Electronic Supplementary Material (ESI) for Chemical Science

Synthesis and Reactivity of Terminal Gold(I) Amides and Phosphides

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Supporting Information

General Information

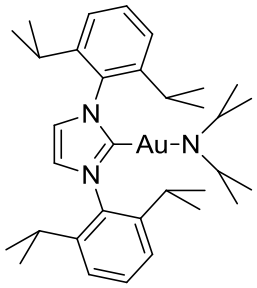
Unless otherwise noted, all manipulations were performed in an inert atmosphere (N_2) glovebox. Glassware was oven-dried overnight or flame-dried under vacuum. All NMR spectra were obtained at ambient temperature using Bruker AV-600, DRX-500, AV-500, AVB-400, AVQ-400, or AV-300 spectrometers. ^{1}H NMR chemical shiftts (δ) are reported in parts per million (ppm) relative to residual solvent peaks (3.58 and 1.73 ppm for THF-d_8, 5.32 ppm for CD_2Cl_2, 7.16 ppm for C_6D_6). ^{13}C NMR chemical shiftts were also reported relative to residual solvent peaks (67.57 and 25.37 ppm for THF-d_8, 54.00 ppm for CD_2Cl_2, 128.06 for C_6D_6). Infrared (IR) spectra were recorded on a Nicolet Avatar FT-IR spectrometer. High-resolution mass spectral data were obtained from the Micromass/Analytical Facillity operated by the College of Chemistry, University of California, Berkeley using Thermo LTQ-FT (ESI) and Fisons VG70 (FAB). X-ray structural analyses were obtained at the University of California, Berkeley CHEXRAY facility (details in the X-ray section below). Combustion analysis data were obtained at the Micro-Mass Facility at the University of California, Berkeley.

Materials

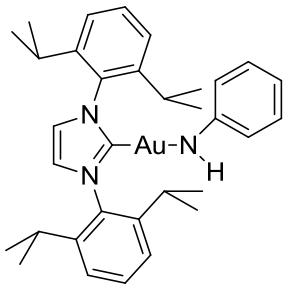
Reagents were purchased from commercial suppliers, checked for purity and used without further purification unless otherwise noted. Pentane, hexane, diethyl ether, toluene, tetrahydrofuran, and methylene chloride were dried and purified by passage through a column of activated alumina (type A2, 12 x 32, UOP LLC), and sparged with N_2 prior to use. Ethyl isocyanate, acrylonitrile, fluorene, benzyl chloride and bromide, and all amines were purified according to literature methods prior to use.[1] Methylene chloride-d_2 was distilled from CaH_2 and degassed prior to use. Tetrahydrofuran-d_8 was passed through a short plug of activated alumina and stored over activated 3 Å molecular sieves prior to use. All lithium amides were prepared by addition of *n*-BuLi in hexane to an excess of amine followed by concentration to yield the

corresponding products as white solids. In purifications utilizing syringe filters, filters of 0.2 μm porosity from National Scientific were used. The compounds IPrAuCl,[2] IPrAuOTf,[3] and BnP(*t*-Bu)$_2$[4] were synthesized by literature methods.

Synthesis of (1,3-bis(2,6-diisopropylphenyl)imidazol-2-ylidene) Gold (I) Complexes

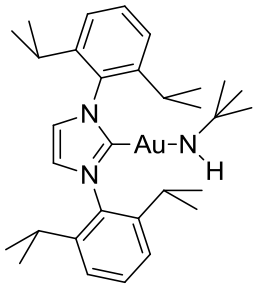


(IPr)gold(I) diisopropylamide (1). To a 20-mL scintillation vial was added IPrAuCl (201 mg, 0.323 mmol) and THF (12 mL). Lithium diisopropylamide (35.5 mg, 0.331 mmol) was added as a solid to the vigorously stirred solution. The reaction mixture immediately turned clear and yellow. After being stirred for 10 min, the solution was concentrated to yield a pale yellow solid. The solid was dissolved in hexane and passed through a syringe filter twice. The hexane solution was concentrated to yield the desired product as a yellow powder (160 mg, 0.23 mmol, 72% yield). X-ray quality crystals were obtained from a concentrated hexane solution of **1** stored at -35 °C. ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.44-7.40 (m, 4 H, aryl), 7.28 (d, 4 H, *J* = 8.0 Hz, *o*-H), 3.16 (sept., 2 H, *J* = 6.5 Hz, amide C(*H*)Me$_2$), 2.73 (sept., 4 H, *J* = 7.0 Hz, IPr C(*H*)Me$_2$), 1.39 (d, 12 H, 7.0 Hz, IPr C(H)*Me*$_2$), 1.20 (d, 12 H, 7.0 Hz, IPr C(H)*Me*$_2$), 0.50 (d, 12 H, *J* = 6.0 Hz, amide C(H)*Me*$_2$). ^{13}C NMR (125 MHz, THF-d_8): δ(ppm) 186.2, 146.9, 136.7, 130.6, 124.7, 123.4, 55.2, 29.8, 28.8, 24.7, 24.6. IR (ATR): ν_{max}(cm^{-1}): 2961, 2867, 1462, 1362,1188, 1061, 946, 804,762. HRMS(*m/z*): calculated for $C_{33}H_{50}AuN_3$ 686.3743, found 686.3743. The instability of this complex and minor aliphatic impurities that could not be removed even upon serial recrystallization prohibited meaningful elemental analysis.

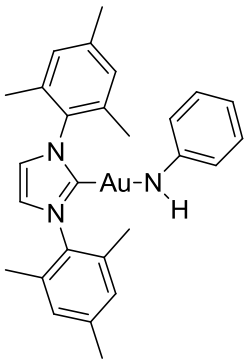


(IPr)gold(I) anilide (2). To a 20-mL scintillation vial was added IPrAuCl (106 mg, 0.170 mmol) and THF (6 mL). Lithium anilide (17.0 mg, 0.172 mmol) was added to the vigorously stirred solution. After being stirred for 10 minutes, the solution was concentrated to a white solid. The solid was dissolved in toluene and passed through a syringe filter. The resulting solution was concentrated to a white solid that that was then recrystallized from diethyl ether to yield the desired product as X-ray quality crystals (71.3 mg, 0.105 mmol, 62% yield). ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.56 (s, 2 H, imidazole), 7.53 (t, 2 H, *J* = 8.0 Hz, *p*-H), 7.56 (d, 4 H, *J* = 7.5 Hz, *m*-H), 6.43 (t, 2 H, *J* = 7.6 Hz, anilide aryl), 585-5.80 (m, 3 H, anilide aryl), 3.49 (s, 1 H, N-*H*), 2.71 (sept., 4 H, J = 7.0 Hz, IPr C(*H*)Me$_2$), 1.36 (d, 12 H, *J* = 6.5 Hz, IPr C(H)*Me*$_2$),

1.23 (d, 12 H, *J* = 6.5 Hz, IPr C(H)*Me*$_2$). ^{13}C NMR (125 MHz, THF-d_8): δ(ppm) 182.0, 160.5, 147.1, 136.2, 131.1, 128.6, 124.9, 124.4, 115.4, 110.8, 29.9, 24.8, 24.4. IR (ATR): ν_{max}(cm^{-1}) 2959, 2926, 2867, 1587, 1486, 1460, 1352, 1182, 802, 743, 689. HRMS(*m/z*): calculated for $C_{33}H_{42}AuN_3$ 678.3117, found 678.3130. Calculated for $C_{33}H_{42}AuN_3$: C, 58.49; H, 6.25; N, 6.20. Found: C, 58.80; H, 6.41; N, 5.88.

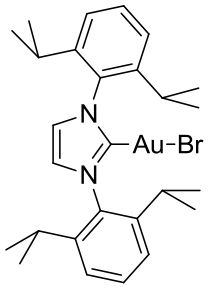


Generation of (IPr)gold(I) *t*-butylamide (3). IPrAuCl (10.0 mg, 0.016 mmol) and hexamethylbenzene (1.1 mg, 0.007 mmol) were dissolved in THF-d_8 and transferred to a J. Young NMR tube. The spectrum of this mixture was then obtained. Lithium *t*-butylamide (1.3 mg, 0.016 mmol) was dissolved in THF-d_8 and transferred to the NMR tube. The reaction mixture immediately changed from colorless to bright orange and then to colorless again. The product was present in 68% yield as determined by reference to the internal standard. ^{1}H NMR (300 MHz, THF-d_8): δ(ppm) 7.45-7.42 (m, 4 H, aryl), 7.29 (d, 4 H, *J* = 7.8 Hz, *m*-H), 2.71 (sept., 4 H, *J* = 6.9 Hz, IPr C(*H*)Me$_2$), 1.38 (d, 12 H, *J* = 6.6 Hz, IPr C(H)*Me*$_2$), 1.20 (d, 12 H, *J* = 6.9 Hz, IPr C(H)*Me*$_2$), 0.68 (s, 9 H, *t*-Bu). The N—H proton was not observed.

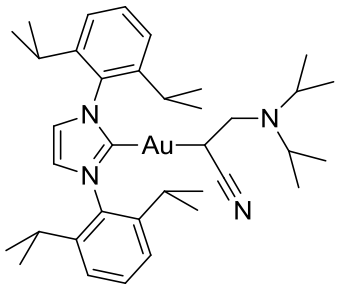


(IMes)gold(I) anilide (4). To a stirred suspension of IMesAuCl (100.9 mg, 0.188 mmol) and THF (7 mL) in a 20-mL scintillation vial was added lithium anilide (20.0 mg, 0.202 mmol). After being stirred for ten min, the homogenous clear solution was concentrated to yield an off-white solid. The solid was dissolved in toluene (10 mL) and filtered through a syringe filter. An overnight recrystallization at -35°C in toluene yielded the desired product as off-white crystals (63.5 mg, 57% yield). ^{1}H NMR (600 MHz, THF-d_8): δ(ppm) 7.41 (s, 2H, imidazole), 7.07 (s, 4H, mes), 6.47 (t, 2H, *J* = 7.7 Hz, anilide *m*-H), 5.90 (d, 2H, *J* = 7.6 Hz, anilide *o*-H), 5.86 (t, 1H, *J* = 7.1 Hz, anilide *p*-H), 3.46 (s, 1H, N-*H*), 2.37 (s, 6H, *p*-Me), 2.16 (s, 12H, *o*-Me). ^{13}C (150 MHz, THF-d_8): δ(ppm) 180.2, 140.1, 138.6, 136.1, 130.1, 128.6, 123.2, 115.5, 110.9,

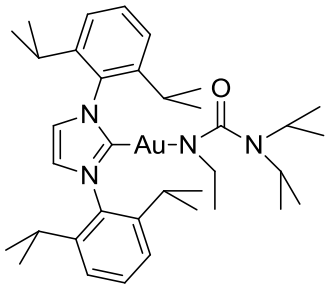
21.4, 18.2. IR (ATR): ν_{max}(cm^{-1}) 3133, 3013, 2913, 1596, 1580. 1485, 1304, 855, 732. HRMS (*m*/*z*): calculated for $C_{27}H_{30}N_3Au$ 593.2105, found 593.2115. Calculated for $C_{27}H_{30}AuN_3$: C, 54.64; H, 5.09; N, 7.08. Found: C, 56.22; H, 5.23; N, 6.64.



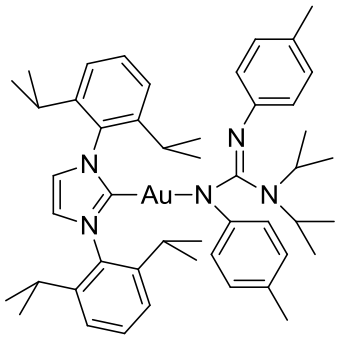
Complex 5. To a weighed vial containing **1** (50 mg, 0.073 mmol) and a Teflon stir bar was added THF (2 mL). Benzyl bromide (25 mg, 0.15 mmol) was added via syringe and the reaction mixture was stirred at 23 °C for 4 h. The reaction mixture was concentrated and the resulting solid washed with pentane (2 x 1 mL). The product was isolated as a white solid (47 mg, 0.072 mmol, 98%). The ^{1}H NMR spectrum of **8** matches that found in the literature.[5] The identity of the organic fragment (N,N-diisopropyl-benzylamine) was confirmed by ^{1}H NMR by comparison to a sample synthesized by a literature method.[6]



Complex 6. To a vial containing **1** (50.1 mg, 0.073 mmol) and a Teflon stir bar was added THF (2 mL). Acrylonitrile (7.8 mg, 0.15 mmol) was added via syringe and the reaction mixture was stirred for 30 min. The reaction mixture was concentrated to yield a crude solid that was washed with hexane (2 mL). Removing the remaining solvent under vacuum yielded a pale yellow solid (48.8 mg, 0.066 mmol, 90% yield). X-ray quality crystals were obtained from a concentrated solution of **9** in diethyl ether stored at -35 °C. ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.54 (s, 2H, imidazole), 7.48 (t, 2 H, *J* = 7.8 Hz, *p*-H), 7.33 (d, 4 H, 7.5 Hz, *m*-H), 2.88 (sept., 2 H, *J* = 6.5 Hz, N-C(*H*)Me_2), 2.65 (sept., 4 H, *J* = 6.8 Hz, IPr C(H)*Me*$_2$), 2.38 (dd, 1 H, *J* = 13.5 Hz, 10.0 Hz, N-C(*H*)$_2$), 2.26 (dd, 1 H, *J* = 14.0 Hz, 5.0 Hz, N-C(*H*)$_2$), 1.50 (dd, 1 H, *J* = 10.0 Hz, 5.0 Hz, Au-C(*H*)), 1.37 (dd, 12 H, *J* = 7.0 Hz, 1.5 Hz, IPr C(*H*)Me_2), 1.22 (dd, 12 H, *J* = 6.5 Hz, 1.5 Hz, IPr C(*H*)Me_2), 0.81 (d, 12 H, *J* = 8.0 Hz, IPr C(*H*)Me_2), 0.75 (d, 12 H, 7.0 Hz, N- C(*H*)Me_2). ^{13}C NMR (125 MHz, THF-d_8): δ(ppm) 193.9, 146.8, 146.8, 136.0, 131.1, 128.5, 124.9, 124.8, 124.5, 48.1, 47.7, 29.8, 29.8, 22.1, 21.0, 20.0. IR (ATR): ν_{max}(cm^{-1}) 2961, 2928, 2868, 2191, 1462, 1415, 1384, 1363, 1329, 1204, 1180, 803, 757. HRMS(*m*/*z*): calculated for $C_{36}H_{53}AuN_4$ 739.4009, found 739.4021. Calculated for $C_{36}H_{53}AuN_4$: C, 58.53; H, 7.22; N, 7.58. Found: C, 58.21; H, 6.68; N, 8.21.

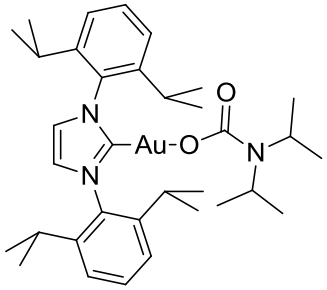


Complex 7. To a weighed vial containing **1** (51.8 mg, 0.076 mmol) and a Teflon stir bar was added THF (2 mL). Ethyl isocyanate (10.8 mg, 0.151 mmol) was added via syringe and the reaction mixture was stirred for 10 min at 23 °C. The product was isolated as a white solid upon concentration (56.6 mg, 0.075 mmol, 99% yield). ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.56 (s, 2 H, imidazole), 7.47 (t, 2 H, J = 7.8 Hz, *p*-H), 7.33 (d, 4 H, J = 8.0 Hz, *m*-H), 3.36 (sept., 2 H, J = 6.8 Hz,), 2.87 (q, 2 H, J = 7.0 Hz, N-CH_2), 2.69 (sept., 4 H, J = 7.0 Hz, IPr C(*H*)Me$_2$), 1.36 (d, 12 H, J = 7.0 Hz, IPr C(H)*Me*$_2$), 1.21 (d, 12 H, J = 7.0 Hz, IPr C(H)*Me*$_2$), 0.75 (d, 12 H, J = 6.5 Hz, N-C(H)*Me*$_2$), 0.45 (t, 3 H, J = 7.3 Hz, NCH$_2$C*H*$_3$). ^{13}C NMR (125 MHz, THF-d_8): δ(ppm) 179.4, 167.9, 146.8, 136.4, 131.2, 125.0, 124.7, 47.1, 44.2, 29.9, 24.8, 24.5, 22.2, 18.3. IR (ATR) ν_{max}(cm^{-1}) 2960, 2926, 2868, 1572, 1552, 1467, 1418, 1328, 1159, 801, 765. HRMS (*m/z*): calculated for $C_{36}H_{55}AuN_4O$ 757.4114, found 757.4118. Anal. Calcd. for $C_{36}H_{55}AuN_4O$: C, 57.13; H, 7.33; N, 7.40. Found: C, 56.96; H, 7.13; N, 7.25.



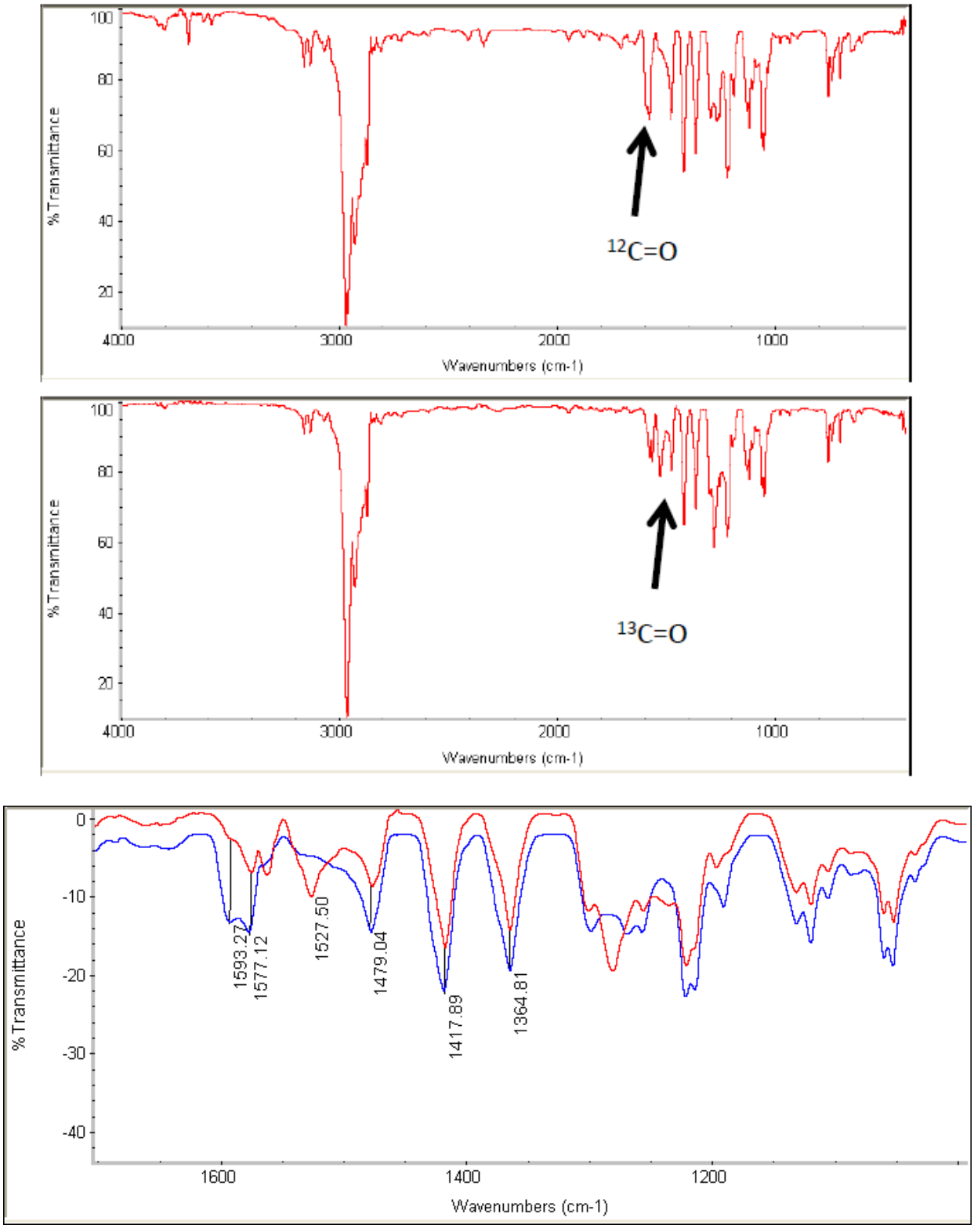
Compound 8. Compound **1** (51.4 mg, 0.750 mmol) and 1,3-*p*-tolylcarbodiimide (16.5 mg, 0.742 mmol) were added to a weighed vial containing a stir bar and THF (2 mL), and the solution was stirred for 2 h. The reaction mixture was concentrated, leaving a solid. The sparingly soluble solid was dissolved in diethyl ether (3 mL) and precipitated upon addition of pentane (10 mL). The mother liquor was decanted and residual solvent removed under vacuum to give the product as a pale yellow powder (39 mg, 0.043 mmol, 57% yield). ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.57 (t, 2 H, J = 7.8 Hz, IPr *p*-H), 7.56 (s, 2 H, imidazole), 7.37 (d, 4 H, 8.0 Hz, IPr *m*-H), 6.44 (d, 2 H, J = 8.0 Hz, *p*-tolyl aryl), 6.38, (d, 2 H, J = 8.0 Hz, *p*-tolyl aryl), 6.33 (d, 2 H, J = 8.0 Hz, *p*-tolyl aryl), 6.05 (d, 2 H, J = 7.5 Hz, *p*-tolyl aryl), 3.70 (sept., 2 H, J = 7.0 Hz, NC(*H*)Me$_2$), 2.65 (sept., 4 H, J = 7.0 Hz, IPr C(*H*)Me$_2$), 2.05 (s, 3 H, *p*-tolyl Me), 2.00 (s, 3 H, *p*-tolyl Me), 1.26 (d, 12 H, J = 7.0 Hz, IPr C(H)*Me*$_2$), 1.20 (d, 12 H, J = 7.0 Hz, IPr C(H)*Me*$_2$), 1.03 (d, 12 H, J = 7.0 Hz, NC(H)*Me*$_2$). IR (ATR) ν_{max}(cm^{-1}): 2961, 2922, 2866, 1551, 1498, 1460, 1288, 1148, 813, 759. ^{13}C NMR (125 MHz, THF-d_8): δ(ppm) 178.5, 156.9, 153.4, 150.3, 146.8, 136.1, 131.2, 129.1, 128.8,126.9, 125.1, 124.7, 123.4, 122.6, 117.6, 46.8, 29.9,

