Catalytic Activity of *trans*-bis(pyridine)gold Complexes

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1. Experimental Procedures

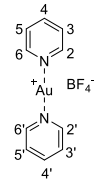
1.1 General Information:

Commercial grade reagents were used as received. Dry solvents were collected from a solvent-purification system. All reactions were monitored by thin-layer chromatography (TLC) using silica gel 60 F254 (0.25-mm thickness) or by ^{1}H-NMR. Flash chromatography was carried out using silica gel 60 (0.040-0.063 mm). High Throughput Flash Purification (HPFP) was performed on pre-packed cartridges. ^{1}H, ^{13}C NMR, ^{1}H, ^{15}N HMBC NMR spectrum were recorded in CD_2Cl_2, CD_3CN or DMSO-d_6 using a 500 or a 600 MHz Bruker Avance Neo spectrometer equipped with TCI or TXI cryogenic probe. ^{1}H and ^{13}C chemical shifts are reported in ppm (δ), using the residual solvent signal as internal standard. Accurate mass determination in either positive or negative mode was performed with a "Synapt G2-S" Q-TOF instrument from Waters. Samples were ionized with an ASAP probe, and no chromatographic separation was used before the mass analysis. Single crystal X-ray data were collected on a Bruker D8 APEX-II equipped with a CCD camera using Mo Kα radiation (λ = 0.71073 Å). Crystals were mounted on a fibre loop and fixated using Fomblin oil. Data reduction was performed with SAINT, Absorption corrections for the area detector were performed using SADABS. Structures were solved by direct methods and refined by least squares methods on F2 using the SHELX and the OLEX2 suit of programs. ORTEP plots are shown in the thesis and all metric data, including reflection data, are contained in the respective cif files. The data [**3**-Au(III)$_2$] (CCDC No: 1982782), [**4**-Au(I)]$_2$(BF$_4$)$_2$ (CCDC No: 1982783) and [**4**-Au(I)]$_2$(AuCl$_4$)$_2$ (CCDC No: 1983592) can be obtained free of charge via http://www.ccdc.cam.ac.uk/conts/retrieving.html, or from the Cambridge Crystallographic Data Centre, 12 Union Road, Cambridge CB2 1EZ, UK. Fax: +44 1223 336 033; or deposit@ccdc.cam.ac.uk. Ligands **2**,[1] **3**[2] and **4**[3] and propargyl ester **5**[4] were prepared according to literature procedures.

1.2 Synthesis and Characterization: Bis(pyridine)gold(III) complexes

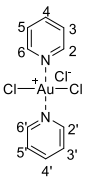
The bis(pyridine)gold(III) complexes were prepared by dissolving K(AuCl$_4$) (1 equiv.) in MeOH, followed by addition of the selected pyridine (2 equiv.). This resulted in immediately precipitation of the bis(pyridine)gold(III) complexes, for all pyridines beside 4-CF$_3$-pyridine. The complexes were filtered, before they were washed with more methanol and dried.

Bis(pyridine)gold(I) complex, [(**1**-H)$_2$-Au(I)]BF$_4$:



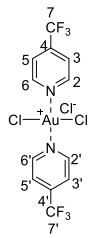
The bis(pyridine)gold(I) complex was prepared by dissolving chloro(dimethylsulfide)gold(I) (6.6 mg, 0.020 mmol) in dichloromethane (2 mL), followed by addition of pyridine (1.6 mg, 0.020 mmol) and AgBF$_4$ (3.8 mg, 0.020 mmol). The coordination mixture was stirred for 15 min, before AgCl precipitate was filtered off. Drying gave [(**1**-H)$_2$-Au(I)]BF$_4$ as a white powder, 6.4 mg (74%, 0,014 mmol). ^{1}H NMR (600 MHz, CD_2Cl_2) δ = 8.74 – 8.72 (m, 4H, H-2, H-2', H-6, H-6'), 8.14 (dddd, *J*=7.8, 7.8, 1.6, 1.6, 2H, H-4, H-4'), 7.76 – 7.66 (m, 4H, H-3, H-3', H-5, H-5'); ^{13}C NMR (151 MHz, CD_2Cl_2) δ = 153.2 (C-2, C-2', C-6, C-6'), 142.0 (C-4, C-4'), 127.7 (C-3, C-3', C-5, C-5'); ^{15}N NMR (61 MHz, CD_2Cl_2) δ = -155.5 (N-1, N-1').

Bis(pyridine)gold(III) complex, [(**1**-H)$_2$-Au(III)]Cl:



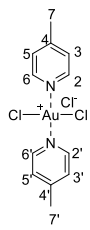
The bis(pyridine)gold(III) complex was prepared according to the general method in 1.2, starting with pyridine (8 mg, 0.106 mmol) and K(AuCl$_4$) (20 mg, 0.053 mmol). Drying gave 19 mg (77%, 0.041 mmol) of [(**1**-H)$_2$-Au(III)]Cl as a yellow powder. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 8.90 – 8.89 (m, 4H, H-2, H-2', H-6, H-6'), 8.21 (dddd, *J*=7.7, 7.7, 1.4,1.4, 2H, H-4, H-4'), 7.79 – 7.76 (m, 4H, H-3, H-3', H-5, H-5'); ^{13}C NMR (126 MHz, CD_2Cl_2) δ 150.5 (C-2, C-2', C-6, C-6'), 143.0 (C-4, C-4'), 128.4 (C-3, C-3', C-5, C-5'); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -154.2 (N-1, N-1'); HRMS (ESI) *m/z* [M+]: calcd. for $C_{10}H_{10}N_2Cl_2Au$: 424.9883, found 424.9987.

Bis(4-CF$_3$-pyridine)gold(III) complex, [(**1**-CF$_3$)$_2$-Au(III)]Cl:



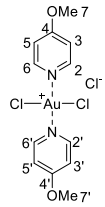
The bis(4-CF$_3$-pyridine)gold(III) complex was prepared according to the general method in 1.2, starting with 4-(trifluoromethyl)pyridine (23 mg, 0.153 mmol) and K(AuCl$_4$) (29 mg, 0.077 mmol). The complex was purified by precipitating from dichloromethane by addition of *n*-pentane. Drying gave 37 mg (80%, 0.061 mmol) of the complex as a yellow powder. ^{1}H NMR (500 MHz, CD_3CN) δ = 9.16 – 9.14 (m, 4H, H-2, H-2', H-6, H-6'), 8.09 – 8.08 (m, 4H, H-3, H-3', H-5, H-5'); ^{13}C NMR (126 MHz, CD_3CN) δ = 152.0 (C-2, C-2', C-6, C-6'), 142.6 (q, $^2J_{CF}$ =35.8, C-4, C-4'), 124.7 (q, $^3J_{CF}$ =3.4, C-3, C-3', C-5, C-5'), 121.5 (q, $^1J_{CF}$ =273.9, C-7, C-7'); ^{15}N NMR (51 MHz, CD_3CN) δ = -148.0 (N-1, N-1').

Bis(4-Me-pyridine)gold(III) complex, [(**1**-CH$_3$)$_2$-Au(III)]Cl



The bis(4-Me-pyridine)gold(III) complex was prepared according to the general method in 1.2, starting with 4-methylpyridine (10 mg, 0.107 mmol) and K(AuCl$_4$) (21 mg, 0.055 mmol). Drying gave 24 mg (92%, 0.049 mmol) of the complex as a yellow powder. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 8.65 – 8.63 (m, 4H, H-2, H-2', H-6, H-6'), 7.51 (d, *J*=6.1, 4H, H-3, H-3', H-5, H-5'), 2.55 (s, 6H, H-7, H-7'); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 156.6 (C-4, C-4'), 149.4 (C-2, C-2', C-6, C-6'), 129.0 (C-3, C-3', C-5, C-5'), 21.9 (C-7, C-7'); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -162.6 (N-1, N-1').

Bis(4-OMe-pyridine)gold(III) complex, [(**1**-OCH_3)$_2$-Au(III)]Cl:

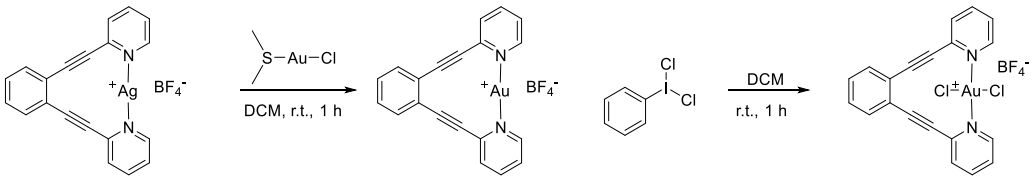


The bis(4-OMe-pyridine)gold(III) complex was prepared according to the general method in 1.2, starting with 4-methoxypyridine (12 mg, 0.108 mmol) and $K(AuCl_4)$ (20 mg, 0.053 mmol). Drying gave 23 mg (82%, 0.044 mmol) of the complex as a yellow powder. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 8.61 – 8.60 (m, 4H, H-2, H-2', H-6, H-6'), 7.13 – 7.11 (m, 4H, H-3, H-3', H-5, H-5'), 4.01 (s, 6H, H-7, H-7'); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 169.8 (C-4, C-4'), 151.1 (C-2, C-2', C-6, C-6'), 113.9 (C-3, C-3', C-5, C-5'9, 57.5 (C-7, C-7'); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -178.2 (N-1, N-1'); HRMS (ESI) *m/z* [M+]: calcd. for $C_{12}H_{14}N_2O_2Cl_2Au$: 485.0100, found 485.0098.

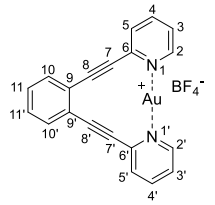
1.3 Synthesis and Characterization: [(1,2-Bis(pyridin-2-ylethynyl)benzene)-type gold complexes

The unsubstituted and para substituted [(1,2-Bis(pyridin-2-ylethynyl)benzene)gold(III)] chloride complexes, [(**2**-R)-Au(III)]Cl, were prepared by dissolving the ligand (1 equiv.) in methanol, followed by addition of $KAuCl_4$ (1 equiv.) dissolved in methanol. Mixing gave immediately precipitate of the gold(III) complexes, which were filtered and washed with more methanol.

The [(1,2-Bis(pyridin-2-ylethynyl)benzene)gold(I)] tetrafluoroborate, [(**2**-H)-Au(I)]BF_4, and [(1,2-Bis(pyridin-2-ylethynyl)benzene)-gold(III)] tetrafluoroborate, [(**2**-H)-Au(III)]BF_4, were prepared starting from the previously reported [(1,2-Bis(pyridin-2-ylethynyl)-benzene)silver(I)] tetrafluoroborate complex[1] following the method described in the scheme below and for each complex.

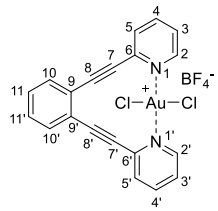


[(1,2-Bis(pyridin-2-ylethynyl)benzene)gold(I)] tetrafluoroborate, [(**2**-H)-Au(I)]BF_4



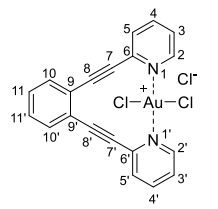
[(1,2-Bis(pyridin-2-ylethynyl)benzene)silver(I)] tetrafluoroborate (8 mg, 0.0016 mmol) was dissolved in dichloromethane (3 mL) under a nitrogen atmosphere. Chloro(dimethylsulfide)gold(I) (5 mg, 0.0017 mmol) was added to the solution, before the reaction was stirred for 1 hour. The reaction mixture was filtered and dried to give the gold(I) complex [(**2**-H)-Au(I)]BF_4as a pale solid, 6 mg (67%, 0.0011 mmol). ^{1}H NMR (600 MHz, CD_2Cl_2) δ = 8.87 (ddd, *J*=5.7, 1.6, 0.8, 2H,H-2, H-2'), 8.14 (td, *J*=7.9, 1.6, 2H, H-4, H-4'), 7.95 (ddd, *J*=8.0, 1.5, 0.8, 2H, H-5, H-5'), 7.78 (dd, *J*=5.8, 3.3, 2H, H-10, H-10'), 7.68 (ddd, *J*=7.5, 5.7, 1.5, 2H, H-3, H-3'), 7.59 (dd, *J*=5.8, 3.3, 2H, H-11, H-11'); ^{13}C NMR (151 MHz, CD_2Cl_2) δ = 154.1 (C-2, C-2'), 144.7 (C-6, C-6'), 141.3 (C-4, C-4'), 133.6 (C-10, C-10'), 131.2 (C-11, C-11'), 130.4 (C-5, C-5'), 126.7 (C-3, C-3'), 124.0 (C-9, C-9'), 94.5 (C-8, C-8'), 90.6 (C-7, C-7'); ^{15}N NMR (61 MHz, CD_2Cl_2) δ = -150.1 (N-1, N-1').

[(1,2-Bis(pyridin-2-ylethynyl)benzene)gold(III)] tetrafluoroborate, [(**2**-H)-Au(III)]BF_4



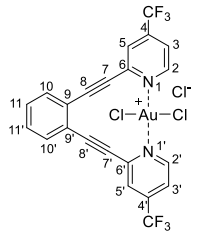
[(1,2-Bis(pyridin-2-ylethynyl)benzene)gold(I)] tetrafluoroborate (4 mg, 0.007 mmol) was dissolved in dichloromethane (2 mL) and added dichloro(phenyl)-λ^3-iodane (3 mg, 0.010 mmol). Precipitate of [(1,2-Bis(pyridin-2-ylethynyl)benzene)gold(III)] tetrafluoroborate was observed during the reaction. The reaction mixture was stirred for 1 hour, before *n*-pentane was added to the reaction mixture to ensure complete precipitate of the gold(III) complex. The organic phase was removed from the precipitate, which upon drying gave 5 mg (79%, 0.008 mmol) of [(**2**-H)-Au(III)]BF_4 as a yellow solid. ^{1}H NMR (600 MHz, MeOD) δ = 9.10 (ddd, *J*=6.1, 1.4, 0.6, 2H, H-2, H-2'), 8.28 (td, *J*=7.8, 1.4, 2H, H-4, H-4'), 8.12 (ddd, *J*=7.9, 1.7, 0.6, 2H, H-5, H-5'), 7.84 (ddd, *J*=7.7, 6.1, 1.6, 2H, H-3, H-3'), 7.82 (dd, *J*=5.8, 3.3, 2H, H-11, H-11'), 7.60 (dd, *J*=5.8, 3.3, 2H, H-10, H-10'); ^{13}C NMR (151 MHz, MeOD) δ = 152.1 (C-2, C-2'), 144.2 (C-4, C-4'), 142.6 (C-6, C-6'), 134.0 (C-10, C-10'), 133.0 (C-11, C-11'), 132.3 (C-5, C-5'), 128.9 (C-3, C-3'), 123.8 (C-9, C-9'), 99.2 (C-8, C-8'), 89.3 (C-7, C-7'); ^{15}N NMR (61 MHz, MeOD) δ = -178.9 (N-1, N-1').

[(1,2-Bis(pyridin-2-ylethynyl)benzene)gold(III)] chloride, [(**2**-H)-Au(III)]Cl



Following the general method described in Section 1.3, the complex was prepared starting from 1,2-bis(pyridin-2-ylethynyl)benzene (19 mg, 0.068 mmol) and $KAuCl_4$ (26 mg, 0.068 mmol), to give 24 mg (60%, 0.041 mmol) of the complex as a yellow solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 8.80 (d, *J*=5.3, 2H, H-2, H-2'), 8.38 (t, *J*=7.7, 2H, H-4, H-4'), 8.06 (d, *J*=8.0, 2H, H-5, H-5'), 7.89 (t, *J*=6.2, 2H, H-3, H-3'), 7.83 (dd, *J*=5.7, 3.3, 2H, H-11, H-11'), 7.63 (dd, *J*=5.8, 3.2, 2H, H-10, H-10'); ^{15}N NMR (51 MHz, DMSO-d_6) δ = -179.8 (N-1, N-1'). Poor solubility of the complex hindered measurement of ^{13}C NMR chemical shift for [(**2**-H)-Au(III)]$^+$ possessing Cl^- as counterion, see [(**2**-H)-Au(III)]BF_4 for ^{13}C chemical shifts.

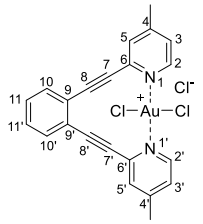
[(1,2-Bis(4-trifluoromethylpyridin-2-yl)ethynyl)benzene)gold(III)] chloride, [(**2**-CF_3)-Au(III)]Cl



Following the general method described in Section 1.3, the complex was prepared starting from 1,2-bis(pyridin-2-ylethynyl)benzene (6 mg, 0.014 mmol) and $KAuCl_4$ (5 mg, 0.014 mmol). The complex was purified by precipitation from dichloromethane in *n*-pentane to give 5 mg (53%, 0.007 mmol) of the complex as a yellow solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 9.40 (d, *J*=6.0, 2H, H-2, H-2'), 8.20 (s, 2H, H-5, H-5'), 7.96 – 7.94 (m, 2H, H-3, H-3'), 7.88 (dd, *J*=5.8, 3.3, 2H, H-11, H-11'), 7.69 (dd, *J*=6.1, 3.3, 2H, H-10, H-10'); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 156.0 (C-2, C-2'), 146.0 (C-6, C-6'), 142.3 (q, $^2J_{CF}$ = 34.5, C-4, C-4'), 134.0 (C-10, C-10'), 132.8 (C-9, C-9'), 131.9 (C-11, C-11'), 126.3 (q, $^3J_{CF}$ = 3.5, C-5,

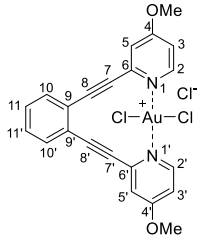
C-5'), 125.3 (q, $^{1}J_{CF}$ = 273.6, CF_3), 122.6 (q, $^{3}J_{CF}$ = 2.6, C-3, C-3'), 96.7(C-8, C-8'), 90.1 (C-7, C-7'); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -142.6 (N-1, N-1').

[(1,2-Bis(4-methylpyridin-2-yl)ethynyl)benzene)gold(III)] chloride, [(**2**-CH_3)-Au(III)]Cl



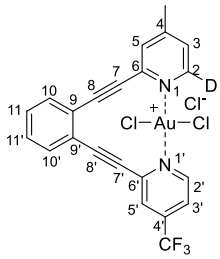
Following the general method described in Section 1.3, the complex was prepared starting from 1,2-bis((4-methylpyridin-2-yl)ethynyl)benzene (11 mg, 0.035 mmol) and $KAuCl_4$ (13 mg, 0.035 mmol), to give 15 mg (72%, 0.026 mmol) of the complex as a yellow solid. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 9.13 (d, *J*=6.3, 2H, H-2, H-2'), 7.88 – 7.85 (m, 2H, H-11, H-11'), 7.85 – 7.83 (m, 2H, H-5, H-5'), 7.67 (dd, *J*=5.8, 3.3, 2H, H-10, H-10'), 7.65 – 7.62 (m, 2H, H-3, H-3'), 2.65 (s, 6H, H-12, H-12'); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 156.6 (C-4, C-4'), 150.9 (C-2, C-2'), 140.9 (C-6, C-6'), 133.3 (C-10, C-10'), 132.4 (C-11, C-11'), 131.5 (C-5, C-5'), 129.0 (C-3, C-3'), 123.2 (C-9, C-9'), 98.5 (C-8, C-8'), 88.6 (C-7, C-7'), 30.6 (C-12, C-12'); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -186.5 (N-1, N-1').

[(1,2-Bis(4-methoxypyridin-2-yl)ethynyl)benzene)gold(III)] chloride, [(**2**-OCH_3)-Au(III)]Cl



The complex was prepared according to the general method described in Section 1.3, starting with 1,2-bis((4-methoxypyridin-2-yl)ethynyl)benzene (5 mg, 0.015 mmol) and $KAuCl_4$ (6 mg, 0.015 mmol). This method yielded 6 mg (68%, 0.010 mmol) of the complex as a yellow powder. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 8.90 (d, *J*=7.2, 2H, H-2, H-2'), 7.85 (dd, *J*=5.8, 3.3, 2H, H-11, H-11'), 7.66 (dd, *J*=5.8, 3.3, 2H, H-10, H-10'), 7.47 (d, *J*=3.1, 2H, H-5, H-5'), 7.28 (dd, *J*=7.2, 3.1, 2H, H-3, H-3'), 4.11 (s, 6H, H-12, H-12'); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 170.1 (C-4, C-4'), 152.4 (C-2, C-2'), 142.7 (C-6, C-6'), 133.7 (C-10, C-10'), 131.9 (C-11, C-11'), 123.6 (C-9, C-9'), 118.1 (C-5, C-5'), 114.5 (C-3, C-3'), 98.6 (C-8, C-8'), 88.8 (C-7, C-7'), 58.1 (C-12, C-12'); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -202.4 (N-1, N-1').

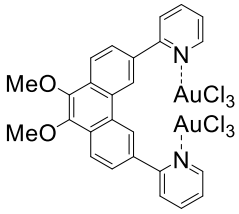
[4-methyl-2-((2-((4-(trifluoromethyl)pyridin-2-yl)ethynyl)phenyl)ethynyl)pyridine)gold(III)] chloride, [(**2**-CH_3/CF_3)-Au(III)]Cl



The complex was prepared according to the general method described in Section 1.3, starting with 4-methyl-2-((2-((4-(trifluoromethyl)pyridin-2-yl)ethynyl)phenyl)ethynyl)pyridine-6-*d* (11 mg, 0.031 mmol) and $KAuCl_4$ (12 mg, 0.031 mmol). This method yielded 14 mg (66%, 0.020 mmol) of the complex as a yellow powder. ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 8.86 (d, *J*=5.1, 1H, H-2'), 8.10 (m, 1H, H-3), 7.92 – 7.91 (m, 1H, H-10'), 7.85 - 7.84 (m, 1H, H-3'), 7.74 – 7.73 (m, 1H, H-10), 7.57 – 7.54 (m, 3H, H-5, H-11, H-11'), 7.49 (d, *J*=2.2, 1H, H-5'), 2.58 (s, 3H, CH_3); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 155.7 (C-4), 151.6 (C-2'), 151.5 (C-2), 144.7 (C-6'), 143.7 (C-6), 138.9 (q, $^{2}J_{CF}$ =34.6, C-4'), 133.4 (C-10 or C-10'), 133.2 (C-3), 132.9 (C-10 or C-10'), 131.4 (C-11 or C-11'), 130.3 (C-11 or C-11'), 128.4 (C-5), 125.5 (C-9' or C-9), 124.1 (C-9' or C-9), 123.5 (q, $^{3}J_{CF}$ =3.4, C-3'), 123.0 (q, $^{1}J_{CF}$ = 273.8, CF_3), 119.1 (q, $^{3}J_{CF}$=3.5, C-5'), 99.7 (C-8), 98.6 (C-8'), 89.3 (C-7), 88.6 (C-7'), 21.7 (CH_3); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -159.4 (N-1), -189.6 (N-1').

1.4 Synthesis and Characterization: 2,2'-(9,10-dimethoxyphenanthrene-3,6-diyl)dipyridine gold complexes

2,2'-(9,10-dimethoxyphenanthrene-3,6-diyl)dipyridine (12 mg, 0.031 mmol) was dissolved in dichloromethane (1,5 mL) and added $KAuCl_4$ (12 mg, 0.031 mmol) dissolved in methanol (0.5 mL). The reaction mixture was allowed to stir for 15 min, before solvent was removed. Judging from ^{1}H and ^{15}N NMR of the crude product, a mixture of two different Au complexes were obtained. One of the complexes was easily crystalized by diffusion of *n*-pentane into the product mixture dissolved in dichloromethane, allowing for isolation of 7 mg (23%, 0.007 mmol) of this complex as yellow crystals, [**3**-Au(III)$_2$]. The other complex, [**3**-Au(III)]$_2$$Cl_2$, was only obtained as a mixture, hence only ^{1}H and ^{15}N NMR shifts are reported.

