.95680700	-0.28365000	-2.96784300
H	1.95374500	-0.67252800	-3.99235600
H	2.56793200	0.62135700	-2.94838700
H	0.93354100	0.00486800	-2.70920100
C	1.69186000	-2.66902500	-2.23522600
H	1.83247500	-3.00801700	-3.26783500
H	0.62228500	-2.50300400	-2.08018900
H	2.00573300	-3.48145500	-1.57689200
C	3.98023700	-1.66343100	-2.37476900
H	4.39926500	-2.46963100	-1.76804000
H	4.61743100	-0.78254800	-2.28056000

H	4.03296900	-1.98484900	-3.42121000
C	3.25111200	-1.61317100	1.08782800
C	4.76841000	-1.35568200	1.02893900
H	5.24911300	-1.95954400	1.80682000
H	5.01087500	-0.31113500	1.23421600
H	5.21617000	-1.64171800	0.07557200
C	2.72824700	-1.08406500	2.44234300
H	1.68273500	-1.35993600	2.61067600
H	2.80569100	0.00398900	2.50997900
H	3.32711400	-1.52530800	3.24722500
C	2.98061400	-3.12760900	0.99108700
H	3.44135000	-3.57211000	0.10502100
H	1.90922700	-3.35334200	0.97850600
H	3.41578000	-3.62163200	1.86691000
P	2.20699700	-0.73541500	-0.24550200
C	-3.25253700	-0.96137800	0.23921600
C	-3.37273100	-0.68088800	-1.17902300
C	-4.43468000	-0.82542500	1.07406600
C	-4.59684900	-0.26792600	-1.68223000
C	-5.62041700	-0.38761600	0.51095300
C	-5.72627600	-0.10655000	-0.86301800
H	-4.69309600	-0.06805900	-2.74560400
H	-6.49765000	-0.26230300	1.13916800
O	0.95277300	1.68001100	2.59550500
O	-0.16948900	2.25407900	-1.90685500
C	0.63216300	1.51609000	3.97411900
H	1.58386700	1.36628100	4.48390000
H	0.13906200	2.40713700	4.37959900
H	-0.00634400	0.63802700	4.13254600
C	-1.05110400	2.70428300	-2.93243100
H	-0.44564500	2.76846900	-3.83681500
H	-1.87284700	1.99673300	-3.09915200
H	-1.46477800	3.69168600	-2.69677300
C	-4.39708600	-1.09503600	2.55800100
H	-4.05177600	-2.11010200	2.77892400
H	-3.72494100	-0.39828800	3.07046800
H	-5.39104100	-0.98089800	2.99436300
C	-7.04080800	0.31898200	-1.44898900
H	-7.64734400	-0.56843500	-1.67291600
H	-7.61416900	0.93115200	-0.74744300
H	-6.91153400	0.87186000	-2.38254200
C	-2.23204800	-0.85257200	-2.14462400
H	-1.43776200	-0.12664300	-1.94768800
H	-1.78543800	-1.84664100	-2.06333300
H	-2.57544600	-0.71318900	-3.17244700

Gold(I) Carbene 5d'



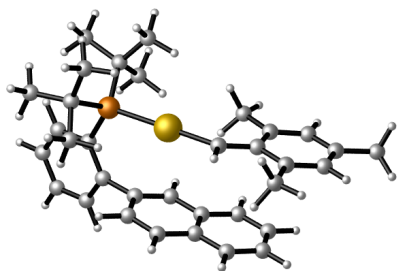
E = -1987.38360385

G = -1986.749420

Au	-0.14109800	-1.11477100	-0.32862500
C	1.79136500	-1.50916700	-0.79478600
H	1.92754000	-1.76065700	-1.84812300
C	-2.86008100	1.10374600	0.25753800
C	-4.19736800	1.46029300	0.52210800
H	-4.95694000	0.69413800	0.58797500
C	-4.58239500	2.78404700	0.70909300
H	-5.62238600	3.02060200	0.91110900
C	-3.62389600	3.79368100	0.63631000
H	-3.90521700	4.83278800	0.77704000
C	-2.29710100	3.45849400	0.38811600
H	-1.54324900	4.23820900	0.34054300
C	-1.88682200	2.12788500	0.20130600
C	-0.41879600	1.93930400	-0.01788600
C	0.47274700	1.96074900	1.07551800
C	1.85404800	1.99663200	0.89007800
H	2.55178600	2.01189500	1.71531900
C	2.36980500	2.00957100	-0.41073400
C	1.52424500	1.98579500	-1.52360500
H	1.92423800	2.00894700	-2.52563200
C	0.13400300	1.96785800	-1.31226100
C	-2.93845200	-1.51720100	1.72484100
C	-2.44048600	-0.57672200	2.84321500
H	-2.54316000	-1.09019000	3.80597600
H	-3.01777500	0.34942800	2.88753200
H	-1.38918500	-0.30225900	2.71272200
C	-2.18534500	-2.86089100	1.84153500
H	-2.45644700	-3.33453100	2.79189500
H	-1.10126200	-2.71704800	1.83653500
H	-2.43706200	-3.55841000	1.04054800
C	-4.44472500	-1.78102800	1.90045800
H	-4.82908200	-2.49187200	1.16496100
H	-5.04246400	-0.86877600	1.85466000
H	-4.60874300	-2.21954600	2.89139100
C	-3.41993300	-1.32769300	-1.43923400

C	-4.91975000	-0.97802300	-1.47071700
H	-5.36706500	-1.46451200	-2.34477600
H	-5.08239100	0.09616200	-1.57840200
H	-5.46146500	-1.33057400	-0.59146400
C	-2.75175500	-0.67634800	-2.67186300
H	-1.72138200	-1.01980100	-2.80504500
H	-2.73662800	0.41412300	-2.59706300
H	-3.31799200	-0.95475500	-3.56805400
C	-3.24553000	-2.85811400	-1.51218200
H	-3.80657800	-3.37537300	-0.72925600
H	-2.19424200	-3.15647900	-1.44224800
H	-3.62949000	-3.21227600	-2.47548700
P	-2.44951300	-0.68299600	0.07114400
C	3.00916600	-1.34699800	-0.12426600
C	3.08006100	-1.08598300	1.30174700
C	4.24141300	-1.32208700	-0.89501000
C	4.29274100	-0.70973000	1.85435200
C	5.41641100	-0.92648100	-0.28275100
C	5.46039300	-0.59208600	1.08228000
H	4.35075000	-0.50433200	2.91961600
H	6.33215200	-0.87144600	-0.86433100
O	-0.77257200	1.98494000	-2.32392800
O	-0.11671300	1.91494900	2.30421100
C	-0.31255900	1.93282600	-3.66997400
H	-1.20917900	1.92029900	-4.28978300
H	0.29043100	2.81273800	-3.92360700
H	0.26942500	1.02110000	-3.85564700
C	0.68191700	2.16553000	3.45793500
H	-0.01049500	2.18091700	4.29994300
H	1.42385700	1.37326300	3.61632600
H	1.19395500	3.13192200	3.38455000
O	3.72981400	2.02205300	-0.48663400
C	4.34071500	2.16830800	-1.76181200
H	5.41490300	2.20553200	-1.57783700
H	4.12076900	1.31524100	-2.41590200
H	4.02372300	3.09472800	-2.25563900
C	4.27481700	-1.68375100	-2.36028600
H	5.30085000	-1.67376900	-2.73310000
H	3.86621400	-2.68407200	-2.53589200
H	3.69462100	-0.98302300	-2.96993000
C	6.75181700	-0.17578400	1.72271700
H	7.25249400	-1.05385200	2.15165000
H	7.43799100	0.27088800	0.99906300
H	6.58418900	0.53204100	2.53895100
C	1.89965700	-1.26438200	2.21783400
H	1.13447300	-0.50497100	2.03769300
H	1.42582800	-2.23768700	2.06633800
H	2.21295800	-1.19198200	3.26220600

Gold(I) Carbene 5e'



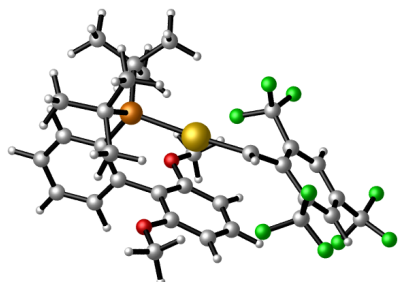
E = -1797.41542281

G = -1796.854818

Au	-0.13788500	-0.72298600	-0.51314600
C	1.84189400	-0.79028100	-0.97833000
H	2.00702700	-0.62673000	-2.04396900
C	-3.08103900	0.97717800	0.59309600
C	-4.39643500	1.05421500	1.09286700
H	-5.03539900	0.18310300	1.06192500
C	-4.91416100	2.22794500	1.63264600
H	-5.93244000	2.24528300	2.00809000
C	-4.11753500	3.37026000	1.68609900
H	-4.50380700	4.29359900	2.10638800
C	-2.81822400	3.32018300	1.18968100
H	-2.19362100	4.20774700	1.21838200
C	-2.27956200	2.14506600	0.63967000
C	-0.88051200	2.25127400	0.12238000
C	0.20143200	2.15579000	0.97943700
C	1.75214100	2.56689600	-0.88508900
C	0.62401700	2.70144900	-1.73809900
H	0.78331300	2.93195800	-2.78811800
C	-0.65362700	2.55126100	-1.25095800
C	-2.80790700	-1.94798100	1.33117300
C	-2.32565100	-1.29939800	2.64687700
H	-2.34760400	-2.05233000	3.44248200
H	-2.95974000	-0.46470900	2.95429500
H	-1.29572700	-0.93465200	2.56228000
C	-1.93324200	-3.19184700	1.05131300
H	-2.08675200	-3.91585700	1.85937900
H	-0.86906100	-2.94466100	1.02143500
H	-2.18908500	-3.68620000	0.11275700
C	-4.26592000	-2.42023600	1.48181000
H	-4.62289100	-2.94056400	0.59016600
H	-4.95981900	-1.61254000	1.71811900
H	-4.31463000	-3.13305900	2.31270700
C	-3.45817600	-0.97847500	-1.65090200

C	-4.98349400	-0.80780200	-1.52684800
H	-5.43705000	-1.04140800	-2.49649200
H	-5.25765000	0.21939400	-1.27714100
H	-5.43000900	-1.47738500	-0.79020400
C	-2.94050200	0.05119900	-2.67932100
H	-1.86556400	-0.04623200	-2.85789400
H	-3.14787000	1.07644800	-2.35912100
H	-3.45823900	-0.10913600	-3.63152900
C	-3.12651800	-2.40072300	-2.14339400
H	-3.57584500	-3.16983700	-1.51000100
H	-2.04688800	-2.57684800	-2.19343500
H	-3.53399600	-2.53186000	-3.15194500
P	-2.48054300	-0.65228400	-0.04874000
C	3.04482000	-0.93747400	-0.27905800
C	3.09541500	-1.16215100	1.15488000
C	4.30326800	-0.84616000	-1.00583700
C	4.32772100	-1.29955000	1.77419100
C	5.49808400	-0.99026800	-0.32402100
C	5.53512700	-1.22497100	1.06160300
H	4.36604800	-1.46976500	2.84614900
H	6.43579900	-0.92126700	-0.86771600
C	4.34919100	-0.58359800	-2.48920500
H	5.38194100	-0.55288700	-2.84130200
H	3.82765300	-1.35935100	-3.05877200
H	3.88478100	0.37869500	-2.72673100
C	6.84768700	-1.41656700	1.76340600
H	7.13791300	-2.47453500	1.71694600
H	7.64720400	-0.84198000	1.28811400
H	6.78838000	-1.14114000	2.81934800
C	1.86270000	-1.26314600	2.00851900
H	1.25416800	-0.35829800	1.93006500
H	1.23400000	-2.10172300	1.69618500
H	2.13157500	-1.41034900	3.05687500
H	-1.50501300	2.66464000	-1.91284000
H	0.03447600	1.95981800	2.03562100
C	1.53532000	2.30061400	0.50709200
C	2.65940900	2.17073700	1.36364300
C	3.08459100	2.69588200	-1.36216900
C	3.94006400	2.28578700	0.86703900
C	4.15538700	2.55361500	-0.50697800
H	2.49524000	1.97438900	2.41981800
H	3.24506400	2.91915700	-2.41387600
H	4.79120100	2.17614200	1.53174900
H	5.16941900	2.65269800	-0.88179100

Gold(I) Carbene 5c'-CF₃



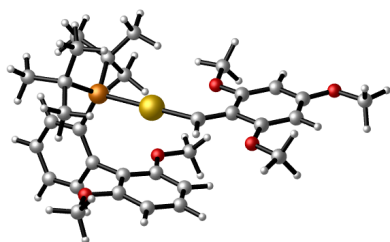
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G = -2765.439993

Au	-0.70086600	0.71647800	-0.71126600
C	1.14818200	1.41288600	-0.99170700
H	1.23967800	2.49707300	-1.03870600
C	-3.43941900	-0.66942400	1.04296600
C	-4.77786200	-1.03800500	1.27964100
H	-5.53069500	-0.85494500	0.52525100
C	-5.16916700	-1.64458500	2.46926500
H	-6.20901200	-1.91673900	2.62006300
C	-4.21787100	-1.89814200	3.45645800
H	-4.50642700	-2.36595100	4.39254400
C	-2.88770700	-1.55967900	3.22953100
H	-2.13956500	-1.77474300	3.98614000
C	-2.47233400	-0.95346000	2.03281300
C	-0.99715900	-0.71949300	1.91916400
C	-0.14987200	-1.80055400	1.59419100
C	1.24179900	-1.68435600	1.71498900
H	1.89070400	-2.51797900	1.48094900
C	1.79018600	-0.48341000	2.16661600
H	2.86788500	-0.40795700	2.27522800
C	0.99231100	0.61220800	2.47809200
H	1.44391400	1.53477000	2.81418900
C	-0.40630100	0.48870700	2.36874200
C	-3.41423300	-1.13798400	-1.93433800
C	-2.91563000	-2.50768500	-1.42718800
H	-2.99806600	-3.23176600	-2.24551100
H	-3.50765100	-2.87516600	-0.58610100
H	-1.87039400	-2.47268200	-1.10921000
C	-2.61819700	-0.76345300	-3.20464700
H	-2.86288500	-1.48404400	-3.99312000
H	-1.53940400	-0.81043700	-3.03585900
H	-2.86365100	0.23153100	-3.58181600
C	-4.90936200	-1.22483800	-2.28820600
H	-5.28633700	-0.29475200	-2.72046500
H	-5.53276400	-1.49447700	-1.43306500

H	-5.04315100	-2.00974700	-3.04095000
C	-3.98416400	1.75817300	-0.65968800
C	-5.49814800	1.64450900	-0.39677900
H	-5.94700800	2.63174800	-0.55290500
H	-5.70885000	1.35416800	0.63426800
H	-6.00326600	0.95016200	-1.07019100
C	-3.37999300	2.67664900	0.42711100
H	-2.33244700	2.91818900	0.22201600
H	-3.43368600	2.22279000	1.42003700
H	-3.94334200	3.61625800	0.44619800
C	-3.74578700	2.38297100	-2.04883900
H	-4.24838900	1.82631800	-2.84406900
H	-2.68019700	2.45234200	-2.29063600
H	-4.15528700	3.39905000	-2.05321800
P	-3.00508700	0.12350800	-0.55808200
C	2.41919100	0.75487800	-0.88148000
C	2.64093300	-0.60743100	-1.24349500
C	3.48657100	1.43823000	-0.21714800
C	3.82243900	-1.24974100	-0.89808500
C	4.63783300	0.76723100	0.16909100
C	4.79381100	-0.57970000	-0.15589000
H	3.99405200	-2.27482900	-1.20154800
H	5.41727000	1.28463800	0.71410000
O	-1.27996700	1.46995800	2.69003600
O	-0.78512900	-2.92120000	1.16892000
C	-0.77360500	2.75885000	3.03914200
H	-1.65001500	3.38839000	3.19020200
H	-0.18865400	2.71960200	3.96465200
H	-0.15876300	3.17105900	2.23022800
C	-0.01724000	-4.09445800	0.90354400
H	-0.73951800	-4.85931600	0.61838100
H	0.68262100	-3.92990400	0.07748500
H	0.52877700	-4.42333200	1.79536400
C	3.35666900	2.90544400	0.16677100
C	5.98747900	-1.34446100	0.37383600
C	1.65599300	-1.39409500	-2.10008700
F	6.32832700	-2.35181400	-0.44621900
F	7.05164200	-0.54400700	0.54008900
F	5.66940800	-1.87339500	1.57532400
F	3.14597800	3.67453900	-0.91980800
F	2.30762100	3.10123000	1.00764400
F	4.45510700	3.35614700	0.78486500
F	2.26768200	-2.42276300	-2.71228900
F	1.09557800	-0.62632900	-3.05330600
F	0.65465200	-1.92676700	-1.35703900

Gold(I) Carbene 5c'-OMe

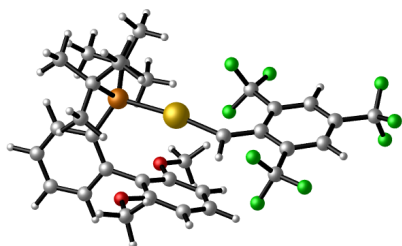


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G = -2097.874195

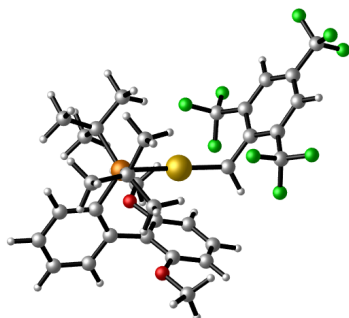
Au	-0.01057500	-0.16218800	-0.74386000
C	1.89449100	0.51617800	-0.95331100
H	2.00377500	1.42537000	-1.54612200
C	-3.27223000	-0.09336500	0.71037000
C	-4.55234800	-0.60454300	1.00225500
H	-4.91951900	-1.47318100	0.47390100
C	-5.38073100	-0.01734300	1.95346700
H	-6.36065000	-0.44075900	2.15089900
C	-4.94270800	1.11334500	2.64118300
H	-5.57621100	1.58669000	3.38504700
C	-3.68298200	1.63407400	2.36525900
H	-3.33414600	2.51597300	2.89334600
C	-2.83072900	1.05159000	1.41347900
C	-1.50938200	1.72841400	1.23392100
C	-0.38937900	1.33286300	1.98931000
C	0.81590600	2.04831600	1.91965900
H	1.67870900	1.74738100	2.49895000
C	0.89360100	3.15795000	1.07995300
H	1.82493100	3.71359000	1.02128200
C	-0.19438800	3.57205900	0.31435500
H	-0.10575600	4.44207300	-0.32317300
C	-1.40044600	2.86257200	0.40683000
C	-2.14226900	-2.79433100	-0.02461000
C	-1.83419600	-2.77250900	1.48834800
H	-1.57348900	-3.78687300	1.81370800
H	-2.69188800	-2.43935600	2.07707400
H	-1.00031100	-2.10253800	1.72055600
C	-0.95039400	-3.45090000	-0.75934000
H	-0.85251100	-4.48639700	-0.41199800
H	-0.01033000	-2.93105700	-0.55857700
H	-1.08972100	-3.47970000	-1.84154500
C	-3.39431800	-3.64866200	-0.29229500
H	-3.61792100	-3.72879100	-1.35868600
H	-4.28196500	-3.28234400	0.22526100
H	-3.20873500	-4.66421600	0.07638100
C	-3.13572200	-0.69279200	-2.22330900

C	-4.64552400	-0.99310900	-2.20955800
H	-5.03687500	-0.84330000	-3.22219100
H	-5.18657400	-0.31495500	-1.54649000
H	-4.87512800	-2.02081400	-1.92149700
C	-2.93986200	0.80207400	-2.56229900
H	-1.88345000	1.04722200	-2.70914400
H	-3.33166900	1.45403800	-1.77743000
H	-3.47246500	1.02518600	-3.49412400
C	-2.43994300	-1.55212000	-3.29664800
H	-2.64102000	-2.61902400	-3.16762700
H	-1.35584100	-1.39801600	-3.30161800
H	-2.82293200	-1.26585600	-4.28269200
P	-2.24526300	-0.95473300	-0.55952000
C	3.11029900	0.07510200	-0.46064100
C	3.25918900	-1.11741100	0.36925300
C	4.34354700	0.79066900	-0.77975000
C	4.50075400	-1.55384200	0.78340900
C	5.58702900	0.34273700	-0.36006000
C	5.65518800	-0.83128900	0.41394000
H	4.64142300	-2.43664800	1.39066600
H	6.48676700	0.87968000	-0.61642200
O	-2.53541200	3.19661100	-0.26735500
O	-0.57165300	0.21682700	2.75304800
C	-2.49940000	4.30255700	-1.16333600
H	-3.50028200	4.37119000	-1.59040800
H	-2.26470000	5.23670900	-0.63911800
H	-1.77127500	4.14195000	-1.96830600
C	0.52464000	-0.26570500	3.51836300
H	0.16138800	-1.16051700	4.02585600
H	1.37042600	-0.52824700	2.87151000
H	0.84791700	0.46640600	4.26837100
O	4.18034700	1.89888400	-1.50698800
O	6.79609500	-1.35066000	0.86682200
O	2.12256900	-1.73964200	0.70237800
C	2.17336900	-2.94869000	1.46928200
H	2.73348800	-3.72447900	0.93738900
H	2.62153800	-2.76977300	2.45249100
H	1.13612000	-3.25685600	1.58836500
C	5.31841700	2.66429800	-1.92103600
H	5.86226900	3.05624300	-1.05476500
H	5.98716200	2.06261600	-2.54570600
H	4.91548100	3.49044900	-2.50525300
C	8.05186800	-0.72400600	0.56409400
H	8.22191900	-0.69437300	-0.51700800
H	8.09480400	0.28674000	0.98285100
H	8.80796400	-1.34884100	1.03725100

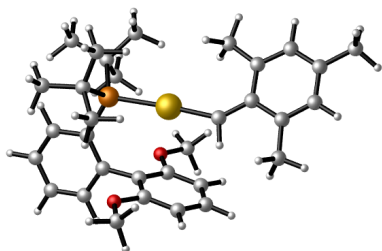
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Au	0.53455000	-0.14460200	-0.68371600
C	-1.32165400	0.63666700	-0.55624200
H	-1.27091300	1.70265000	-0.75089100
C	3.88232600	0.06931500	0.49870000
C	5.26947400	-0.17710600	0.46375900
H	5.68038700	-0.85629500	-0.27014000
C	6.14673200	0.42996000	1.35699100
H	7.20921400	0.21570700	1.29881800
C	5.64955300	1.30727900	2.31924200
H	6.31864900	1.78694900	3.02680500
C	4.28443500	1.57059000	2.36282900
H	3.88973100	2.25943500	3.10308000
C	3.38488900	0.97458700	1.46558700
C	1.95526600	1.38541300	1.61700400
C	1.47092200	2.52587400	0.94466900
C	0.15483200	2.96824400	1.14057300
H	-0.22937600	3.83826900	0.62485200
C	-0.67463500	2.25645600	2.01165900
H	-1.69490100	2.59575800	2.15915400
C	-0.21866700	1.13342000	2.70294600
H	-0.88052700	0.60915300	3.37935800
C	1.10601000	0.70929300	2.51255500
C	3.48696100	-0.31368700	-2.47587900
C	3.76050800	1.20384400	-2.41825800
H	3.96947700	1.56203200	-3.43242700
H	4.61872100	1.44415300	-1.78701500
H	2.89897100	1.75549700	-2.03012900
C	2.37289100	-0.57214300	-3.51666100
H	2.75330900	-0.30728200	-4.50954900
H	1.48991200	0.04606600	-3.32654900
H	2.05630600	-1.61645100	-3.55197500
C	4.75527700	-1.06066400	-2.92431100
H	4.58471200	-2.13312200	-3.04433500

H	5.59922800	-0.91115100	-2.24915200
H	5.05882700	-0.67014800	-3.90222600
C	2.93797900	-2.66005200	-0.35455200
C	4.36798700	-3.20962600	-0.19786100
H	4.30345300	-4.29133600	-0.03576000
H	4.87368600	-2.78105700	0.66965800
H	4.98861400	-3.05163100	-1.08132100
C	2.19590000	-2.85735200	0.98607400
H	1.13255700	-2.62130200	0.90543300
H	2.62049200	-2.24203200	1.78329900
H	2.28328400	-3.90917700	1.28133000
C	2.20131200	-3.43442900	-1.46543500
H	2.74461700	-3.41494400	-2.41376200
H	1.18943200	-3.05198700	-1.63232500
H	2.11216700	-4.48376800	-1.16305500
P	2.82688200	-0.79767300	-0.74239200
C	-2.67227600	0.21515700	-0.30437800
C	-3.02742100	-1.09892900	0.14246900
C	-3.75154700	1.12470800	-0.56369100
C	-4.35722000	-1.45837300	0.30960900
C	-5.07655700	0.74140300	-0.41389800
C	-5.37502200	-0.54644500	0.02639700
H	-4.61505500	-2.45314400	0.64887500
H	-5.87844300	1.43265700	-0.63883400
O	1.66071700	-0.36393300	3.13457500
O	2.35549600	3.11478400	0.09596800
C	0.87746500	-1.09979100	4.07229600
H	1.53178800	-1.88542500	4.45047300
H	0.55350300	-0.46560600	4.90586700
H	0.00385900	-1.55450000	3.59220300
C	1.94495700	4.27375800	-0.62480500
H	2.80701700	4.57245400	-1.22131100
H	1.10148000	4.05141300	-1.29110400
H	1.67035800	5.09090500	0.05237800
C	-3.49139700	2.54877400	-1.04591300
C	-6.81930600	-0.95127500	0.25932300
C	-1.99288600	-2.16481100	0.47828900
F	-7.14805200	-0.73040400	1.54464200
F	-7.65194300	-0.24068800	-0.51772000
F	-6.99606400	-2.25751200	-0.00010700
F	-2.79643700	3.25181000	-0.12079300
F	-2.77157500	2.55478000	-2.18801800
F	-4.63186000	3.20923900	-1.27929900
F	-2.56500100	-3.25932000	1.00679200
F	-1.09842400	-1.71168200	1.38575300
F	-1.31836400	-2.56080400	-0.62004600

5c'-CF₃-TSC1C2**E = -2765.95775925****G = -2765.433400**

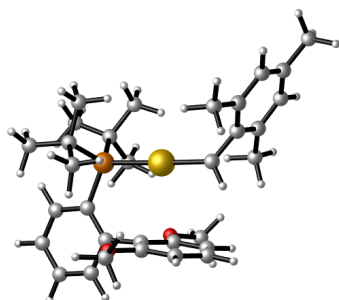
Au	0.32246000	-0.01263700	-0.05404500	H	3.92535600	3.05391300	-2.59340200
C	-1.28126100	-0.78962400	0.81210400	H	2.68747900	4.28851400	-2.75849700
H	-1.16383600	-1.64261700	1.48521100	C	2.29519300	-0.28577900	-2.89519500
C	3.79930500	0.47736400	-0.39545000	C	3.58695700	-0.08097700	-3.70740200
C	4.98049200	0.99939800	-0.95795000	H	3.51936200	-0.68455100	-4.61933100
H	4.94205800	1.52538600	-1.90202100	H	4.46816500	-0.41765300	-3.15731500
C	6.21524800	0.85528900	-0.33307800	H	3.73974600	0.95486500	-4.01558800
H	7.10539600	1.27114600	-0.79430900	C	2.22485200	-1.76448300	-2.45191600
C	6.29517000	0.17536500	0.88136200	H	1.25748700	-2.00861400	-2.00072000
H	7.25041500	0.05247200	1.38210500	H	3.01027700	-2.01539300	-1.73501100
C	5.13851000	-0.34668500	1.45153100	H	2.34934900	-2.40133800	-3.33492800
H	5.19393100	-0.87752900	2.39669900	C	1.06529200	0.04442900	-3.76224700
C	3.88304100	-0.20653400	0.83996800	H	1.11823900	1.04593400	-4.19665300
C	2.73389800	-0.81755500	1.57908000	H	0.13083300	-0.04546100	-3.19825600
C	2.00303600	-0.06698700	2.52468800	H	1.02017200	-0.66813000	-4.59331600
C	1.01314000	-0.67833700	3.32080900	P	2.21437500	0.74306800	-1.29390600
H	0.46135900	-0.10752500	4.05507100	C	-2.65615800	-0.44211000	0.48843000
C	0.77289800	-2.04343500	3.17072000	C	-3.43748800	-1.31069800	-0.30858400
H	0.02874900	-2.52253400	3.80061600	C	-3.22440500	0.78356600	0.89641700
C	1.46697100	-2.80804800	2.23443600	C	-4.73045200	-0.95567300	-0.68038300
H	1.26170600	-3.86657900	2.14434200	C	-4.53330800	1.10777000	0.55820200
C	2.46110000	-2.19467400	1.45228700	C	-5.28556100	0.24170800	-0.23396700
C	2.01455100	2.62419100	-1.57080300	H	-5.30448400	-1.61743400	-1.31827000
C	2.40999600	3.29283200	-0.23644300	H	-4.96461500	2.03865400	0.90784200
H	2.14448600	4.35464600	-0.28308800	O	3.22256100	-2.85185700	0.54160500
H	3.48148500	3.21681000	-0.03916600	O	2.32350300	1.24894300	2.59181500
H	1.88306700	2.84494800	0.61207200	C	2.97531800	-4.23731700	0.30444000
C	0.52416700	2.92990200	-1.84852100	H	3.68481200	-4.53531200	-0.46741400
H	0.41739800	4.00818300	-2.01155000	H	3.14904600	-4.83465000	1.20662200
H	-0.11383900	2.66087300	-1.00328200	H	1.95266700	-4.40123300	-0.05658700
H	0.14485400	2.42407700	-2.73820700	C	1.61610600	2.08924600	3.50617000
C	2.85278300	3.20586500	-2.72384300	H	2.03417000	3.08653100	3.36983800
H	2.55587800	2.80233200	-3.69475800	H	0.54450000	2.10427800	3.27958200
				H	1.77220100	1.76920300	4.54252000
				C	-2.40571500	1.73863600	1.72848200
				C	-6.72150100	0.58322000	-0.56181400
				C	-2.79843700	-2.54512900	-0.90004800
				F	-7.10842400	0.00270600	-1.71250600
				F	-7.54370400	0.15474900	0.41468300
				F	-6.88386400	1.91478500	-0.68024900
				F	-1.63992500	1.05387200	2.62757400
				F	-1.54375400	2.45749500	0.96902700
				F	-3.16462400	2.60379900	2.40828100
				F	-3.69767700	-3.37595900	-1.43448400
				F	-2.09278900	-3.23214400	0.03651700
				F	-1.91065200	-2.20474900	-1.86761100

5c'-TSAuCl**E = -1872.84898542****G = -1872.243720**

Au	0.43860500	-0.36163100	-0.21285400
C	2.29276700	0.46008400	-0.35194800
H	2.19442600	1.49825000	-0.67197600
C	-3.08368300	-0.00873300	0.29106600
C	-4.41260400	-0.46257800	0.40819200
H	-4.65257700	-1.49248400	0.18310900
C	-5.44575000	0.38115500	0.80283600
H	-6.45714100	-0.00472200	0.88332400
C	-5.16922800	1.71748400	1.08875600
H	-5.96293100	2.39165800	1.39546800
C	-3.86327100	2.18257300	0.98056400
H	-3.63866900	3.22089300	1.20351800
C	-2.80618100	1.34354000	0.59154900
C	-1.46041500	1.99423800	0.54363200
C	-0.60355000	1.95142500	1.66080700
C	0.58330300	2.70321100	1.68764600
H	1.23390900	2.68977900	2.55204400
C	0.89996000	3.50105500	0.58846300
H	1.79798200	4.11144500	0.61927700
C	0.08588000	3.54715600	-0.54180000
H	0.35698400	4.17986900	-1.37688200
C	-1.10183100	2.79951100	-0.55451600
C	-1.92089500	-2.72954900	0.91450000
C	-2.10868700	-2.17559500	2.34280800
H	-1.99606900	-2.99802300	3.05823200
H	-3.09694000	-1.73326800	2.48551400
H	-1.36494800	-1.40867200	2.57957400
C	-0.57702700	-3.48927500	0.85843900
H	-0.64868900	-4.38076800	1.49168300
H	0.24319600	-2.87573000	1.23683700
H	-0.31875700	-3.81822300	-0.15063600
C	-3.04937700	-3.72472200	0.58639900
H	-2.91758900	-4.19372000	-0.39130100
H	-4.04294200	-3.27615900	0.62702800

H	-3.03257500	-4.52511500	1.33480900
C	-2.18683200	-1.60920400	-2.07224300
C	-3.65449000	-1.98329800	-2.34953400
H	-3.75454200	-2.22021300	-3.41484400
H	-4.33048100	-1.15291200	-2.13560900
H	-3.98786100	-2.85912200	-1.79084500
C	-1.86126400	-0.32034100	-2.86129200
H	-0.79280500	-0.08352400	-2.82999200
H	-2.41019000	0.54482900	-2.48049400
H	-2.14039700	-0.47027900	-3.91053700
C	-1.25740300	-2.74389700	-2.54562200
H	-1.50552200	-3.70495100	-2.08739900
H	-0.20495800	-2.52045700	-2.34084100
H	-1.36715100	-2.86209000	-3.62944000
P	-1.79244900	-1.21005200	-0.24741200
C	3.63010100	0.08221700	-0.17971100
C	4.01488600	-1.23946800	0.28183100
C	4.68291400	1.03739100	-0.49350600
C	5.35989700	-1.55077700	0.39220000
C	6.00767500	0.65913600	-0.36654600
C	6.36984800	-0.62790400	0.06878700
H	5.64957200	-2.53752700	0.74168900
H	6.79316200	1.36994600	-0.60599100
O	-1.98618000	2.79293600	-1.58840300
O	-1.01485400	1.14047500	2.67358200
C	-1.69546600	3.56934400	-2.74706700
H	-2.52931400	3.40580100	-3.43001800
H	-1.62710100	4.63701900	-2.50758900
H	-0.76434200	3.24030600	-3.22514500
C	-0.21350500	1.05241500	3.84810400
H	-0.73465700	0.36138900	4.51115100
H	0.78490300	0.65715900	3.62086600
H	-0.11781200	2.02614800	4.34259700
C	4.37488700	2.43633000	-0.96682600
H	3.83479900	2.42968500	-1.91943800
H	3.75517200	2.97709500	-0.24525300
H	5.29571300	3.00426000	-1.11161200
C	7.81456100	-1.02147300	0.16283400
H	8.12824400	-1.48955900	-0.77976600
H	8.46165200	-0.15668700	0.32890600
H	7.98300400	-1.75236500	0.95810600
C	3.00684600	-2.28471000	0.66762000
H	2.37175200	-1.93066700	1.48478100
H	2.34124100	-2.52441200	-0.16639900
H	3.50407000	-3.20198300	0.99014100

5c'-TSC1C2



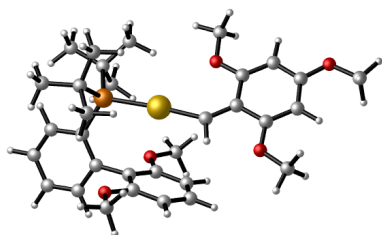
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G = -1872.211560

Au	0.51042800	0.06711600	0.34933400
C	2.17222600	-1.00254300	0.53028000
H	2.09714600	-2.06324500	0.81047300
C	-2.94873700	0.43749500	-0.43844500
C	-4.12500700	1.13464600	-0.77851000
H	-4.13017900	2.21592800	-0.78970100
C	-5.30352800	0.46910200	-1.10109700
H	-6.19119400	1.03813300	-1.35870500
C	-5.33189000	-0.92466200	-1.08760000
H	-6.24394800	-1.45971500	-1.33308700
C	-4.17777300	-1.62934100	-0.76110700
H	-4.19006900	-2.71473800	-0.75492200
C	-2.97723700	-0.97635900	-0.44114200
C	-1.81540700	-1.87109500	-0.14526900
C	-0.97172600	-2.30939300	-1.18667100
C	0.03843100	-3.25954000	-0.94466100
H	0.67078500	-3.61640300	-1.74706600
C	0.18042500	-3.78164000	0.34157400
H	0.93837800	-4.53770400	0.52565000
C	-0.63192400	-3.36248700	1.39306700
H	-0.50300800	-3.79154000	2.37812800
C	-1.64119200	-2.41628500	1.14201300
C	-1.05697300	2.52894400	-1.53740700
C	-1.21910400	1.63034200	-2.78169600
H	-0.85390700	2.17475300	-3.65957700
H	-2.26161500	1.35668800	-2.95832300
H	-0.64578100	0.70266200	-2.68871300
C	0.41555800	2.99337100	-1.45523500
H	0.62708300	3.62980800	-2.32168700
H	1.11426400	2.15190400	-1.48507100
H	0.62773400	3.57780300	-0.55820500
C	-1.95429500	3.77315500	-1.66757800
H	-1.82550600	4.46785200	-0.83407000

H	-3.01302800	3.52619200	-1.75947400
H	-1.67335800	4.30949200	-2.58094200
C	-1.80403900	2.35343700	1.58298800
C	-3.13872100	3.12052800	1.58828900
H	-3.22291700	3.65788000	2.53947400
H	-3.99453700	2.44632500	1.51737500
H	-3.20695600	3.86100100	0.78943700
C	-1.85519900	1.27625800	2.69014700
H	-0.88299200	0.79184500	2.83207700
H	-2.59161100	0.49823700	2.47327200
H	-2.12962700	1.75621500	3.63628500
C	-0.64176600	3.32446400	1.86595900
H	-0.62902600	4.16874700	1.17204400
H	0.33229400	2.82532400	1.82539100
H	-0.76331900	3.73417900	2.87476200
P	-1.43846200	1.40941600	-0.03333500
C	3.50732300	-0.51088300	0.23731800
C	3.99673900	-0.54944500	-1.08593200
C	4.26328400	0.06052300	1.28472400
C	5.26374900	-0.01988600	-1.33187000
C	5.52400800	0.57230200	0.97824200
C	6.04838600	0.54131400	-0.31852900
H	5.64541500	-0.04603800	-2.35003700
H	6.11124700	1.01071300	1.78202500
O	-2.51001900	-1.96333200	2.08126700
O	-1.20910800	-1.74496000	-2.39928200
C	-2.39506900	-2.44486000	3.41933200
H	-3.18403600	-1.94526800	3.98144900
H	-2.54543400	-3.52935100	3.46853200
H	-1.42051900	-2.18794500	3.85230200
C	-0.48792200	-2.21817300	-3.53614600
H	-0.88357100	-1.66408500	-4.38735600
H	0.58575500	-2.01844200	-3.44059300
H	-0.64994000	-3.29078200	-3.69180200
C	3.69233300	0.11057200	2.68153100
H	2.73495400	0.64944800	2.69657700
H	3.50510700	-0.89653300	3.07693000
H	4.37050000	0.61276200	3.37520200
C	7.43010000	1.07317600	-0.60984400
H	7.51229200	1.43382400	-1.63901300
H	7.69248700	1.89556000	0.06172400
H	8.18465700	0.28865600	-0.47637600
C	3.13984900	-1.12081500	-2.18978700
H	2.84259700	-2.15506000	-1.97511700
H	2.21549700	-0.53877900	-2.30628200
H	3.66459100	-1.11669000	-3.14791400

5c'-OMe-TSAuCl



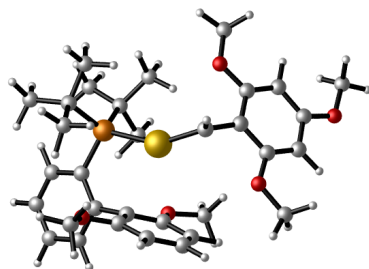
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G = -2097.871147

Au	0.03684500	-0.32724900	-0.42084100
C	1.90268300	0.47309200	-0.54076500
H	1.88486000	1.50899800	-0.88041500
C	-3.41226500	0.03947800	0.46565300
C	-4.73560100	-0.40508400	0.65674800
H	-5.03180800	-1.38281200	0.30377300
C	-5.69389500	0.38209400	1.28715700
H	-6.70308300	0.00371200	1.41694000
C	-5.34595800	1.65234400	1.74415500
H	-6.08046000	2.28222300	2.23656800
C	-4.04473700	2.10876300	1.56456500
H	-3.76436700	3.09670600	1.91619100
C	-3.06259300	1.32566100	0.93670200
C	-1.71238100	1.95814700	0.82609300
C	-0.73478800	1.75038900	1.81716500
C	0.48459900	2.44622800	1.78319600
H	1.23684800	2.29178000	2.54527100
C	0.71633300	3.35167800	0.74898100
H	1.65926200	3.88941300	0.71871000
C	-0.22693400	3.57325900	-0.25205700
H	-0.02053100	4.28467900	-1.04102700
C	-1.44702500	2.88264700	-0.20133600
C	-2.27661700	-2.75042600	0.58618400
C	-2.24594600	-2.37309800	2.08253500
H	-2.07443200	-3.27892200	2.67542500
H	-3.18499600	-1.92389400	2.41291600
H	-1.44451600	-1.66007600	2.29829900
C	-0.98466900	-3.53130300	0.25768000
H	-0.97728200	-4.46094400	0.83941000
H	-0.09887100	-2.94920800	0.52148900
H	-0.90862500	-3.79969700	-0.79824100
C	-3.47886500	-3.66688300	0.29776400
H	-3.50675400	-3.99872000	-0.74278800
H	-4.43723600	-3.20755500	0.54389200
H	-3.38900500	-4.56395500	0.92141700

C	-2.81651100	-1.23744500	-2.17981700
C	-4.31635100	-1.54131000	-2.34706400
H	-4.53348300	-1.63342600	-3.41739900
H	-4.93884800	-0.73414600	-1.95555900
H	-4.61820400	-2.47718700	-1.87353500
C	-2.52624200	0.13563300	-2.82812800
H	-1.45352700	0.35054100	-2.86149600
H	-3.01875800	0.95282500	-2.29451500
H	-2.89996100	0.12348800	-3.85852700
C	-1.98121500	-2.32180200	-2.88819700
H	-2.23424700	-3.32886000	-2.54558100
H	-0.90645500	-2.16479300	-2.74895900
H	-2.18848200	-2.28287900	-3.96359700
P	-2.21921700	-1.09238600	-0.37408500
C	3.18890000	0.05155300	-0.25960800
C	3.52208700	-1.29607700	0.19459200
C	4.31666100	0.96426700	-0.44402000
C	4.83450700	-1.67977100	0.38998800
C	5.62918700	0.56711300	-0.24550500
C	5.87648500	-0.75728900	0.16551400
H	5.11537300	-2.67087900	0.71564100
H	6.44817100	1.25268100	-0.39637200
O	-2.45050300	3.04074500	-1.10825500
O	-1.06149900	0.83292500	2.77010900
C	-2.25055400	3.92870600	-2.20283500
H	-3.16742200	3.88561300	-2.79134900
H	-2.08820800	4.95794000	-1.86081300
H	-1.40421600	3.61252000	-2.82562600
C	-0.10204300	0.52322700	3.77430400
H	-0.56586100	-0.23730800	4.40337800
H	0.81923800	0.12084400	3.33330400
H	0.13811900	1.40047800	4.38697500
O	3.98398600	2.20393100	-0.81864900
O	7.09796700	-1.24468500	0.38374700
O	2.48840000	-2.11618300	0.40279000
C	2.74383300	-3.46803500	0.80702400
H	3.33813800	-3.99430200	0.05293900
H	3.25508500	-3.49595200	1.77506900
H	1.76594900	-3.93641900	0.89514800
C	5.00403500	3.17770100	-1.06771000
H	5.58760100	3.37391500	-0.16169900
H	5.66500800	2.85363100	-1.87865300
H	4.47549500	4.08225900	-1.36581100
C	8.25671700	-0.41982000	0.19111000
H	8.32706900	-0.08197500	-0.84794200
H	8.24159300	0.43976200	0.86920600
H	9.10749900	-1.05734500	0.42732800

5c'-OMe-TSC1C2



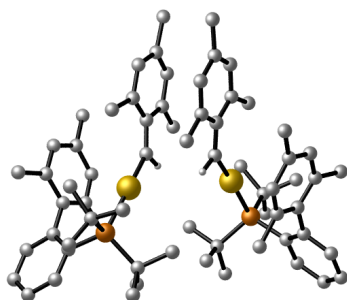
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G = -2097.821877

Au	0.03381000	-0.03588700	-0.78075100
C	-1.70044100	-0.33108800	-1.64615500
H	-1.79749300	-0.48707100	-2.72860000
C	2.97818100	0.42208500	1.06281400
C	4.02925100	1.06206400	1.74615900
H	4.17470400	2.12919500	1.64314900
C	4.90297600	0.34775400	2.56052700
H	5.70501500	0.86554600	3.07705200
C	4.73906200	-1.03000400	2.70649300
H	5.41190600	-1.59915900	3.34035400
C	3.70824600	-1.67613900	2.03121600
H	3.58158200	-2.74928300	2.13599300
C	2.81730800	-0.97139400	1.20669900
C	1.77009700	-1.80048800	0.52314700
C	0.57766700	-2.16698000	1.20843300
C	-0.23653300	-3.20255800	0.72964600
H	-1.14664900	-3.47567100	1.24397700
C	0.13523900	-3.87373900	-0.43074300
H	-0.49693000	-4.67339700	-0.80384400
C	1.28995800	-3.54303200	-1.13846100
H	1.54827800	-4.09057900	-2.03503200
C	2.11929700	-2.52710600	-0.64829800
C	1.00086700	2.68696600	1.20634600
C	0.63752000	1.93916100	2.50666700
H	0.07231300	2.61776000	3.15521800
H	1.52217200	1.60422000	3.05277500
H	0.01636200	1.06157600	2.30667800
C	-0.30302600	3.21392100	0.56891800
H	-0.76223800	3.92508200	1.26536700
H	-1.02195700	2.41547300	0.37693900
H	-0.13191800	3.74043600	-0.37184000
C	1.91105800	3.88588900	1.53034900
H	2.14946500	4.47705600	0.64312000
H	2.84175600	3.59293100	2.01937400
H	1.38023100	4.54580100	2.22586600

C	2.73709900	2.11353800	-1.42387500
C	4.04822500	2.82371900	-1.03914300
H	4.49176400	3.24787800	-1.94684300
H	4.77479500	2.12723000	-0.61527500
H	3.89772900	3.64477800	-0.33615300
C	3.08099600	0.91844700	-2.34011600
H	2.18121000	0.44985200	-2.75218200
H	3.65191100	0.15083800	-1.81249700
H	3.68376900	1.28142300	-3.18017900
C	1.81032900	3.08477100	-2.18019000
H	1.63884600	4.00962100	-1.62346900
H	0.84171000	2.62874300	-2.40971800
H	2.28527900	3.35851500	-3.12879400
P	1.78682100	1.38164600	0.05028700
C	-2.97134700	-0.17259300	-0.92422100
C	-3.62304000	-1.30149000	-0.39592800
C	-3.52839600	1.09295300	-0.70498000
C	-4.77750400	-1.16863300	0.36859300
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C	-5.30647800	0.11249200	0.59334500
H	-5.30044600	-2.01825400	0.78612800
H	-5.11281800	2.23371500	0.21231100
O	3.30185800	-2.17258100	-1.20586400
O	0.31917700	-1.45533300	2.33283200
C	3.71274300	-2.80956300	-2.41598300
H	4.66494300	-2.35075200	-2.68167500
H	3.85517100	-3.88616700	-2.27024100
H	2.98645800	-2.63803900	-3.21929000
C	-0.94353800	-1.63301600	2.97765800
H	-0.96132300	-0.90944300	3.79266900
H	-1.77078300	-1.43052000	2.28575300
H	-1.04279200	-2.64340000	3.38991300
O	-2.84176700	2.11630900	-1.29707400
O	-6.43402100	0.13959100	1.34587700
O	-3.01649500	-2.48611800	-0.70672000
C	-3.32684900	3.44778400	-1.14291500
H	-3.32816600	3.75103900	-0.08902800
H	-2.63640600	4.08170800	-1.69952100
H	-4.33484800	3.55487400	-1.55972600
C	-7.06123300	1.39218200	1.60220400
H	-7.93896700	1.16745600	2.20848500
H	-6.39906500	2.06645500	2.16024800
H	-7.37917600	1.87927800	0.67190700
C	-3.63084700	-3.69361300	-0.26587200
H	-3.66852600	-3.74672500	0.82952800
H	-4.64512400	-3.79487000	-0.66821000
H	-3.00843000	-4.50325000	-0.64739700

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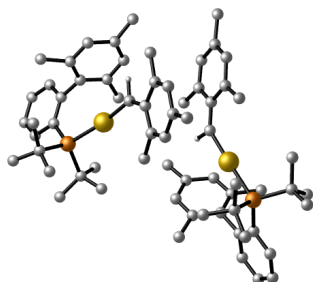
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H	-7.03873200	-4.95291300	0.70862700
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H	-7.62479400	-4.21679500	-1.60908000
C	-6.19192900	-2.61242700	-1.59901700
H	-6.44804100	-2.28233300	-2.60124400
C	-5.18876100	-1.90917100	-0.90746100
C	-4.59643200	-0.75192000	-1.66266900
C	-5.27110400	0.49189600	-1.68474700
C	-4.76156700	1.53210100	-2.46915500
H	-5.29179100	2.48229600	-2.48251000
C	-3.63470000	1.37157300	-3.28033100
C	-3.00867600	0.12140100	-3.28504400
H	-2.16540600	-0.05157500	-3.95043600
C	-3.47019300	-0.94501900	-2.49570300
C	-4.41615500	-0.70269400	2.91058600
C	-5.10949900	0.54219900	2.32108200
H	-5.60119700	1.09399500	3.12996600
H	-5.87679600	0.26515700	1.59746200
H	6.22006400	0.06594200	-3.06843400
C	-3.36203800	-0.25296000	3.93955300
H	-3.84866800	0.38041400	4.68941700
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H	-2.91009600	-1.09298500	4.47106600
C	-5.48756600	-1.56518200	3.60324900
H	-5.08835200	-2.48669900	4.02961000
H	-6.30412300	-1.81856800	2.92431600
H	-5.91631700	-0.98542300	4.42804400
C	-2.36321900	-2.96793000	2.02739400
C	-2.86813400	-3.81681100	3.20994100
H	-2.10939700	-4.57333300	3.43914500
H	-3.79015400	-4.35549300	2.98814700
H	-3.01813800	-3.22569500	4.11507900

C	-2.12384900	-3.87832600	0.80641300
H	-1.77299800	-3.30917000	-0.05789400
H	-3.02446000	-4.42224500	0.51407700
H	-1.35091600	-4.61260400	1.05880300
C	-1.01196000	-2.33507700	2.43227500
H	-1.09945100	-1.65987500	3.28604100
H	-0.55580400	-1.78096700	1.60701100
H	-0.32274900	-3.13701500	2.71566100
P	-3.53128200	-1.55684900	1.44969500
C	-1.04201000	2.53793300	-1.38504600
C	-1.44867900	4.89583300	-0.89919600
C	0.18004500	4.29046400	-2.58600000
H	-1.98350300	5.66978900	-0.35627800
H	0.90172600	4.59300900	-3.33932000
Au	2.23705800	-0.02858200	-0.23859300
C	1.22257600	1.25890700	0.96907400
H	0.52099600	0.70633000	1.59218400
C	4.60246500	-2.63960900	-0.30730300
C	5.24171600	-3.77940300	-0.83751000
H	5.01538100	-4.10475900	-1.84253500
C	6.17803000	-4.50968600	-0.11192500
H	6.64706800	-5.38077300	-0.55802700
C	6.50546800	-4.10837000	1.18159000
H	7.22987000	-4.66595700	1.76683500
C	5.90840900	-2.96900500	1.71305900
H	6.18112100	-2.63565700	2.70998000
C	4.96845600	-2.20708600	0.99657000
C	4.48778300	-0.96943700	1.70312200
C	5.26768400	0.20940000	1.67478400
C	4.83573100	1.33095400	2.39390200
H	5.44143700	2.23455200	2.36106100
C	3.69278600	1.30789900	3.19570500
C	2.97139500	0.11129300	3.26858000
H	2.11349500	0.04456400	3.93390200
C	3.35229200	-1.02846100	2.54488000
C	4.39518400	-1.07410100	-2.87764300
C	5.67325600	-0.45892400	-2.27763600
H	-4.40267900	1.21687100	1.82986800
H	6.33699600	-1.21766100	-1.85830900
H	5.43792500	0.26796600	-1.49508500
C	3.59520700	0.06106800	-3.54791200
H	4.18718800	0.46623300	-4.37604900
H	3.40414300	0.87612900	-2.84515500
H	2.64146600	-0.27229800	-3.95989600
C	4.77708000	-2.11653100	-3.94288500
H	3.90481200	-2.51850700	-4.46314400
H	5.35918300	-2.94512300	-3.53460400
H	5.40527200	-1.62847100	-4.69634700
C	2.05096800	-3.03353500	-1.94598600
C	2.55303300	-4.35723500	-2.55601700
H	1.68171900	-4.92464700	-2.90180100
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H	3.20822600	-4.22050600	-3.41626100
C	1.23013300	-3.38606700	-0.68859900
H	0.73481700	-2.51068600	-0.25889600