26.0, 24.8, 24.6, 21.2, 20.8. HRMS (*m/z*): calculated for $C_{48}H_{65}N_5Au$ 908.4900, found 908.4928. Anal. Calcd. for $C_{48}H_{64}AuN_5$: C, 63.49; H, 7.10; N, 7.71. Found: C, 62.68; H, 7.03; N, 7.31.

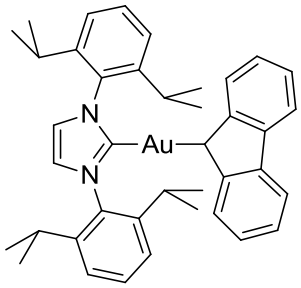


Complex 9. Compound **1** (5.6 mg, 0.008 mmol) and 1,3,5-trimethoxybenzene (1.0 mg, 0.006 mmol) were dissolved in benzene-d_6 and transferred to a J.-Young tube. The reaction mixture was subjected to one freeze-pump-thaw cycle and the evacuated tube opened to carbon dioxide (1 atm). Upon closure and inversion of the tube, the reaction mixture instantly changed from yellow to colorless. The product was present in 88% yield as determined by reference to the internal standard. ^{1}H NMR (500 MHz, Benzene-d_6): δ(ppm) 7.10 (t, 2 H, *J* = 7.7 Hz, IPr *p*-H), 7.00 (d, 4 H, 7.8 Hz, IPr *m*-H), 6.30 (s, 2 H, imidazole), 4.02-3.77 (m, 2 H, NC(*H*)Me_2), 2.61 (sept., 4 H, 6.9 Hz, IPr C(*H*)Me_2), 1.52 (d, 12 H, *J* = 6.9 Hz, IPr C(H)*Me*$_2$), 1.10 (d, 12 H, *J* = 7.8 Hz, C(H)*Me*$_2$), 1.05 (d, 12 H, *J* = 6.8 Hz, IPr C(H)*Me*$_2$).). ^{13}C (150 MHz, Benzene-d_6): 171.3, 161.4, 145.7, 134.7, 130.8, 128.4, 122.7, 29.2, 24.7, 24.1, 21.8. IR (C_6D_6) ν_{max}(cm^{-1}): 2970, 2928, 1577 (C=O), 1478, 1418, 1364, 1299, 1221.

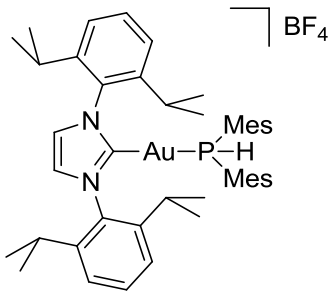
Figure S1. Comparison of ^{12}C-[9] and ^{13}C-[9] IR spectra.



Red: ^{13}C-[9]; Blue ^{12}C-[9]

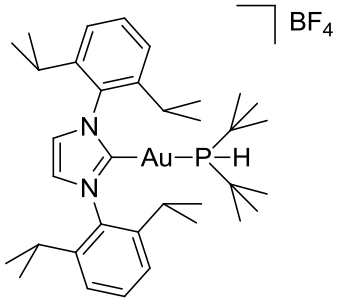


Complex 10. To a weighed vial containing **1** (51.9 mg, 0.076 mmol) and a Teflon stir bar was added THF (2 mL). Fluorene (12.2 mg, 0.073 mmol) was added and the solution immediately turned from yellow to colorless. After being stirred for 10 minutes, the reaction mixture was concentrated and the crude product washed with pentane (1 mL). The product was isolated as a white solid (51.8 mg, 0.069 mmol, 94% yield). ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.61-7.57 (m, 2 H, aryl), 7.42 (t, 2 H, J = 7.8 Hz, aryl), 7.41 (s, 2 H, imidazole), 7.19 (d, 4 H, J = 7.5 Hz, aryl), 6.87-6.81 (m, 6 H, aryl), 3.99 (s, 1 H, Au-C(*H*)), 2.43 (sept., 4 H, J = 6.8 Hz, IPr C(*H*)Me$_2$), 1.11 (d, 12 H, J = 7.0 Hz, IPr C(H)*Me*$_2$), 1.02 (d, 12 H, J = 6.5 Hz, IPr C(H)*Me*$_2$). ^{13}C NMR (125 MHz, THF-d_8): δ(ppm) 193.0, 153.9, 146.6, 138.3, 135.9, 130.8, 124.6, 124.4, 124.2,124.0, 121.3, 119.2, 49.8, 29.6, 24.6, 24.3. IR (ATR) ν_{max}(cm^{-1}): 2963, 2927, 2868, 1471, 1382,1329, 1217, 1191, 903, 743. HRMS(*m/z*): calculated for $C_{40}H_{45}AuN_2Li$ [M-Li$^+$] 757.3403, found 757.3402. Anal. Calcd. for $C_{40}H_{45}AuN_2$: C, 63.99; H, 6.04; N, 3.73. Found: C, 63.58; H, 5.96; N, 3.93.

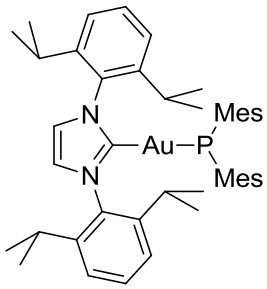


(IPr)gold(I) bis(2,4,6-trimethlyphenyl)phosphine tetrafluoroborate (11). IPrAuCl (99.7 mg, 0.161 mmol) was added to a solution of bis(2,4,6-trimethylphenyl)phosphine (45.0 mg, 0.166 mmol) and $AgBF_4$ (32.4 mg, 0.164) in methylene chloride (5 mL). Silver chloride precipitated immediately. After being stirred for 10 minutes, the reaction mixture was filtered through a syringe filter and the resulting solution was concentrated to a white solid. The solid was dissolved in methylene chloride (~1 mL) and precipitated using pentane. The mother liquor was decanted and the resulting product washed with hexane (1 mL) to leave a white powder (136 mg, 0.144 mmol, 89% yield). X-ray quality crystals were obtained from a methylene chloride solution of **4** layered with hexane and stored at -35 °C. ^{1}H NMR(500 MHz, CD_2Cl_2): δ(ppm) 7.60 (t, 2H, J = 7.3 Hz, IPr *p*-H), 7.44, (s, 2 H, imidazole), 7.31 (d, 4 H, 8.0 Hz, IPr *m*-H), 6.82 (d, 4 H, $J_{H\text{-}P}$ = 4.0 Hz, mes), 6.78, (d, 1 H, $J_{H\text{-}P}$ = 395.5 Hz, P-*H*), 2.45 (sept., 4 H, J = 7.0 Hz, IPr C(*H*)Me$_2$), 2.25 (s, 6 H, mes *p*-H), 1.90 (s, 12 H, *o*-H), 1.22 (d, 12 H, J = 7.0 Hz, IPr C(H)*Me*$_2$), 1.09 (d, 12 H, J = 7.0 Hz, IPr C(H)*Me*$_2$). ^{13}C NMR (125 MHz, CD_2Cl_2): δ(ppm) 191.9, 191.1,

146.3, 133.8, 131.7, 125.0, 125.0, 124.9, 34.3, 34.1, 30.5, 30.4, 29.4, 25.0, 24.4. $^{31}P\{^{1}H\}$ NMR (162 MHz, CD_2Cl_2): δ(ppm) 42.0. $^{19}F\{^{1}H\}$ (376 MHz, CD_2Cl_2) -152.6. IR (ATR): $\nu_{max}(cm^{-1})$ 2963, 1604, 1458, 1422, 1385, 1050, 851, 805, 759, 705. HRMS(*m/z*): calculated for $C_{42}H_{61}AuN_2P$ [M-BF_4] 855.4076, found 855.4093. Anal. Calcd. for $C_{45}H_{59}AuBF_4N_2P$: C, 57.33; H, 6.31; N, 2.97. Found: C, 56.55; H, 6.30; N, 2.90.

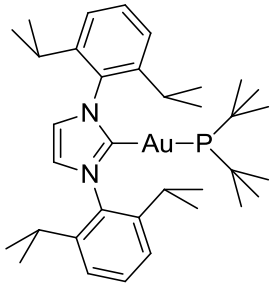


(IPr)gold(I) di-*t*-butylphosphine tetrafluoroborate (12). Compound **5** was synthesized analogously to **4** but with di-*t*-butylphosphine (24.5 mg, 0.167 mmol). The product was isolated as a white solid (125 mg, 0.153 mmol, 95% yield). X-ray quality crystals were grown from a methylene chloride solution layered with pentane and stored at -35 °C. ^{1}H NMR (500 MHz, CD_2Cl_2): δ(ppm) 7.55 (t, 2 H, *J* = 8.0 Hz, *p*-H), 7.45 (s, 2 H, imidazole), 7.34 (d, 4 H, 8.0 Hz, *m*-H), 4.55 (d, 1 H, $J_{H\text{-}P}$ = 359.5 Hz, P-*H*), 2.52 (sept., 4 H, *J* = 7.0 Hz, IPr C(*H*)Me_2) 1.28 (d, 12 H, 7.0 Hz, IPr C(H)*Me*$_2$), 1.26 (d, 12 H, 7.0 Hz, IPr C(H)*Me*$_2$), 1.00 (d, 18 H, $J_{H\text{-}P}$ = 16.5 Hz, *t*-Bu). ^{13}C NMR (125 MHz, CD_2Cl_2): δ(ppm) 146.3, 133.8, 131.7, 125.0 (d, *J* = 3.3 Hz), 124.9, 34.2 (d, *J* = 26.4), 30.4 (d, *J* = 5.4 Hz), 29.4, 25.0, 24.4. $^{31}P\{^{1}H\}$ NMR (162, CD_2Cl_2): δ(ppm) 57.1. $^{19}F\{^{1}H\}$ NMR (376 MHz, CD_2Cl_2): 152.6. IR (ATR): $\nu_{max}(cm^{-1})$ 2964, 2870, 1471, 1420, 1365, 1049, 809, 763. HRMS(*m/z*): calculated for $C_{35}H_{55}AuN_2P$ [M-BF_4] 731.3763, found 731.3744. Anal. Calcd. for $C_{35}H_{55}AuBF_4N_2P$: C, 51.35; H, 6.77; N, 3.42. Found: C, 51.54; H, 6.77; N, 3.43.

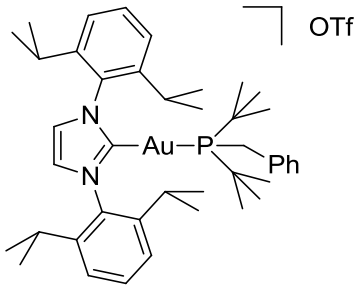


(IPr)gold(I) bis(2,4,6-trimethlyphenyl)phosphide (13). KHMDS (11.6 mg, 0.058 mmol) was stirred vigorously in THF (3 mL). To the basic solution was added **4** (49.7 mg, 0.053 mmol) in THF (2 mL) dropwise. The reaction mixture turned yellow immediately. After being stirred for 5 minutes, the reaction mixture was concentrated to give a yellow solid. The solid was dissolved in diethyl ether and passed through a syringe filter, and the resulting solution was concentrated to a yellow solid. The solid was washed with pentane (~l mL) and the residual solvent removed under vacuum to yield the desired product as a yellow powder (43.6 mg, 0.051 mmol, 96% yield) X-ray quality crystals were grown from a concentrated diethyl ether solution

stored at -35 °C. ^{1}H NMR (600 MHz, THF-d_8): δ(ppm) 7.53 (s, 2 H, imidazole), 7.48 (t, 2 H, J = 7.5 Hz, IPr *p*-H), 7.25 (d, 4 H, J = 7.8 Hz, IPr *m*-H), 6.44 (s, 4 H, mes), 2.59 (sept., 4 H, J = 6.9 Hz, C(*H*)Me$_2$), 2.09 (s, 6 H, mes *p*-Me), 1.80 (s, 12 H, mes *o*-Me), 1.16 (d, 12 H, J = 3.0 Hz, C(H)*Me*$_2$), 1.15 (d, 12 H, J = 2.5 Hz, C(H)*Me*$_2$). ^{13}C NMR (500 MHz, THF-d_8): δ(ppm) 146.7, 143.3, 143.1, 141.8, 141.7, 136.2, 133.0, 131.0, 128.9, 128.8, 124.8, 124.3, 29.8, 24.6, 24.5, 21.1. ^{31}P{^{1}H} NMR (162 MHz, THF-d_8): δ(ppm) -52.7. IR (ATR): ν_{max}(cm^{-1}) 3146, 3024, 2960, 2866, 1554, 1461, 1409, 1350, 847, 802, 758. HRMS (*m*/*z*): calculated for $C_{45}H_{58}N_2AuP$ 854.4003, found 854.4001. Anal. Calcd. for $C_{45}H_{58}AuN_2P$: C, 63.22; H, 6.84; N, 3.28. Found: C, 63.02; H, 6.88; N, 3.17.



Generation of (IPr)gold(I) di-*t*-butyl phosphide (14). Complex **5** (7.2 mg, 0.009 mmol) and hexamethylbenzene (0.6 mg, 0.004 mmol) were transferred to a J. Young NMR tube using THF-d_8 (0.5 mL). The ^{1}H NMR spectrum of the reaction mixture was then obtained. The contents of the tube were added dropwise to a vigorously stirred solution of sodium *t*-amylate (1.3 mg, 0.012 mmol) in THF-d_8 (0.2 mL). The reaction mixture immediately turned pale yellow and was returned to the NMR tube, and a second spectrum was acquired. Complex **7** was present in 85% yield as determined by reference to the internal standard. ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.52 (s, 2 H, imidazole), 7.43 (t, 2 H, J = 7.5 Hz, IPr *p*-H), 7.29 (d, 4 H, J = 7.5 Hz, IPr *m*-H), 2.70 (sept., 4 H, J = 6.8 Hz, C(*H*)Me$_2$), 1.38 (d, 12 H, J = 6.5 Hz, C(H)*Me*$_2$), 1.20 (d, 12 H, J = 7.0 Hz, C(H)*Me*$_2$), 0.89 (d, 18 H, $J_{P\text{-}H}$ = 10.5 Hz, *t*-Bu). ^{31}P{^{1}H} NMR (162 MHz, THF-d_8): δ(ppm): 73.6.



Complex 15. To a weighed vial was added IPrAuOTf (30.1 mg, 0.041 mmol), methylene chloride (2 mL), and di(*t*-butyl)benzylphosphine (13.1 mg, 0.055 mmol). The reaction mixture was stirred for 10 min and then concentrated to a solid. The crude solid was washed with hexane (2 mL) to give the desired product as a white powder (38.2 mg, 0.039 mmol, 95% yield). ^{1}H NMR (500 MHz, THF-d_8): δ(ppm) 7.97 (s, 2 H, imidazole), 7.60 (t, 2 H, J = 7.8 Hz, IPr *p*-H), 7.45 (d, 4 H, J = 8.0 Hz, *m*-H), 7.15-7.03 (m, 5 H, phenyl), 3.36 (d, 2 H, $J_{H\text{-}P}$ = 11.5, PC*H*$_2$), 2.71

(sept., 4 H, J = 7.0 Hz, C(*H*)Me$_2$), 1.32 (d, 12 H, 6.5 Hz, C(H)*Me*$_2$), 1.26 (d, 12 H, J = 7.0 Hz, C(H)*Me*$_2$), 0.99 (d, 18 H, $J_{H\text{-}P}$ = 15.0 Hz, *t*-Bu). ^{13}C NMR (125 MHz, THF-d_8): δ(ppm) 146.8, 135.6 (d, J = 4.1 Hz), 135.4, 132.0, 131.3 (d, J = 5.6 Hz), 129.9, 127.6, 126.9, 125.4, 36.9 (d, J = 23.6), 30.1 (d, J = 17.5 Hz), 30.0, 28.3 (d, J = 23.4 Hz), 24.9, 24.6. ^{31}P{^{1}H} NMR (162 Hz, CD_2Cl_2): δ(ppm) 70.9. IR (ATR) ν_{max}(cm^{-1}): 2963, 2870, 1466, 1455, 1259, 1224, 1149, 1029, 809, 761, 636. HRMS(*m/z*): calculated for $C_{42}H_{61}N_2AuP$ [M-OTf] 821.4233, found 821.4213. Anal. Calc. for $C_{43}H_{61}AuF_3N_2O_3PS$: C, 53.19; H, 6.33; N, 2.89. Found: C, 53.57; H, 6.36; N, 2.81.

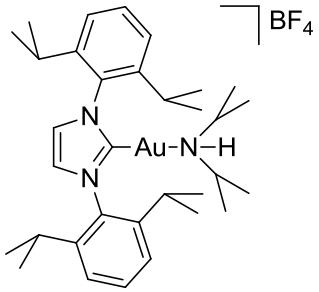
Catalytic Benzylation of Di(*t*-butyl)phosphine

Hexamethylbenzene (2.9 mg, 0.006 mmol) and sodium *t*-amylate (2.9 mg, 0.026 mmol) were dissolved in THF-d_8 and transferred to a J. Young NMR tube. Benzyl chloride (3.0 mg, 0.024 mmol) and di(t-butyl)phosphine (3.6 mg, 0.024 mmol) were added via syringe to the reaction mixture. The ^{1}H NMR spectrum of the mixture was taken. Compound **4** (2.0 mg, 0.002 mmol) in THF-d_8 was added to the tube. The tube was promptly inverted to ensure mixing, resulting in a pale yellow reaction mixture. A ^{1}H NMR spectrum of the mixture was obtained every two hours after heating continuously at 75 °C. Conversion was determined by comparison of the benzyl protons of the starting material and product relative to the internal standard. The identity of the product was confirmed by comparison of the spectra of the reaction mixture to the spectrum of an authentic sample of di(*t*-butyl)benzylphosphine[4] in THF-d_8.