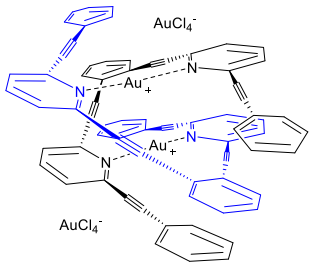


Spectroscopic data for complex [**3**-Au(III)$_2$]: ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 9.40 (d, *J*=1.9, 2H), 8.87 (d, *J*=6.0, 2H), 8.58 (d, *J*=8.5, 2H), 8.29 (tt, *J*=7.7, 1.2, 2H), 8.21 – 8.17 (m, 4H), 7.77 (td, *J*=6.4, 5.4, 1.4, 2H), 4.22 (s, 6H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 160.4, 150.3, 145.8, 142.9, 135.6, 131.9, 130.9, 128.8, 127.4, 126.9, 125.0, 124.6, 61.6 ; ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -153.4; CCDC No: 1982782

Spectroscopic data for complex [**3**-Au(III)] $_2$$Cl_2$: ^{1}H NMR (600 MHz, CD_2Cl_2) δ = 9.57 (d, *J*=1.9, 2H), 9.46 (d, *J*=1.6, 2H), 8.96 (dd, *J*=6.2, 1.4, 2H), 8.79 – 8.76 (m, 2H), 8.56 (d, *J*=8.5, 2H), 8.49 – 8.43 (m, 8H), 8.09 (dd, *J*=7.8, 1.7, 2H), 8.04 (dd, *J*=8.4, 1.8, 2H), 7.94 (td, *J*=7.7, 1.9, 4H), 7.87 – 7.81 (m, 4H), 7.39 – 7.34 (m, 4H), 4.22 (s, 3H), 4.22 (s, 3H); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -152.8, -153.1.

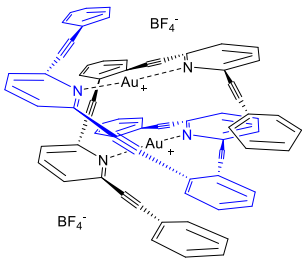
1.5 Synthesis and Characterization:1,2-bis((6-(phenylethynyl)pyridin-2-yl)ethynyl)benzene gold complexes

[**4**-Au(I)]$_2$($AuCl_4$)$_2$



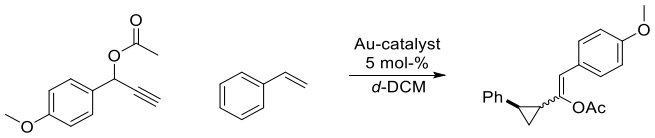
The complex was prepared by dissolving 1,2-bis((6-(phenylethynyl)pyridin-2-yl)ethynyl)benzene, **4**, (7 mg, 0.015 mmol) in dichloromethane (0.5 mL) under a nitrogen atmosphere, followed by addition of $AuCl_3$ (4.5 mg, 0.015 mmol) dissolved in methanol (0.3 mL). After stirring the complex for 10 min, *n*-pentane was added until no more further precipitation was observed. The precipitate was collected and dried, to give [**4**-Au(I)]$_2$($AuCl_4$)$_2$ as a yellow-brown powder, 5.4 mg (46%, 0.07 mmol). ^{1}H NMR (500 MHz, CD_2Cl_2) δ = 8.16 (t, *J*=7.8, 4H), 7.95 (d, *J*=7.7, 4H), 7.89 – 7.83 (m, 8H), 7.64 (dd, *J*=5.7, 3.2, 4H), 7.35 (t, *J*=7.4, 4H), 7.29 (d, *J*=7.6, 8H), 7.19 (t, *J*=7.6, 8H); ^{13}C NMR (126 MHz, CD_2Cl_2) δ = 146.6 (2C), 146.1 (2C), 145.2 (2C), 144.7 (2C), 142.2 (2C), 141.1 (2C), 134.5 (2C), 133.7 (2C), 132.6 (4C), 132.1 (2C), 131.4 (2C), 130.9 (2C), 130.7 (2C), 130.5 (2C), 130.1 (2C), 129.9 (2C), 129.2 (2C), 129.1 (4C), 128.80 (2C), 128.75 (6C), 124.1 (2C), 122.8 (2C), 120.3 (2C), 120.0 (2C), 100.0 (2C), 99.4 (2C), 97.9 (2C), 95.7 (2C), 90.7 (2C), 89.9 (2C), 86.5 (2C), 86.3 (2C); ^{15}N NMR (51 MHz, CD_2Cl_2) δ = -148.1; CCDC No: 1983592

[**4**-Au(I)]$_2$(BF$_4$)$_2$



The complex was prepared by dissolving 1,2-bis((6-(phenylethynyl)pyridin-2-yl)ethynyl)benzene, **4**, (8 mg, 0.017 mmol) and chloro(dimethylsulfide)gold(I) (5 mg, 0.017 mmol) in dichloromethane (1.5 mL) under a nitrogen atmosphere. AgBF$_4$ (4 mg, 0.020 mmol) was added to the reaction mixture after stirring for 10 min, giving immediate precipitation of AgCl. The mixture was stirred for additional 15 min, before AgCl precipitate was filtered of. The complex was purified by diffusion of n-pentane into a dichloromethane solution of the complex, giving the complex, [**4**-Au(I)]$_2$(BF$_4$)$_2$, as a white solid, 7 mg (55%, 0.009 mmol). The spectroscopic data and X-ray crystal structure corresponds to [**4**-Au(I)]$_2$(AuCl$_4$)$_2$. ^{1}H NMR (400 MHz, CD$_2$Cl$_2$) δ = 8.21 (t, *J*=8.0, 4H), 7.99 (d, *J*=7.8, 4H), 7.91 (m, 8H), 7.68 (dd, *J*=5.7, 3.3, 4H), 7.40 (t, *J*=7.5, 4H), 7.32 (d, *J*=7.3, 8H), 7.23 (t, *J*=7.6, 8H); ^{15}N NMR (61 MHz, CD$_2$Cl$_2$) δ = -145.5; CCDC No: 1982783

1.6 General Procedure for Testing of Catalytic Activity.



The propargyl ester (5 mg, 1 equiv.) and styrene (4 equiv.) were dissolved in *d*-DCM (0.6 mL) and added the gold-catalyst (5 mol-%) dissolved in *d*-DCM. The reaction progress was monitored by ^{1}H NMR at 30 min, 1 h, 2 h, 3h, 5 h, 8 h, and up to 24 hours, depending on the conversion. Reactivity data for the different Au-catalyst is presented in the main text and Tables 1 and 3.

2. X-ray Crystallography

Single crystals of [**3**-Au(III)$_2$], [**4**-Au(III)]$_2$(AuCl$_4$)$_2$ and [**4**-Au(III)]$_2$(BF$_4$)$_2$ were crystallized by slow diffusion of *n*-pentane into a dichloromethane solution of the complexes. A suitable crystal was selected and Bruker D8 APEX-II diffractometer equipped with a CCD camera using Mo Kα radiation (λ = 0.71073 Å). Data reduction was performed with SAINT,[5] Absorption corrections for the area detector were performed using SADABS.[5] The crystals were kept at 150(2) K during data collection. Using Olex2,[6] the structure was solved with the SHELXT[7] structure solution program using Intrinsic Phasing and refined with the SHELXL[8] refinement package using Least Squares minimization. [**4**-Au(III)]$_2$(AuCl$_4$)$_2$ was refined a two-component twin.

Table S1. Crystallographic data for [**3**-Au(III)$_2$], [**4**-Au(III)]$_2$(AuCl$_4$)$_2$ and [**4**-Au(III)]$_2$(BF$_4$)$_2$.

Compound	[**3**-Au(III)$_2$]	[**4**-Au(III)]$_2$(AuCl$_4$)$_2$	**4**-Au(III)]$_2$(BF$_4$)$_2$
CCDC	**1982782**	**1983592**	**1982783**
Chemical formula	$C_{26}H_{20}Au_2Cl_6N_2O_2$	$C_{72}H_{40}Au_2N_4{\cdot}2(AuCl_4){\cdot}CH_2Cl_2$	$C_{72}H_{40}Au_2N_4{\cdot}2(BF_4){\cdot}2CH_2Cl_2$
Formula weight	999.08	2117.47	1698.49
Temperature (K)	150	150	150
Wavelength (Å)	0.71073	0.71073	0.71073
Crystal system	Orthorhombic	Monoclinic	Monoclinic
Space group	$Pna2_1$	*Cc*	C2/c
a (Å); α (°)	32.117(15), 90	26.339 (3), 90	26.4032(9), 90
b (Å); β(°)	2.282(6), 90	15.8633 (15), 125.911 (2)	17.2822(9), 113.881(2)
c (Å); γ (°)	8.293(4), 90	20.316 (2), 90	15.4213(6), 90
V (Å3); Z	3271(3)	6875.1 (12)	6434.4(5)
Z	4	4	4
ρ (calc.) mg m-3	2.029	2.046	1.753
μ(Mo Kα) mm-1	9.474	8.94	4.793
2θmax (°)	50	50	50
R(int)	0.12	0.166	0.0693
Completeness to θ	100 %	100 %	99 %
GOF	1.030	1.050	1.034
R1 [F>4σ(F)]	0.069	0.065	0.028
wR2 (all data)	0.1566 (5748)	0.1656 (20636)	0.0718(9153)
Absolute structure parameter	-	0.010 (7)	-
Max. peak/hole (e.Å-3)	2.77, -2.39	1.62, -1.15	1.509, -1.138

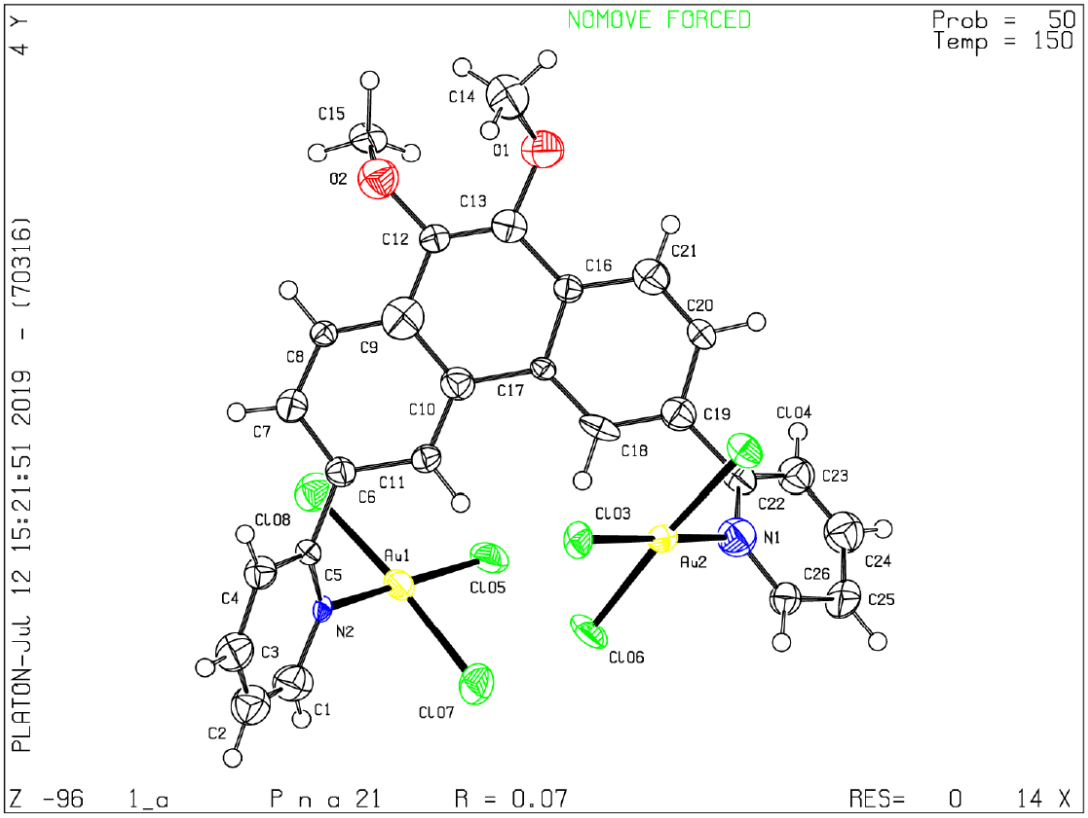


Figure S1. ORTEP plot of [**3**-Au(III)$_2$].

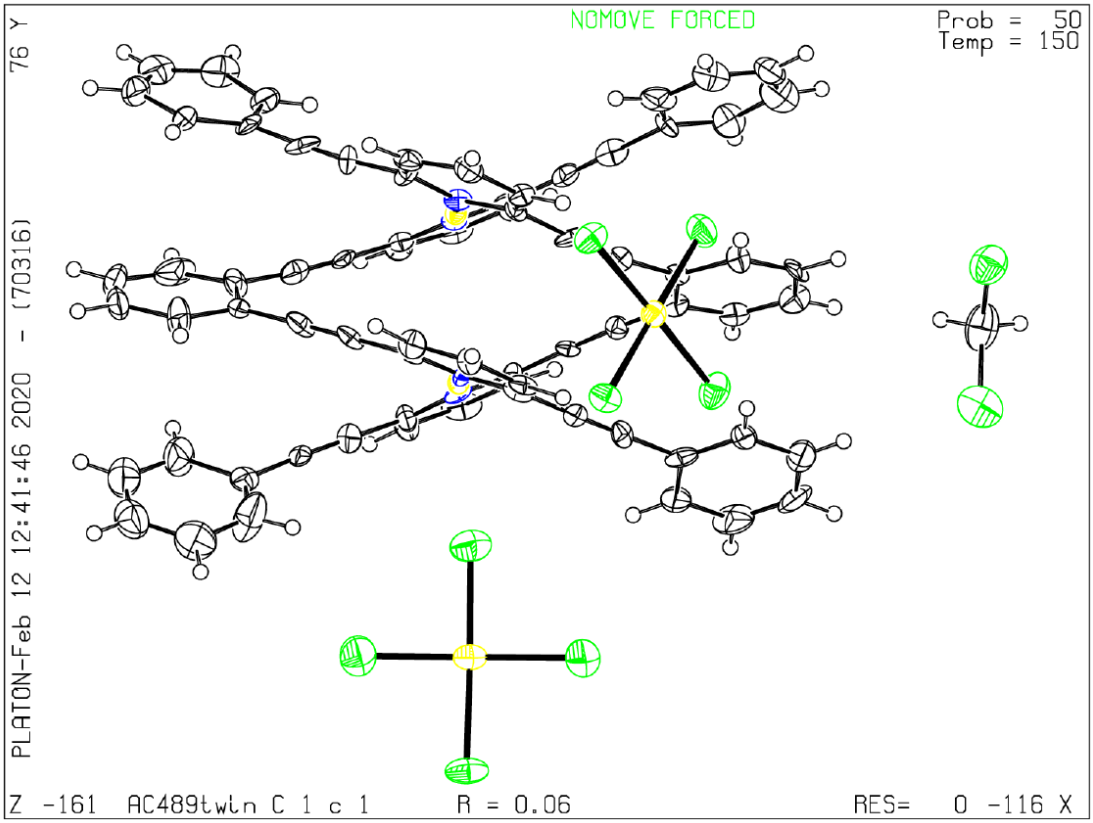


Figure S2. ORTEP plot of [**4**-Au(III)]$_2$(AuCl$_4$)$_2$.

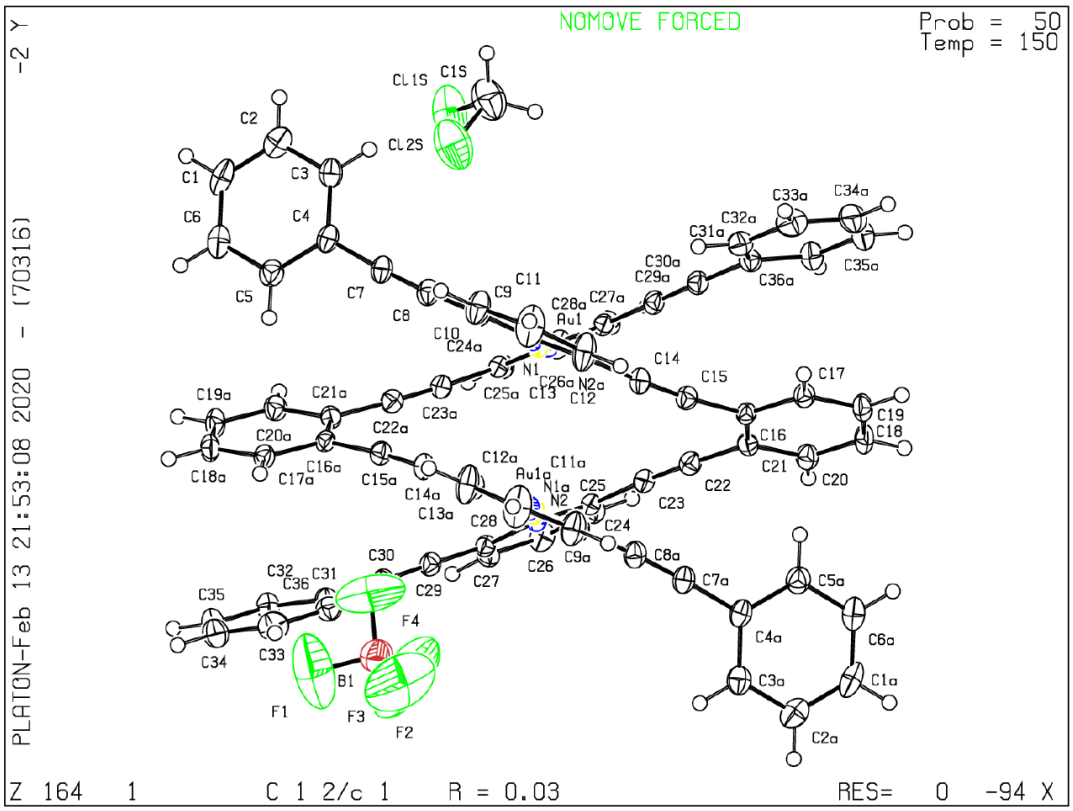


Figure S3. ORTEP plot of [**4**-Au(III)]$_2$(BF$_4$)$_2$.

3. Computational details

To gain structural parameters of the Au(III)/ Au(I)-complexes and insights into the process of acyloxy migration, we performed DFT calculations with the *Gaussian 16* suite of programs (Revision A.03).[9] The calculations were carried out with dispersion-corrected ωB97X-D exchange-correlation functional.[10-11] The SMD implicit solvation model was used to take into account the global solvation effects.[12] The solvent used in our calculations was dichloromethane following the reaction conditions. The ultrafine integration was employed to increase the accuracy of the numerical integration in all electronic structure calculations. Harmonic vibrational frequency calculations were utilized to identify the nature of the obtained structures. The vibrational analysis revealed that all located transition states have only one negative Hessian eigenvalue, while no imaginary frequencies were found for the reported minima.

The reported Gibbs free energies were obtained from ωB97X-D/Def2TZVPP electronic energies and all the additional terms computed at the ωB97X-D/Def2SVP level according to the following formula:

$$G = E_0' + (G_0 - E_0) + (G_{sol} - E_0) + \Delta G_{conc}.$$

In this formula, E_0' and E_0 are electronic energies obtained using Def2TZVPP and Def2SVP basis sets,[13] respectively, G_0 and G_{sol} are gas-phase and solution-phase Gibbs free energies obtained from ωB97X-D/Def2SVP calculations (T = 298.15 K, following the experimental conditions). The thermal and entropic contributions to the Gibbs free energies were computed by employing Grimme's quasi-RRHO approximation. This approach seems more appropriate than the standard ideal gas RRHO (rigid rotor – harmonic oscillator) model, because most of the optimized structures possessed numerous low harmonic frequency modes.[14] The value of ΔG_{conc} (0.003019 Hartree) corresponds to concentration correction to the Gibbs free energy when shifting from ideal gas standard state (p = 1 atm) to the standard concentration in solution phase (c = 1 mol/dm3).

The natural population analysis implemented in *Gaussian 16* was performed at the ωB97X-D/Def2TZVPP level of theory.

4. Computational results

4.1. *Trans* bis(R-pyridine) (1) Au complexes

We first performed structural optimization on each complex at the ωB97X-D/Def2SVP DFT level to determine N-Au bond lengths and calculate the relative stabilities of the different pyridine-ligated Au complexes. The latter was calculated according to $[(\mathbf{1}\text{-H})_2\text{-Au(III)}]^+ + 2\ \mathbf{1}\text{-R} = [(\mathbf{1}\text{-R})_2\text{-Au(III)}]^+ + 2\ \mathbf{1}\text{-H}$ isodesmic reaction. The obtained structures are depicted in Figure S4.

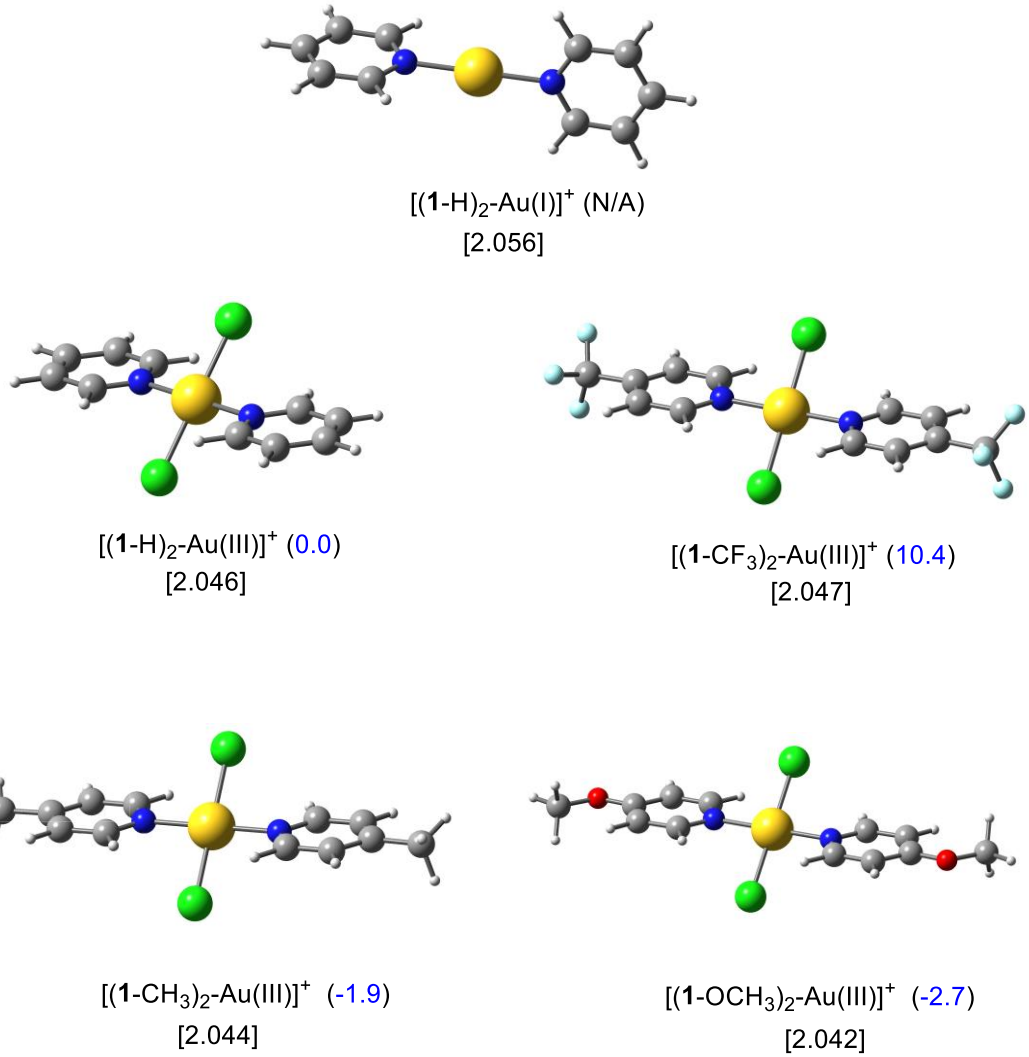


Figure S4. Optimized structure of the *trans* bis(pyridine) Au(I)/Au(III) complexes. Relative stabilities are given in parenthesis (in kcal/mol). Au-N bond length is indicated in square bracket (in Å).