H	1.84997300	-3.85327500	0.08194100	H	3.62319600	4.01025100	-0.86218200
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C	1.12947100	-2.32376100	-2.95887000	H	3.82318400	2.46287200	-0.01651100
H	1.62403900	-2.14936400	-3.91723100	C	-0.10074900	2.94599300	-2.41080500
H	0.76234300	-1.36688600	-2.57316500	C	-0.45929200	5.28072900	-1.82069800
H	0.25972600	-2.96035900	-3.15275200	C	-1.76690800	3.56681800	-0.66924600
P	3.38749500	-1.76722900	-1.39921400	C	2.07498700	3.57303700	0.56056300
C	1.22931300	2.63094600	1.26164800	C	1.05589300	5.41210400	1.80861300
C	1.96245300	4.92491000	0.85235000	C	0.33363900	3.13606600	2.28510300
C	0.25924100	4.49778300	2.52009800	C	-6.56960600	0.73158000	-0.94705100
H	2.59935800	5.63314800	0.32998600	H	-6.50753800	1.62549800	-0.31779300
H	-0.41793500	4.87470000	3.28111900	H	-7.38108500	0.90234700	-1.66301900
C	-0.08516000	6.72501000	-1.97634300	H	-6.86255100	-0.11192100	-0.32234500
H	0.27084400	6.94857100	-2.98509900	C	-3.13902100	2.50871100	-4.13824600
H	0.73289000	6.96281600	-1.28267600	H	-2.71850900	3.31364900	-3.52337300
H	-0.91885400	7.39047500	-1.73823000	H	-2.36426200	2.18176700	-4.83706800
C	0.58047600	1.93791900	-3.29552400	H	-3.95409300	2.94509000	-4.72390200
H	1.24866400	2.42961400	-4.00495100	C	-2.73892000	-2.26551500	-2.57146200
H	-0.15470700	1.36094600	-3.86633800	H	-1.82726400	-2.23451800	-1.96248800
H	1.17169500	1.22514800	-2.71466300	H	-3.34619800	-3.09830500	-2.21446100
C	-2.87617100	3.25196100	0.29399700	H	-2.43358600	-2.48015300	-3.60000900
H	-3.34896600	4.16903200	0.65243600	C	6.60593900	0.28887800	0.97430200
H	-2.50650500	2.69987200	1.16161800	H	6.80167200	-0.56890300	0.33379300
H	-3.63712200	2.63005300	-0.18518700	H	6.68860300	1.19933100	0.37184400
C	0.92224100	6.88630200	2.05601900	H	7.40888700	0.32866100	1.71918500
H	0.07742300	7.28189900	1.47623700	C	3.28834400	2.52548100	3.98917100
H	1.81659400	7.43541800	1.75228700	H	3.16904200	3.39925200	3.33920600
H	0.71472100	7.10107600	3.10787700	H	2.34678200	2.36833200	4.52162100
C	-0.51515300	2.20683300	3.11176300	H	4.05114500	2.77903300	4.73313700
H	-1.15699900	1.58250500	2.48218300	C	2.56086800	-2.30391200	2.69434800
H	-1.15291200	2.76588300	3.79923800	H	3.21525600	-3.16900000	2.83426000
H	0.10661800	1.52813000	3.70536400	H	1.88199100	-2.24619300	3.54855100
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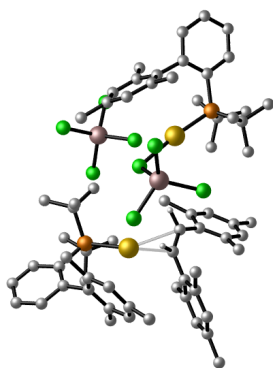
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C	7.47599000	-4.04357600	-0.61873800
H	8.45899800	-4.46530200	-0.43564800
C	6.53289500	-4.73617100	-1.37697200
H	6.76865200	-5.70921200	-1.79624600
C	5.28122800	-4.16880200	-1.59439200
H	4.54269800	-4.70573900	-2.18188400
C	4.92624300	-2.90888600	-1.07745100
C	3.52440700	-2.47322100	-1.40658100
C	1.13434600	-2.72521400	-1.06877200
H	0.31831700	-3.14952400	-0.49108500
C	1.92900600	-1.53080600	-2.98191000
H	1.74118500	-1.00610700	-3.91645400
C	5.60082400	-0.71208100	2.29582500
C	4.31780800	-1.49830500	2.63551100
H	4.21211000	-1.55907800	3.72474100
H	4.36332700	-2.51786000	2.25013100
H	3.42063200	-1.02167400	2.22857400
C	5.51476500	0.69461800	2.92055700
H	5.36169200	0.59484700	4.00137100
H	4.67788400	1.26963700	2.51148100
H	6.43015200	1.27299400	2.77717300
C	6.79126800	-1.48338100	2.89672300
H	7.75292700	-1.00299300	2.71813700
H	6.83712900	-2.50953600	2.52627800
H	6.65298400	-1.53679200	3.98256000
C	7.06685300	0.58873400	-0.21735900
C	8.35811500	0.49626900	0.61791500
H	9.11308300	1.14060700	0.15449100
H	8.77927900	-0.50979600	0.64835100
H	8.22038300	0.84818700	1.64223200
C	7.37636100	0.20184600	-1.67769300
H	6.48337300	0.23893200	-2.30627600
H	7.81168600	-0.79571900	-1.76136200
H	8.09763300	0.91915500	-2.08387600
C	6.57925700	2.05511000	-0.20254900
H	6.21285900	2.37342700	0.77639400
H	5.78210500	2.20991000	-0.93508000

H	7.41413200	2.70932900	-0.47612000
P	5.61522400	-0.52121400	0.39276900
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C	-6.24128500	-1.67086500	-0.32371000
C	-7.13941300	-2.74792500	-0.47723500
H	-6.91284200	-3.70592300	-0.03013800
C	-8.32731700	-2.62522400	-1.19006300
H	-8.99123400	-3.47834800	-1.28556200
C	-8.64997400	-1.40192200	-1.77540800
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C	-6.57618100	-0.42346300	-0.90867600
C	-5.78947200	0.85695200	-0.83366400
C	-5.51771500	3.08892400	0.08616000
H	-5.80868000	3.83706200	0.82072800
C	-4.28191300	2.45884200	-1.86349800
H	-3.60178100	2.71405100	-2.67270800
C	-5.14659300	-2.30331500	2.42637500
C	-5.61230000	-0.94873300	2.99835900
H	-5.87291900	-1.08238800	4.05410000
H	-6.50119800	-0.58405300	2.48324700
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C	-3.88914700	-2.76383800	3.18985100
H	-4.11634100	-2.78384300	4.26125300
H	-3.04869200	-2.07705900	3.04118400
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C	-6.28693200	-3.31883600	2.62862700
H	-6.05836900	-4.30870800	2.23269200
H	-7.22226400	-2.97160300	2.18471300
H	-6.45983300	-3.43189000	3.70448100
C	-3.84850400	-3.53023800	-0.20723800
C	-4.43144900	-4.89853100	0.19265400
H	-3.88005700	-5.67681200	-0.34686200
H	-5.48161700	-5.01458700	-0.07777200
H	-4.31866400	-5.10491900	1.25881700
C	-3.96265300	-3.34799600	-1.73396700
H	-3.55329100	-2.38740500	-2.05524100
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H	-3.38914000	-4.13877000	-2.23026700
C	-2.35174000	-3.51874200	0.17390400
H	-2.18777700	-3.61422100	1.24866900
H	-1.85921100	-2.60532200	-0.16460800
H	-1.85907100	-4.36729600	-0.31451000
P	-4.67614900	-1.99252000	0.59795100
C	1.80519300	1.32004200	-0.88022200
H	1.14276200	0.54041400	-1.25914600
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C	1.30096400	2.60762000	-1.10937900
C	0.09411700	2.76036600	-1.90845500
C	1.95121200	3.80636500	-0.61257500
C	-0.36901900	4.02786000	-2.21118800
C	1.40935400	5.04621100	-0.91860900
C	0.27050700	5.18597100	-1.72827400

H	-1.24737600	4.13927900	-2.83995800	H	-0.12555400	-0.75824700	0.48021400
H	1.88830300	5.94279600	-0.53606200	H	0.90534500	-1.16591400	1.85217100
C	-0.82503100	1.83604600	1.49155200	C	-7.22929500	1.62240700	1.15416600
C	-0.56230900	3.22940700	1.82206200	H	-8.03515800	2.34842500	1.00148500
C	0.13289100	0.83421300	1.91951600	H	-6.84876700	1.77642500	2.16895800
C	0.52934900	3.54749600	2.61026400	H	-7.67327700	0.62891700	1.09844700
C	1.21902800	1.22666100	2.69061400	C	-4.07988800	4.84335800	-1.03201500
C	1.41654000	2.56174000	3.07842800	H	-3.09544700	4.86690400	-1.50893500
H	0.70365000	4.58250000	2.89063700	H	-4.00168500	5.33129700	-0.05641900
H	1.93220500	0.47864300	3.01983700	H	-4.75081100	5.45511700	-1.64628200
C	3.19728600	3.76689400	0.22491700	C	-4.44224700	0.19351100	-2.91381400
H	3.12795200	3.02643900	1.02226200	H	-4.36439500	0.68572500	-3.88800600
H	4.05968400	3.48903800	-0.38770100	H	-5.14645400	-0.63384200	-3.00919000
H	3.39831500	4.74687400	0.66378100	H	-3.45707400	-0.23201500	-2.68665800
C	-0.25022100	6.54420600	-2.09283200	C	-4.60848600	3.43300400	-0.91597800
H	0.06520800	7.30941200	-1.37996100	C	-6.14009000	1.83407300	0.12602900
H	0.13853400	6.83242000	-3.07843300	C	-4.84975000	1.17937800	-1.84244600
H	-1.34148500	6.55098400	-2.16645200	C	4.36355900	-1.20620900	-3.46822500
C	-0.66178000	1.57071900	-2.43706800	H	4.09241200	-1.27224200	-4.52554800
H	-0.01986100	0.90034600	-3.01271300	H	5.30550900	-1.73767100	-3.32491500
H	-1.09941800	0.98768000	-1.61823200	H	4.54091500	-0.14680700	-3.24614700
H	-1.48138300	1.88891800	-3.08178300	C	-0.57706000	-1.87217900	-2.71706600
C	-1.47571800	4.33836600	1.37021600	H	-0.63439100	-1.34698400	-3.67405700
H	-1.60387600	4.32742600	0.28589000	H	-1.19184700	-1.32365800	-1.99377000
H	-2.47067600	4.24967300	1.81805800	H	-1.04643300	-2.85207800	-2.84939100
H	-1.06833000	5.31085600	1.65239800	C	2.63064400	-3.84128100	0.58072900
C	2.55640800	2.94992100	3.97406100	H	2.09039600	-4.78675300	0.46608900
H	3.18318500	3.71191200	3.49684600	H	2.22657500	-3.34910500	1.47245300
H	2.17224500	3.39594600	4.89876200	H	3.67613100	-4.08286100	0.77089700
H	3.18346700	2.09747600	4.23877100	C	2.44366900	-2.97638300	-0.64664200
C	0.00954700	-0.61778400	1.55396200	C	3.25846600	-1.74842600	-2.59186500
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IntIII



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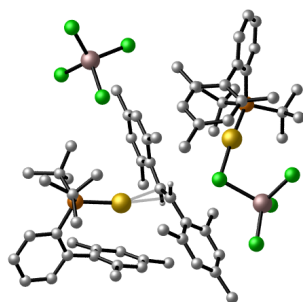
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C	-8.70163700	-1.70446200	-0.27205100
H	-9.57085800	-2.19434500	0.15617300
C	-8.83492400	-0.82297100	-1.34373300
H	-9.81194900	-0.61644500	-1.77058700
C	-7.70411700	-0.19443700	-1.85442900
H	-7.80054700	0.51101400	-2.67404700
C	-6.41710300	-0.42093300	-1.33550000
C	-5.30974500	0.38728500	-1.94451000
C	-3.99861300	2.42373000	-2.00667700
H	-3.76452100	3.39876600	-1.58969400
C	-3.57682300	0.69134900	-3.61072900
H	-3.01015400	0.29975000	-4.45109800
C	-4.80298500	-1.26615400	2.38130200
C	-5.47438400	0.12073000	2.40813000
H	-5.45000100	0.50114500	3.43553900
H	-6.51810800	0.08024700	2.08725300
H	-4.93791800	0.83996700	1.78683700
C	-3.37987900	-1.12477200	2.96236300
H	-3.46470900	-0.85188100	4.02083100
H	-2.82575500	-0.32745400	2.46624500
H	-2.79226000	-2.04177900	2.90657600
C	-5.59986400	-2.24604600	3.26134000
H	-5.11797700	-3.22341000	3.33806100
H	-6.62921700	-2.38361600	2.92425100
H	-5.65089000	-1.82863500	4.27348400
C	-4.40009400	-3.65999800	0.30322900
C	-5.58681500	-4.55735400	0.70595900
H	-5.27844500	-5.60125000	0.57741600
H	-6.45427700	-4.39526800	0.06287400
H	-5.89165100	-4.43571500	1.74618500
C	-4.13839700	-3.88227800	-1.20177600
H	-3.24091900	-3.36542400	-1.54716200
H	-4.98754600	-3.56049600	-1.80966900
H	-3.98593500	-4.95347700	-1.37666700

C	-3.14732200	-4.07023200	1.10501700
H	-3.32080700	-4.04459500	2.18394700
H	-2.28297200	-3.44359000	0.87053400
H	-2.88440200	-5.09994200	0.83749200
P	-4.66657900	-1.77725700	0.53835300
C	-4.91040200	-1.42511900	-3.71821200
H	-5.05214000	-1.29929400	-4.79672000
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H	-4.07958000	-2.12491900	-3.59197100
C	-2.09588500	2.74234900	-3.64016500
H	-1.25119400	2.09242200	-3.89113400
H	-1.75564800	3.49762200	-2.92593900
H	-2.39265900	3.26366000	-4.55859400
C	-5.88152600	2.33116100	-0.36542300
H	-6.52283400	1.62212300	0.15803400
H	-6.53403200	3.09404200	-0.80721200
H	-5.25219700	2.83755600	0.37054400
C	-5.04599000	1.68349600	-1.44616200
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Ga	-0.09405000	-1.87080000	-2.73006200
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C	1.39657000	-1.80699000	0.99713600
H	0.67604900	-1.32126200	0.34428600
H	4.89873200	3.54063000	3.45160600
C	0.88200700	-2.13500600	2.33605500
C	0.45896400	-3.65006200	4.17830600
C	-0.28185200	-1.37712800	4.33162200
H	0.51800100	-4.65208600	4.59740100
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Au	2.97132600	0.25413200	0.34706600
C	2.62156800	-2.09648500	0.42658300
H	2.63102200	-2.02796100	-0.66200500
C	4.83205800	3.07419100	-0.71434700
C	5.11224200	4.45698200	-0.74975600
H	4.40860000	5.15501200	-0.31999100
C	6.27158100	4.96615300	-1.32251900
H	6.44661600	6.03757400	-1.32723500
C	7.19736100	4.08672200	-1.88169000
H	8.11481100	4.45806100	-2.32860800
C	6.92914300	2.72305900	-1.87298500
H	7.63442400	2.03293900	-2.32583100
C	5.75490300	2.18294700	-1.30998000
C	5.64337000	0.69176900	-1.48122700
C	6.18218900	-0.18829400	-0.51217800
C	6.36316100	-1.53639700	-0.83563500
H	6.78644000	-2.20318500	-0.08872700

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C	5.46576200	-1.16973900	-3.02469600	H	-0.58383800	0.90295200	3.08444500
H	5.19206800	-1.54436100	-4.00820100	H	-0.70992900	0.11018000	1.52345800
C	5.26701000	0.18618300	-2.74708900	H	0.84501600	0.68571900	2.07012200
C	3.39146500	3.36860200	1.92176800	C	1.50842600	-4.63139200	2.14124400
C	4.83822300	3.17870400	2.41902400	H	0.95835900	-5.53023200	2.43525000
H	5.56520300	3.73641200	1.82475000	H	2.56708900	-4.80646700	2.35564600
H	5.12950500	2.12515700	2.42101800	H	1.40202200	-4.51433200	1.06212900
C	2.45049000	2.61362100	2.88147600	C	7.09261100	-5.28805900	2.36154300
H	2.55917100	3.04973700	3.88096400	H	7.29765300	-5.14386200	3.42613400
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H	1.40147700	2.71520500	2.60482100	H	6.91795300	-6.35525300	2.18967800
C	3.00289600	4.85954800	1.98657600	C	3.54191000	-4.33189800	-1.07729500
H	1.95412700	5.02411300	1.73553800	H	2.46990500	-4.51261500	-0.94947300
H	3.63074300	5.50200600	1.36792400	H	3.98843400	-5.23283000	-1.50425400
H	3.13339800	5.19311400	3.02232100	H	3.63288500	-3.53157600	-1.81872000
C	1.82037600	3.22828700	-0.87949600	C	3.92014400	-1.49296900	3.18049400
C	1.86370500	4.73146200	-1.21436100	H	4.75323400	-1.14172400	3.79615000
H	0.95489000	4.96961600	-1.77671500	H	3.13439600	-1.85738800	3.85083900
H	2.72211000	4.98618300	-1.84110500	H	3.50425000	-0.62805000	2.65637800
H	1.85897000	5.37144600	-0.33298000	C	0.18334900	-1.12113400	3.04425300
C	1.84731400	2.44810500	-2.20869600	C	-0.13977800	-2.63598000	4.92705700
H	1.83502700	1.36473200	-2.07034100	C	0.97156600	-3.43539900	2.89266400
H	2.72258300	2.71011900	-2.80676500	C	4.37488300	-2.58390300	2.23867600
H	0.95278500	2.71393400	-2.78195000	C	5.91742800	-4.45889000	1.90351700
C	0.53512300	2.90458000	-0.10511500	C	4.21375600	-3.96397900	0.22489400
H	0.44331000	3.49759700	0.80490100	C	6.59318500	0.28901500	0.86160400
H	0.46571900	1.84936600	0.15596800	H	6.88385900	1.34172600	0.86258900
H	-0.32905400	3.13850800	-0.73062400	H	5.76449500	0.17227300	1.56975200
P	3.28301400	2.57608000	0.15810100	H	7.42858500	-0.30168100	1.24771700
C	3.75656600	-2.86561400	1.00022300	C	6.41396200	-3.44825200	-2.49742500
C	5.45462100	-3.37724200	2.65142600	H	6.45830900	-4.10805800	-1.62869900
C	5.26590100	-4.74584200	0.69847100	H	5.69923900	-3.86498400	-3.21256400
H	5.93751900	-3.14377600	3.59776000	H	7.40122800	-3.46402600	-2.97568900
H	5.58853900	-5.60391000	0.11296800	C	4.69237600	1.05434200	-3.84426400
C	-0.64338700	-2.88443100	6.32727400	H	5.17234200	0.83117900	-4.80247700
H	0.03690400	-2.44915700	7.06944600	H	3.62349100	0.85184700	-3.96435800
H	-0.72791700	-3.95326300	6.54278800	H	4.81741500	2.11966400	-3.64746300
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IntIV



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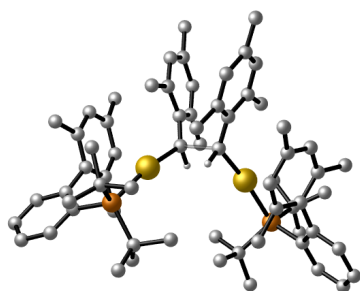
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H	-7.71258400	4.80892000	-0.54938300
C	-6.28702400	3.27846200	-1.05100400
H	-6.22653700	3.57217800	-2.09452100
C	-5.48787700	2.20244000	-0.62673200
C	-4.56424700	1.62756100	-1.65997200
C	-2.44762300	1.74797900	-2.83526300
H	-1.49106700	2.24276600	-2.98821500
C	-4.04366200	0.05839000	-3.42972900
H	-4.33436700	-0.79821300	-4.03329800
C	-3.48456600	1.11245000	2.84601000
C	-2.88435900	2.41301700	2.28313400
H	-2.12722600	2.78959500	2.97736300
H	-3.63737100	3.19201700	2.14617000
H	-2.38436200	2.24314500	1.32819900
C	-2.33390700	0.11691800	3.11698200
H	-1.66018000	0.55668000	3.86111700
H	-1.74229400	-0.07074300	2.21913300
H	-2.68506300	-0.84292100	3.50039800
C	-4.19932500	1.41351600	4.17577700
H	-4.59820200	0.51426900	4.65020100
H	-5.00460700	2.14271100	4.06687900
H	-3.46686900	1.84916000	4.86485000
C	-5.89675200	-0.86274200	2.14230600
C	-7.00854000	-0.26272500	3.02539200
H	-7.62768300	-1.08889700	3.39321200
H	-7.66164500	0.40442000	2.45919100
H	-6.63045400	0.27163700	3.89864800
C	-6.56923700	-1.51000000	0.91384100
H	-5.86352700	-2.06177100	0.28846600
H	-7.07800500	-0.76704900	0.29486000
H	-7.32269400	-2.22452700	1.26467400
C	-5.13723300	-1.94758000	2.93049300
H	-4.73501900	-1.56836900	3.87339300

H	-4.32629600	-2.38900500	2.34653200
H	-5.83738000	-2.75466800	3.17336200
P	-4.61685500	0.39515300	1.47121000
Au	3.07027300	-0.61719600	0.09474700
C	6.44957100	-0.26468900	-0.83344700
C	7.49294100	0.30037500	-1.59353500
H	7.32249800	1.22213500	-2.13292400
C	8.75159800	-0.28683700	-1.67533600
H	9.52777300	0.18017900	-2.27364700
C	8.99904500	-1.47244500	-0.98562000
H	9.97269000	-1.95020700	-1.03973100
C	7.98732000	-2.03703700	-0.21492600
H	8.17780400	-2.95104900	0.33986400
C	6.71007200	-1.45861200	-0.11084600
C	5.75263400	-2.17005200	0.80136100
C	4.95658800	-2.67681200	3.03029500
H	5.00930800	-2.50440000	4.10367600
C	4.05067600	-3.87003600	1.15883400
H	3.37260100	-4.61436500	0.75130200
C	4.97683100	2.21899500	0.11073700
C	5.05768300	1.83399900	1.60163800
H	5.17011300	2.75215900	2.18878800
H	5.91603700	1.19508000	1.81170100
H	4.14866800	1.33438100	1.94730700
C	3.71421300	3.06755700	-0.11027800
H	3.74120800	3.92925800	0.56229300
H	2.79723500	2.51820500	0.11544400
H	3.62978100	3.46899600	-1.11995000
C	6.23884700	3.02540200	-0.24909200
H	6.26945800	3.32573000	-1.29719500
H	7.15507400	2.47735900	-0.01363700
H	6.23610100	3.94327200	0.34843700
C	4.35289400	0.90837400	-2.72287700
C	5.02946800	2.14047400	-3.35715200
H	4.69460400	2.21286800	-4.39784500
H	6.11875400	2.07088700	-3.37952200
H	4.74496300	3.07096600	-2.86446100
C	4.72975600	-0.35268900	-3.52430200
H	4.23069300	-1.24246700	-3.13182100
H	5.80631600	-0.53749300	-3.54038000
H	4.39350100	-0.22135300	-4.55877900
C	2.82102600	1.10201600	-2.81618700
H	2.45568800	1.94420700	-2.22841000
H	2.28348000	0.20221500	-2.50633700
H	2.56110000	1.29916500	-3.86240100
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C	0.85877900	-1.62881000	0.37821400
H	0.38261100	-1.07412300	-0.41714700
C	1.26637900	-0.98318800	1.53963200
H	1.67405800	-1.65502000	2.28542200
C	0.82173200	-3.09732700	0.22841500
C	1.16739200	-3.66636100	-1.02516400
C	0.36481900	-3.93650100	1.27176600
C	1.15615200	-5.05012400	-1.17451500
C	0.35613200	-5.32175200	1.06599300

C	0.76066600	-5.90168200	-0.13573600	H	7.34837600	-0.40409300	2.10981000
H	1.41797800	-5.47898900	-2.13816400	C	3.20009300	-4.43355100	3.47992100
H	-0.02622200	-5.96211800	1.85671100	H	2.38164300	-4.92223400	2.94766400
C	1.11112900	0.40707600	2.00673400	H	2.77513300	-3.79914300	4.26512600
C	1.65756800	0.71322500	3.28626300	H	3.78663300	-5.21298000	3.98116400
C	0.49199500	1.44876800	1.25853800	C	4.92039200	-3.53358900	-1.17761800
C	1.57759900	2.01722400	3.77534200	H	4.07367400	-4.17192400	-1.43788300
C	0.45392900	2.73729900	1.78829200	H	5.84434500	-4.07163100	-1.42088200
C	0.98901400	3.05224200	3.04173300	H	4.89766200	-2.65001700	-1.81730700
H	1.99290700	2.23596900	4.75634300	C	4.06748400	-3.63406200	2.53785800
H	-0.01784200	3.52215400	1.20958400	C	5.81315400	-1.95145900	2.19276800
C	-0.21321300	-3.41583200	2.57216700	C	4.89005300	-3.16773800	0.28679700
H	-0.75585300	-2.47820800	2.42816100	C	-6.31355900	-0.10047300	-2.37962000
H	-0.92158600	-4.14326000	2.97427700	H	-6.77196500	-0.16470400	-3.37202800
H	0.55283000	-3.24531700	3.33648700	H	-6.99088000	0.46351400	-1.73537900
C	0.66964100	-7.38893700	-0.35803300	H	-6.23852900	-1.12206000	-1.99803900
H	0.65118400	-7.93960100	0.58666700	C	-1.78643600	0.02819900	-4.56932000
H	-0.25194900	-7.62347500	-0.90387100	H	-1.21756800	-0.77492800	-4.08487000
H	1.50837600	-7.75802200	-0.95700600	H	-1.07293100	0.77801400	-4.92436600
C	1.53542900	-2.80150600	-2.20550900	H	-2.28614600	-0.41052400	-5.43847100
H	0.73321300	-2.09534500	-2.44514400	C	-2.98401800	3.58136500	-1.20681900
H	2.43659800	-2.21151700	-2.00934100	H	-3.23271600	3.59356200	-0.14653300
H	1.71729700	-3.41033200	-3.09437200	H	-3.54638300	4.40656400	-1.66017500
C	2.34837500	-0.33165100	4.13679700	H	-1.92686300	3.82369100	-1.31227300
H	1.68167300	-1.16168800	4.39912600	C	-3.32830100	2.27950800	-1.88815500
H	3.21671600	-0.76368600	3.62705900	C	-4.94983900	0.54419100	-2.47717500
H	2.69982000	0.11005500	5.07237600	C	-2.77867400	0.62398200	-3.60030800
C	0.93970200	4.46510200	3.55886400	Ga	0.59823300	6.13327700	-0.60709500
H	-0.03800000	4.91899900	3.37271200	Cl	2.44068400	6.37685500	0.65121100
H	1.16042200	4.51120300	4.62925300	Cl	-1.17670700	5.89145000	0.75758000
H	1.66489500	5.09033600	3.02579600	Cl	0.31953700	7.83134600	-1.99365000
C	-0.13423300	1.24104400	-0.09528200	Cl	0.81777400	4.21334100	-1.80049400
H	0.60301600	0.94593800	-0.84944500	Ga	-3.13117200	-4.16494800	-1.28703500
H	-0.91228900	0.46973400	-0.07428700	Cl	-1.97348200	-2.11330100	-1.58000100
H	-0.59052100	2.16178200	-0.45090300	Cl	-2.02548000	-5.64957800	-2.47016600
C	6.82260400	-1.02544300	2.83546700	Cl	-3.14386500	-4.49288300	0.90334600
H	7.58144300	-1.60966700	3.36964600	Cl	-5.15749700	-3.70924900	-2.04491200
H	6.34486000	-0.37076400	3.57116200				

TSIntI-IntIII



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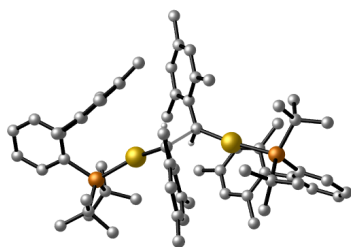
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C	-4.76432400	-2.30344500	0.11255600
C	-5.53817700	-3.45243900	0.38092300
H	-5.28790000	-4.08632300	1.21923800
C	-6.63291000	-3.80654500	-0.39936900
H	-7.20303100	-4.69809600	-0.15907800
C	-6.98487800	-3.00575800	-1.48465300
H	-7.83648800	-3.26120300	-2.10726300
C	-6.23294500	-1.87020200	-1.76689400
H	-6.50553000	-1.24418500	-2.61097400
C	-5.11773600	-1.49255700	-0.99396400
C	-4.45572900	-0.23164400	-1.48685600
C	-5.00163200	1.02749000	-1.12235200
C	-4.63465600	2.16609100	-1.84326400
H	-5.07865900	3.12104500	-1.57050100
C	-3.79206300	2.10363800	-2.95837700
C	-3.24743400	0.86218100	-3.29448700
H	-2.61382900	0.78309500	-4.17462100
C	-3.55227200	-0.30169900	-2.58343400
C	-3.95111700	-1.63329100	2.96080800
C	-4.50981300	-0.19601400	2.95208200
H	-4.86122400	0.05548700	3.95883200
H	-5.36064000	-0.10534900	2.27566900
H	6.21568400	1.09784900	-2.97604500
C	-2.77774800	-1.72165700	3.95544400
H	-3.10413500	-1.31686800	4.91946000
H	-1.91100000	-1.14472100	3.63035400
H	-2.46113500	-2.75198400	4.12970300
C	-5.07783500	-2.57765500	3.42326900
H	-4.77814500	-3.62728900	3.43390000
H	-5.97538300	-2.47419500	2.81062500
H	-5.34886700	-2.30852400	4.45005300
C	-2.18096600	-3.52729900	1.11309900
C	-2.69216600	-4.74300600	1.91043900
H	-1.96506300	-5.55582700	1.80458700
H	-3.64372700	-5.12301000	1.53657300

H	-2.79106300	-4.53799400	2.97787300
C	-2.05578300	-3.91035100	-0.37497900
H	-1.65201100	-3.08680000	-0.97001600
H	-3.01195000	-4.21434300	-0.80680300
H	-1.36377700	-4.75510300	-0.46370800
C	-0.77315600	-3.15549200	1.62895400
H	-0.75935100	-2.90357700	2.68956000
H	-0.34248800	-2.31717400	1.07348900
H	-0.11278300	-4.01794300	1.48972500
P	-3.30688700	-1.97160000	1.19023100
C	-0.93729700	2.47392000	-1.15815200
C	-1.68326300	4.77624000	-0.84254000
C	-0.44513400	4.19372700	-2.83216100
H	-2.21132300	5.52261700	-0.25588000
H	-0.00630000	4.48645800	-3.78193000
Au	2.07525600	0.08254500	-0.39285100
C	0.68958300	0.97523300	0.90708600
H	0.27927800	0.16232700	1.50007600
C	4.80885000	-2.06798900	-0.62606600
C	5.69079600	-2.98020600	-1.24414700
H	5.58315400	-3.20493800	-2.29562600
C	6.71743700	-3.60724600	-0.54711100
H	7.37416900	-4.30242900	-1.06004700
C	6.89302800	-3.32637800	0.80676600
H	7.68931400	-3.80085700	1.37152400
C	6.04093800	-2.42169100	1.43130500
H	6.18122900	-2.19463500	2.48382100
C	4.99385300	-1.77160000	0.74877400
C	4.20812400	-0.83067300	1.62839500
C	4.70395800	0.46512000	1.90976500
C	4.14140300	1.20209400	2.95880300
H	4.54651700	2.18815400	3.17558500
C	3.15196300	0.67694900	3.79170000
C	2.66661500	-0.60324800	3.50018900
H	1.92392700	-1.05246900	4.15571800
C	3.17039400	-1.36364700	2.44294900
C	4.52952400	-0.24573100	-3.00667500
C	5.68815700	0.44903100	-2.26870500
H	-3.75844700	0.54466300	2.66179800
H	6.41104900	-0.26071200	-1.86127500
H	5.32035700	1.07764200	-1.45511300
C	3.61851400	0.85277300	-3.58785800
H	4.19523500	1.43929200	-4.31171000
H	3.27161300	1.53821400	-2.80974000
H	2.75107400	0.45101900	-4.11349000
C	5.09340300	-1.08573200	-4.16746300
H	4.30890700	-1.53865100	-4.77716300
H	5.77788200	-1.86644900	-3.83204200
H	5.66721300	-0.42155500	-4.82321500
C	2.44890100	-2.61672200	-2.48948500
C	3.19746600	-3.76875100	-3.18927300
H	2.45345300	-4.42409800	-3.65550900
H	3.75885600	-4.37677900	-2.47778600
H	3.87188500	-3.43764100	-3.97842400
C	1.61094100	-3.23543100	-1.35404100

H	0.98066000	-2.49323200	-0.85590100	H	2.54818500	4.33630400	-0.45941100
H	2.24374600	-3.71857800	-0.60532500	H	1.66644100	2.89608900	-0.97414700
H	0.95216300	-4.00273900	-1.77544800	H	3.18043500	2.72809100	-0.08481800
C	1.49721400	-1.93489000	-3.49353600	C	-0.38474600	2.86794300	-2.43480400
H	2.02172800	-1.56183400	-4.37574400	C	-1.07638200	5.17175000	-2.04613200
H	0.94465200	-1.10606400	-3.03918800	C	-1.64233100	3.46609500	-0.38627600
H	0.76400300	-2.67170200	-3.84039600	C	1.52718000	3.33400700	1.14507000
P	3.54745500	-1.25265300	-1.69286000	C	0.99241000	4.58086700	3.18228200
C	0.81271200	2.18830900	1.65054800	C	0.21382400	2.28222300	2.96080000
C	1.59603200	4.48462100	1.91659200	C	-6.02356800	1.18294400	-0.01896900
C	0.30556500	3.46463700	3.68088700	H	-5.57864900	1.65759000	0.86285400
H	2.14320600	5.34278800	1.53604200	H	-6.84674500	1.82489000	-0.34554800
H	-0.15974900	3.52750700	4.66040500	H	-6.44953800	0.22793100	0.29060100
C	-1.15666400	6.59410500	-2.51937100	C	-3.57509000	3.32051000	-3.82053600
H	-1.97864600	6.70147700	-3.23936400	H	-3.46784900	4.22345900	-3.21315100
H	-0.24090400	6.89708500	-3.03502000	H	-2.68691200	3.22196800	-4.44862000
H	-1.34751900	7.28806800	-1.69744700	H	-4.43555100	3.47308300	-4.48237100
C	0.27460300	1.86464200	-3.33940000	C	-2.94071300	-1.60528000	-3.04535700
H	0.68385100	2.34577700	-4.22979200	H	-1.87969300	-1.65000100	-2.76953600
H	-0.43930500	1.10122400	-3.66427800	H	-3.43242900	-2.47443200	-2.60929100
H	1.09000900	1.34398000	-2.83265900	H	-2.99443300	-1.69539400	-4.13447300
C	-2.38938200	3.12583000	0.87112200	C	5.88294500	1.06869800	1.18121600
H	-2.74844400	4.02912700	1.36896600	H	6.37423900	0.35810100	0.51852100
H	-1.76838200	2.57723100	1.57802700	H	5.57700900	1.93685400	0.58580000
H	-3.25430500	2.49898200	0.63488700	H	6.62831700	1.42652200	1.89824600
C	1.11817300	5.83567900	3.99754800	C	2.71712500	1.41699600	5.03231600
H	0.28369000	5.95272300	4.69355200	H	2.72450400	2.49887900	4.87883400
H	1.17920400	6.72472200	3.36407000	H	1.71519700	1.12328400	5.35574900
H	2.03844800	5.80184700	4.59539700	H	3.40194300	1.19711100	5.85975300
C	-0.54879100	1.13175600	3.55590900	C	2.65937700	-2.76666900	2.22993800
H	-1.39108000	0.84082300	2.91846300	H	3.47711700	-3.49294100	2.19766900
H	-0.94516500	1.38848900	4.54007200	H	1.97403500	-3.06115200	3.02805900
H	0.08693900	0.24881600	3.66401800	H	2.12228400	-2.84537200	1.28299800
C	2.26377600	3.32283500	-0.16715500				

TSIntII-IntIV



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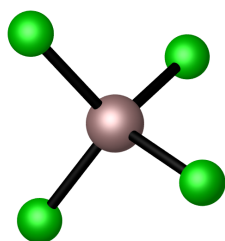
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H	7.34491200	-1.14078600	0.53706100
C	7.84762700	-1.39755100	-1.50712800
H	8.86020900	-1.71390400	-1.27849600
C	7.40980100	-1.30281400	-2.82659200
H	8.07725100	-1.53714400	-3.64985200
C	6.09840800	-0.91624300	-3.08089300
H	5.74586600	-0.86271200	-4.10656500
C	5.18741200	-0.60043700	-2.05430100
C	3.79893800	-0.31109800	-2.56280500
C	1.79872100	-1.19925800	-3.62345300
H	1.19515800	-2.05831100	-3.90879400
C	2.24018100	1.15142700	-3.71601400
H	1.99393400	2.14707300	-4.07883900
C	4.58032500	-1.71421400	1.93782400
C	4.23324000	-2.93006900	1.05858700
H	4.09895500	-3.80676500	1.70194800
H	5.02537000	-3.15919500	0.34194500
H	3.29652500	-2.77523300	0.51485000
C	3.43973200	-1.51728000	2.95598600
H	3.33694600	-2.43279300	3.54839100
H	2.48485200	-1.34012700	2.46114600
H	3.62495200	-0.69711100	3.64988400
C	5.88074700	-1.99330600	2.71361600
H	6.14703900	-1.17544600	3.38532600
H	6.72904300	-2.20839500	2.06283600
H	5.72539500	-2.88269400	3.33452000
C	5.50663500	1.30765100	1.58393500
C	7.02609700	1.16124900	1.80206800
H	7.38062200	2.05945400	2.31948000
H	7.56907200	1.09705100	0.85765700
H	7.29576800	0.30605100	2.42273800
C	5.29392900	2.50953900	0.64154600
H	4.23615900	2.71876200	0.45886400
H	5.78143200	2.35046500	-0.32205300
H	5.74055700	3.40051500	1.09631300
C	4.82841100	1.58969200	2.94026000
H	5.10571500	0.85395400	3.69842400
H	3.73795900	1.61699800	2.86721500
H	5.16306000	2.56729900	3.30394200

P	4.63761400	-0.19245600	0.76208100
Au	-2.18329100	-0.33045600	-0.10729500
C	-5.73867100	-0.44163100	-0.53099300
C	-6.91463700	-0.85468700	-1.19000400
H	-6.87278200	-1.65814100	-1.91197500
C	-8.14979900	-0.26880500	-0.93337900
H	-9.03202900	-0.61397800	-1.46265800
C	-8.23892900	0.75478300	0.00883500
H	-9.19344000	1.22403900	0.22526600
C	-7.09040900	1.17110800	0.67517600
H	-7.15442000	1.96554600	1.41269900
C	-5.83024100	0.59666100	0.43074100
C	-4.69622500	1.18180600	1.22051200
C	-3.52417100	1.51494500	3.31475100
H	-3.41718600	1.27752400	4.37162300
C	-2.95807700	2.86949500	1.42073900
H	-2.39338900	3.68399600	0.98033100
C	-4.28865000	-3.04388800	-0.13986000
C	-4.13816900	-2.82525400	1.38000400
H	-4.22877400	-3.79354600	1.88468600
H	-4.92098000	-2.17626100	1.77122500
H	-3.16608800	-2.39812800	1.64580900
C	-3.12870500	-3.93423200	-0.62453400
H	-3.14156300	-4.86528400	-0.04729800
H	-2.15680800	-3.45980900	-0.46266400
H	-3.21633100	-4.20788000	-1.67777600
C	-5.63802800	-3.74606800	-0.38876900
H	-5.83862600	-3.93374100	-1.44406200
H	-6.47288500	-3.17842700	0.02760200
H	-5.61806200	-4.71816600	0.11574000
C	-4.02976600	-1.44417600	-2.87585800
C	-4.87878200	-2.55206300	-3.53145900
H	-4.70790900	-2.51772700	-4.61309700
H	-5.95098500	-2.42387200	-3.38017900
H	-4.59651000	-3.54997200	-3.19270200
C	-4.42645200	-0.07519000	-3.46238500
H	-3.79754900	0.72717600	-3.06719800
H	-5.47063000	0.17881300	-3.26821000
H	-4.28239900	-0.10035500	-4.54804400
C	-2.54825500	-1.71004600	-3.23190500
H	-2.17025800	-2.64629500	-2.81824700
H	-1.89444600	-0.90326800	-2.89013000
H	-2.45880400	-1.77121400	-4.32197300
P	-4.17169500	-1.31652700	-0.95899100
C	0.60884300	1.24637600	-0.44101500
H	0.27073600	0.74970700	-1.34679000
C	-0.54602700	-0.08151100	1.14849500
H	-0.61891100	0.76123400	1.83175400
C	0.16036000	2.58943200	-0.31693000
C	-0.65025800	3.15886700	-1.37431300
C	0.55958600	3.45621900	0.76924300
C	-0.94961600	4.51202900	-1.36389300
C	0.21169300	4.79990300	0.73041800
C	-0.52059200	5.35927700	-0.32867700
H	-1.53915000	4.93151900	-2.17421100

H	0.52010400	5.44661500	1.54717100	H	0.62791300	-3.38356900	-0.94424500
C	-0.05311800	-1.27825800	1.74199300	C	-5.39529600	-0.13916400	3.31186100
C	-0.03528500	-1.37645200	3.18512600	H	-5.95090800	0.37604800	4.10312800
C	0.28260100	-2.45184800	0.96448800	H	-4.80222700	-0.92123900	3.79707400
C	0.17952100	-2.61272200	3.77585400	H	-6.12920700	-0.61513500	2.66138700
C	0.53514700	-3.64702600	1.62038400	C	-1.74492400	3.28407300	3.61100700
C	0.46090800	-3.76281000	3.01891300	H	-1.36826800	4.16766200	3.09071400
H	0.15290300	-2.69298800	4.85892000	H	-0.88441700	2.66188700	3.87997100
H	0.80044300	-4.52340800	1.03597900	H	-2.20268600	3.61420900	4.54866600
C	1.37995400	3.00516100	1.94984500	C	-4.24283800	2.72977500	-0.74069400
H	1.19933600	1.96878500	2.22880000	H	-3.55118700	3.51982500	-1.03758600
H	2.44660300	3.09789900	1.72295300	H	-5.26124000	3.12986200	-0.79154000
H	1.17670800	3.63821400	2.81629100	H	-4.18881600	1.92995800	-1.48110900
C	-0.83327500	6.82631000	-0.35930900	C	-2.73982000	2.52907300	2.76115400
H	-0.84883500	7.26016400	0.64345700	C	-4.51065700	0.84459900	2.57751700
H	-0.06237700	7.35656200	-0.93378500	C	-3.93493400	2.23039300	0.65021700
H	-1.79131000	7.02426700	-0.84747800	C	4.28312600	2.19915200	-2.72380300
C	-1.16806300	2.31948400	-2.50756500	H	4.27414600	2.86771900	-3.58925700
H	-0.34831500	1.93324700	-3.11545600	H	5.32053600	1.93100300	-2.51816500
H	-1.73281000	1.45769400	-2.13530300	H	3.90722800	2.77080500	-1.86863900
H	-1.82803600	2.90034400	-3.15419600	C	0.25382800	0.24504100	-5.00956700
C	-0.27953900	-0.18147200	4.07004000	H	0.17698000	1.27111100	-5.37884600
H	0.42868700	0.62387100	3.84904300	H	-0.69464800	-0.01269300	-4.52898400
H	-1.28843300	0.22042200	3.94053000	H	0.35823100	-0.41135500	-5.87979900
H	-0.15666600	-0.44969300	5.12095700	C	3.40224600	-2.83186000	-2.60070400
C	0.67827800	-5.08634800	3.69317700	H	4.19059300	-3.14793700	-3.29314700
H	1.13807200	-4.96691200	4.67807200	H	2.56726400	-3.52823600	-2.71151900
H	-0.28597200	-5.58801000	3.84804600	H	3.81219000	-2.93855800	-1.59693300
H	1.29872700	-5.75358200	3.08971600	C	2.97350200	-1.41419900	-2.89970500
C	0.46477000	-2.38980000	-0.52318300	C	3.42372100	0.98435100	-2.97838300
H	-0.38738100	-1.92743600	-1.02843300	C	1.43079500	0.07389800	-4.07709600
H	1.33002200	-1.76692300	-0.77903800				

GaCl₄⁻

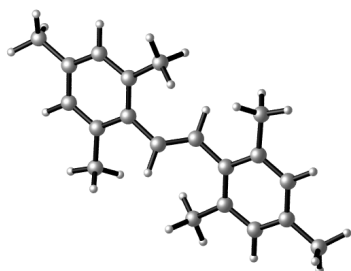


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G = -1843.208109

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Cl	1.83481000	0.00000000	-1.29771100

E-2a'



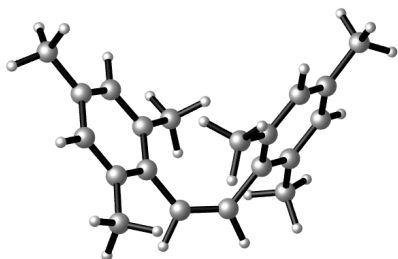
H	6.53918000	0.18848600	-1.28954300
H	6.61451800	1.22807700	0.13556800
H	6.79063500	-0.52699800	0.30294900
C	2.17637600	-2.66536400	0.17622800
H	1.65468500	-2.85278600	1.12314500
H	1.44202500	-2.81653300	-0.62227600
H	2.95132500	-3.42929200	0.07154900

E = -776.661926601

G = -776.330594

C	-0.48669600	0.33353000	-0.32359500
H	-0.19072100	1.12451000	-1.00868400
C	0.48666800	-0.33345300	0.32375500
H	0.19066600	-1.12441800	1.00884000
C	-1.94291900	0.12722000	-0.18485800
C	-2.77305000	1.27670100	-0.12576800
C	-2.54454500	-1.15378200	-0.14977000
C	-4.15383100	1.13110100	0.00340400
C	-3.93625000	-1.25079400	-0.02653400
C	-4.75952600	-0.12827200	0.06250800
H	-4.77516700	2.02268500	0.05859700
H	-4.38959800	-2.23990900	-0.01112700
C	1.94290700	-0.12727200	0.18492900
C	2.77294500	-1.27675100	0.12650000
C	2.54465100	1.15375900	0.14918500
C	4.15382900	-1.13128100	-0.00270400
C	3.93626100	1.25062000	0.02580000
C	4.75954100	0.12794200	-0.06264500
H	4.77508500	-2.02294200	-0.05732100
H	4.38970600	2.23969900	0.00993200
C	-1.75301400	-2.43635100	-0.28400800
H	-0.90344200	-2.31570500	-0.96085700
H	-1.34920800	-2.77418700	0.67799600
H	-2.38886400	-3.24053700	-0.66555400
C	-2.17645400	2.66532300	-0.17470600
H	-1.44198600	2.81597000	0.62378400
H	-1.65488300	2.85328600	-1.12158600
H	-2.95136600	3.42920900	-0.06945700
C	-6.25383900	-0.26249400	0.23177000
H	-6.61249600	-1.23477900	-0.11933700
H	-6.54157000	-0.16895100	1.28668200
H	-6.79082500	0.51666800	-0.31907000
C	1.75321900	2.43643000	0.28305300
H	1.34923000	2.77391200	-0.67900200
H	0.90380200	2.31610600	0.96014200
H	2.38921000	3.24071800	0.66414600
C	6.25373300	0.26280900	-0.23246400

Z-2a'



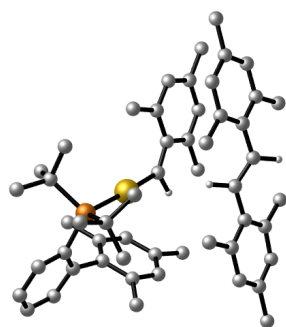
H	-3.19564100	2.92707100	-0.99753400
H	-2.20506500	2.11584300	-2.20281500
H	-3.93672300	1.75590600	-2.09423800
C	-0.17587800	-0.17970400	2.14239800
H	0.68672200	-0.68707100	1.69835300
H	0.14774900	0.83156200	2.39934600
H	-0.43396900	-0.70567200	3.06664700

E = -776.664356897

G = -776.331611

C	-0.66441700	2.02950800	0.10967000
C	0.66440900	2.02951600	-0.10965200
H	1.14241600	3.00901000	-0.14357700
C	1.58142200	0.88043200	-0.27203900
C	2.75330000	0.85482400	0.52680100
C	1.35418100	-0.16339900	-1.19673400
C	3.63510300	-0.22039300	0.42893400
C	2.27135900	-1.22093100	-1.26466600
C	3.40644100	-1.27972800	-0.45685400
H	4.52249400	-0.23501200	1.05853700
H	2.09164900	-2.01914700	-1.98202400
H	-1.14242700	3.00900200	0.14362700
C	-1.58142000	0.88041900	0.27204600
C	-1.35417200	-0.16343200	1.19671600
C	-2.75331000	0.85483200	-0.52677900
C	-2.27135200	-1.22096400	1.26464200
C	-3.63511300	-0.22038400	-0.42892100
C	-3.40644300	-1.27973900	0.45684300
H	-2.09163200	-2.01919300	1.98198400
H	-4.52251400	-0.23499000	-1.05851000
C	3.03885300	1.96829800	1.50780700
H	3.19566200	2.92704600	0.99759600
H	2.20504200	2.11582400	2.20284600
H	3.93669200	1.75585300	2.09430200
C	4.35576000	-2.45233000	-0.52138900
H	5.39695800	-2.13147700	-0.41191200
H	4.15232500	-3.16877000	0.28457500
H	4.26449900	-2.99173100	-1.46887200
C	0.17590300	-0.17965100	-2.14243300
H	-0.68668700	-0.68708100	-1.69844000
H	-0.14775800	0.83162100	-2.39931700
H	0.43403100	-0.70554600	-3.06671300
C	-4.35576600	-2.45233900	0.52136900
H	-5.39695200	-2.13150100	0.41175100
H	-4.15223400	-3.16884500	-0.28451200
H	-4.26460700	-2.99166200	1.46890600
C	-3.03886500	1.96832600	-1.50776200

IntV



E = -2538.46370751

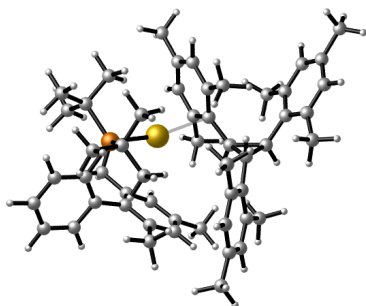
G = -2537.478038

Au	-0.88591600	-0.69873300	0.23586100
C	0.87595300	-0.11224100	1.06754800
H	0.85680800	0.95882700	1.26701900
C	-4.43865800	-0.47180500	0.06983300
C	-5.73245900	-0.88495400	-0.30915200
H	-5.85220800	-1.71401100	-0.99244300
C	-6.87952600	-0.25895900	0.16813400
H	-7.85749600	-0.60727300	-0.14876500
C	-6.75592800	0.80832200	1.05606700
H	-7.63780000	1.30186500	1.45280900
C	-5.48753600	1.25730700	1.41017800
H	-5.38451700	2.11586000	2.06702700
C	-4.31276100	0.65781700	0.92073100
C	-3.04255500	1.38170600	1.27368200
C	-1.27293100	1.96485500	2.83131100
H	-0.77041700	1.79067700	3.78080800
C	-1.53946000	3.23195500	0.81872300
H	-1.23325700	4.05275300	0.17737600
C	-3.23699900	-3.22951100	0.14922800
C	-2.96803800	-3.12630900	1.66538600
H	-3.09912900	-4.11512900	2.11922900
H	-3.66407100	-2.43974400	2.15386600
H	-1.94879900	-2.79098600	1.87793100
C	-2.17567200	-4.14775900	-0.48964000
H	-2.16532400	-5.10261400	0.04792800
H	-1.17213000	-3.72016800	-0.42737100
H	-2.39426200	-4.36825000	-1.53705200
C	-4.63107700	-3.85930000	-0.03379200
H	-4.94454200	-3.92453800	-1.07644700
H	-5.39656900	-3.32418700	0.53094100
H	-4.59531900	-4.88219600	0.35774100
C	-3.05431300	-1.43080000	-2.47115300
C	-4.07517200	-2.39133000	-3.10801800
H	-4.03362900	-2.26884300	-4.19619000
H	-5.10233000	-2.17855600	-2.80449500
H	-3.85541400	-3.43892700	-2.89307000
C	-3.38275300	0.01245800	-2.89722900
H	-2.68102700	0.73144700	-2.46767600
H	-4.39733800	0.30275000	-2.61394700

H	-3.30445000	0.08537500	-3.98780400
C	-1.64347200	-1.77657100	-2.99732600
H	-1.29851300	-2.76232600	-2.68009300
H	-0.90498100	-1.03860100	-2.67594300
H	-1.66543700	-1.77022100	-4.09308100
P	-3.00336200	-1.45620300	-0.55241300
C	2.05217800	-0.72617900	1.50911700
C	2.33590500	-2.13470200	1.30397200
C	3.06481200	0.08859100	2.16691700
C	3.56170100	-2.64267600	1.70222500
C	4.26690800	-0.48032300	2.53564000
C	4.54463000	-1.83954200	2.29624400
H	3.78246700	-3.69032100	1.52721100
H	5.02477400	0.13102000	3.01718600
C	3.78043100	0.96543900	-1.43380800
H	4.59013600	1.66704200	-1.60386700
C	2.53553200	1.46475600	-1.28601300
H	1.72550800	0.75814200	-1.14165500
C	4.19240000	-0.44831600	-1.36771900
C	5.91586400	-2.05456500	-0.74129500
C	3.90540800	-2.83265100	-1.77221300
H	6.89198400	-2.25598900	-0.30566600
H	3.29814800	-3.64550200	-2.16458800
C	2.10805700	2.87470300	-1.30936800
C	0.35939300	4.46798300	-1.90027900
C	2.32540200	5.23748100	-0.77778800
H	-0.60703500	4.66906000	-2.35774700
H	2.90313700	6.04633100	-0.33619700
C	1.35017500	-3.08650500	0.68880900
H	0.44076000	-3.15143400	1.29359700
H	1.05066400	-2.76211100	-0.30938700
H	1.78304900	-4.08566600	0.60790700
C	5.86626400	-2.41667300	2.70912200
H	6.04439600	-3.39359400	2.25543500
H	6.68588900	-1.74571900	2.43495200
H	5.89908600	-2.53541100	3.79960200
C	2.82215600	1.54065700	2.47741400
H	2.57021700	2.11200300	1.58092500
H	1.98985900	1.65425700	3.17842300
H	3.70646300	1.99451700	2.92889100
C	5.66847100	-4.54027000	-1.14531100
H	4.86030200	-5.27253200	-1.22982700
H	6.20112300	-4.72629800	-0.20631600
H	6.37711400	-4.73919700	-1.95815200
C	6.34697400	0.36489400	-0.26389200
H	7.25533100	-0.04637400	0.18381500
H	5.82439000	0.94683100	0.50286900
H	6.65957500	1.07012600	-1.04293400
C	2.07610900	-1.32392800	-2.53920300
H	1.80901600	-2.20007200	-3.13642000
H	2.08176400	-0.44790600	-3.19385500
H	1.27079700	-1.16747000	-1.81068300
C	4.23193000	3.76904700	-0.14042500
H	4.44557000	4.58470900	0.55569100
H	5.01965700	3.78380900	-0.90329900