Ligand Exchange of Complex 4 with d_5-Aniline

A J. Young tube was charged with complex **4** (6.8 mg, 0.010 mmol), C_6D_6 (0.5 mL), and hexamethylbenzene (0.8 mg, 0.005 mmol). A ^{1}H NMR spectrum of the mixture was taken. Aniline-d_5 (5.0 μL, 5.5 equiv.) was added to the reaction mixture via syringe. A second spectrum was collected immediately following addition. A statistical amount (~80%) of free aniline was observed relative to the internal standard.

Synthesis of the Conjugate Acid of (1)



To a vial was added $AgBF_4$ (70.6 mg, 0.357 mmol), diisopropylamine (42.7 mg, 0.422 mmol), and methylene chloride (10 mL). IPrAuCl (200 mg, 0.322 mmol) was added to the reaction mixture, leading to the immediate precipitation of AgCl. Following 10 min. of stirring, the reaction mixture was filtered through two syringe filters and concentrated to yield the product as a white solid (237 mg, 0.306 mmol, 95% yield). X-ray quality crystals were grown from a

methylene chloride solution layered with pentane and stored at -35 °C. ^{1}H NMR (500 MHz, CD_2Cl_2): δ(ppm) 7.54 (t, 2 H, *J* = 7.5 Hz, *p*-H), 7.39(s, 2 H, imidazole), 7.35 (d, 4 H, *J* = 10 Hz, *m*-H), 3.50 (br s,1 H, N-*H*), 3.18-3.09 (m, 2 H, NC(*H*)Me_2), 2.51 (sept., 4 H, *J* = 5.0 Hz, IPr NC(*H*)Me_2), 1.31 (d, 12 H, *J* = 5.0 Hz, C(H)*Me*$_2$), 1.24 (d, 12 H, *J* = 10 Hz, C(H)*Me*$_2$), 0.85 (d, 3 H, 5.0 Hz, NC(H)*Me*$_2$), 0.78 (d, 3 H, 5.0 Hz, NC(H)*Me*$_2$). ^{13}C NMR (125 MHz, CD_2Cl_2): δ(ppm) 173.1, 146.3, 134.2, 131.5, 124.9, 124.6, 51.6, 29.4, 24.6, 24.5, 22.8, 22.3. ^{19}F{^{1}H} NMR (376 MHz, CD_2Cl_2): δ(ppm) 151.4. HRMS(*m/z*): calculated for $C_{33}H_{51}AuN_3$ 686.3743, found 686.3744.

DFT Calculations

Density functional calculations were performed at the UC Berkeley Molecular Graphics and Computional Facility using the Gaussian09 suite.[7] Calculations were conducted using the BPV86 functional and LANL2DZ basis set for Au. The 6-311++G(d,p) basis set was used for all other atoms during geometry optimization, frequency, energy, NBO, and NLMO calculations. Optimized XYZ coordinates for all calculated molecules are enumerated below.

(IPr)gold(I) diisopropylamide (1)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.000089	1.033261	0.000091
2	7	0	1.086069	-1.809786	-0.022296
3	7	0	-1.086473	-1.809603	0.021704
4	7	0	0.000394	3.059113	0.000294
5	6	0	-0.000133	-0.954227	-0.000161
6	6	0	-0.681130	-3.144977	0.013334
7	1	0	-1.394881	-3.960699	0.028048
8	6	0	0.680497	-3.145088	-0.014341
9	1	0	1.394105	-3.960931	-0.029334
10	6	0	2.471767	-1.397017	-0.066644
11	6	0	3.091073	-1.241231	-1.327586
12	6	0	4.445948	-0.870601	-1.342392
13	1	0	4.952951	-0.736128	-2.300814
14	6	0	5.151836	-0.664403	-0.155178
15	1	0	6.204254	-0.372549	-0.189936
16	6	0	4.514035	-0.827482	1.076471
17	1	0	5.074582	-0.662127	1.999718
18	6	0	3.160971	-1.198166	1.151255
19	6	0	2.347286	-1.455939	-2.642521
20	1	0	1.308457	-1.728785	-2.400945
21	6	0	2.958289	-2.619620	-3.451911
22	1	0	3.998329	-2.402999	-3.744114
23	1	0	2.381172	-2.788768	-4.374957
24	1	0	2.961676	-3.557288	-2.874599
25	6	0	2.297991	-0.160044	-3.477697
26	1	0	1.819736	0.653391	-2.912629
27	1	0	1.721870	-0.323778	-4.402388
28	1	0	3.308539	0.170291	-3.767410
29	6	0	2.495004	-1.378491	2.511846
30	1	0	1.440242	-1.640837	2.337551
31	6	0	3.141191	-2.536319	3.302298
32	1	0	4.198843	-2.325559	3.528014
33	1	0	3.101477	-3.482549	2.740568

34	1	0	2.618449	-2.685624	4.260520
35	6	0	2.510124	-0.069333	3.327133
36	1	0	3.539087	0.255658	3.550391
37	1	0	1.989514	-0.211936	4.287491
38	1	0	2.004769	0.739957	2.779639
39	6	0	-2.472104	-1.396640	0.066367
40	6	0	-3.161489	-1.197468	-1.151374
41	6	0	-4.514499	-0.826646	-1.076289
42	1	0	-5.075185	-0.661050	-1.999409
43	6	0	-5.152067	-0.663726	0.155500
44	1	0	-6.204447	-0.371762	0.190495
45	6	0	-4.445996	-0.870221	1.342555
46	1	0	-4.952823	-0.735863	2.301087
47	6	0	-3.091169	-1.241011	1.327449
48	6	0	-2.495752	-1.377549	-2.512108
49	1	0	-1.441023	-1.640168	-2.338034
50	6	0	-3.142284	-2.534994	-3.302830
51	1	0	-4.199917	-2.323941	-3.528365
52	1	0	-3.102713	-3.481405	-2.741394
53	1	0	-2.619687	-2.684123	-4.261159
54	6	0	-2.510712	-0.068134	-3.326995
55	1	0	-3.539642	0.257126	-3.550015
56	1	0	-1.990251	-0.210546	-4.287463
57	1	0	-2.005131	0.740889	-2.779318
58	6	0	-2.347200	-1.456101	2.642218
59	1	0	-1.308377	-1.728776	2.400425
60	6	0	-2.958028	-2.620127	3.451251
61	1	0	-3.998059	-2.403691	3.743620
62	1	0	-2.380811	-2.789567	4.374181
63	1	0	-2.961392	-3.557583	2.873596
64	6	0	-2.297899	-0.160510	3.477857
65	1	0	-1.819766	0.653165	2.913031
66	1	0	-1.721649	-0.324549	4.402413
67	1	0	-3.308427	0.169655	3.767833
68	6	0	1.219325	3.858644	0.131201
69	1	0	1.076923	4.801920	-0.439684
70	6	0	2.444521	3.157897	-0.469079
71	1	0	2.631673	2.198543	0.042165
72	1	0	3.347890	3.781161	-0.362793
73	1	0	2.285658	2.945552	-1.536959
74	6	0	1.489855	4.257367	1.601565
75	1	0	0.611671	4.757590	2.039415
76	1	0	2.351288	4.943049	1.689457
77	1	0	1.695664	3.354560	2.199718
78	6	0	-1.218249	3.859063	-0.130755
79	1	0	-1.075400	4.802469	0.439783

80	6	0	-2.443603	3.158919	0.469912
81	1	0	-2.630979	2.199401	-0.040940
82	1	0	-3.346832	3.782349	0.363431
83	1	0	-2.284706	2.946958	1.537863
84	6	0	-1.488783	4.257388	-1.601223
85	1	0	-0.610411	4.757059	-2.039326
86	1	0	-2.349928	4.943413	-1.689272
87	1	0	-1.695055	3.354460	-2.199036

(IPr)gold(I) anilide (2)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-0.272905	-0.936341	0.000112
2	6	0	0.752376	0.764120	0.000049
3	6	0	1.298629	2.982155	-0.000069
4	1	0	1.108163	4.049156	-0.000145
5	6	0	2.465374	2.276615	0.000049
6	1	0	3.498575	2.604281	0.000088
7	6	0	3.078774	-0.160348	0.000040
8	6	0	3.535143	-0.660452	1.240647
9	6	0	4.486537	-1.693800	1.210049
10	1	0	4.855663	-2.107492	2.151459
11	6	0	4.960361	-2.205054	0.000115
12	1	0	5.698854	-3.010351	0.000144
13	6	0	4.486693	-1.693745	-1.209859
14	1	0	4.855942	-2.107397	-2.151239
15	6	0	3.535306	-0.660392	-1.240536
16	6	0	3.028897	-0.137074	2.581734
17	1	0	2.297470	0.660605	2.380535
18	6	0	4.172190	0.479481	3.415608
19	1	0	4.930940	-0.274931	3.677482
20	1	0	3.778336	0.895981	4.356228
21	1	0	4.680927	1.289453	2.870048
22	6	0	2.293630	-1.242952	3.367531
23	1	0	2.967390	-2.082061	3.603796
24	1	0	1.443638	-1.637507	2.790597
25	1	0	1.908379	-0.844479	4.319435
26	6	0	3.029241	-0.136955	-2.581672
27	1	0	2.297745	0.660675	-2.380539
28	6	0	4.172616	0.479725	-3.415342
29	1	0	4.681239	1.289679	-2.869647
30	1	0	3.778869	0.896280	-4.355981
31	1	0	4.931439	-0.274626	-3.677178

32	6	0	2.294150	-1.242828	-3.367644
33	1	0	1.909080	-0.844339	-4.319616
34	1	0	1.444051	-1.637418	-2.790893
35	1	0	2.967980	-2.081916	-3.603792
36	6	0	-1.144832	2.400749	-0.000164
37	6	0	-1.797962	2.576876	1.240842
38	6	0	-3.151502	2.951593	1.209820
39	1	0	-3.688659	3.090717	2.150796
40	6	0	-3.822245	3.139982	-0.000397
41	1	0	-4.875755	3.429526	-0.000489
42	6	0	-3.151394	2.951214	-1.210496
43	1	0	-3.688465	3.090052	-2.151564
44	6	0	-1.797855	2.576479	-1.241281
45	6	0	-1.100919	2.360497	2.580686
46	1	0	-0.052377	2.092475	2.377535
47	6	0	-1.093607	3.647641	3.432290
48	1	0	-0.619961	4.485614	2.897526
49	1	0	-0.538510	3.482254	4.369275
50	1	0	-2.115752	3.957429	3.702425
51	6	0	-1.735730	1.183538	3.351172
52	1	0	-1.195556	1.008701	4.295280
53	1	0	-1.704460	0.256683	2.759036
54	1	0	-2.788348	1.390964	3.601407
55	6	0	-1.100681	2.359723	-2.580996
56	1	0	-0.052121	2.091900	-2.377674
57	6	0	-1.093471	3.646583	-3.433029
58	1	0	-2.115642	3.956171	-3.703301
59	1	0	-0.538321	3.480946	-4.369939
60	1	0	-0.619936	4.484784	-2.898525
61	6	0	-1.735278	1.182420	-3.351130
62	1	0	-1.704009	0.255795	-2.758635
63	1	0	-1.194949	1.007271	-4.295091
64	1	0	-2.787877	1.389648	-3.601603
65	6	0	-2.632710	-2.934675	0.000045
66	6	0	-3.585046	-1.879621	0.000131
67	1	0	-3.221706	-0.847358	0.000122
68	6	0	-4.955566	-2.142727	0.000229
69	1	0	-5.657137	-1.303260	0.000301
70	6	0	-5.444026	-3.459343	0.000245
71	1	0	-6.517557	-3.658053	0.000328
72	6	0	-4.517473	-4.513345	0.000158
73	1	0	-4.869021	-5.549246	0.000175
74	6	0	-3.144337	-4.262757	0.000066
75	1	0	-2.438947	-5.100597	0.000018
76	7	0	2.119844	0.925162	0.000022
77	7	0	0.261825	2.049597	-0.000051

78	7	0	-1.278047	-2.691386	-0.000021
79	1	0	-0.727150	-3.548662	-0.000054

(IPr)gold(I) bis(2,4,6-trimethlyphenyl)phosphide(13)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.092697	-0.273240	-0.219365
2	15	0	-2.021486	-1.004680	-1.037556
3	6	0	1.989530	0.452166	0.133164
4	6	0	4.256884	0.731653	0.062896
5	1	0	5.279779	0.473962	-0.186406
6	6	0	3.733239	1.811560	0.710089
7	1	0	4.206618	2.685140	1.143271
8	6	0	1.442903	2.568076	1.372070
9	6	0	0.891557	3.602365	0.583509
10	6	0	0.060086	4.531595	1.230454
11	1	0	-0.389015	5.340413	0.650126
12	6	0	-0.209116	4.433055	2.596849
13	1	0	-0.861325	5.165807	3.077959
14	6	0	0.347090	3.396103	3.348259
15	1	0	0.123799	3.323461	4.415256
16	6	0	1.186799	2.438428	2.755702
17	6	0	1.182690	3.749313	-0.906581
18	1	0	1.715775	2.844251	-1.236621
19	6	0	2.105251	4.959986	-1.169487
20	1	0	2.342573	5.037336	-2.242567
21	1	0	3.053512	4.878236	-0.615492
22	1	0	1.619238	5.900471	-0.863637
23	6	0	-0.110378	3.844652	-1.739695
24	1	0	-0.780280	2.994684	-1.544499
25	1	0	0.133353	3.855275	-2.813796
26	1	0	-0.668085	4.769235	-1.521398
27	6	0	1.782087	1.320663	3.607531
28	1	0	2.368494	0.664710	2.945597
29	6	0	2.744017	1.882165	4.676795
30	1	0	3.555317	2.472161	4.222784
31	1	0	3.199893	1.061379	5.252989
32	1	0	2.213920	2.535884	5.387728
33	6	0	0.681485	0.452344	4.250056
34	1	0	0.069012	1.034370	4.956959
35	1	0	1.131612	-0.383107	4.809477
36	1	0	0.010923	0.033186	3.485862

37	6	0	3.342694	-1.357087	-0.966172
38	6	0	3.158554	-1.404519	-2.366519
39	6	0	3.365489	-2.640611	-3.001417
40	1	0	3.226633	-2.714114	-4.082286
41	6	0	3.743599	-3.773080	-2.278208
42	1	0	3.897582	-4.723639	-2.794411
43	6	0	3.924225	-3.693256	-0.895889
44	1	0	4.218739	-4.586138	-0.339610
45	6	0	3.727000	-2.485797	-0.205726
46	6	0	2.778619	-0.182536	-3.196910
47	1	0	2.566961	0.646390	-2.504312
48	6	0	3.950398	0.251422	-4.104675
49	1	0	4.859269	0.465095	-3.520735
50	1	0	3.683423	1.160280	-4.667118
51	1	0	4.198963	-0.534241	-4.836082
52	6	0	1.495916	-0.425360	-4.016997
53	1	0	1.213444	0.492139	-4.557089
54	1	0	0.658209	-0.714477	-3.364789
55	1	0	1.636653	-1.219564	-4.767761
56	6	0	3.950667	-2.430168	1.303635
57	1	0	3.623238	-1.440560	1.658914
58	6	0	5.449144	-2.577173	1.648238
59	1	0	5.833993	-3.559602	1.331018
60	1	0	5.604038	-2.490311	2.735457
61	1	0	6.059667	-1.805650	1.154284
62	6	0	3.111865	-3.484759	2.053217
63	1	0	2.041495	-3.380633	1.826182
64	1	0	3.246267	-3.372764	3.140807
65	1	0	3.417048	-4.509265	1.787813
66	6	0	-3.001099	0.589211	-0.919124
67	6	0	-3.230036	1.302996	-2.129772
68	6	0	-3.980302	2.490723	-2.109104
69	1	0	-4.149829	3.021279	-3.052563
70	6	0	-4.523553	3.009127	-0.925866
71	6	0	-4.265558	2.314385	0.263465
72	1	0	-4.651954	2.713492	1.207937
73	6	0	-3.513533	1.126930	0.295347
74	6	0	-2.677161	0.829329	-3.456400
75	1	0	-2.915156	-0.229937	-3.638929
76	1	0	-1.576996	0.900827	-3.484955
77	1	0	-3.077200	1.435827	-4.283344
78	6	0	-5.373963	4.259380	-0.934181
79	1	0	-5.099500	4.928986	-1.763778
80	1	0	-5.273614	4.821291	0.007394
81	1	0	-6.443642	4.013760	-1.053466
82	6	0	-3.247130	0.488088	1.636051

83	1	0	-3.531553	1.167084	2.453858
84	1	0	-2.176623	0.239665	1.732812
85	1	0	-3.798217	-0.456615	1.762279
86	6	0	-2.949296	-2.219286	0.032837
87	6	0	-2.341440	-3.034216	1.029014
88	6	0	-3.113286	-3.982018	1.725894
89	1	0	-2.624845	-4.583504	2.500407
90	6	0	-4.472867	-4.184615	1.467504
91	6	0	-5.049488	-3.418400	0.445160
92	1	0	-6.103321	-3.574027	0.188870
93	6	0	-4.323056	-2.463969	-0.282709
94	6	0	-0.877863	-2.947886	1.382566
95	1	0	-0.584809	-1.916120	1.649128
96	1	0	-0.236308	-3.237656	0.533373
97	1	0	-0.644008	-3.612515	2.228464
98	6	0	-5.278729	-5.212724	2.228386
99	1	0	-5.516065	-6.086683	1.597570
100	1	0	-6.237678	-4.796502	2.577005
101	1	0	-4.729150	-5.579191	3.108414
102	6	0	-5.036626	-1.748886	-1.407368
103	1	0	-5.985165	-2.254484	-1.642866
104	1	0	-4.412421	-1.733367	-2.316606
105	1	0	-5.259435	-0.698526	-1.163136
106	7	0	2.352250	1.625664	0.746957
107	7	0	3.183774	-0.088945	-0.280376

(IPr)gold(I) di-*t*-butyl phosphide (14)

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.099265	0.724407	-0.193715
2	15	0	0.358564	3.033098	-0.729611
3	6	0	-0.169783	-1.322643	0.010706
4	6	0	-1.126021	-3.397989	0.129023
5	1	0	-1.939180	-4.114668	0.150665
6	6	0	0.225617	-3.569496	0.186551
7	1	0	0.830672	-4.465090	0.271016
8	6	0	2.221382	-2.054047	0.140740
9	6	0	2.928021	-2.041373	-1.082574
10	6	0	4.315602	-1.829236	-1.022997
11	1	0	4.892022	-1.804236	-1.950524
12	6	0	4.966786	-1.642820	0.197941
13	1	0	6.046496	-1.476748	0.219988
14	6	0	4.240757	-1.663984	1.390779