4.2. Cis bis(pyridine) Au complexes

DFT calculations at the ωB97X-D/Def2SVP level predicts that the *cis* arrangement of the bis(pyridine) Au(III) complexes is higher in energy in all cases. The optimized structures are shown in Figure S5.

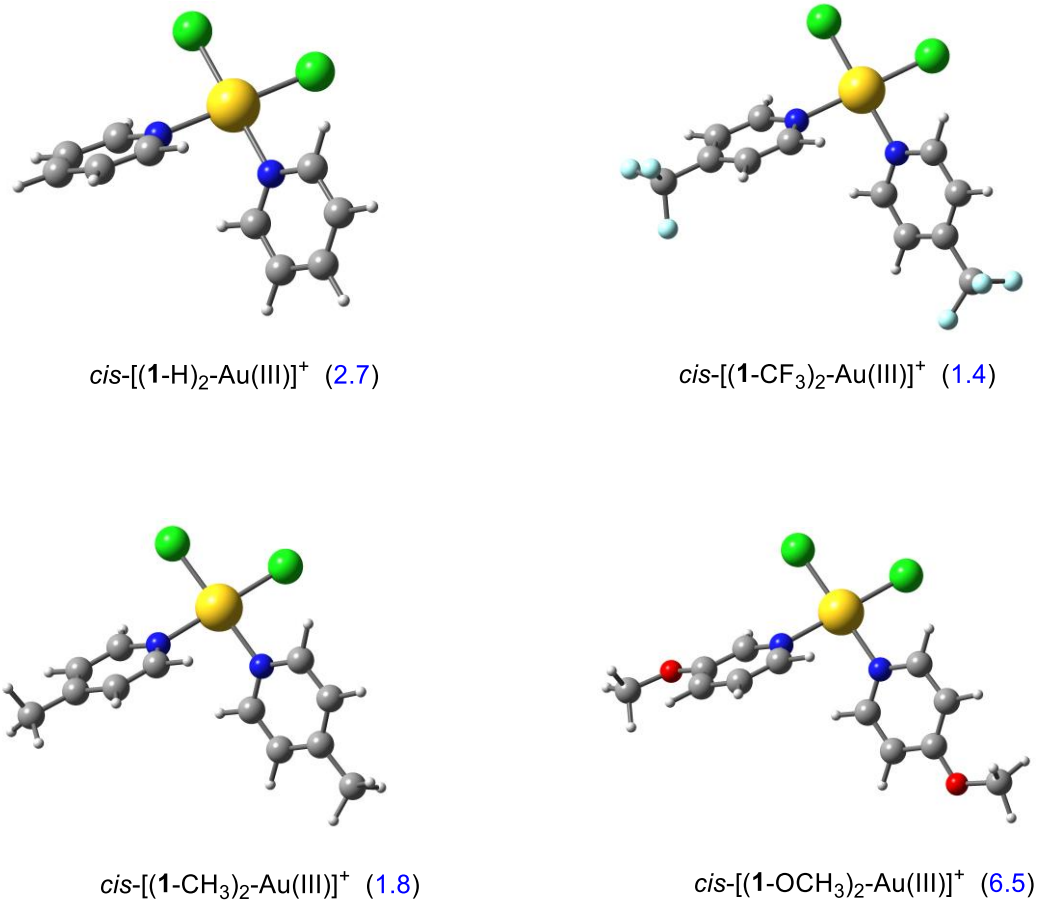


Figure S5. Optimized structure of the *cis* bis(pyridine) Au(III) complexes. Relative stabilities compared to the corresponding *trans* complexes are given in parenthesis (in kcal/mol).

4.3. NBO charges of pyridine ligands

Natural population analysis was carried out to determine the net atomic charges of the pyridine N atoms (n(N)) at the ωB97X-D/Def2TZVPP level of theory (Table S2). We then calculated the change of the net atomic charge (Δn(N)) with respect to the unsubstituted pyridine (**1**-H).

Table S2 Calculated NBO charges of the pyridine N atoms and the relative NBO charge with respect to 1-H.

Structure	n(N)	$10^3 \times \Delta n(N)$
1-H	-0.417	0.0
1-CF_3	-0.400	17.0
1-CH_3	-0.425	-8.0
1-OCH_3	-0.444	-27.0

The quality of the correlations was examined by determining the regression coefficients R^2 for the correlation of the change of the measured N chemical shift ($\Delta\delta^{15}N$) with the change of the natural atomic population of N atom (Δn(N)) (Figure S6). The change in both cases was defined to the unsubstituted pyridine (**1**-H). The regression coefficients R^2 was found to be high (0.993). Consequently, the calculated NBO charge of the pyridine N atom adequately reflects the electronic effects of the substituents on the pyridine ring as the calculated changes upon substitution correlates excellently with the measured $\delta\Delta^{15}N$ data.

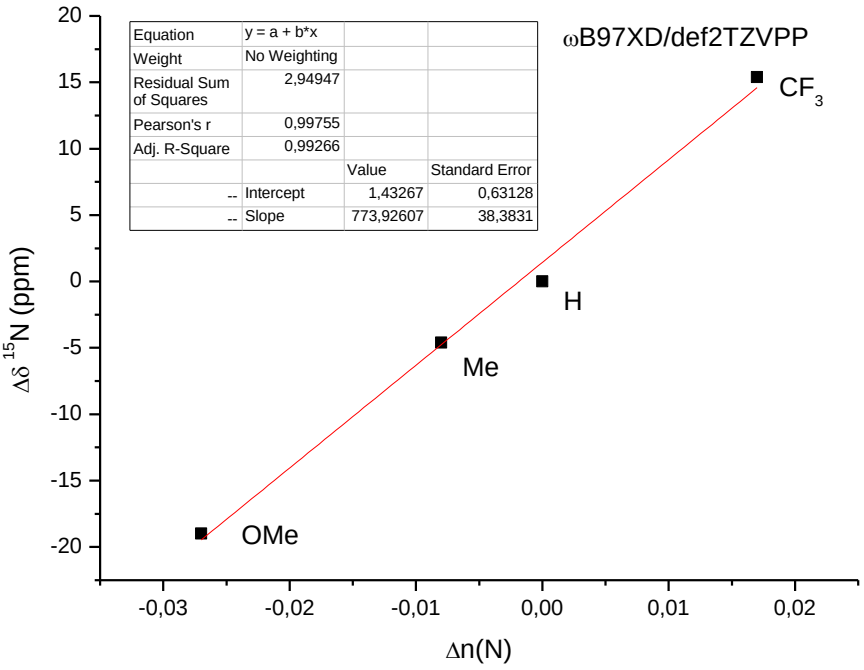


Figure S6. The change of the N chemical shift ($\Delta\delta^{15}N$) versus the change of the natural atomic population of N atom (Δn(N)) for substituted pyridines.

4.4. 1,2-bis(4-R-pyridin-2-yl)ethynyl)benzene (2) Au complexes

The structures of the different **2**-R -ligated Au complexes were optimized at the ωB97X-D/Def2SVP level to determine N-Au bond lengths and compare their relative stabilities. The latter was calculated according to $[(\mathbf{2}\text{-H})\text{-Au(III)}]^+ + \mathbf{2}\text{-R} = [(\mathbf{2}\text{-R})\text{-Au(III)}]^+ + \mathbf{2}\text{-H}$ isodesmic reaction. The DFT-optimized structures can be seen in Figure S7.

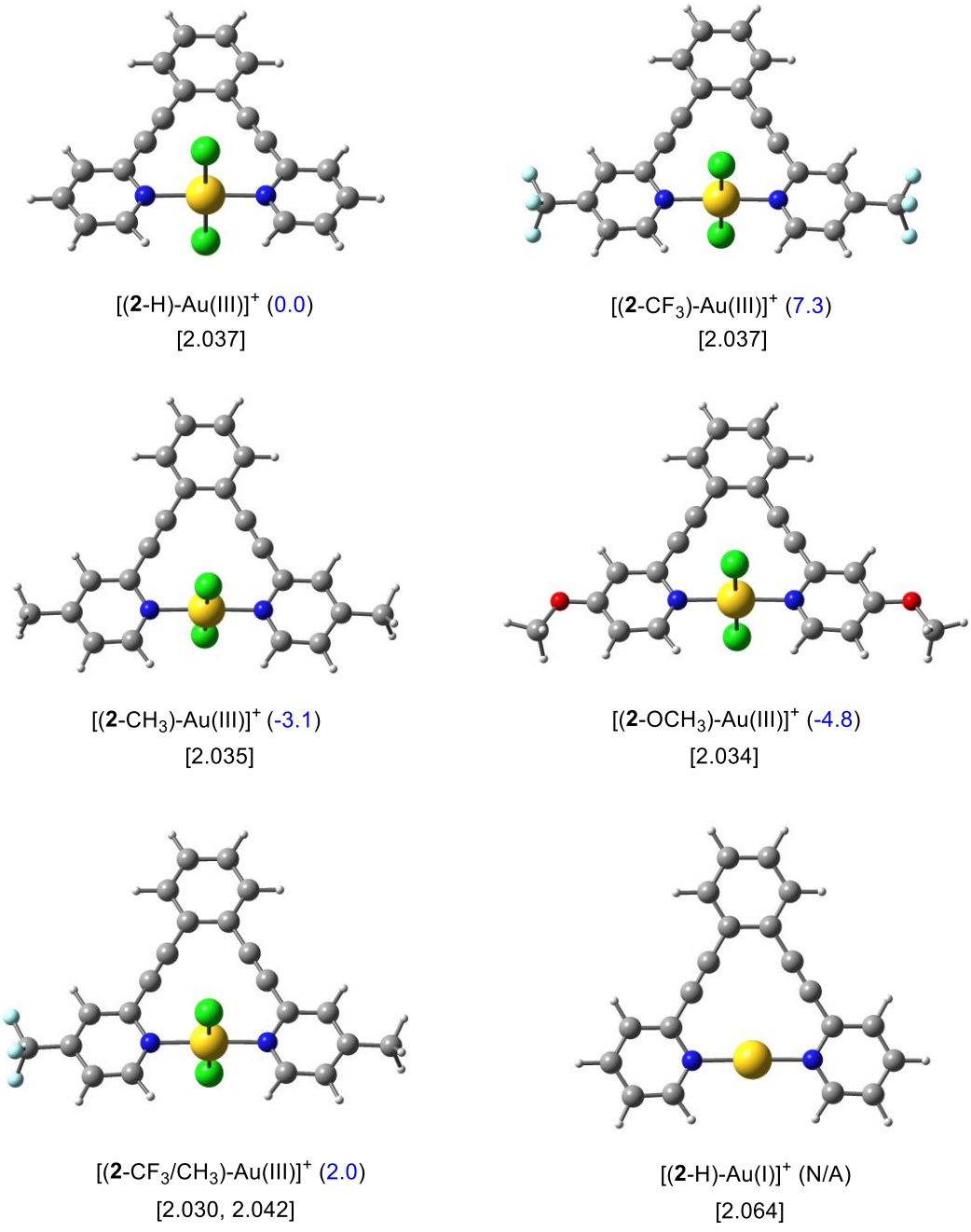


Figure S7. Optimized structure of the investigated 1,2-bis(4-R-pyridin-2-yl)ethynyl)benzene Au(III)/Au(I) complexes. Relative stabilities are given in parenthesis (in kcal/mol). Au-N bond length is indicated in square bracket (in Å).

4.5. Substrate exchange with ligands

In the course of the reaction, the first step is expected to be the coordination of the propargyl ester **5** to the Au(III) center. The formation of such a complex could take place via either the exchange of a Cl^- anion or a pyridine ligand **1**-H. To examine the possibility of the two pathways, we first calculated the relative stability of the Au(III)(**1**-H)$_2$Cl-**5** complex with respect to the reactant state ([(**1**-H)$_2$-Au(III)]$^+$ + **5**). The formation of the [(**1**-H)$_2$-Au(III)Cl]-**5** complex was computed to be highly exergonic (46.2 kcal/mol), rendering this pathway highly unlikely (Figure S8). Therefore, only the pathway involving the exchange of a pyridine **1**-H was considered in the further computational investigations (see below section **4.6.**).

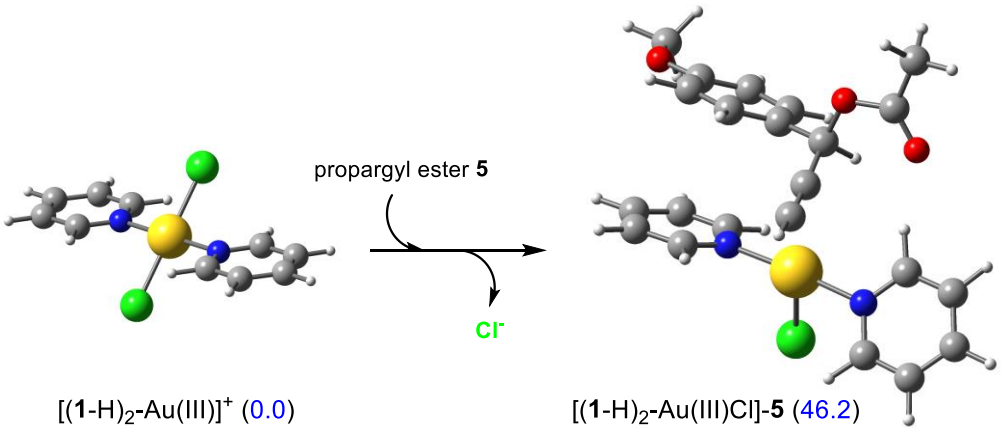


Figure S8 The formation of the reactive intermediate formed via the exchange of a Cl^- with propargyl ester **5**. Relative stabilities are given in parenthesis (in kcal/mol) with respect to [(**1**-H)$_2$-Au(III)]$^+$ + **5** reactant state.

4.6. Conformation of the reactive intermediate

Given that several orientations of the aromatic group are feasible, the conformational space was explored by generating possible rotamers along the Au-C_1-C_3-O dihedral angles (see **A** in Figure S9) which were then subjected to optimization at the ωB97X-D/Def2SVP level of theory. The *cis* and the *trans* geometry of the chlorides were both considered in our calculations. Various conformers were identified as minima. The most stable and additional conformers of the *cis* and the *trans* complexes are presented in Figure S9 and S10, respectively. The most stable arrangement was found to be **A** (Figure S9) wherein geometry of the chlorides is *cis* and the activated triple bond is in close proximity to the ester group. This complex is predicted to be 23.2 kcal/mol above the reactant state, indicating that the formation of such an intermediate upon pyridine dissociation is still thermodynamically unfavored, leading to a highly reactive species. The second most stable conformer **A-1** lying 24.1 kcal/mol above the reactant state was derived through rotating the aromatic moiety by about 180°. The orientation of the aromatic moiety found in complex **A-2** and **A-3** significantly decreased the stability.

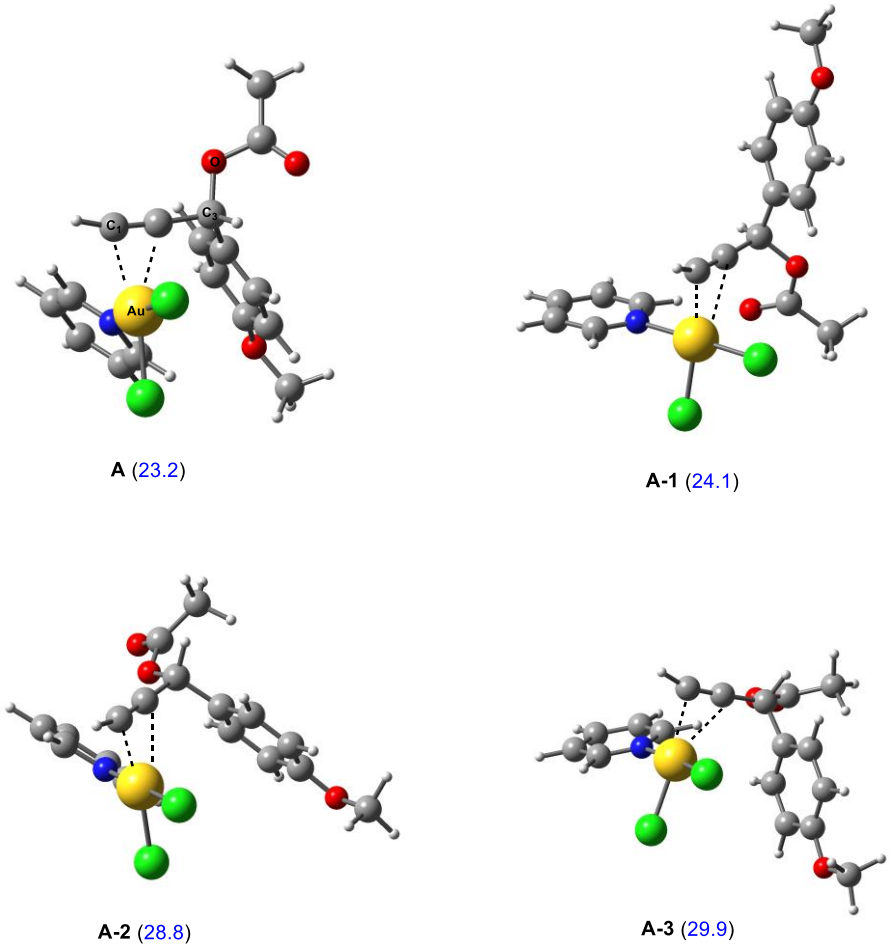


Figure S9. *Cis* coordination complexes of the reactive intermediate formed upon the exchange of an **1**-H with propargyl ester **5**. The coordinative bond is highlighted by a dashed line. Relative stabilities are given in parenthesis (in kcal/mol) with respect to [(**1**-H)$_2$-Au(III)]$^+$ + **5** reactant state.

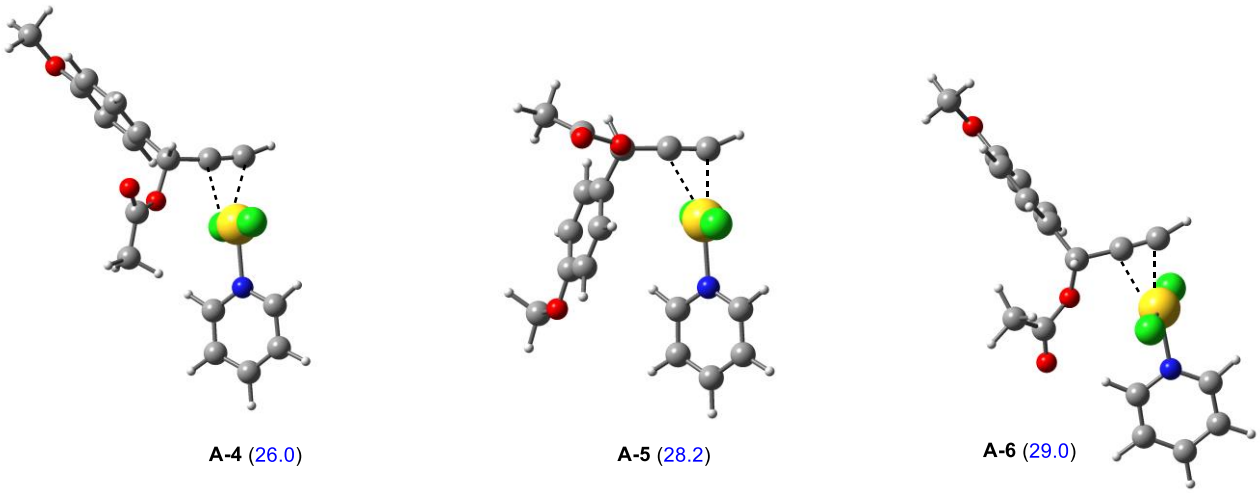


Figure S10. Selected *trans* coordination complexes of the reactive intermediate formed upon the exchange of an **1**-H with propargyl ester **5**. The coordinative bond is highlighted by a dashed line. Relative stabilities are given in parenthesis (in kcal/mol) with respect to $[(\mathbf{1}\text{-H})_2\text{-Au(III)}]^+$ + **5** reactant state.

In the case of the *trans* geometry (Figure S10), complex **A-4** was computed to be the most stable, in which the oxygen atom of the ester group is facing towards the Au(III) center. However, complex **A** remained favored over **A-4** by 2.8 kcal/mol, being the most stable conformer identified in our analysis. Consequently, we used complex **A** to study the process of the acyloxy migration which is a key step in the formation of the substituted-cyclopropane product.

4.7. Acyloxy migration

To model the migration of the acyloxy group, we performed a series of constrained geometry optimizations (energy scans) departing from the most stable structure **A** while the dihedral angle that rotates the acyloxy group towards the triple bond (C_2-C_3-O-C_4) in the less hindered direction was gradually altered by 1° (Figure S11). By carrying out the constrained optimizations in this fashion, the obtained potential energy curve revealed an energy barrier of 0.2 kcal/mol for this motion.

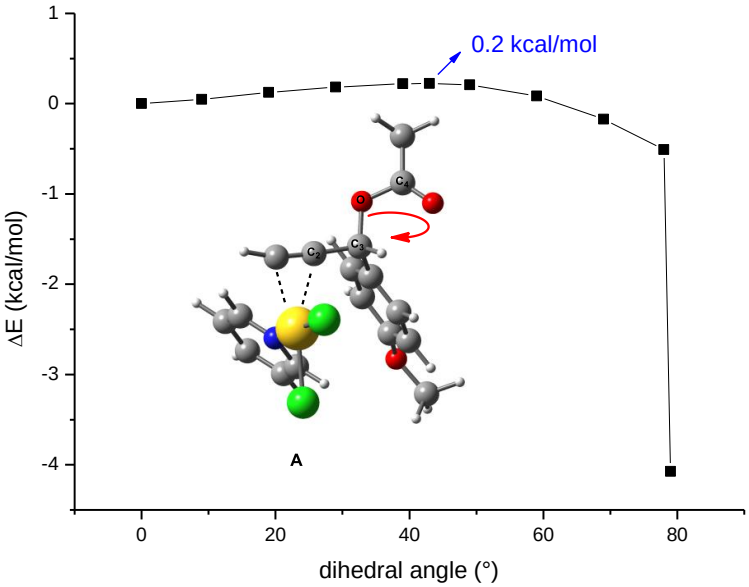


Figure S11. Potential energy curve derived via constrained optimizations along the C_2-C_3-O-C_4 dihedral angle.

Using the structure found as the energy maximum on the potential energy curves as initial geometry, we identified a transition state that was found to be 24.4 kcal/mol above the reactant state. The structure of the obtained transition state is shown in Figure S12.

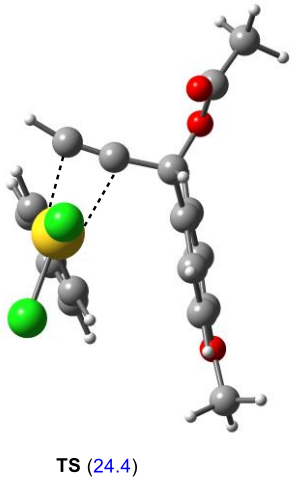
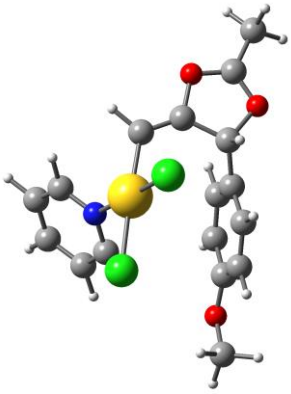


Figure S12. Transition state giving rise to acyloxy migration. Relative stabilities are given in parenthesis (in kcal/mol) with respect to [(**1**-H)$_2$-Au(III)]$^+$ + **5** reactant state.