H	4.33125200	2.82398400	0.39743300	C	-2.76682600	0.04290200	3.43666900
C	0.55546800	6.94066200	-1.38953900	H	-2.63409400	0.35643500	4.47614000
H	0.93541500	7.53692400	-0.55481000	H	-2.14786700	-0.84782200	3.28375600
H	-0.53809100	6.96157700	-1.35417900	H	-3.80979200	-0.25177600	3.30292300
H	0.86026100	7.44414300	-2.31509900	C	0.27971400	3.94103400	2.40060400
C	-0.01063800	2.05860500	-2.47576900	H	1.03423600	4.00281200	1.60905800
H	-0.89103200	2.47201300	-2.97416700	H	0.76710200	3.62935200	3.32770000
H	-0.36577600	1.36142000	-1.70513100	H	-0.09854900	4.95790800	2.55460300
H	0.54540300	1.46941500	-3.21219900	C	-3.43107700	2.88613100	-0.76962900
C	0.83599400	3.15788000	-1.87665400	H	-4.07995900	3.73339800	-0.51674300
C	2.86257500	3.94410600	-0.75918400	H	-4.07414900	2.09899900	-1.15821600
C	1.08444400	5.52825300	-1.34706100	H	-2.76411300	3.21936200	-1.56980700
C	3.41154500	-1.52396600	-1.86518700	C	-2.36027100	1.14602200	2.48697500
C	5.46928300	-0.73573000	-0.81402600	C	-0.84649600	3.01261500	2.01215300
C	5.14850300	-3.12558900	-1.21466200	C	-2.64196700	2.45990700	0.44827200

IntVI



E = -2538.47450977

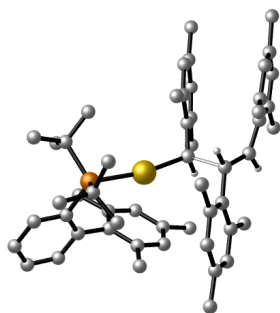
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H	1.53936800	1.03273800	1.48374700
C	-4.10290000	-0.30734500	-0.42295500
C	-5.32281800	-0.63077300	-1.05451800
H	-5.34271200	-1.37661000	-1.83704400
C	-6.52046100	-0.01754100	-0.70592800
H	-7.43870900	-0.29573100	-1.21322000
C	-6.52287300	0.95223500	0.29591800
H	-7.44545300	1.44678800	0.58364000
C	-5.33076300	1.27758200	0.93345300
H	-5.32854800	2.02350100	1.72219700
C	-4.10517900	0.66573600	0.60559500
C	-2.94743000	1.11852600	1.45159200
C	-1.79958800	1.01189900	3.58610400
H	-1.63029500	0.50363900	4.53298700
C	-1.39518900	2.85927600	2.12142700
H	-0.90773800	3.80408800	1.90022100
C	-2.96617800	-3.07637700	-1.02706200
C	-3.74142500	-3.39199000	0.26643400
H	-3.85508200	-4.47826800	0.35137400
H	-4.73847600	-2.94669400	0.27450200
H	-3.20371100	-3.04399000	1.15143800
C	-1.61993500	-3.83609700	-0.98365900
H	-1.82699500	-4.91151800	-1.02765000
H	-1.07151700	-3.63992500	-0.05936300
H	-0.96460100	-3.59007100	-1.82167300
C	-3.75899800	-3.59314500	-2.24397100
H	-3.20805900	-3.47628600	-3.17923600
H	-4.73970900	-3.12872700	-2.35423500
H	-3.93294700	-4.66575900	-2.10429400
C	-2.27164200	-0.49884700	-2.78481200
C	-3.47848400	-0.55436400	-3.74216400
H	-3.16676000	-0.12889300	-4.70253600
H	-4.31339200	0.04760100	-3.37827500
H	-3.83270400	-1.56643000	-3.93656900
C	-1.89850500	0.98431900	-2.59558700
H	-1.07072300	1.13389600	-1.89926100

H	-2.75196200	1.56031200	-2.23622700
H	-1.59827100	1.40265500	-3.56201200
C	-1.08600300	-1.26757000	-3.40037500
H	-1.34559900	-2.30021900	-3.64695100
H	-0.21491100	-1.28196500	-2.73930100
H	-0.79016700	-0.77372600	-4.33219700
P	-2.60221200	-1.18197300	-1.03099300
C	1.73090200	-0.95083500	0.71010700
C	2.07348500	-1.89691200	-0.33004200
C	1.23455000	-1.49047100	1.95582100
C	1.93363200	-3.26110000	-0.08379900
C	1.07836800	-2.88176400	2.11518400
C	1.44321000	-3.78311800	1.12221700
H	2.21419900	-3.95478200	-0.87201200
H	0.70731600	-3.25315200	3.06625500
C	3.52107300	1.10399200	0.60353600
H	3.72736400	1.84800400	1.36516900
C	2.45230800	1.43422100	-0.42376400
H	2.65888800	0.91097200	-1.34045600
C	4.73563600	0.32372700	0.17262100
C	6.26969600	-1.54127800	0.42265900
C	6.56775900	-0.01063000	-1.38753200
H	6.59675700	-2.41166600	0.98783400
H	7.13240200	0.32811800	-2.25352700
C	1.72952700	2.72798500	-0.67945300
C	0.44212700	4.05448400	-2.27855500
C	0.78933200	4.88909700	-0.07579400
H	0.03510000	4.16882700	-3.28056500
H	0.65548600	5.67070500	0.66887100
C	2.60057900	-1.50221000	-1.68975100
H	2.68418600	-2.38376600	-2.32924600
H	1.93755900	-0.79570300	-2.19014900
H	3.59067100	-1.04581200	-1.62124100
C	1.29297900	-5.27076900	1.30664500
H	2.18950700	-5.80189400	0.97204300
H	1.10805300	-5.53219500	2.35138100
H	0.45299900	-5.65024500	0.71230700
C	1.06056800	-0.62942100	3.18575900
H	2.03954900	-0.31064700	3.55885100
H	0.46591100	0.26150800	3.00031800
H	0.56490100	-1.19229100	3.97933200
C	8.10970000	-2.01371200	-1.25295400
H	8.56938200	-2.60575000	-0.45645900
H	8.88633800	-1.38825700	-1.70342800
H	7.76858100	-2.71331100	-2.02620800
C	4.55574200	-1.23327900	2.20665100
H	5.33252500	-1.56190400	2.90335900
H	3.86729500	-2.07477700	2.07430800
H	4.00801300	-0.42029400	2.68534300
C	5.16894100	2.03678000	-1.69347600
H	6.08043300	2.45147200	-2.13201600
H	4.72735700	2.79932500	-1.04889400
H	4.46754700	1.87088900	-2.51963000
C	2.14342800	3.75801200	1.66409900
H	1.74846400	4.59431200	2.24585800

H	3.23053600	3.88269100	1.62731700	C	-3.31873000	-0.88597200	3.01136700
H	1.93077900	2.85040000	2.23369400	H	-3.50523200	-0.96263300	4.08621700
C	-0.63357700	6.26128600	-1.65896200	H	-2.64690800	-1.71008600	2.74150100
H	-0.36327000	7.12307800	-1.04216500	H	-4.26376100	-1.04764100	2.48991800
H	-1.69452100	6.04770300	-1.47625000	C	-0.19477800	2.80649400	4.35459800
H	-0.53747800	6.55109500	-2.70953000	H	-0.64508100	2.81234500	5.35242100
C	1.40404000	1.90795700	-3.09617900	H	0.08534300	3.83180500	4.10193400
H	0.90709200	2.23977500	-4.01093500	H	0.72964200	2.21959100	4.42557300
H	1.00622800	0.91779600	-2.85575600	C	-2.60822500	3.19227800	-0.03067600
H	2.46559000	1.78216600	-3.33466200	H	-2.79635700	4.22970200	0.26382600
C	1.18633900	2.90911600	-1.97946400	H	-3.48314500	2.84078600	-0.57856900
C	1.53983200	3.75857200	0.27338300	H	-1.75227200	3.20876200	-0.71143900
C	0.21745900	5.05846500	-1.33614200	C	-2.67878600	0.43920300	2.66659600
C	5.48262500	0.75467600	-0.95057700	C	-1.14089700	2.22143200	3.33389400
C	5.18014600	-0.80202900	0.89758300	C	-2.31117000	2.35018800	1.18960800
C	6.96243600	-1.18164200	-0.73381400				

TSIntV-IntVI



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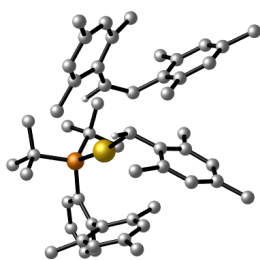
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C	-4.12220900	-1.05753600	0.13483800
C	-5.33748300	-1.65373200	-0.26355800
H	-5.36513500	-2.28833100	-1.13701100
C	-6.52398700	-1.45937500	0.43548200
H	-7.43693000	-1.93668700	0.09335900
C	-6.52405100	-0.64996200	1.57005100
H	-7.44024600	-0.47649900	2.12615200
C	-5.32996600	-0.07959800	1.99760400
H	-5.31507100	0.52752200	2.89766600
C	-4.11380600	-0.27541700	1.31644800
C	-2.91971400	0.33939400	1.99025600
C	-1.34733500	0.31463400	3.83615600
H	-0.92246400	-0.20361100	4.69373200
C	-1.54078200	2.27506500	2.47824300
H	-1.26266800	3.29943000	2.24980800
C	-2.31472200	-3.27279900	-0.81403800
C	-2.44322000	-3.66043100	0.67155500
H	-2.13449900	-4.70448000	0.79559800
H	-3.46975300	-3.56801100	1.03262400
H	-1.79609400	-3.04321400	1.30138000
C	-0.86654000	-3.57529100	-1.25642700
H	-0.69795500	-4.65576100	-1.17939900
H	-0.13966000	-3.07596300	-0.61113700
H	-0.66624400	-3.28333200	-2.28843400
C	-3.27658500	-4.13072100	-1.65495000
H	-3.16863400	-3.94677700	-2.72631200
H	-4.32278500	-3.99278300	-1.37627000
H	-3.03910200	-5.18685600	-1.48332900
C	-3.04117100	-0.79311700	-2.67867700
C	-4.38071800	-1.26591300	-3.27798900
H	-4.42698200	-0.91899100	-4.31674400
H	-5.23571300	-0.83222500	-2.75663600
H	-4.49105800	-2.35109500	-3.29630100
C	-3.07927500	0.74800400	-2.62037000
H	-2.13475700	1.17949500	-2.28548200

H	-3.87148200	1.10380900	-1.95639100
H	-3.28892800	1.13606600	-3.62413100
C	-1.89572800	-1.24821900	-3.60583100
H	-1.93849400	-2.32083100	-3.81090300
H	-0.91130100	-1.01449700	-3.19323500
H	-1.98779100	-0.72863500	-4.56618100
P	-2.62411200	-1.37706900	-0.90044100
C	2.25476700	-0.83139300	0.67910700
C	2.69806500	-1.73282900	-0.32952000
C	2.73588000	-1.03163500	2.01554600
C	3.63940200	-2.71641100	-0.01277700
C	3.64812300	-2.04653900	2.28354900
C	4.14455900	-2.88349000	1.27529200
H	3.98646300	-3.37471000	-0.80631600
H	3.99381000	-2.18851300	3.30475800
C	3.20438200	1.84847400	-0.25075200
H	3.24321900	2.50988500	0.60082400
C	1.96141400	1.68637400	-0.88948100
H	1.99624700	1.04562200	-1.75383200
C	4.39033800	1.08680500	-0.50449100
C	6.27064600	-0.12320100	0.45701200
C	5.77377100	-0.35864500	-1.88422100
H	6.89576800	-0.36428600	1.31228100
H	6.03596200	-0.75812200	-2.86072100
C	0.89826000	2.73285900	-0.98293400
C	-0.88291300	3.70314400	-2.33789100
C	-0.39142500	4.63902400	-0.20118700
H	-1.45988900	3.70179300	-3.25935100
H	-0.58546800	5.37905900	0.57167400
C	2.21697300	-1.71706000	-1.76306200
H	1.76028600	-2.67986900	-2.01153800
H	1.47256400	-0.94858200	-1.96018300
H	3.05879100	-1.58040300	-2.44709500
C	5.20012700	-3.91461300	1.58041100
H	6.17928200	-3.43596500	1.70940300
H	4.98225500	-4.45029400	2.50973100
H	5.29308700	-4.64989500	0.77650300
C	2.20391700	-0.22270900	3.17482700
H	2.29556500	0.85811500	3.02311800
H	1.13797200	-0.41485500	3.32893500
H	2.73352200	-0.47018500	4.09784700
C	7.56844600	-1.83022800	-0.87758500
H	8.40020500	-1.65117300	-0.19031600
H	7.96574800	-1.90484300	-1.89325900
H	7.13782600	-2.80625900	-0.61992600
C	5.11919700	1.53790000	1.92448700
H	5.89214300	1.20991300	2.62236700
H	4.15409200	1.36764500	2.40169100
H	5.23453000	2.62015700	1.79101400
C	4.08708600	1.02718600	-3.07755600
H	4.82110200	0.99128300	-3.88691000
H	3.72738000	2.05502000	-2.99839700
H	3.24452000	0.40041800	-3.38608100
C	1.40994600	3.84118100	1.30074400
H	0.89223200	4.51400200	1.98778700

H	2.40375800	4.27234900	1.13036100	C	-2.78756500	-1.70063600	3.55219500
H	1.53901700	2.88752800	1.81778200	H	-3.26176500	-1.62483200	4.53741800
C	-2.30192000	5.63534900	-1.52906700	H	-1.93615000	-2.38103000	3.65985900
H	-2.13935300	6.54595800	-0.94585400	H	-3.50854800	-2.16032400	2.87885100
H	-3.24712100	5.19265400	-1.19004300	C	0.02109200	2.33703300	4.47674700
H	-2.43353200	5.91929200	-2.57726500	H	-0.51622800	2.82522900	5.29861600
C	0.38075900	1.79215200	-3.31851700	H	0.58263100	3.11478700	3.95344000
H	-0.37525500	1.91290300	-4.09729100	H	0.73592700	1.64292400	4.92814900
H	0.34603500	0.74773300	-2.99543300	C	-3.14292000	2.44772500	0.56154500
H	1.35784800	1.96377100	-3.78203700	H	-3.24163800	3.50289700	0.83121800
C	0.12622000	2.75176300	-2.17539000	H	-4.13177100	2.07033200	0.29340500
C	0.63182600	3.70765600	0.00990300	H	-2.50905900	2.40670400	-0.32844400
C	-1.16855900	4.65606100	-1.35869100	C	-2.33367100	-0.33389000	3.08593900
C	4.72801600	0.55273100	-1.78993100	C	-0.94747600	1.62453000	3.56311100
C	5.25851200	0.81718400	0.60435700	C	-2.52327400	1.66211400	1.69272200
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IntVII



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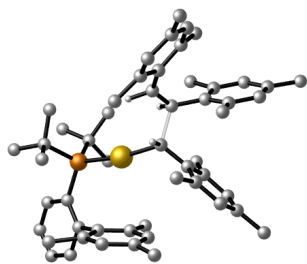
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C	4.57841500	0.52607900	0.30947800
C	5.74106800	1.16519600	0.78796400
H	5.65478400	2.05281300	1.39810200
C	7.01905600	0.69638500	0.50014400
H	7.88660600	1.21990900	0.88935200
C	7.16824700	-0.44104700	-0.29053000
H	8.15604600	-0.81898700	-0.53552700
C	6.03436800	-1.10270000	-0.75145300
H	6.14242300	-2.00580900	-1.34459600
C	4.73186100	-0.65884300	-0.46023700
C	3.63422200	-1.56026900	-0.95598400
C	3.26161400	-2.68062400	-0.17462900
C	2.29986000	-3.56706700	-0.66635700
H	2.01820800	-4.42336800	-0.05629300
C	1.71628000	-3.40751700	-1.92677200
C	2.13207700	-2.32501600	-2.70384000
H	1.72145300	-2.19768200	-3.70345300
C	3.08653900	-1.40373900	-2.24788500
C	2.80224100	1.29069200	2.64902900
C	3.21791700	-0.11883100	3.11235000
H	3.03777900	-0.20863600	4.18942900
H	4.27790700	-0.31247700	2.93234900
H	2.63305400	-0.89518800	2.60997800
C	1.32199800	1.50460800	3.03977700
H	1.23583000	1.44563600	4.13065100
H	0.67856600	0.73198900	2.61239900
H	0.93149200	2.47509900	2.73181700
C	3.65965400	2.34362300	3.37280200
H	3.37093700	3.36453500	3.11360000
H	4.72760800	2.21953000	3.18447900
H	3.51203200	2.23066300	4.45286400
C	2.94448400	3.05661800	0.00140700
C	4.19524000	3.91061900	0.28617400
H	4.02366900	4.91224400	-0.12398100
H	5.08313700	3.50861500	-0.20527000
H	4.40521700	4.02998900	1.35036600
C	2.82972100	2.88868000	-1.52817500
H	1.89968500	2.39195400	-1.82002800

H	3.67150800	2.32228000	-1.93372100
H	2.84041200	3.88006300	-1.99519300
C	1.69636500	3.79793200	0.51842100
H	1.78638900	4.07999900	1.57008700
H	0.78678200	3.20491200	0.39367600
H	1.57051200	4.72219500	-0.05638400
P	2.94291500	1.28579200	0.73672500
C	-1.27158000	-1.98084200	-0.80368200
C	-1.31199700	-2.63211300	0.49072900
C	-2.18889700	-2.44162400	-1.83254400
C	-2.28534400	-3.58734200	0.73647000
C	-3.12896600	-3.40668300	-1.52556600
C	-3.21919900	-3.96750800	-0.23858200
H	-2.34324600	-4.04431500	1.71939100
H	-3.82626400	-3.73729300	-2.29007500
C	-2.13206000	-1.90733500	-3.24195100
H	-2.38583600	-0.84360600	-3.28515500
H	-1.13332500	-2.02715400	-3.67328100
H	-2.83988000	-2.43855900	-3.88133600
C	-4.25966700	-5.00488200	0.06791000
H	-5.16158300	-4.85703400	-0.53160500
H	-3.87165200	-6.00491800	-0.16552100
H	-4.53439100	-4.99404600	1.12494400
C	-0.32085600	-2.33177000	1.57783700
H	0.69854000	-2.52038900	1.22920100
H	-0.36218100	-1.28397400	1.87996800
H	-0.51430400	-2.94800700	2.45857200
C	-2.11719200	1.98015700	0.39320300
C	-2.25693900	0.82846400	1.08695000
H	-1.34589200	0.50774100	1.58561500
C	-3.39218500	-0.08112800	1.29532500
C	-3.53463500	-0.65409700	2.59115100
C	-4.28162700	-0.48126900	0.26729900
C	-4.53472300	-1.59372800	2.82937500
C	-5.26585000	-1.43471200	0.55491400
C	-5.41564100	-2.00277600	1.82083800
H	-4.64091600	-2.01178000	3.82791700
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H	-1.09277300	2.34454100	0.34229500
C	-3.10124200	2.81218300	-0.31370600
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C	-2.75878200	3.26509700	-1.61418200
C	-5.20873300	3.99027600	-0.50276400
C	-3.66439400	4.04012600	-2.33527200
C	-4.90339500	4.41131300	-1.79853100
H	-6.15398400	4.29455700	-0.05891600
H	-3.40136500	4.36756900	-3.33860600
C	-2.64448300	-0.21790000	3.73280600
H	-1.59783500	-0.50630000	3.57695900
H	-2.65580300	0.87059400	3.85275000
H	-2.96890100	-0.66596800	4.67503100
C	-6.51502700	-2.99485500	2.10976200
H	-6.19048100	-3.75889000	2.82376700
H	-7.38569200	-2.49435300	2.55043000
H	-6.85518400	-3.49770400	1.19992000

C	-4.21342400	0.05539700	-1.14031500	H	-3.89260000	2.72200800	2.32410300
H	-4.79584100	0.97576500	-1.24384700	H	-5.44065900	3.54819900	2.07048300
H	-3.18967900	0.29893800	-1.42851200	C	0.69942100	-4.40285700	-2.42945000
H	-4.61256700	-0.67603400	-1.84815100	C	3.48334700	-0.26913200	-3.16235400
C	-5.88298600	5.22858500	-2.60472700	C	3.90908300	-2.99700100	1.15568200
H	-5.36890100	5.92401500	-3.27510700	H	3.15675200	-3.24845300	1.91090400
H	-6.51173300	4.58099800	-3.22848700	H	4.56598500	-3.86897800	1.05746500
H	-6.55042700	5.80688000	-1.95950900	H	4.51453900	-2.17634600	1.53638800
C	-1.43770600	2.87904400	-2.24083800	H	-0.14019300	-4.49655500	-1.73201300
H	-0.58670500	3.29881100	-1.69002100	H	0.29715900	-4.11330300	-3.40403500
H	-1.29397600	1.79179000	-2.24494300	H	1.14389700	-5.39861500	-2.53617800
H	-1.37067400	3.23596400	-3.27171600	H	2.72118900	0.51706300	-3.15158100
C	-4.75223700	2.80755700	1.65458800	H	4.43325800	0.18325500	-2.87204300
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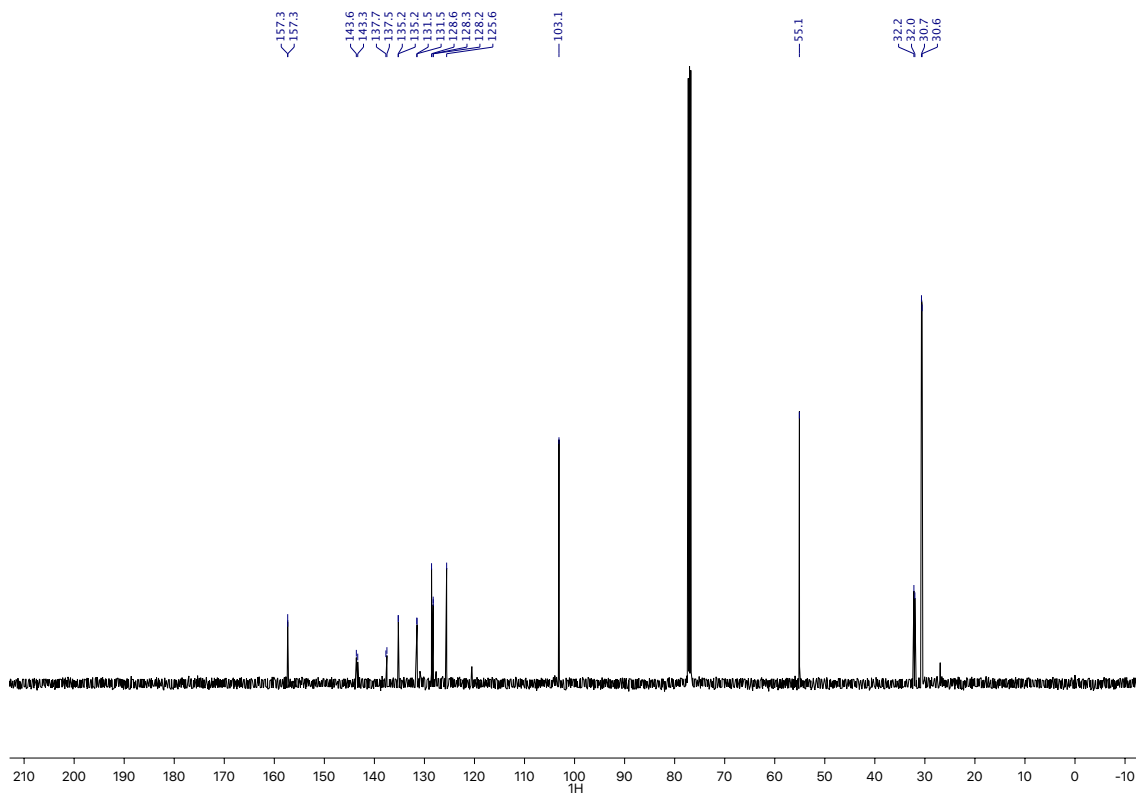
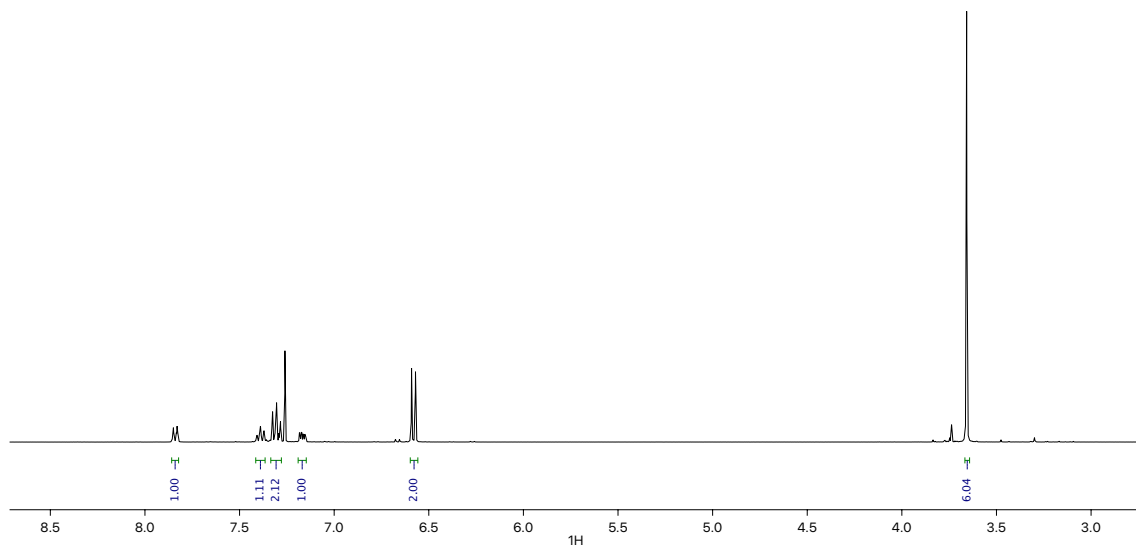
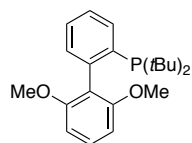
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C	-1.05403500	0.33428700	0.29994100
H	-1.28289900	0.06523100	1.32978800
C	4.51295000	-0.45723100	-0.50321400
C	5.66520400	-0.98148000	-1.12445300
H	5.63616000	-1.97017000	-1.55869000
C	6.85810700	-0.27053800	-1.19949200
H	7.72054700	-0.71210900	-1.68892000
C	6.92842300	1.00658100	-0.64516500
H	7.84615100	1.58401200	-0.70105000
C	5.81303700	1.52897900	0.00078600
H	5.86838800	2.50935600	0.46456800
C	4.60041900	0.82218000	0.10163300
C	3.54496700	1.49716200	0.92800100
C	2.61360100	2.37673100	0.33177200
C	1.75036700	3.11567900	1.14702900
H	1.03612100	3.78915400	0.68144300
C	1.80040100	3.02394800	2.54219600
C	2.72613200	2.14773800	3.11205900
H	2.79650400	2.08100200	4.19616900
C	3.61919500	1.40292900	2.33368700
C	2.76542800	-2.02935700	-2.42228700
C	3.06641600	-0.81082100	-3.31962100
H	2.86709700	-1.08236400	-4.36250900
H	4.10591800	-0.48448500	-3.25004000
H	2.42201700	0.03867400	-3.07296900
C	1.29107100	-2.43352600	-2.66368600
H	1.18266000	-2.75488900	-3.70592800
H	0.61617100	-1.58989200	-2.50383100
H	0.96228200	-3.25712700	-2.02742400
C	3.64774200	-3.21893200	-2.85236100
H	3.43940000	-4.12187000	-2.27542900
H	4.71612900	-3.01022000	-2.79437400
H	3.42990700	-3.44835400	-3.90161600
C	3.17681000	-2.93219700	0.59751300
C	4.55170400	-3.61674300	0.49337900
H	4.58931000	-4.44129400	1.21450000
H	5.36462500	-2.92891000	0.73775800
H	4.74325100	-4.04006500	-0.49421700
C	3.01710400	-2.37055500	2.02587600
H	2.03033200	-1.92468900	2.18309500

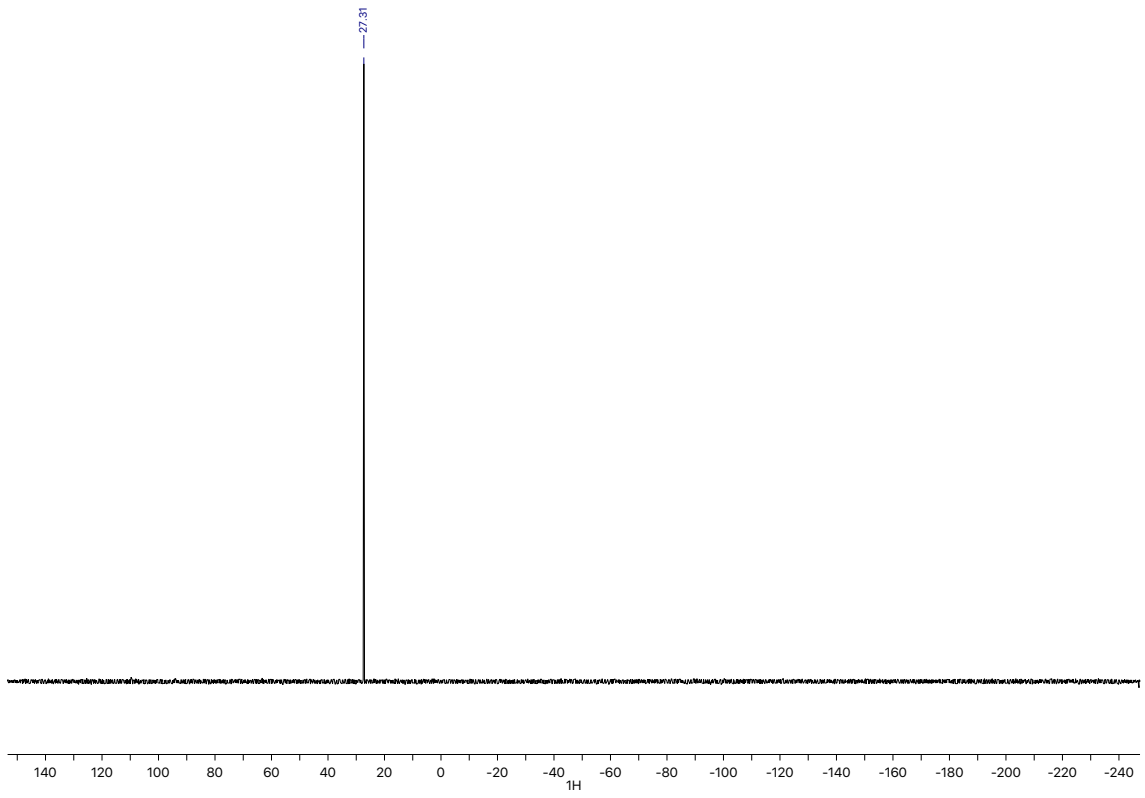
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H	3.14368800	-3.18776100	2.74547400
C	2.05335200	-3.95808800	0.35126600
H	2.15777500	-4.47576300	-0.60443800
H	1.06514300	-3.48736800	0.38598000
H	2.09154500	-4.71830400	1.13970300
P	2.95278200	-1.44962300	-0.58563500
C	-1.33875600	1.77764800	0.12637200
C	-1.17014900	2.45072000	-1.11430100
C	-1.67838500	2.55277700	1.27636300
C	-1.39918400	3.82688300	-1.18997700
C	-1.91252500	3.92017600	1.14479900
C	-1.79726500	4.58072000	-0.08436700
H	-1.26041700	4.32614700	-2.14644600
H	-2.18072300	4.49538700	2.02781900
C	-1.71319000	1.95548700	2.66629200
H	-2.44932600	1.15191300	2.77026700
H	-0.73289000	1.54667600	2.93685600
H	-1.96380200	2.71889900	3.40580800
C	-2.09384100	6.05368800	-0.20442200
H	-3.16825000	6.22259700	-0.34893700
H	-1.80008200	6.59729000	0.69864300
H	-1.57571900	6.50028800	-1.05767000
C	-0.72662600	1.76027400	-2.38172400
H	-0.05056600	2.40739800	-2.94792700
H	-0.19738900	0.82626400	-2.18331700
H	-1.58374200	1.53874500	-3.02276700
C	-2.33183800	-1.69410900	0.34732600
C	-2.15636200	-0.72971600	-0.70517900
H	-1.40865900	-1.08008000	-1.40497100
C	-3.29071600	-0.06574600	-1.43953100
C	-3.36114000	-0.28297600	-2.84346700
C	-4.27641100	0.73240100	-0.82608400
C	-4.36731900	0.32900800	-3.58869400
C	-5.26179800	1.33812800	-1.61893800
C	-5.32329200	1.16506000	-2.99873100
H	-4.41292000	0.14868700	-4.65997100
H	-6.00778500	1.95924400	-1.12789900
H	-1.37060800	-2.05646800	0.70742100
C	-3.45566000	-2.13204300	1.10775400
C	-4.75521900	-2.38969700	0.56052400
C	-3.23699200	-2.33253000	2.51886000
C	-5.79574800	-2.70022500	1.43230900
C	-4.32060200	-2.61858000	3.33447000
C	-5.61651500	-2.78338400	2.81718100
H	-6.77604800	-2.91516900	1.01496300
H	-4.16449600	-2.72443800	4.40464500
C	-2.40029900	-1.20380000	-3.56820900
H	-1.36715800	-0.84167300	-3.53027900
H	-2.40171000	-2.21766800	-3.15027600
H	-2.67277000	-1.28808000	-4.62255200
C	-6.37228000	1.85206400	-3.83713300
H	-5.94348400	2.70854100	-4.37117600
H	-6.78537000	1.17604600	-4.59261200
H	-7.19766300	2.22513700	-3.22483200

C	-4.40305100	0.94094900	0.66527600	H	-4.12548400	-2.63036500	-1.50474000
H	-5.33889500	0.49697800	1.02356400	H	-5.69196300	-3.34143200	-1.10821300
H	-3.59915800	0.48582600	1.23229700	C	0.95330400	3.91495300	3.41900700
H	-4.42237300	2.00673000	0.90796300	C	4.71036900	0.62718600	3.04139600
C	-6.77158300	-3.06535300	3.73796300	C	2.59491700	2.58380100	-1.16434800
H	-7.64127800	-3.44505200	3.19683400	H	2.43022000	1.64396300	-1.69770600
H	-6.49635800	-3.79044200	4.51014600	H	1.80031300	3.27582400	-1.45097700
H	-7.07468000	-2.14605800	4.25452300	H	3.55049800	2.98586300	-1.51905300
C	-1.87545000	-2.16014000	3.15308200	H	0.10986600	4.33288900	2.86687500
H	-1.10744700	-2.76062200	2.65241300	H	0.56460900	3.37521100	4.28821400
H	-1.53797300	-1.11915400	3.12437700	H	1.54867800	4.75326100	3.80003200
H	-1.90239400	-2.46888200	4.19997500	H	4.31894800	0.10391200	3.91921800
C	-5.03302600	-2.48838600	-0.92001400	H	5.20551100	-0.09883300	2.39528900
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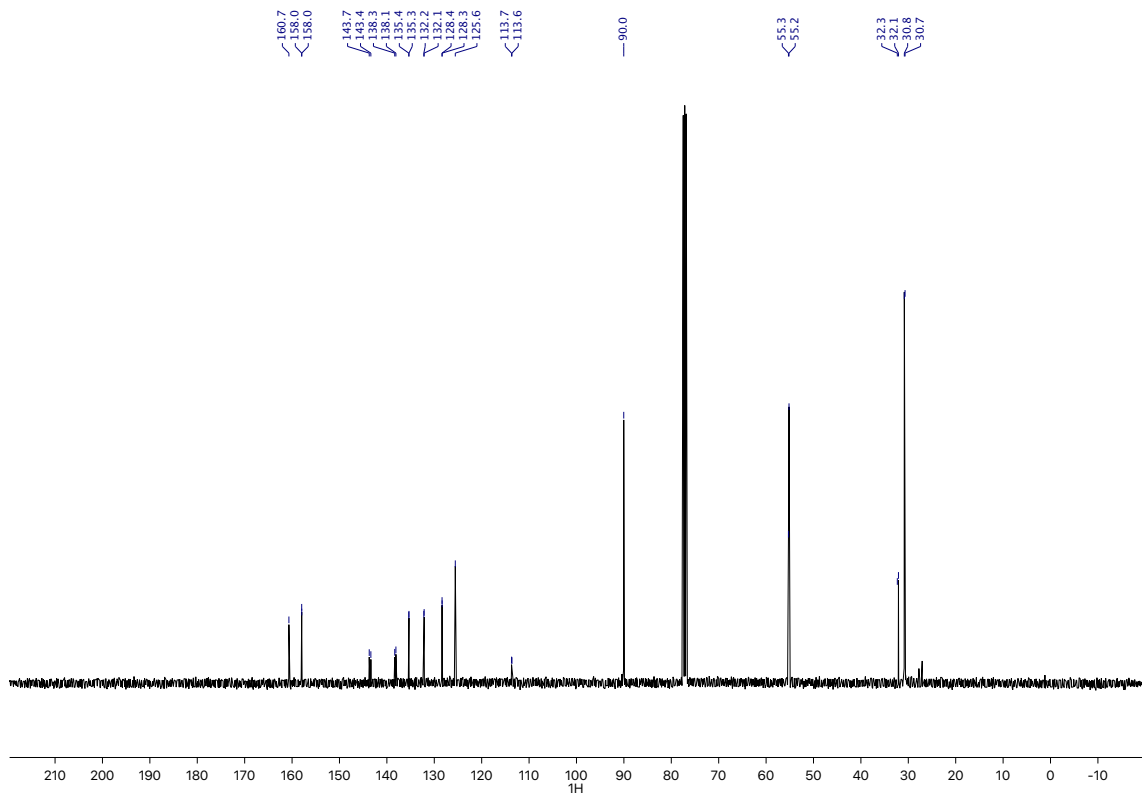
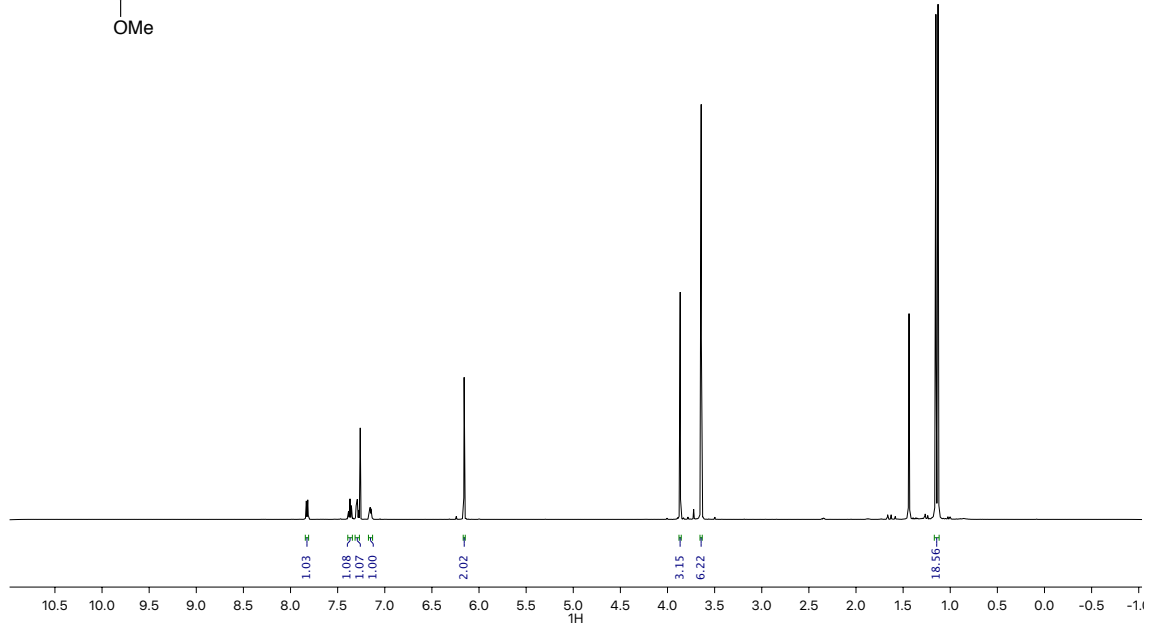
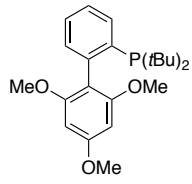
13. NMR Spectra

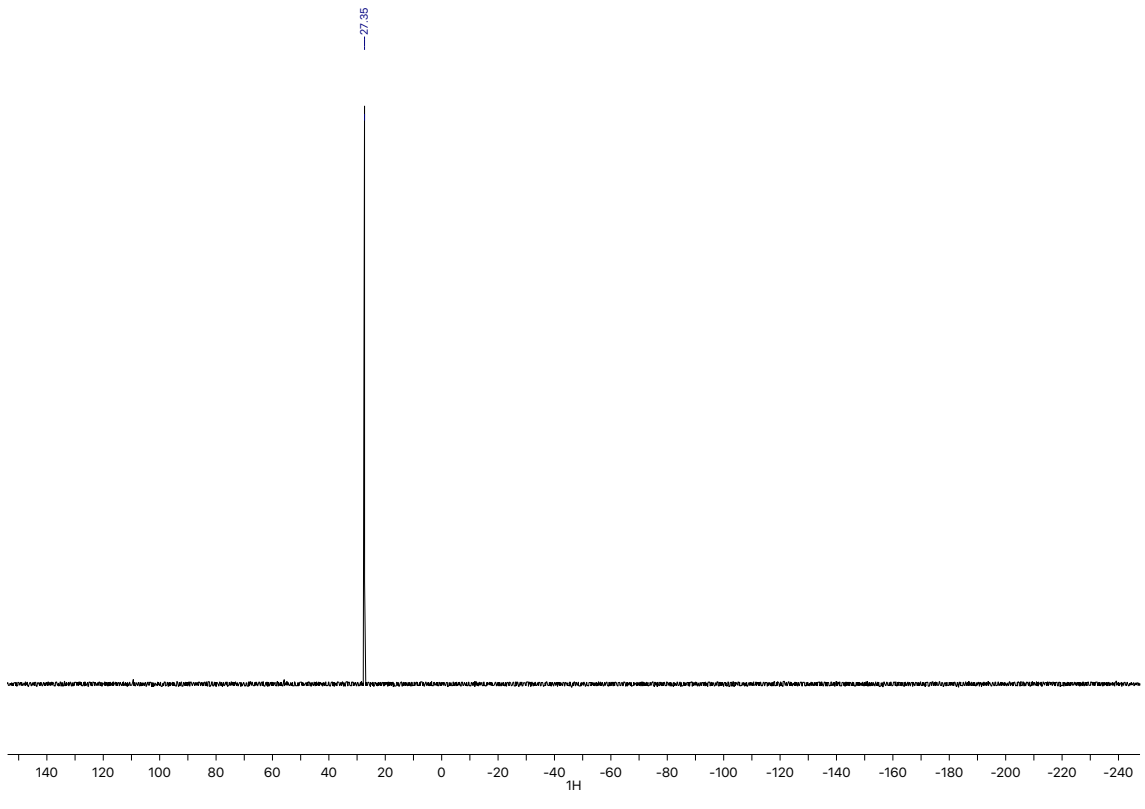
2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl (L1)



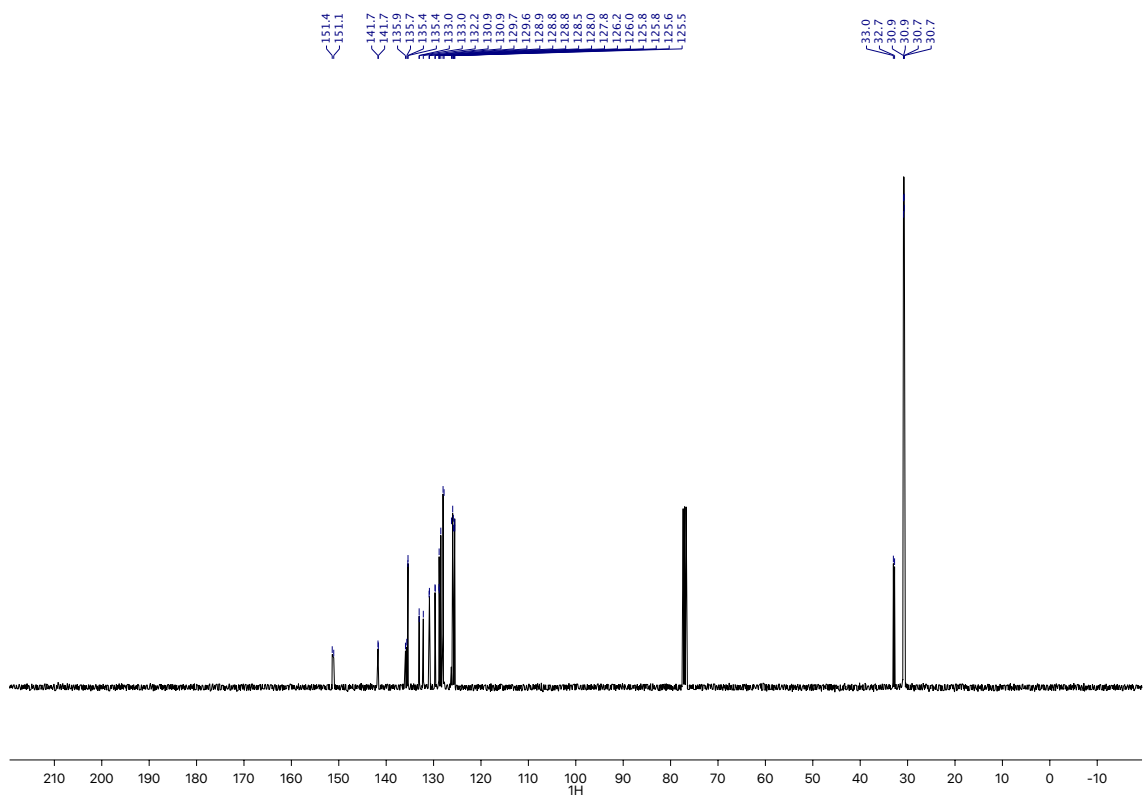
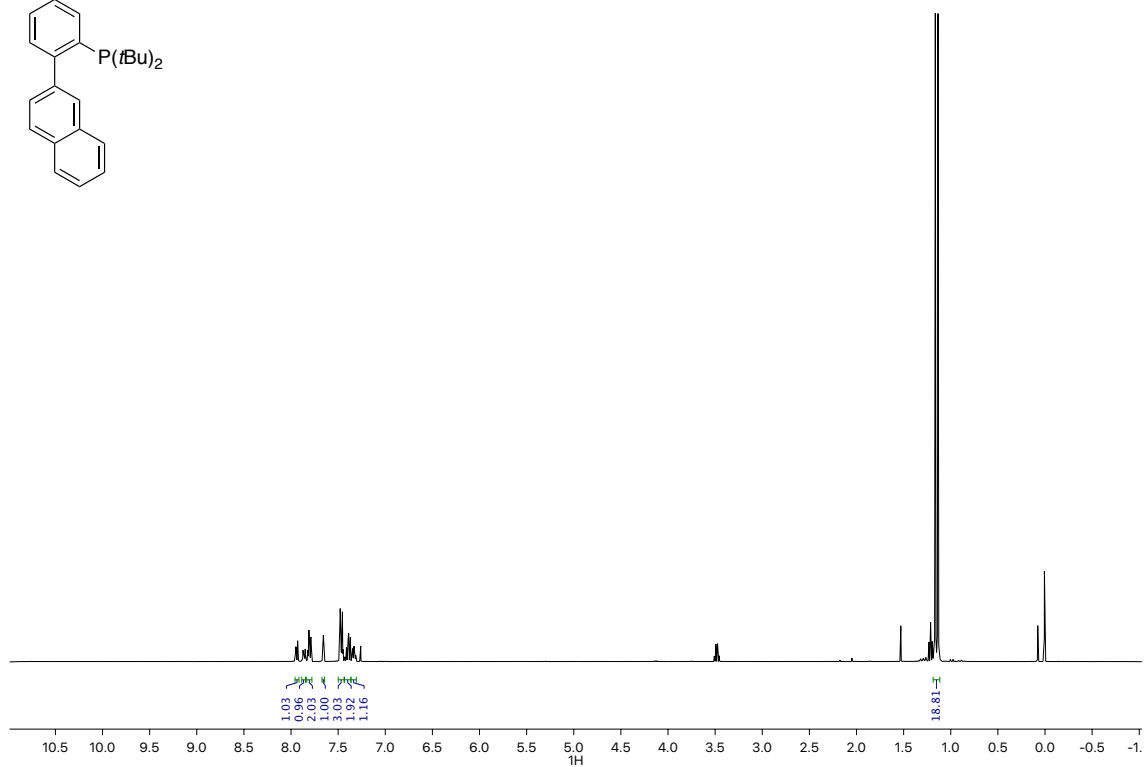
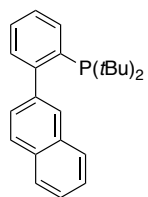


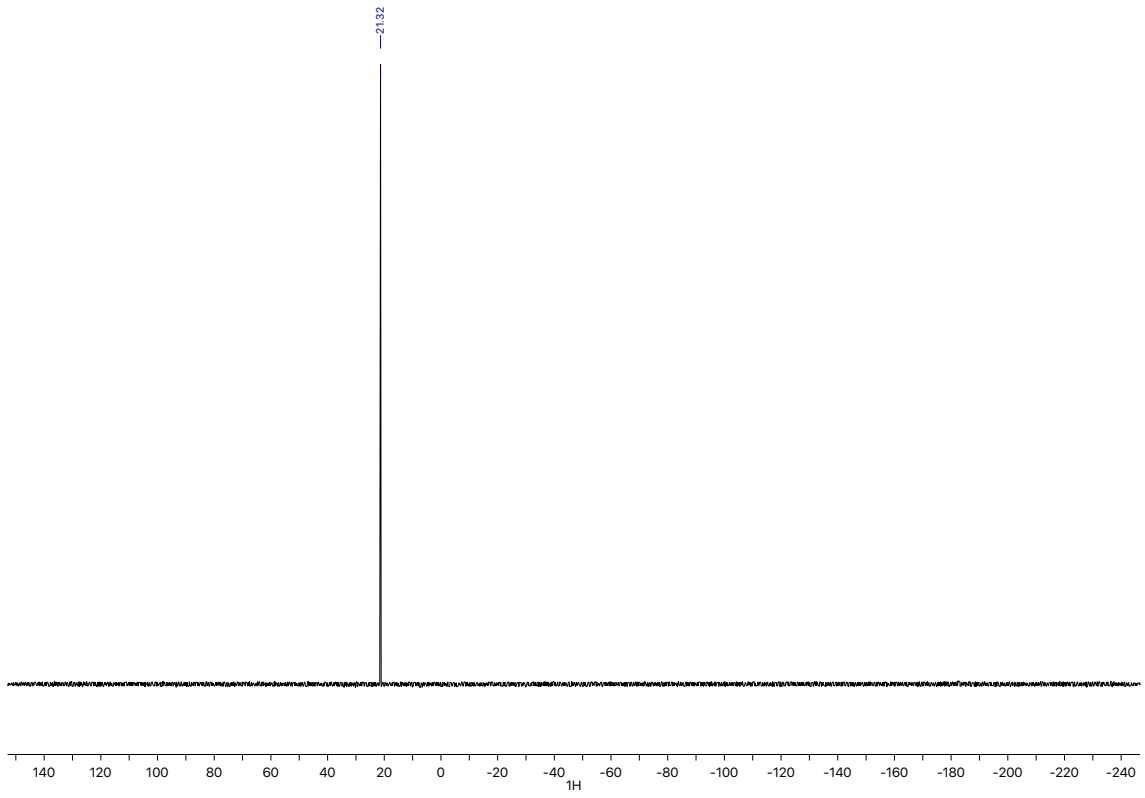
2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl (L2)