15	1	0	4.759755	-1.511844	2.339828
16	6	0	2.851518	-1.872816	1.392496
17	6	0	2.243030	-2.224860	-2.433270
18	1	0	1.180596	-2.446625	-2.247345
19	6	0	2.831714	-3.416516	-3.217100
20	1	0	3.888590	-3.247353	-3.477684
21	1	0	2.278820	-3.563364	-4.158406
22	1	0	2.774858	-4.351297	-2.637835
23	6	0	2.300623	-0.923681	-3.260999
24	1	0	1.830545	-0.089753	-2.717790
25	1	0	1.771736	-1.055098	-4.218469
26	1	0	3.341300	-0.641317	-3.487711
27	6	0	2.081137	-1.869855	2.710039
28	1	0	1.040312	-2.156771	2.493499
29	6	0	2.644275	-2.899844	3.710939
30	1	0	2.662755	-3.913992	3.282580
31	1	0	2.024038	-2.924174	4.620952
32	1	0	3.671172	-2.647165	4.019139
33	6	0	2.048583	-0.453374	3.321765
34	1	0	3.064753	-0.099943	3.559326
35	1	0	1.463198	-0.450529	4.255123
36	1	0	1.591096	0.265304	2.624301
37	6	0	-2.671763	-1.432333	-0.045183
38	6	0	-3.210060	-1.113945	-1.312488
39	6	0	-4.501385	-0.560696	-1.342842
40	1	0	-4.946638	-0.298307	-2.305319
41	6	0	-5.223090	-0.340846	-0.168011
42	1	0	-6.225210	0.091882	-0.216493
43	6	0	-4.666493	-0.672518	1.069061
44	1	0	-5.239571	-0.494596	1.982221
45	6	0	-3.378769	-1.225809	1.161541
46	6	0	-2.460407	-1.358863	-2.618913
47	1	0	-1.470601	-1.770687	-2.368849
48	6	0	-3.191714	-2.401943	-3.491532
49	1	0	-4.188987	-2.043696	-3.793029
50	1	0	-3.326127	-3.355759	-2.957812
51	1	0	-2.617567	-2.601908	-4.410183
52	6	0	-2.226707	-0.045845	-3.393197
53	1	0	-1.655596	-0.243979	-4.314058
54	1	0	-1.659322	0.677000	-2.787684
55	1	0	-3.179362	0.423514	-3.686504
56	6	0	-2.799402	-1.574763	2.530416
57	1	0	-1.791505	-1.989816	2.375950
58	6	0	-3.641776	-2.656876	3.239037
59	1	0	-4.662132	-2.298155	3.448425
60	1	0	-3.181148	-2.932065	4.201117

61	1	0	-3.728174	-3.568732	2.627971
62	6	0	-2.646840	-0.321264	3.415976
63	1	0	-2.006711	0.431178	2.932985
64	1	0	-2.193089	-0.589968	4.383275
65	1	0	-3.622277	0.146542	3.623565
66	6	0	2.082286	3.576509	-0.033280
67	6	0	3.084779	2.544012	-0.591410
68	1	0	4.118230	2.863870	-0.362593
69	1	0	2.995701	2.452168	-1.686215
70	1	0	2.927011	1.546450	-0.151992
71	6	0	2.215103	3.623105	1.498375
72	1	0	1.944727	2.657459	1.951943
73	1	0	1.578178	4.401540	1.945119
74	1	0	3.259951	3.855604	1.782027
75	6	0	2.448016	4.954518	-0.629254
76	1	0	1.782668	5.753785	-0.273009
77	1	0	2.391164	4.936204	-1.728660
78	1	0	3.480915	5.228255	-0.342801
79	6	0	-1.072438	3.914399	0.233935
80	6	0	-2.336998	3.533019	-0.567575
81	1	0	-3.228409	4.000905	-0.110771
82	1	0	-2.493455	2.441981	-0.572378
83	1	0	-2.266270	3.871835	-1.612928
84	6	0	-1.271179	3.469611	1.696099
85	1	0	-0.402243	3.703956	2.326509
86	1	0	-1.439661	2.383282	1.748363
87	1	0	-2.150882	3.980514	2.134471
88	6	0	-0.909359	5.446380	0.180586
89	1	0	-1.829493	5.934108	0.553026
90	1	0	-0.731768	5.799796	-0.847315
91	1	0	-0.078523	5.795710	0.812585
92	7	0	0.792832	-2.297321	0.114381
93	7	0	-1.351122	-2.025500	0.024725

IPrAuO*t*-Bu

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-0.071339	-1.131751	0.025034
2	7	0	1.465908	1.452233	-0.026031
3	7	0	-0.669925	1.841953	-0.045529
4	6	0	0.245266	0.814323	-0.017898
5	6	0	-0.032095	3.082332	-0.069699

6	1	0	-0.589450	4.011631	-0.092586
7	6	0	1.308991	2.837385	-0.057398
8	1	0	2.159157	3.509665	-0.067929
9	6	0	2.752388	0.784923	-0.007957
10	6	0	3.352090	0.504306	1.240458
11	6	0	4.614822	-0.111028	1.225975
12	1	0	5.104301	-0.348296	2.173392
13	6	0	5.248436	-0.433358	0.024268
14	1	0	6.229089	-0.914983	0.037028
15	6	0	4.626755	-0.150780	-1.193597
16	1	0	5.125407	-0.419107	-2.127876
17	6	0	3.364315	0.463417	-1.240508
18	6	0	2.675092	0.815864	2.571698
19	1	0	1.719009	1.317784	2.356118
20	6	0	3.520336	1.779213	3.431047
21	1	0	4.484510	1.327330	3.713565
22	1	0	2.986421	2.029520	4.361538
23	1	0	3.734494	2.717857	2.896626
24	6	0	2.348378	-0.482628	3.339625
25	1	0	1.713879	-1.149955	2.737119
26	1	0	1.816039	-0.249811	4.275673
27	1	0	3.266317	-1.031895	3.603624
28	6	0	2.699275	0.729212	-2.587650
29	1	0	1.743678	1.242484	-2.398183
30	6	0	3.554894	1.657245	-3.475021
31	1	0	4.519525	1.192000	-3.733146
32	1	0	3.768418	2.614113	-2.973682
33	1	0	3.029231	1.875128	-4.418271
34	6	0	2.373213	-0.595441	-3.309904
35	1	0	3.290987	-1.157688	-3.545638
36	1	0	1.849489	-0.395358	-4.258310
37	1	0	1.731145	-1.237526	-2.688315
38	6	0	-2.108613	1.674115	-0.047398
39	6	0	-2.786293	1.638335	1.192147
40	6	0	-4.183360	1.494535	1.159736
41	1	0	-4.738744	1.456505	2.099806
42	6	0	-4.871931	1.394791	-0.051044
43	1	0	-5.958550	1.280321	-0.052405
44	6	0	-4.174524	1.439224	-1.260050
45	1	0	-4.723095	1.358452	-2.201412
46	6	0	-2.777135	1.580815	-1.288880
47	6	0	-2.063894	1.742791	2.532221
48	1	0	-0.989643	1.872252	2.328560
49	6	0	-2.534628	2.975130	3.333402
50	1	0	-3.600118	2.897787	3.602488
51	1	0	-2.401034	3.906206	2.760939

52	1	0	-1.961176	3.064043	4.269739
53	6	0	-2.220872	0.446775	3.354079
54	1	0	-3.276963	0.255127	3.602947
55	1	0	-1.662813	0.524299	4.300765
56	1	0	-1.837820	-0.421904	2.798314
57	6	0	-2.045413	1.626463	-2.627113
58	1	0	-0.970119	1.742446	-2.421075
59	6	0	-2.489549	2.840572	-3.470537
60	1	0	-3.555888	2.774727	-3.739480
61	1	0	-1.912241	2.887190	-4.407585
62	1	0	-2.339291	3.787479	-2.929006
63	6	0	-2.221520	0.308105	-3.408377
64	1	0	-1.861326	-0.549979	-2.822001
65	1	0	-1.653338	0.344280	-4.351477
66	1	0	-3.278712	0.129428	-3.662092
67	8	0	-0.179243	-3.154679	0.069906
68	6	0	-1.396257	-3.890858	0.083936
69	6	0	-0.982310	-5.377420	0.105250
70	1	0	-1.859448	-6.045509	0.117567
71	1	0	-0.375175	-5.607995	-0.783555
72	1	0	-0.370645	-5.581207	0.997491
73	6	0	-2.225340	-3.563310	1.344653
74	1	0	-1.617550	-3.737277	2.246286
75	1	0	-2.527051	-2.502906	1.330717
76	1	0	-3.137566	-4.181202	1.411239
77	6	0	-2.232404	-3.601198	-1.181280
78	1	0	-2.530555	-2.539802	-1.198451
79	1	0	-1.630989	-3.805363	-2.080879
80	1	0	-3.146826	-4.218047	-1.222499

IPrAuNTf$_2$

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.178301	-0.004169	-0.002341
2	16	0	3.119421	0.809101	1.199206
3	16	0	3.086075	-0.915009	-1.213845
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5	9	0	3.970311	3.332395	1.341488
6	9	0	4.195138	2.464390	-0.658170
7	9	0	3.849027	-3.466100	-1.359567
8	9	0	2.118060	-3.148432	-0.049780
9	9	0	4.125630	-2.602315	0.635372

10	8	0	2.139994	1.047693	2.273287
11	8	0	4.453704	0.269469	1.474315
12	8	0	4.435059	-0.417882	-1.497207
13	8	0	2.093610	-1.124068	-2.282149
14	7	0	-2.616479	1.116765	-0.159768
15	7	0	-2.651953	-1.030948	0.162552
16	7	0	2.290415	-0.039399	-0.005721
17	6	0	-1.800797	0.028979	0.000248
18	6	0	-3.955455	0.740049	-0.097833
19	1	0	-4.756649	1.462132	-0.203661
20	6	0	-3.977749	-0.609678	0.104252
21	1	0	-4.802342	-1.304571	0.212377
22	6	0	-2.161582	2.479958	-0.369155
23	6	0	-1.999154	3.314966	0.759176
24	6	0	-1.585100	4.636435	0.523147
25	1	0	-1.442717	5.310270	1.370899
26	6	0	-1.343581	5.098407	-0.772081
27	1	0	-1.017469	6.128977	-0.930582
28	6	0	-1.511167	4.245719	-1.865004
29	1	0	-1.312161	4.616422	-2.873033
30	6	0	-1.925858	2.914635	-1.692917
31	6	0	-2.250547	2.842211	2.188287
32	1	0	-2.534656	1.778655	2.151020
33	6	0	-0.975044	2.945263	3.050393
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38	1	0	-3.194471	4.684429	2.927596
39	1	0	-3.627211	3.223033	3.842705
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41	6	0	-2.093923	2.009122	-2.909885
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78	1	0	-0.906338	-1.075780	4.482590
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80	6	0	3.397053	2.539173	0.414268
81	6	0	3.313493	-2.652018	-0.427851

X-ray Crystallography

Low-temperature diffraction data were collected at the UC-Berkeley CHEXRAY crystallographic facility. Measurements were made with a Bruker-AXS Smart Apex CCDdetector with graphite-monochromated Mo Kα radiation (λ = 0.71073 Å). The structures were solved by direct methods using SHELXS[8] and refined against *F*2 on all data by full-matrix least squares with SHELXL-97[9] using established methods.[10] All non-hydrogen atoms were refined anisotropically. All hydrogen atoms were included into the model at geometrically calculated positions and refined using a riding model. The isotropic displacement parameters of all hydrogen atoms were fixed to 1.2 times the *U* value of the atoms they are linked to (1.5 times for methyl groups). Crystallographic data for **1**, **2**, **6**, **11**, **12**, **13**, and the conjugate acid of **1** can be obtained free of charge from the Cambridge Crystallographic Data Centre via www.ccdc.cam.ac.uk/data_request/cif.

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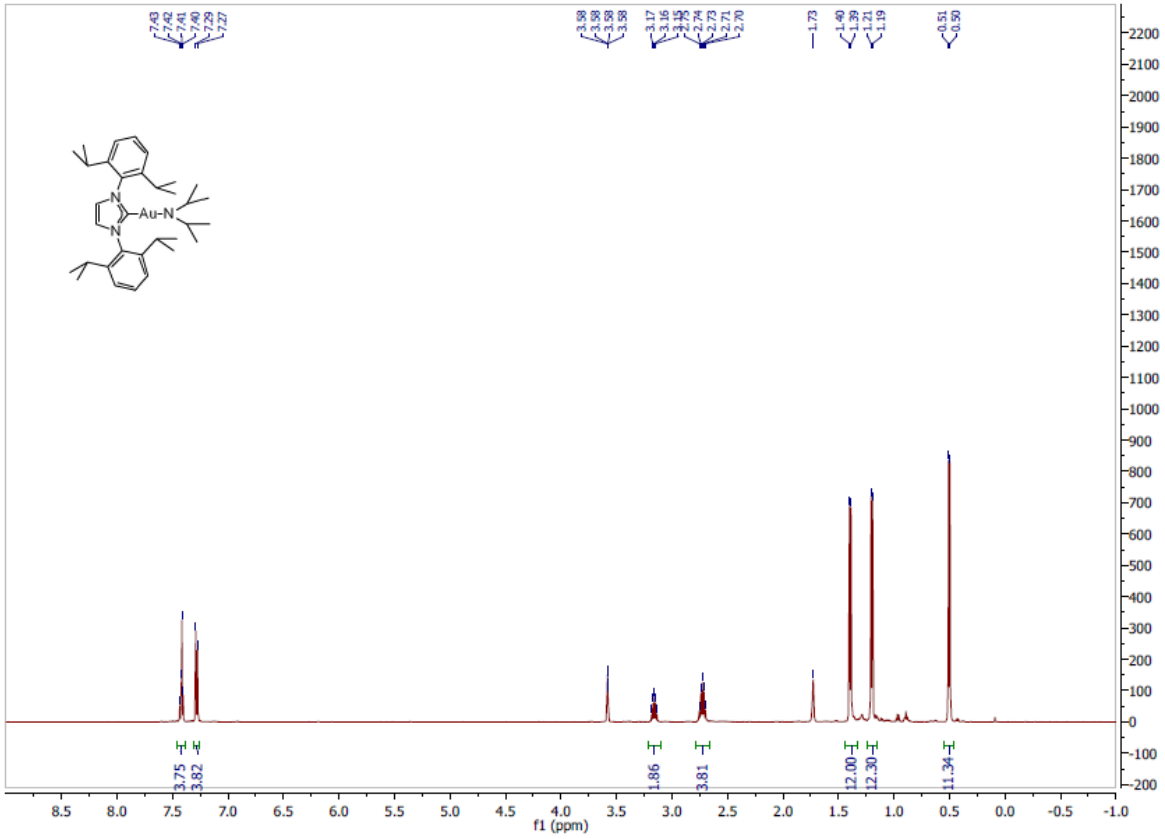
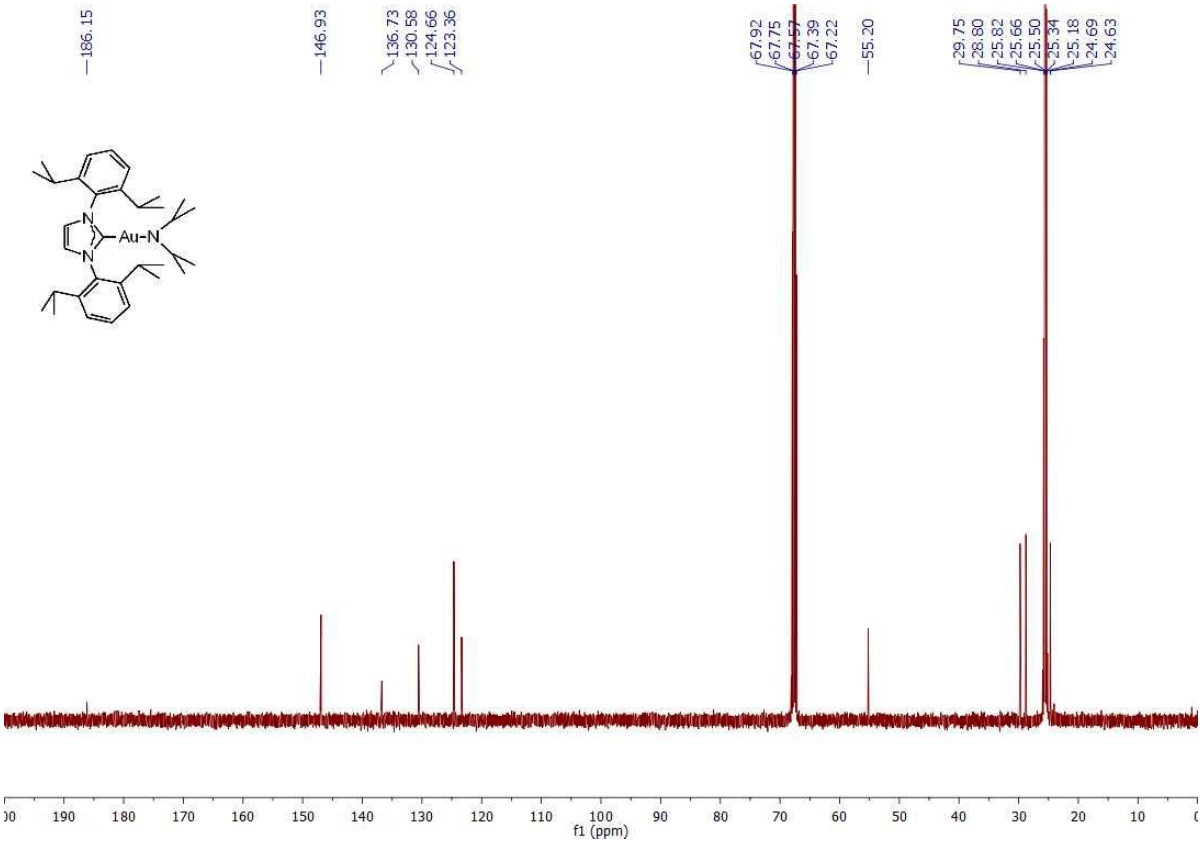
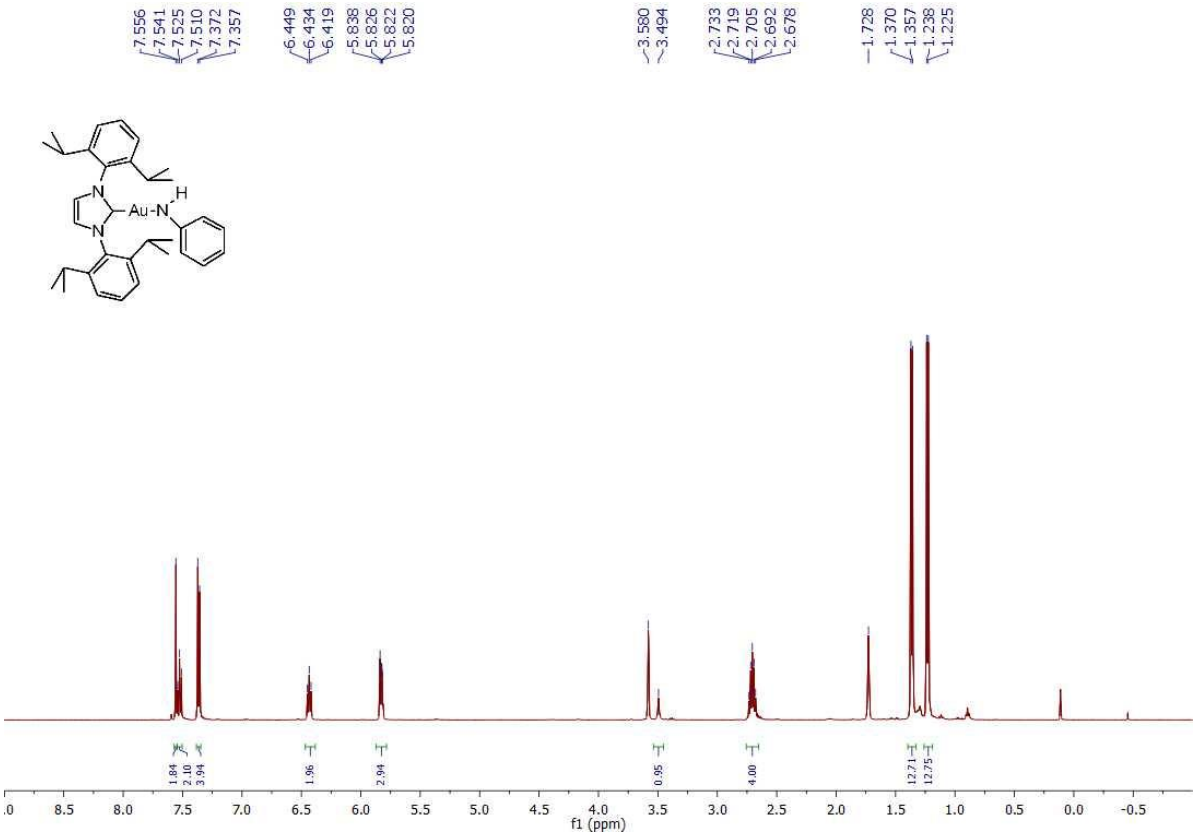
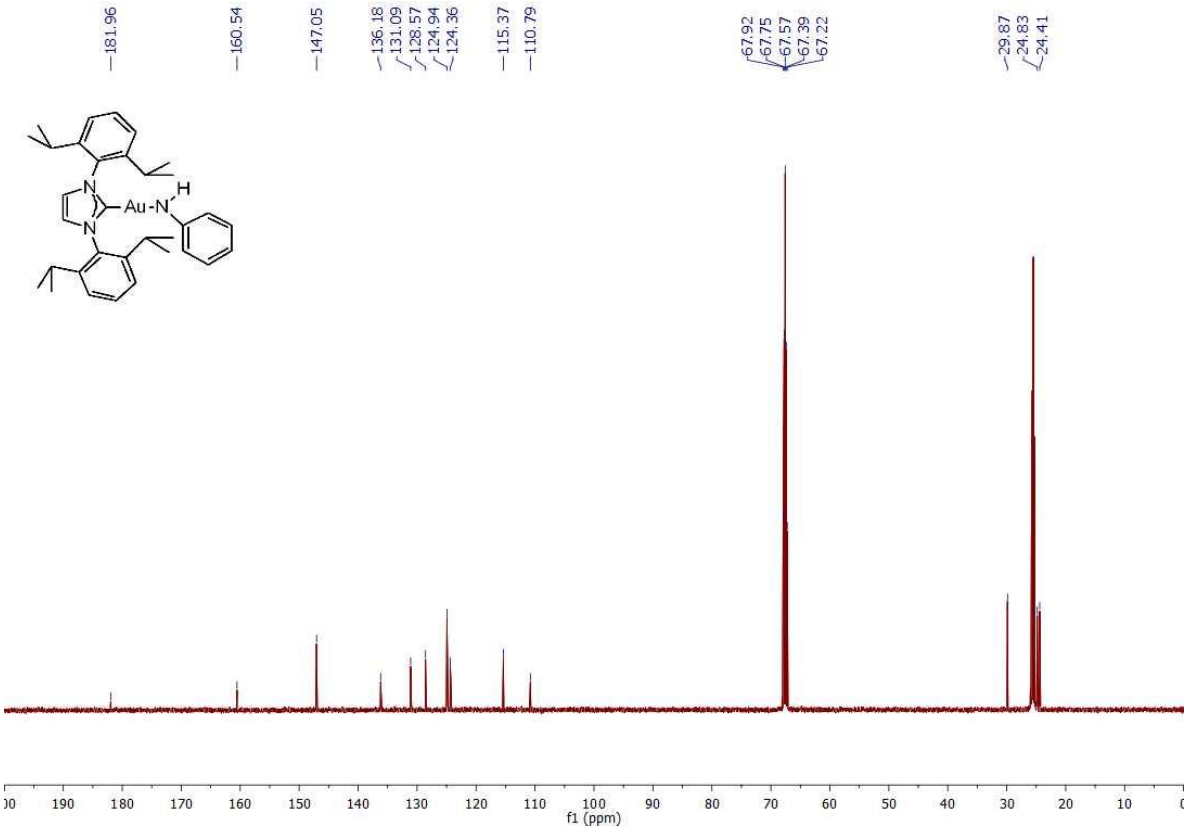
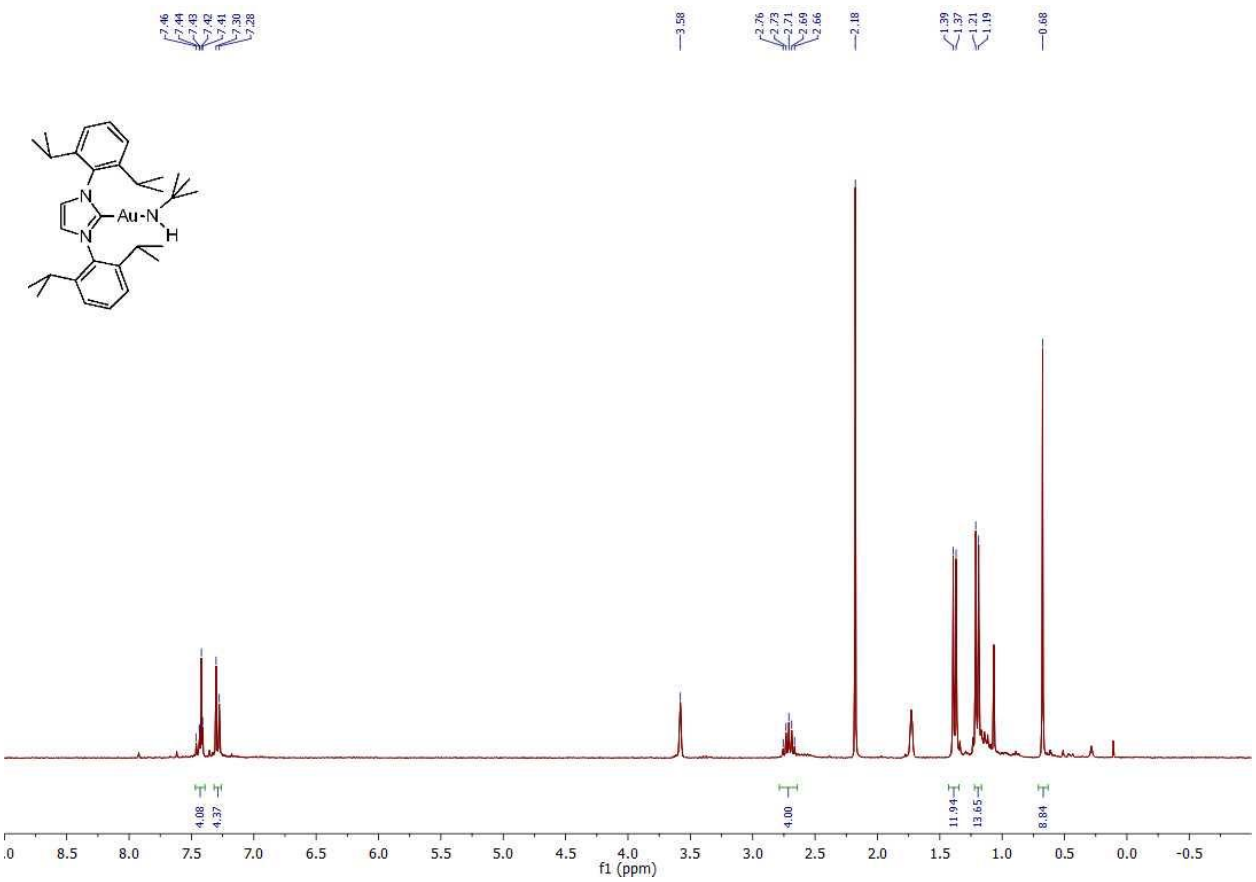
^{1}H and ^{13}C NMR Spectra