The normal mode associated with the imaginary frequency computed for this transition state corresponded to rotational motion. The IRC calculation towards the product side showed the formation of a cyclic product **B** having the acyloxy group enclosed in a ring (Figure S13). This intermediate **B** was predicted to be more stable than the reactant state by 4.8 kcal/mol. These computational experiments indicated that the coordinated propargyl ester **5** is highly activated and undergoes practically spontaneous intramolecular cyclisation with the acyloxy group by a simple rotational displacement of that group.



B (-4.8)

Figure S13. The DFT-optimized structure of the cyclic intermediate **B**. Relative stabilities are given in parenthesis (in kcal/mol) with respect to $[(\mathbf{1}\text{-H})_2\text{-Au(III)}]^+$ + **5** reactant state.

The same series of calculations were performed rotating the acyloxy group in the opposite direction (Figure S14). In this case, the rotation gave rise to a cyclisation involving the acyloxy group through an energy barrier of 9.2 kcal/mol. The total barrier of such a cyclisation process, therefore, would be 32.1 kcal/mol, which is prohibitively high at ambient conditions. The resultant product of the energy scan was found to be the same product that we obtained in the previous case (Figure S13).

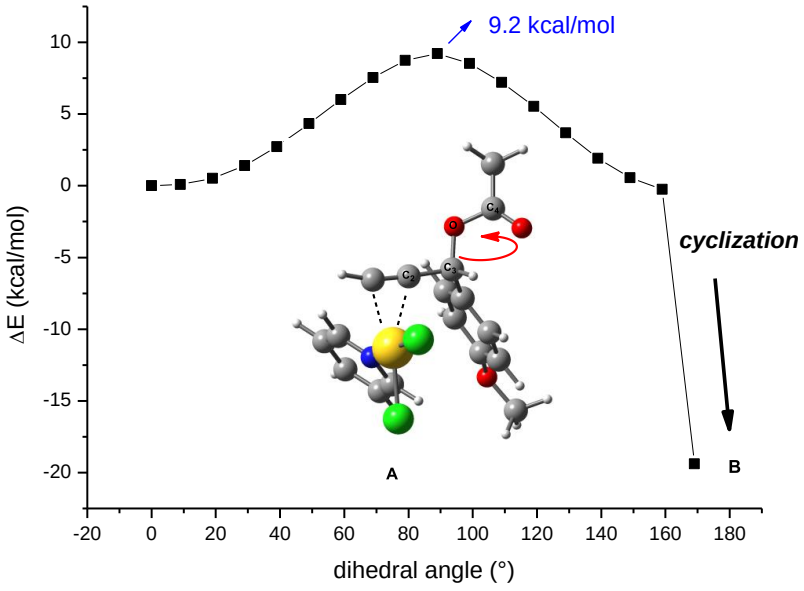


Figure S14. Potential energy curve derived via constrained optimizations along the C_2-C_3-O-C_4 dihedral angle.

4.8. Substitution effect

Next, we examined the relative stabilities of structures **A**, **TS** and the cyclic intermediate **B** when the pyridine ligand was substituted with CF_3-, CH_3-, OCH_3-groups. The obtained minima and transition states along with the energy data are shown in Figure S15, S16, S17 respectively.

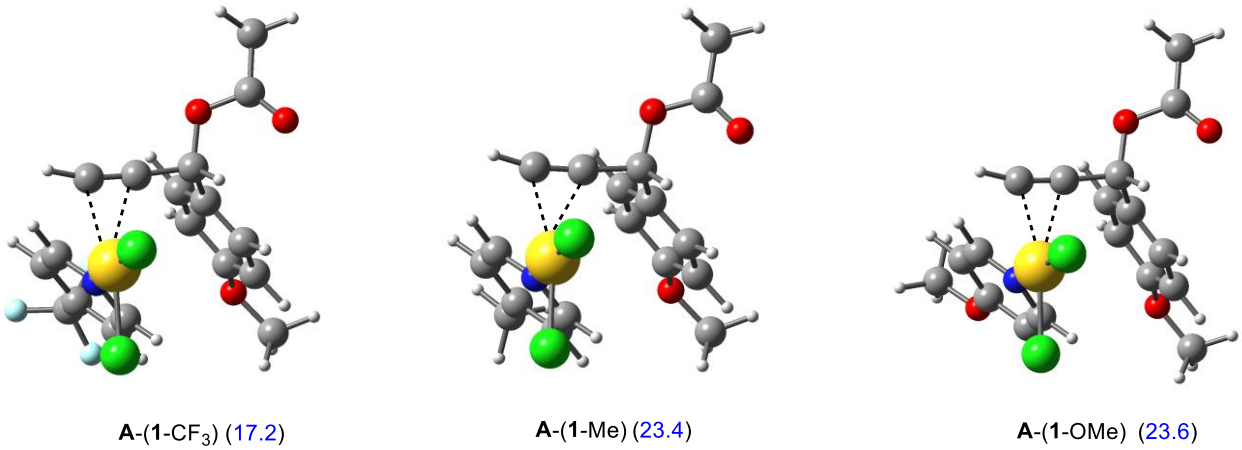


Figure S15. Coordination complexes of the reactive intermediate with CF_3-, CH_3-, OCH_3-substituted pyridines. The coordinative bond is highlighted by a dashed line. Relative stabilities are given in parenthesis (in kcal/mol) with respect to the corresponding $[(\mathbf{1}\text{-R})_2\text{-Au(III)}]^+$ + **5** reactant state.

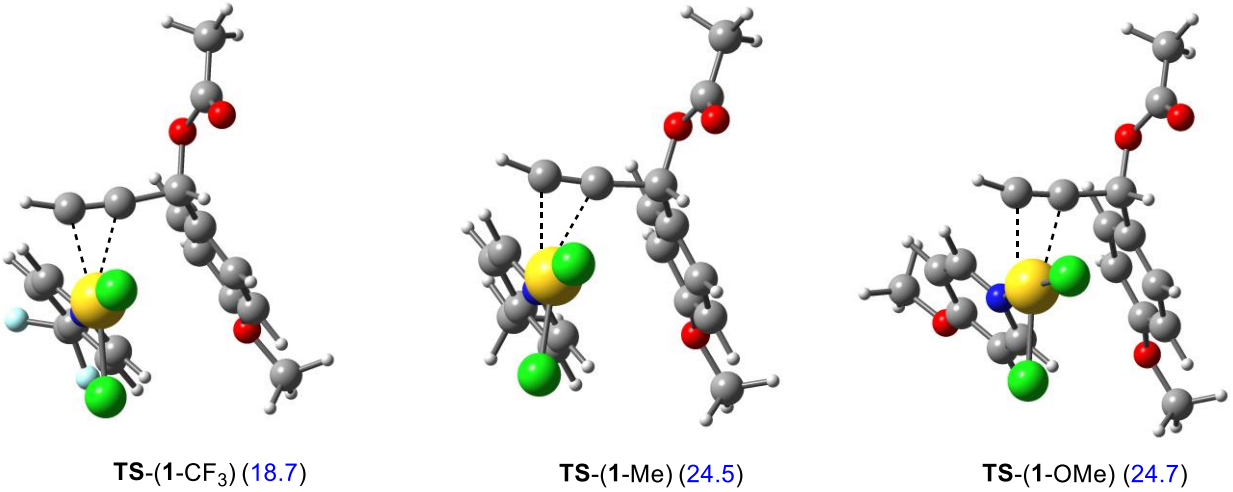


Figure S16. Transition states for the rotation when the pyridine ligand is substituted with CF_3-, CH_3-, OCH_3-groups. Relative stabilities are given in parenthesis (in kcal/mol) with respect to the corresponding $[(\mathbf{1}\text{-R})_2\text{-Au(III)}]^+$ + **5** reactant state.

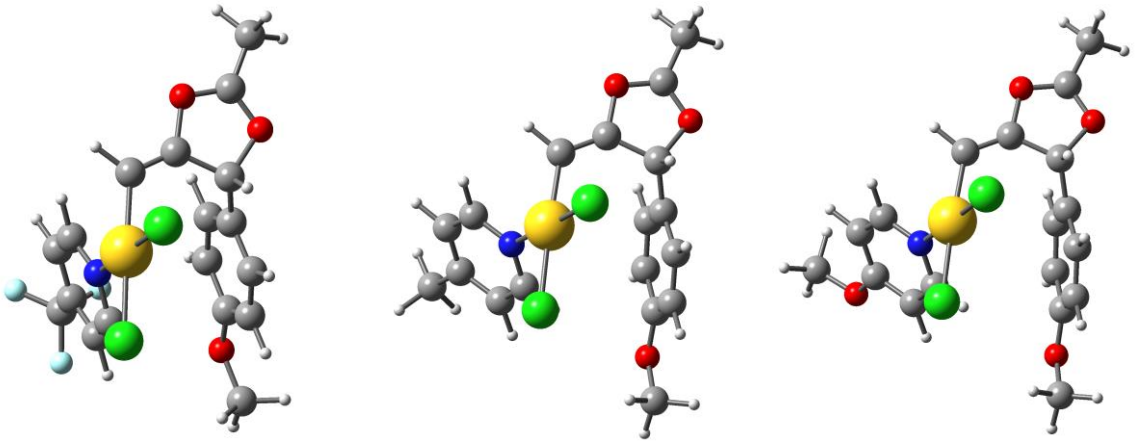


Figure S17. Cyclic intermediates when the pyridine ligand is substituted with CF_3-, CH_3-, OCH_3-groups. Relative stabilities are given in parenthesis (in kcal/mol) with respect to the corresponding $[(\mathbf{1}\text{-R})_2\text{-Au(III)}]^+$ + **5** reactant state.

4.9. Structures of the dimeric complex

In our study, a ligand having two pyridines linked by a phenanthrene ring was also examined. Following the synthetic protocol applied for the preparation of the $[(\mathbf{1}\text{-H})_2\text{-Au(III)}]^+$ complex, a mixture of two Au(III)-complexes was formed based on the ^{15}N-NMR data (for the analysis of the ^{15}N-NMR data see section 1). From the mixture, we obtained a crystal structure which was assigned as the $[\mathbf{3}\text{-Au(III)}_2]$ complex by single crystal X-ray crystallography (for crystallographic data see section 2). Due to the lack of a crystal structure of the other complex detected in the mixture, we performed DFT-calculations to identify its plausible structure. Its NMR spectrum suggests that the Au(III)-complex has a high degree of symmetry. Keeping that in mind, the following two symmetrical complexes could be obtained as minima at DFT level (Figure S18). Complex $[\mathbf{3}\text{-Au(III)}^+]_2$was computed to be the most stable form of a dimeric structure. This is likely to be a result of the stabilizing π-π stacking between the phenanthrene rings in $[\mathbf{3}\text{-Au(III)}^+]_2$ complex. The second most probable structure $[\mathbf{3}\text{-Au(III)}^+]_2$-a, in which π-π stacking is absent, was predicted to be 5.9 kcal/mol higher in free energy.

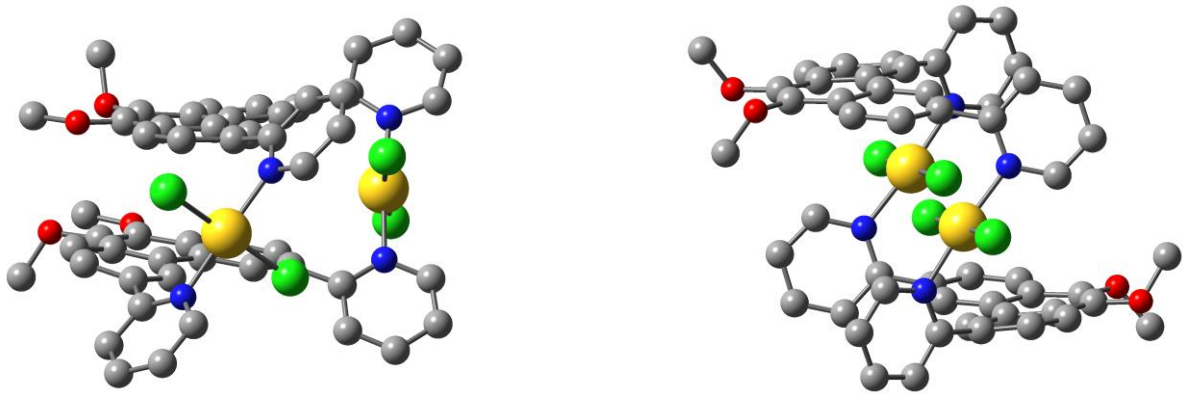


Figure S18. The identified structures of the dimeric complex formed with ligand **3**. Hydrogen atoms are omitted for clarity. Relative stabilities are given in parenthesis (in kcal/mol) with respect to $[\mathbf{3}\text{-Au(III)}^+]_2$.

The dimeric complex shown above is not the only symmetrical structure that could be envisioned. First, we did not exclude the possibility of a monomeric complex in which the $AuCl_2^+$ fragment was situated between the two pyridines resulting in a highly symmetrical structure. DFT calculations were carried out to assess the relative stability of such a complex. The optimized structure of the monomeric complex is shown in Figure S19. It is apparent from the relative free energy that the presence of a monomeric complex is highly unlikely compared to the dimeric counterpart. Inspection of complex [(**3**-Au(III))]$^+$ reveals that the phenanthrene ring is highly distorted, which may explain its high instability.

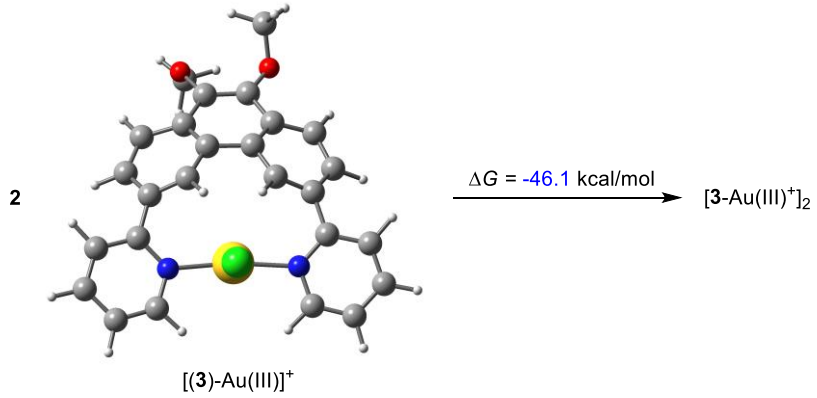


Figure S19. The optimized structure of the monomeric complex. The free energy of dimerization (ΔG) is shown on the reaction arrow.

4.10. Helix structures

DFT computations predicted the preferential formation of dimeric and helical structure for Au(I) (see **Scheme 4**), instead of a monomeric helix wherein both of the pyridines belong to two different ligands. The predicted preference was corroborated by the obtained single crystal structure of [**4**-Au(I)]$^+$ (see crystallographic data in section 2). We suggest that the difference found in the relative stabilities of the weakly interacting monomeric helix and the dimeric helix structures of [**4**-Au(I)]$^+$ and [**4**-I(I)]$^+$ systems could be associated with the difference in the ionic radii of Au^+ and I^+ ions. Indeed these radii are notably different ($r(Au^+)$ = 1.99 Å and $r(I^+)$ = 2.21 Å).[10] The shorter Au···Au distance in [**4**-Au(I)]$^+$ allows closer van der Waals contacts (π-stacking interactions) between the aromatic rings of the ligand as compared to those in [**4**-I(I)]$^+$. To demonstrate the more favorable stacking interaction in [**4**-Au(I)]$^+$, we selected two characteristic distances between the aromatic groups, highlighted in red in Figure S20. The distance between C_α and N as well as C_1 and C_2 atoms (indicated in red) is 0.21 and 0.12 Å shorter, respectively, in the preferred structure of Au(I) complex. This significant difference indicates the presence of a stronger π-π stacking in complex [**4**-Au(I)]$^+$.

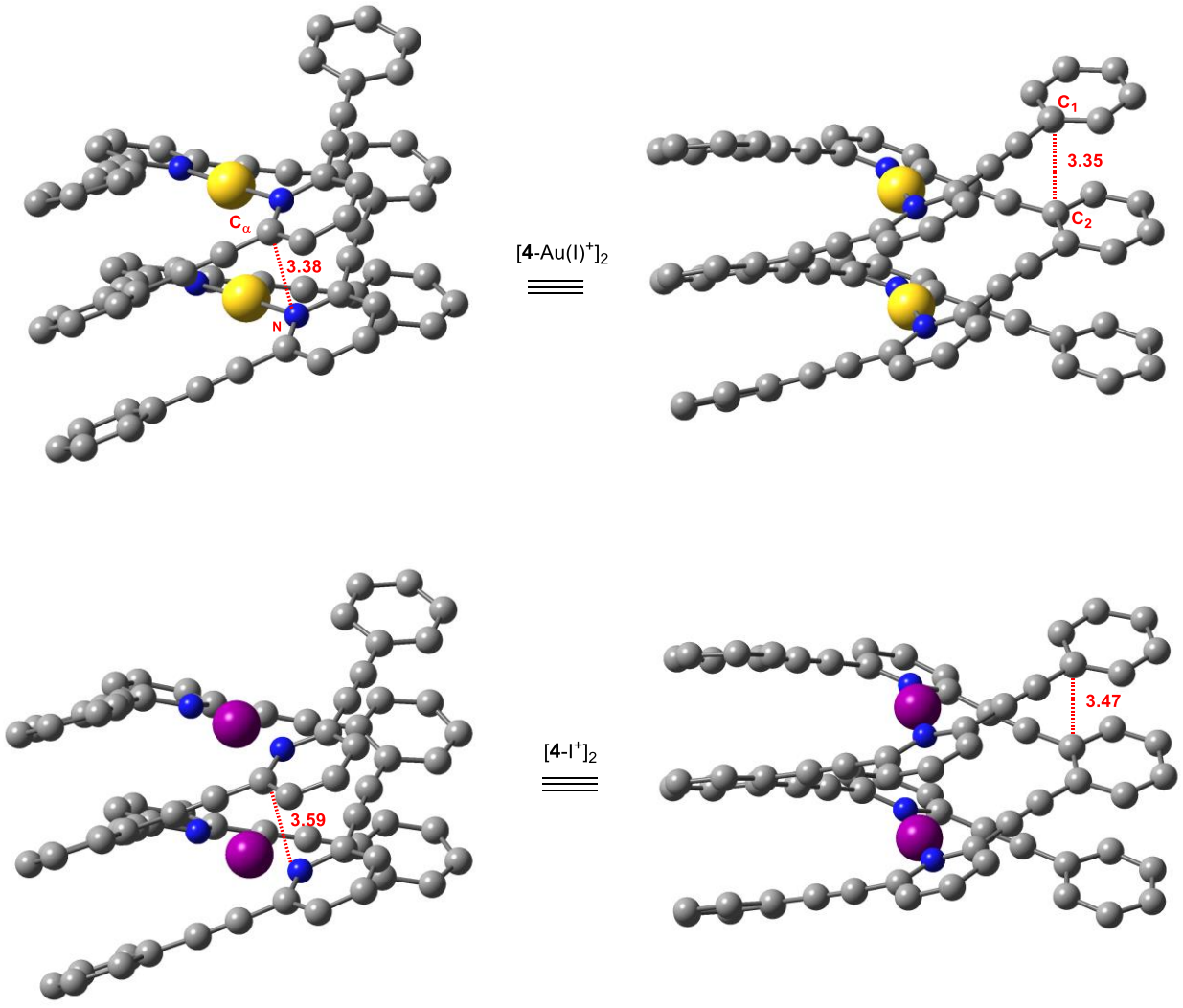


Figure S20. Computationally identified dimeric helix structures of ligand **4** with Au(I) and I^+ cations. Selected characteristic distances for π-stacking interaction are highlighted by a red dashed line and given in Å.

5. Computed energy components of the reported structures.

Table S3 Summary of energy data (given in Hartree) computed for optimized structures at the ωB97X-D/Def2SVP level of theory. Note that *G* contains concentration correction (0.003019 Hartree**).** For the definition of various energy components, see Computational details section.

Structure	E_0'	G_0	E_0	G_{sol} (DCM)	G
[(**1**-H)$_2$-Au(I)]$^+$	-632.2320	-631.5474	-631.6924	-631.7690	-632.1604
[(**1**-H)$_2$-Au(III)]$^+$	-1552.6527	-1551.6430	-1551.7872	-1551.8762	-1552.5945
[(**1**-CF$_3$)$_2$-Au(III)]$^+$	-2226.8381	-2225.0191	-2225.1651	-2225.2590	-2226.7831
[(**1**-CH$_3$)$_2$-Au(III)]$^+$	-1631.3060	-1630.1613	-1630.3576	-1630.4437	-1631.1929
[(**1**-OMe)$_2$-Au(III)]$^+$	-1781.7459	-1780.4129	-1780.6193	-1780.7025	-1781.6197
cis-[(**1**-H)$_2$-Au(III)]$^+$	-1552.6399	-1551.6302	-1551.7752	-1551.8735	-1552.5902
cis-[(**1**-CF$_3$)$_2$-Au(III)]$^+$	-2226.8249	-2225.0080	-2225.1528	-2225.2564	-2226.7808
cis-[(**1**-CH$_3$)$_2$-Au(III)]$^+$	-1631.2933	-1630.1500	-1630.3457	-1630.4411	-1631.1899
cis-[(**1**-OMe)$_2$-Au(III)]$^+$	-1781.7250	-1780.3943	-1780.5992	-1780.6914	-1781.6093
1-H	-248.2850	-247.9542	-248.0165	-248.0268	-248.2300
1-CF$_3$	-585.3878	-584.6540	-584.7155	-584.7247	-585.3326
1-CH$_3$	-287.6069	-287.2094	-287.2969	-287.3080	-287.5276
1-OCH$_3$	-362.8238	-362.3322	-362.4243	-362.4360	-362.7404
[(**2**-H)-Au(III)]$^+$	-1934.8137	-1933.3306	-1933.5500	-1933.6436	-1934.6849
[(**2**-CF$_3$)-Au(III)]$^+$	-2609.0009	-2606.7094	-2606.9296	-2607.0259	-2608.8739
[(**2**-CH$_3$)-Au(III)]$^+$	-2013.4660	-2011.8495	-2012.1192	-2012.2112	-2013.2853
[(**2**-OMe)-Au(III)]$^+$	-2163.9040	-2162.0989	-2162.3790	-2162.4693	-2163.7111
[(**2**-CH$_3$/CF$_3$)-Au(III)]$^+$	-2311.2338	-2309.2798	-2309.5247	-2309.6187	-2311.0798
[(**2**-H)-Au(I)]$^+$	-1014.3928	-1013.2349	-1013.4550	-1013.5348	-1014.2495
2-H	-878.7298	-877.5788	-877.7969	-877.8276	-878.5395
2-CF$_3$	-1552.9368	-1550.9775	-1551.1975	-1551.2238	-1552.7401
2-CH$_3$	-957.3749	-956.0895	-956.3590	-956.3913	-957.1348
1-OCH$_3$	-1107.8073	-1106.3341	-1106.6135	-1106.6467	-1107.5580
2-CH$_3$/CF$_3$	-1255.1570	-1253.5350	-1253.7801	-1253.8087	-1254.9375
5	-690.1363	-689.1994	-689.3735	-689.3906	-689.9767
[(**1**-H)$_2$-Au(III)]-**5**	-1782.2213	-1780.4090	-1780.7546	-1780.9966	-1782.1147
Cl$^-$	-460.2698	-460.0958	-460.0808	-460.1816	-460.3825
A	-1994.4665	-1992.8493	-1993.1060	-1993.2031	-1994.3038
A-1	-1994.4706	-1992.8554	-1993.1115	-1993.2025	-1994.3024
A-2	-1994.4583	-1992.8407	-1993.0989	-1993.1969	-1994.2950
A-3	-1994.4570	-1992.8404	-1993.0980	-1993.1949	-1994.2932
A-4	-1994.4671	-1992.8502	-1993.1070	-1993.1990	-1994.2994
A-5	-1994.4592	-1992.8415	-1993.0985	-1993.1952	-1994.2959
A-6	-1994.4637	-1992.8470	-1993.1043	-1993.1955	-1994.2946
TS	-1994.4660	-1992.8477	-1993.1057	-1993.2027	-1994.3020
B	-1994.5161	-1992.8998	-1993.1622	-1993.2601	-1994.3485
A-(1-CF$_3$)	-2331.5610	-2329.5395	-2329.7976	-2329.8971	-2331.3994
A-(1-Me)	-2033.7936	-2032.1087	-2032.3918	-2032.4885	-2033.6043
A-(1-OMe)	-2109.0128	-2107.2343	-2107.5216	-2107.6171	-2108.8179
TS-(1-CF$_3$)	-2331.5602	-2329.5380	-2329.7971	-2329.8960	-2331.3971
TS-(1-Me)	-2033.7927	-2032.1072	-2032.3910	-2032.4874	-2033.6024
TS-(1-OMe)	-2109.0122	-2107.2330	-2107.5212	-2107.6164	-2108.8161
B-(1-CF$_3$)	-2331.6113	-2329.5906	-2329.8544	-2329.9561	-2331.4460
B-(1-Me)	-2033.8418	-2032.1586	-2032.4465	-2032.5436	-2033.6480
B-(1-OMe)	-2109.0609	-2107.2833	-2107.5764	-2107.6727	-2108.8610
[**3**-Au(III)]$^+$	-2318.8276	-2316.8020	-2317.1548	-2317.2466	-2318.5636
[**3**-Au(III)$^+$]$_2$	-4637.7236	-4633.6509	-4634.3897	-4634.6087	-4637.2008
[**3**-Au(III)$^+$]$_2$-a	-4637.6966	-4633.6258	-4634.3572	-4634.5825	-4637.1875
[**4**-Au(I)]$^+$	-3257.6343	-3253.6703	-3254.4822	-3254.6980	-3257.0350

[**4**-Au(I)$^+$]$_2$	-3257.6370	-3253.6725	-3254.4853	-3254.7039	-3257.0398
[**4**-I(I)]$^+$	-3581.4313	-3577.4792	-3578.2775	-3578.4931	-3580.8405
[**4**-I(I)$^+$]$_2$	-3581.4441	-3577.4672	-3578.2902	-3578.5006	-3580.8336

6. Cartesian coordinates of the reported structures

Cartesian coordinates of the optimized geometries are given below in standard XYZ format (units are in Å). The first line indicates the total number of atoms and the second line is the molecule name (as defined above in Table S3).