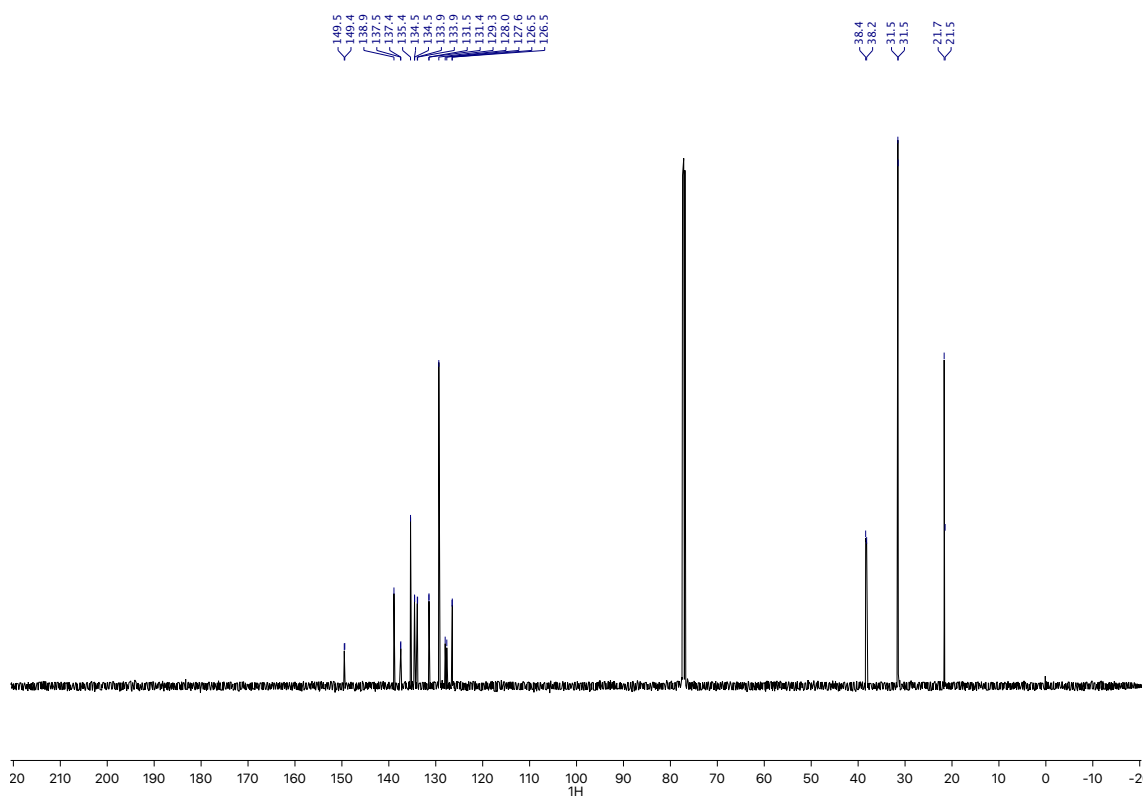
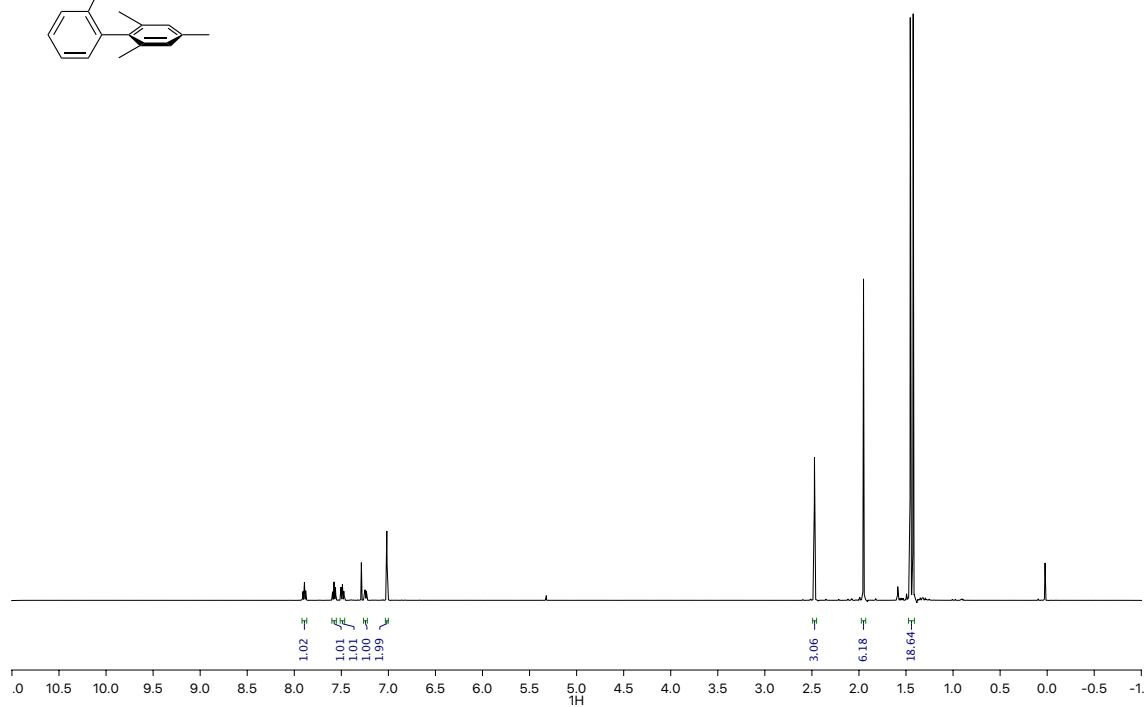
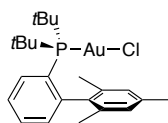


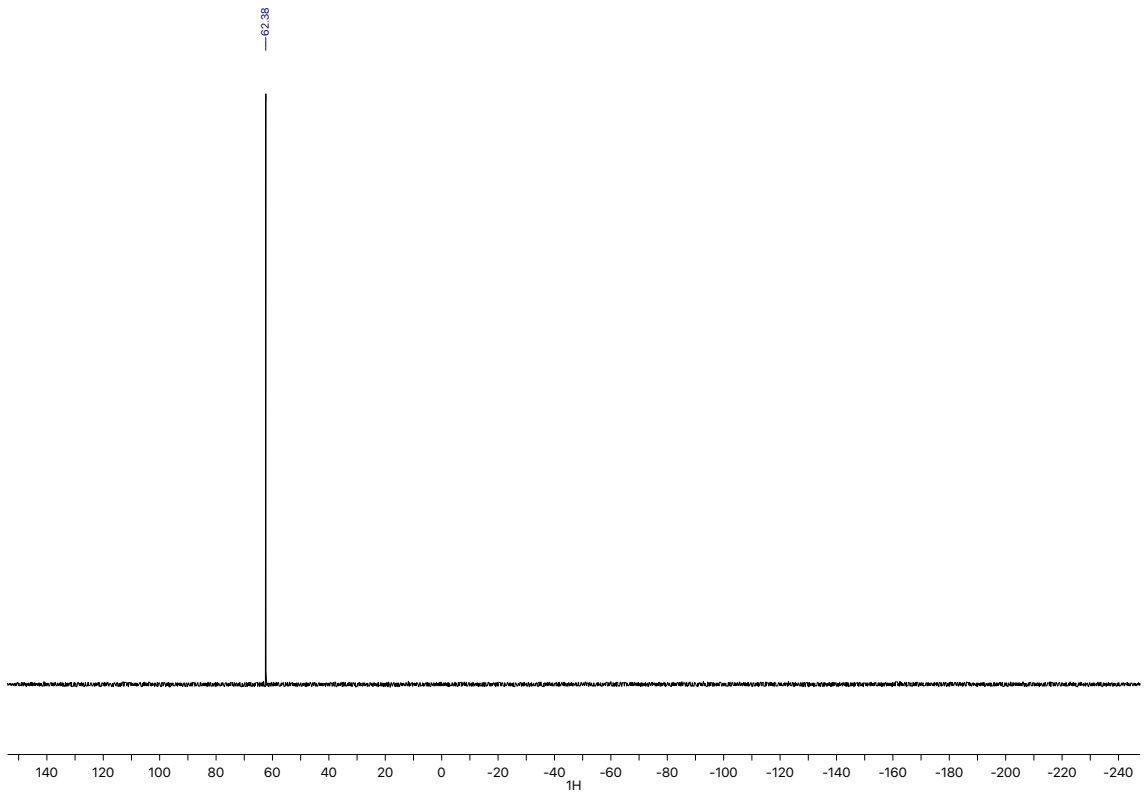
2-Di-*t*-butylphosphino-2-naphthyl (L3)



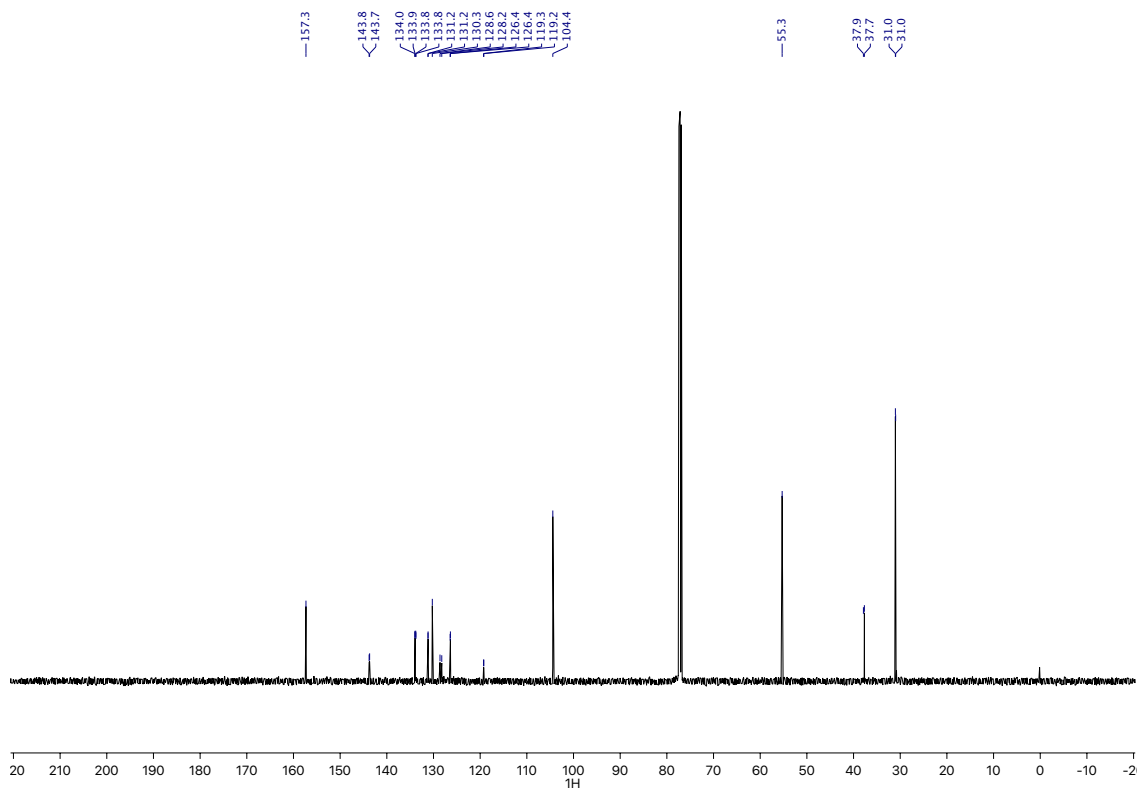
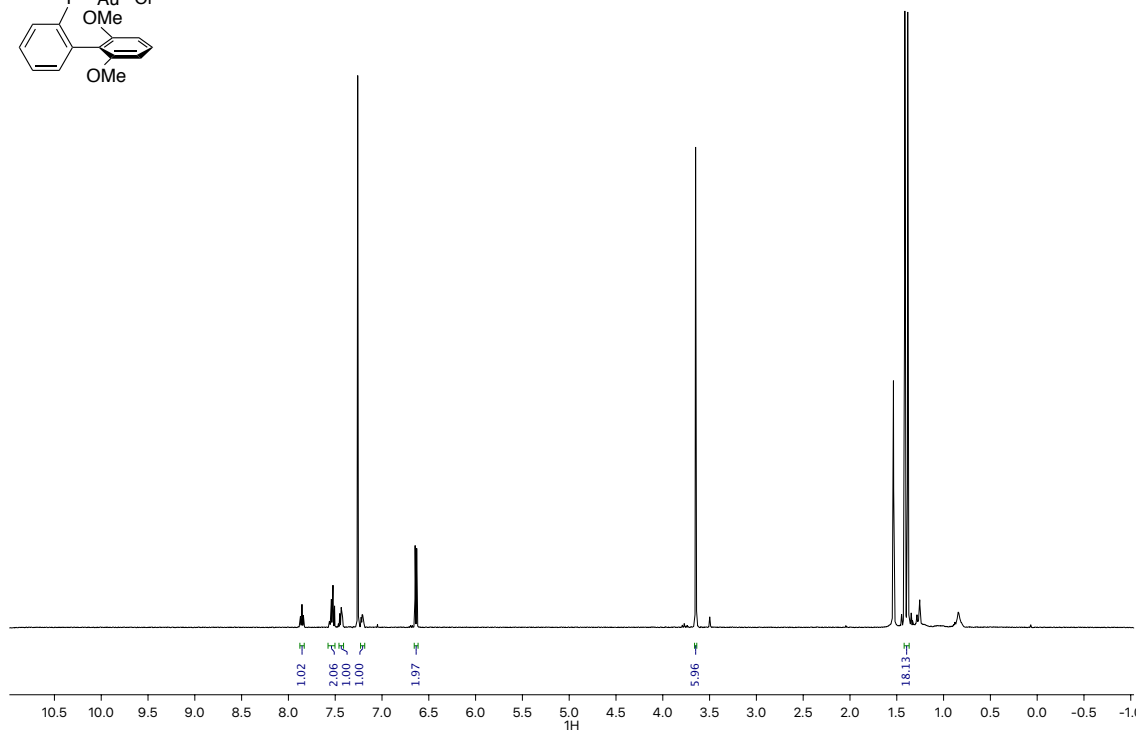
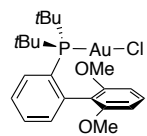


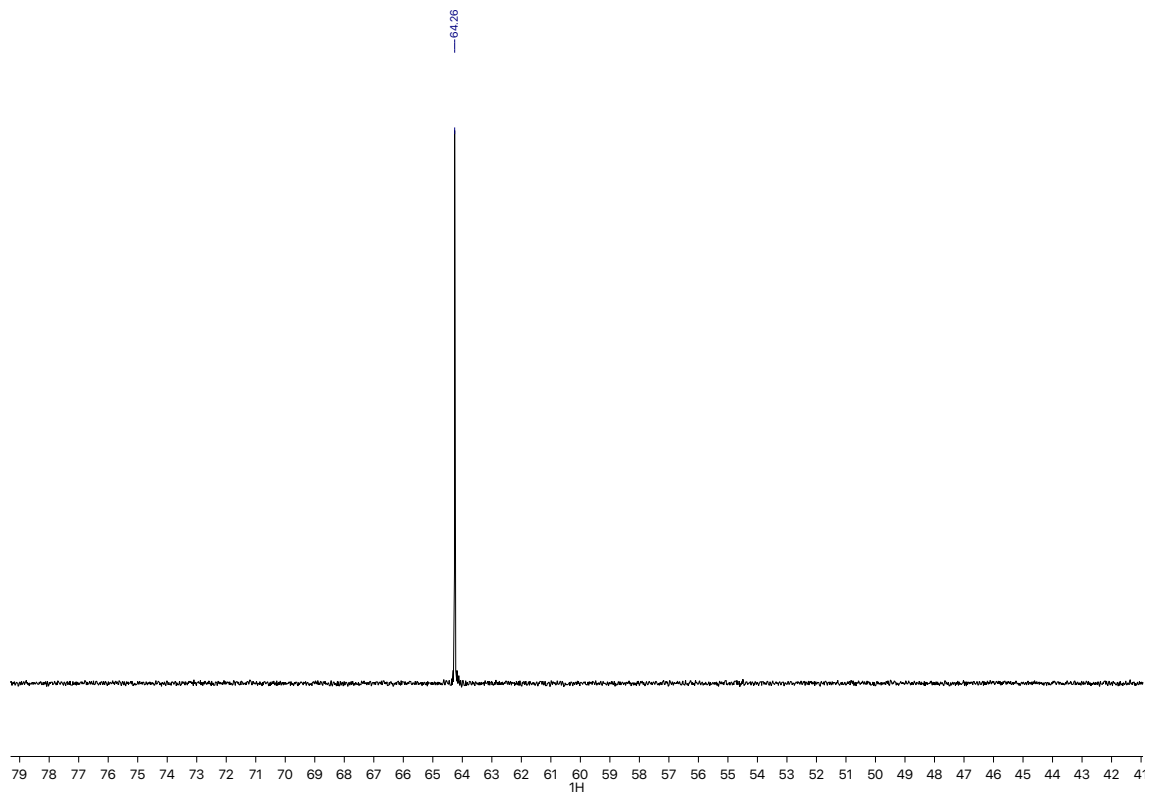
2-Di-*t*-butylphosphino-2',4,6'-trimethylbiphenyl gold(I) chloride (6b)



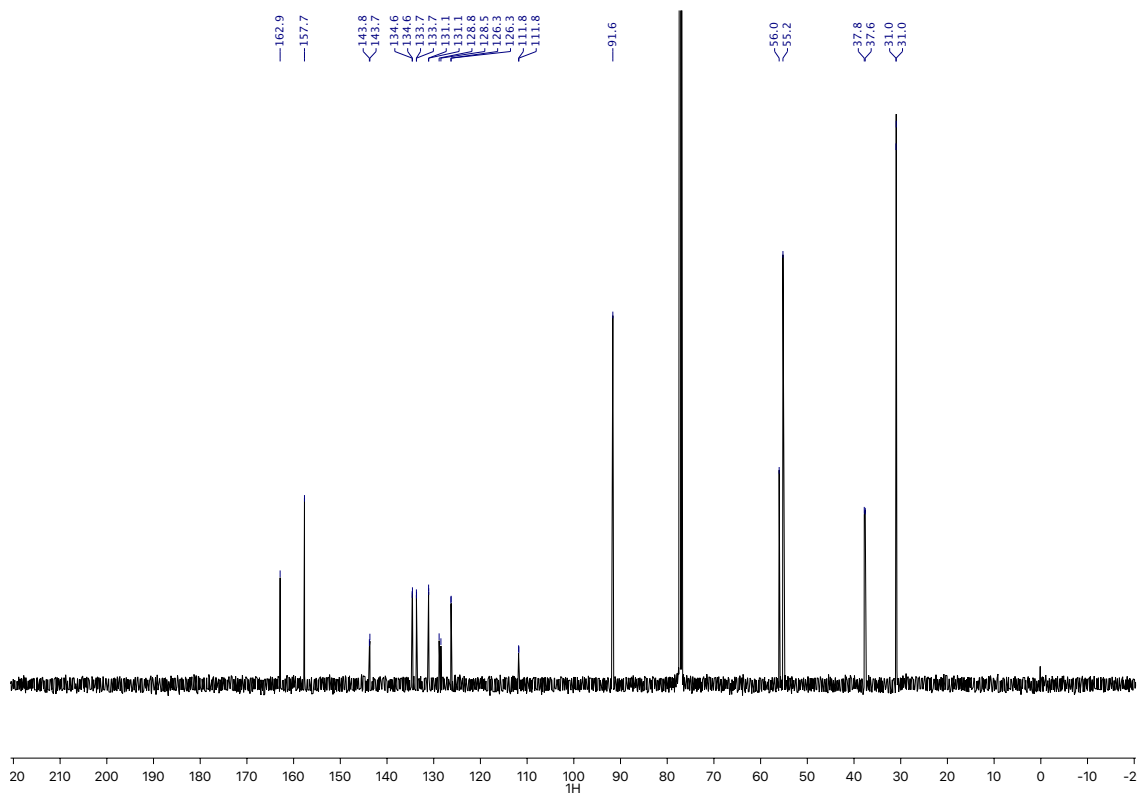
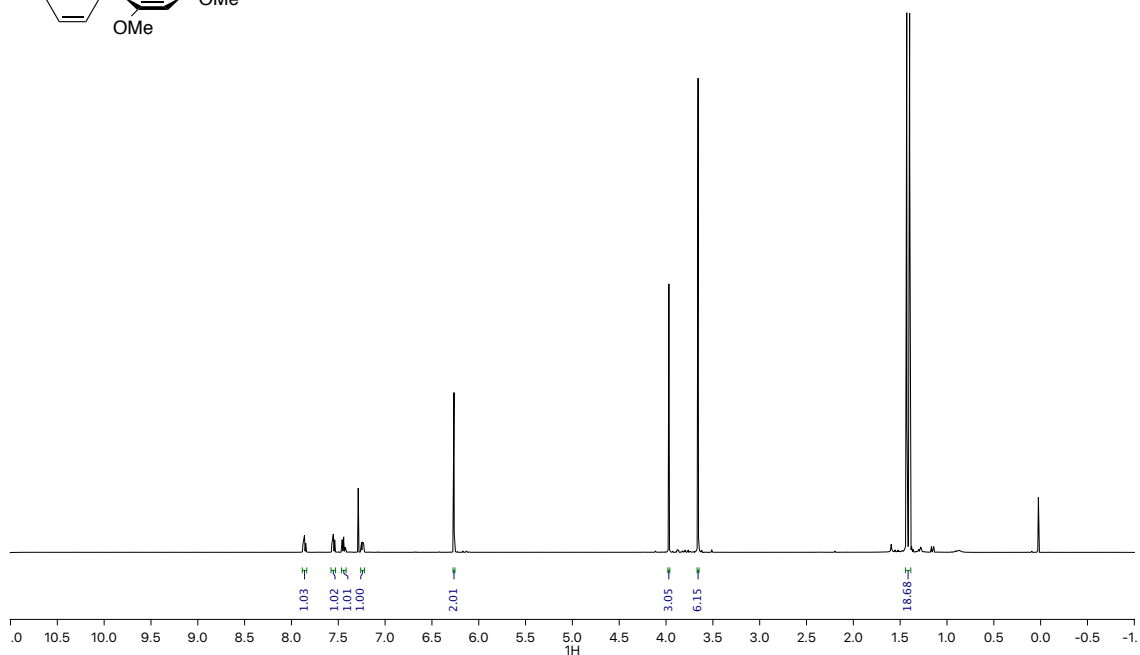
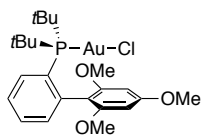


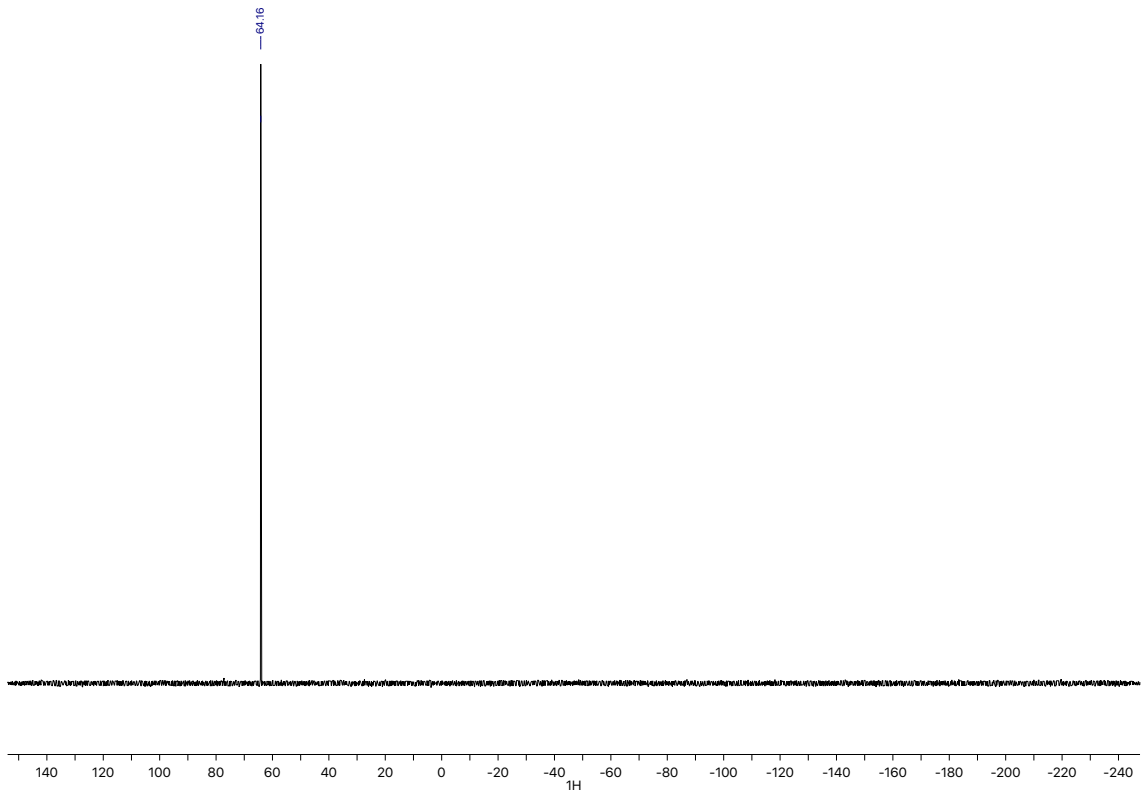
2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl gold(I) chloride (6c)



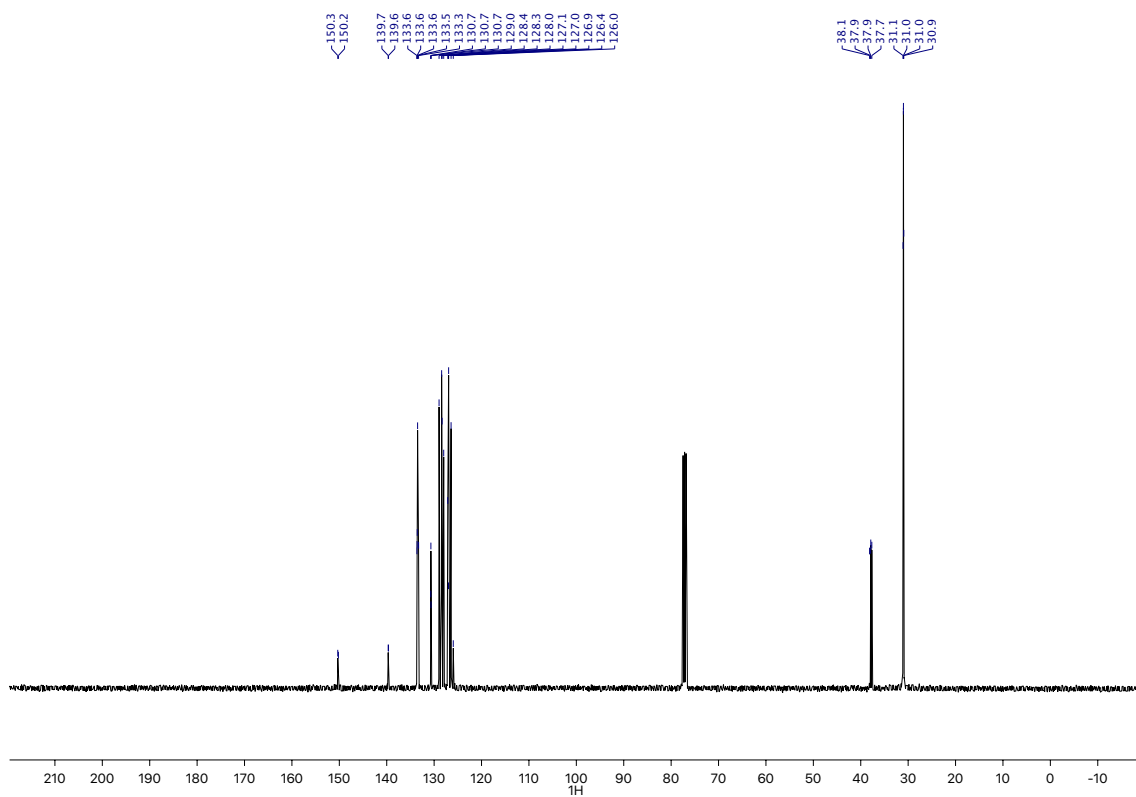
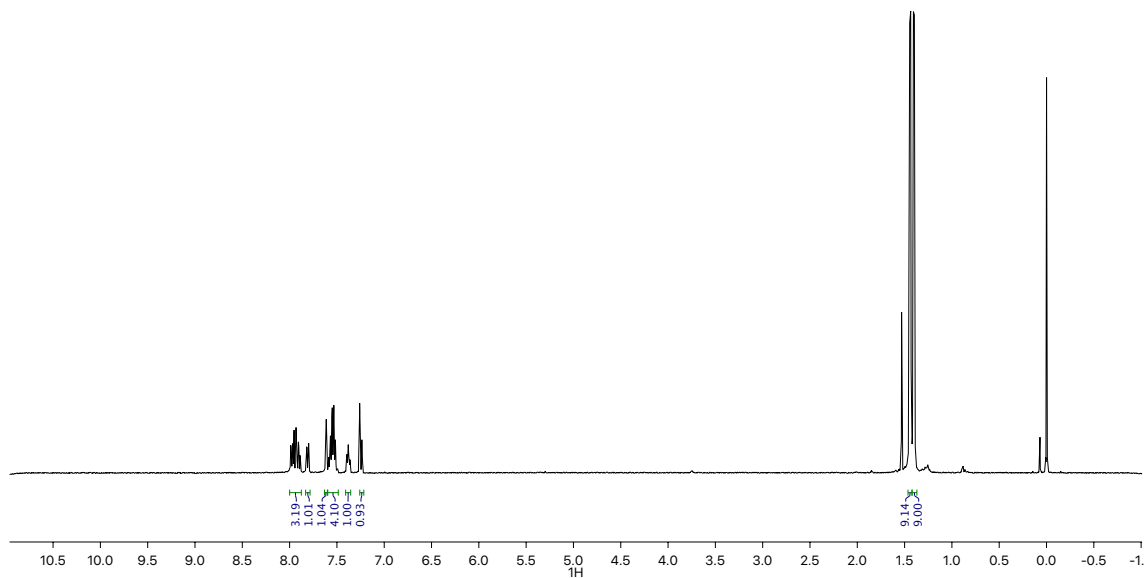
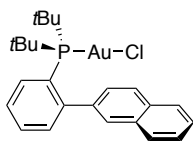


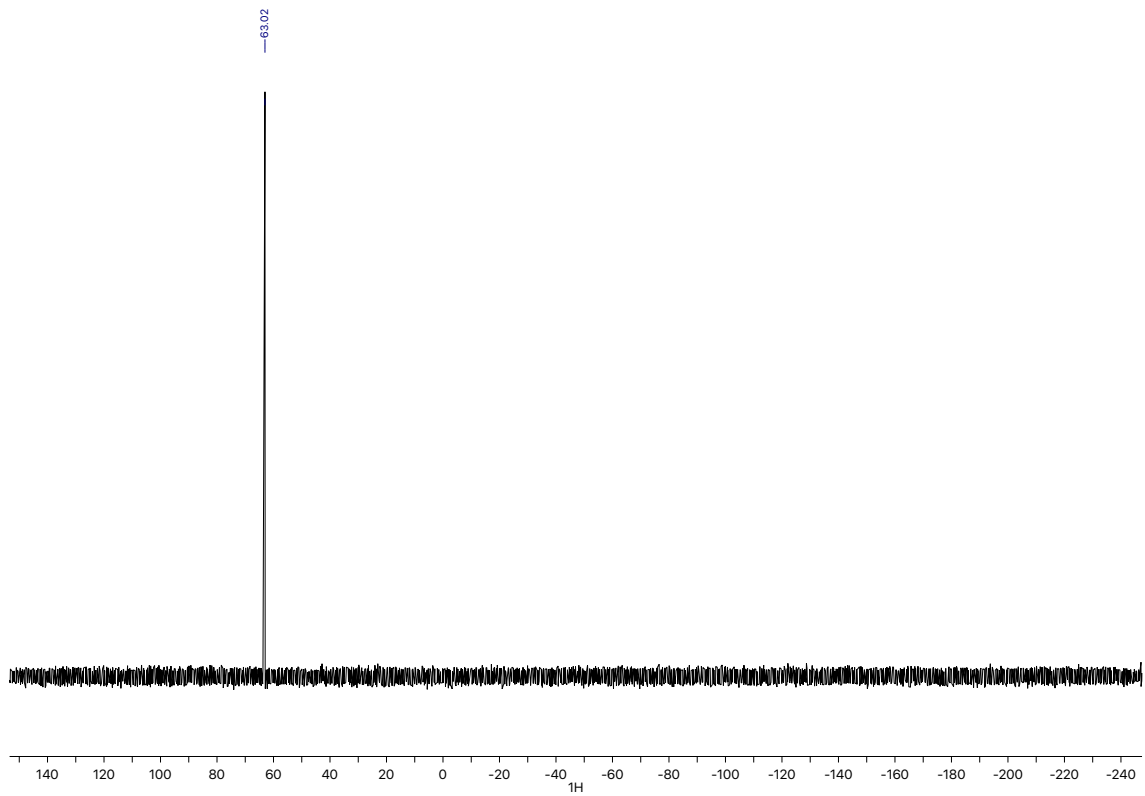
2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl gold(I) chloride (6d)



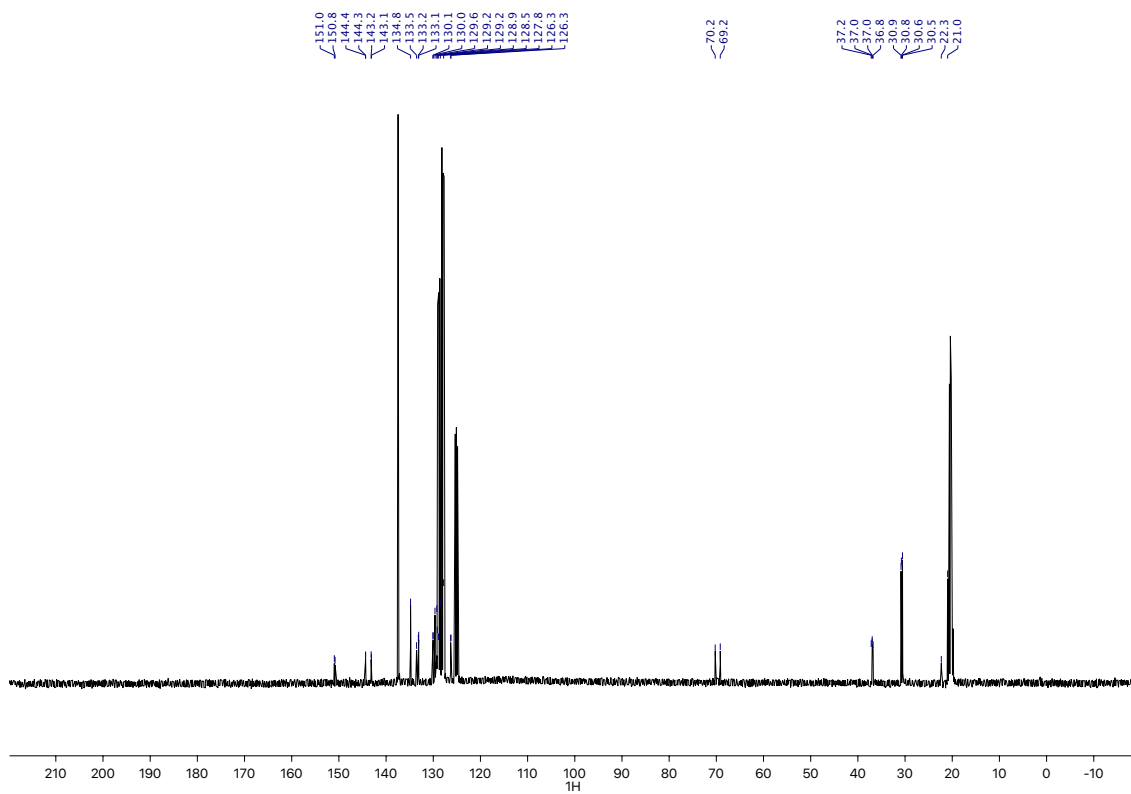
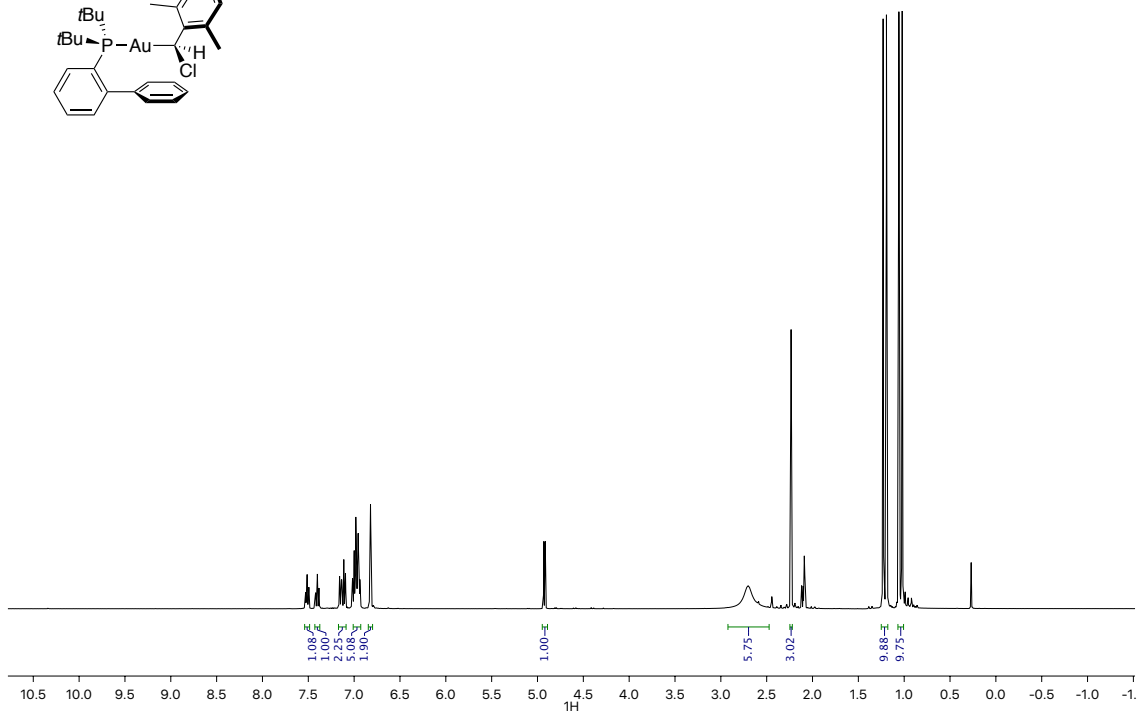
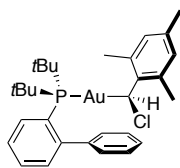


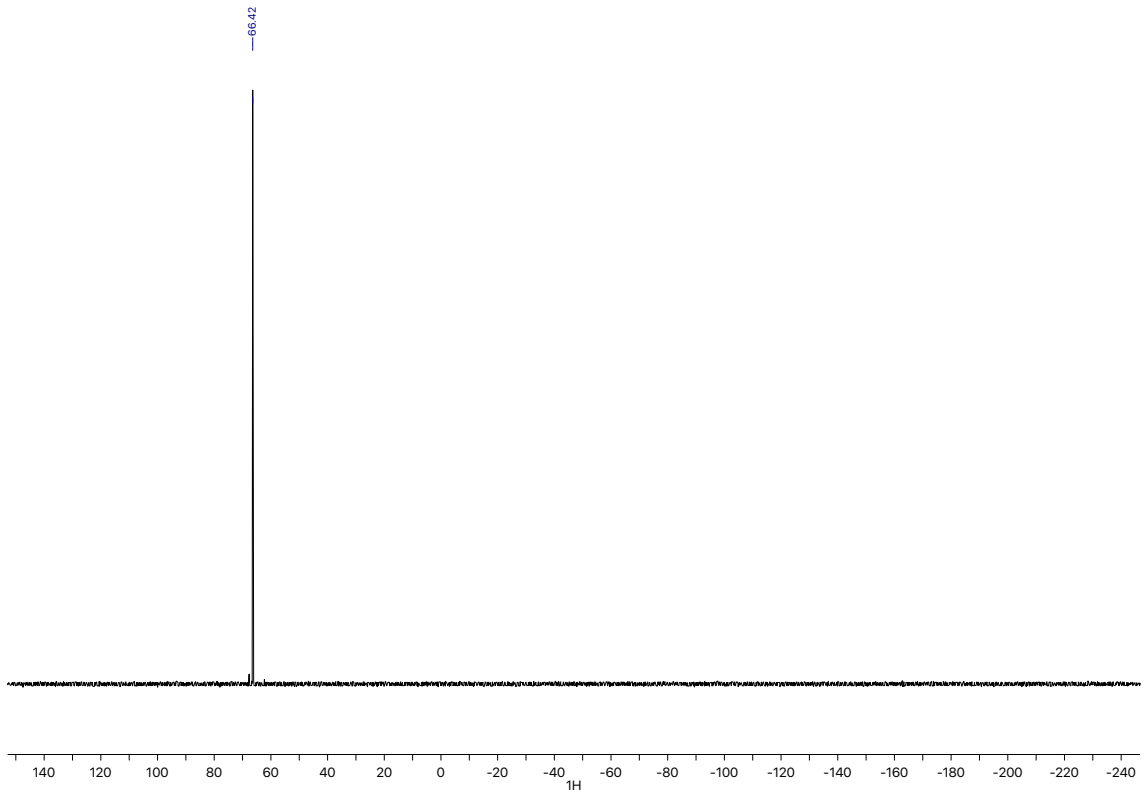
2-Di-*t*-butylphosphino-2-naphthyl gold(I) chloride (6e)



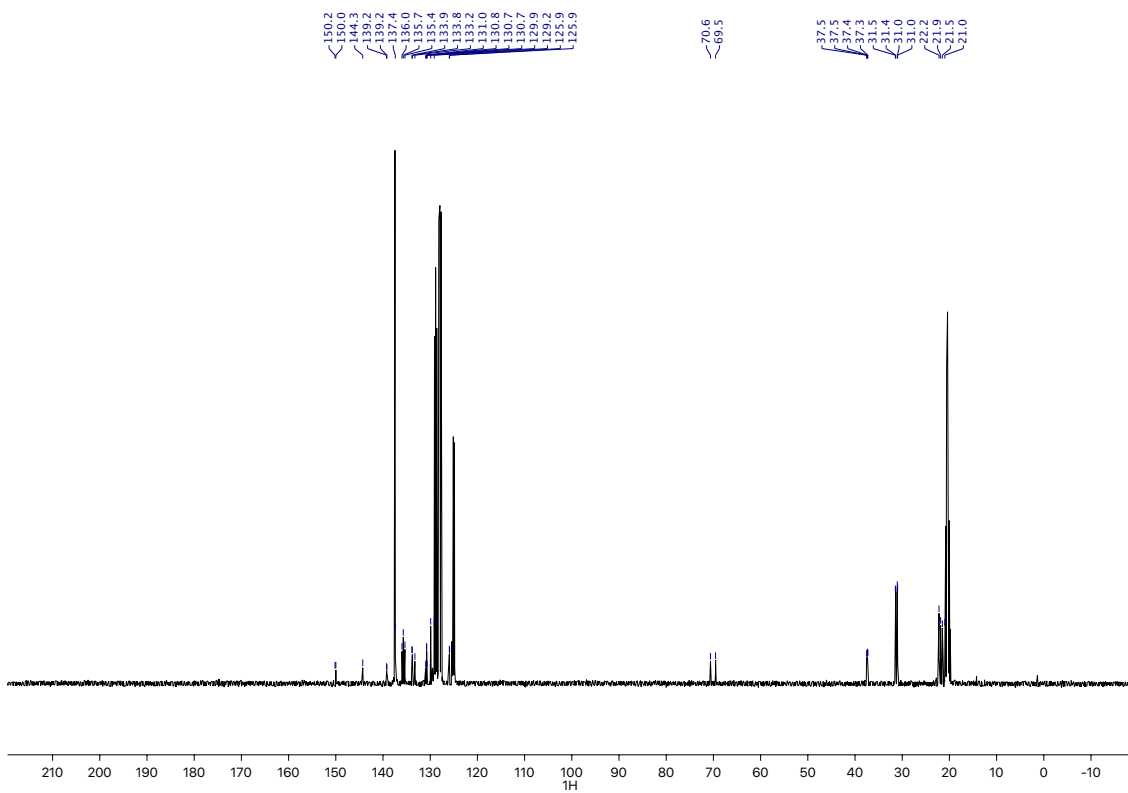
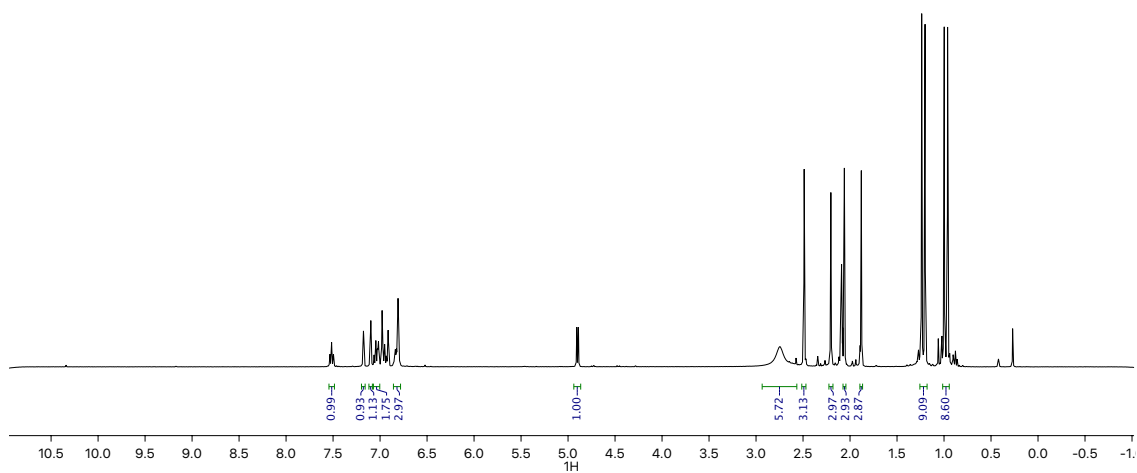
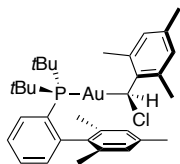


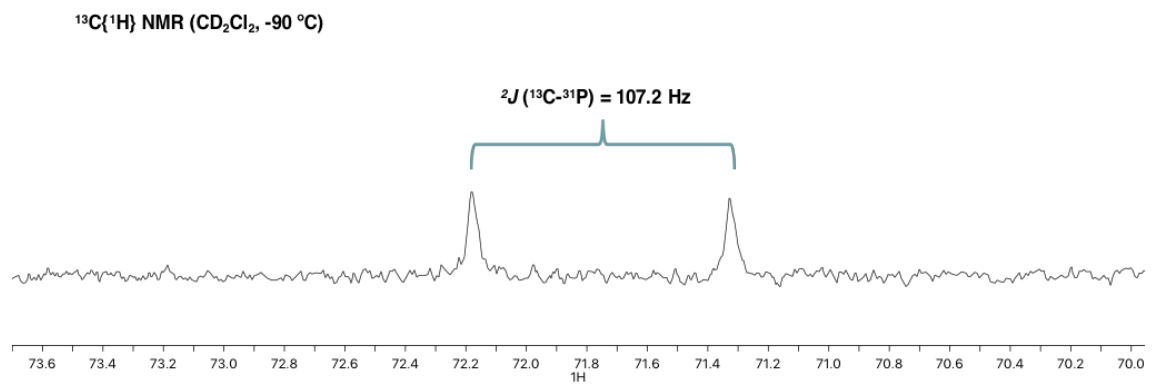
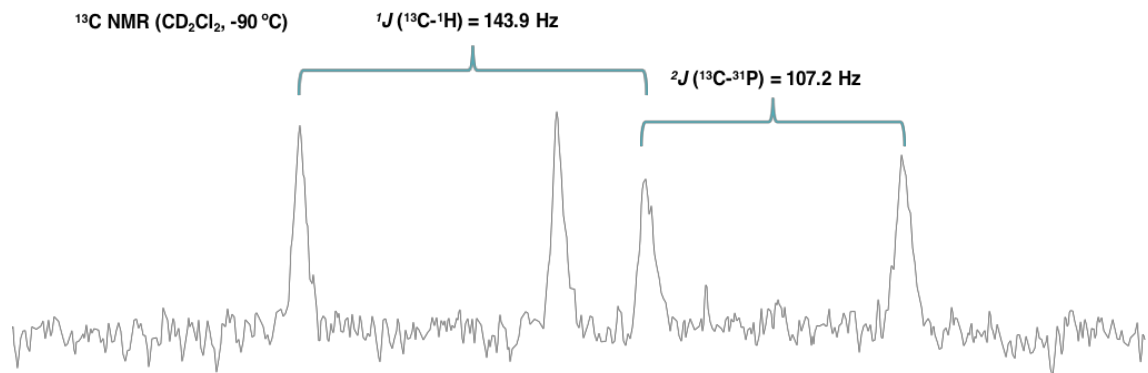
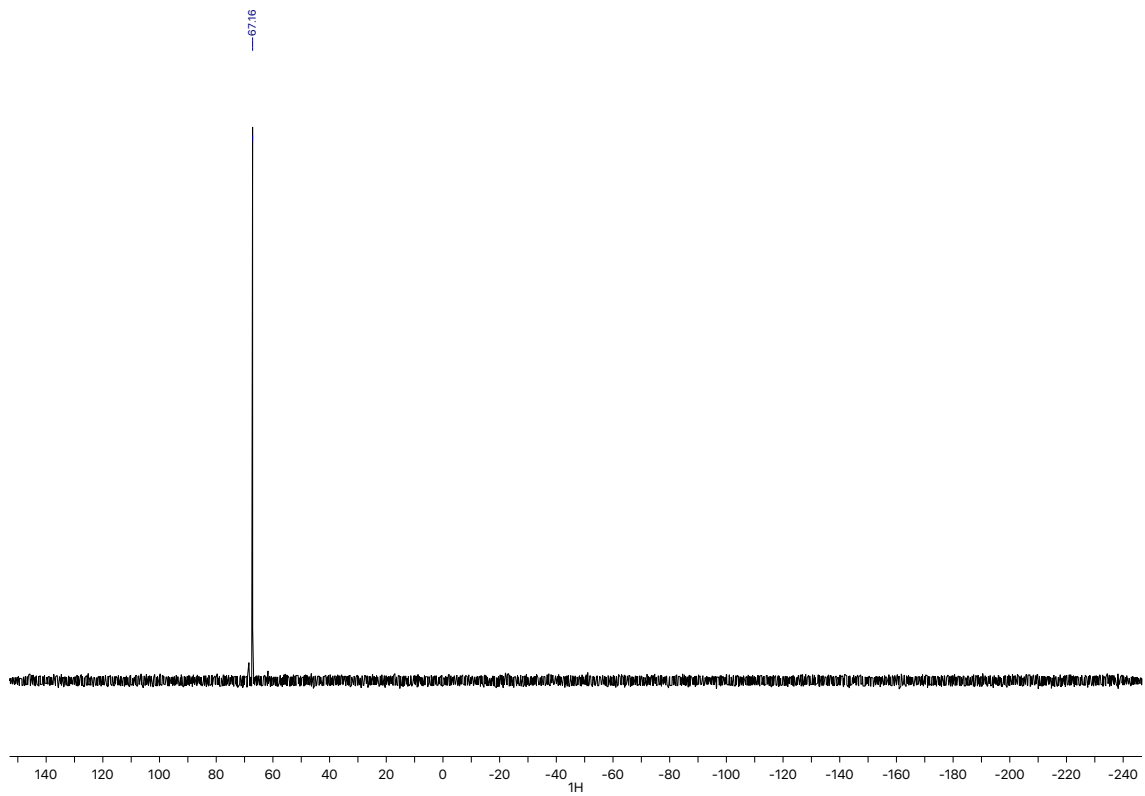
2-Di-*t*-butylphosphinobiphenyl chloromesityl(methyl) gold(I) carbenoid (1a)



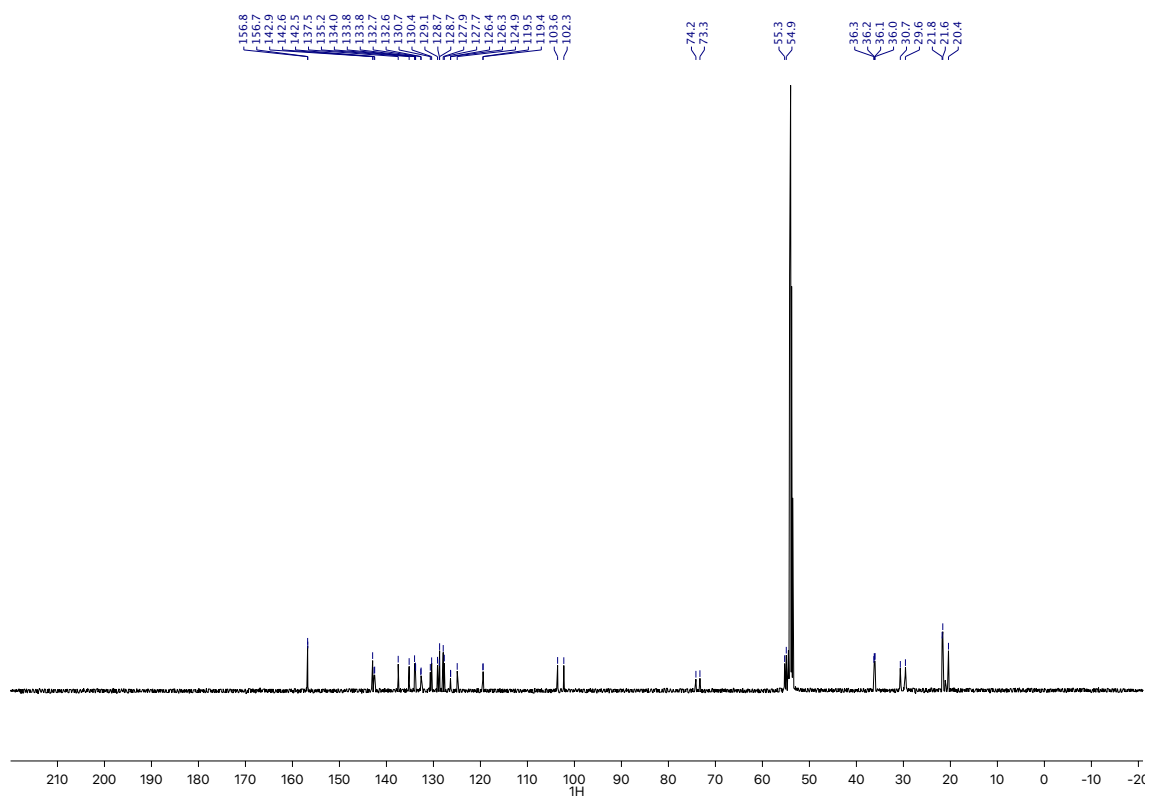
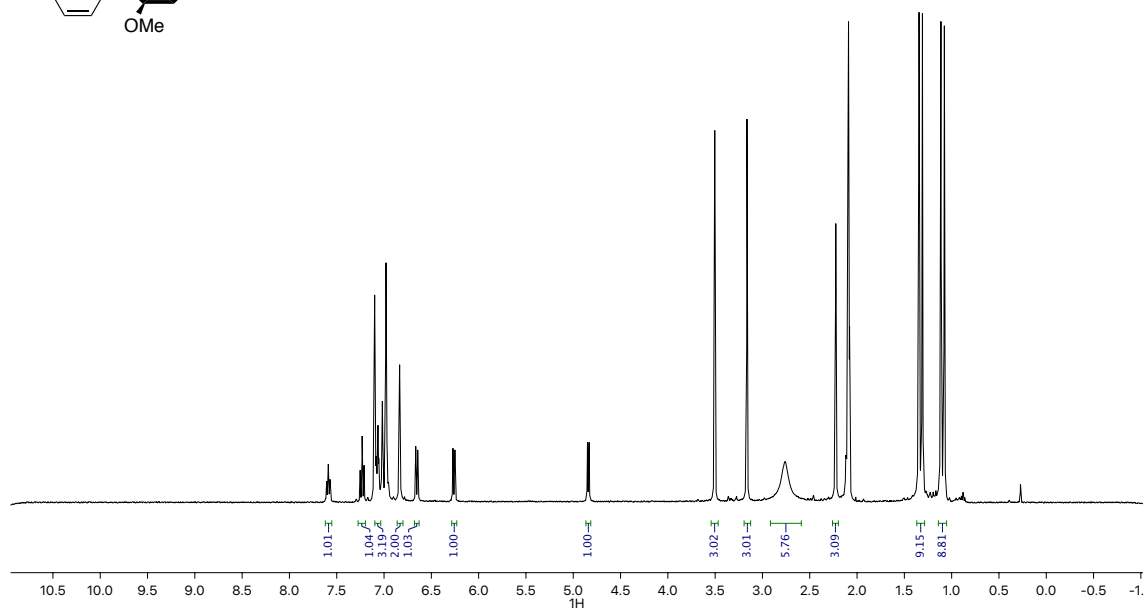
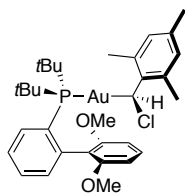