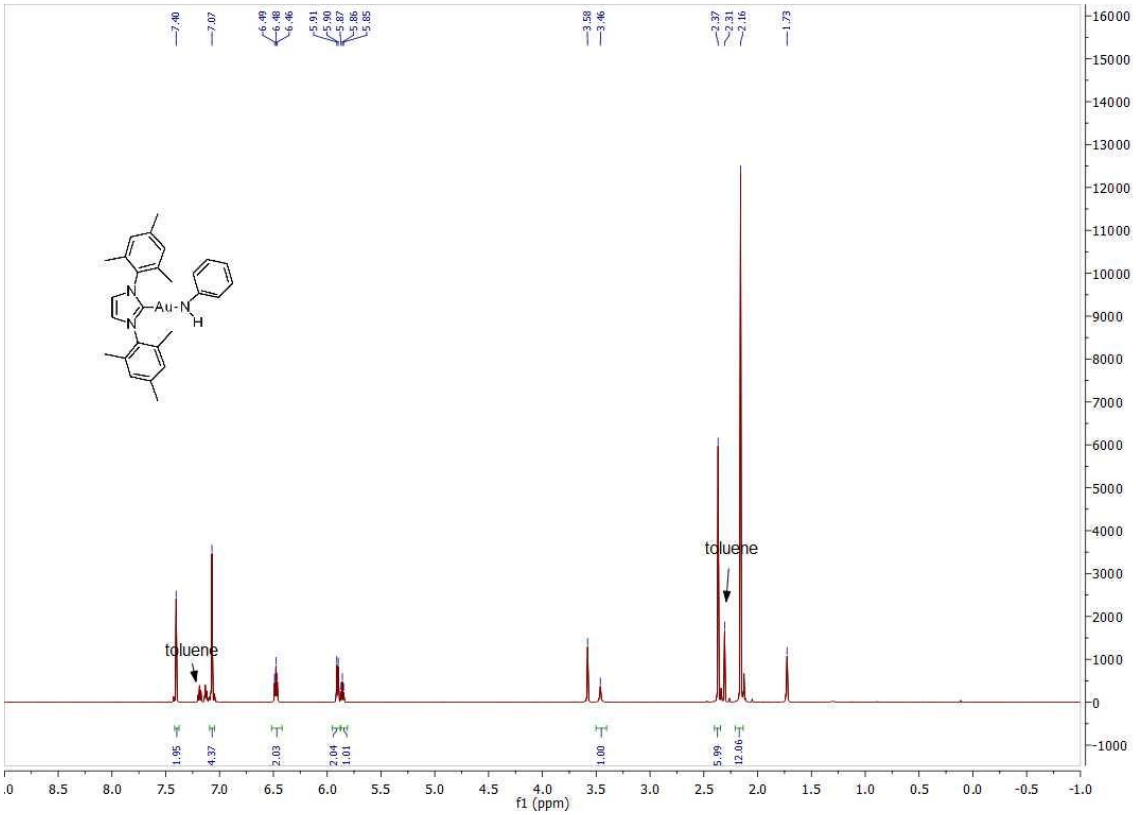








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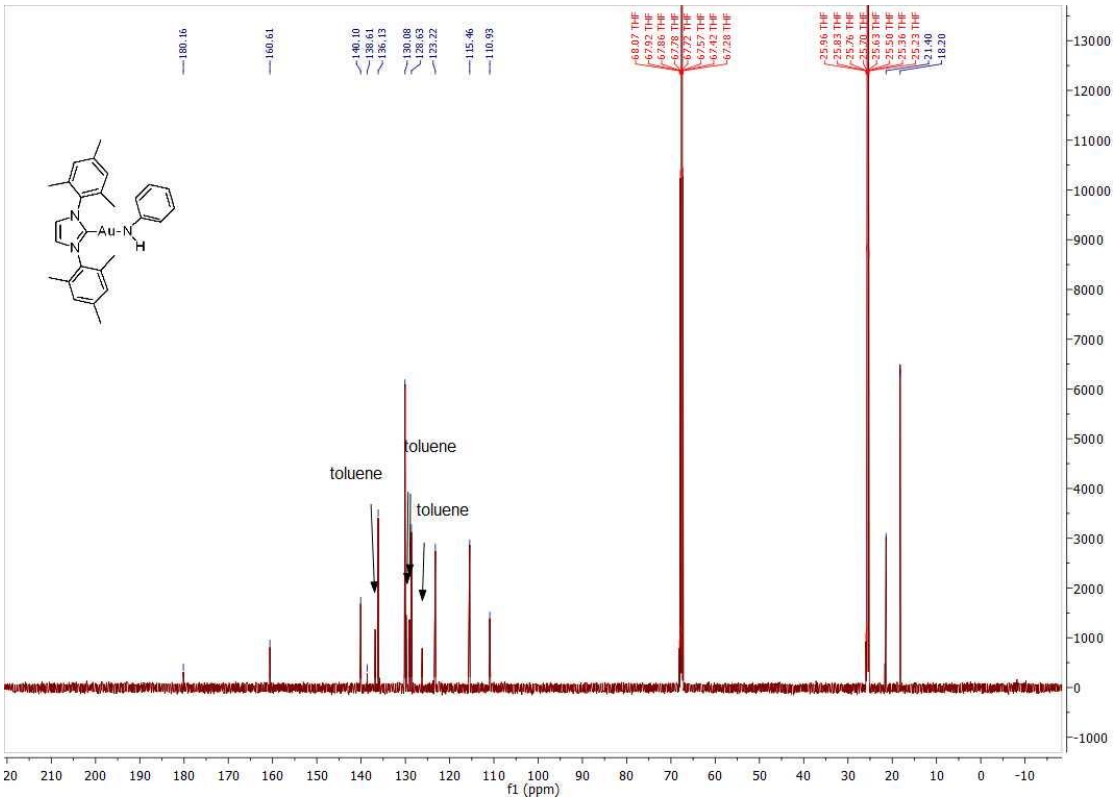
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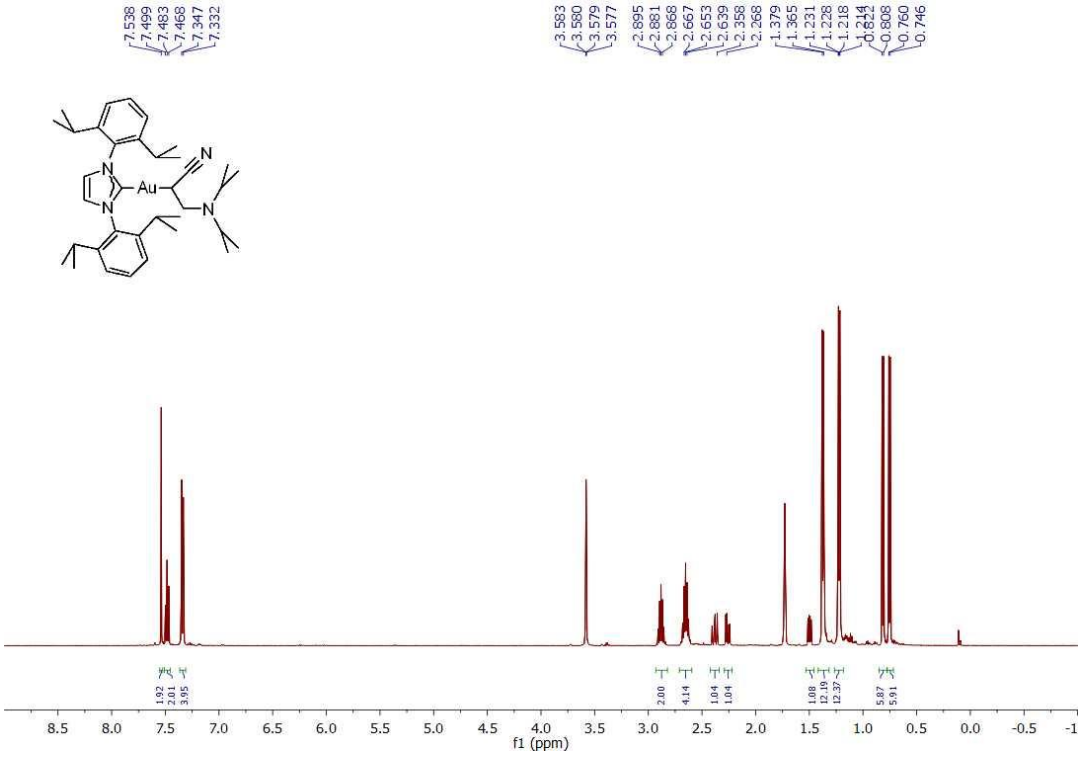
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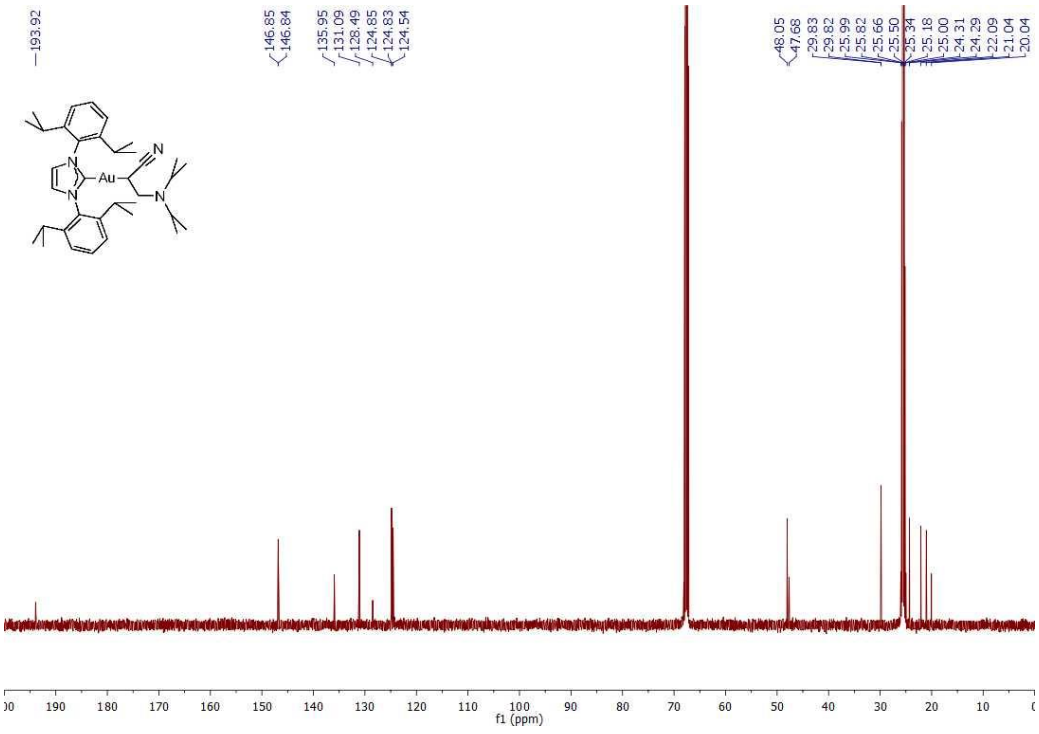
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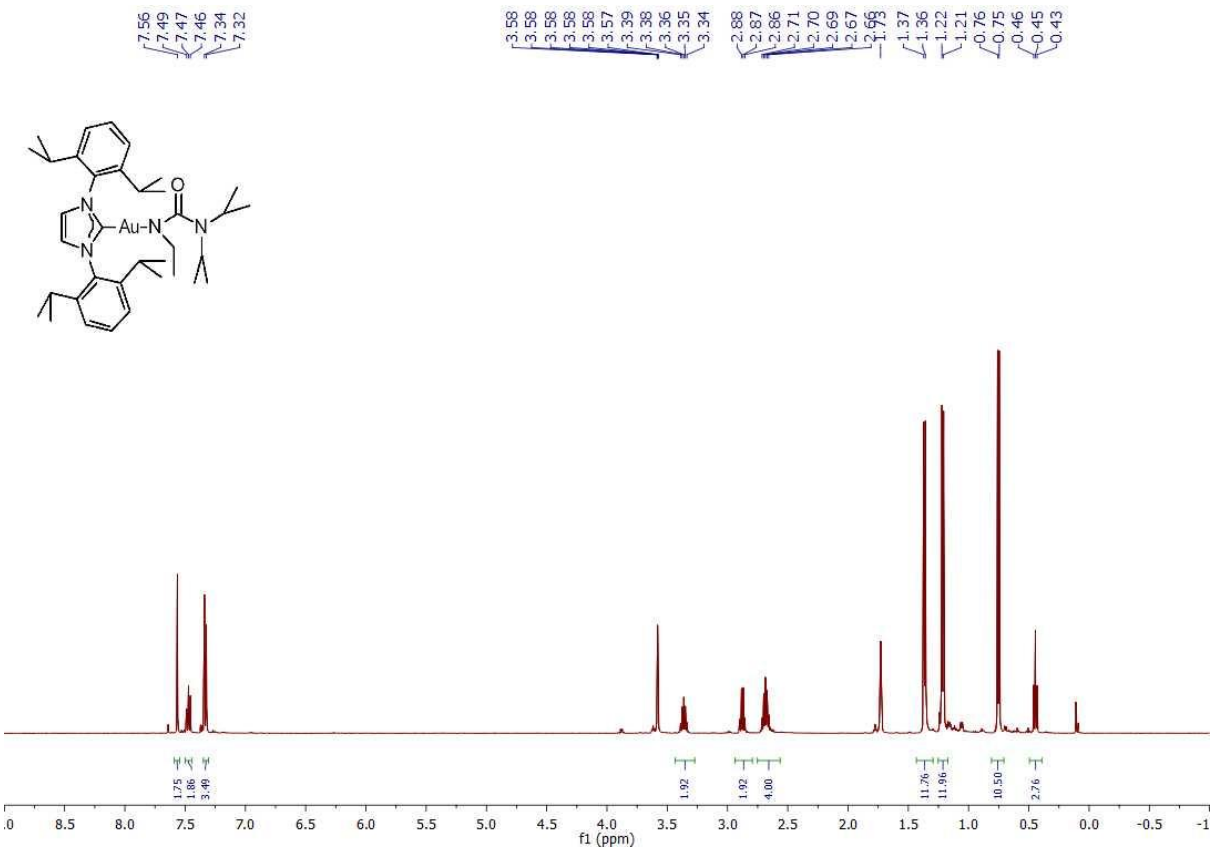
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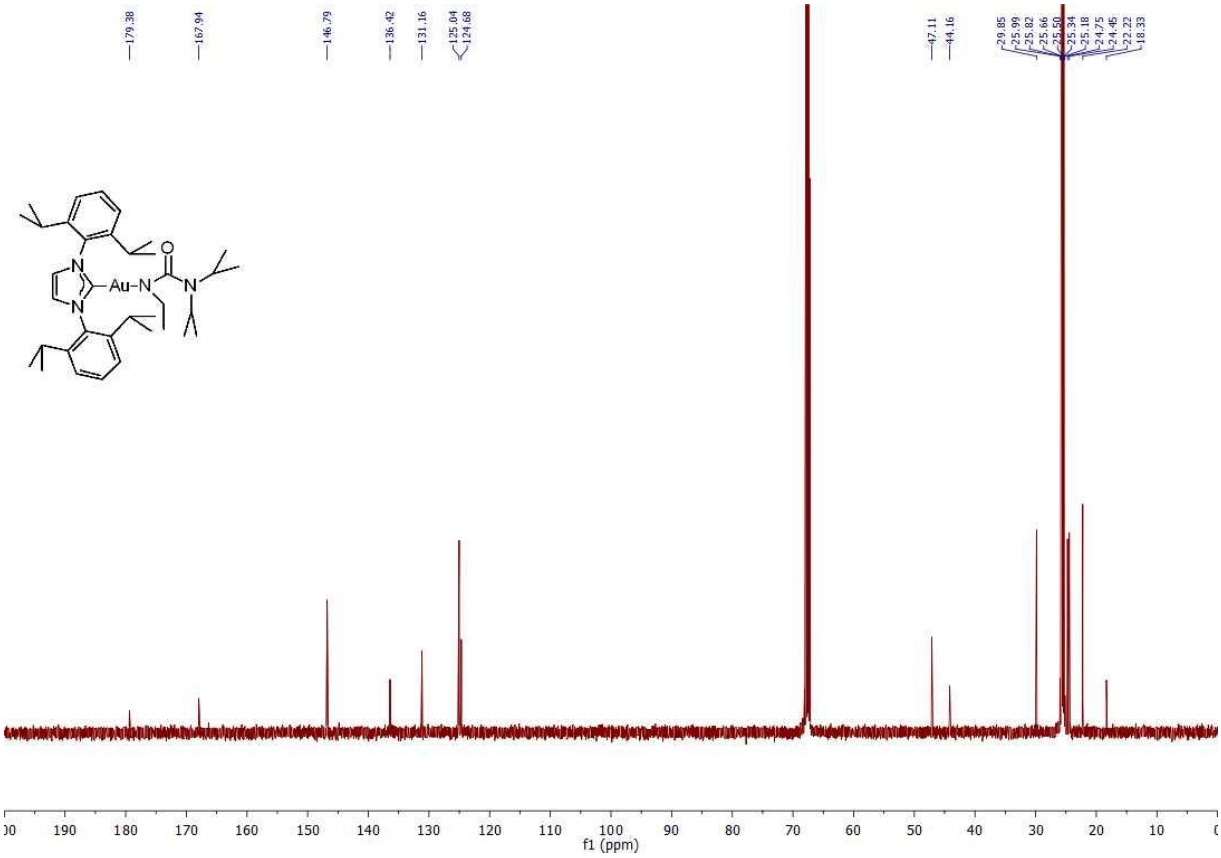
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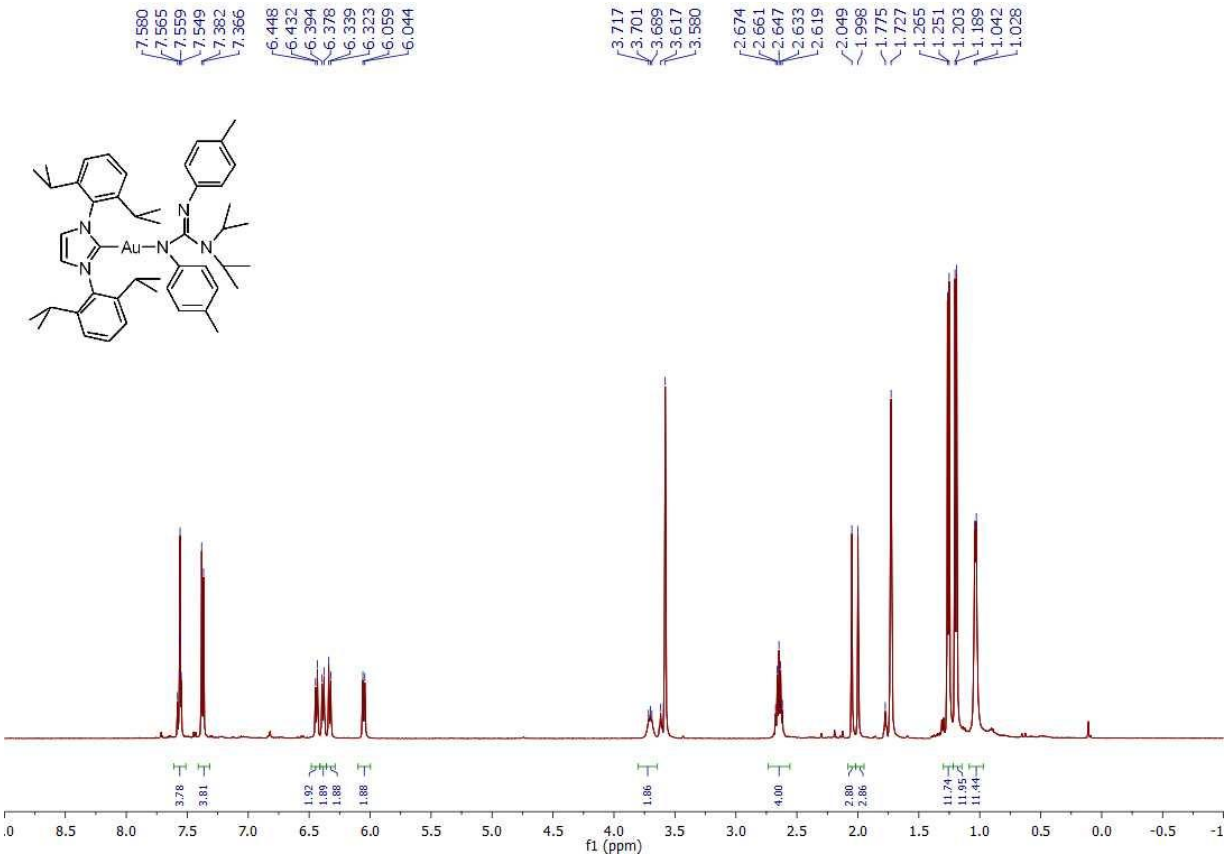
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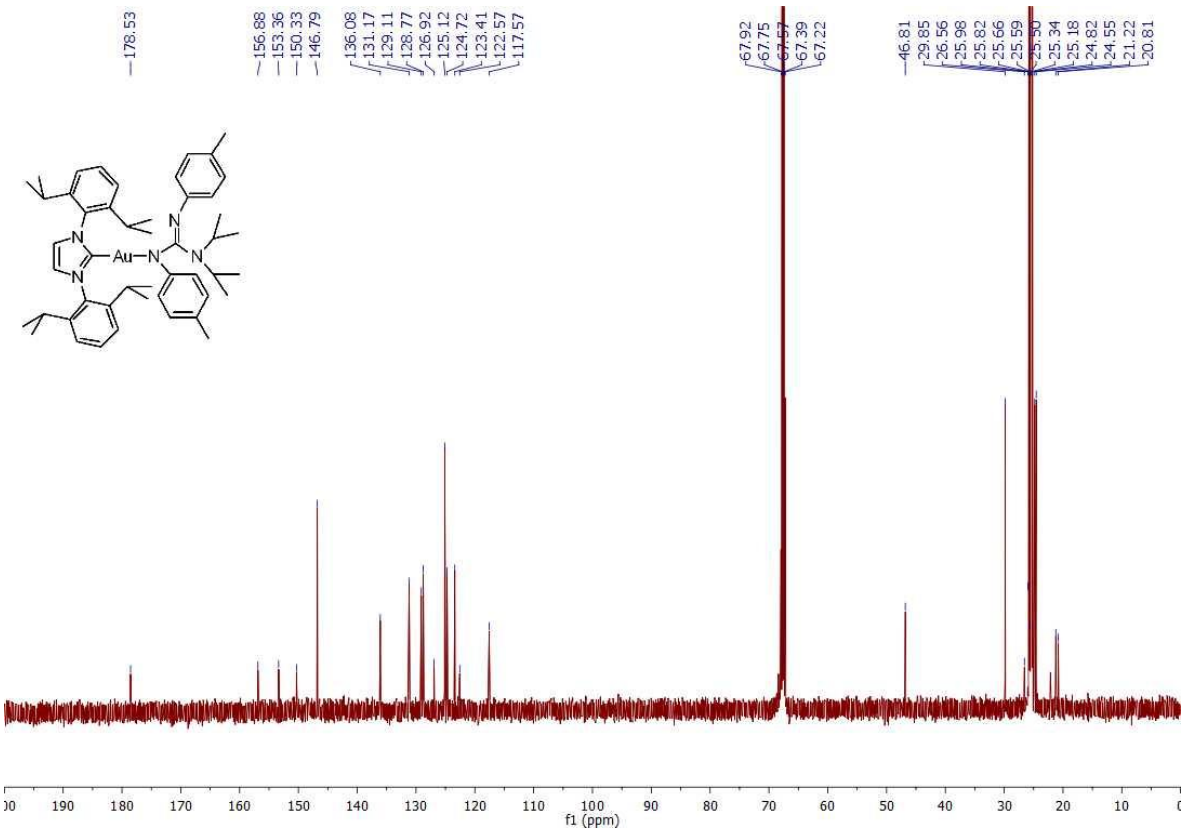
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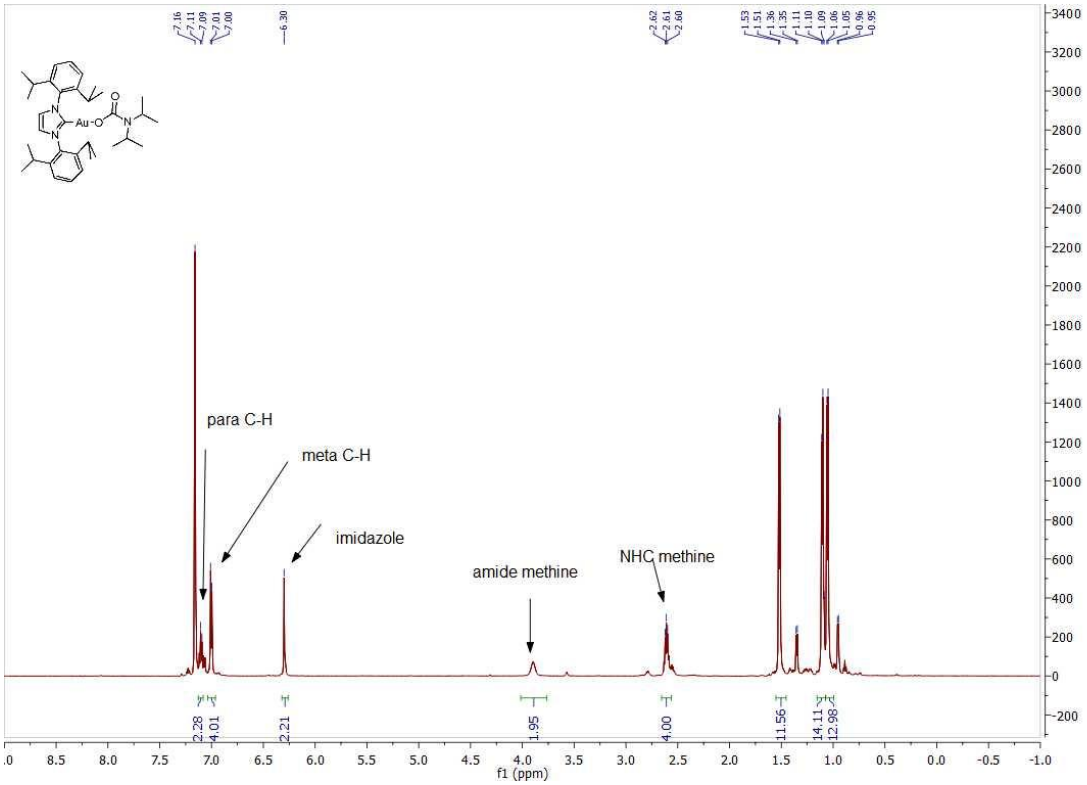