23
[(**1**-H)$_2$-Au(I)]$^+$
Au -1.119293 0.163452 -0.050270
N -1.117340 -1.892936 -0.049571
C -0.170839 -2.574946 -0.723502
C -2.062682 -2.576231 0.624711
C -0.138987 -3.961082 -0.745040
H 0.576755 -1.985899 -1.256744
C -2.092220 -3.962400 0.646884
H -2.811245 -1.988190 1.157703
C -1.115008 -4.669908 -0.048916
H 0.646061 -4.471000 -1.304025
H -2.876416 -4.473379 1.206097
H -1.114112 -5.761604 -0.048691
N -1.121288 2.219847 -0.051010
C -0.447638 2.903555 0.894468
C -1.796251 2.901443 -0.997090
C -0.427114 4.289745 0.924571
H 0.086228 2.315843 1.642666
C -1.819393 4.287558 -1.028408
H -2.329013 2.312059 -1.744760
C -1.123917 4.996816 -0.052233
H 0.131603 4.801068 1.708896
H -2.379078 4.797143 -1.813175
H -1.124952 6.088512 -0.052720

25
[(**1**-H)$_2$-Au(III)]$^+$
Au -1.119367 0.163708 -0.050387
N -1.118821 -1.882383 -0.049724
C -0.919168 -2.551535 -1.201057
C -1.318194 -2.550874 1.102035
C -0.920892 -3.936299 -1.233307
H -0.739577 -1.958402 -2.097872
C -1.315928 -3.935618 1.135170
H -1.498041 -1.957233 1.998465
C -1.118277 -4.642037 -0.048842
H -0.761738 -4.446525 -2.183467
H -1.474886 -4.445294 2.085659
H -1.118070 -5.733721 -0.048497
N -1.119893 2.209317 -0.051094
C -1.305317 2.878398 1.102568
C -0.934780 2.877654 -1.205240
C -1.303406 4.263167 1.134742
H -1.472857 2.285612 2.001928
C -0.937440 4.262395 -1.238429
H -0.766861 2.284285 -2.104148
C -1.120622 4.968828 -0.052103
H -1.450863 4.773451 2.086755
H -0.790228 4.772062 -2.190810
H -1.120913 6.060511 -0.052505
Cl -3.096397 0.164842 1.144383
Cl 0.857648 0.165141 -1.245169

31
[(**1**-CF$_3$)$_2$-Au(III)]$^+$
Au -1.132338 0.163576 -0.043146
N -1.130840 -1.883398 -0.043708
C -1.229076 -2.551712 -1.208667
C -1.034202 -2.551893 1.119370
C -1.224272 -3.934905 -1.243121
H -1.331220 -1.960347 -2.118527
C -1.037381 -3.936895 1.153572
H -0.937441 -1.961671 2.030651
C -1.127196 -4.638763 -0.044387
H -1.306482 -4.448853 -2.201487

H	-0.968452	-4.452680	2.111485
N	-1.133095	2.210543	-0.042669
C	-1.037269	2.878540	1.120768
C	-1.232037	2.879354	-1.207279
C	-1.042002	4.263517	1.155689
H	-0.939874	2.287937	2.031738
C	-1.228782	4.262567	-1.241015
H	-1.333487	2.288342	-2.117450
C	-1.132524	4.965908	-0.041910
H	-0.973715	4.778889	2.113870
H	-1.311545	4.776916	-2.199120
Cl	-2.987199	0.162918	-1.419156
Cl	0.721244	0.164238	1.334396
C	-1.085682	-6.160587	-0.063265
C	-1.092738	6.487782	-0.060047
F	0.131263	-6.567894	-0.404632
F	-1.951541	-6.634480	-0.950448
F	-1.380127	-6.659110	1.129890
F	-1.959446	6.961079	-0.946735
F	-1.387329	6.985396	1.133456
F	0.123622	6.896603	-0.401654

31

[(**1**-CH_3)$_2$-Au(III)]$^+$

Au	-1.129426	0.163585	-0.050557
N	-1.129059	-1.880035	-0.050883
C	-0.987393	-2.555458	-1.207257
C	-1.273477	-2.556459	1.104627
C	-0.992707	-3.937069	-1.237849
H	-0.853393	-1.967060	-2.115068
C	-1.271532	-3.938068	1.133619
H	-1.410492	-1.968783	2.012448
C	-1.131034	-4.670729	-0.052340
H	-0.883487	-4.440206	-2.199734
H	-1.390132	-4.442010	2.093975
N	-1.129014	2.207190	-0.050700
C	-1.273065	2.883499	1.104860
C	-0.987700	2.882717	-1.207111
C	-1.271065	4.265158	1.133977
H	-1.409805	2.295777	2.012695
C	-0.993004	4.264280	-1.237582
H	-0.854024	2.294371	-2.115001
C	-1.130934	4.997880	-0.051917
H	-1.389339	4.769007	2.094414
H	-0.884086	4.767504	-2.199463
Cl	-3.044045	0.163590	1.242913
Cl	0.785169	0.163646	-1.344298
C	-1.101348	-6.167193	-0.049253
H	-0.062782	-6.512240	0.081312
H	-1.694362	-6.579840	0.777362
H	-1.471456	-6.579460	-0.996961
C	-1.101111	6.494340	-0.049271
H	-0.060775	6.839314	0.066566
H	-1.483990	6.906219	-0.992127
H	-1.682785	6.907448	0.785064

33

[(**1**-OMe)$_2$-Au(III)]$^+$

Au	-1.142819	0.163510	-0.056716
N	-1.225102	-1.876045	-0.006441
C	-1.331923	-2.583416	-1.155948
C	-1.170692	-2.530921	1.167817
C	-1.378980	-3.954844	-1.159925
H	-1.396312	-2.014882	-2.083572
C	-1.226410	-3.907532	1.247828
H	-1.062149	-1.926534	2.068633
C	-1.329264	-4.656644	0.061451
H	-1.461016	-4.504987	-2.096985
H	-1.181173	-4.374108	2.230386
N	-1.060637	2.203066	-0.107068
C	-0.954216	2.910504	1.042442
C	-1.114887	2.857869	-1.281372
C	-0.907387	4.281940	1.046359

H	-0.889997	2.342008	1.970098
C	-1.059337	4.234481	-1.361436
H	-1.223210	2.253414	-2.182173
C	-0.956886	4.983656	-0.175068
H	-0.825706	4.832163	1.983404
H	-1.104432	4.701025	-2.344017
Cl	-2.948868	0.201845	-1.498809
Cl	0.663296	0.125137	1.385325
O	-1.383017	-5.967424	-0.001369
O	-0.903349	6.294436	-0.112310
C	-1.339327	-6.750082	1.182676
H	-1.398460	-7.793552	0.857923
H	-0.394488	-6.588501	1.723722
H	-2.195934	-6.521085	1.834863
C	-0.946502	7.076990	-1.296444
H	-1.891060	6.915260	-1.837936
H	-0.887634	8.120487	-0.971731
H	-0.089548	6.848045	-1.948191

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cis-[(**1**-H)$_2$-Au(III)]$^+$

Au	-0.778678	-0.222772	-0.000457
N	-0.767621	-2.307093	0.166805
C	-1.382422	-3.053189	-0.769080
C	-0.104867	-2.901407	1.175032
C	-1.360456	-4.437517	-0.721860
H	-1.894977	-2.521340	-1.572938
C	-0.053776	-4.283047	1.287840
H	0.407220	-2.249590	1.884600
C	-0.687560	-5.065010	0.325676
H	-1.861378	-5.010109	-1.502912
H	0.489862	-4.731179	2.120046
H	-0.652892	-6.154491	0.386941
N	-2.862721	-0.209518	-0.171015
C	-3.454842	0.455223	-1.179221
C	-3.610835	-0.824956	0.762832
C	-4.836260	0.507770	-1.294093
H	-2.801485	0.967678	-1.887100
C	-4.995072	-0.801643	0.713489
H	-3.080708	-1.339137	1.566788
C	-5.620310	-0.126663	-0.334055
H	-5.282592	1.053016	-2.126216
H	-5.569346	-1.303152	1.492927
H	-6.709661	-0.090895	-0.396963
Cl	-0.779275	2.043720	-0.208901
Cl	1.487444	-0.225825	0.211739

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cis-[(**1**-CF_3)$_2$-Au(III)]$^+$

Au	-0.785460	-0.241388	0.067869
N	-0.779399	-2.331081	-0.104844
C	-0.082806	-2.925781	-1.089711
C	-1.432389	-3.076126	0.803060
C	-0.035884	-4.305712	-1.207831
H	0.458570	-2.276804	-1.779843
C	-1.419386	-4.460775	0.753141
H	-1.973204	-2.547320	1.590114
C	-0.711142	-5.084884	-0.270796
H	0.528514	-4.758234	-2.024328
H	-1.956646	-5.038415	1.505662
N	-2.880058	-0.208752	0.160285
C	-3.598977	-0.819548	-0.799783
C	-3.502222	0.463447	1.142269
C	-4.981830	-0.788188	-0.800941
H	-3.046551	-1.336757	-1.586358
C	-4.887243	0.526114	1.210997
H	-2.873166	0.976354	1.871649
C	-5.636828	-0.109830	0.227769
H	-5.535528	-1.282183	-1.600503
H	-5.364825	1.077750	2.021145
Cl	-0.774913	2.021647	0.285245
Cl	1.484244	-0.259633	-0.060033
C	-0.637367	-6.603525	-0.357146

C	-7.158878	-0.099875	0.265723
F	0.536639	-7.021174	0.097233
F	-1.597682	-7.166524	0.365258
F	-0.766156	-6.997165	-1.618387
F	-7.599548	-1.305593	0.611654
F	-7.611237	0.784541	1.142123
F	-7.644713	0.195024	-0.933106

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cis-[(**1**-CH_3)$_2$-Au(III)]$^+$

Au	-0.794729	-0.237513	-0.001579
N	-0.782896	-2.318106	0.133333
C	-1.422352	-3.054992	-0.793364
C	-0.095688	-2.936450	1.110796
C	-1.398506	-4.436878	-0.767349
H	-1.961055	-2.514837	-1.574257
C	-0.044431	-4.316545	1.196738
H	0.436325	-2.301437	1.820823
C	-0.697179	-5.109172	0.243954
H	-1.927454	-4.990040	-1.545067
H	0.520802	-4.771762	2.011614
N	-2.875194	-0.225925	-0.138890
C	-3.492583	0.462266	-1.116257
C	-3.612970	-0.866453	0.786354
C	-4.872592	0.513491	-1.203568
H	-2.856908	0.995066	-1.825100
C	-4.994833	-0.842711	0.758935
H	-3.073571	-1.405955	1.567218
C	-5.666145	-0.140345	-0.252298
H	-5.327019	1.079550	-2.018313
H	-5.548753	-1.372558	1.535500
Cl	-0.800593	2.033832	-0.176927
Cl	1.476408	-0.243112	0.176429
C	-0.618459	-6.603512	0.282272
H	0.269771	-6.936351	-0.279032
H	-0.517469	-6.975225	1.310386
H	-1.497910	-7.067501	-0.182903
C	-7.160448	-0.061682	-0.292090
H	-7.493887	0.826329	0.269207
H	-7.531111	0.039716	-1.320547
H	-7.624888	-0.941330	0.172252

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cis-[(**1**-OMe)$_2$-Au(III)]$^+$

Au	-0.935007	-0.379835	0.099295
N	-0.893412	-2.464141	0.196987
C	-1.411206	-3.183820	-0.817270
C	-0.317004	-3.064661	1.240424
C	-1.356049	-4.566340	-0.794254
H	-1.860374	-2.636339	-1.646286
C	-0.236114	-4.463721	1.331702
H	0.125711	-2.446972	2.023433
C	-0.768510	-5.224394	0.283905
H	-1.770871	-5.132319	-1.628917
H	-0.723673	-6.313709	0.296482
N	-2.996053	-0.411246	-0.193441
C	-3.566808	0.326033	-1.162384
C	-3.786475	-1.136945	0.630032
C	-4.933415	0.356622	-1.363479
H	-2.900299	0.927105	-1.782906
C	-5.153358	-1.155622	0.504851
H	-3.291305	-1.712105	1.414484
C	-5.764985	-0.395056	-0.514074
H	-5.329043	0.974462	-2.168057
H	-5.770650	-1.741133	1.185941
Cl	-0.967116	1.894070	-0.033171
Cl	1.317488	-0.351103	0.444333
O	0.351527	-4.935670	2.420567
O	-7.074940	-0.446489	-0.589598
C	0.515809	-6.332905	2.583440
H	1.033327	-6.469841	3.538258
H	-0.459095	-6.844774	2.622289
H	1.131301	-6.755358	1.773338

C	-7.772612	0.307473	-1.571328
H	-7.482952	-0.007631	-2.585387
H	-8.835239	0.097815	-1.414661
H	-7.588808	1.384570	-1.439772

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1-H

C	-0.171916	0.067859	0.000228
C	1.223018	0.061379	0.000124
C	1.890810	1.283638	-0.000089
C	1.135735	2.453987	-0.000211
C	-0.255042	2.345941	-0.000124
N	-0.901978	1.181784	0.000111
H	2.982462	1.323463	-0.000137
H	-0.726689	-0.876886	0.000386
H	1.769499	-0.883394	0.000225
H	1.611831	3.436113	-0.000359
H	-0.877178	3.247755	-0.000176

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1-CF_3

C	-0.169664	0.067794	-0.008333
C	1.224573	0.059367	0.014451
C	1.887806	1.284117	0.024128
C	1.136641	2.456814	0.014397
C	-0.253388	2.346148	-0.008350
N	-0.897484	1.181833	-0.021026
H	-0.722121	-0.877679	-0.015235
H	1.775759	-0.881679	0.030385
H	1.617377	3.435677	0.030316
H	-0.873669	3.248586	-0.015265
C	3.397859	1.338339	-0.001578
F	3.860552	2.443440	0.587007
F	3.937630	0.288332	0.621453
F	3.854895	1.334367	-1.257321

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1-CH_3

C	-0.176319	0.072100	-0.005868
C	1.217344	0.068544	0.010321
C	1.907473	1.284471	0.016041
C	1.130443	2.446624	0.009935
C	-0.259379	2.341377	-0.006180
N	-0.912099	1.181399	-0.014446
H	-0.724463	-0.876748	-0.009102
H	1.760213	-0.879846	0.021085
H	1.602582	3.432130	0.020393
H	-0.875267	3.247726	-0.009734
C	3.410346	1.338927	0.001405
H	3.848819	0.469887	0.512079
H	3.782928	1.336366	-1.035674
H	3.784327	2.252368	0.485015

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1-OCF_3

C	-0.167628	0.325142	-0.751351
C	1.216280	0.309091	-0.657905
C	1.845376	1.260657	0.156892
C	1.037306	2.179676	0.834439
C	-0.345702	2.092971	0.658223
N	-0.951941	1.196355	-0.110134
H	-0.674249	-0.411908	-1.383966
H	1.820122	-0.420403	-1.199055
H	1.449894	2.949777	1.485732
H	-0.993157	2.805433	1.182174
O	3.183899	1.216703	0.225105
C	3.858186	2.150770	1.028650
H	4.927947	1.930416	0.934054
H	3.674153	3.185089	0.691645
H	3.566765	2.060861	2.089001

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[(**2**-H)-Au(III)]$^+$

C	-0.867083	0.857701	-1.810969
C	0.550910	0.858562	-1.810095
C	1.239663	2.078712	-1.802800
C	0.538041	3.279927	-1.796471
C	-0.857157	3.279081	-1.797333
C	-1.557319	2.077017	-1.804527
H	2.330473	2.075885	-1.802158
H	1.084365	4.224559	-1.790828
H	-1.404634	4.223048	-1.792366
H	-2.648125	2.072871	-1.805233
C	-1.585446	-0.375319	-1.818424
C	-2.184089	-1.430939	-1.824897
C	-2.895922	-2.662194	-1.832469
C	-4.294974	-2.701684	-1.833622
C	-2.817202	-5.008926	-1.846005
C	-4.947232	-3.926309	-1.841148
H	-4.844644	-1.761026	-1.828546
C	-4.197407	-5.102219	-1.847457
H	-2.185277	-5.897937	-1.850707
H	-6.037967	-3.965531	-1.842097
H	-4.669539	-6.084377	-1.853450
N	-2.191907	-3.820583	-1.838724
C	1.270789	-0.373584	-1.816662
C	1.870917	-1.428368	-1.822393
C	2.584281	-2.658751	-1.829083
C	3.983378	-2.696522	-1.828513
C	2.508497	-5.005596	-1.842710
C	4.637170	-3.920331	-1.835238
H	4.531875	-1.755182	-1.822758
C	3.888814	-5.097171	-1.842467
H	1.877677	-5.895386	-1.848185
H	5.727952	-3.958192	-1.834850
H	4.362170	-6.078745	-1.847878
N	1.881707	-3.818030	-1.836202
Au	-0.155115	-3.784502	-1.837234
Cl	-0.156533	-3.844852	0.470614
Cl	-0.153674	-3.817381	-4.145642

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[(**2**-CF_3)-Au(III)]$^+$

C	-0.185222	-0.393112	-0.029109
C	1.233377	-0.392736	-0.028515
C	1.923035	0.826682	-0.027351
C	1.221003	2.028006	-0.026769
C	-0.174129	2.027637	-0.027352
C	-0.875525	0.825942	-0.028521
H	3.013837	0.824070	-0.026899
H	1.767456	2.972556	-0.025854
H	-0.721082	2.971897	-0.026893
H	-1.966326	0.822753	-0.028983
C	-0.902921	-1.625725	-0.030310
C	-1.500151	-2.682477	-0.031321
C	-2.210461	-3.912420	-0.032403
C	-3.611334	-3.946462	-0.033520
C	-2.140710	-6.259258	-0.033138
C	-4.262814	-5.167950	-0.034529
H	-4.164143	-3.007896	-0.033518
C	-3.518358	-6.350057	-0.034196
H	-1.513117	-7.151093	-0.032895
H	-3.997049	-7.329656	-0.034697
N	-1.511601	-5.071607	-0.032334
C	1.951736	-1.624965	-0.029096
C	2.549544	-2.681390	-0.029574
C	3.260516	-3.910952	-0.029995
C	4.661406	-3.944251	-0.029912
C	3.192010	-6.257829	-0.030549
C	5.313533	-5.165394	-0.030254
H	5.213727	-3.005396	-0.029496
C	4.569707	-6.347897	-0.030389
H	2.564889	-7.149997	-0.030738
H	5.048923	-7.327240	-0.030305
N	2.562274	-5.070511	-0.030441
C	6.832805	-5.243889	-0.031726

C	-5.782043	-5.247262	-0.036966
F	7.379821	-4.034978	-0.022384
F	7.250654	-5.890461	-1.114022
F	7.252330	-5.908001	1.039227
F	-6.329716	-4.038634	-0.029928
F	-6.198822	-5.895808	-1.118491
F	-6.201925	-5.909870	1.034781
Au	0.525327	-5.039086	-0.031265
Cl	0.524263	-5.086355	2.276207
Cl	0.526419	-5.082807	-2.338815

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[(**2**-CH_3)-Au(III)]$^+$

C	-1.545107	-0.819185	0.055494
C	-0.127299	-0.818796	0.056173
C	0.561517	0.401318	0.075936
C	-0.139274	1.602732	0.094729
C	-1.534494	1.602350	0.094063
C	-2.234609	0.400551	0.074600
H	1.652335	0.397786	0.076371
H	0.407479	2.547026	0.109995
H	-2.081779	2.546343	0.108805
H	-3.325425	0.396422	0.073991
C	-2.264978	-2.051608	0.035302
C	-2.866226	-3.105415	0.017791
C	-3.576562	-4.338731	-0.002792
C	-4.973402	-4.376429	-0.003154
C	-3.505078	-6.677228	-0.040309
C	-5.655657	-5.592286	-0.023369
H	-5.513805	-3.429685	0.013638
C	-4.881929	-6.763244	-0.041499
H	-2.880034	-7.571011	-0.053757
H	-5.351043	-7.747912	-0.055819
N	-2.869581	-5.493577	-0.021680
C	0.593273	-2.050821	0.036674
C	1.195127	-3.104292	0.019736
C	1.906167	-4.337212	-0.000164
C	3.303029	-4.374141	0.000821
C	1.836005	-6.675750	-0.037759
C	3.985969	-5.589623	-0.018735
H	3.842894	-3.427101	0.018129
C	3.212902	-6.761008	-0.037622
H	1.211461	-7.569874	-0.051815
H	3.682576	-7.745416	-0.051500
N	1.199841	-5.492446	-0.019734
C	5.482398	-5.653677	-0.030019
H	5.833494	-6.068232	-0.987556
H	5.935328	-4.663644	0.103545
H	5.846687	-6.318336	0.766690
C	-7.152039	-5.657156	-0.036115
H	-7.605638	-4.667403	0.097260
H	-7.501969	-6.071643	-0.994110
H	-7.516750	-6.322226	0.760056
Au	-0.834879	-5.461494	-0.020213
Cl	-0.835941	-5.549212	2.287195
Cl	-0.833792	-5.468652	-2.329290