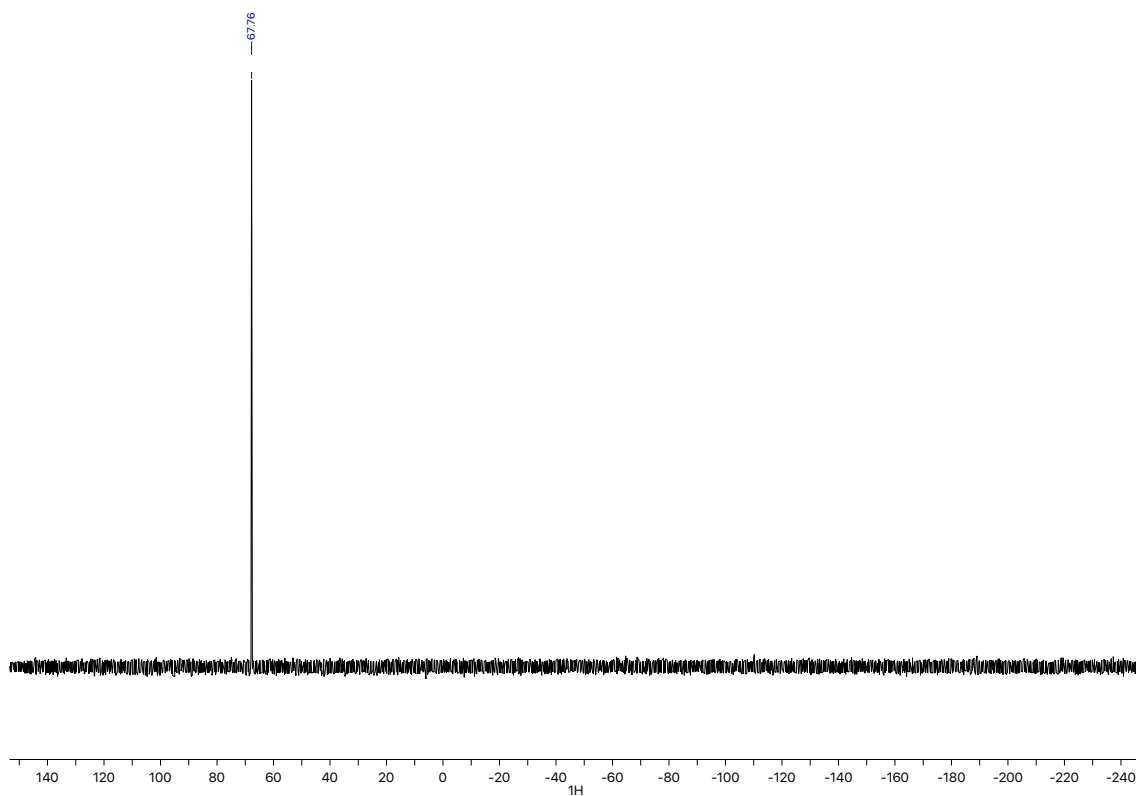
2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl chloromesityl(methyl) gold(I) carbenoid (1b)





2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (1c)

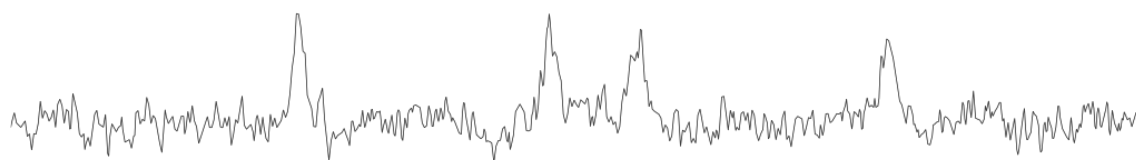




13C NMR (CD₂Cl₂, -90 °C)

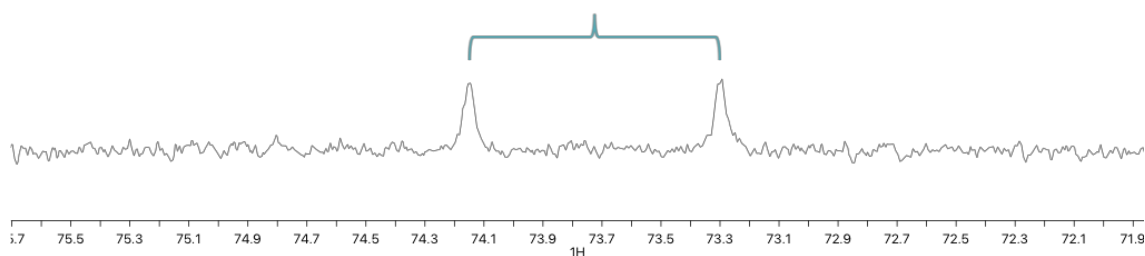
$^1J(^{13}\text{C}-^1\text{H}) = 144.3 \text{ Hz}$

$^2J(^{13}\text{C}-^{31}\text{P}) = 107.4 \text{ Hz}$

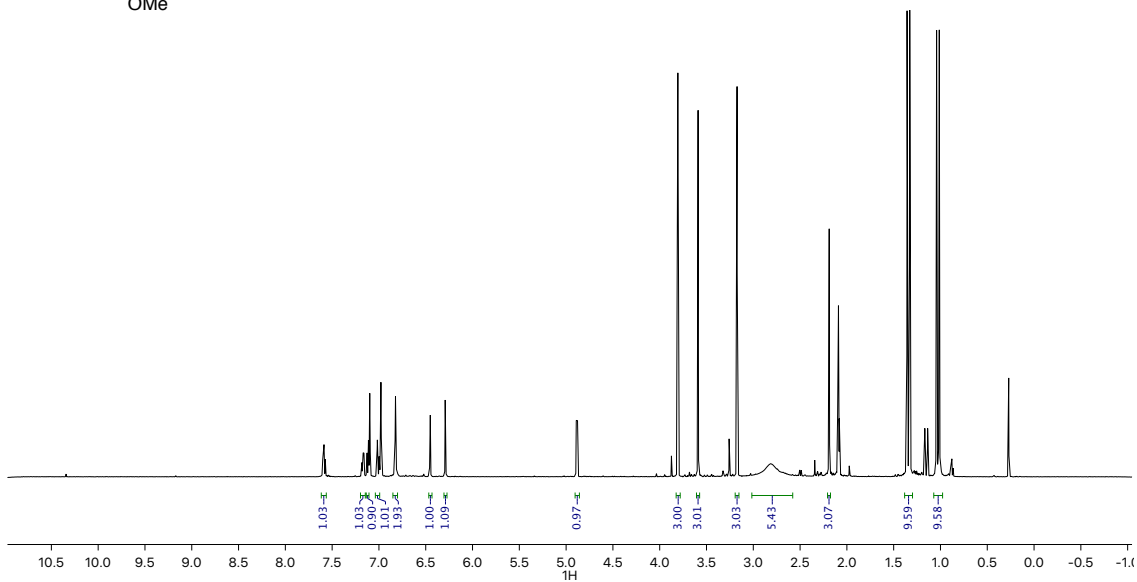
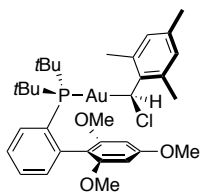


13C{¹H} NMR (CD₂Cl₂, -90 °C)

$^2J(^{13}\text{C}-^{31}\text{P}) = 107.4 \text{ Hz}$

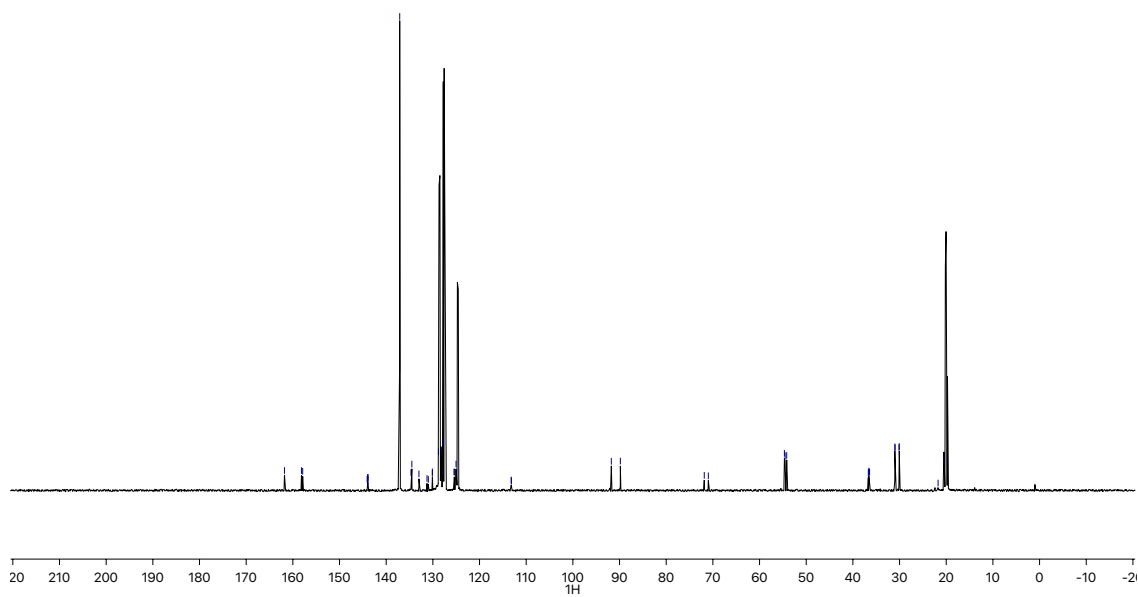


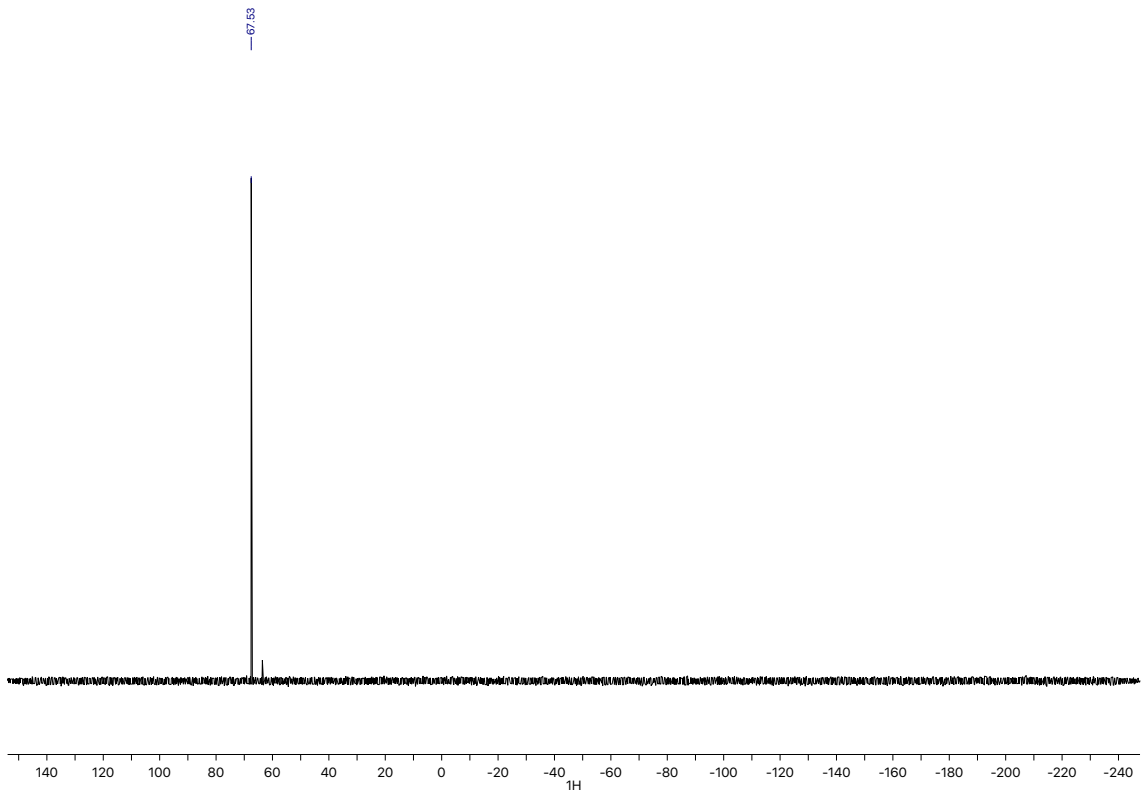
2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl chloromesityl(methyl) gold(I) carbenoid (1d)



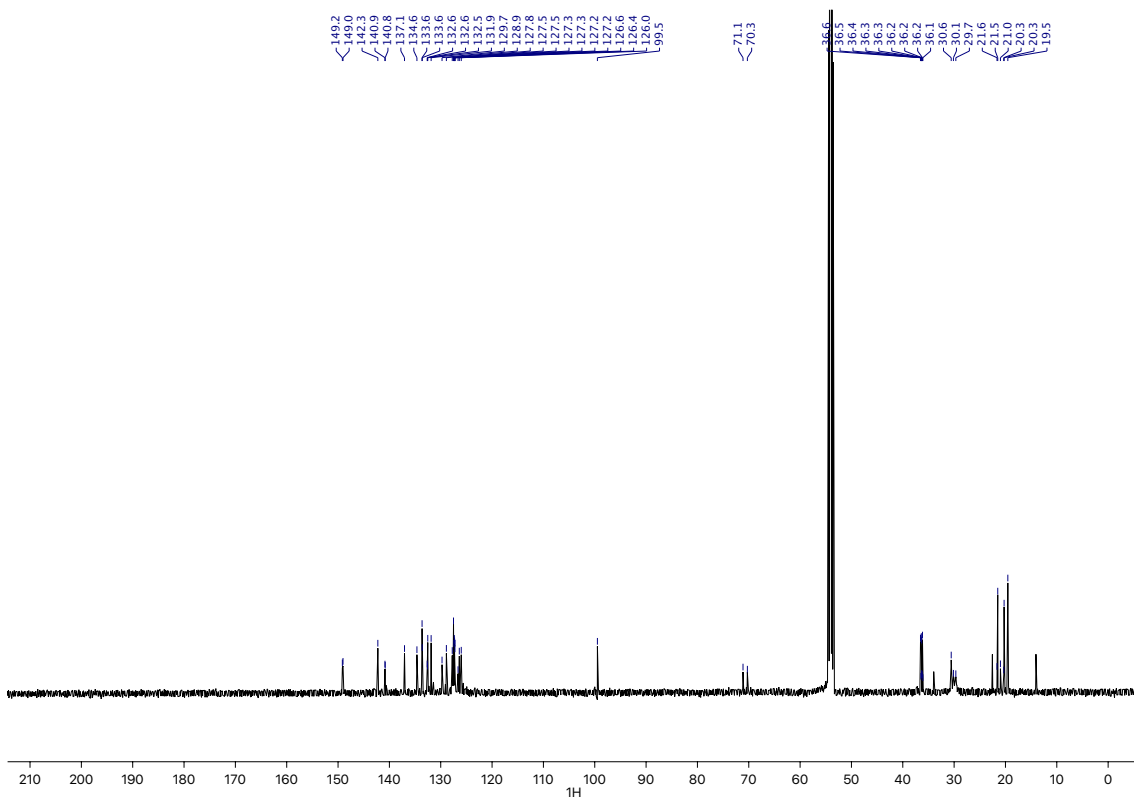
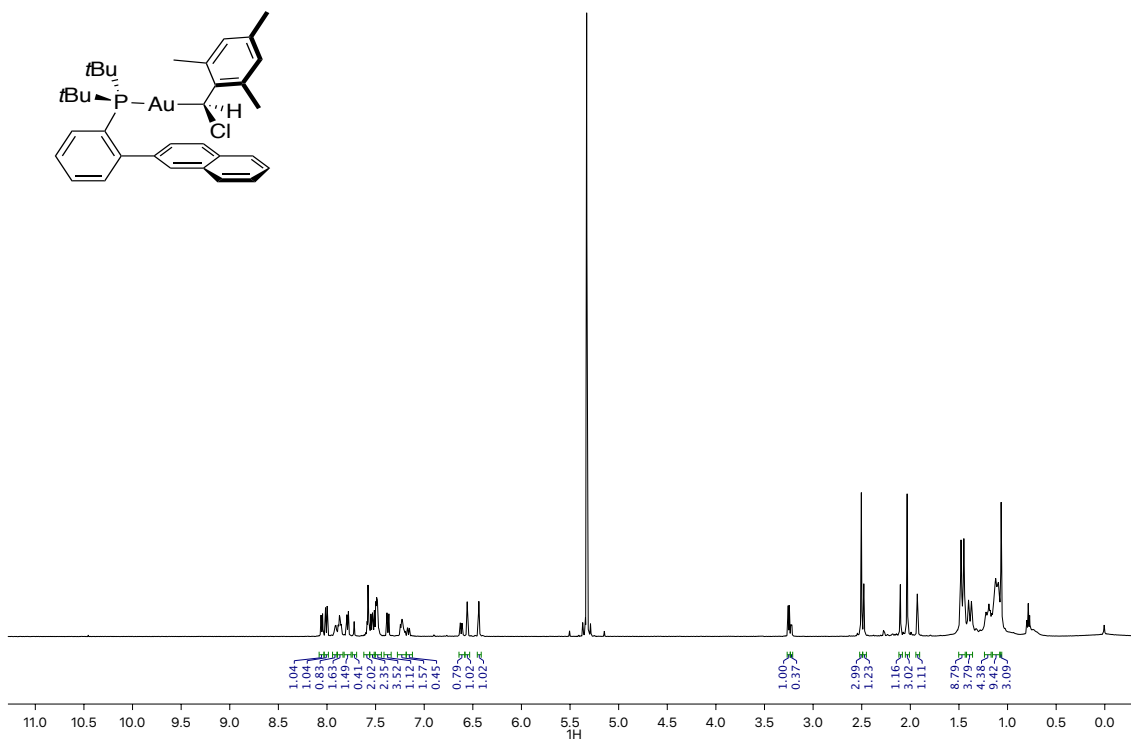
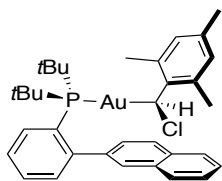
Chemical shifts (ppm) for the ¹H NMR spectrum:

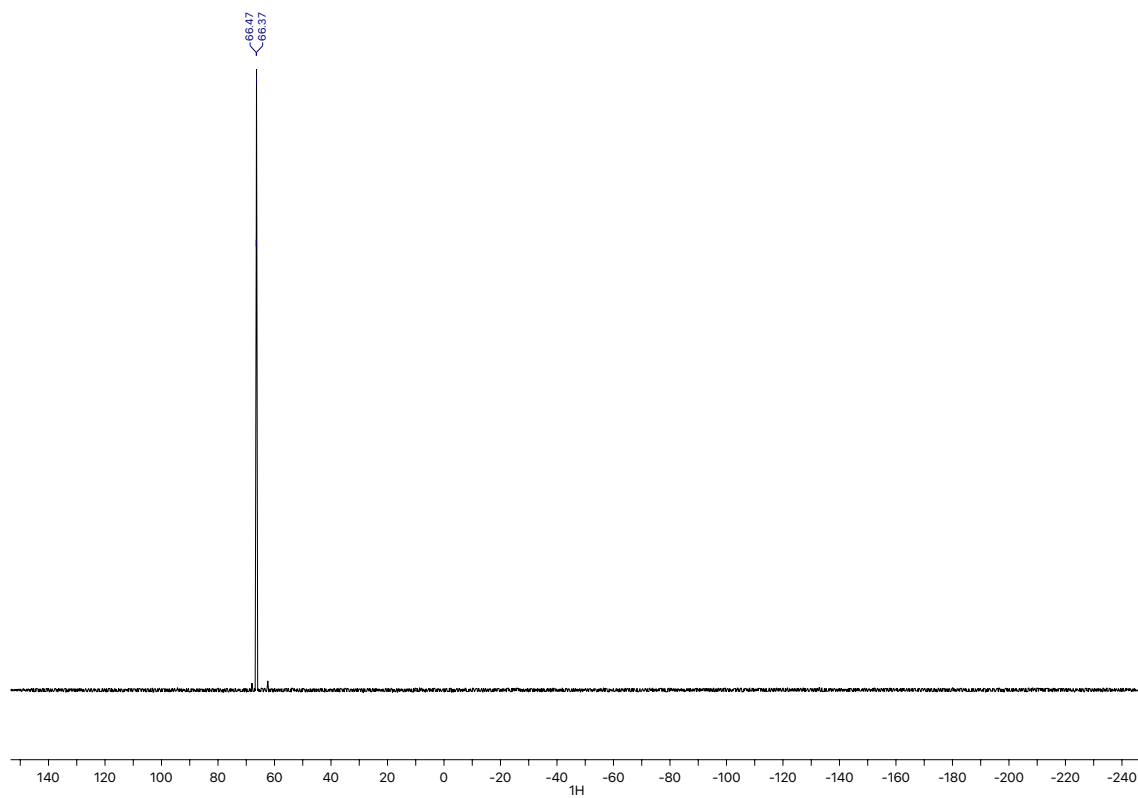
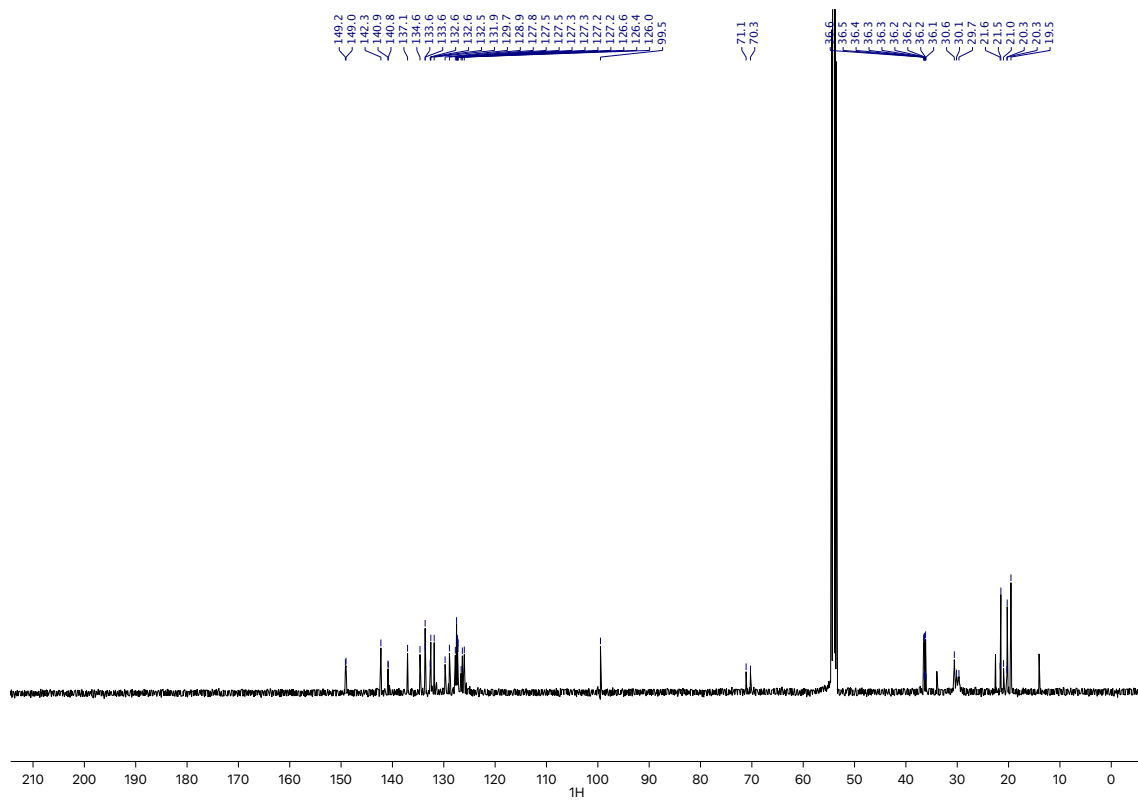
- 161.8
- 159.2
- 157.9
- 144.1
- 143.9
- 143.9
- 143.9
- 137.1
- 134.5
- 133.0
- 131.3
- 131.0
- 130.1
- 128.8
- 127.9
- 125.4
- 125.4
- 113.2
- 113.2
- 81.8
- 80.8
- 71.8
- 71.0
- 54.7
- 54.5
- 54.2
- 36.7
- 36.6
- 36.5
- 36.4
- 31.0
- 30.7
- 30.1
- 30.1
- 21.7
- 20.6





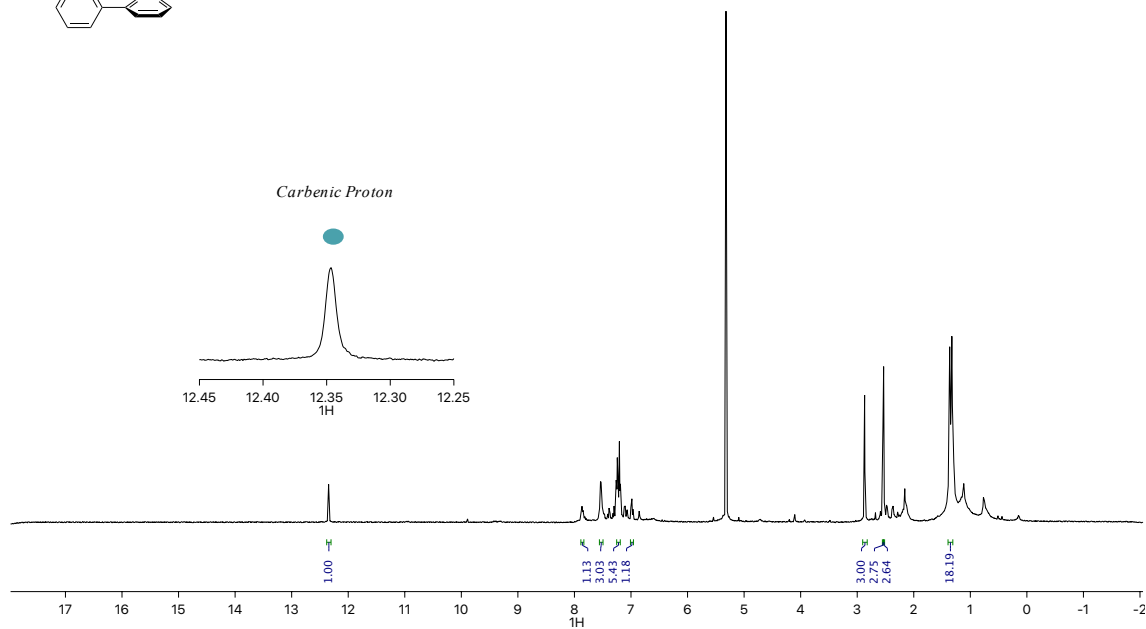
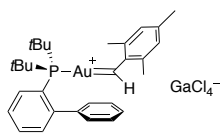
2-Di-*t*-butylphosphino-2-naphthyl chloromesityl(methyl) gold(I) carbenoid (1e)



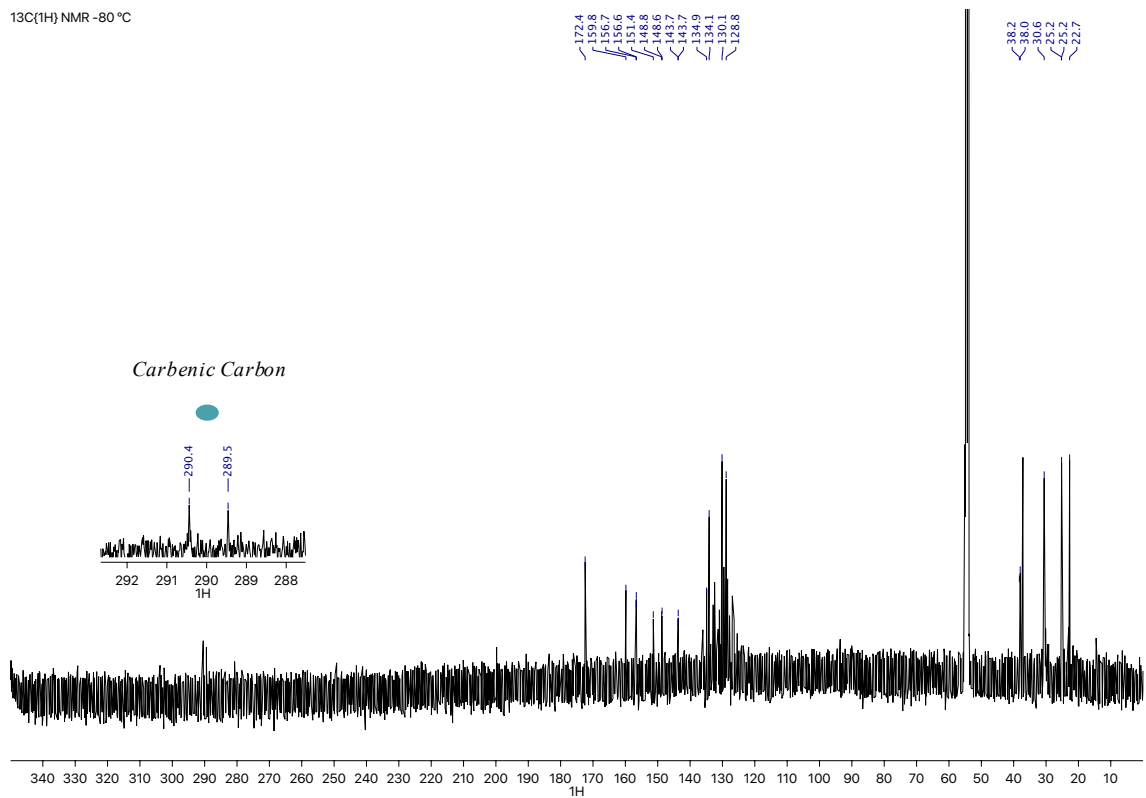


2-Di-*t*-butylphosphinobiphenyl mesityl(methyl) gold(I) carbene (5a)

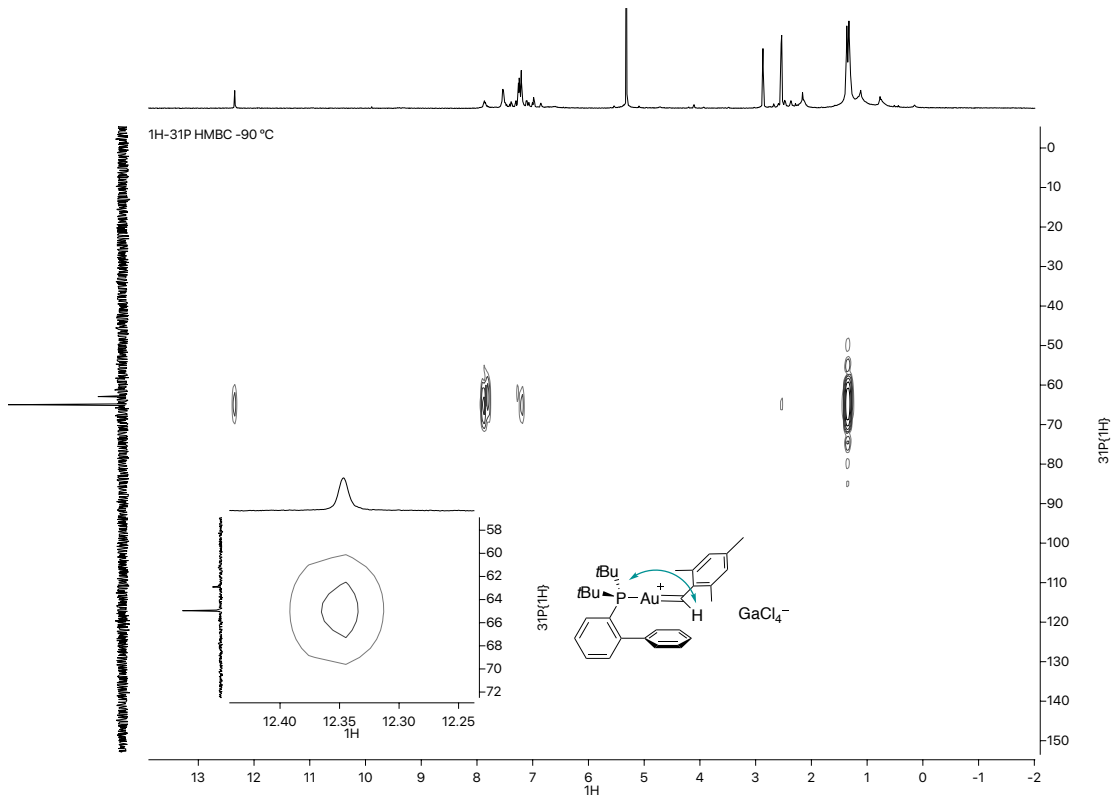
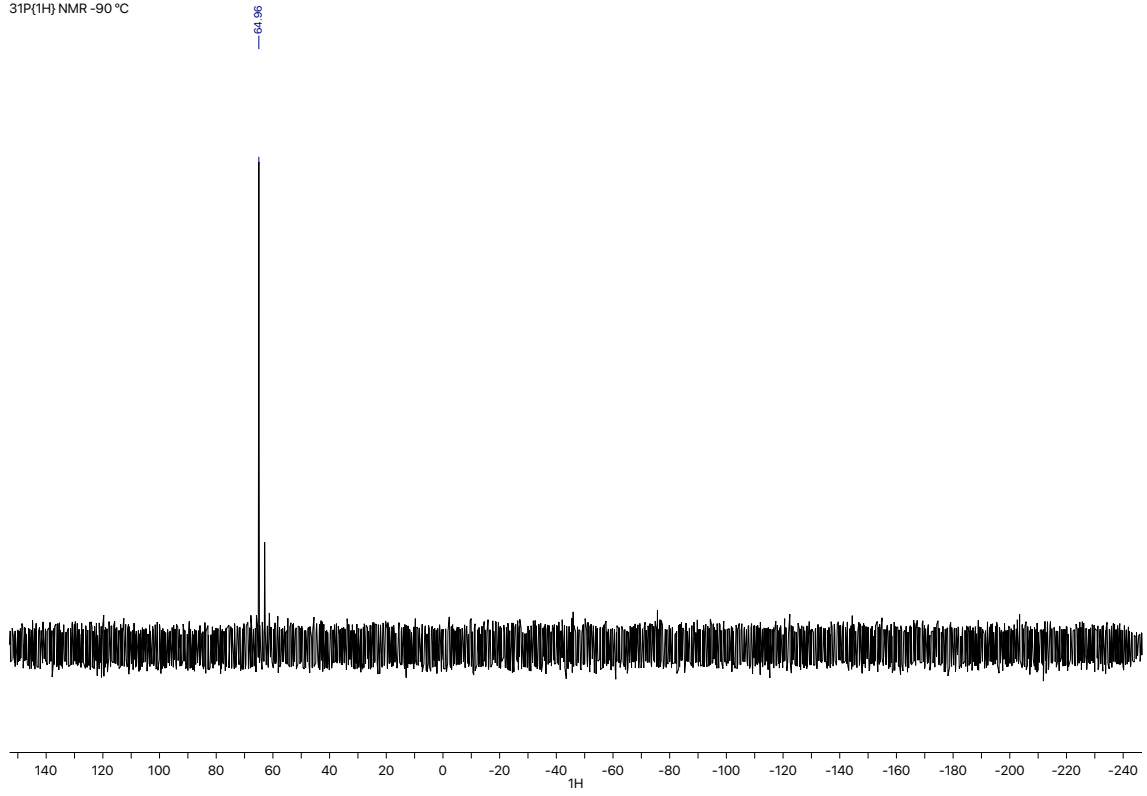
$^1\text{H NMR}$ -90 °C

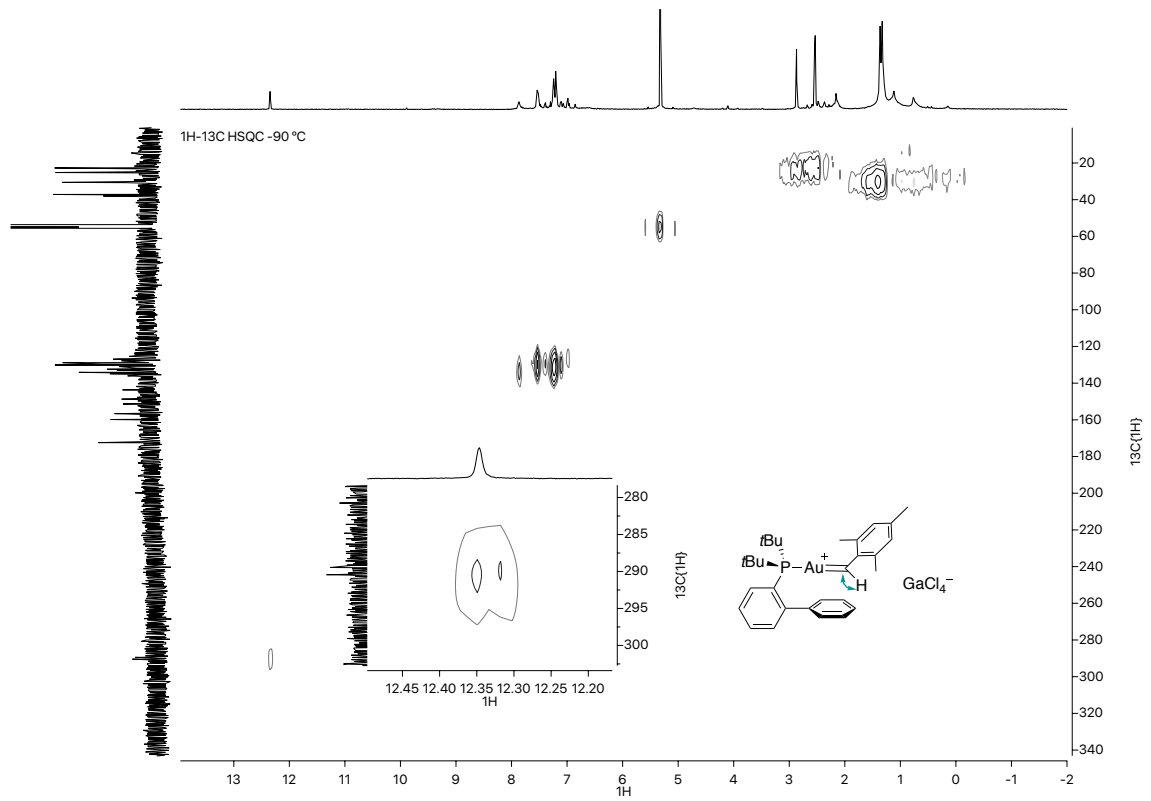


$^{13}\text{C}(^1\text{H})\text{ NMR}$ -80 °C



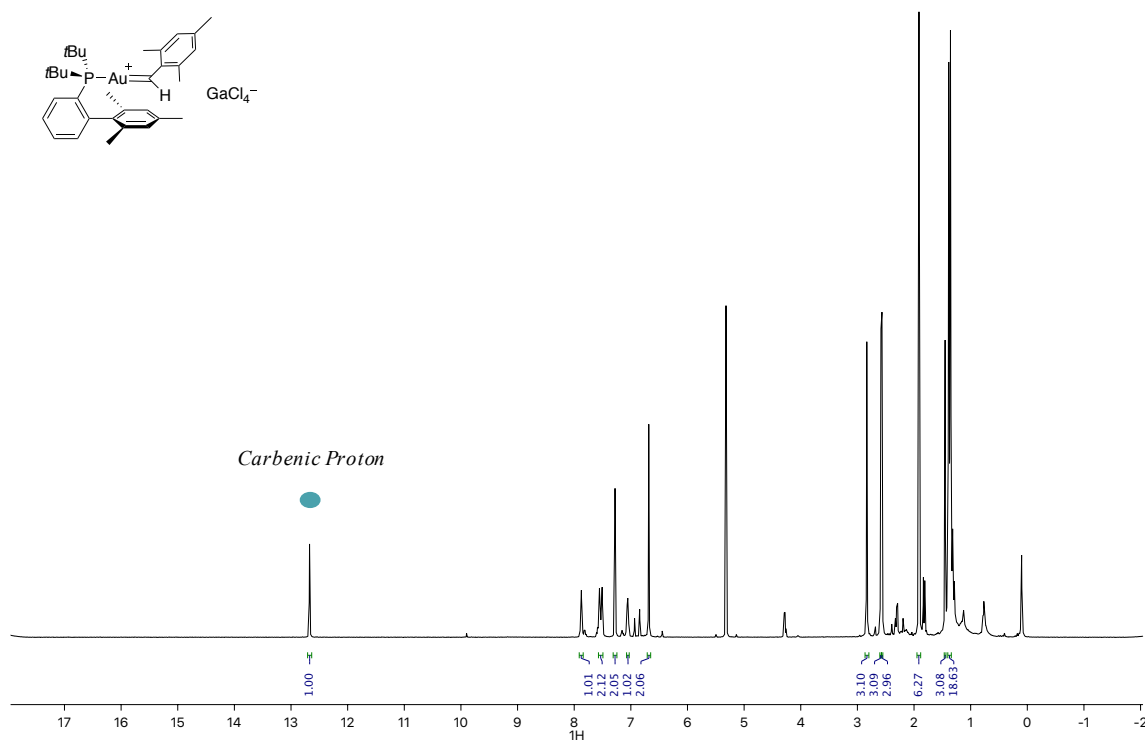
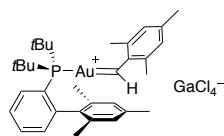
31P(1H) NMR -90 °C



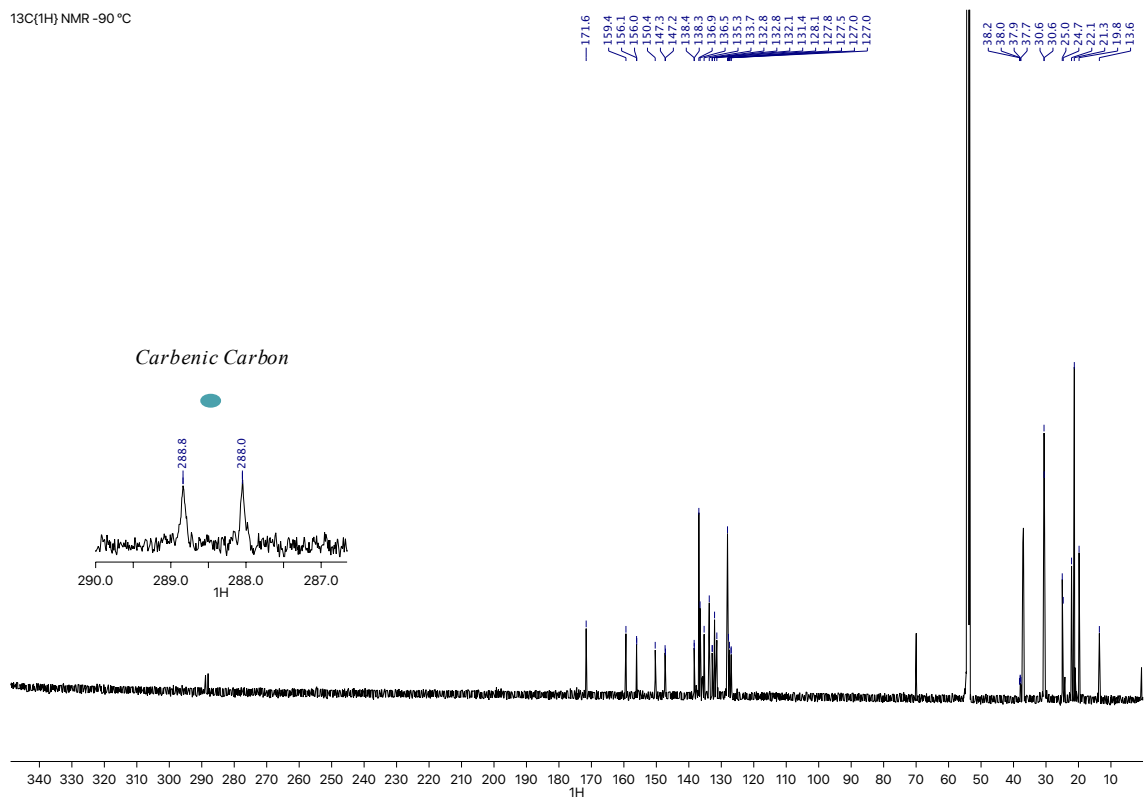


2-Di-*t*-butylphosphino-2',4',6'-trimethylbiphenyl mesityl(methyl) gold(I) carbene (5b)

¹H NMR -90 °C

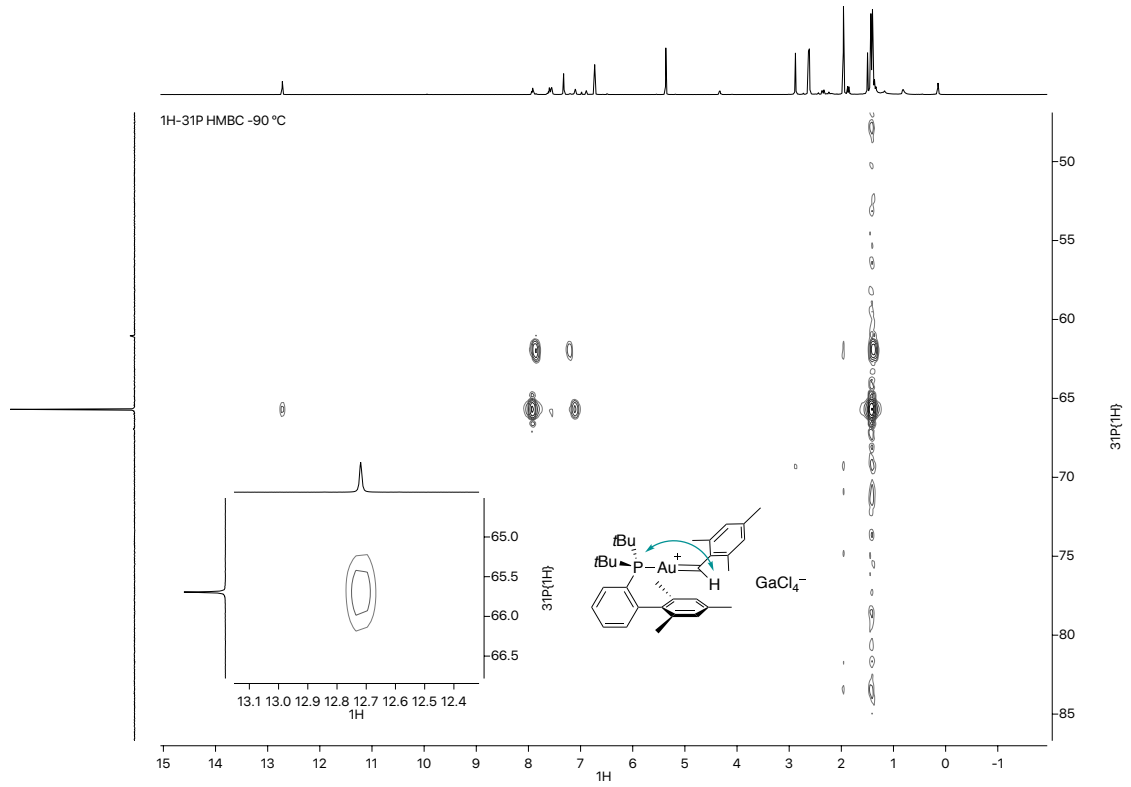
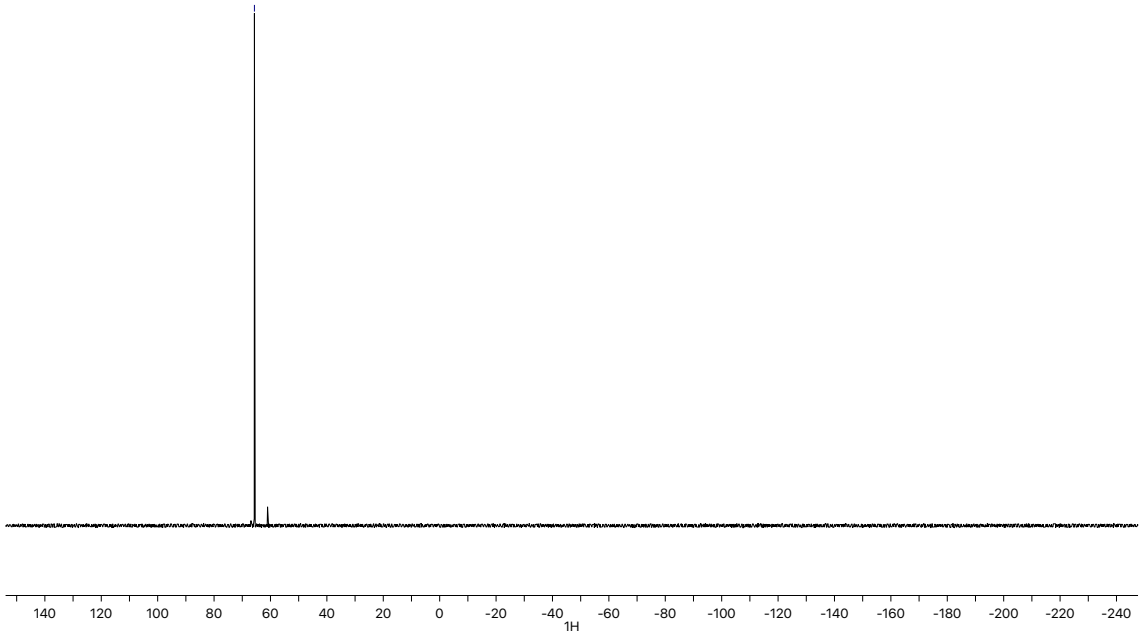


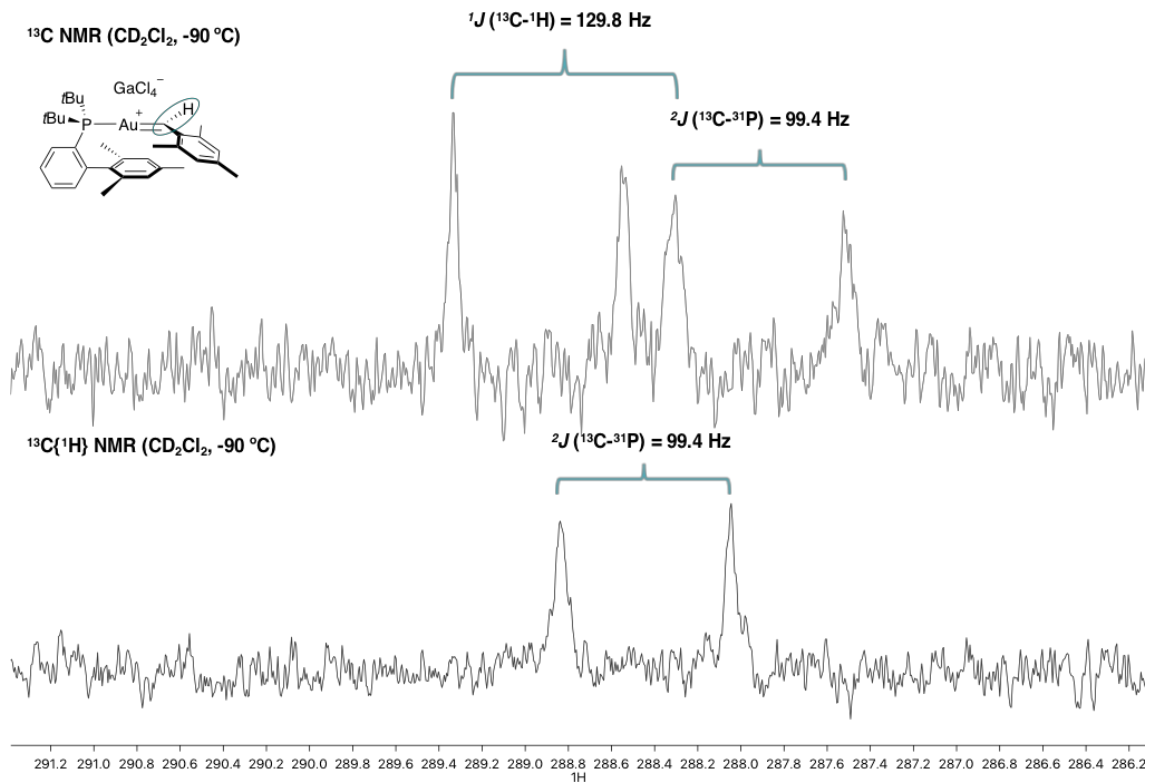
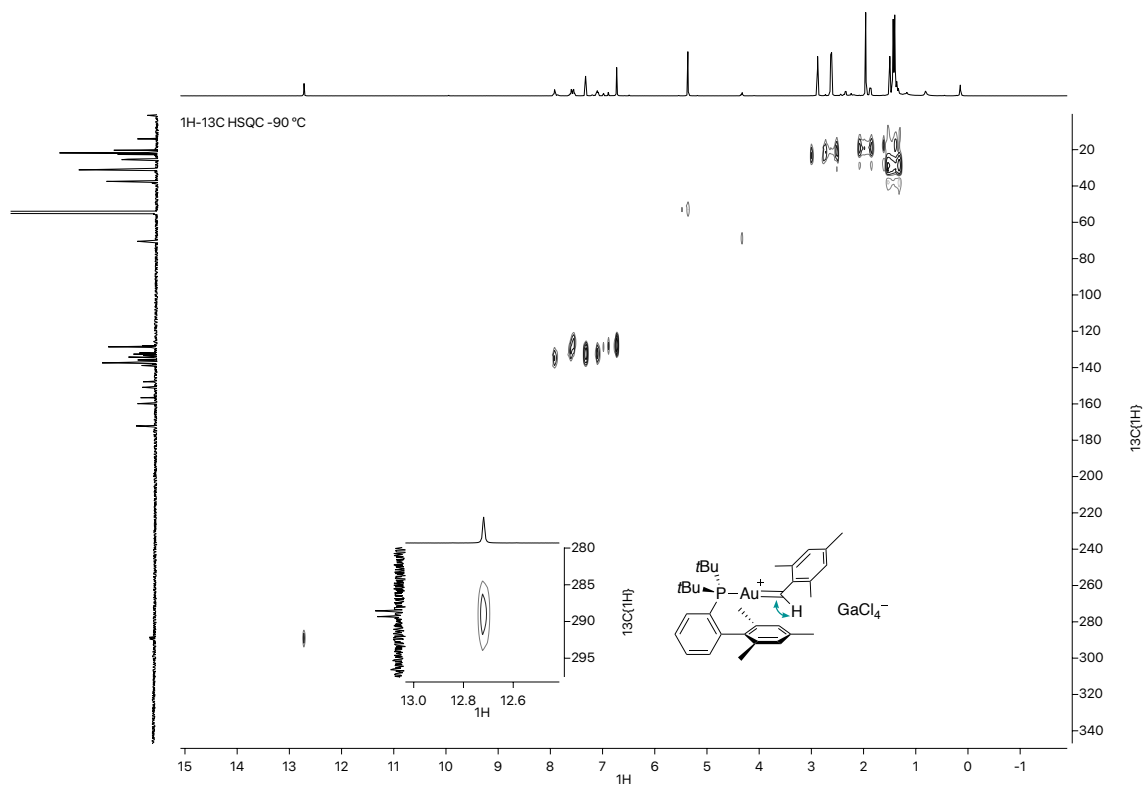
¹³C(¹H) NMR -90 °C