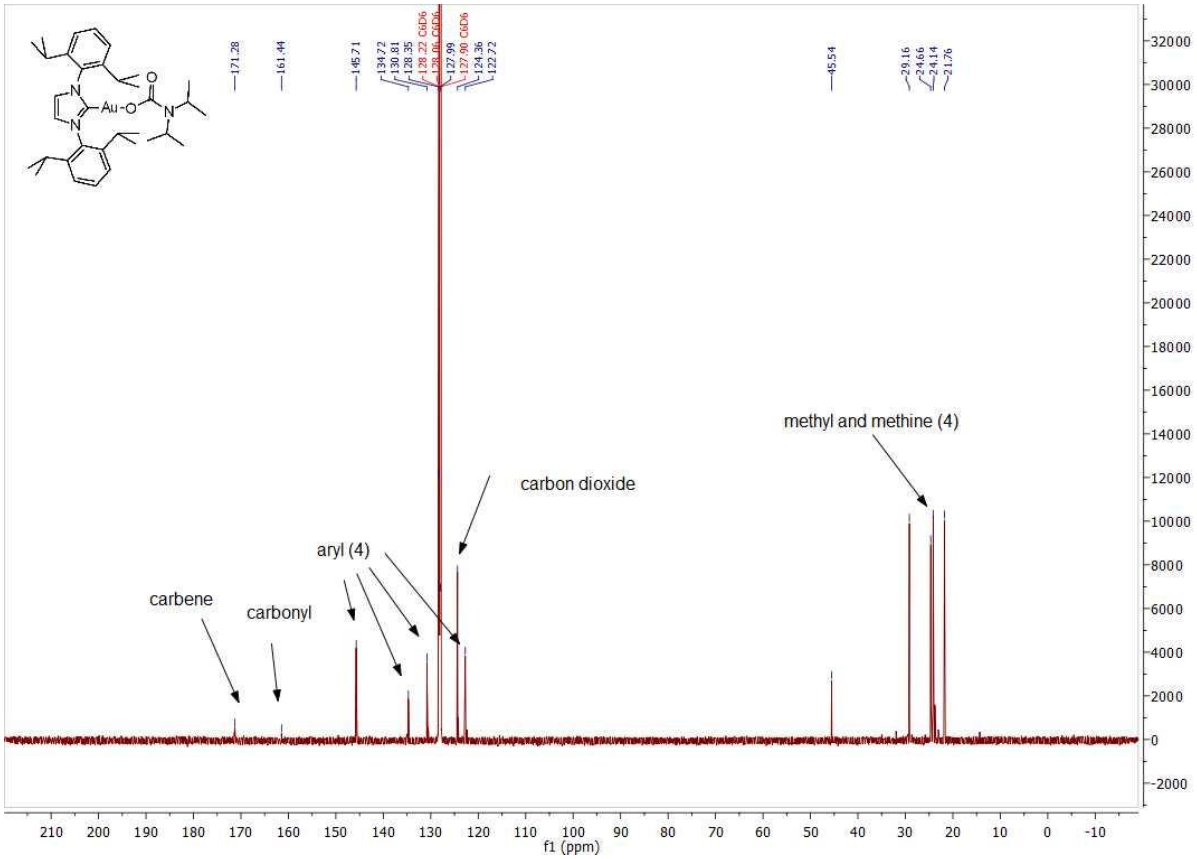

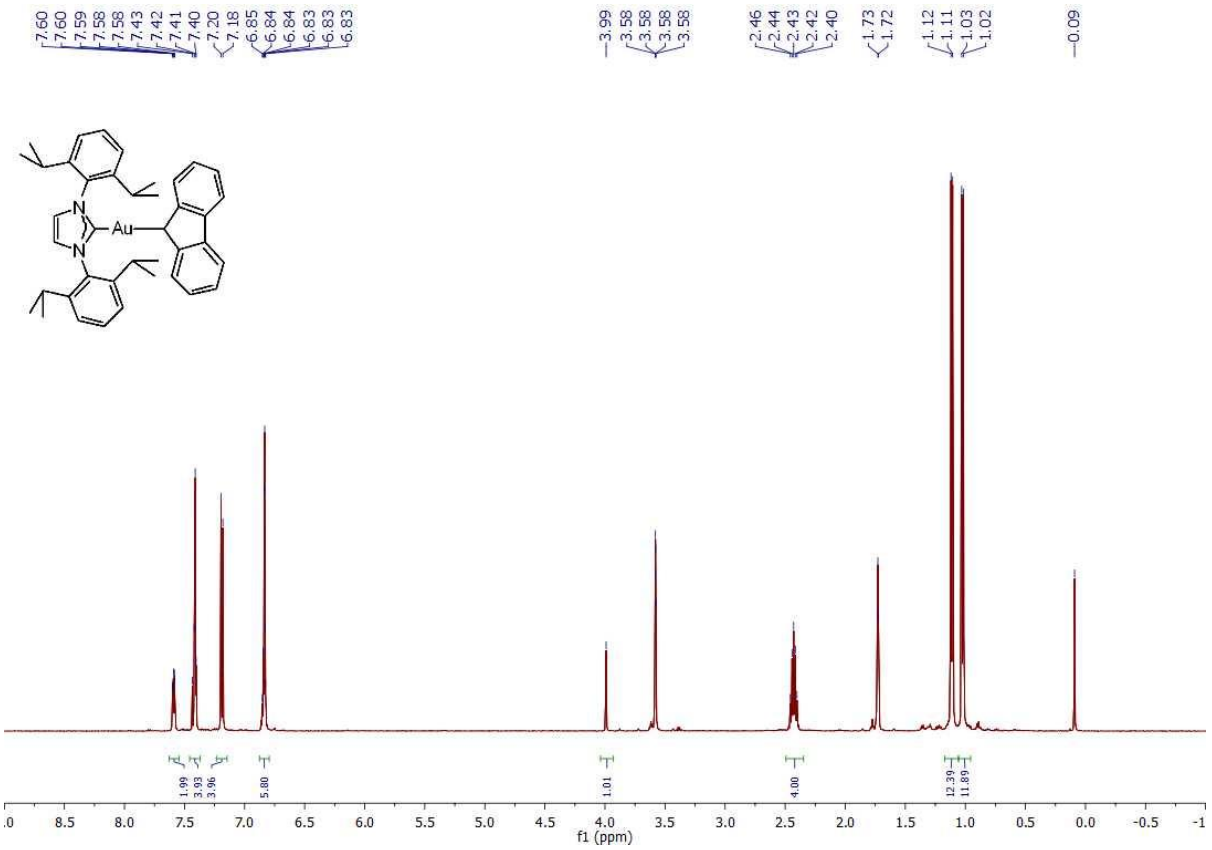
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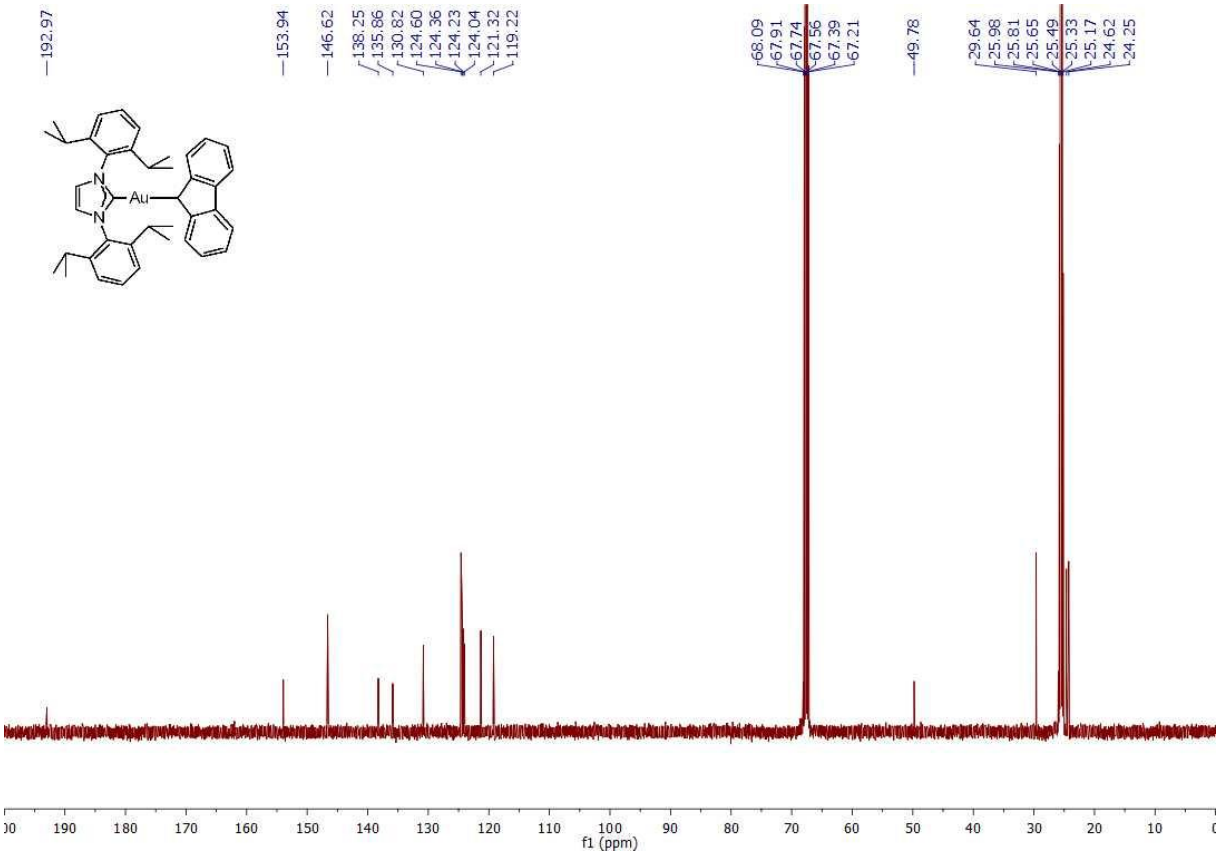
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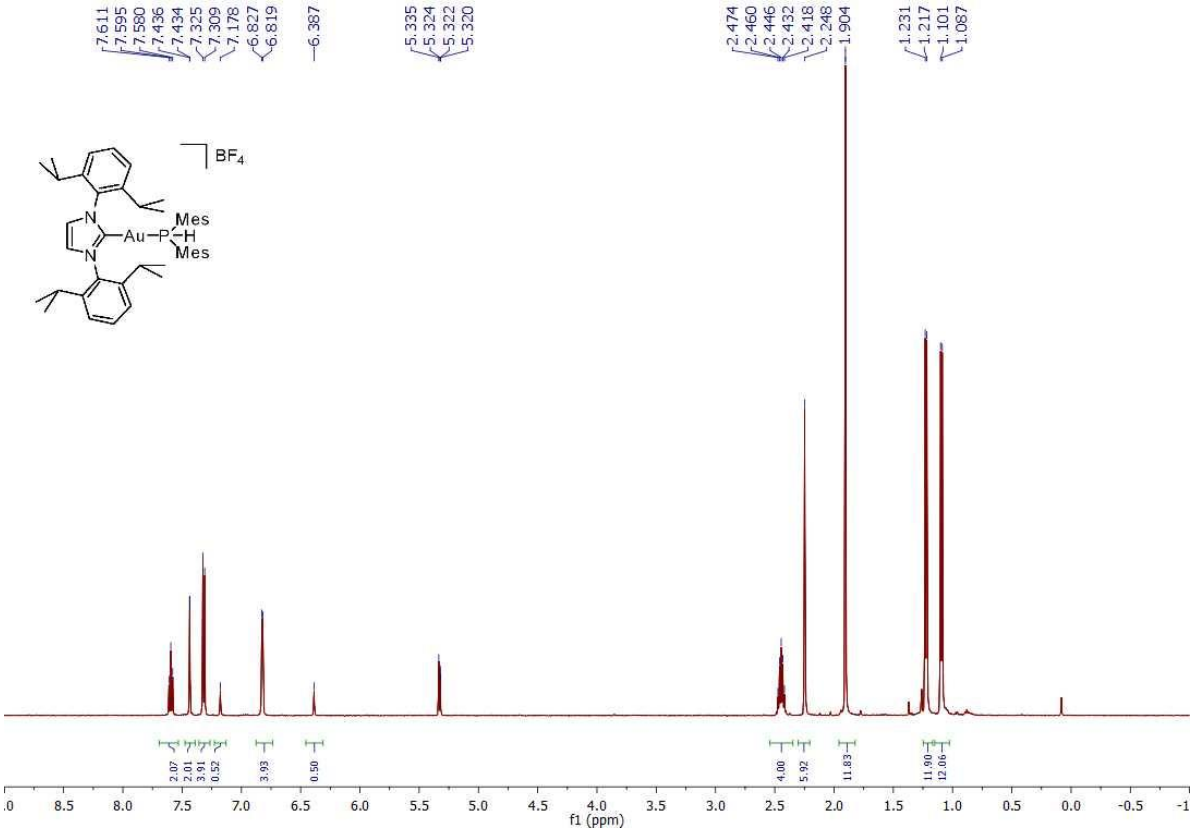