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[(**2**-OMe)-Au(III)]$^+$

C	-0.868809	0.828129	-1.828016
C	0.548546	0.829125	-1.823990
C	1.237022	2.049055	-1.858959
C	0.535974	3.249847	-1.897283
C	-0.859203	3.248868	-1.901245
C	-1.558779	2.047094	-1.866897
H	2.327854	2.045639	-1.855691
H	1.082528	4.194009	-1.924241
H	-1.406918	4.192263	-1.931308
H	-2.649606	2.042149	-1.869828
C	-1.588611	-0.404416	-1.792429
C	-2.192205	-1.456129	-1.761675
C	-2.905492	-2.688705	-1.725786
C	-4.290749	-2.719872	-1.728884

C	-2.829271	-5.025864	-1.653458
C	-4.968720	-3.949752	-1.692917
H	-4.858914	-1.791338	-1.759204
C	-4.205069	-5.130583	-1.654289
H	-2.206723	-5.921212	-1.624164
H	-4.656782	-6.120248	-1.625145
N	-2.190726	-3.847863	-1.687851
C	1.269889	-0.402391	-1.784305
C	1.874909	-1.453176	-1.750095
C	2.589844	-2.684659	-1.710148
C	3.975136	-2.713744	-1.705445
C	2.516729	-5.021937	-1.638224
C	4.654747	-3.942606	-1.665691
H	4.542075	-1.784363	-1.732592
C	3.892673	-5.124584	-1.631318
H	1.895371	-5.918219	-1.612421
H	4.345702	-6.113568	-1.599615
N	1.876619	-3.844899	-1.676237
O	-6.283915	-3.901056	-1.698295
O	5.969881	-3.891913	-1.663752
C	6.735384	-5.085774	-1.625012
H	6.534529	-5.709678	-2.509533
H	7.784418	-4.773530	-1.632180
H	6.530280	-5.653927	-0.704639
C	-7.047784	-5.096095	-1.663672
H	-8.097240	-4.785454	-1.676367
H	-6.841293	-5.719638	-2.547148
H	-6.846663	-5.663979	-0.742255
Au	-0.157074	-3.814702	-1.682955
Cl	-0.163692	-3.794622	0.626306
Cl	-0.150368	-3.940247	-3.988936

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[(**2**-CH_3/CF_3)-Au(III)]$^+$

C	-0.866993	0.870327	-1.819492
C	0.551204	0.869198	-1.818124
C	1.239795	2.089113	-1.814318
C	0.538251	3.290683	-1.811907
C	-0.856938	3.291395	-1.813260
C	-1.557553	2.089745	-1.817026
H	2.330575	2.086238	-1.813270
H	1.085198	4.235000	-1.808952
H	-1.403698	4.235744	-1.811367
H	-2.648386	2.085879	-1.818096
C	-1.586056	-0.361451	-1.823384
C	-2.185759	-1.416806	-1.826770
C	-2.896923	-2.646268	-1.830756
C	-4.298069	-2.678831	-1.832085
C	-2.828860	-4.991784	-1.837107
C	-4.950351	-3.899735	-1.835984
H	-4.850059	-1.739835	-1.830043
C	-4.206633	-5.082282	-1.838593
H	-2.201564	-5.883851	-1.838969
H	-4.686002	-6.061489	-1.841760
N	-2.198541	-3.805222	-1.833303
C	1.270423	-0.363768	-1.820635
C	1.870022	-1.418654	-1.822828
C	2.580187	-2.652198	-1.825519
C	3.976703	-2.690666	-1.823530
C	2.508147	-4.992396	-1.830923
C	4.658913	-3.907053	-1.826115
H	4.517358	-1.743923	-1.819019
C	3.884867	-5.078076	-1.829082
H	1.883223	-5.886329	-1.832933
H	4.353663	-6.063001	-1.829135
N	1.873316	-3.807817	-1.829421
C	6.155030	-3.972149	-1.836764
H	6.505356	-4.391581	-2.792533
H	6.608724	-2.981828	-1.708306
H	6.518912	-4.633512	-1.037203
C	-6.469127	-3.978141	-1.837126
F	-7.017030	-2.769329	-1.837191
F	-6.889685	-4.633861	-0.760987

F -6.888213 -4.633344 -2.914147
Au -0.156676 -3.774743 -1.831265
Cl -0.162303 -3.828329 0.476603
Cl -0.157704 -3.814110 -4.139448

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[(**2**-H)-Au(I)]$^{+}$
C -0.870754 0.843210 -1.829949
C 0.547473 0.843382 -1.829275
C 1.235614 2.064551 -1.830143
C 0.535726 3.266432 -1.831644
C -0.859567 3.266269 -1.832299
C -1.559176 2.064224 -1.831462
H 2.326505 2.060810 -1.829627
H 1.082901 4.210636 -1.832307
H -1.406960 4.210346 -1.833474
H -2.650066 2.060236 -1.831973
C -1.594583 -0.387949 -1.829099
C -2.197488 -1.441478 -1.828330
C -2.924110 -2.668866 -1.827607
C -4.323969 -2.673523 -1.828153
C -2.892268 -5.001982 -1.825568
C -5.004762 -3.882937 -1.827391
H -4.853463 -1.721166 -1.829173
C -4.276080 -5.070792 -1.826088
H -2.285831 -5.908568 -1.824555
H -6.096110 -3.899594 -1.827799
H -4.767276 -6.043837 -1.825458
N -2.225506 -3.833672 -1.826290
C 1.271561 -0.387608 -1.827740
C 1.874328 -1.441209 -1.826370
C 2.601187 -2.668423 -1.824614
C 4.001050 -2.672868 -1.823684
C 2.569661 -5.001517 -1.822161
C 4.682019 -3.882176 -1.821958
H 4.530363 -1.720408 -1.824342
C 3.953484 -5.070128 -1.821181
H 1.963358 -5.908191 -1.821607
H 5.773367 -3.898690 -1.821217
H 4.444788 -6.043119 -1.819824
N 1.902733 -3.833292 -1.823831
Au -0.161411 -3.815736 -1.825148

34
2-H
C -0.734249 1.029956 -1.751085
C 0.672319 1.100295 -1.580284
C 1.287953 2.357379 -1.492183
C 0.533641 3.522783 -1.570791
C -0.850443 3.453038 -1.738971
C -1.478797 2.216062 -1.828322
H 2.370138 2.403973 -1.360746
H 1.028392 4.493546 -1.500353
H -1.442587 4.368173 -1.800617
H -2.560334 2.152915 -1.959771
C -1.375791 -0.245183 -1.842333
C -1.872670 -1.349622 -1.914010
C -2.463113 -2.656993 -1.999323
C -3.851151 -2.796070 -2.161125
C -2.170135 -4.929409 -1.995633
C -4.389730 -4.074678 -2.240214
H -4.480577 -1.907491 -2.221726
C -3.534537 -5.170580 -2.156267
H -1.467658 -5.766857 -1.925733
H -5.465555 -4.213686 -2.366057
H -3.911515 -6.192849 -2.213400
N -1.641432 -3.713620 -1.918499
C 1.437095 -0.103713 -1.500714
C 2.032968 -1.158046 -1.439637
C 2.643309 -2.460233 -1.379968
C 1.825644 -3.597524 -1.494644
C 4.531375 -3.727447 -1.162144
C 2.433646 -4.846674 -1.434624

H 0.744263 -3.491971 -1.626836
C 3.814110 -4.920375 -1.265079
H 5.618580 -3.749279 -1.028127
H 1.832579 -5.754875 -1.519661
H 4.331006 -5.880295 -1.212814
N 3.971117 -2.524787 -1.216782

40
2-CF_3
C -0.073673 -0.212338 0.334882
C 1.297849 -0.042788 0.654124
C 1.781289 1.241886 0.939546
C 0.928597 2.339992 0.910951
C -0.421235 2.172894 0.596715
C -0.918677 0.906353 0.310821
H 2.837453 1.364739 1.184286
H 1.319227 3.334437 1.135379
H -1.089833 3.035566 0.574528
H -1.972668 0.768025 0.064361
C -0.575742 -1.518920 0.042338
C -0.948848 -2.647896 -0.197244
C -1.394992 -3.982588 -0.481990
C -2.741868 -4.214782 -0.807080
C -0.889266 -6.209704 -0.682678
C -3.141151 -5.516032 -1.076073
H -3.447838 -3.385582 -0.842058
C -2.200231 -6.542607 -1.013605
H -0.122823 -6.986086 -0.623123
H -2.475330 -7.578959 -1.214017
N -0.490316 -4.968045 -0.423358
C 2.161316 -1.180772 0.679462
C 2.842320 -2.183605 0.684490
C 3.568033 -3.424334 0.665921
C 2.881685 -4.608399 0.354028
C 5.548865 -4.534009 0.933794
C 3.609754 -5.794757 0.344059
H 1.809711 -4.590669 0.127328
C 4.969372 -5.768978 0.637842
H 6.616454 -4.474704 1.169934
H 5.566823 -6.680609 0.638196
N 4.876990 -3.391348 0.949972
C 2.904449 -7.087820 0.013319
C -4.569595 -5.834765 -1.454382
F 3.728988 -8.135232 0.046736
F 2.358912 -7.045359 -1.207851
F 1.909621 -7.332518 0.874174
F -4.647548 -6.224969 -2.729126
F -5.374103 -4.782659 -1.303631
F -5.052976 -6.828236 -0.705187

40
2-CH_3
C -1.980037 0.469473 -0.634846
C -0.611725 0.283747 -0.309277
C 0.241428 1.396129 -0.261133
C -0.242364 2.671709 -0.528816
C -1.588776 2.854762 -0.849185
C -2.449341 1.763940 -0.901655
H 1.292586 1.244461 -0.009921
H 0.433397 3.528207 -0.487641
H -1.970346 3.855897 -1.059634
H -3.502897 1.899140 -1.151308
C -2.853337 -0.659657 -0.685369
C -3.538740 -1.659646 -0.710699
C -4.246277 -2.913399 -0.709129
C -3.532451 -4.080775 -0.405958
C -6.186319 -4.069291 -0.990744
C -4.204739 -5.305369 -0.400260
H -2.462633 -4.029588 -0.177199
C -5.567692 -5.287237 -0.702120
H -7.255590 -4.043875 -1.229008
H -6.150834 -6.211128 -0.714524
N -5.555176 -2.902793 -0.998194

C	-0.115409	-1.029584	-0.034091
C	0.266442	-2.158729	0.192542
C	0.733490	-3.491031	0.464232
C	2.081462	-3.704748	0.790442
C	0.277276	-5.720967	0.639201
C	2.535592	-4.996789	1.053929
H	2.762428	-2.852466	0.832084
C	1.594523	-6.028050	0.970351
H	-0.469548	-6.519046	0.569316
H	1.882095	-7.064790	1.158879
N	-0.156626	-4.490381	0.390604
C	3.964451	-5.266056	1.436329
H	4.631343	-4.462105	1.096299
H	4.058584	-5.338104	2.531572
H	4.318591	-6.216160	1.011981
C	-3.469632	-6.577757	-0.078818
H	-2.644626	-6.735910	-0.790129
H	-3.028373	-6.523376	0.928145
H	-4.132692	-7.452747	-0.118552

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2-OCH_3

C	-0.094085	0.329007	0.083379
C	1.324527	0.314794	0.043229
C	2.025226	1.529580	0.030206
C	1.343178	2.740848	0.056216
C	-0.052164	2.755792	0.095741
C	-0.763707	1.561253	0.109186
H	3.115922	1.508806	-0.000740
H	1.902079	3.678680	0.045679
H	-0.589384	3.706148	0.116222
H	-1.854436	1.564996	0.140128
C	-0.818996	-0.902833	0.097083
C	-1.384149	-1.975793	0.107226
C	-1.955822	-3.298132	0.115999
C	-1.089545	-4.392869	0.085266
C	-3.796840	-4.630333	0.160386
C	-1.643971	-5.676866	0.093607
H	-0.002336	-4.261268	0.055408
C	-3.035672	-5.802788	0.132263
H	-4.889613	-4.707590	0.190865
H	-3.537952	-6.769657	0.141082
N	-3.295383	-3.405554	0.153127
C	2.017998	-0.935807	0.016711
C	2.542585	-2.029131	-0.004069
C	3.095358	-3.356383	-0.026979
C	4.474647	-3.556951	-0.067643
C	2.687643	-5.605025	-0.027252
C	4.965822	-4.868547	-0.088800
H	5.169994	-2.717929	-0.083184
C	4.046685	-5.923333	-0.067951
H	1.935805	-6.402074	-0.010007
H	4.355865	-6.967728	-0.082451
N	2.212306	-4.370018	-0.007079
O	6.296944	-5.012044	-0.127968
O	-0.782634	-6.710993	0.063415
C	-1.291531	-8.018970	0.069855
H	-1.925556	-8.214287	-0.811892
H	-0.426886	-8.692811	0.041020
H	-1.874266	-8.225377	0.983868
C	6.846514	-6.305289	-0.150869
H	6.524264	-6.867376	-1.043704
H	7.935178	-6.181032	-0.181765
H	6.576392	-6.877063	0.753032

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2-CH_3/CF_3

C	-1.886067	-1.033995	0.474632
C	-0.514366	-1.184469	0.146269
C	0.315648	-0.054293	0.131461
C	-0.195555	1.202779	0.434735
C	-1.545572	1.350436	0.757812
C	-2.383969	0.241290	0.777582

H 1.369973 -0.176805 -0.121941
H 0.462664 2.073675 0.419259
H -1.947143 2.337348 0.995911
H -3.440403 0.347765 1.029012
C -2.735425 -2.182798 0.490951
C -3.402564 -3.194945 0.487112
C -4.115438 -4.442791 0.458136
C -3.419636 -5.618051 0.132347
C -6.086700 -5.571088 0.721308
C -4.139140 -6.809730 0.113016
H -2.347624 -5.590027 -0.097584
C -5.498140 -6.797958 0.411263
H -7.154037 -5.522793 0.961436
H -6.087810 -7.714611 0.404324
N -5.423973 -4.423322 0.746637
C 0.001116 -2.481801 -0.163984
C 0.381047 -3.605525 -0.417708
C 0.836448 -4.935626 -0.719576
C 2.179367 -5.152170 -1.061007
C 0.356993 -7.157947 -0.932453
C 2.619826 -6.442991 -1.352982
H 2.866693 -4.304548 -1.092124
C 1.669912 -7.466214 -1.280523
H -0.394767 -7.949083 -0.871288
H 1.946304 -8.501722 -1.491136
N -0.063330 -5.927017 -0.656868
C 4.042876 -6.718128 -1.752331
H 4.124286 -6.787724 -2.848731
H 4.718002 -5.918980 -1.417195
H 4.396345 -7.671563 -1.334869
C -3.426976 -8.095080 -0.233333
F -2.891689 -8.040154 -1.457731
F -4.246148 -9.148367 -0.202948
F -2.426533 -8.341949 0.619379

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5
C 0.322037 1.275873 -0.651302
C 1.522184 1.586875 -1.306759
C 2.280127 2.673162 -0.898501
C 1.865192 3.474600 0.174261
C 0.671112 3.160359 0.819720
C -0.102881 2.071502 0.419080
H 1.838047 0.955134 -2.138389
H 3.204537 2.919164 -1.425590
H 0.336914 3.770730 1.662117
H -1.028791 1.853889 0.951327
C 2.681566 4.691011 0.562635
H 3.726472 4.530412 0.255642
O -0.348266 0.201734 -1.114241
C -1.554790 -0.166049 -0.503645
H -1.918505 -1.053630 -1.035344
H -1.414388 -0.421388 0.561250
H -2.313923 0.631826 -0.581700
O 2.198292 5.857936 -0.130555
C 2.751910 6.136732 -1.320948
O 3.640135 5.491007 -1.812347
C 2.104327 7.342947 -1.941525
H 1.058633 7.104705 -2.184334
H 2.095436 8.177586 -1.227621
H 2.643225 7.620785 -2.853566
C 2.651196 4.993730 1.996799
C 2.646950 5.225143 3.181955
H 2.646262 5.433778 4.235564

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[(**1**-H)$_2$-Au(III)]-**5**
Au -0.789050 0.305997 1.132628
N -0.406249 -1.679206 1.458736
C 0.869394 -2.113674 1.426395
C -1.420916 -2.541812 1.657373
C 1.172761 -3.452278 1.599860
H 1.652878 -1.374445 1.250415

C	-1.177909	-3.892088	1.845119
H	-2.435420	-2.142480	1.652161
C	0.134197	-4.357344	1.816050
H	2.214001	-3.774118	1.561843
H	-2.019731	-4.565590	2.005199
H	0.347113	-5.418670	1.959086
N	-1.153594	2.277771	0.688830
C	-0.847412	2.745793	-0.542384
C	-1.721934	3.085792	1.607972
C	-1.102708	4.061184	-0.887328
H	-0.407719	2.048346	-1.256134
C	-2.009290	4.408427	1.310539
H	-1.926795	2.690659	2.606721
C	-1.698813	4.907546	0.047651
H	-0.840487	4.407746	-1.887715
H	-2.469393	5.029549	2.079907
H	-1.917117	5.946718	-0.207563
Cl	-1.886303	-0.302320	-0.767228
C	-1.447045	-4.011830	5.219513
C	-0.214946	-3.329895	5.138444
C	-0.181294	-1.976100	4.866594
C	-1.371915	-1.263063	4.653059
C	-2.591346	-1.936469	4.744053
C	-2.641178	-3.299864	5.024520
H	0.699580	-3.896846	5.319854
H	0.784089	-1.463396	4.835533
H	-3.530950	-1.392997	4.609380
H	-3.609693	-3.793320	5.103317
C	-1.364372	0.222066	4.419777
H	-2.336113	0.546098	4.008261
O	-1.374920	-5.314983	5.466363
C	-2.554420	-6.064972	5.694215
H	-2.229903	-7.083023	5.933089
H	-3.124476	-5.657828	6.543791
H	-3.193080	-6.090297	4.796078
O	-1.114162	0.924437	5.623224
C	-1.511497	2.227602	5.656014
O	-1.945657	2.760715	4.666956
C	-1.348443	2.827364	7.009812
H	-2.077663	2.366943	7.693343
H	-0.347734	2.609682	7.406372
H	-1.522987	3.906930	6.960052
C	-0.313198	0.638077	3.445069
C	0.633593	1.017311	2.752440
H	1.563107	1.450338	2.399916

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A

C	-0.694350	1.610119	4.260079
C	0.497726	1.309375	4.300036
C	1.949508	1.039361	4.403789
H	2.155226	0.757656	5.451666
H	-1.648919	2.119447	4.279965
C	3.786478	2.461165	4.732122
O	4.217605	1.665237	5.511290
O	2.581810	2.262899	4.100053
C	4.413834	3.745517	4.293888
H	4.663765	3.682549	3.225013
H	3.706375	4.575877	4.422223
H	5.322826	3.922976	4.877647
C	2.362609	-0.093557	3.488906
C	2.679599	-1.344843	4.011828
C	2.428245	0.109564	2.102512
C	3.037193	-2.401780	3.172730
H	2.663449	-1.506149	5.093130
C	2.790780	-0.926643	1.262045
H	2.208156	1.095519	1.685582
C	3.088154	-2.198445	1.788078
H	3.287596	-3.366872	3.612386
H	2.859002	-0.786249	0.182167
O	3.383256	-3.147792	0.891988
C	3.808437	-4.418359	1.335756
H	4.044231	-4.997973	0.436599

H 4.711535 -4.341989 1.962297
H 3.014996 -4.936485 1.900364
Cl -0.808095 -0.334663 6.750681
Au -0.821752 -0.649307 4.493563
Cl -1.509168 -2.796998 4.818500
N -0.799119 -0.999567 2.423150
C -0.227178 -2.123536 1.960921
C -1.325932 -0.112208 1.559503
C -0.156422 -2.394632 0.602320
H 0.179663 -2.812952 2.700435
C -1.295290 -0.323933 0.191933
H -1.787184 0.783144 1.976621
C -0.698474 -1.485201 -0.298195
H 0.337698 -3.306808 0.267826
H -1.740208 0.415216 -0.474692
H -0.658004 -1.675620 -1.372327

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A-1
C -0.554969 -1.559412 3.766830
C 0.212250 -1.583240 4.736183
C 1.184336 -1.725402 5.835369
Cl 0.782311 1.205832 3.047826
H 0.632592 -1.852122 6.779360
H -1.005666 -1.954285 2.863192
C 1.548676 0.517185 6.441903
O 0.387609 0.582129 6.777764
O 2.059327 -0.615800 5.926607
C 2.538544 1.629138 6.474670
H 3.543678 1.260586 6.711619
H 2.561582 2.068359 5.464617
H 2.212179 2.393735 7.187401
C 1.951891 -2.974951 5.483430
C 1.797110 -4.140132 6.234060
C 2.822528 -2.973053 4.379302
C 2.504138 -5.294429 5.909991
H 1.124991 -4.154622 7.095918
C 3.532075 -4.110760 4.052548
H 2.949516 -2.064077 3.785991
C 3.381001 -5.286924 4.814092
H 2.373641 -6.187685 6.519784
H 4.221915 -4.127878 3.207902
O 4.105983 -6.333011 4.421424
C 4.029903 -7.550198 5.129127
H 4.711103 -8.243814 4.624458
H 4.352401 -7.426392 6.175920
H 3.009154 -7.965945 5.104496
Au -1.060629 0.538991 4.228598
Cl -1.840531 2.686071 4.310372
N -2.743578 -0.035282 5.296050
C -2.658999 -0.175349 6.629423
C -3.917528 -0.193636 4.661097
C -3.777638 -0.501257 7.382817
H -1.676704 -0.003137 7.076329
C -5.069784 -0.522499 5.356535
H -3.927226 -0.039664 3.580456
C -5.000045 -0.679144 6.739956
H -3.682047 -0.602310 8.464147
H -6.007886 -0.643454 4.814324
H -5.894928 -0.930666 7.312489

41
A-2
C -2.511741 -3.249949 4.287236
C -1.739531 -3.057742 5.224040
C -0.826321 -2.889177 6.374015
Cl -0.546231 -3.781818 2.022150
H -1.072409 -3.720745 7.061643
H -3.307560 -3.601549 3.643239
C -0.804130 -1.277080 8.217716
O -0.950223 -0.129477 8.504364
Au -1.006233 -1.900204 3.234904
O -1.136616 -1.637922 6.932397

C -0.310204 -2.359808 9.133190
H -1.092153 -3.116970 9.296389
H 0.576211 -2.860361 8.716587
H -0.053001 -1.904316 10.095047
C 0.615719 -3.001772 5.890740
C 1.056709 -4.188124 5.304399
C 1.484003 -1.904337 5.946007
C 2.331929 -4.286369 4.758575
H 0.392053 -5.054220 5.242387
C 2.758754 -1.992483 5.409821
H 1.166465 -0.970406 6.412872
C 3.195287 -3.180424 4.798677
H 2.639756 -5.223919 4.297475
H 3.449741 -1.149325 5.450472
O 4.428934 -3.164470 4.295735
C 4.940436 -4.309804 3.650122
H 5.951721 -4.050987 3.318439
H 4.996893 -5.167908 4.339734
H 4.331136 -4.580370 2.772232
Cl 0.204750 -0.660508 1.761937
C -2.645848 0.067398 4.797260
C -0.385149 0.620516 4.706944
C -2.906131 1.113413 5.665127
H -3.442393 -0.599173 4.463971
C -0.575360 1.675425 5.583402
H 0.592691 0.396571 4.279044
C -1.850459 1.917963 6.085393
H -3.924926 1.278491 6.015595
H 0.276739 2.291170 5.871333
N -1.404379 -0.177944 4.344501
H -2.021039 2.729539 6.794364