31P(1H) NMR -90 °C

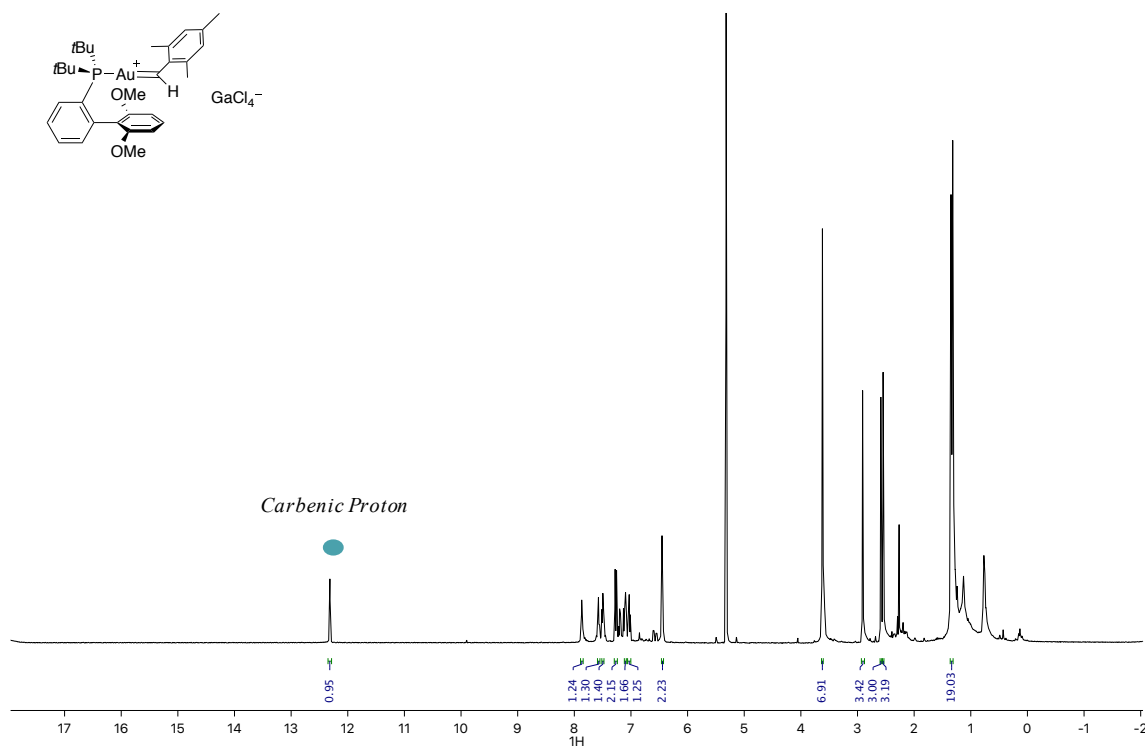
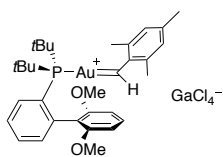
65.89



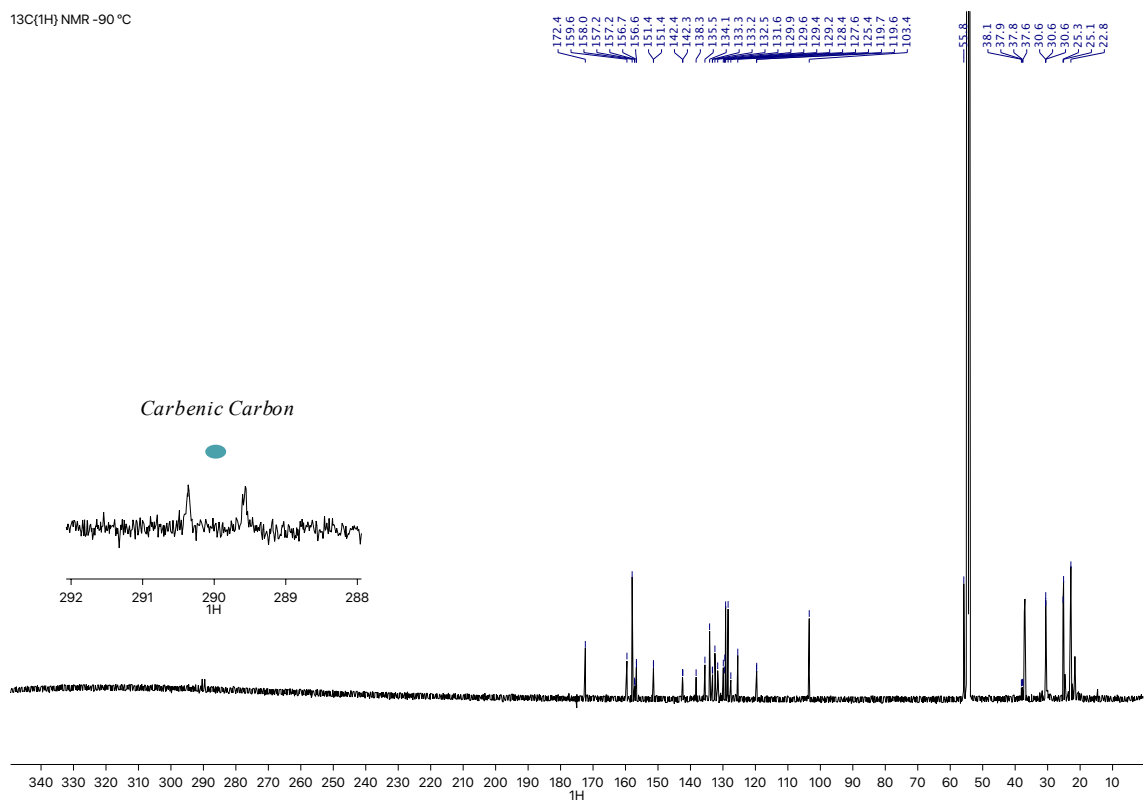


2-Di-*t*-butylphosphino-2',6'-dimethoxybiphenyl mesityl(methyl) gold(I) carbene (5c)

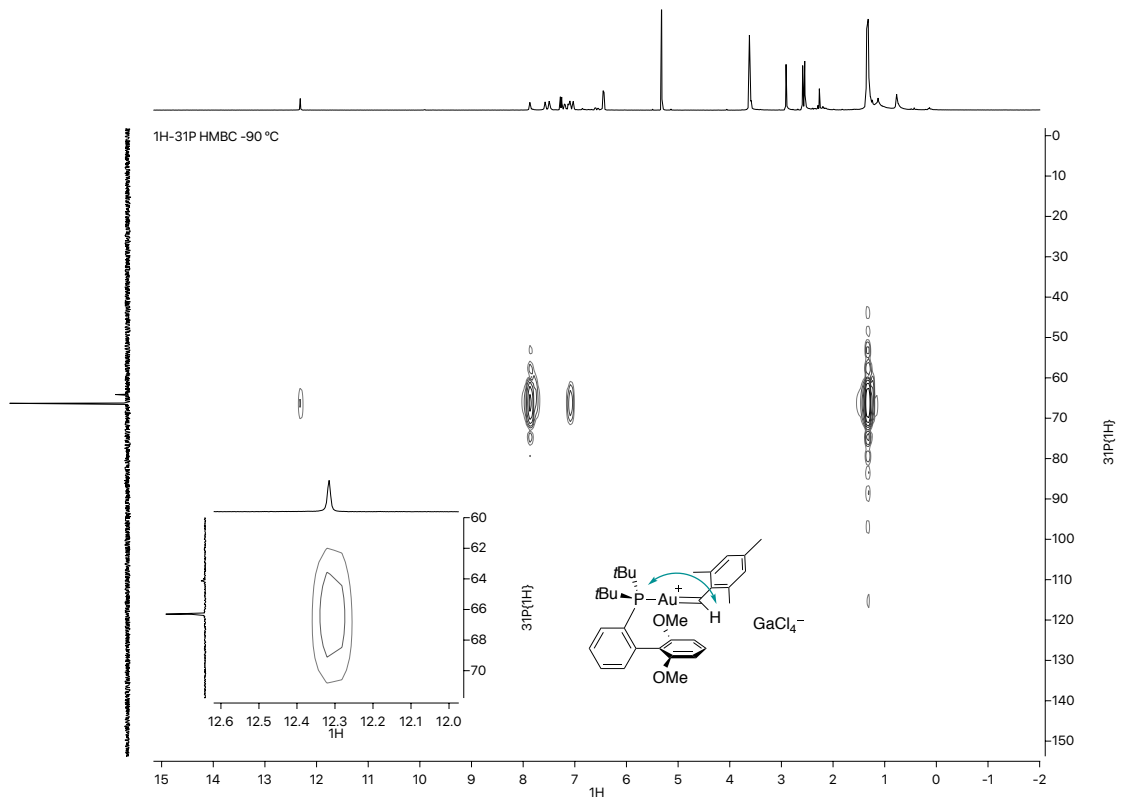
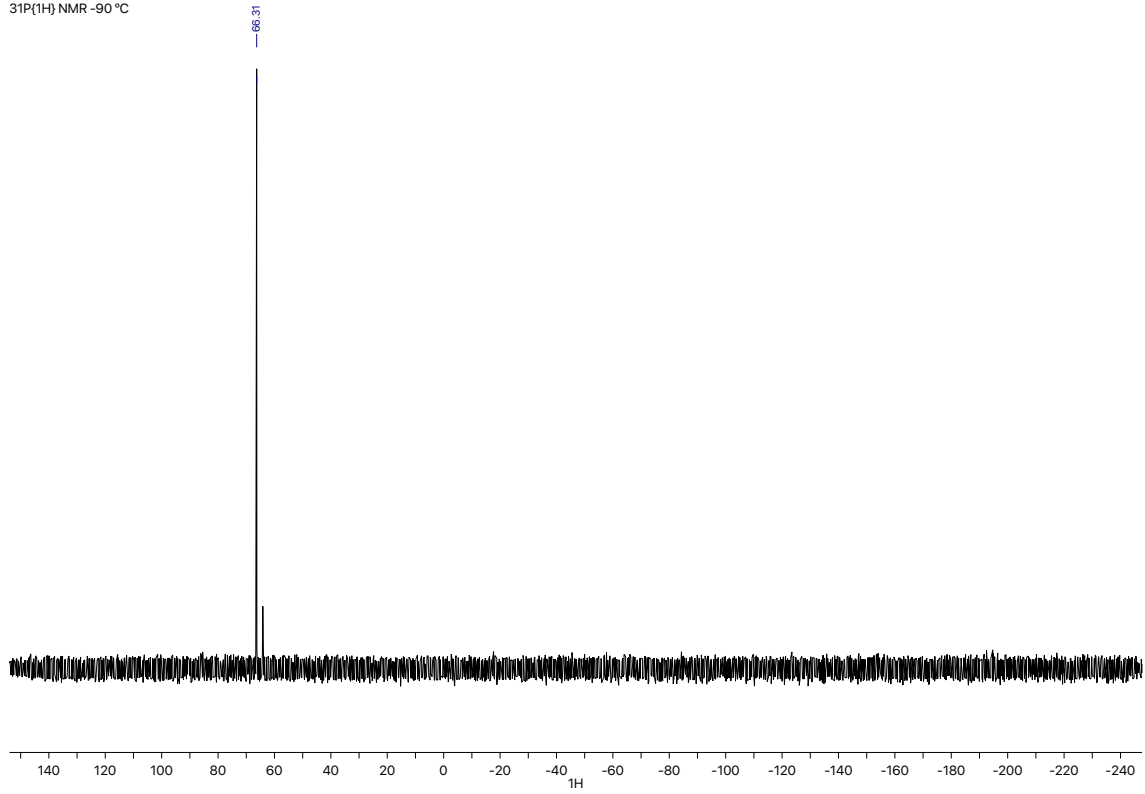
$^1\text{H NMR}$ -90 °C

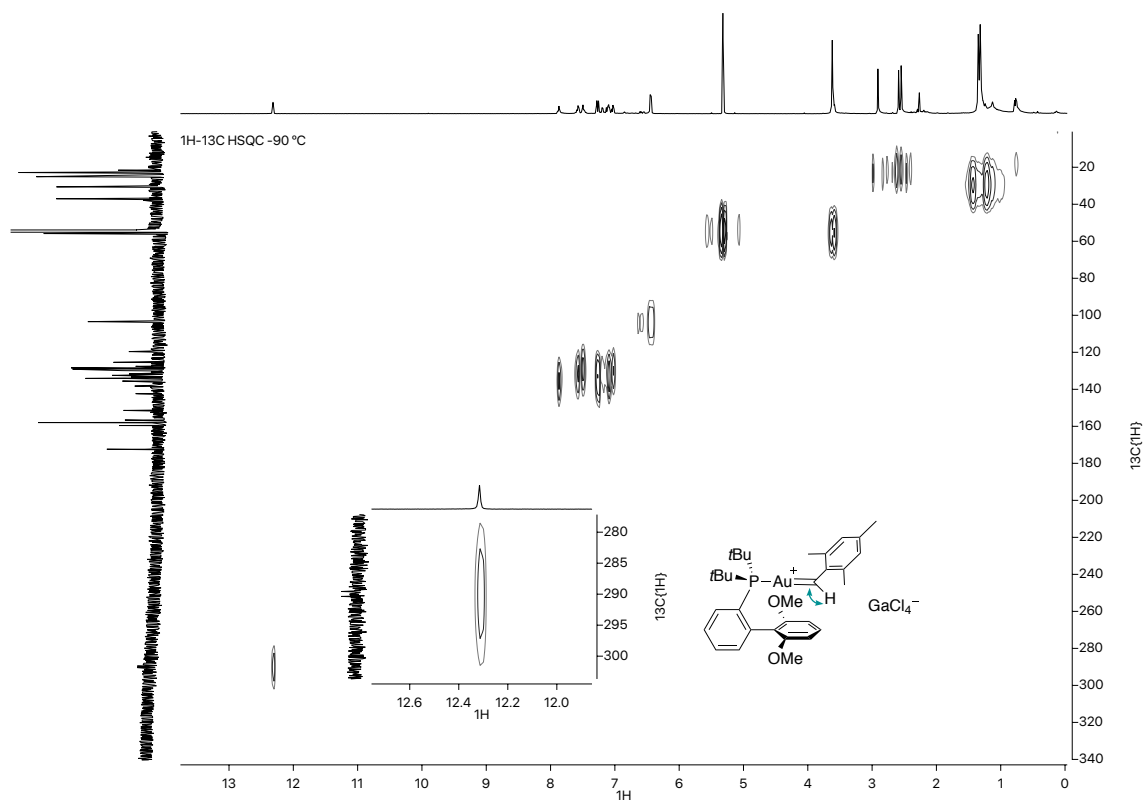


$^{13}\text{C}(^1\text{H})\text{NMR}$ -90 °C



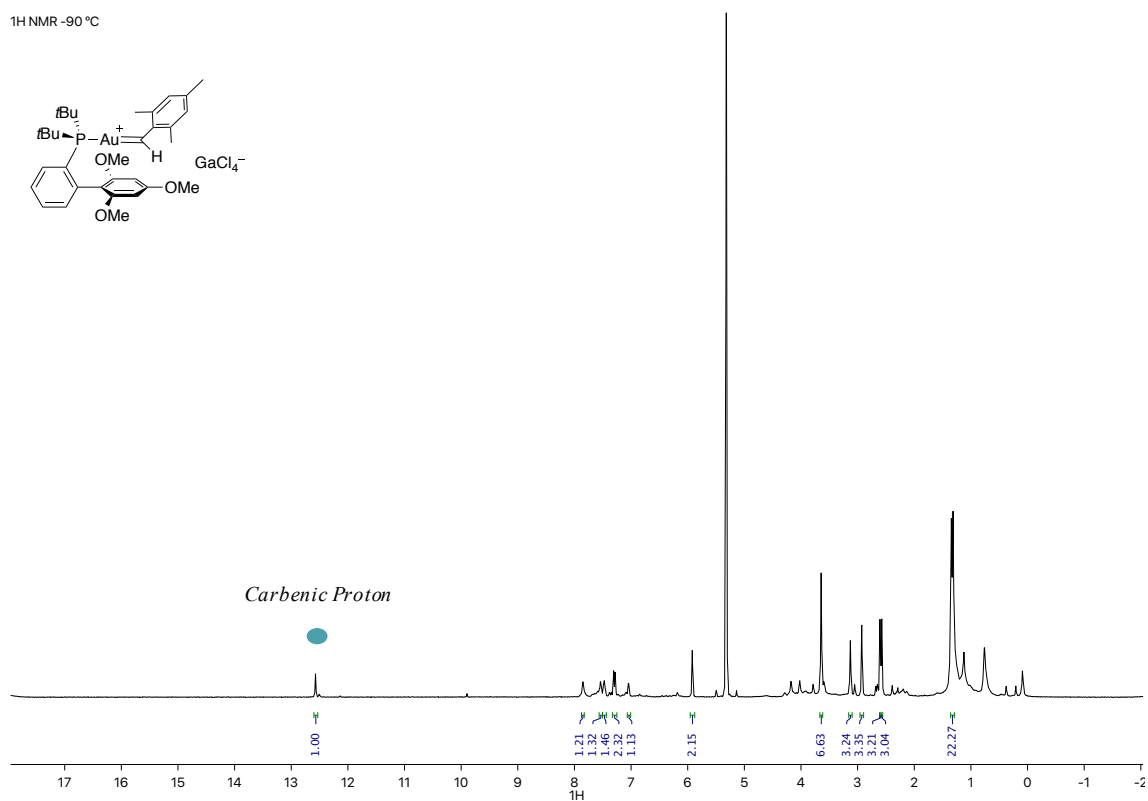
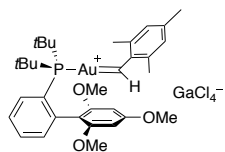
31P{1H} NMR -90 °C



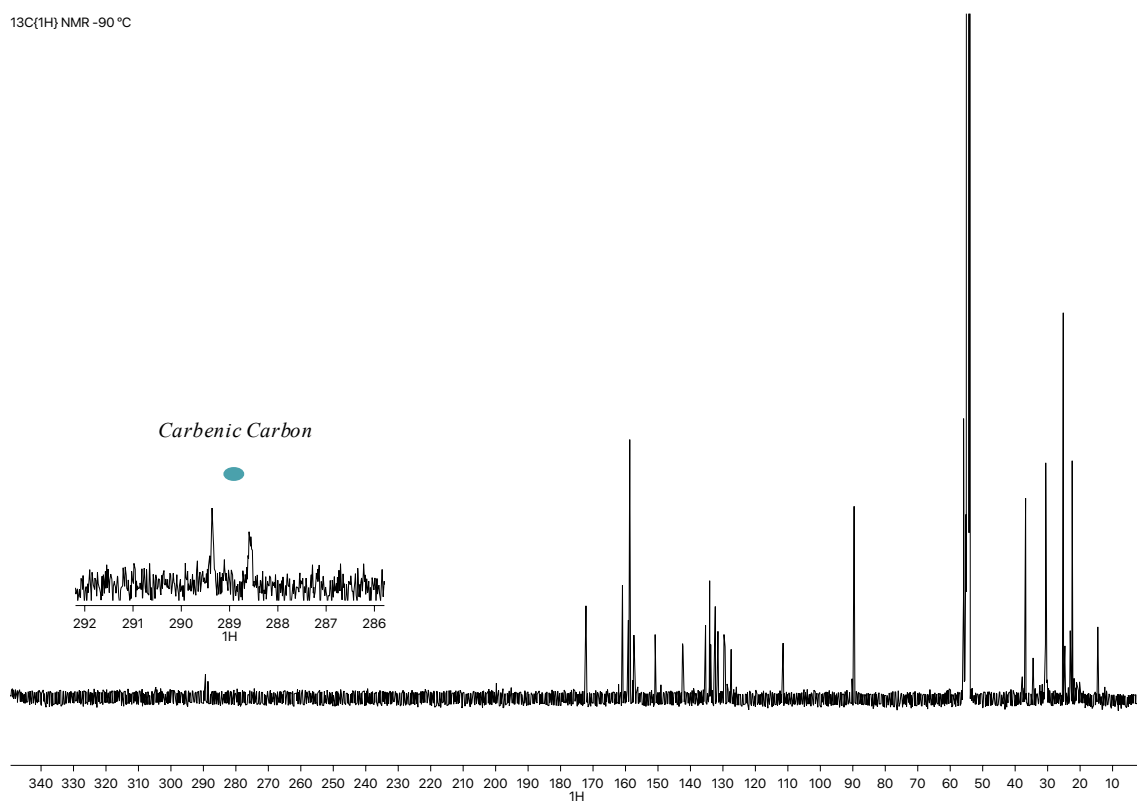


2-Di-*t*-butylphosphino-2',4',6'-trimethoxybiphenyl mesityl(methyl) gold(I) carbene (5d)

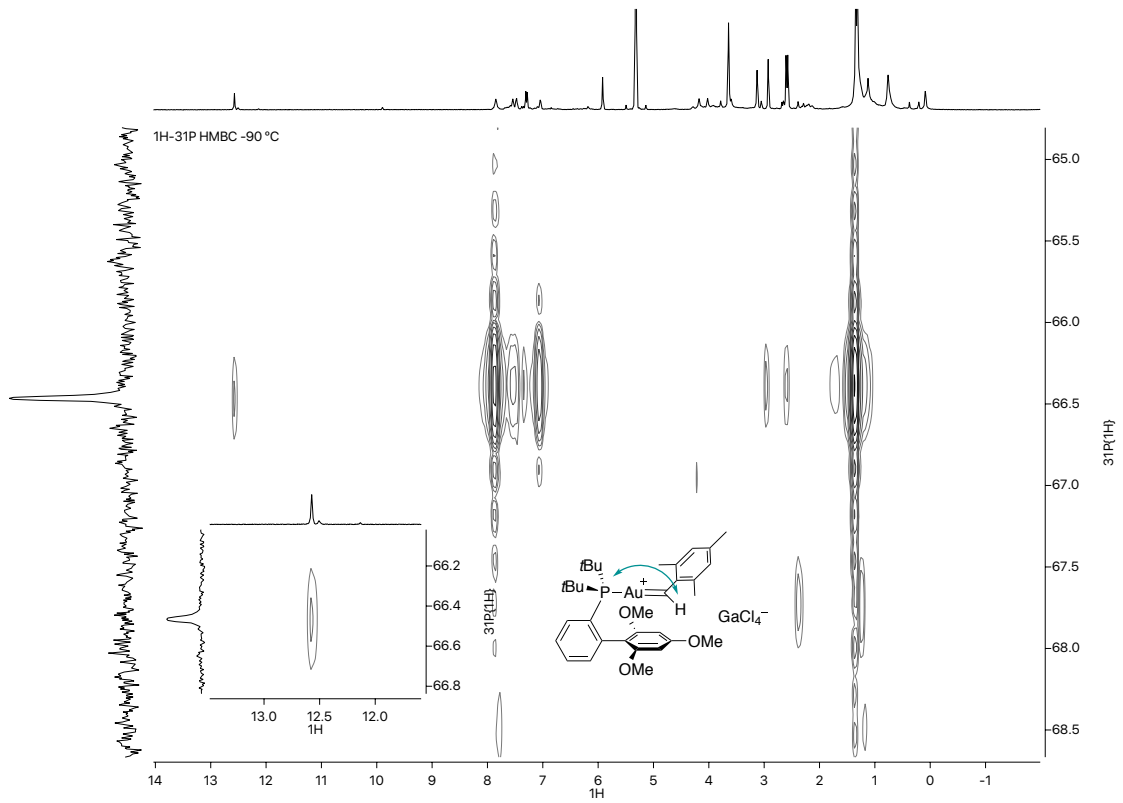
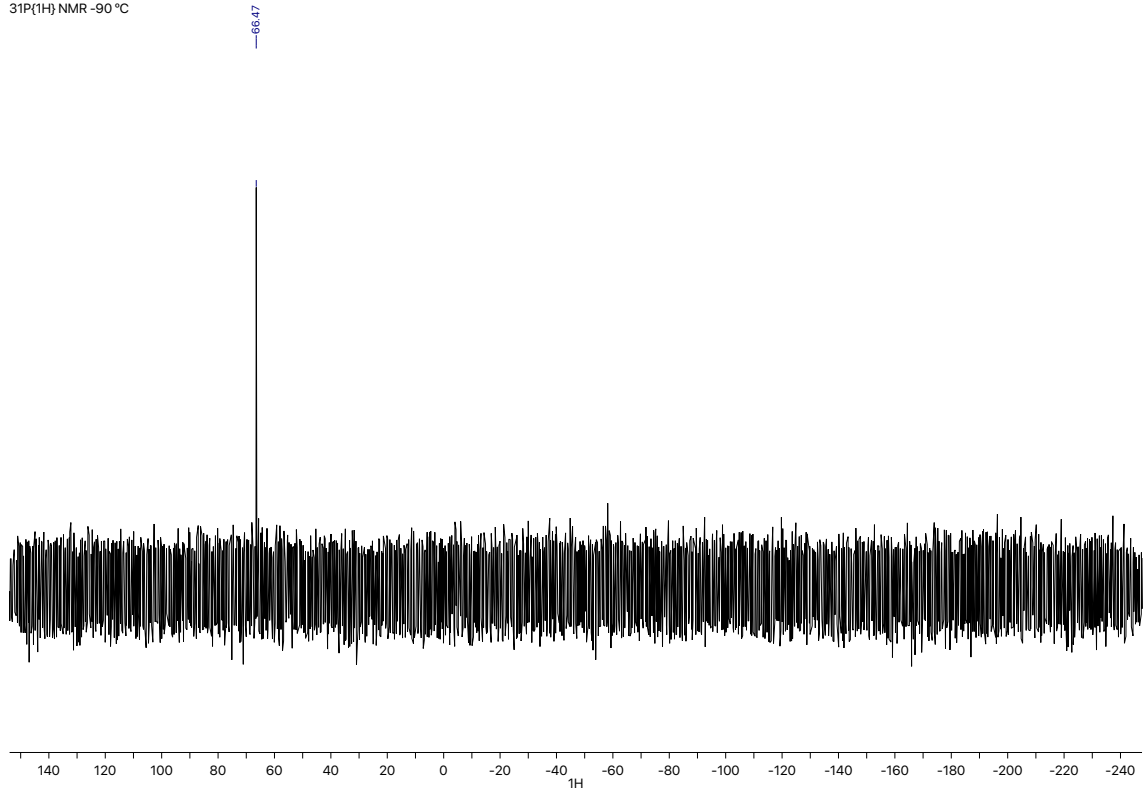
¹H NMR -90 °C

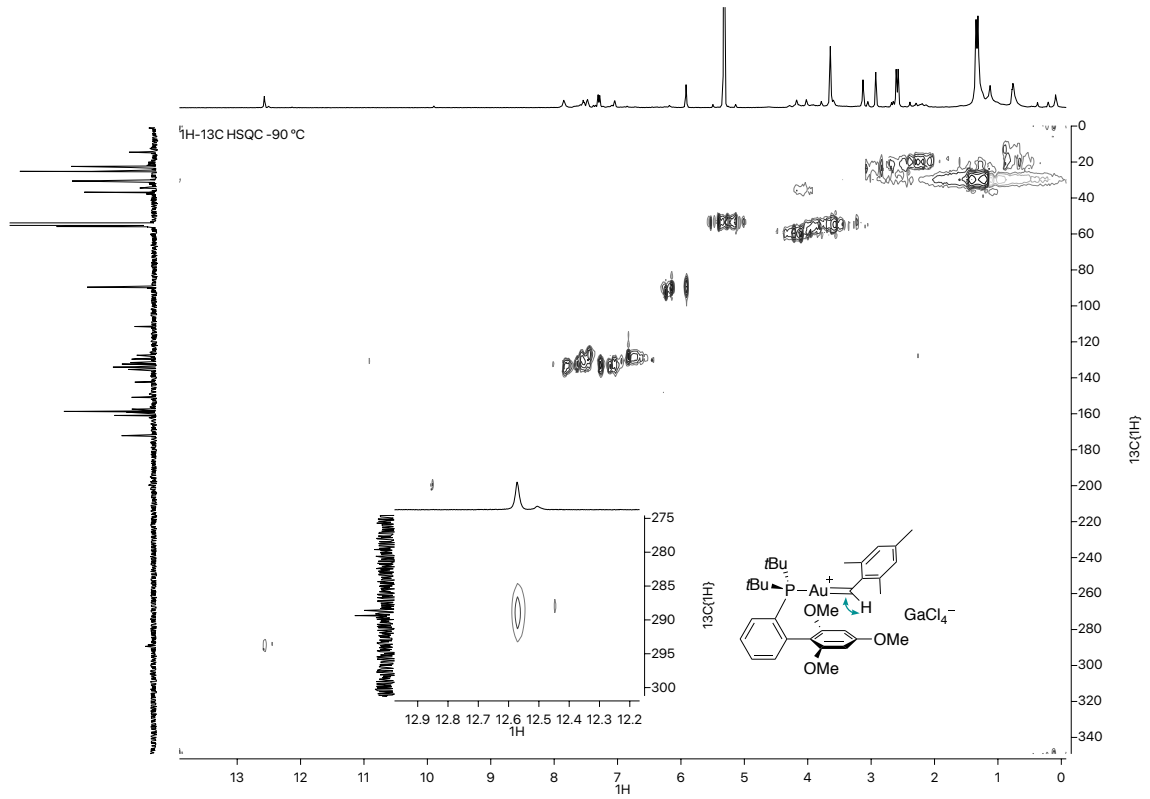


¹³C{¹H} NMR -90 °C

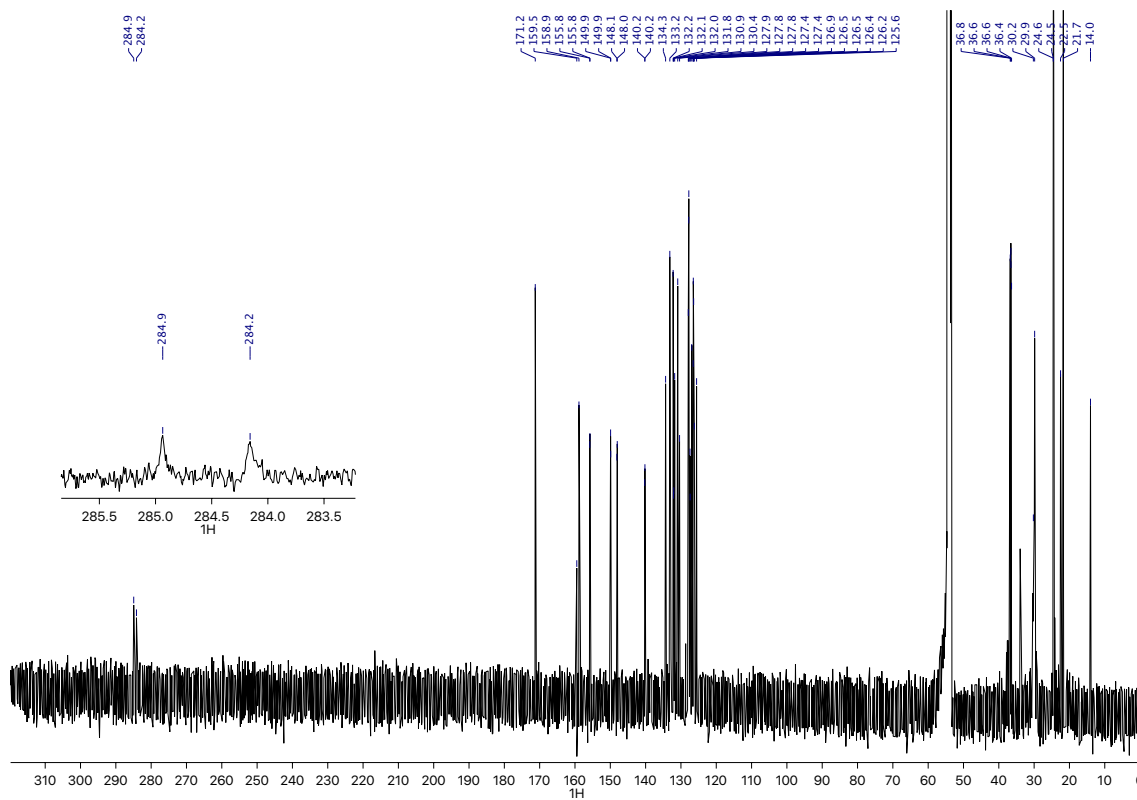
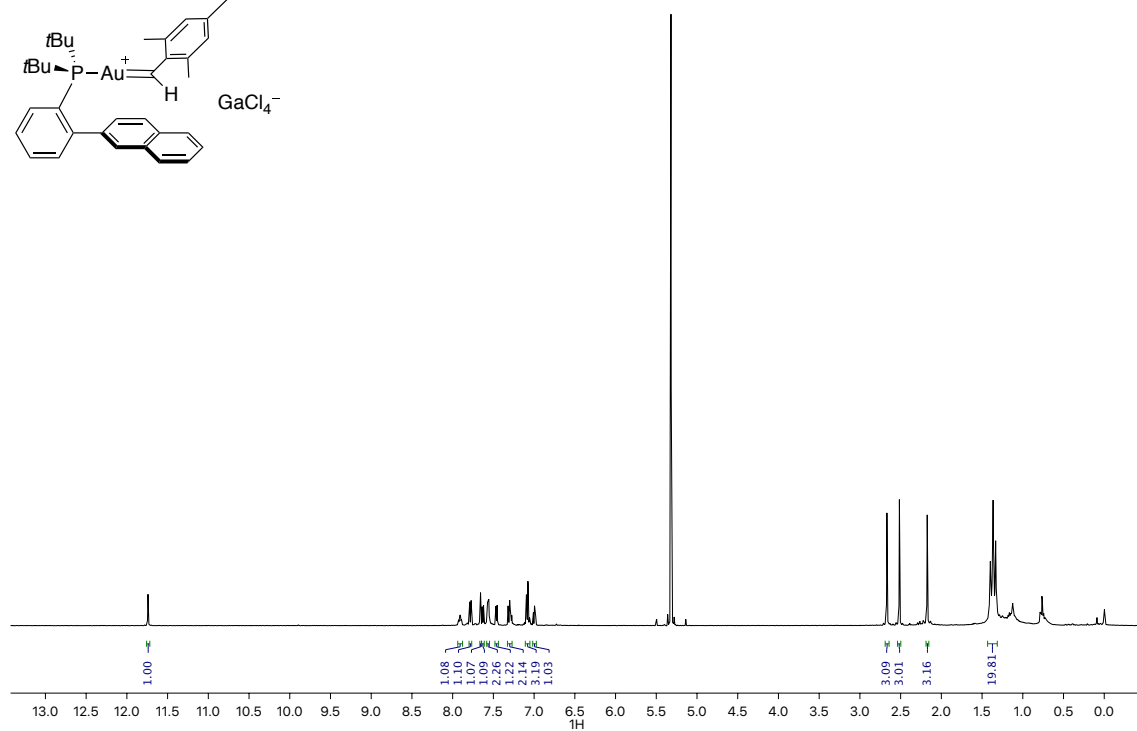
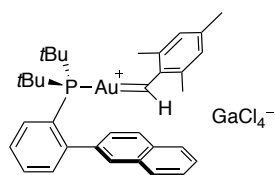


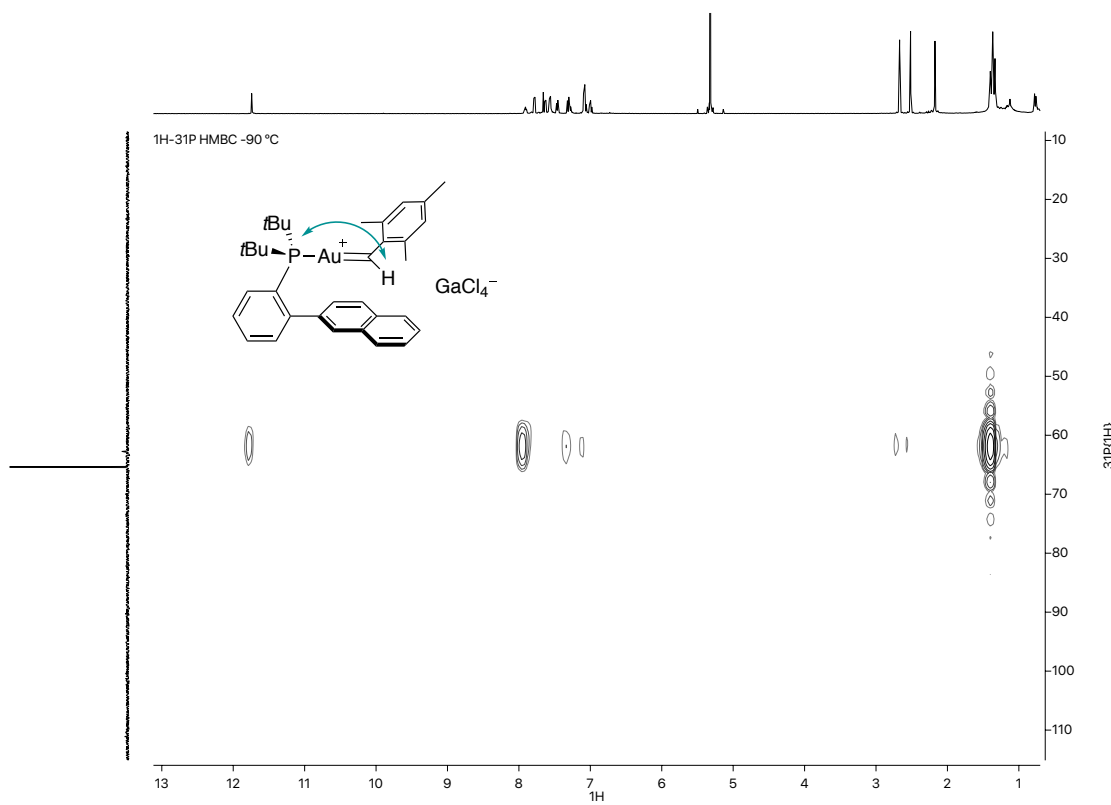
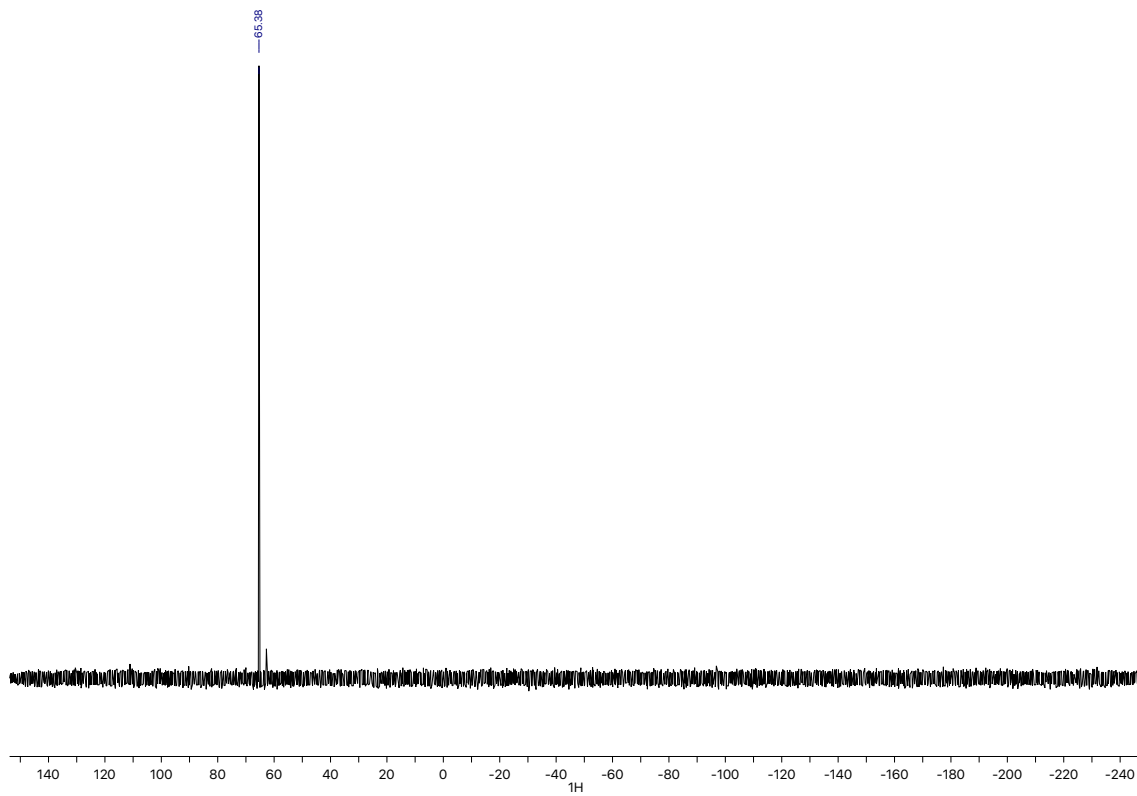
31P(1H) NMR -90 °C



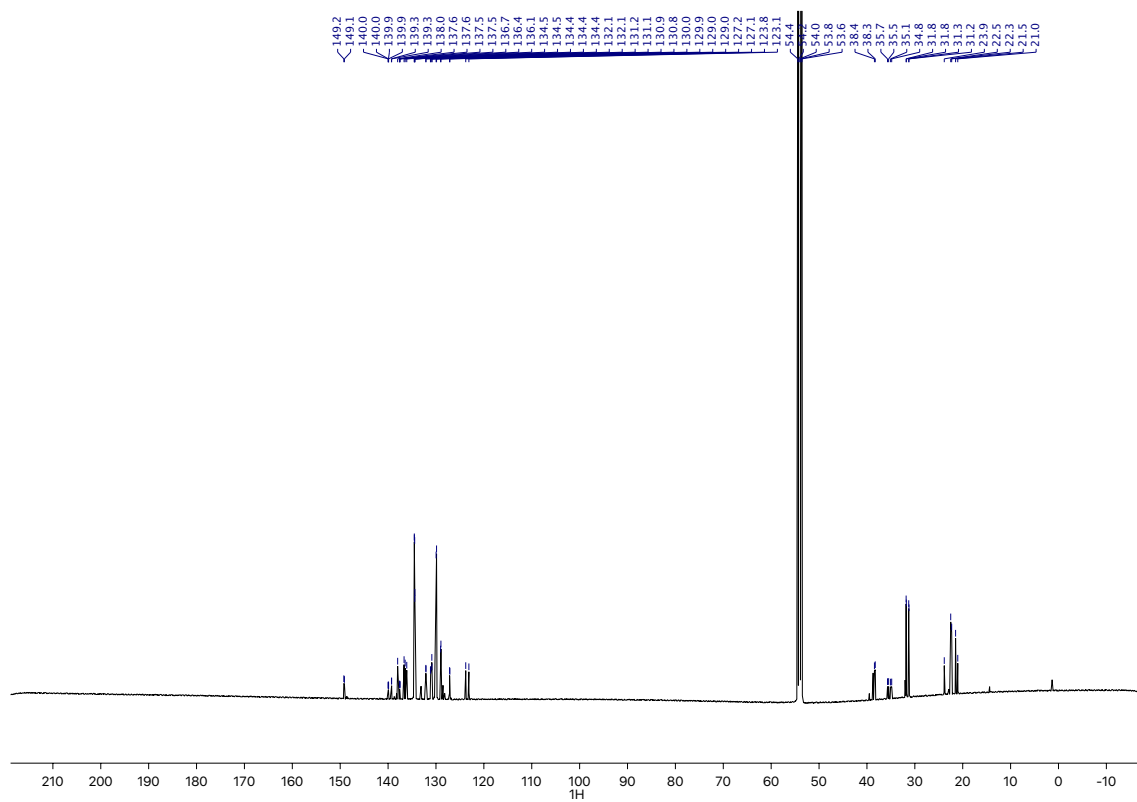
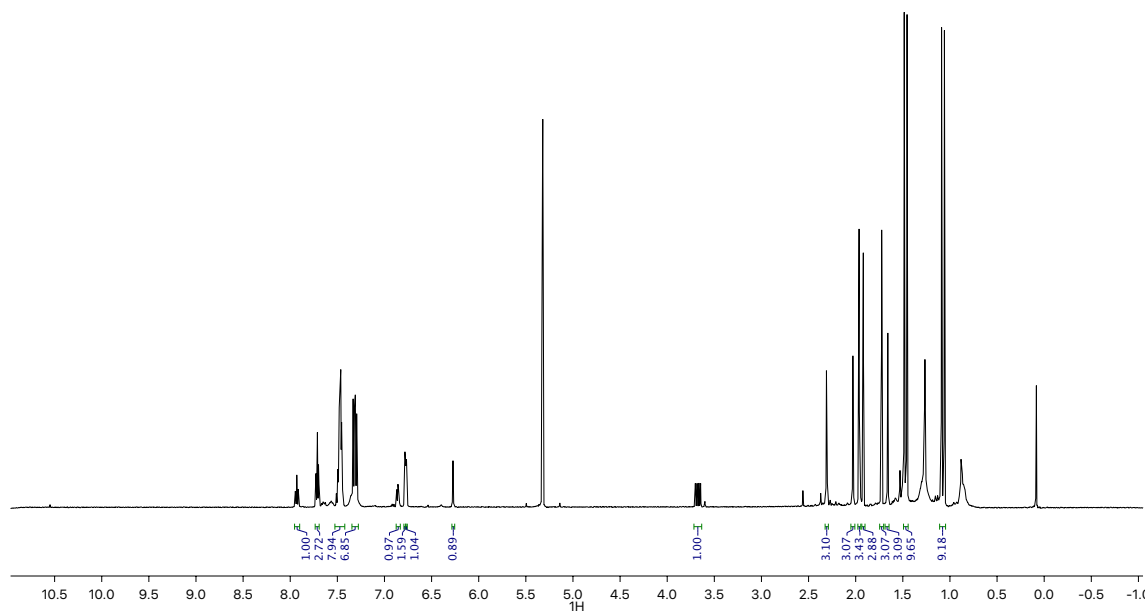
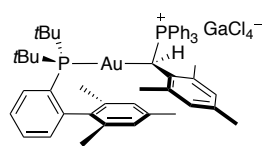


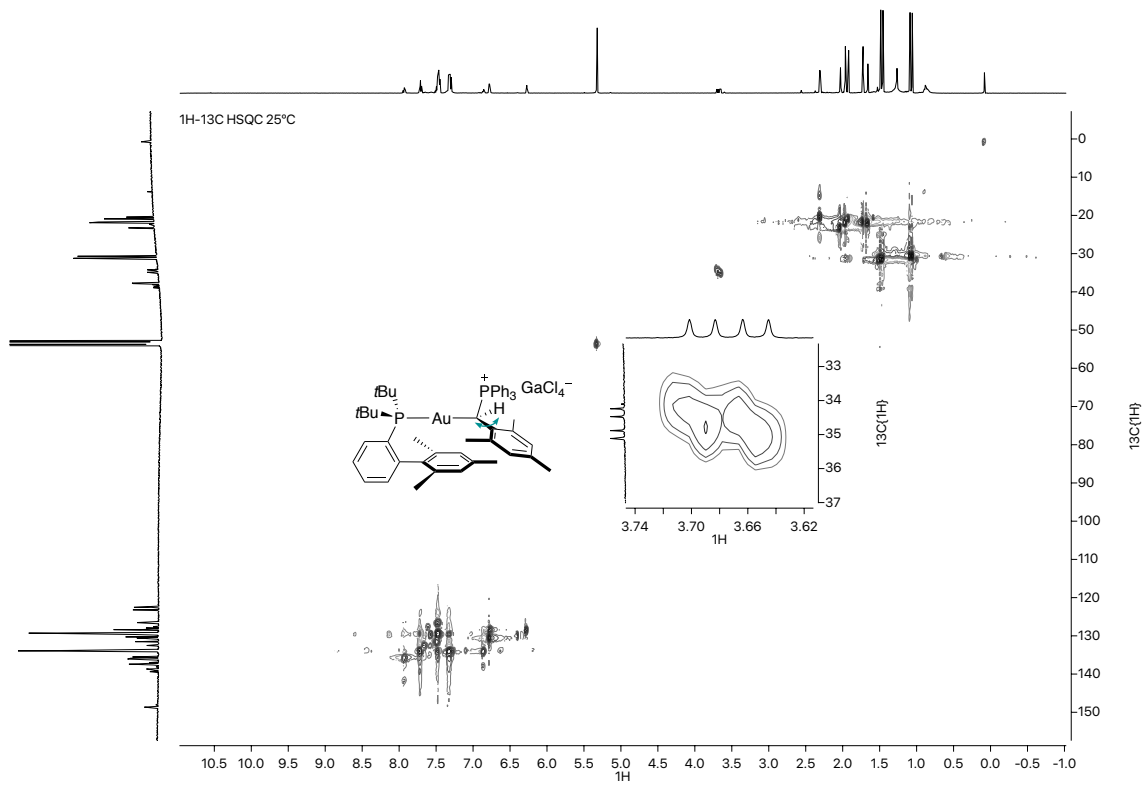
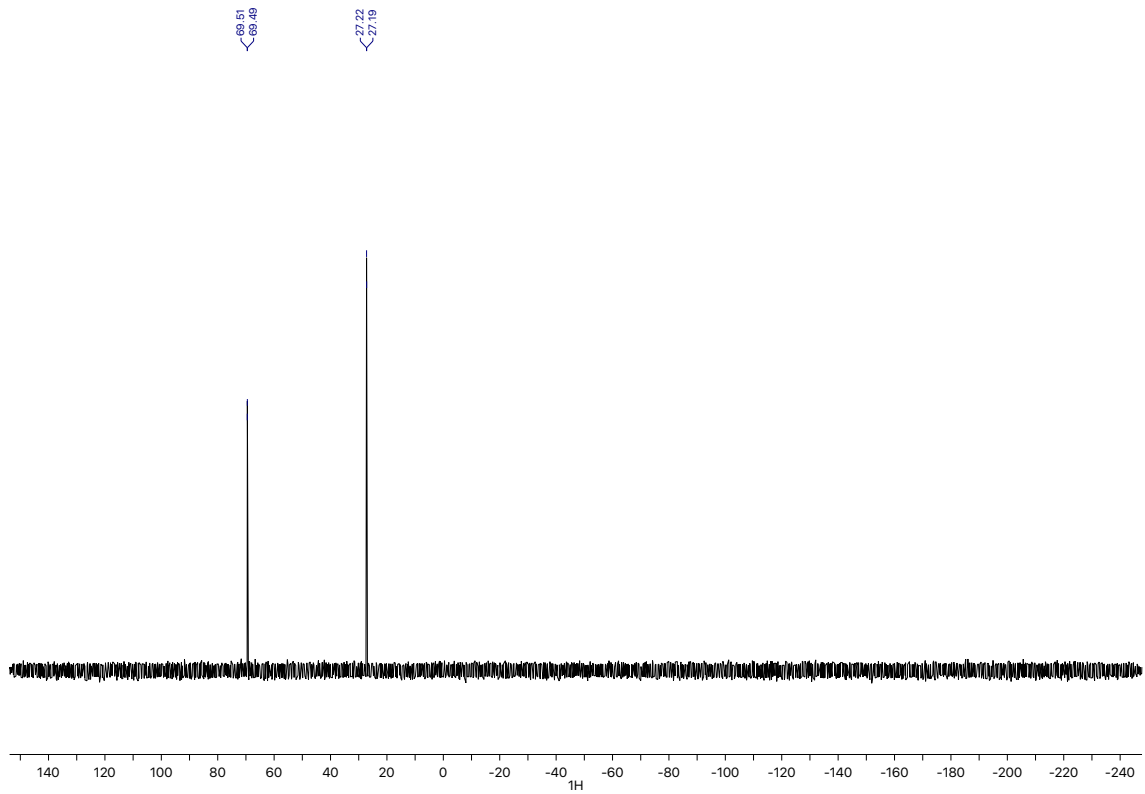
2-Di-*t*-butylphosphino-naphthylphenyl mesityl(methyl) gold(I) carbene (5e)