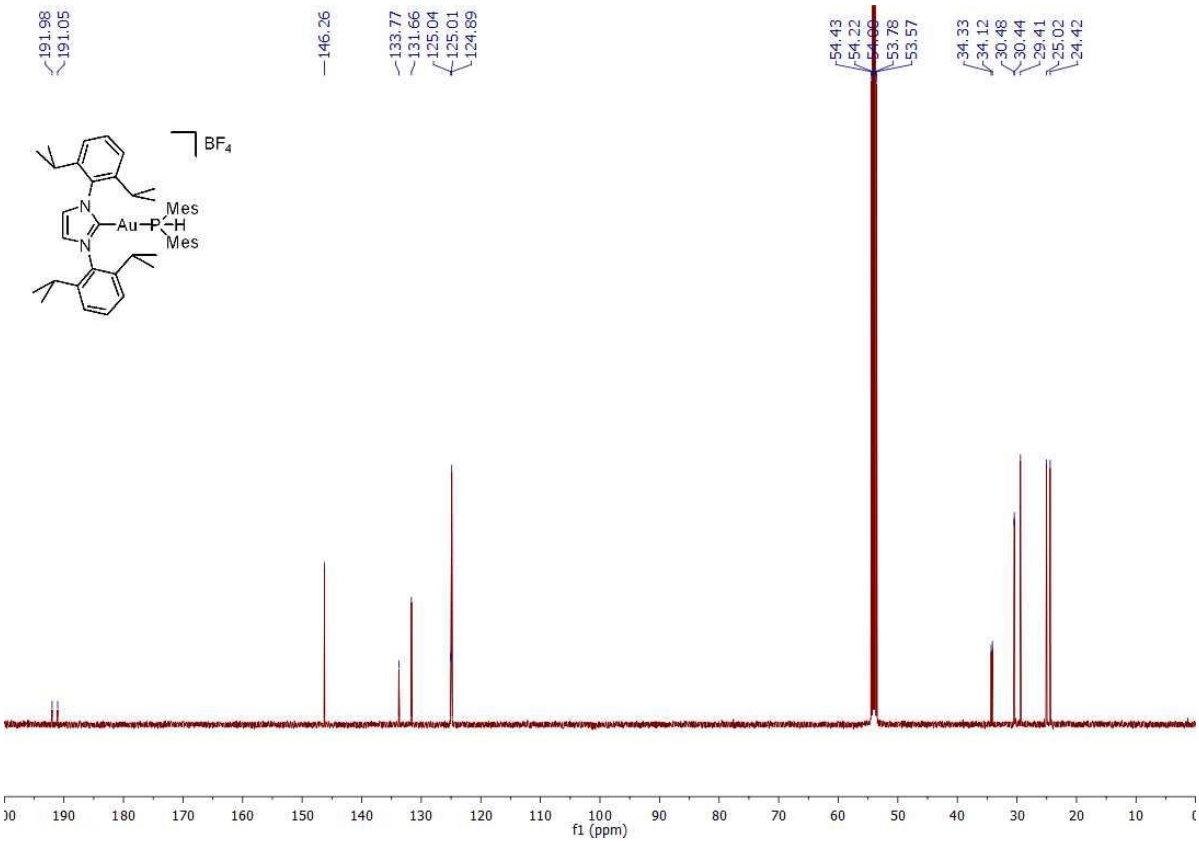

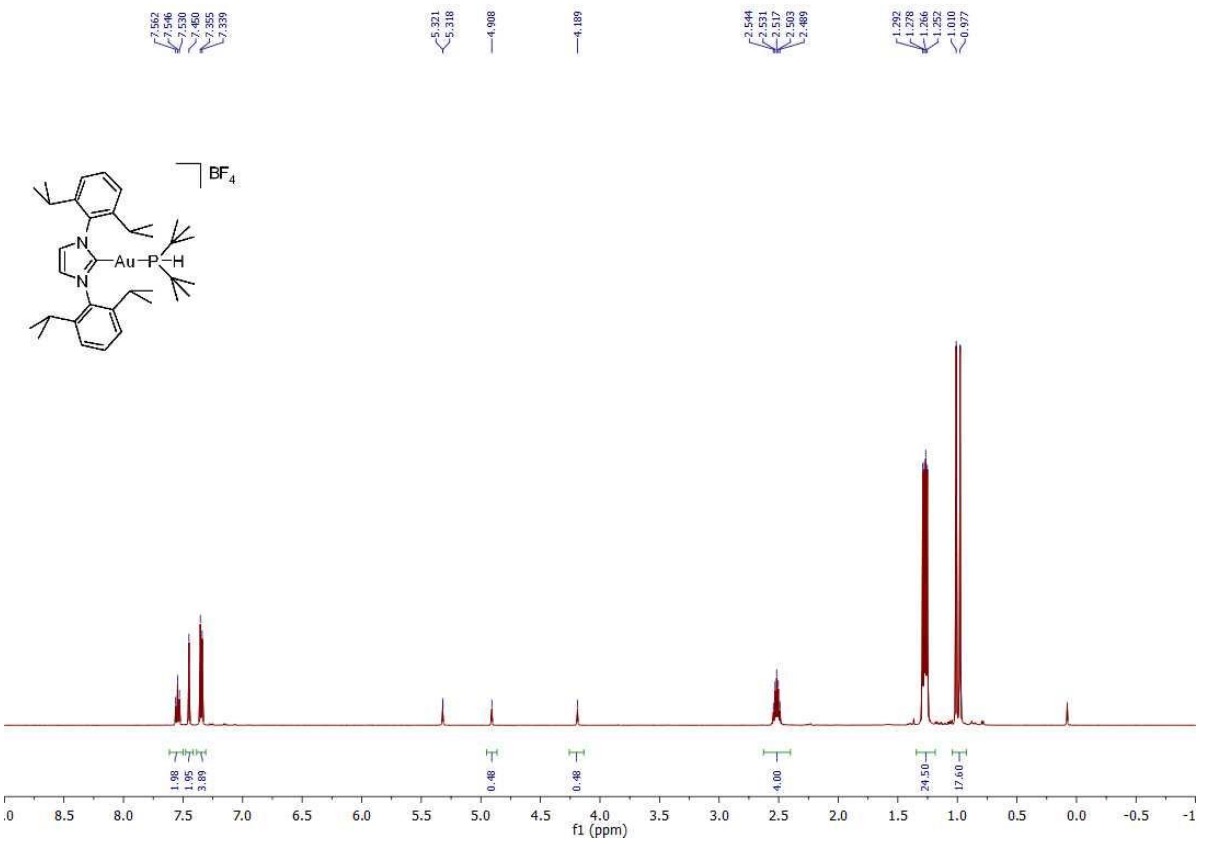

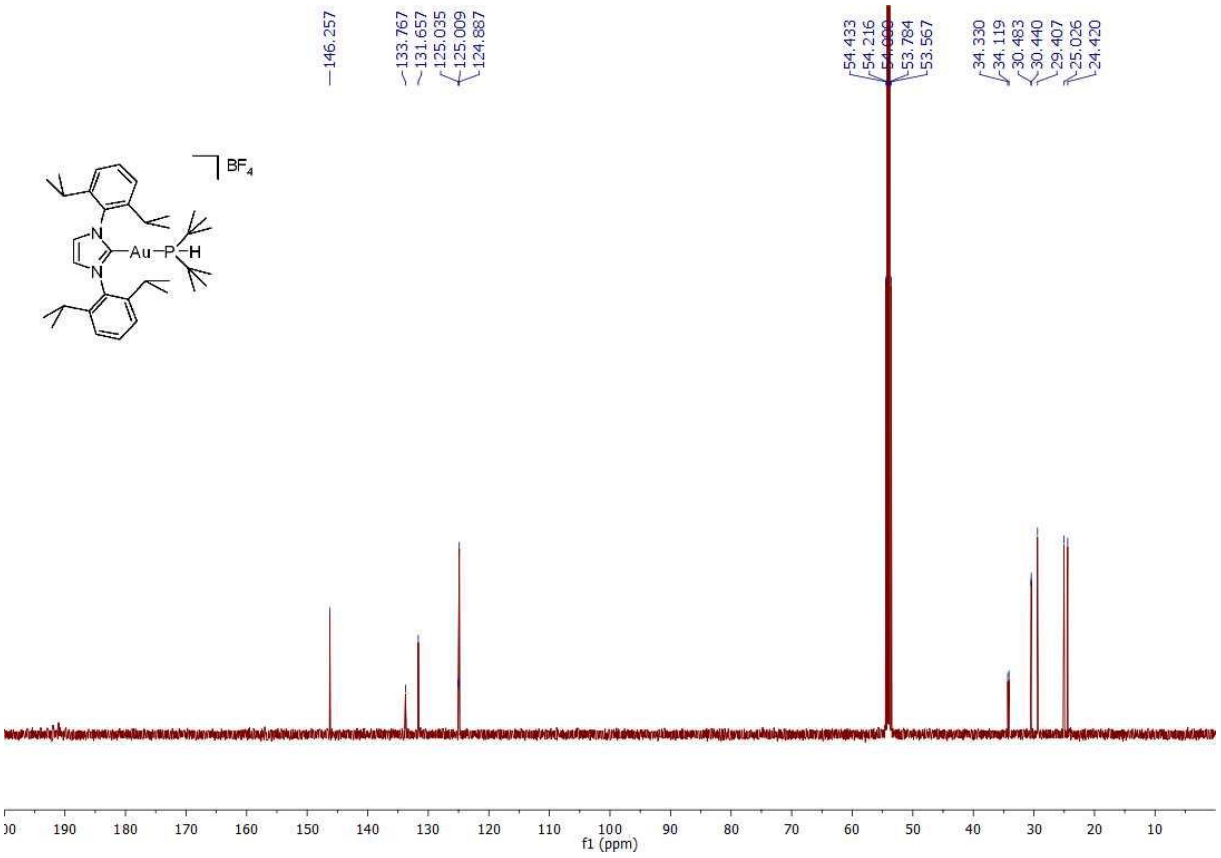

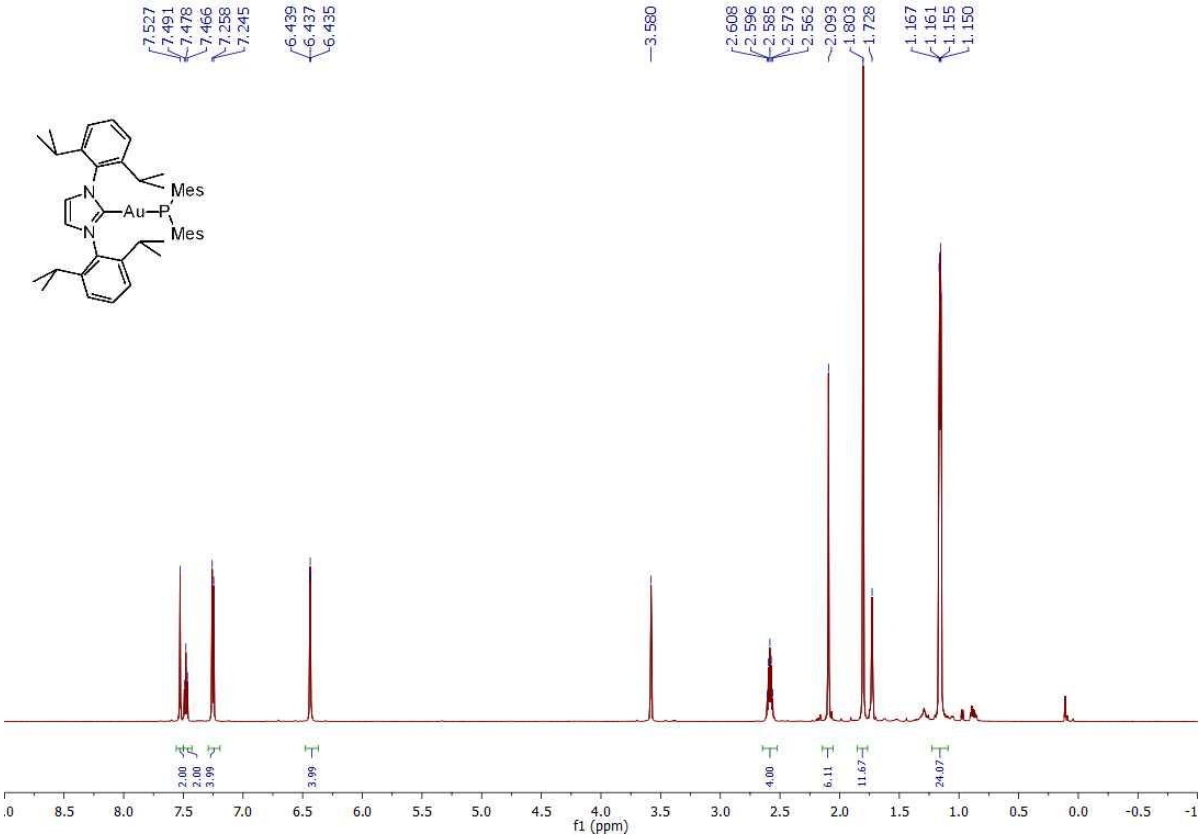
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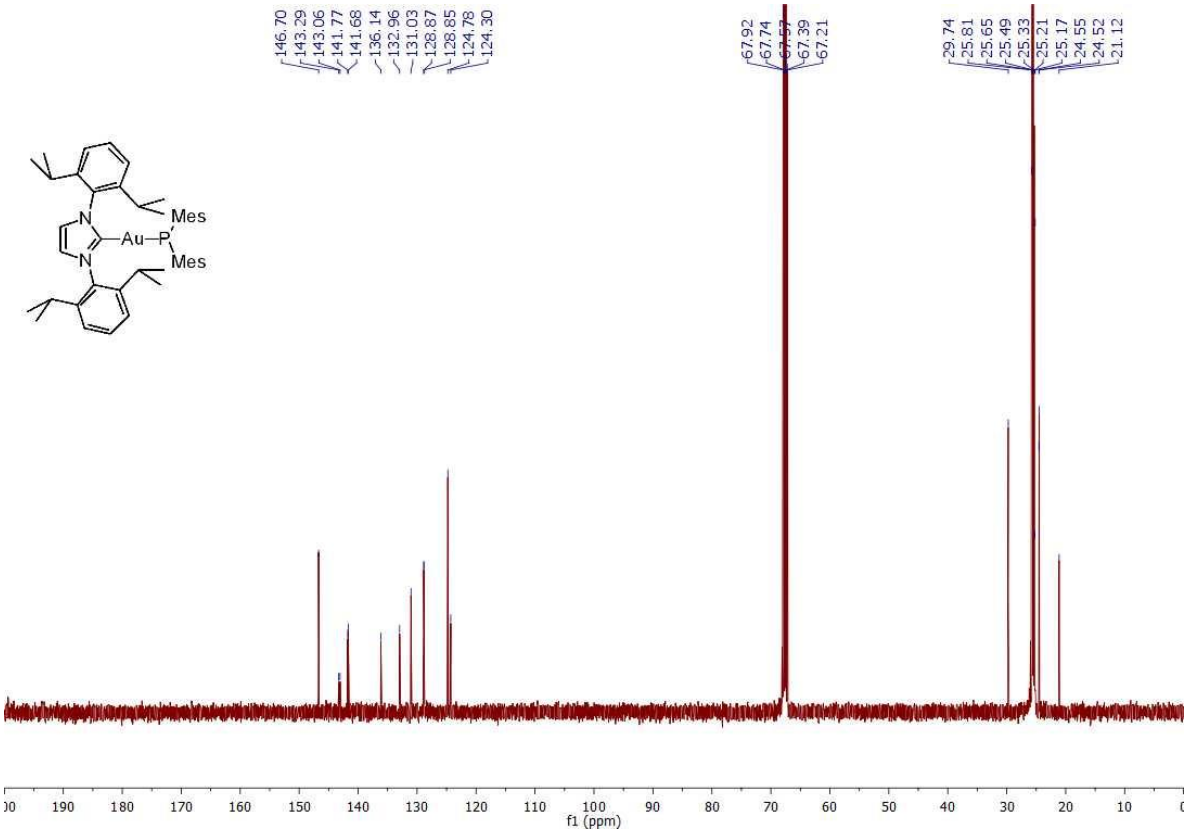
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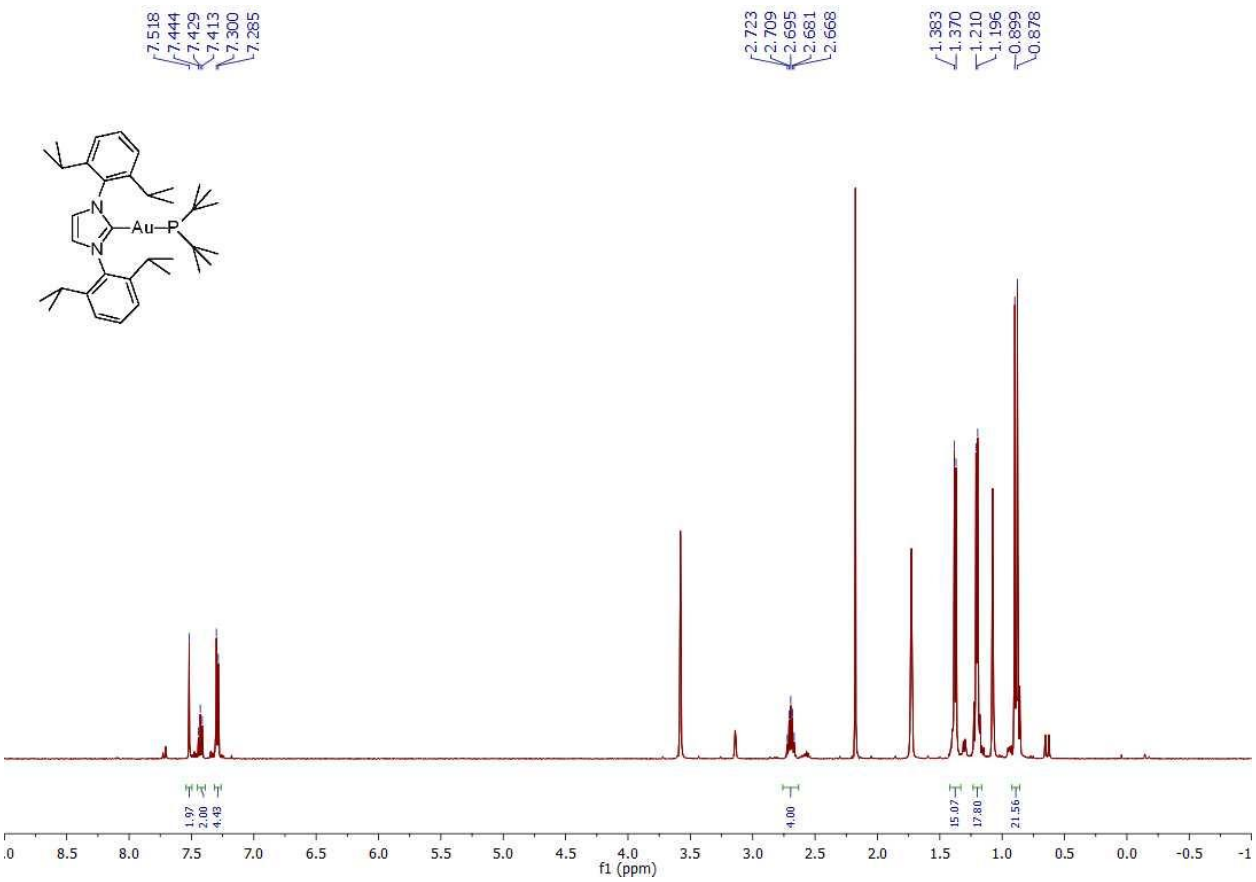
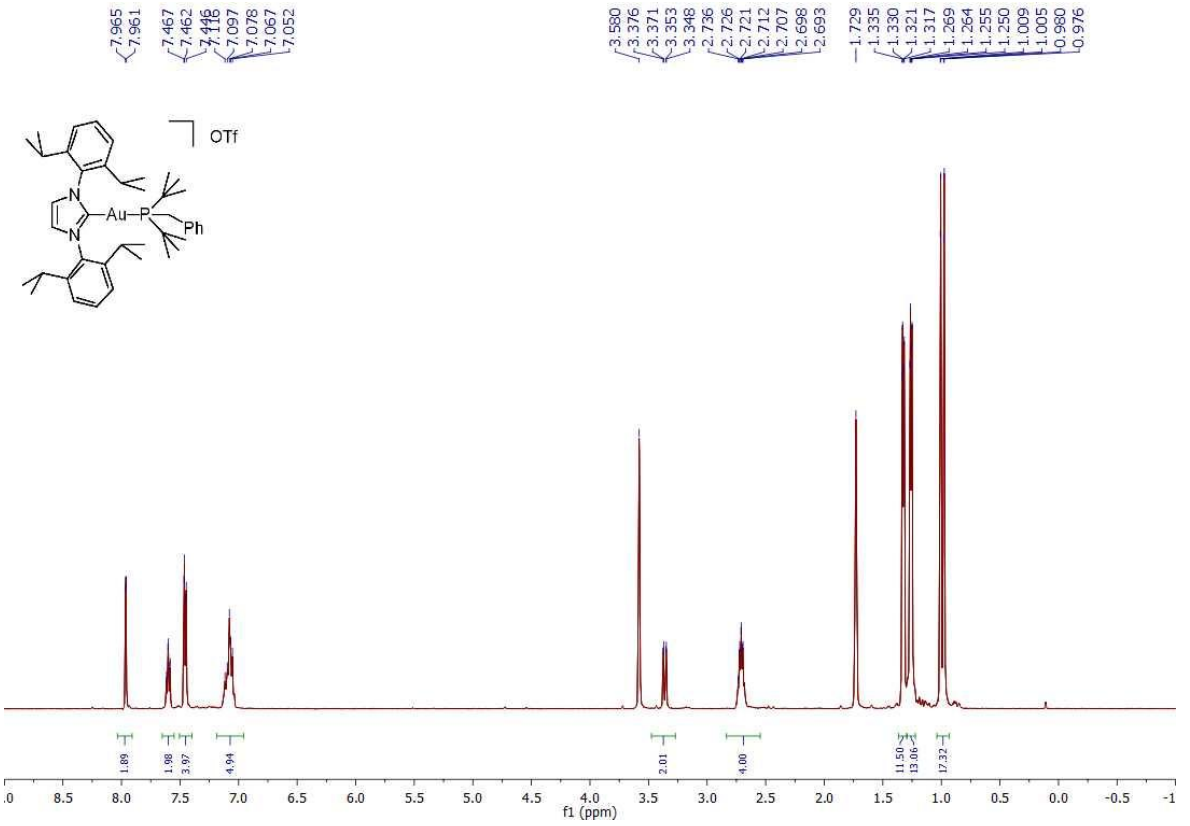
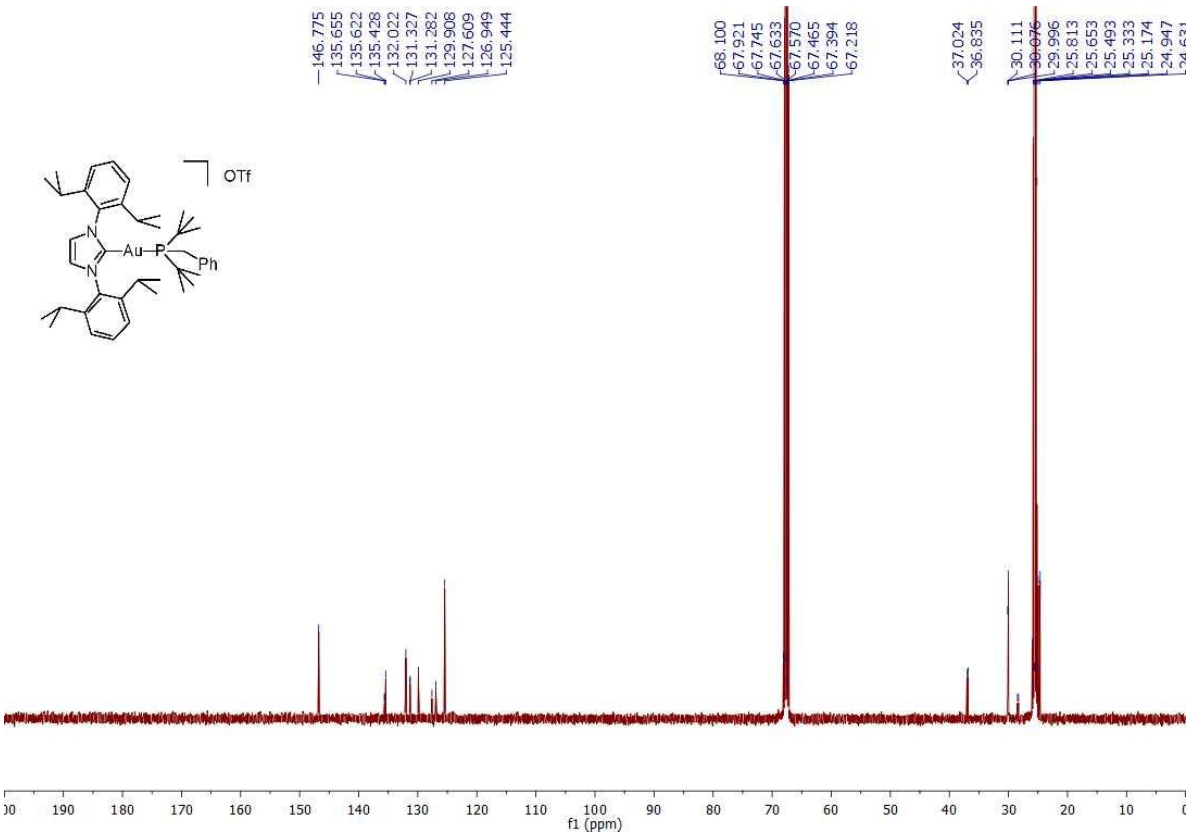