41
A-3
C -2.012670 -3.396119 6.554282
C -0.913941 -2.933219 6.860147
C 0.410454 -2.416248 7.266845
Cl -0.564538 -4.824554 4.124778
H 0.645700 -2.944812 8.210327
H -2.979030 -3.880408 6.621587
C 1.154082 -0.201767 8.048228
O 0.967121 0.966507 7.918683
O 0.217008 -1.035670 7.469439
C 2.276307 -0.853759 8.798969
H 1.884671 -1.480923 9.613926
H 2.874532 -1.489889 8.130416
H 2.910950 -0.068498 9.222647
C 1.451261 -2.739960 6.212113
C 2.129126 -3.954807 6.242708
C 1.652261 -1.866279 5.131862
C 2.987909 -4.318052 5.209074
H 1.980777 -4.648334 7.074724
C 2.500565 -2.218235 4.097787
H 1.154007 -0.893408 5.102333
C 3.168792 -3.456282 4.117425
H 3.502980 -5.276621 5.259268
H 2.667234 -1.552807 3.250098
O 3.950946 -3.715221 3.070478
C 4.643965 -4.940938 2.996094
H 5.198120 -4.925479 2.051401
H 5.357311 -5.050587 3.829431
H 3.947353 -5.795328 2.991513
Au -1.468064 -2.756127 4.464636
Cl -1.294651 -2.328433 2.232848
N -2.426405 -0.906265 4.686444
C -1.945222 0.044551 5.506817
C -3.526848 -0.667109 3.946753
C -2.558812 1.284082 5.612835
H -1.062066 -0.189301 6.104585
C -4.192960 0.545230 4.017773
H -3.861830 -1.460277 3.276822
C -3.700722 1.541342 4.859811
H -2.127568 2.025956 6.285791

H -5.082914 0.701015 3.407465
H -4.202918 2.508522 4.925217

41
A-4
C -0.992636 -1.730140 3.017645
C -0.396686 -1.894474 4.085633
C 0.317100 -2.210924 5.343314
Cl 1.024703 0.414320 2.062066
H -0.417445 -2.612639 6.060080
H -1.472252 -1.860131 2.056042
C 0.696417 -0.773092 7.192785
O 0.276869 -1.620452 7.921040
Au -0.635186 0.369883 3.671131
O 0.801683 -0.962540 5.840141
C 1.135684 0.609923 7.562223
H 2.081191 0.860989 7.063833
H 0.362039 1.317536 7.226072
H 1.242090 0.683146 8.649614
C 1.406151 -3.213376 5.083622
C 1.521658 -4.341433 5.895368
C 2.349721 -2.997635 4.064972
C 2.556381 -5.253346 5.704825
H 0.803226 -4.510056 6.701118
C 3.381192 -3.894724 3.867957
H 2.272358 -2.117926 3.419190
C 3.496098 -5.035125 4.686694
H 2.623064 -6.124606 6.355418
H 4.122632 -3.746945 3.081786
O 4.522439 -5.844609 4.419466
C 4.714017 -7.011769 5.185777
H 5.605278 -7.504199 4.781670
H 4.885763 -6.771936 6.248075
H 3.853972 -7.696025 5.098612
Cl -2.313328 0.328406 5.263775
C -1.572107 3.177795 3.918029
C 0.753677 2.953006 4.051116
C -1.478979 4.551581 4.071708
H -2.534641 2.675399 3.819037
C 0.906972 4.318393 4.225902
H 1.609720 2.278990 4.007540
C -0.223456 5.132855 4.232300
H -2.390493 5.149690 4.069533
H 1.909227 4.730122 4.346721
H -0.126348 6.212675 4.360603
N -0.468746 2.406296 3.905486

41
A-5
C 0.268493 -3.562243 3.284558
C 0.185907 -3.079039 4.420575
C 0.150973 -2.501901 5.773505
Cl 3.258297 -2.859843 2.797498
H 0.311608 -3.365479 6.448594
H 0.133946 -4.317642 2.517719
C -1.579176 -1.560900 7.196580
O -2.543658 -0.870666 7.234514
Au 1.246011 -1.726136 2.649266
O -1.100508 -1.908575 5.944328
C -0.846590 -2.115512 8.388586
H -0.880364 -3.215709 8.393209
H 0.206509 -1.798148 8.396222
H -1.342078 -1.744162 9.291659
C 1.320392 -1.529797 5.903623
C 2.592254 -1.987460 6.236917
C 1.129791 -0.175490 5.590030
C 3.682103 -1.119980 6.243194
H 2.755213 -3.041121 6.477474
C 2.206887 0.695415 5.599668
H 0.132504 0.191346 5.336111
C 3.497204 0.228775 5.908994
H 4.666690 -1.507872 6.501614
H 2.077727 1.753976 5.368776

O 4.483869 1.130770 5.831031
C 5.788403 0.774968 6.236218
H 6.399578 1.679300 6.142145
H 5.804172 0.439193 7.285526
H 6.210869 -0.015199 5.593034
Cl -0.781891 -0.650909 2.405838
C 1.716527 0.459407 0.689296
C 3.308319 0.366077 2.401487
C 2.338034 1.564622 0.131331
H 0.807687 0.034997 0.262523
C 3.957517 1.483530 1.903610
H 3.667569 -0.161268 3.284589
C 3.469849 2.091886 0.749545
H 1.922522 2.006695 -0.774444
H 4.835812 1.860588 2.427415
H 3.967460 2.970273 0.333991
N 2.205079 -0.118208 1.802521

41
A-6
C -0.874431 -1.843402 3.080592
C -0.215624 -1.960385 4.114554
C 0.587635 -2.171125 5.343163
Cl 0.618173 0.559267 1.853500
H -0.124365 -2.411313 6.148636
H -1.381430 -2.005360 2.138505
C 1.453715 -0.408879 6.816621
O 1.735224 0.752517 6.883883
Au -0.671202 0.297175 3.748303
O 1.209207 -0.910235 5.571328
C 1.343688 -1.342407 7.984478
H 0.281145 -1.530448 8.205037
H 1.839155 -2.302661 7.786635
H 1.793912 -0.856343 8.856407
C 1.555024 -3.303012 5.127162
C 1.429178 -4.492102 5.843620
C 2.600282 -3.163817 4.198114
C 2.328834 -5.538807 5.654162
H 0.618506 -4.615657 6.567245
C 3.500503 -4.192494 4.005587
H 2.707340 -2.236870 3.628441
C 3.375309 -5.394131 4.731568
H 2.207957 -6.455887 6.229584
H 4.321980 -4.103645 3.293582
O 4.290681 -6.328088 4.475406
C 4.243997 -7.564312 5.151594
H 5.086557 -8.154405 4.775078
H 4.355943 -7.431146 6.240219
H 3.305007 -8.102149 4.940968
Cl -2.008071 0.095486 5.633265
C -1.422776 3.113188 3.314867
C 0.252072 2.802271 4.930550
C -1.385150 4.485454 3.490264
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H -0.445161 6.103791 4.571611
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41
TS
C -0.469830 1.538298 4.381708
C 0.716147 1.213176 4.329005
C 2.178991 0.948793 4.328794
H 2.448131 0.729491 5.377600
H -1.409680 2.063602 4.490343
C 3.466061 2.858169 4.892754
O 3.452682 2.521148 6.037662
O 2.811944 2.137311 3.917235
C 4.151300 4.045554 4.297354

H 4.918772 3.705753 3.587384
H 3.429195 4.655810 3.737797
H 4.613971 4.636285 5.094482
C 2.527163 -0.215092 3.429339
C 2.739570 -1.481268 3.971824
C 2.615338 -0.039359 2.040737
C 3.018395 -2.575943 3.151036
H 2.696088 -1.629043 5.054805
C 2.901461 -1.114090 1.218939
H 2.477511 0.954321 1.608891
C 3.093637 -2.397828 1.763985
H 3.185069 -3.551440 3.607038
H 2.987630 -0.994938 0.137778
O 3.316091 -3.380756 0.883346
C 3.630634 -4.675883 1.347808
H 3.822266 -5.286215 0.458558
H 4.533323 -4.666243 1.979556
H 2.793246 -5.117395 1.914017
Cl -0.484910 -0.529281 6.768802
Au -0.627542 -0.724439 4.502947
Cl -1.335147 -2.876751 4.753802
N -0.721084 -0.962070 2.417020
C -0.198988 -2.070308 1.866803
C -1.267314 -0.017381 1.629336
C -0.196366 -2.266335 0.493482
H 0.223558 -2.808970 2.547501
C -1.305880 -0.153348 0.252431
H -1.686874 0.862901 2.116705
C -0.758326 -1.296933 -0.328863
H 0.260258 -3.169349 0.087940
H -1.764692 0.630495 -0.350700
H -0.772141 -1.427386 -1.412604

41
B
C 0.127540 1.181699 3.897745
C 1.336075 1.598529 4.225667
C 2.560584 0.861929 4.718970
H 2.464904 0.604972 5.784623
H -0.625451 1.924285 3.613743
C 2.975324 3.061817 4.400835
O 1.719240 2.975151 4.162606
O 3.565253 1.969811 4.674983
C 3.680126 4.353268 4.380385
H 3.653110 4.767662 5.401734
H 4.728803 4.201400 4.098725
H 3.173841 5.052927 3.705694
C 2.951914 -0.329183 3.915171
C 2.995670 -1.579842 4.530949
C 3.093168 -0.249165 2.519811
C 3.115533 -2.745139 3.779505
H 2.863088 -1.661256 5.611738
C 3.246977 -1.395083 1.765317
H 3.058193 0.719108 2.012563
C 3.214198 -2.660312 2.386033
H 3.089698 -3.707313 4.288102
H 3.352995 -1.352969 0.680369
O 3.236379 -3.713035 1.564813
C 3.145055 -5.016705 2.104954
H 3.156074 -5.704759 1.252793
H 4.003684 -5.239791 2.758075
H 2.206697 -5.146536 2.668837
Cl -0.089604 -0.713563 6.218617
Au -0.341991 -0.803578 3.939477
Cl -0.761372 -3.110726 3.979117
N -0.597103 -0.848047 1.868978
C 0.005997 -1.809997 1.151400
C -1.383801 0.051742 1.253902
C -0.139856 -1.884048 -0.226467
H 0.590036 -2.543143 1.706038
C -1.586243 0.026564 -0.116465
H -1.871774 0.798220 1.881724
C -0.947471 -0.954363 -0.873577

H 0.373288 -2.676754 -0.771409
H -2.241986 0.766321 -0.576212
H -1.087136 -0.997040 -1.955485

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A-(**1**-CF_3)
C -0.709001 1.743930 4.189143
C 0.464921 1.384328 4.268577
C 1.903113 1.051732 4.376900
H 2.085747 0.687197 5.403288
H -1.637725 2.298981 4.160371
C 3.794776 2.365660 4.815178
O 4.192195 1.487681 5.521606
O 2.583030 2.271753 4.173892
C 4.475074 3.655529 4.486982
H 4.713071 3.678910 3.413831
H 3.805752 4.500549 4.698000
H 5.395218 3.740136 5.074074
C 2.284367 -0.021222 3.382152
C 2.720570 -1.270279 3.814392
C 2.212240 0.243680 2.005484
C 3.053851 -2.268742 2.896497
H 2.818322 -1.474283 4.883789
C 2.545096 -0.732792 1.086509
H 1.901415 1.231822 1.655690
C 2.955305 -2.006991 1.524618
H 3.398411 -3.235095 3.263975
H 2.493036 -0.549368 0.012354
O 3.194667 -2.902645 0.560241
C 3.713722 -4.171449 0.895687
H 3.872458 -4.701009 -0.049945
H 4.675100 -4.083149 1.426434
H 3.006097 -4.746775 1.516734
Cl -1.049430 0.050181 6.809204
Au -0.951040 -0.481561 4.598853
Cl -1.750308 -2.557644 5.089721
N -0.831711 -1.037907 2.570194
C -0.306194 -2.230705 2.253965
C -1.242144 -0.207030 1.594852
C -0.150240 -2.628020 0.933875
H -0.005107 -2.877952 3.077217
C -1.118624 -0.537746 0.258025
H -1.677897 0.746018 1.895311
C -0.546865 -1.764977 -0.077323
H 0.299983 -3.594281 0.709412
H -1.463940 0.158689 -0.506871
C -0.303110 -2.109917 -1.536882
F -0.059407 -3.403200 -1.693053
F 0.750623 -1.425551 -1.980994
F -1.353233 -1.778621 -2.277652

44
A-(**1**-Me)
C -0.656033 1.913562 4.040251
C 0.477592 1.458616 4.183567
C 1.883587 1.028125 4.352899
H 1.989354 0.609319 5.369046
H -1.536479 2.534788 3.942412
C 3.824279 2.200288 4.952050
O 4.133626 1.265873 5.630821
O 2.647453 2.212921 4.247531
C 4.595237 3.461828 4.729473
H 4.878035 3.534461 3.669573
H 3.969564 4.332921 4.967144
H 5.493089 3.454112 5.355784
C 2.262845 -0.017589 3.329581
C 2.726389 -1.268400 3.726953
C 2.183235 0.281234 1.960871
C 3.076804 -2.235124 2.782169
H 2.832469 -1.497227 4.790259
C 2.531762 -0.664474 1.015975
H 1.850714 1.270844 1.636128
C 2.965893 -1.940937 1.418373

H 3.438775 -3.204467 3.123885
H 2.480318 -0.446970 -0.052040
O 3.218769 -2.809315 0.429012
C 3.766983 -4.072827 0.735126
H 3.938098 -4.577902 -0.221837
H 4.726770 -3.974866 1.267207
H 3.074027 -4.678524 1.343560
Cl -1.261386 0.404214 6.725979
Au -1.090592 -0.261966 4.552688
Cl -2.067734 -2.246068 5.095124
N -0.906250 -0.934272 2.583006
C -0.372377 -2.148442 2.355830
C -1.282996 -0.174718 1.540654
C -0.179415 -2.623146 1.073892
H -0.097703 -2.742505 3.227230
C -1.115363 -0.596033 0.233715
H -1.727156 0.796896 1.761310
C -0.534661 -1.841998 -0.031901
H 0.277143 -3.604524 0.939398
H -1.433625 0.059820 -0.577895
C -0.268687 -2.323832 -1.423142
H -0.796706 -3.270937 -1.609904
H -0.581808 -1.594661 -2.180332
H 0.807960 -2.521389 -1.541606

45
A-(**1**-OMe)
C -0.676938 1.699487 4.296429
C 0.502244 1.352523 4.337554
C 1.945542 1.038728 4.430951
H 2.141383 0.699959 5.463599
H -1.615771 2.236847 4.310584
C 3.821599 2.389824 4.826736
O 4.234844 1.540586 5.558566
O 2.610785 2.261011 4.192323
C 4.483614 3.678815 4.457393
H 4.725938 3.669156 3.384980
H 3.800918 4.520311 4.637114
H 5.400256 3.797229 5.044161
C 2.333533 -0.054006 3.460089
C 2.706569 -1.312550 3.923006
C 2.326726 0.196832 2.079467
C 3.050163 -2.330503 3.031261
H 2.746524 -1.509624 4.997539
C 2.673936 -0.799613 1.187015
H 2.059642 1.189386 1.707581
C 3.030001 -2.079326 1.654290
H 3.345109 -3.303155 3.424087
H 2.683808 -0.624018 0.110137
O 3.308590 -2.988135 0.712580
C 3.764591 -4.267865 1.091900
H 3.969057 -4.812287 0.163515
H 4.691754 -4.204267 1.684034
H 3.000260 -4.815139 1.669210
Cl -0.875719 -0.173015 6.827803
Au -0.872399 -0.551464 4.578051
Cl -1.634400 -2.665335 4.952458
N -0.833656 -0.954668 2.528939
C -0.307596 -2.120497 2.090443
C -1.306130 -0.077390 1.627512
C -0.232932 -2.430762 0.755066
H 0.059291 -2.812719 2.847613
C -1.271994 -0.311089 0.267682
H -1.733837 0.851259 2.006826
C -0.717037 -1.517599 -0.199137
H 0.216827 -3.367023 0.426465
H -1.678438 0.442739 -0.404544
O -0.611250 -1.859971 -1.463597
C -1.093644 -1.003367 -2.487408
H -0.893947 -1.518041 -3.432452
H -2.177133 -0.839575 -2.383148
H -0.560425 -0.040242 -2.476890

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TS-(**1**-CF_3)
C -0.488064 1.598478 4.368409
C 0.691572 1.248338 4.327438
C 2.150171 0.962281 4.303069
H 2.429818 0.688786 5.336182
H -1.419201 2.143650 4.455050
C 3.445796 2.839701 4.948734
O 3.421556 2.456626 6.078967
O 2.794919 2.160793 3.940640
C 4.141399 4.045768 4.405890
H 4.907057 3.731065 3.682561
H 3.424773 4.685026 3.872186
H 4.606904 4.598299 5.228350
C 2.464181 -0.158172 3.340765
C 2.770287 -1.430965 3.815919
C 2.423243 0.066766 1.955883
C 3.016298 -2.485787 2.933752
H 2.827093 -1.615965 4.892380
C 2.670901 -0.966752 1.072568
H 2.211502 1.068260 1.573787
C 2.957918 -2.259086 1.553667
H 3.260442 -3.468799 3.335795
H 2.644533 -0.812812 -0.007259
O 3.126009 -3.203315 0.620820
C 3.525860 -4.501707 1.003559
H 3.650478 -5.073242 0.077427
H 4.484061 -4.481520 1.546881
H 2.761571 -4.992361 1.630013
Cl -0.615275 -0.277156 6.874015
Au -0.684626 -0.649562 4.630565
Cl -1.449331 -2.757242 5.042937
N -0.709492 -1.057214 2.556608
C -0.280890 -2.252021 2.122433
C -1.097657 -0.124972 1.667390
C -0.202396 -2.549512 0.769478
H 0.004693 -2.982866 2.878236
C -1.048181 -0.352013 0.304261
H -1.453973 0.827698 2.058780
C -0.575841 -1.582013 -0.152332
H 0.173325 -3.521556 0.451319
H -1.374752 0.425377 -0.387189
C -0.406248 -1.825040 -1.642525
F -0.385548 -3.121167 -1.918631
F 0.746454 -1.290690 -2.046256
F -1.389153 -1.255539 -2.328215

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TS-(**1**-Me)
C -0.426787 1.738126 4.238884
C 0.726865 1.310182 4.265076
C 2.165163 0.936321 4.310263
H 2.367831 0.605306 5.344052
H -1.326005 2.339660 4.258051
C 3.455665 2.753184 5.116890
O 3.281717 2.368839 6.233992
O 2.902948 2.105988 4.034941
C 4.260380 3.931375 4.670859
H 5.085429 3.589799 4.029833
H 3.635086 4.608035 4.072252
H 4.656677 4.454250 5.547219
C 2.470802 -0.156769 3.316152
C 2.776892 -1.443926 3.748942
C 2.433573 0.113172 1.939484
C 3.027306 -2.468468 2.832680
H 2.828281 -1.664831 4.818696
C 2.684833 -0.889940 1.023564
H 2.219570 1.125743 1.589056
C 2.970727 -2.196742 1.461277
H 3.268696 -3.464554 3.202829
H 2.670437 -0.695633 -0.050040
O 3.142738 -3.110335 0.496593
C 3.535233 -4.420725 0.841430

H 3.663928 -4.965119 -0.100521
H 4.490262 -4.421988 1.390916
H 2.765646 -4.927488 1.448356
Cl -0.777162 -0.001578 6.822664
Au -0.769515 -0.480133 4.594741
Cl -1.673102 -2.520507 5.057930
N -0.733889 -0.978788 2.556812
C -0.310809 -2.201052 2.186071
C -1.098586 -0.097203 1.609594
C -0.226668 -2.566622 0.856503
H -0.038866 -2.894042 2.981452
C -1.035296 -0.403812 0.262510
H -1.448147 0.881176 1.940576
C -0.579103 -1.661702 -0.150492
H 0.142661 -3.562283 0.607686
H -1.341603 0.349138 -0.465118
C -0.453511 -2.033490 -1.594692
H -1.117236 -2.879232 -1.830175
H -0.707240 -1.198408 -2.259096
H 0.575979 -2.358212 -1.808872

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TS-(**1**-OMe)
C -0.462311 1.551844 4.412477
C 0.720433 1.217261 4.351721
C 2.182248 0.948554 4.337490
H 2.457044 0.707466 5.379869
H -1.400095 2.079647 4.524280
C 3.465435 2.850897 4.933949
O 3.449788 2.497688 6.074157
O 2.816404 2.144555 3.946296
C 4.150964 4.048550 4.358897
H 4.919957 3.720906 3.644897
H 3.429265 4.667106 3.807985
H 4.611547 4.626883 5.166270
C 2.522940 -0.196123 3.412299
C 2.769491 -1.466061 3.929178
C 2.568171 0.000820 2.024112
C 3.042777 -2.543983 3.084367
H 2.757011 -1.630439 5.010509
C 2.848006 -1.056463 1.178668
H 2.400373 0.998077 1.611336
C 3.077047 -2.344310 1.699215
H 3.236526 -3.523560 3.520462
H 2.898716 -0.922472 0.096980
O 3.292736 -3.309777 0.797905
C 3.624418 -4.609481 1.234477
H 3.799301 -5.204948 0.331751
H 4.540811 -4.605334 1.846470
H 2.802196 -5.064611 1.812176
Cl -0.473552 -0.475404 6.828975
Au -0.626151 -0.709138 4.565019
Cl -1.350110 -2.850711 4.856669
N -0.722264 -0.977960 2.493109
C -0.232326 -2.114493 1.949414
C -1.233294 -0.039176 1.678463
C -0.228490 -2.334485 0.593971
H 0.166037 -2.858183 2.638709
C -1.273744 -0.181685 0.306270
H -1.630575 0.864858 2.140997
C -0.754603 -1.356942 -0.269694
H 0.196709 -3.249411 0.182456
H -1.708542 0.617647 -0.291561
O -0.719577 -1.613493 -1.558338
C -1.250014 -0.687740 -2.494471
H -1.106007 -1.138385 -3.481420
H -2.324936 -0.526809 -2.320449
H -0.709500 0.270265 -2.448528

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B-(**1**-CF_3)
C 0.036884 1.168246 4.575773
C 1.293926 1.557910 4.503203

C	2.577268	0.761970	4.527924
H	2.755375	0.325862	5.522924
H	-0.765436	1.912471	4.616302
C	2.967064	2.984881	4.370834
O	1.688372	2.928304	4.430181
O	3.573301	1.866793	4.396567
C	3.683962	4.267383	4.303419
H	3.915280	4.577305	5.336094
H	4.629184	4.139656	3.762693
H	3.050189	5.033793	3.842832
C	2.716770	-0.260803	3.451361
C	2.982600	-1.588161	3.782977
C	2.478363	0.073195	2.106977
C	2.998634	-2.581801	2.805116
H	3.151457	-1.869125	4.825559
C	2.511948	-0.895482	1.125123
H	2.251166	1.105093	1.823321
C	2.758288	-2.240490	1.468553
H	3.188879	-3.612721	3.101127
H	2.325039	-0.656188	0.077313
O	2.706074	-3.113970	0.460570
C	2.979060	-4.479082	0.700111
H	2.903258	-4.983715	-0.269091
H	3.995353	-4.619126	1.101234
H	2.246531	-4.919252	1.397298
Cl	0.103858	-0.516510	6.972960
Au	-0.406800	-0.812361	4.764563
Cl	-0.890495	-3.076668	5.126122
N	-0.726671	-1.045336	2.687678
C	-0.466110	-2.230967	2.117094
C	-1.074723	-0.001799	1.913801
C	-0.507984	-2.404820	0.739754
H	-0.231108	-3.051678	2.797159
C	-1.137789	-0.099614	0.535548
H	-1.303974	0.937495	2.415578
C	-0.824451	-1.319341	-0.063468
H	-0.272740	-3.378346	0.311188
H	-1.426171	0.768340	-0.058140
C	-0.762412	-1.425760	-1.575574
F	-0.863227	-2.684359	-1.979570
F	-1.729745	-0.715557	-2.143673
F	0.407771	-0.942940	-2.003213