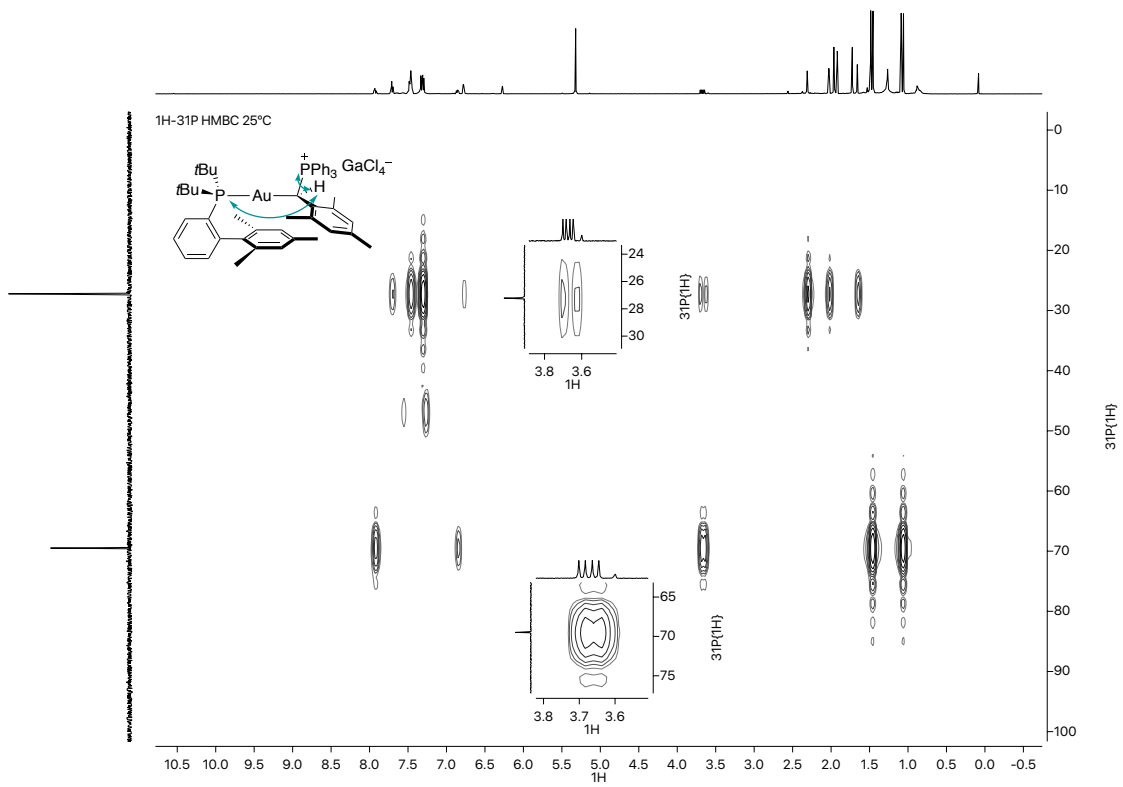




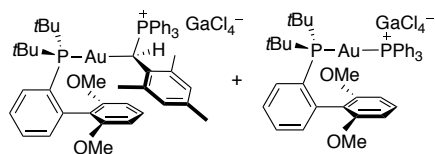
Phosponium ylid complex 7a



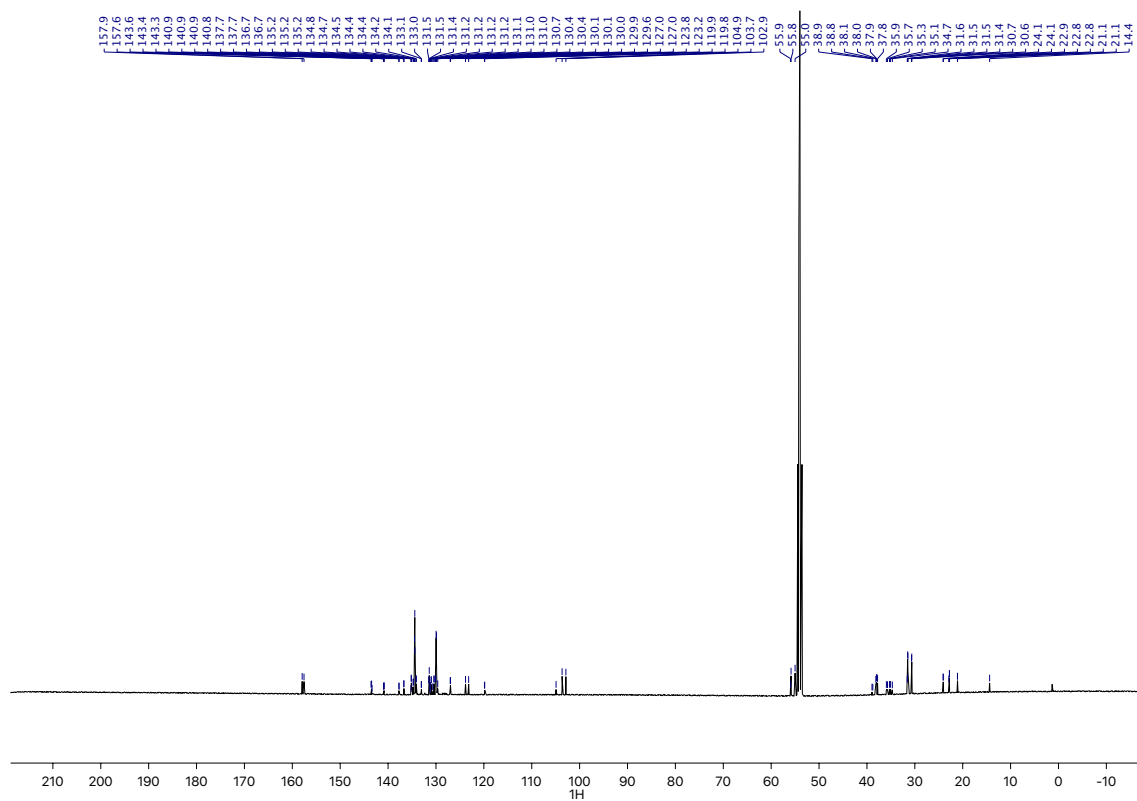
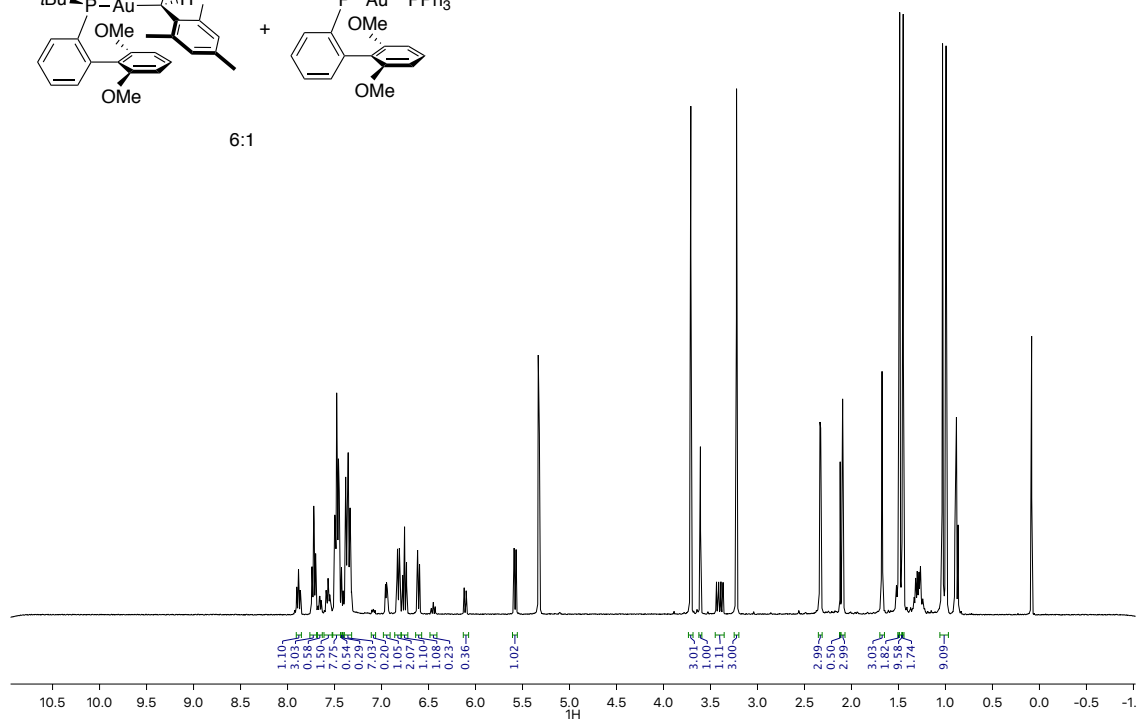


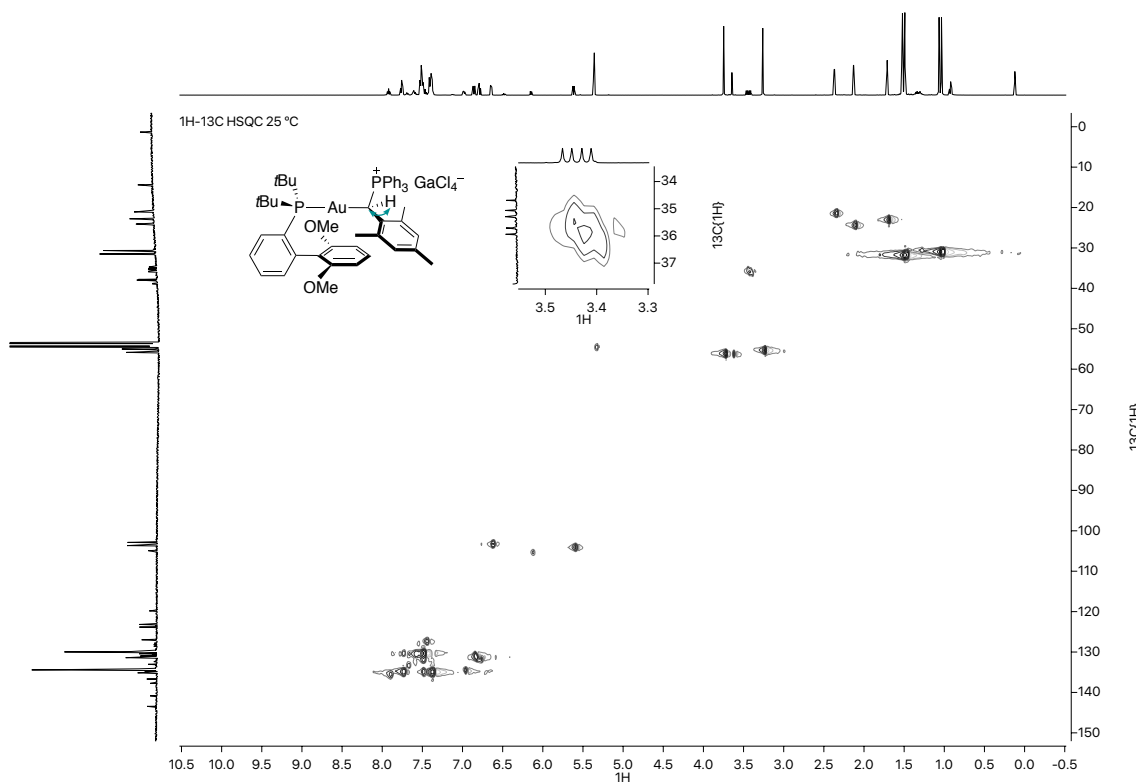
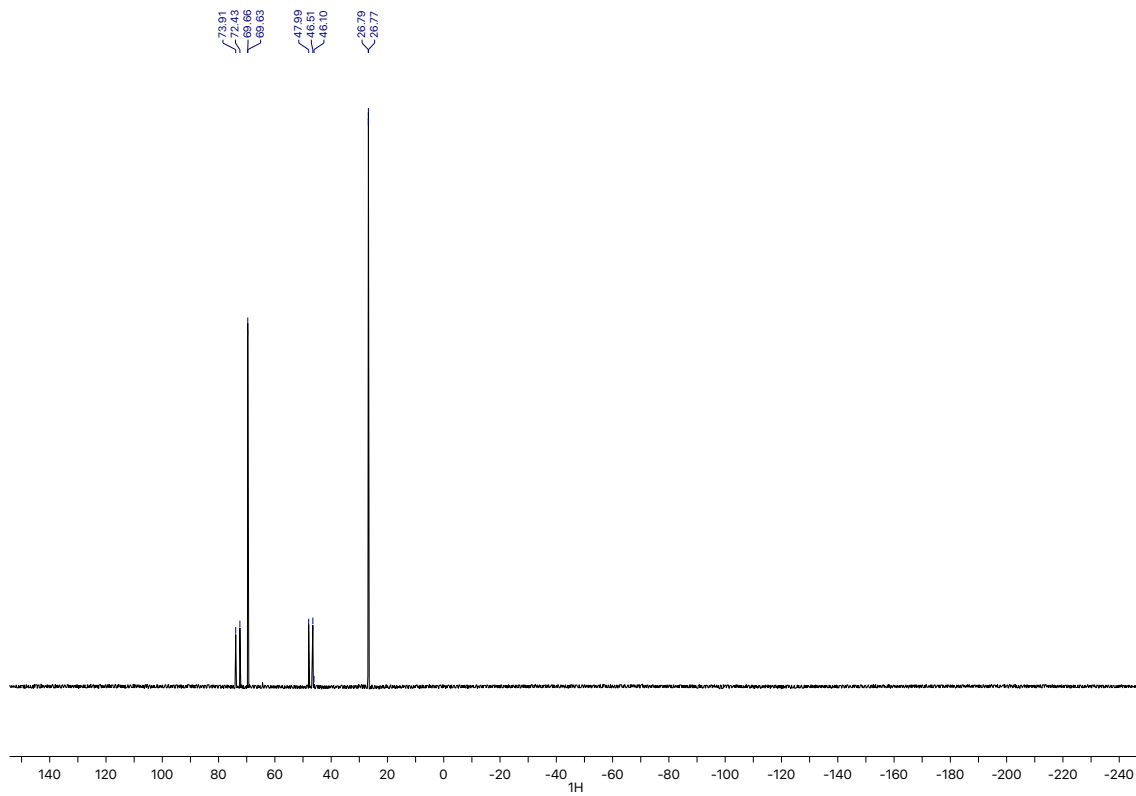


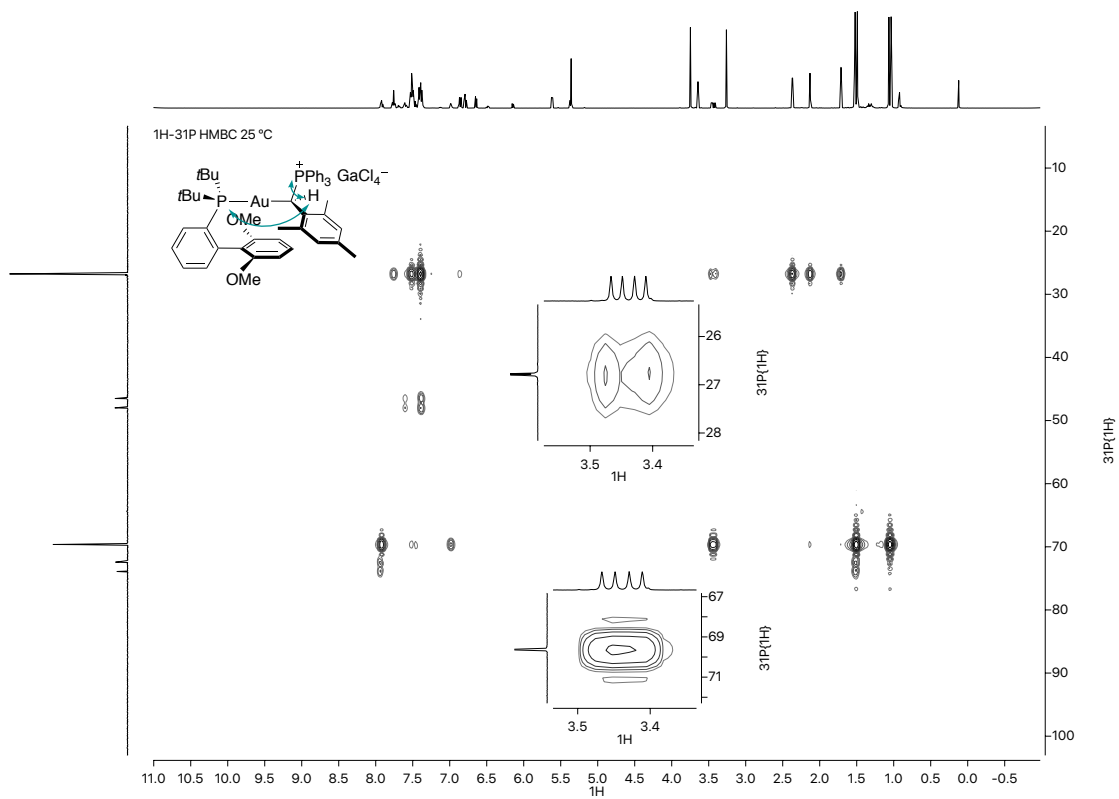
Phosponium ylid complex 7b



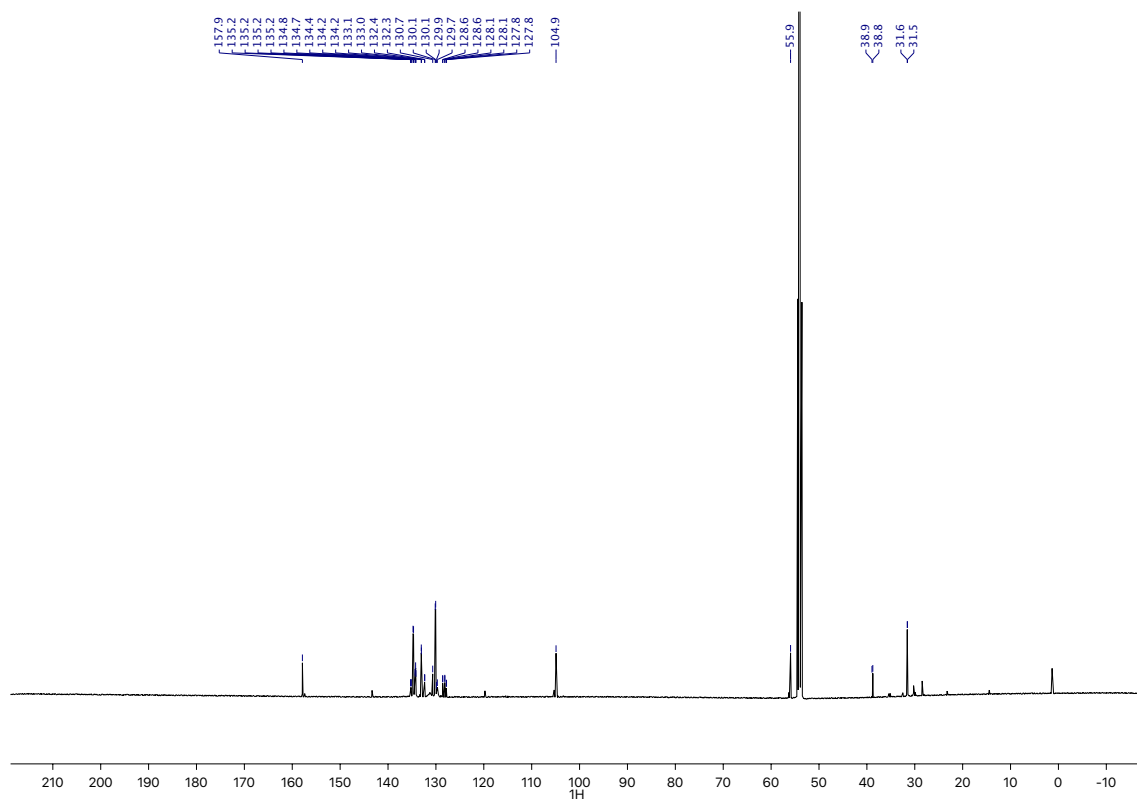
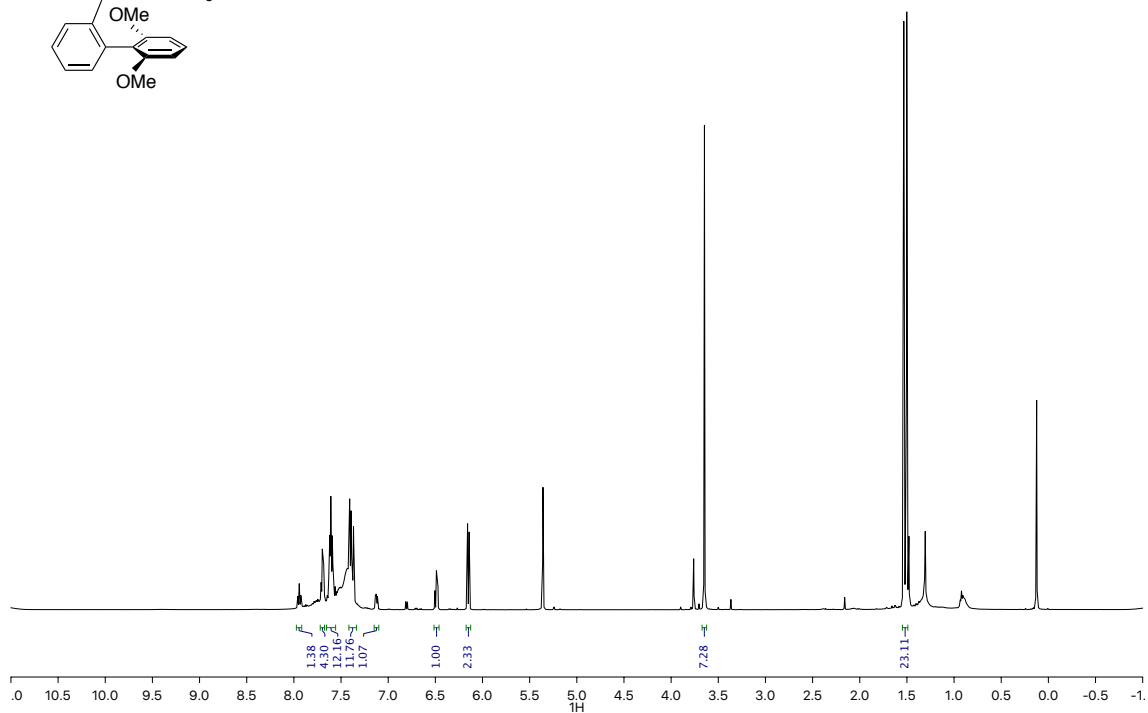
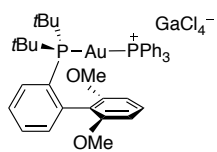
6:1

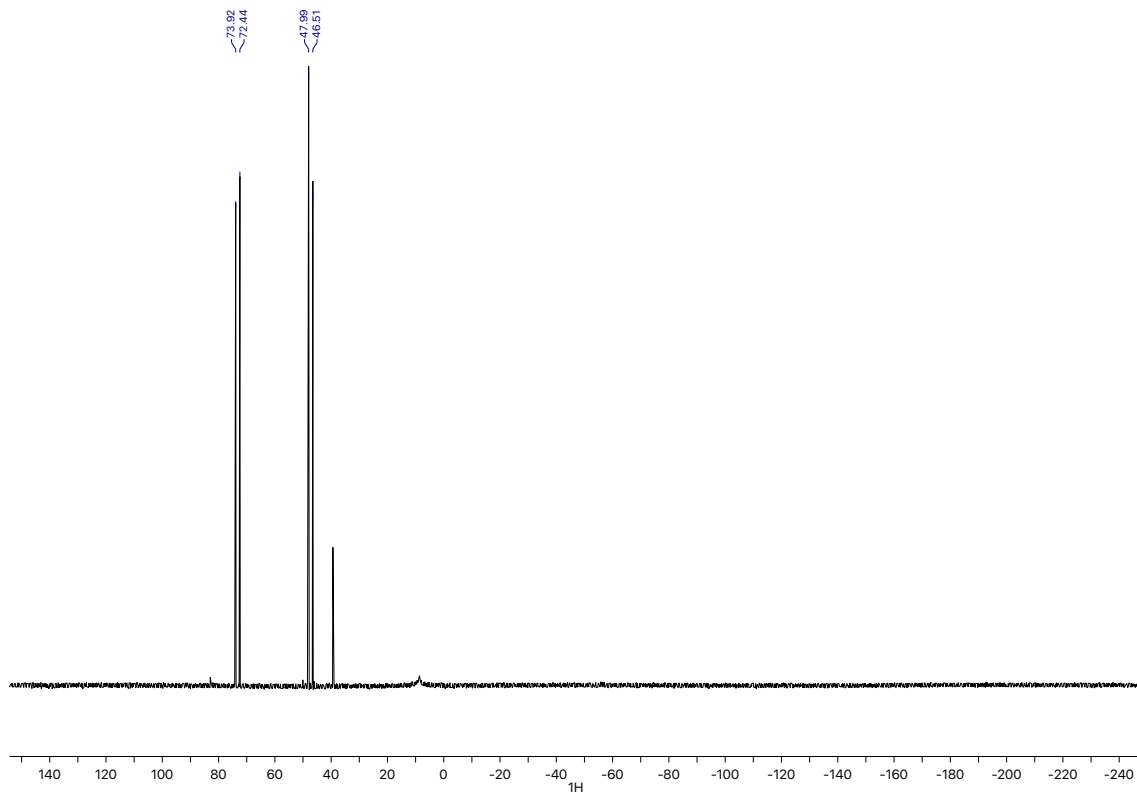




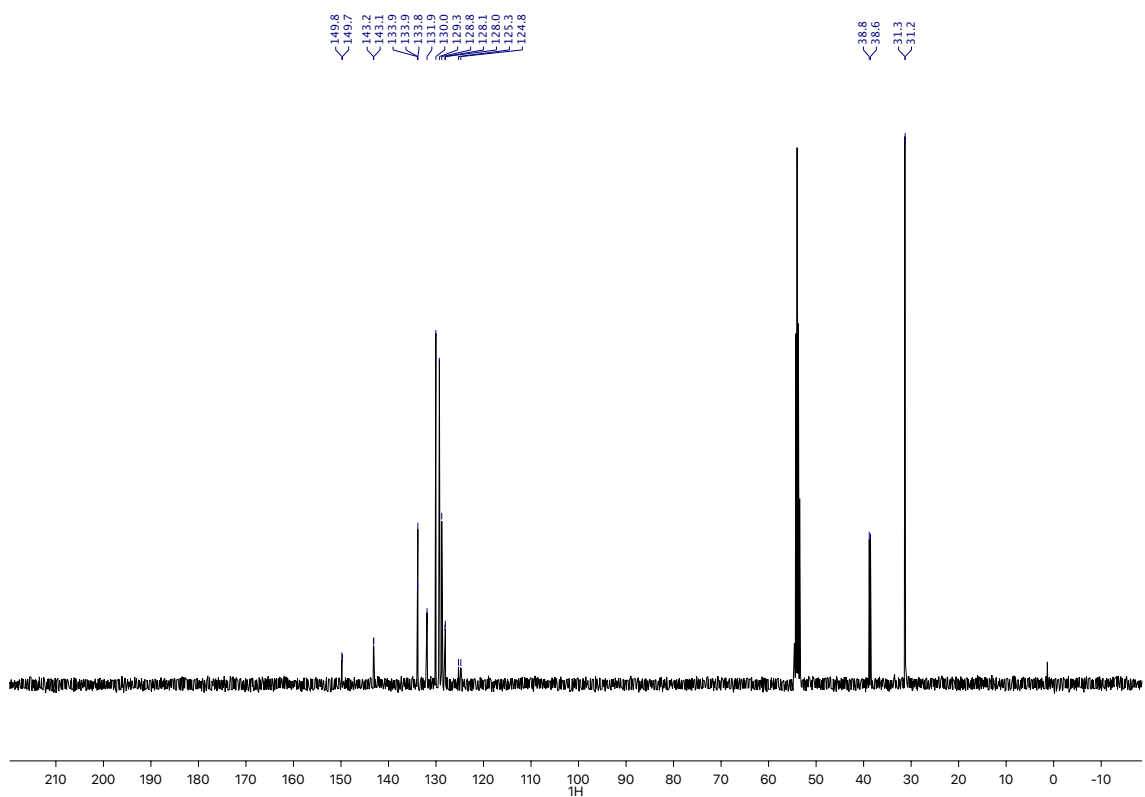
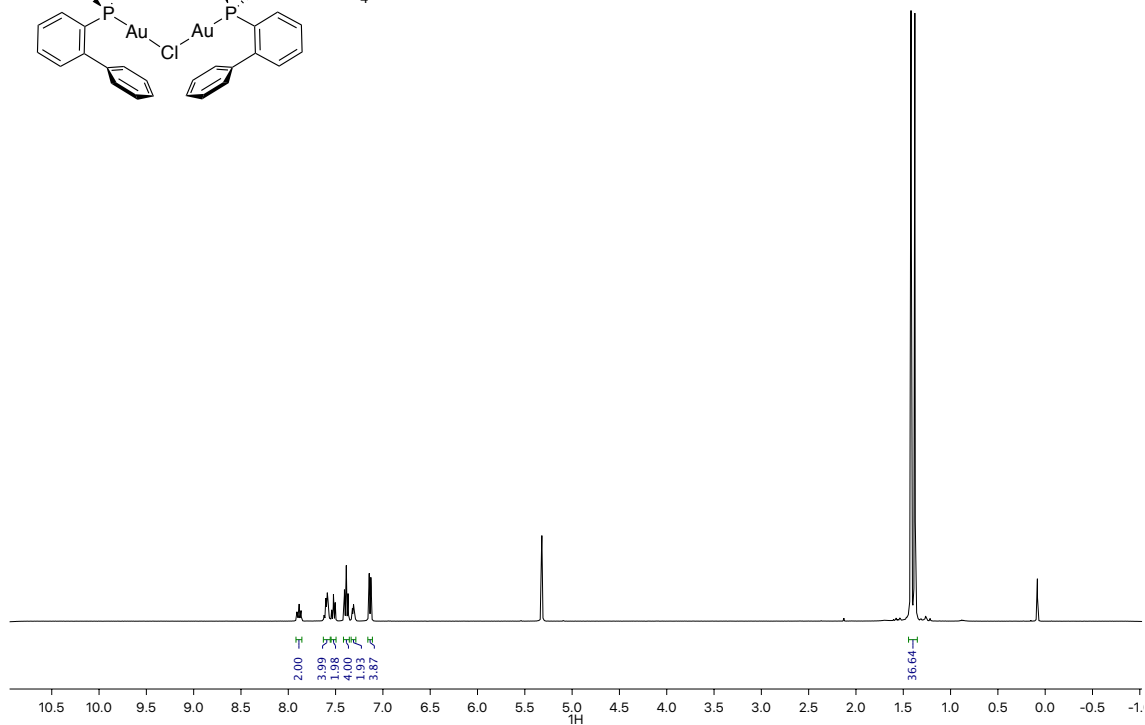
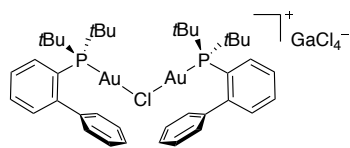


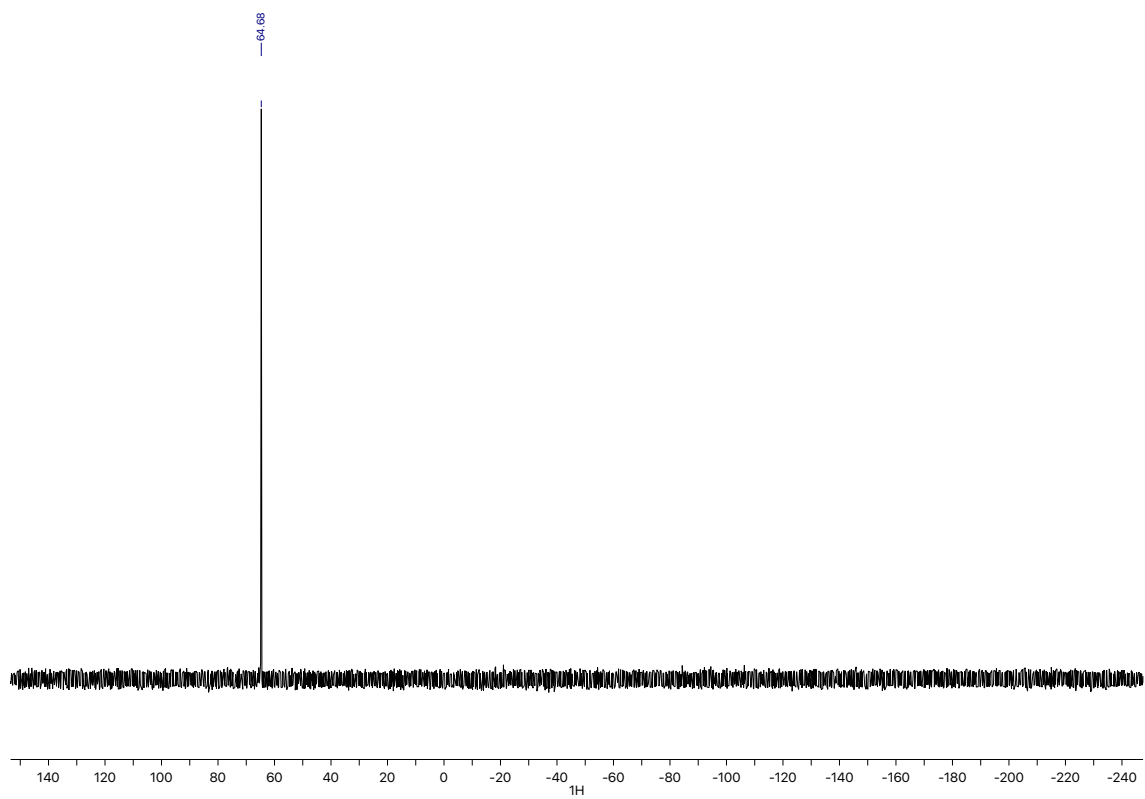
[oMeOJPAuPPh₃][GaCl₄] (S2)



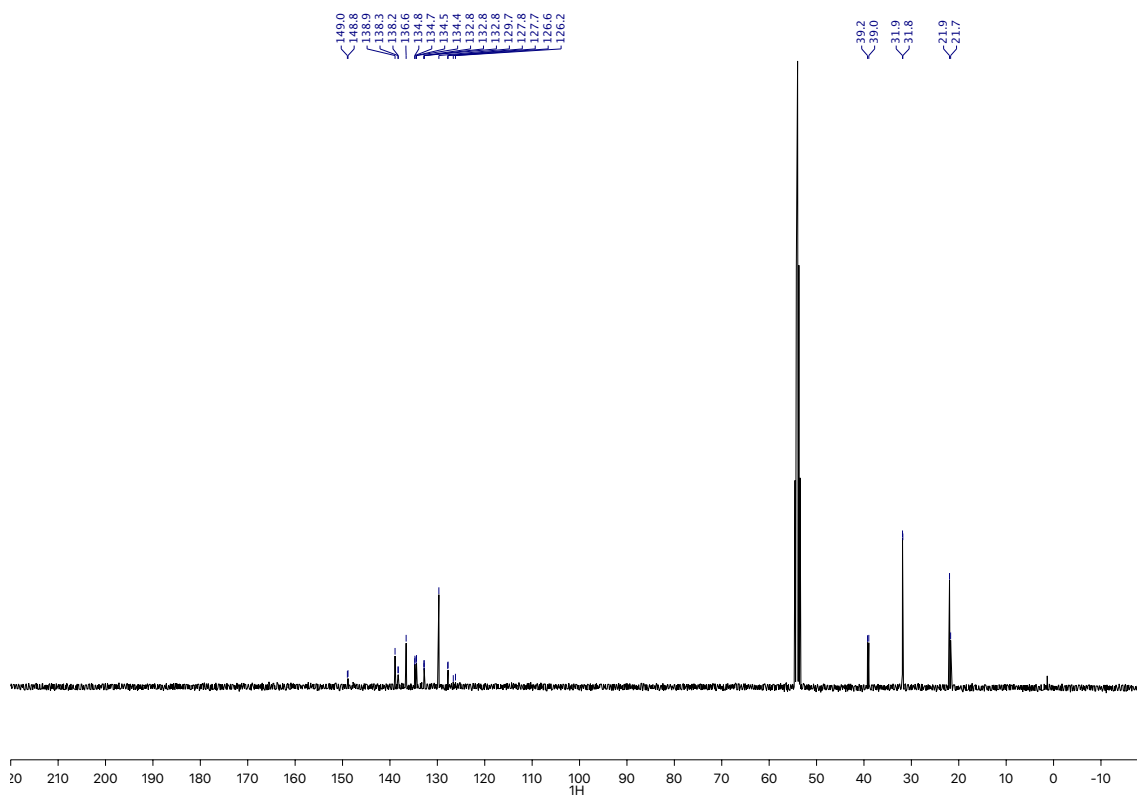
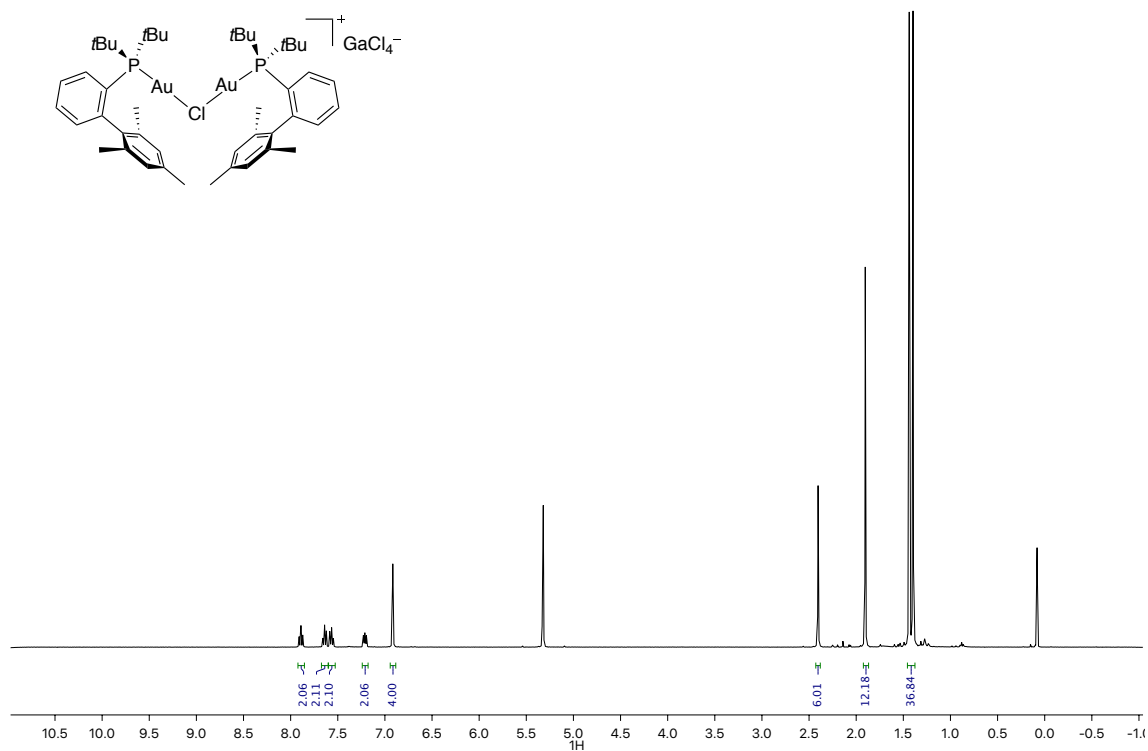
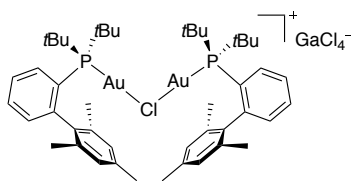


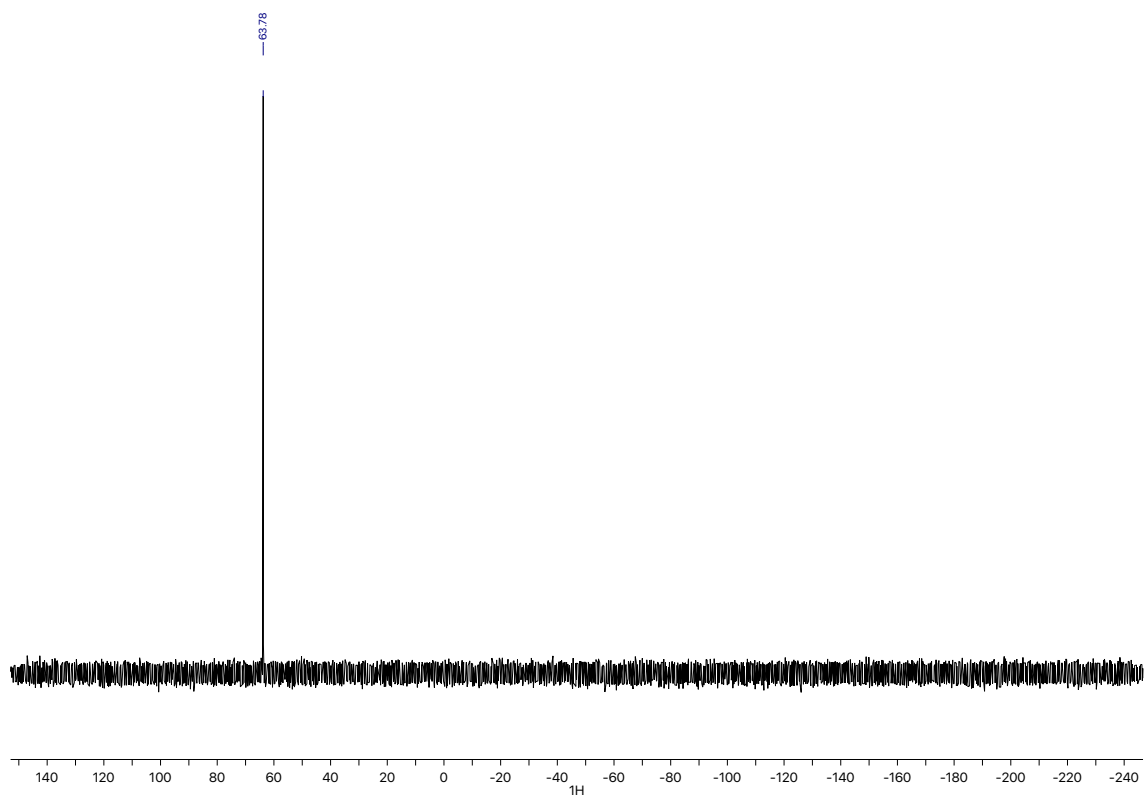
[(2-Di-*t*-butylphosphinobiphenyl)Au]₂Cl][GaCl₄]⁻ (10a)



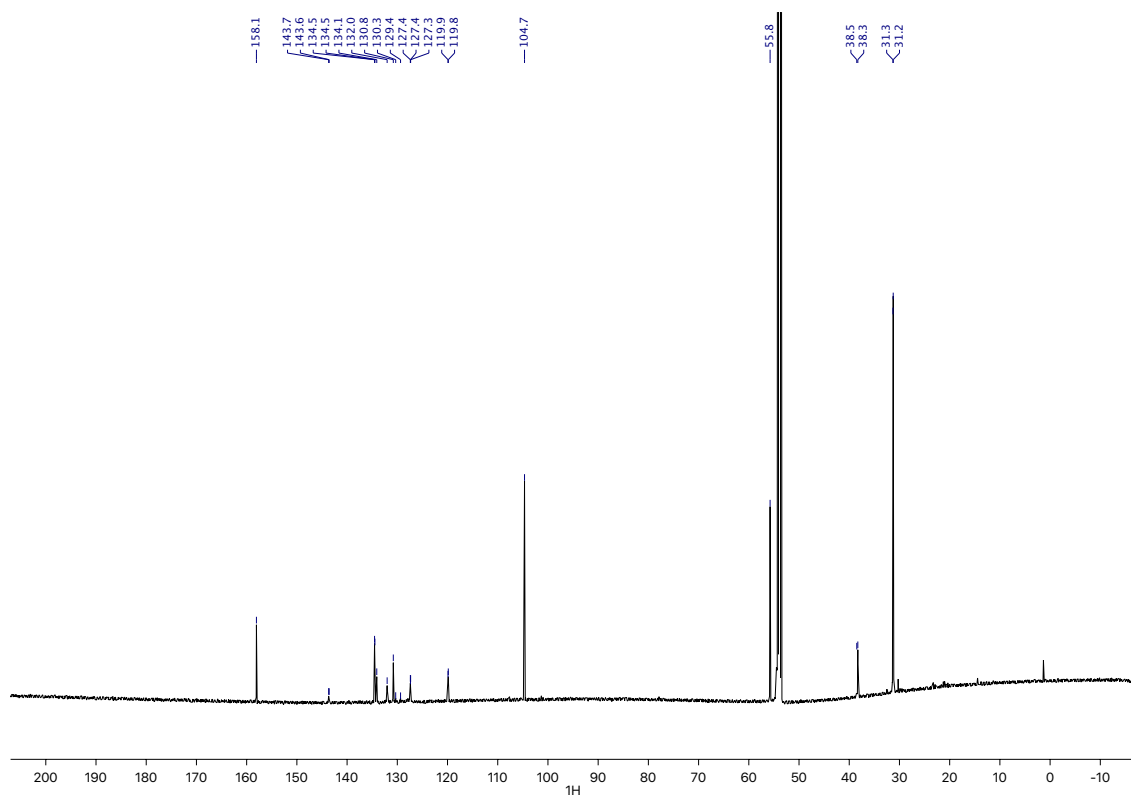
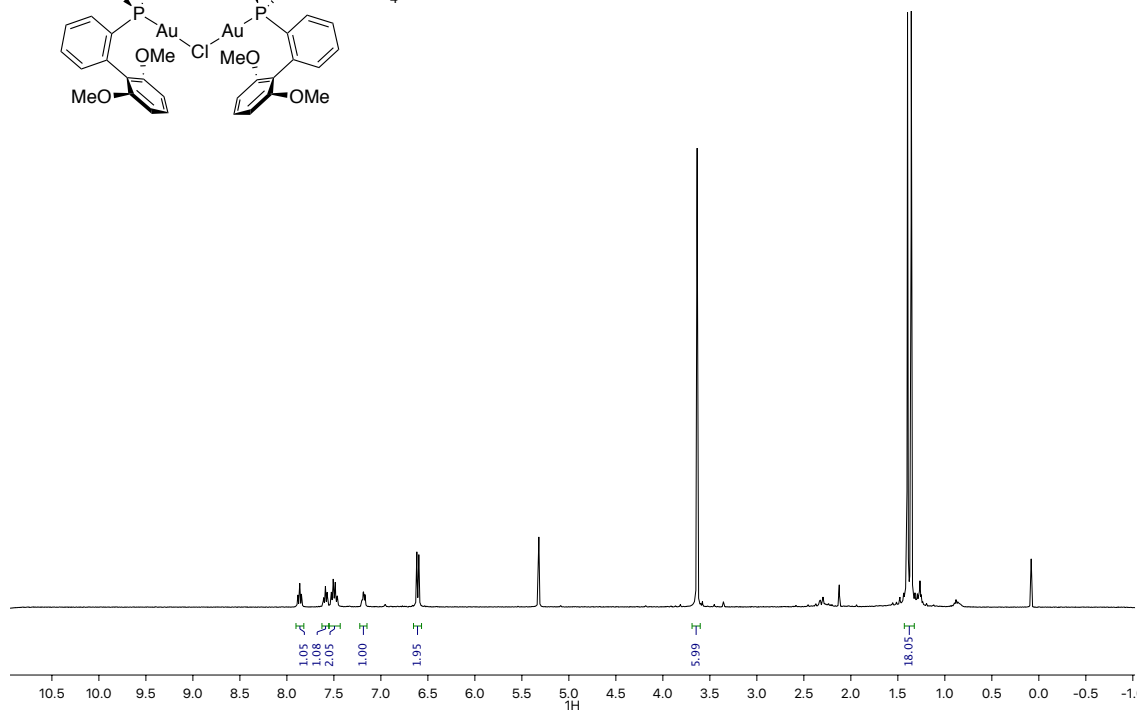
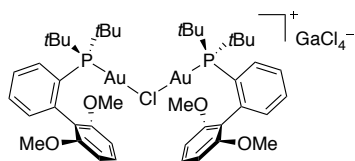


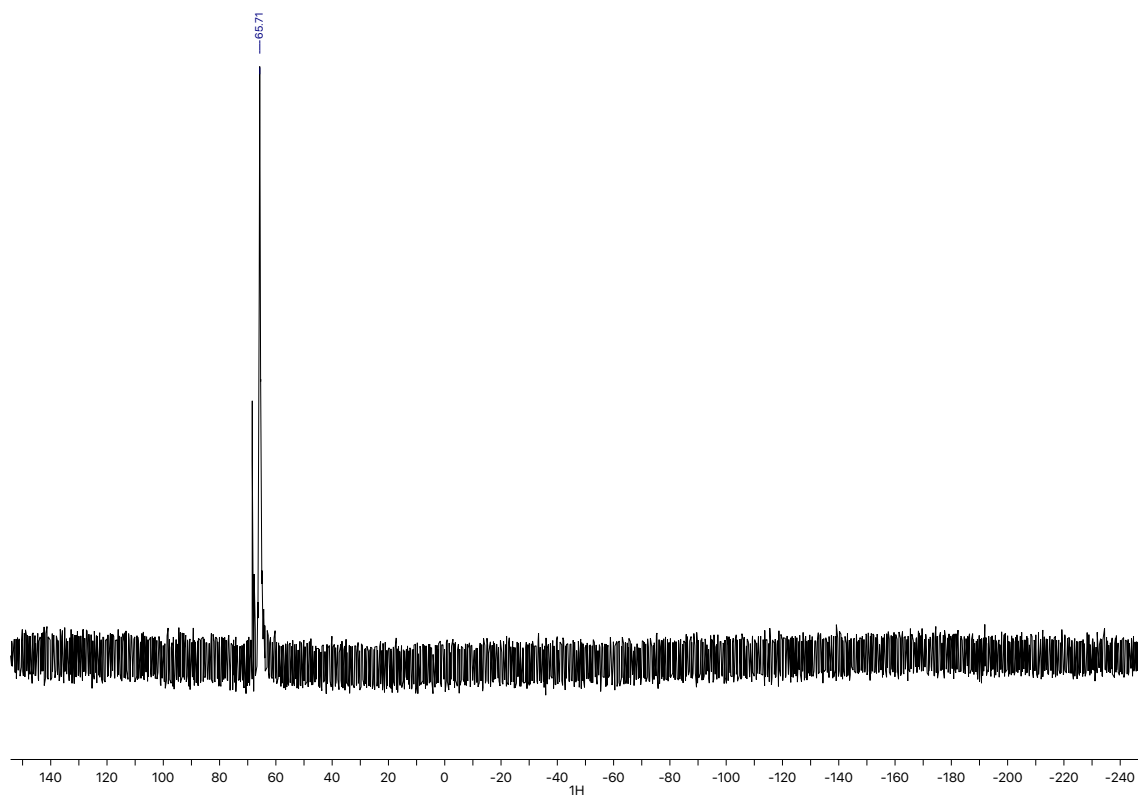
[(2-Di-*t*-butyl-2',4',6'-trimethylphosphinobiphenyl)Au]₂Cl][GaCl₄]⁻ (10b)



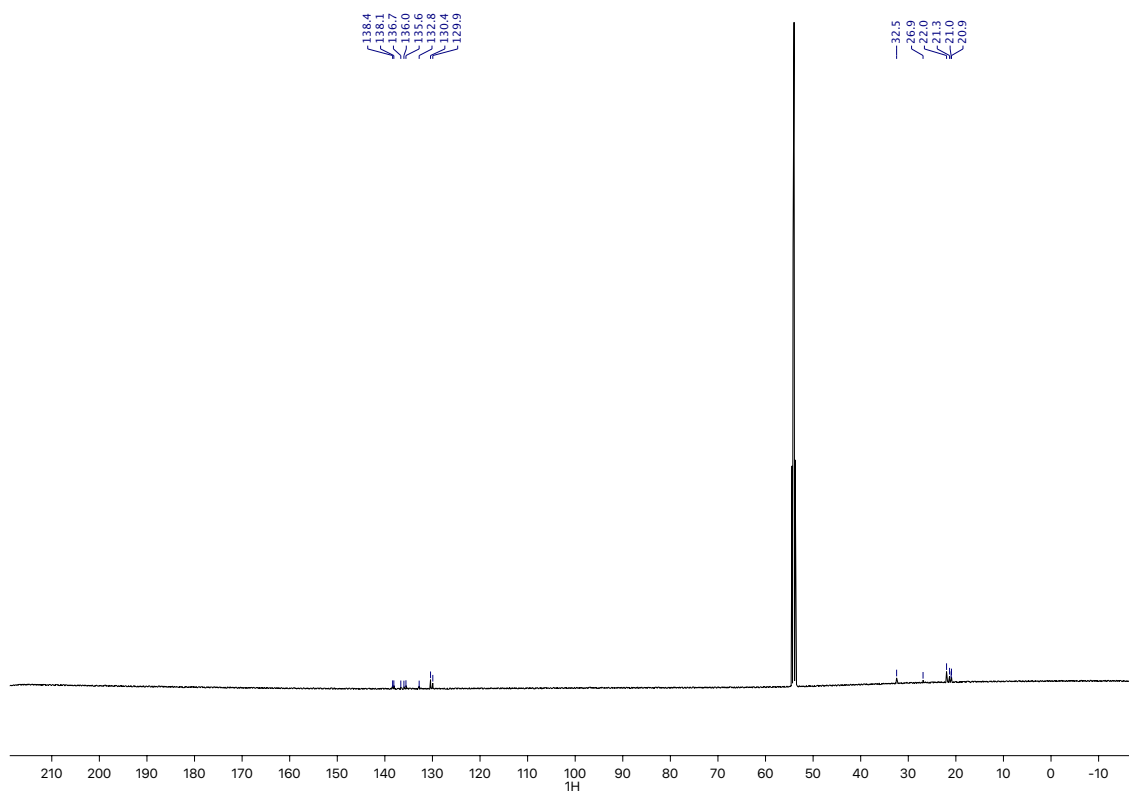
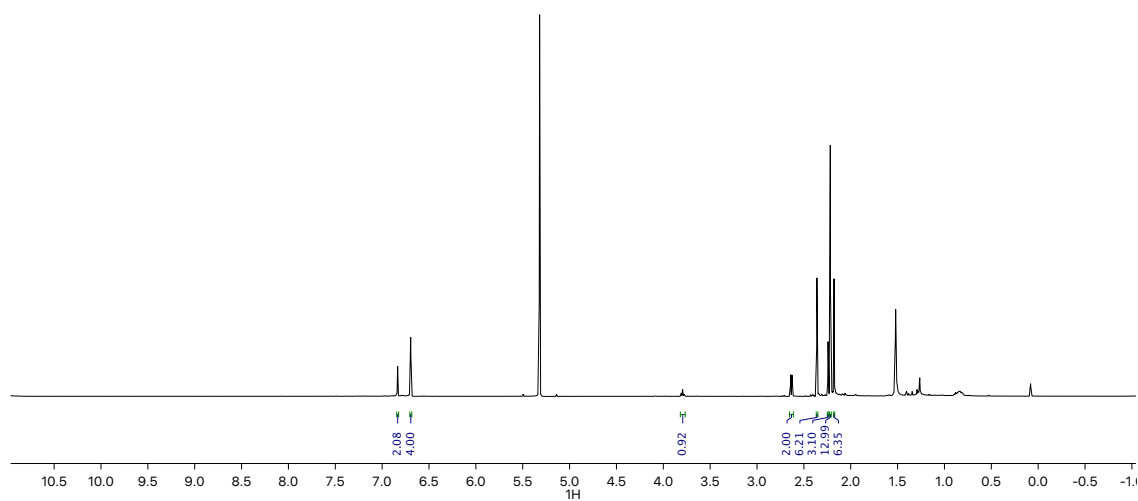
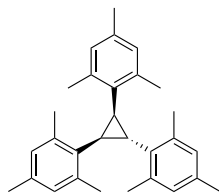