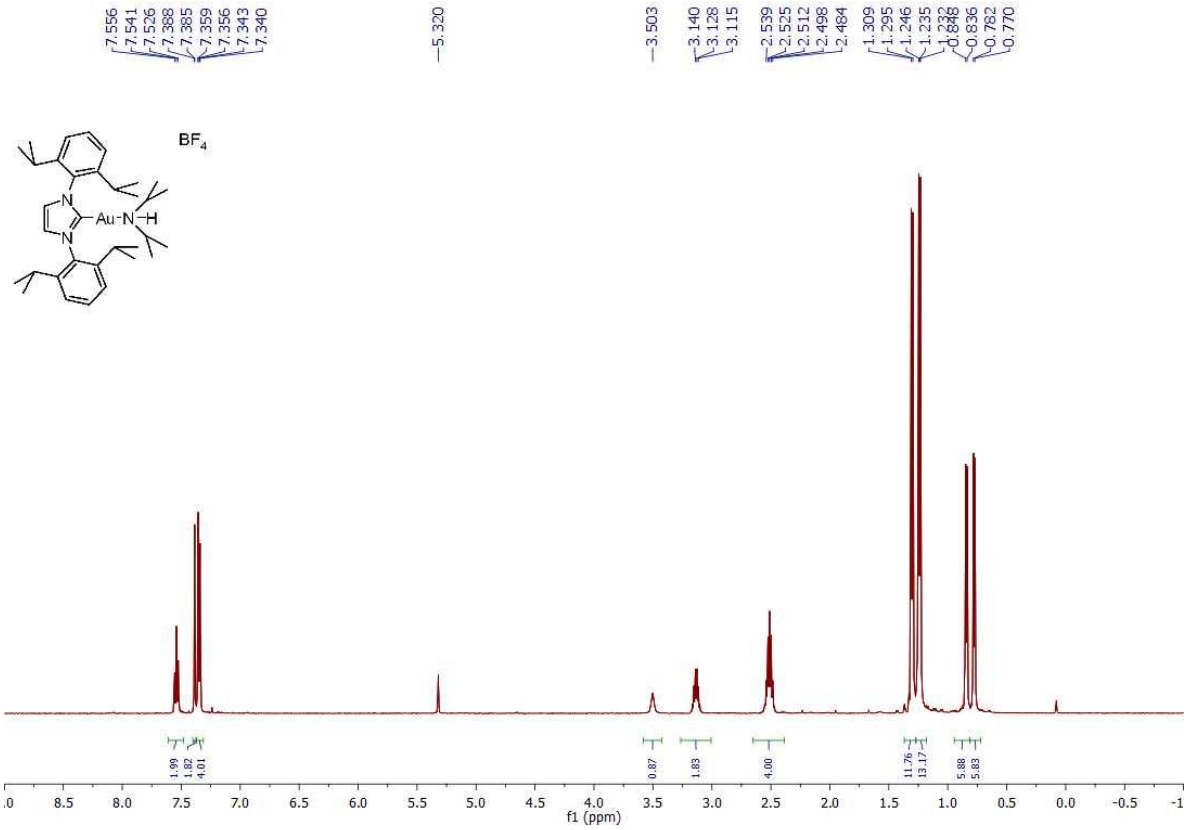
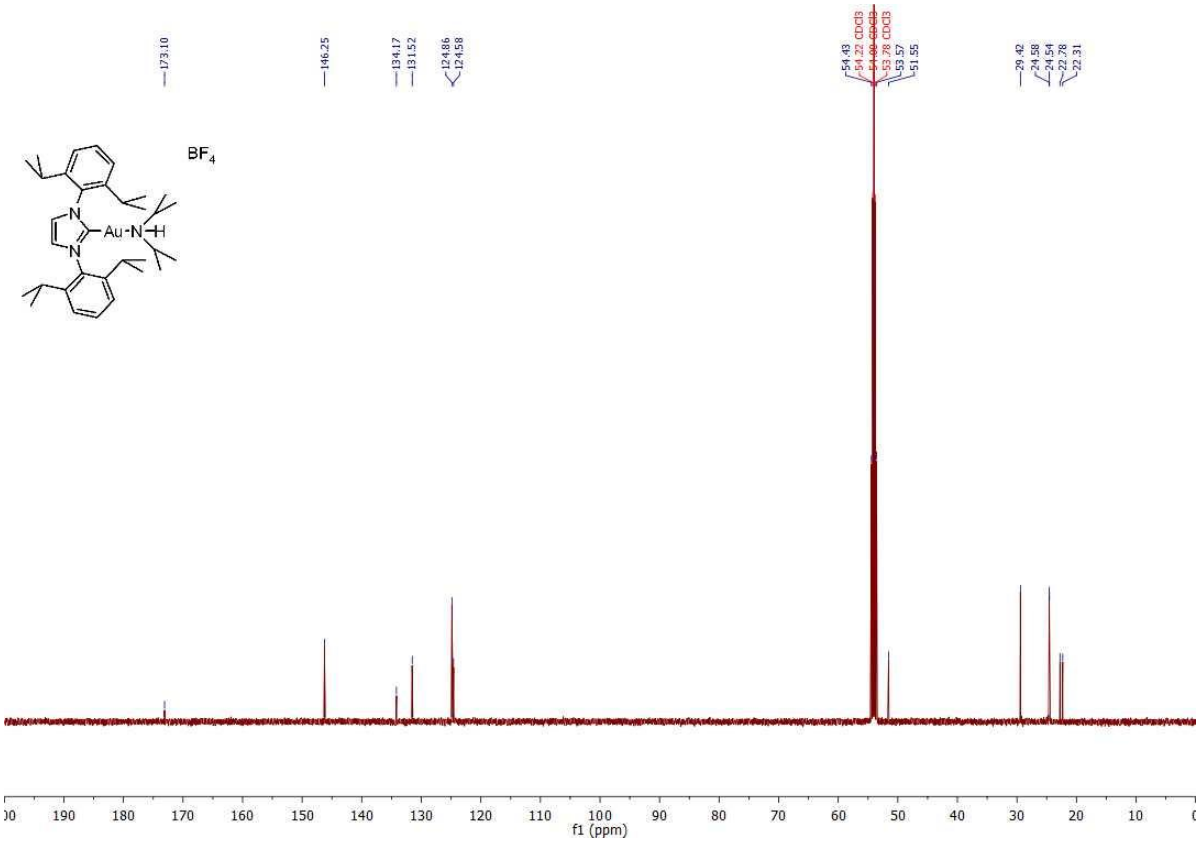
Au
P
Mes
f1 (ppm)








7.556
7.541
7.526
7.388
7.385
7.359
7.356
7.343
7.340
5.320
3.503
3.140
3.128
3.115
2.539
2.525
2.512
2.498
2.484
1.309
1.295
1.246
1.235
1.232
0.836
0.782
0.770
BF4
Au-N-H
1.99
1.82
4.01
0.87
1.83
4.00
11.76
13.17
5.88
5.83
f1 (ppm)


173.10
146.25
134.17
131.52
124.86
124.58
54.43
54.22 CDCl3
53.78 CDCl3
53.57
51.55
29.42
24.58
24.54
22.78
22.31
BF4
Au-N-H
f1 (ppm)