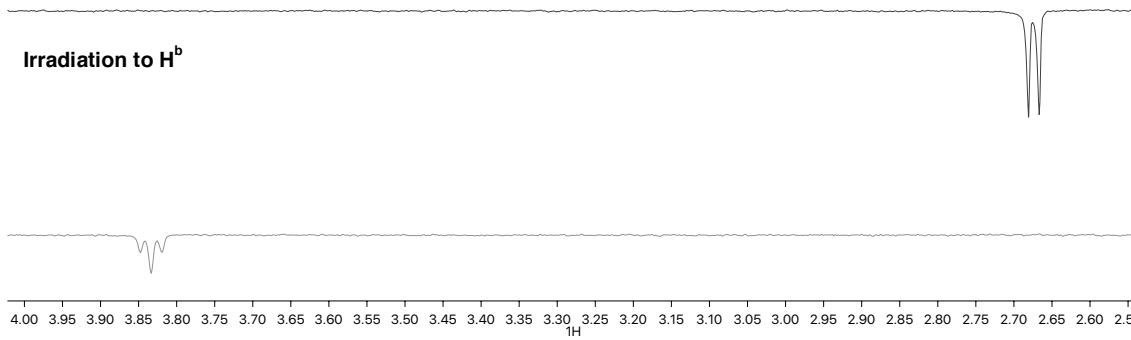
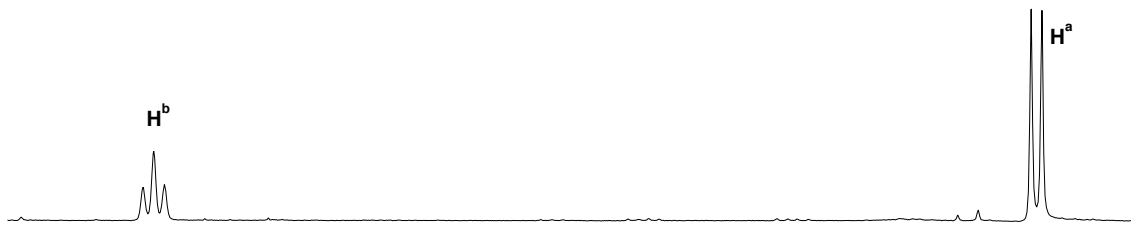
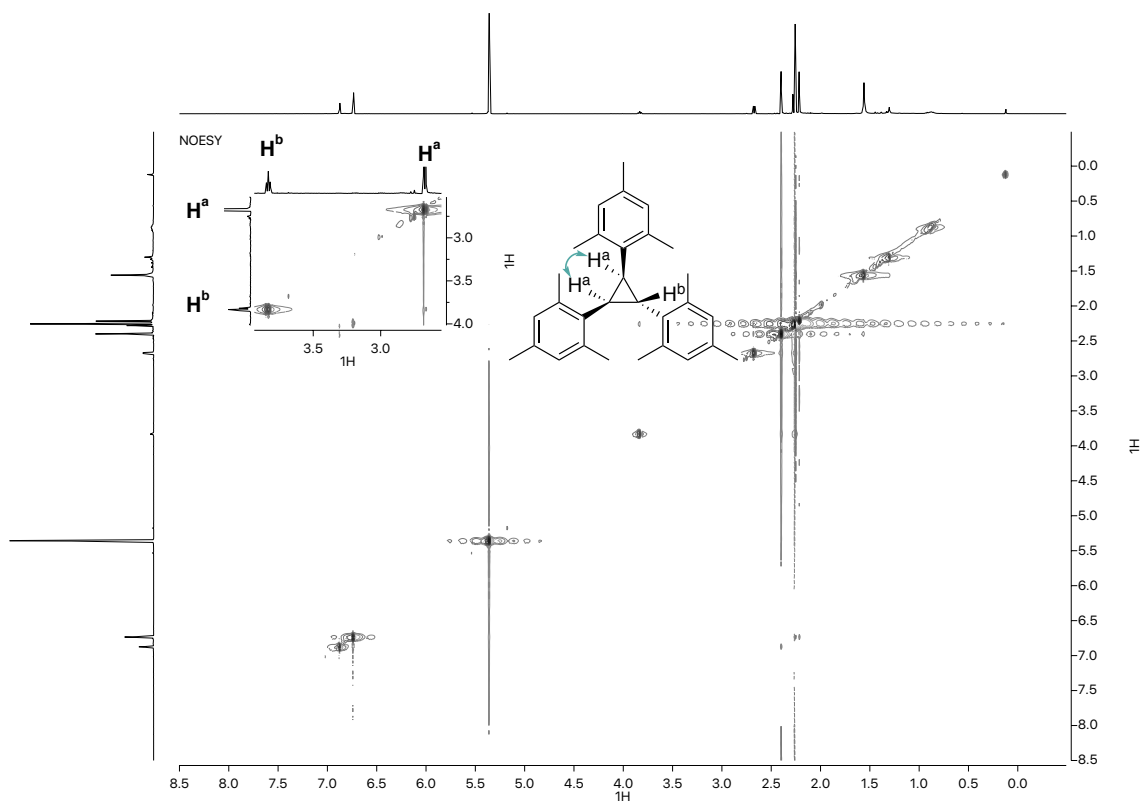
[(2-Di-*t*-butyl-2',6'-dimethoxyphosphinobiphenyl)Au]₂Cl][GaCl₄] (10c)



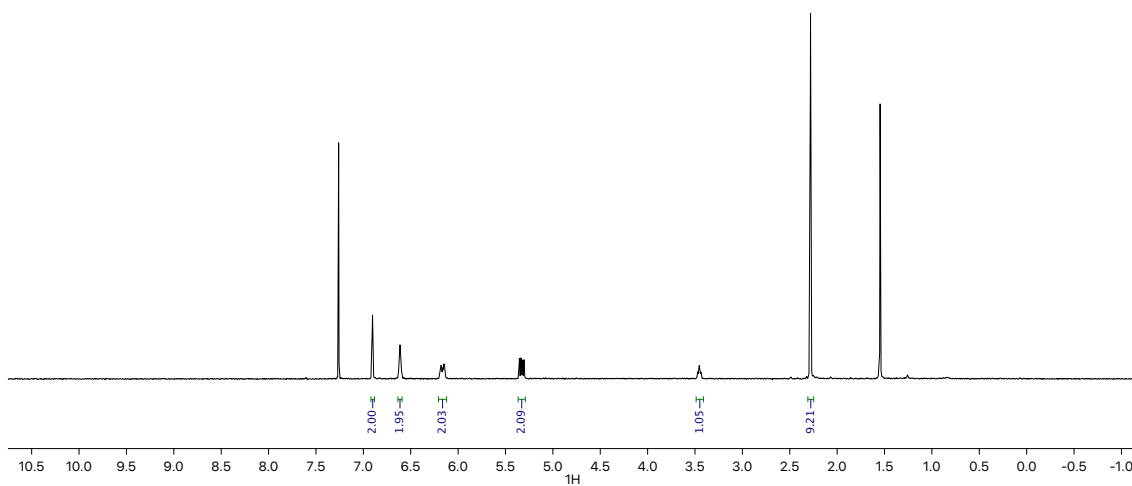
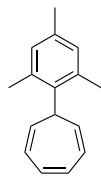


1,2,3-trimesitylcyclopropane (3b)





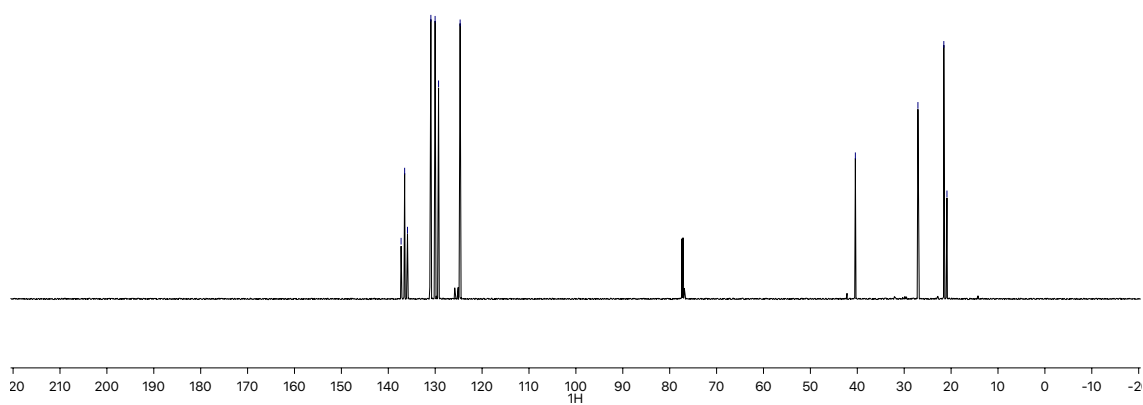
7-mesitylcyclohepta-1,3,5-triene (4a)



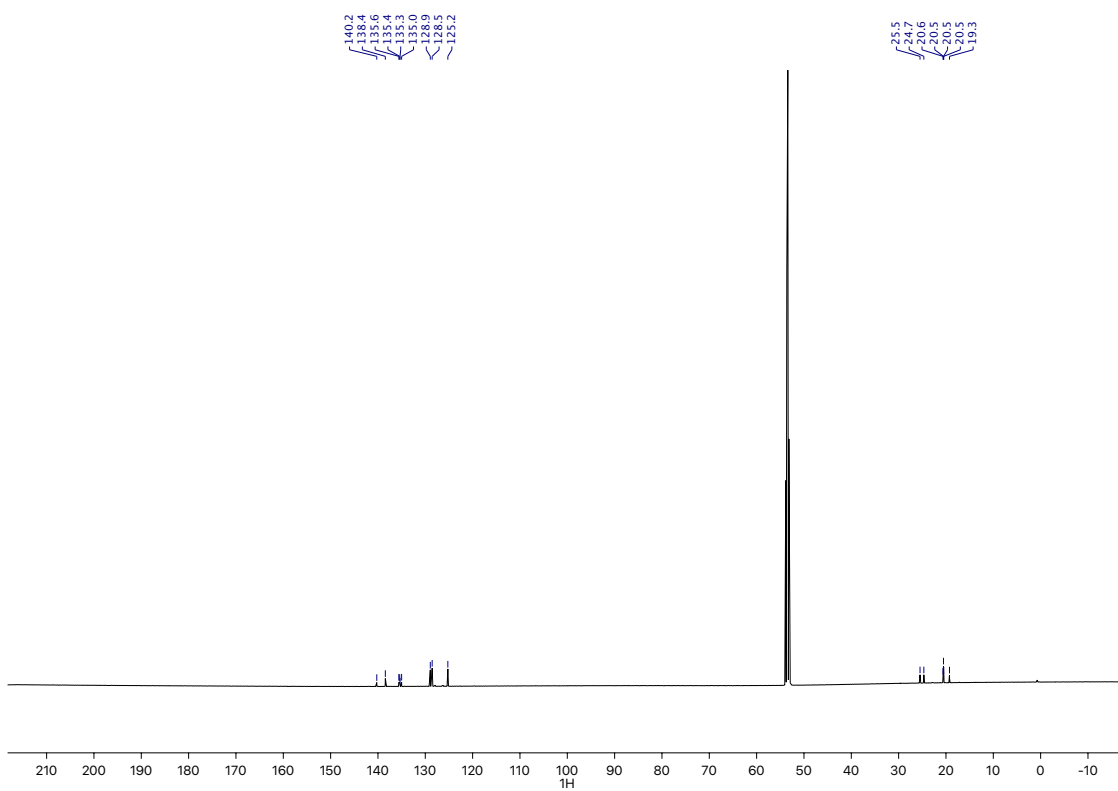
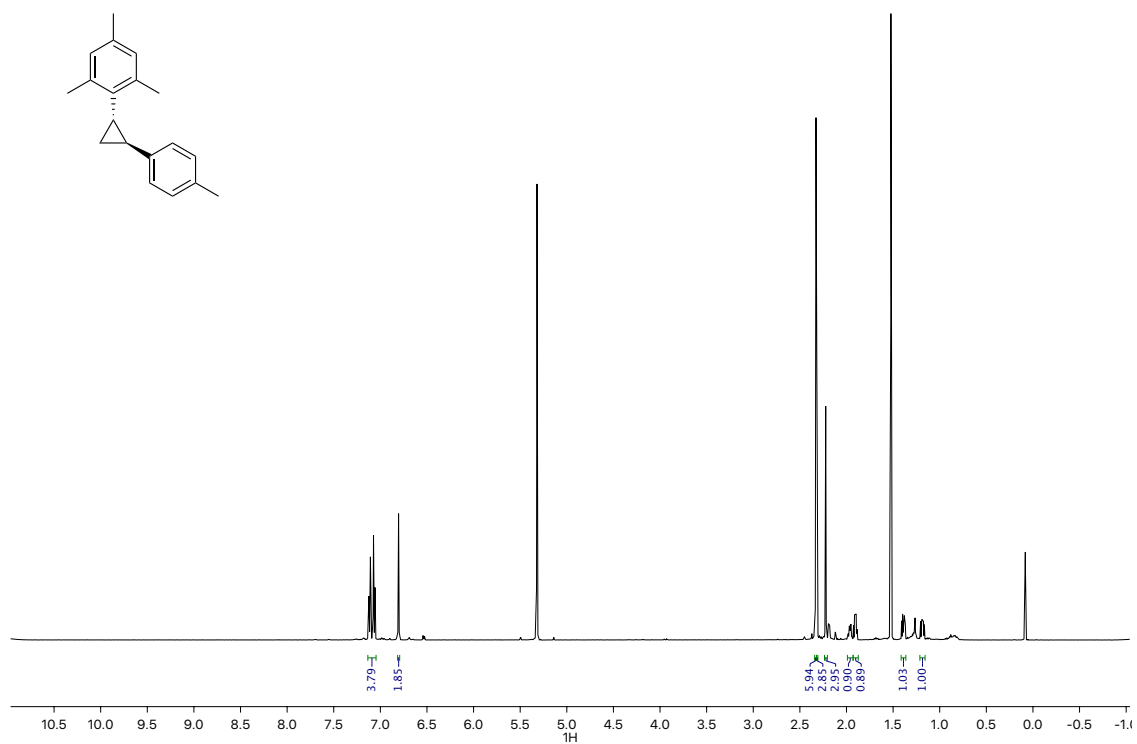
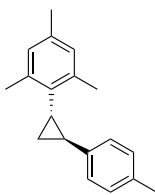
137.3
136.5
136.0
130.9
130.0
129.3
124.7

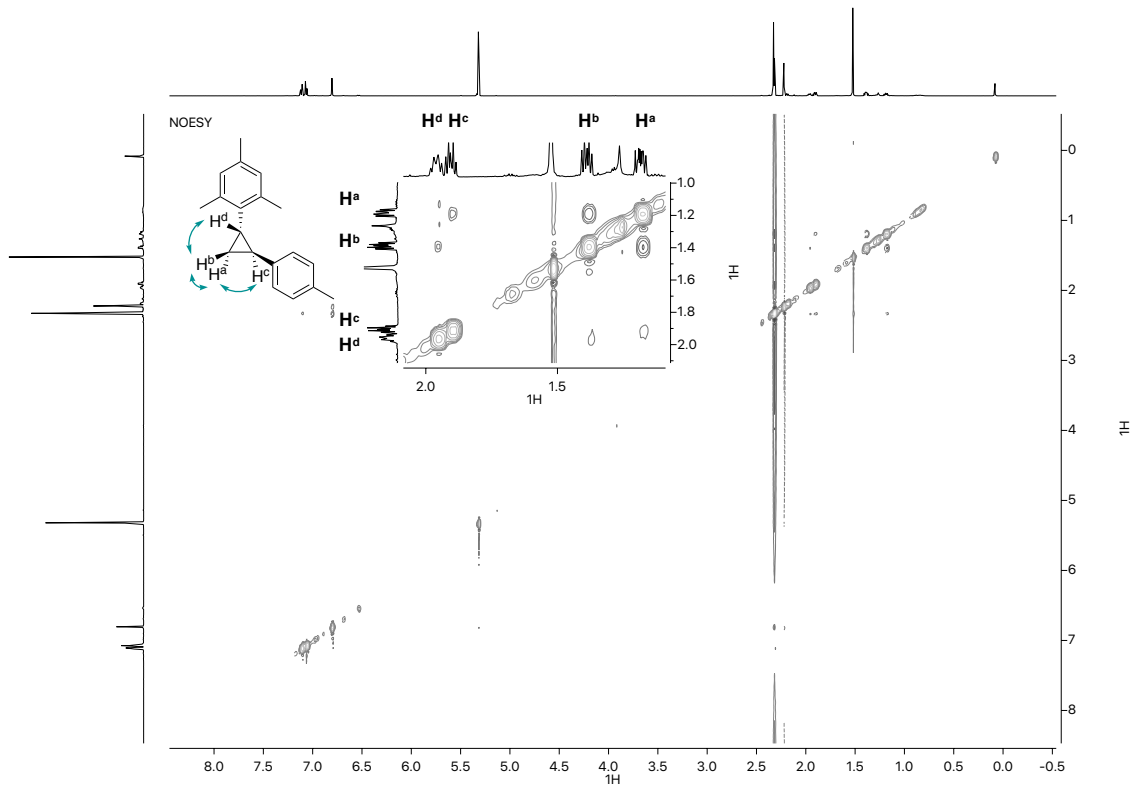
40.4

27.1
21.6
20.9

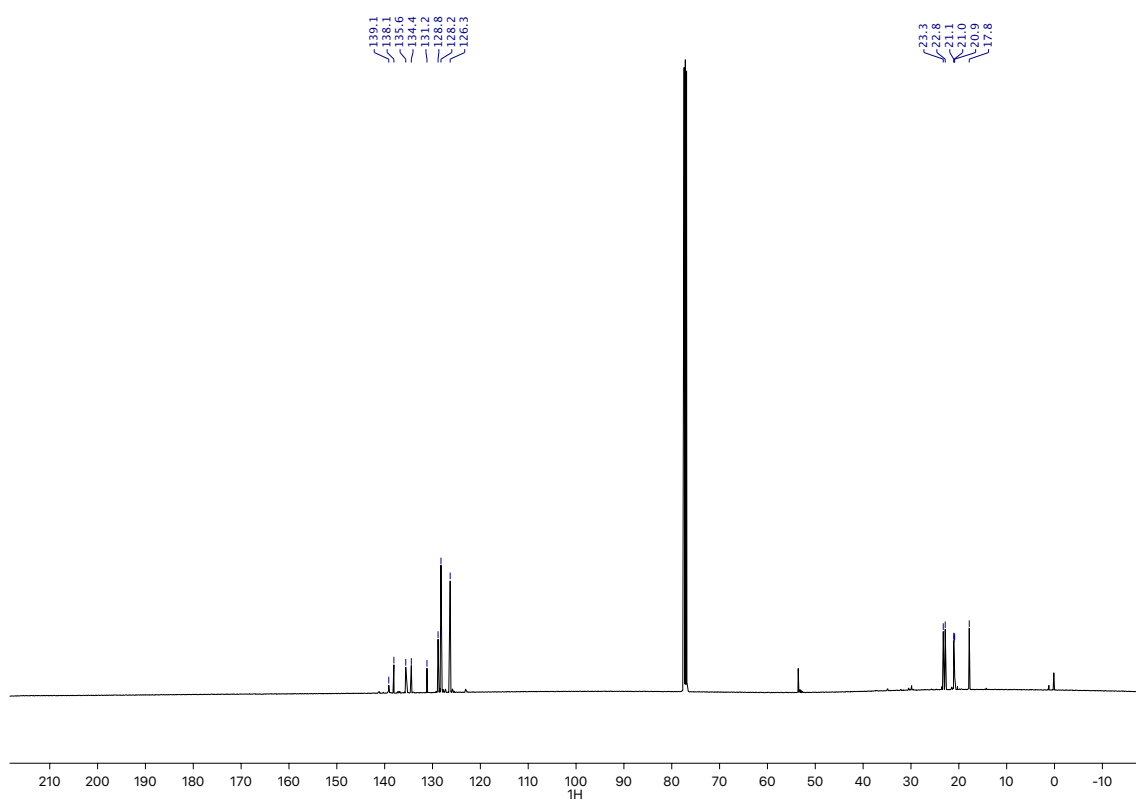
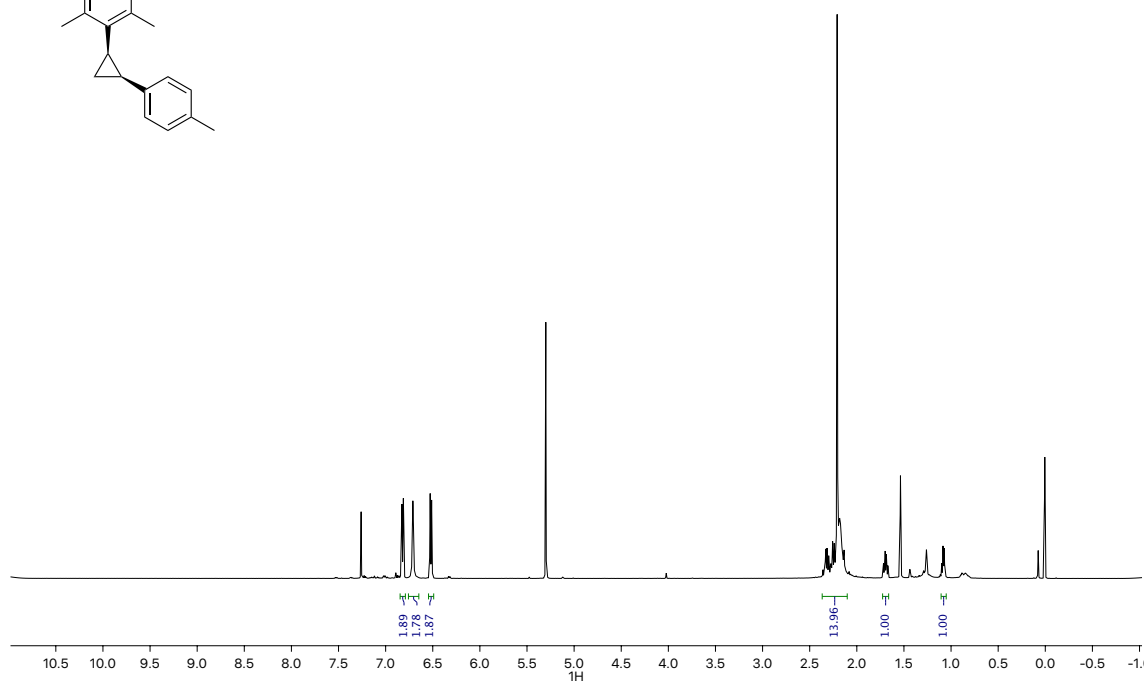
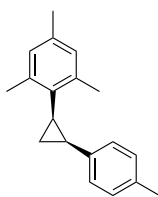


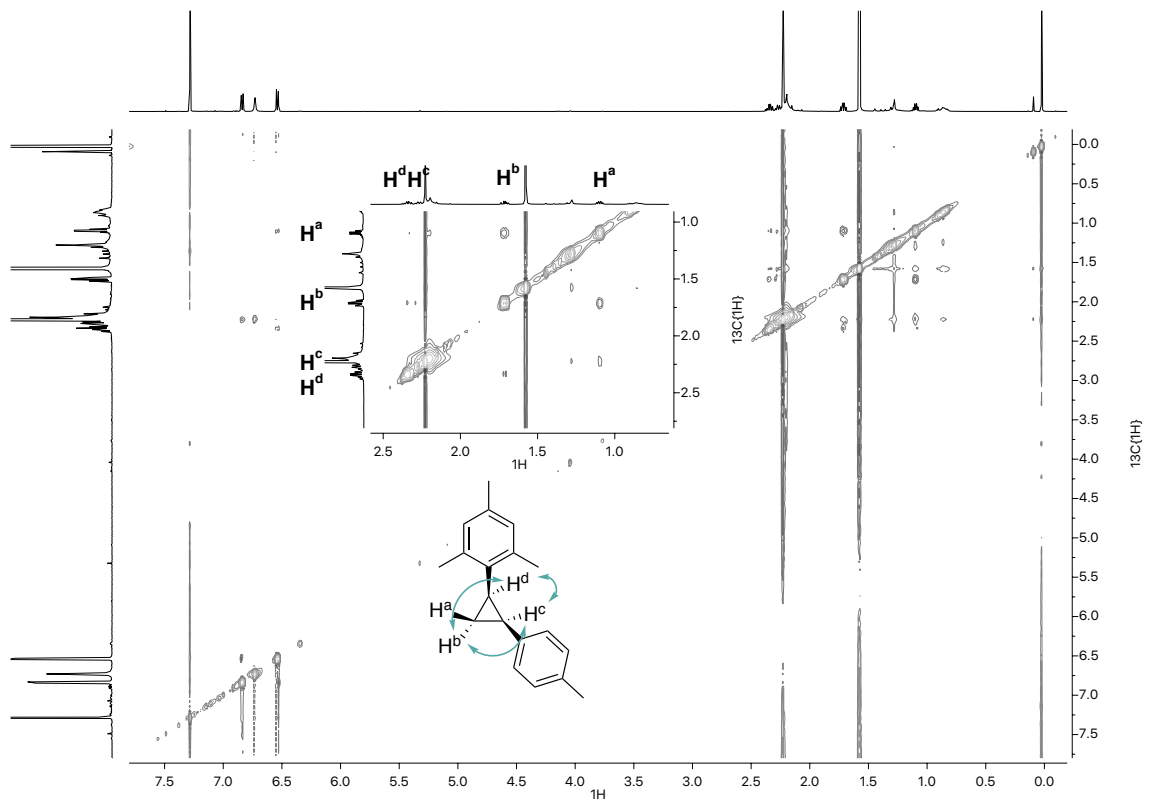
Cyclopropane *trans*-3c



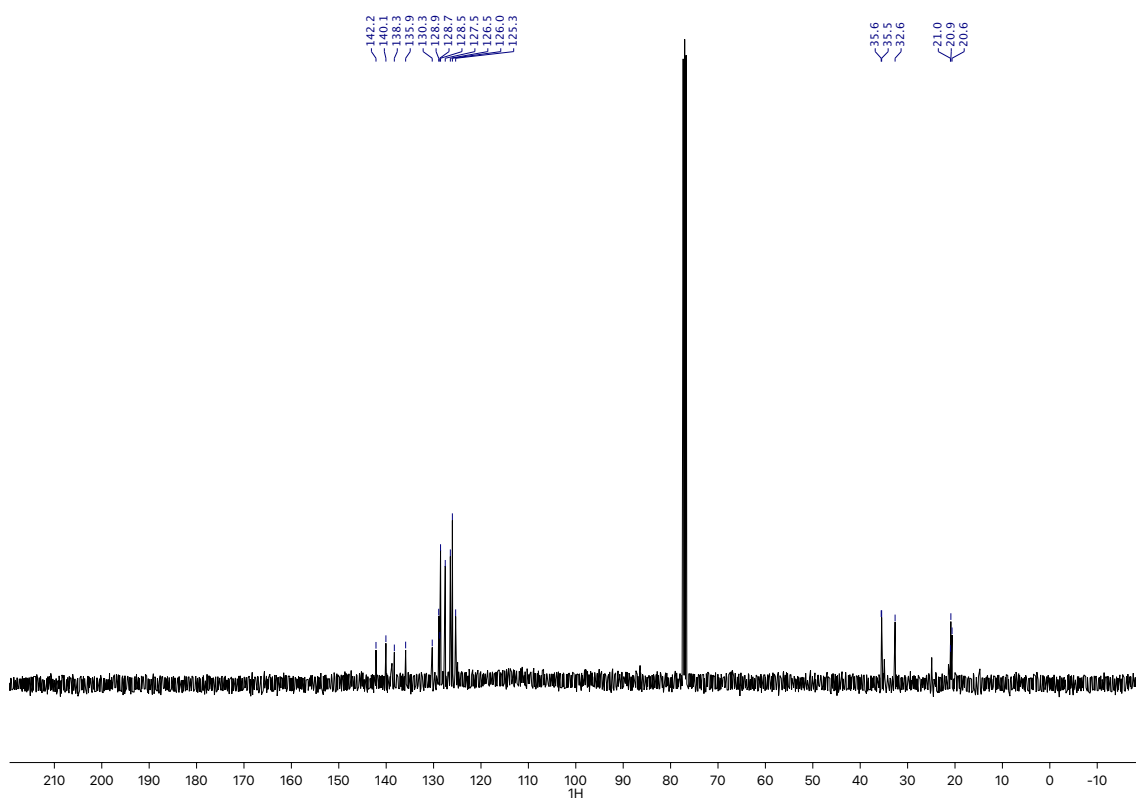
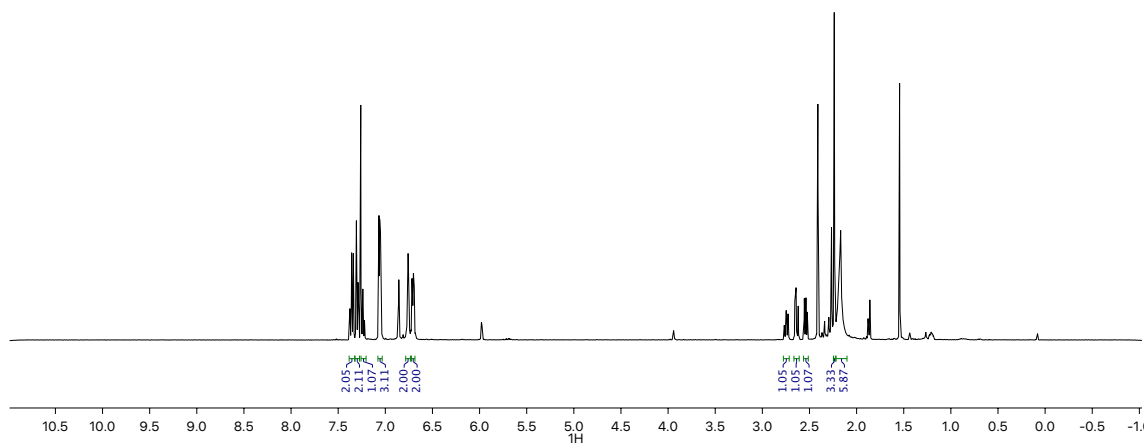
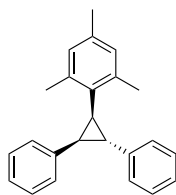


Cyclopropane *cis*-3c

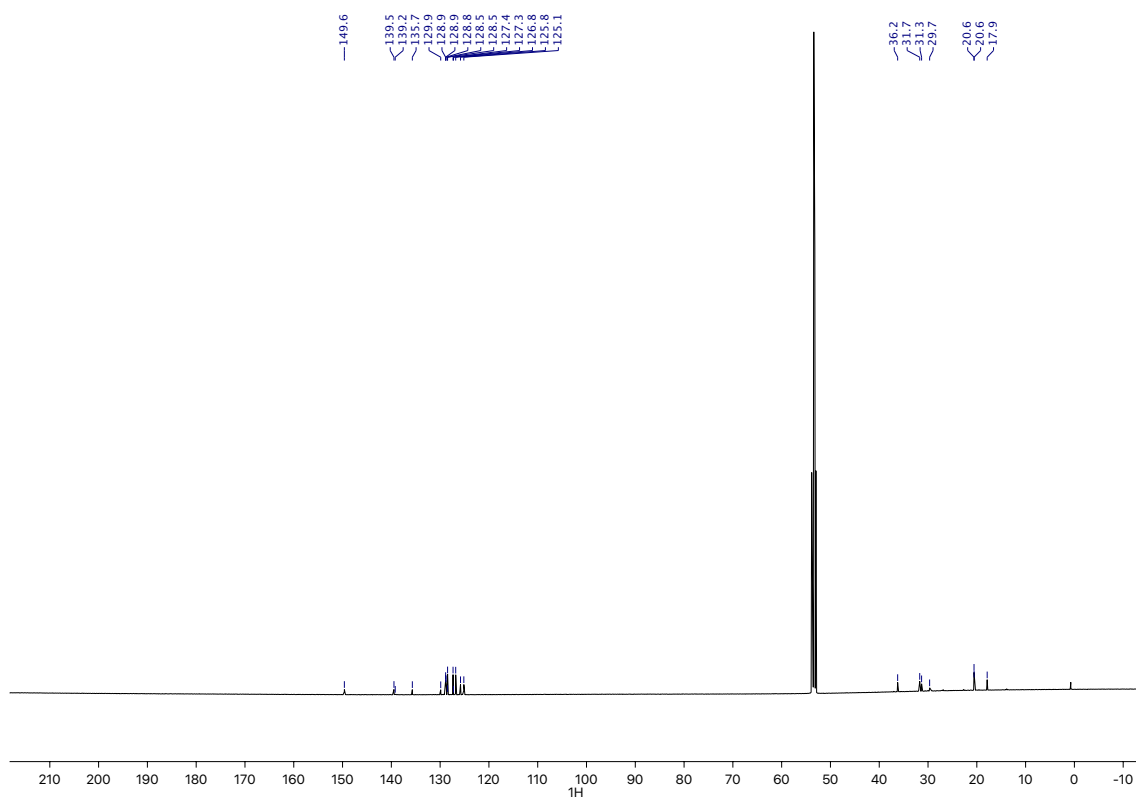
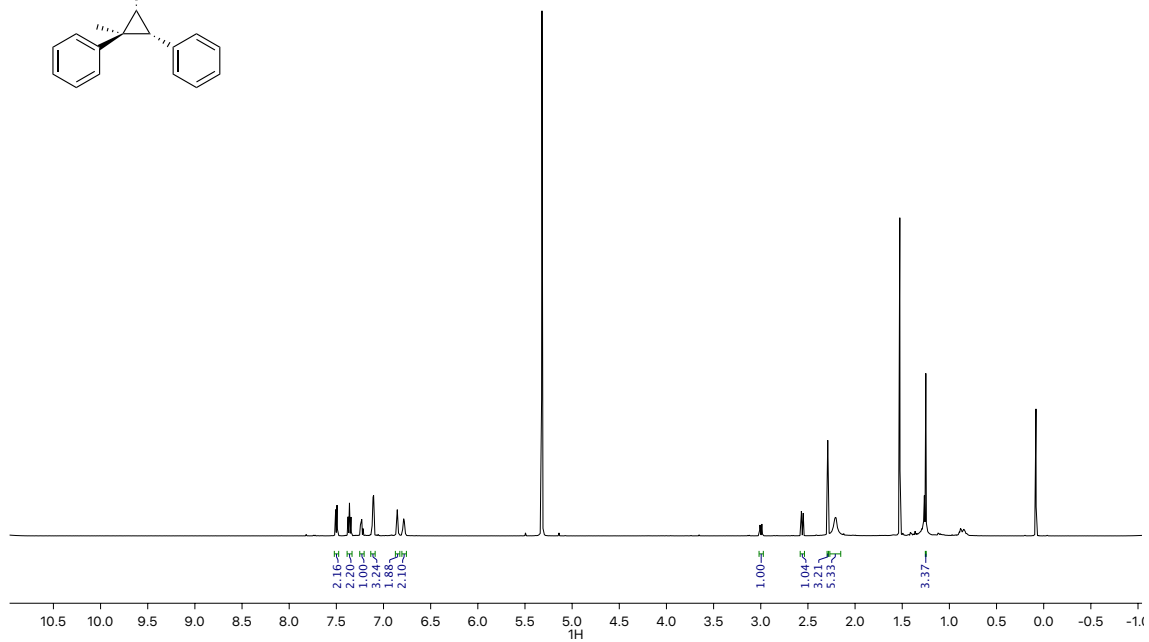
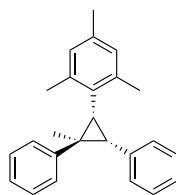


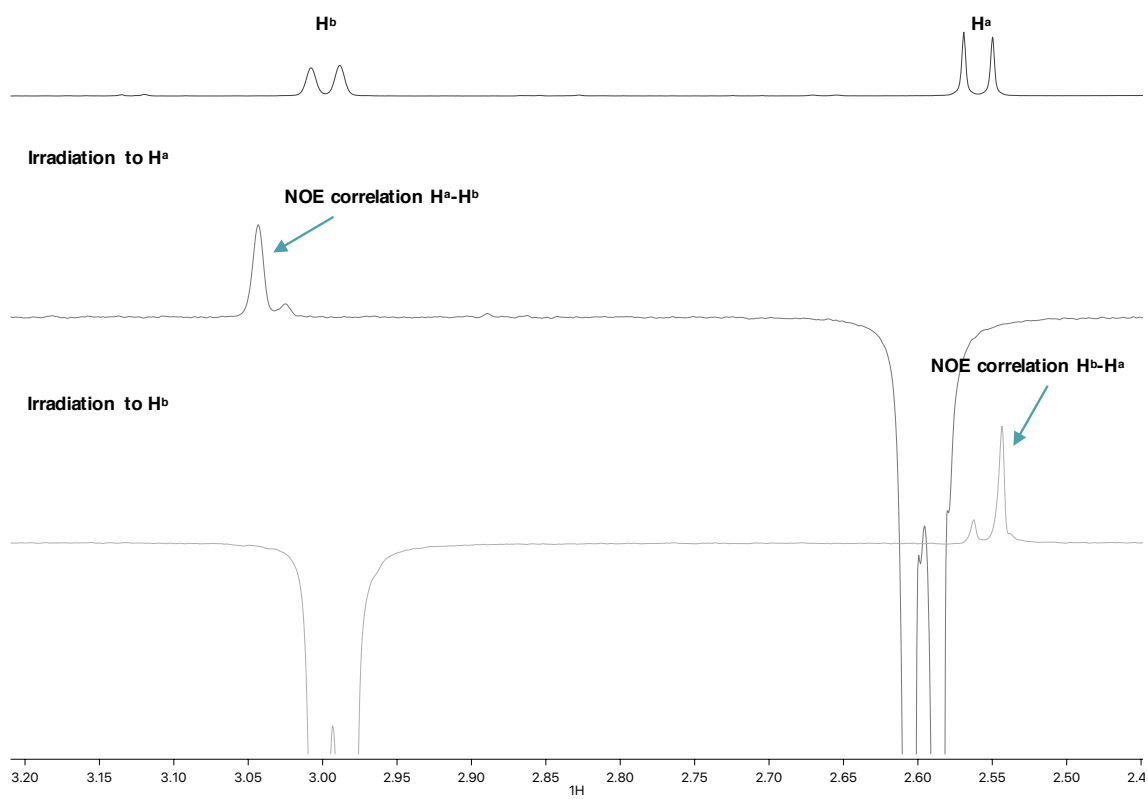
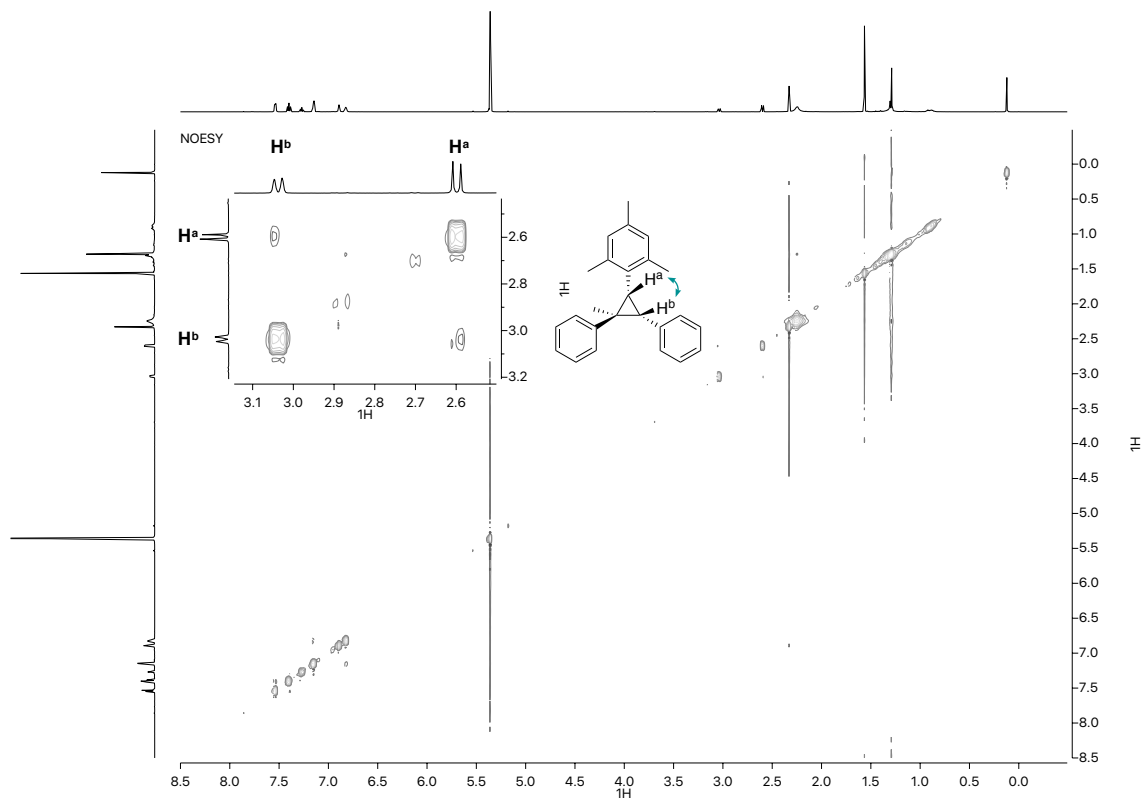


Cyclopropane 3d

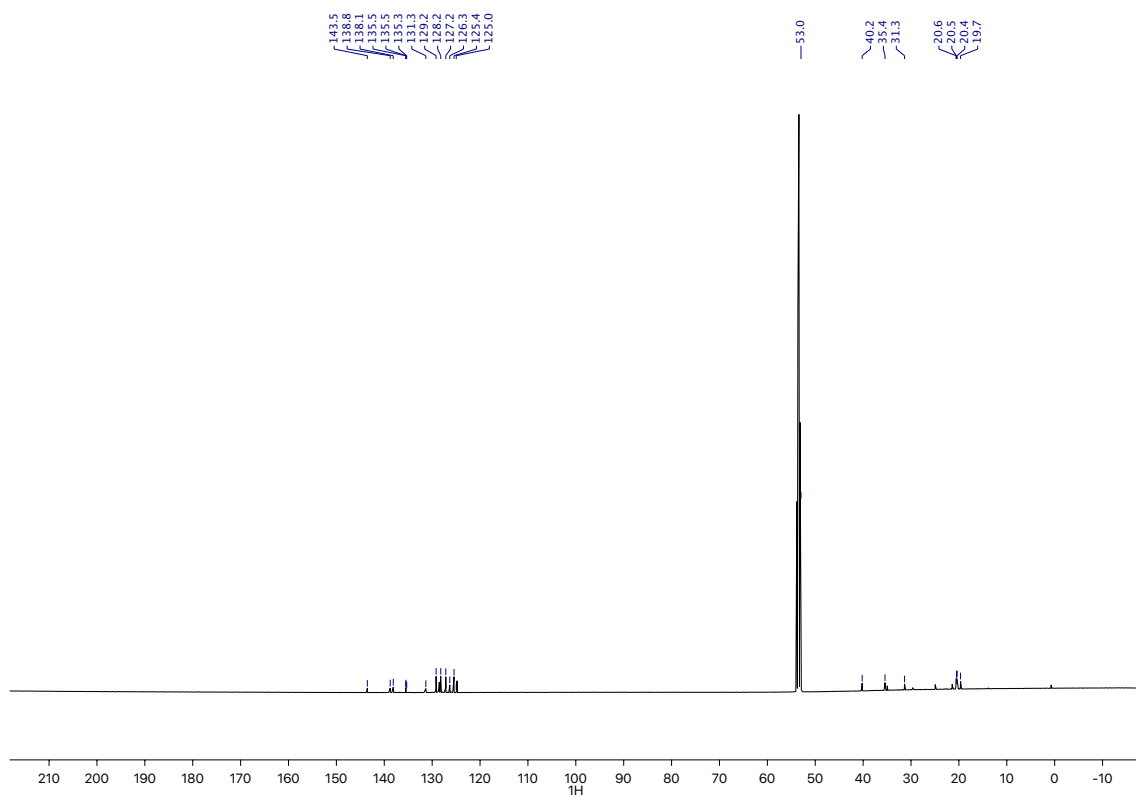
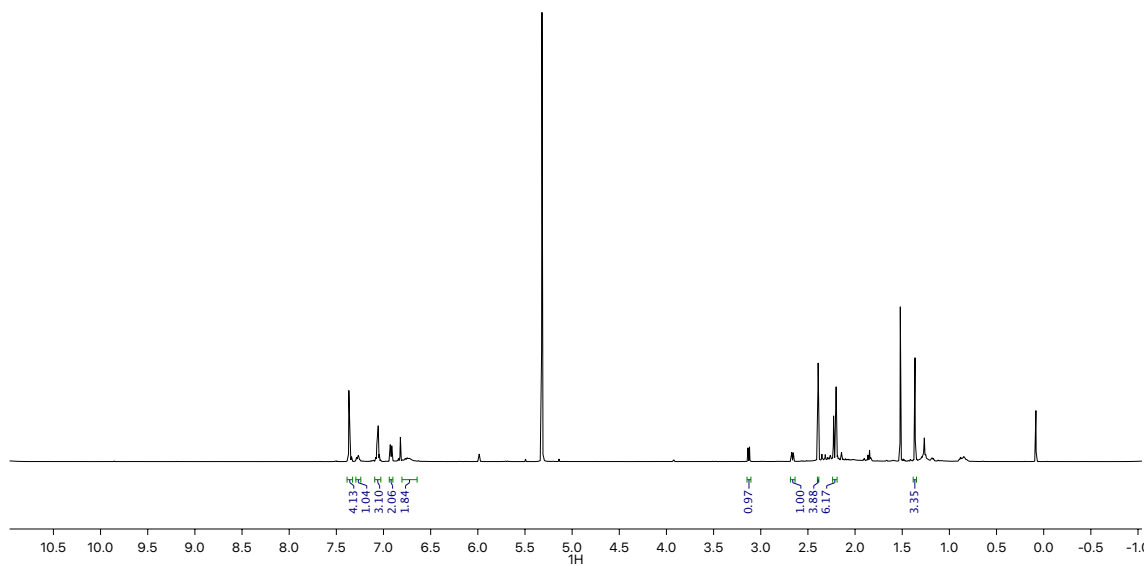
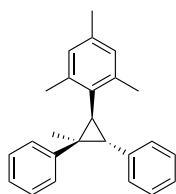


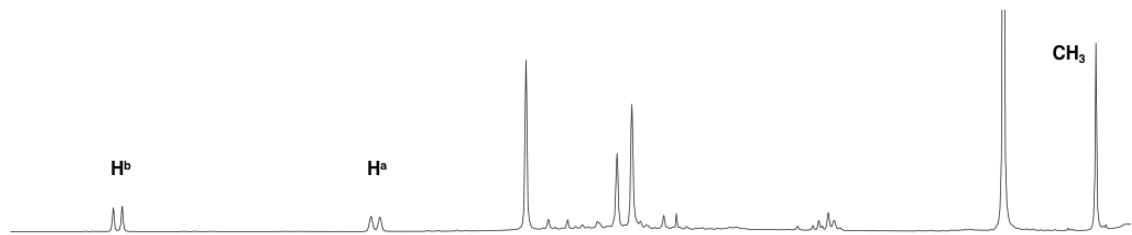
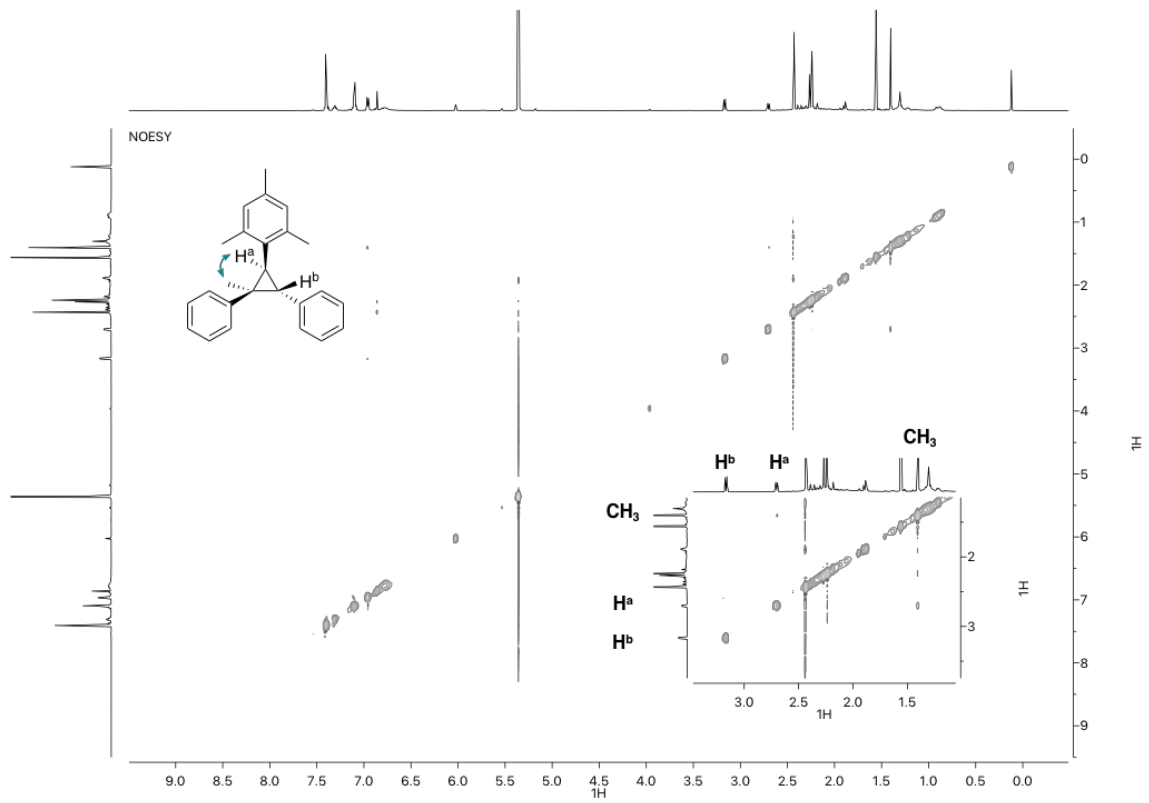
Cyclopropane 3e





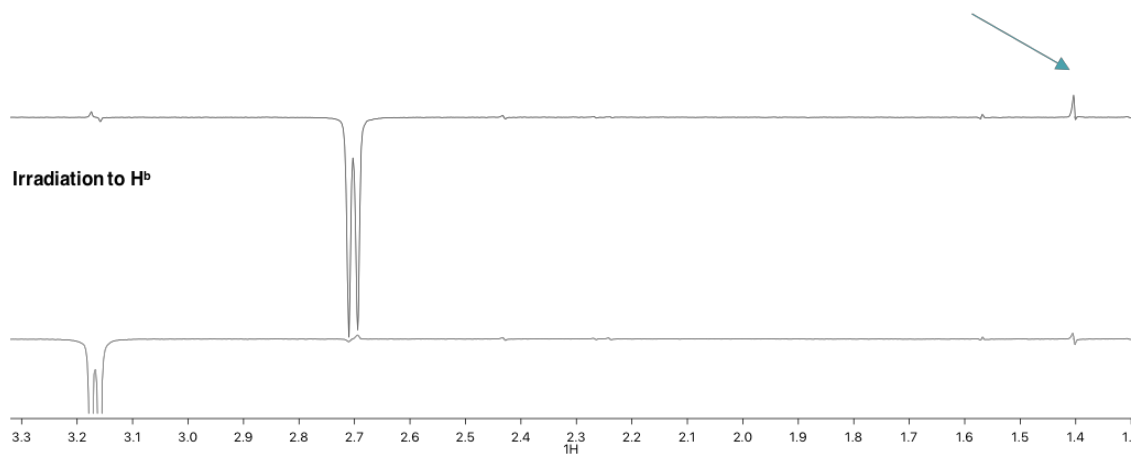
Cyclopropane 3e





Irradiation to H^a

NOE correlation H^a-CH_3



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- ¹ C. H. Burgos, T. E. Barder, X. Huang, S. L. Buchwald, *Angew. Chem. Int. Ed.* **2006**, *45*, 4321-4326.
- ² J.-M. Becht, S. Ngouela, A. Wagner, C. Mioskowski, *Tetrahedron* **2004**, *60*, 6853-6857.
- ³ V. K. Aggarwal, E. Alonso, I. Bae, G. Hynd, M. K. Lydon, M. J. Palmer, M. Patel, P. Marina, J. Richardson, R. A. Stenson, J. R. Studley, J.-L. Vasse, C. Winn, *J. Am. Chem. Soc.* **2003**, *125*, 10926-10940.
- ⁴ Admasu, A.; Platz, M. S.; Marcinek, A.; Michalak, J.; Gudmundsdóttir, A. D.; Gebicki, J. *Journal of physical organic chemistry* **1997**, *10*, 207-220.
- ⁵ Y.-P. Zhao, Y.-L. Yang, R. S. H. Liu, *Green Chem.* **2009**, *11*, 837-842.
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