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B-(**1**-Me)

C	0.245901	1.035863	4.204261
C	1.473938	1.486620	4.378215
C	2.782733	0.777874	4.642826
H	2.852396	0.454217	5.692168
H	-0.566597	1.758748	4.076674
C	3.068337	3.008645	4.407372
O	1.795183	2.880497	4.344993
O	3.730328	1.930091	4.526793
C	3.716750	4.329015	4.367116
H	3.834152	4.678480	5.406143
H	4.714031	4.240930	3.920005
H	3.088911	5.045382	3.825332
C	3.095065	-0.344749	3.715222
C	3.271508	-1.626810	4.234983
C	3.028300	-0.175240	2.322348
C	3.323061	-2.738430	3.398977
H	3.298937	-1.778832	5.315954
C	3.111937	-1.265737	1.479934
H	2.883836	0.818921	1.890135
C	3.216339	-2.565869	2.014311
H	3.405372	-3.729315	3.842192
H	3.055597	-1.154190	0.396244
O	3.159281	-3.565602	1.130445
C	3.195937	-4.901773	1.591029
H	3.110520	-5.536569	0.702477
H	4.147286	-5.123201	2.100519
H	2.354085	-5.109378	2.271908
Cl	0.445442	-0.987921	6.416895

Au	-0.140104	-0.967300	4.196184
Cl	-0.465522	-3.289885	4.160479
N	-0.694904	-0.910937	2.191018
C	-0.174888	-1.802936	1.331744
C	-1.594062	-0.017045	1.744369
C	-0.522327	-1.808542	-0.008440
H	0.513238	-2.539153	1.744668
C	-1.994443	0.018689	0.421449
H	-2.011051	0.677692	2.474493
C	-1.455203	-0.889679	-0.500219
H	-0.061276	-2.549154	-0.663874
H	-2.734886	0.758171	0.112294
C	-1.889874	-0.900347	-1.933784
H	-2.778574	-1.542667	-2.043108
H	-2.164654	0.105052	-2.279530
H	-1.107136	-1.302990	-2.589879

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B-(**1**-OMe)

C	0.284468	1.025461	4.235167
C	1.511206	1.477367	4.416559
C	2.823349	0.770432	4.669974
H	2.898775	0.437680	5.715963
H	-0.528347	1.749242	4.114648
C	3.100246	3.005289	4.458481
O	1.827239	2.873288	4.400407
O	3.766926	1.928449	4.562096
C	3.743355	4.328785	4.430823
H	3.858933	4.669130	5.473031
H	4.740938	4.248974	3.982934
H	3.112698	5.047640	3.895634
C	3.135845	-0.342129	3.731111
C	3.327422	-1.626614	4.239700
C	3.049249	-0.163860	2.340350
C	3.370129	-2.732469	3.396112
H	3.370975	-1.785518	5.319040
C	3.124488	-1.248526	1.489748
H	2.893160	0.832302	1.916867
C	3.239021	-2.551736	2.014547
H	3.462258	-3.726008	3.831306
H	3.049960	-1.130700	0.407817
O	3.166676	-3.545934	1.126102
C	3.187294	-4.884639	1.580399
H	3.078482	-5.513719	0.690346
H	4.141912	-5.124577	2.075247
H	2.351304	-5.079642	2.272030
Cl	0.516382	-1.050253	6.403871
Au	-0.096750	-0.977915	4.190234
Cl	-0.409038	-3.300961	4.097712
N	-0.695032	-0.874199	2.204222
C	-0.179725	-1.733847	1.298745
C	-1.635292	-0.002499	1.808329
C	-0.566558	-1.722855	-0.020455
H	0.542689	-2.460004	1.668136
C	-2.094271	0.065137	0.506344
H	-2.050075	0.661091	2.568584
C	-1.549001	-0.811527	-0.448841
H	-0.131879	-2.426230	-0.730302
H	-2.869539	0.788401	0.259060
O	-1.891400	-0.851171	-1.720684
C	-2.901271	0.009736	-2.218597
H	-2.610778	1.065864	-2.105043
H	-3.003721	-0.224831	-3.282926
H	-3.860929	-0.174699	-1.711401

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[**3**-Au(III)]$^{+}$

N	10.188089	3.874007	4.794268
O	17.030370	7.889690	5.521335
N	9.860023	7.824350	6.114105
O	17.282441	5.176166	4.727019
C	16.049500	6.978057	5.707938
C	13.194533	9.271266	6.437519

H 12.945181 10.320809 6.268675
C 13.909067 5.167901 6.159606
C 17.420916 8.148960 4.178950
H 17.878446 7.266238 3.708667
H 18.150258 8.966252 4.219523
H 16.550899 8.464813 3.580335
C 12.181150 8.335109 6.767337
C 14.493879 8.846105 6.264744
H 15.280772 9.557778 6.013343
C 11.217119 2.979368 4.795871
C 12.585444 3.414854 5.141453
C 8.958652 10.287549 7.013658
H 8.611278 11.255756 7.378675
C 12.541087 7.028827 7.009370
H 11.792305 6.349172 7.408308
C 14.800799 7.461341 6.251911
C 12.754457 4.367053 6.120550
H 11.929103 4.566777 6.798573
C 15.023875 4.784316 5.391193
C 10.747639 8.682610 6.692233
C 10.288785 9.924287 7.147958
H 11.003078 10.591284 7.630770
C 8.562202 8.174062 5.989577
H 7.897749 7.444197 5.526413
C 10.966713 1.660628 4.397694
H 11.791465 0.948561 4.427505
C 13.798994 6.540395 6.614199
C 16.168634 5.664201 5.318677
C 18.459444 5.150123 5.523582
H 18.772748 6.164420 5.814216
H 19.240415 4.684213 4.911640
H 18.298304 4.545902 6.430551
C 8.073935 9.392774 6.415168
H 7.017766 9.624944 6.280761
C 9.700840 1.261980 4.000593
H 9.516764 0.229448 3.698383
C 14.930838 3.627454 4.575787
H 15.804962 3.325978 3.997931
C 13.715778 3.004358 4.388569
H 13.620486 2.233159 3.621531
C 8.952591 3.484712 4.414512
H 8.168217 4.241573 4.440225
C 8.668743 2.198099 4.003787
H 7.654047 1.942750 3.699449
Au 10.191254 5.869110 5.437925
Cl 9.224289 5.127216 7.419294
Cl 11.116612 6.605410 3.465467

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[**3**-Au(III)$^{+}$]$_2$
N 9.925150 1.889150 6.327019
O 17.383164 6.683821 6.346298
N 10.708642 9.849799 7.496649
O 16.726621 3.885684 5.878968
C 16.113859 6.186585 6.376175
C 14.317225 9.362410 7.210438
H 14.559288 10.394541 7.472935
C 13.405856 5.277137 6.387626
C 17.751391 7.357268 5.153823
H 17.699959 6.681872 4.283758
H 18.784538 7.700487 5.286308
H 17.101889 8.226532 4.960258
C 12.970752 8.977656 7.018327
C 15.325708 8.439727 7.051754
H 16.365017 8.735558 7.194876
C 10.427040 3.030565 5.805119
C 11.830279 3.448263 6.042150
C 11.091246 12.031676 5.858237
H 11.254698 12.897616 5.213932
C 12.680090 7.645196 6.765825
H 11.646955 7.356183 6.581716
C 15.042171 7.099039 6.693611
C 12.090761 4.774957 6.351348

H	11.250594	5.434473	6.570956
C	14.476279	4.386248	6.151053
C	11.909152	10.001013	6.891981
C	12.111319	11.116452	6.070607
H	13.076596	11.229956	5.576985
C	9.700475	10.719472	7.278759
H	8.760447	10.524830	7.796969
C	9.606159	3.805780	4.977042
H	10.019196	4.716556	4.544431
C	13.693949	6.678755	6.640201
C	15.852177	4.858467	6.136128
C	18.132029	4.054409	5.796172
H	18.408641	4.710504	4.959670
H	18.528442	3.050914	5.602840
H	18.542265	4.431130	6.739537
C	9.850345	11.819312	6.459113
H	9.012306	12.499874	6.310039
C	8.313337	3.400519	4.681508
H	7.682522	4.006658	4.028697
C	14.201538	3.031734	5.867952
H	15.033807	2.359467	5.667353
C	12.907211	2.568586	5.794890
H	12.726669	1.535875	5.495777
C	8.676680	1.473135	6.031450
H	8.349036	0.535251	6.481912
C	7.840627	2.199388	5.208054
H	6.839964	1.826271	4.990952
N	9.935233	7.281477	10.573694
O	17.896489	3.746819	8.921699
N	11.726263	-0.470944	9.128663
O	16.910067	6.410490	9.562372
C	16.585654	4.032735	9.164988
C	15.189608	0.595544	8.668829
H	15.534733	-0.388595	8.344511
C	13.823990	4.494733	9.731822
C	18.608484	3.162407	9.999963
H	18.630461	3.835438	10.873117
H	19.633126	2.988590	9.649756
H	18.162736	2.202989	10.309409
C	13.868116	0.762144	9.142026
C	16.047331	1.670848	8.630723
H	17.068166	1.543704	8.270312
C	10.710814	6.244177	10.960645
C	12.082238	6.052557	10.429288
C	12.787569	-2.535006	10.613744
H	13.218776	-3.352330	11.194892
C	13.425783	2.034698	9.471698
H	12.420266	2.156557	9.870302
C	15.632397	2.954505	9.062207
C	12.482099	4.779804	10.050025
H	11.731606	3.990319	9.999495
C	14.762833	5.549922	9.755658
C	13.034510	-0.416443	9.468119
C	13.579967	-1.470877	10.210022
H	14.632145	-1.418823	10.490262
C	10.939162	-1.488174	9.536033
H	9.893173	-1.456566	9.227816
C	10.215356	5.362591	11.929046
H	10.849581	4.537100	12.250916
C	14.274809	3.153562	9.400935
C	16.169378	5.305467	9.476275
C	18.310152	6.471372	9.346363
H	18.857411	5.881459	10.094158
H	18.571839	7.528500	9.470919
H	18.568602	6.150486	8.331249
C	11.431290	-2.535587	10.287437
H	10.763389	-3.339795	10.595429
C	8.964958	5.561692	12.494709
H	8.589397	4.874260	13.254907
C	14.339371	6.847329	10.113012
H	15.076707	7.647421	10.147172
C	13.031469	7.097918	10.461766
H	12.754346	8.092983	10.810356

C 8.725995 7.498244 11.130328
H 8.166084 8.363862 10.773804
C 8.207214 6.662624 12.098276
H 7.227558 6.875145 12.525800
Au 10.388586 8.511978 9.008373
Au 10.886841 0.772707 7.740828
Cl 11.634124 -0.706203 6.131028
Cl 9.890237 2.102395 9.373682
Cl 9.300598 7.010282 7.598240
Cl 11.207418 10.120264 10.450661

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[**3**-Au(III)$^{+}$]$_2$-a
N 10.359584 1.566221 4.964815
O 16.491216 7.103456 6.856125
N 9.710104 8.720661 8.000106
O 16.751274 4.431403 5.967864
C 15.447663 6.397545 6.361929
C 12.747455 8.898436 7.064545
H 12.632741 9.878036 7.536875
C 13.193505 5.047428 5.261760
C 17.530139 7.416412 5.933621
H 18.016318 6.506416 5.550862
H 18.261446 8.023242 6.479708
H 17.131285 7.999038 5.088198
C 11.622563 8.223144 6.546992
C 13.994077 8.317179 6.960548
H 14.879013 8.819694 7.351573
C 10.991817 2.272029 3.998042
C 12.236016 2.997942 4.367705
C 8.081974 9.340679 5.857421
H 7.448392 9.600248 5.007099
C 11.779889 7.011657 5.899411
H 10.887669 6.498907 5.541023
C 14.154179 7.042746 6.368734
C 12.118146 4.333052 4.704399
H 11.142928 4.806341 4.599837
C 14.443698 4.395438 5.376011
C 10.230910 8.689923 6.751597
C 9.416554 9.010206 5.663035
H 9.859210 9.003197 4.666673
C 8.413154 9.033523 8.199811
H 8.060356 9.039984 9.231570
C 10.429035 2.342168 2.725623
H 10.953538 2.906015 1.953712
C 13.034183 6.382897 5.811505
C 15.577873 5.103546 5.925789
C 17.337921 4.234379 7.244542
H 17.623102 5.186680 7.715151
H 18.231685 3.619598 7.086299
H 16.639294 3.700159 7.910615
C 7.566582 9.339856 7.151742
H 6.525230 9.586465 7.358140
C 9.227838 1.692643 2.460064
H 8.787009 1.737944 1.462267
C 14.568189 3.044693 4.974578
H 15.546479 2.569481 5.051241
C 13.478352 2.341568 4.501476
H 13.575882 1.289368 4.222944
C 9.198628 0.932101 4.723763
H 8.759524 0.372751 5.550956
C 8.597842 0.980463 3.478530
H 7.657372 0.454445 3.314430
N 12.297531 0.977277 8.531411
O 5.285251 5.353318 10.686735
N 11.738190 8.151354 11.516894
O 5.544195 2.753519 9.614190
C 6.464852 4.688353 10.672707
C 8.617530 7.414190 12.086052
H 8.534861 8.463679 12.378786
C 8.998148 3.383524 10.716387
C 4.278124 4.820968 11.541608
H 3.980025 3.808914 11.228715

H	3.418005	5.496748	11.471931
H	4.634199	4.790076	12.583615
C	9.860177	6.750388	12.171120
C	7.511162	6.724202	11.632523
H	6.536141	7.209316	11.578968
C	11.759714	1.028196	9.772138
C	10.376845	1.525390	9.961311
C	12.927706	8.042452	13.994651
H	13.391919	8.004282	14.982087
C	9.961099	5.420182	11.810092
H	10.937766	4.943308	11.875247
C	7.617830	5.380340	11.203377
C	10.239079	2.728794	10.628413
H	11.138272	3.212635	11.008461
C	7.868761	2.756023	10.140654
C	11.120320	7.466033	12.507487
C	11.711564	7.405759	13.767012
H	11.199189	6.858364	14.558637
C	12.913616	8.770926	11.720252
H	13.341381	9.310398	10.874093
C	12.551406	0.696724	10.874888
H	12.093764	0.719027	11.864224
C	8.866209	4.719273	11.273801
C	6.588101	3.427229	10.148491
C	4.911789	3.330182	8.482068
H	4.428468	4.287066	8.727732
H	4.154936	2.611237	8.147310
H	5.644580	3.493060	7.674034
C	13.543542	8.730611	12.951568
H	14.495990	9.243462	13.085306
C	13.880608	0.335542	10.703626
H	14.494967	0.066884	11.565157
C	8.008099	1.489556	9.526564
H	7.115049	1.006007	9.130497
C	9.242646	0.883556	9.422547
H	9.339257	-0.092237	8.938447
C	13.590661	0.633542	8.354706
H	13.958065	0.608425	7.328521
C	14.414724	0.315818	9.416839
H	15.452370	0.041341	9.227340
Au	10.796463	8.380980	9.715637
Au	11.253702	1.328845	6.789581
Cl	11.739961	-0.842333	6.149394
Cl	10.662682	3.485620	7.398022
Cl	10.314537	10.551410	10.360054
Cl	11.378563	6.224305	9.097731

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[4-Au(I)]$^{+}$

N	-2.306121	-1.057676	2.074585
N	-2.419562	-0.330641	-2.015197
C	0.260291	-4.726214	-0.986171
H	-0.630490	-4.211459	-1.342899
C	0.922912	-5.646648	-1.788491
H	0.544937	-5.867042	-2.788972
C	2.064172	-6.292299	-1.310633
H	2.588303	-7.013461	-1.941153
C	2.541511	-6.013006	-0.029262
H	3.440494	-6.510765	0.338978
C	1.883570	-5.091284	0.778976
H	2.261063	-4.859923	1.776262
C	0.733960	-4.442102	0.303495
C	0.036890	-3.494554	1.114035
C	-0.589449	-2.695934	1.780024
C	-1.346582	-1.837857	2.629850
C	-1.117334	-1.838214	4.009167
H	-0.331511	-2.475751	4.411988
C	-1.904661	-1.044585	4.831460
H	-1.742721	-1.035755	5.910915
C	-2.923071	-0.289008	4.266472
H	-3.586424	0.323825	4.875517
C	-3.109215	-0.321044	2.881893
C	-4.187188	0.399328	2.285504

C	-5.151405	0.968585	1.817487
C	-6.306657	1.583679	1.247629
C	-7.303325	2.118699	2.075704
H	-7.164766	2.098094	3.157799
C	-8.454923	2.671314	1.524304
H	-9.222704	3.088448	2.178247
C	-8.624936	2.699676	0.139037
H	-9.526354	3.138445	-0.292345
C	-7.641908	2.180210	-0.697788
H	-7.767116	2.212096	-1.781235
C	-6.476190	1.618192	-0.159249
C	-5.467937	1.081989	-1.016261
C	-4.589827	0.630677	-1.721672
C	-3.524471	0.220128	-2.579632
C	-3.611082	0.431189	-3.955817
H	-4.519539	0.868057	-4.368714
C	-2.528802	0.098982	-4.763588
H	-2.575360	0.257184	-5.842098
C	-1.381576	-0.411459	-4.178294
H	-0.499808	-0.659360	-4.767344
C	-1.348839	-0.616321	-2.793303
C	0.894872	-1.443259	-1.679138
C	2.130777	-1.824118	-1.069813
C	3.028330	-2.665107	-1.746941
H	2.785953	-3.017778	-2.750717
C	4.215578	-3.047787	-1.133095
H	4.913072	-3.700150	-1.661452
C	4.518204	-2.593649	0.151101
H	5.455805	-2.889718	0.625938
C	3.632110	-1.752127	0.825277
H	3.877473	-1.387586	1.824538
C	2.440840	-1.366121	0.221327
H	1.741528	-0.707982	0.739785
C	-0.167006	-1.111233	-2.167638
N	-2.455761	-5.842831	1.090968
N	-5.395243	-2.906497	0.923590
C	-5.850409	-5.958794	-3.185136
H	-6.251897	-5.745646	-2.193012
C	-6.661004	-5.874389	-4.311446
H	-7.712377	-5.600864	-4.204638
C	-6.135590	-6.151099	-5.574606
H	-6.776970	-6.090488	-6.456188
C	-4.796450	-6.517582	-5.712978
H	-4.389311	-6.740491	-6.700812
C	-3.978010	-6.607107	-4.592635
H	-2.929654	-6.892103	-4.694665
C	-4.500675	-6.323523	-3.320770
C	-3.663207	-6.390101	-2.164233
C	-2.968812	-6.429435	-1.167923
C	-2.184399	-6.610184	0.008749
C	-1.175736	-7.581464	0.040599
H	-0.987624	-8.173157	-0.854084
C	-0.445963	-7.767153	1.203320
H	0.348521	-8.513801	1.243948
C	-0.756077	-7.006793	2.325655
H	-0.232326	-7.143361	3.270984
C	-1.777502	-6.059979	2.246715
C	-2.167106	-5.327682	3.409155
C	-2.534290	-4.799709	4.438135
C	-2.999530	-4.175016	5.634625
C	-2.314776	-4.356449	6.844168
H	-1.426325	-4.989538	6.864142
C	-2.767324	-3.743202	8.008453
H	-2.228059	-3.895377	8.945039
C	-3.912934	-2.945949	7.982677
H	-4.271576	-2.474055	8.899091
C	-4.605845	-2.756653	6.791160
H	-5.504111	-2.137693	6.767657
C	-4.159319	-3.360594	5.607466
C	-4.840703	-3.122333	4.376033
C	-5.378074	-2.892970	3.312373
C	-5.999881	-2.534337	2.078954
C	-7.178874	-1.783916	2.078913

H -7.634905 -1.515099 3.030932
C -7.733549 -1.392269 0.868118
H -8.652508 -0.803616 0.845121
C -7.085014 -1.729333 -0.311686
H -7.462955 -1.412331 -1.282726
C -5.906194 -2.478926 -0.257256
C -5.191644 -2.778950 -1.453256
C -4.578043 -2.951275 -2.486278
C -3.794066 -3.156500 -3.662339
C -4.338924 -2.981743 -4.943282
H -5.385921 -2.694127 -5.051080
C -3.544404 -3.193082 -6.065761
H -3.971403 -3.065887 -7.062250
C -2.210898 -3.579519 -5.922200
H -1.595460 -3.748239 -6.808280
C -1.665722 -3.755620 -4.649515
H -0.620737 -4.050886 -4.534071
C -2.452951 -3.544288 -3.524745
H -2.048612 -3.674684 -2.521701
Au -2.383872 -0.770146 0.014297
Au -3.871591 -4.326586 0.973629

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[**4**-Au(I)$^{+}$]$_2$
Au 6.966159 10.514544 6.875666
Au 7.059618 10.138538 10.304908
C 6.108300 3.534789 8.104562
H 6.399473 2.485746 8.179327
N 5.043542 10.593242 10.446859
N 9.077603 9.677380 10.231789
C 9.545016 15.545158 8.596524
H 10.518974 15.357780 8.142862
C 3.279163 12.212261 10.326969
H 2.979885 13.241061 10.130079
C 4.826165 3.878617 7.679611
H 4.109346 3.100850 7.411051
N 8.980960 10.054071 6.735342
N 4.950141 10.984787 6.950253
C 6.694171 5.016708 4.679956
H 7.666037 4.599592 4.948964
C 4.642276 8.330168 11.073964
C 9.192550 16.828819 8.996875
H 9.900347 17.649160 8.866716
C 3.164143 12.558152 6.666143
H 2.857734 13.571848 6.410073
C 2.358466 11.242388 10.709129
H 1.303645 11.499728 10.822190
C 7.369223 14.986546 5.698689
C 2.239007 11.574558 6.986082
H 1.171880 11.804489 6.990474
C 7.019944 4.528237 8.442652
H 8.018412 4.263405 8.792568
C 6.664478 5.881601 8.361244
C 4.952798 7.589200 7.762105
C 9.124921 12.789398 11.802409
C 4.457749 5.215875 7.588421
H 3.461629 5.490068 7.239021
C 6.482248 6.401560 4.772155
C 9.993602 10.529568 10.753029
C 9.381677 8.901881 6.144821
C 5.062131 7.212110 11.294477
C 6.938581 5.764972 11.920337
H 7.554120 6.655619 12.059384
C 2.791350 9.946663 10.952845
H 2.103088 9.161109 11.263100
C 4.624841 11.859214 10.202425
C 5.596219 5.907555 11.530161
C 8.648367 14.478405 8.747277
C 7.377279 14.718134 9.322367
C 7.937468 17.066624 9.554366
H 7.658908 18.072913 9.871647
C 9.524994 11.749909 11.318245
C 4.151800 9.642600 10.818492

C 9.040771 13.189860 8.272132
C 7.522359 7.264183 5.237560
C 11.268947 10.674678 7.094629
H 11.979515 11.406509 7.477069
C 5.365134 6.230994 7.921246
C 2.680581 10.292034 7.293649
H 1.986103 9.491551 7.546030
C 9.475339 8.499127 9.692169
C 6.348330 14.039845 6.021343
C 11.357834 10.213399 10.741082
H 12.066453 10.916496 11.177596
C 10.824084 8.137322 9.660417
H 11.106572 7.179148 9.225831
C 4.527193 12.236994 6.650275
C 6.436061 13.669742 9.557088
C 5.607724 12.826959 9.834592
C 11.687705 9.494821 6.488841
H 12.752518 9.279057 6.382615
C 4.547746 8.714262 7.553528
C 10.742290 8.597043 6.013605
H 11.029973 7.666900 5.524613
C 4.794029 4.768511 11.356006
H 3.751233 4.882758 11.055376
C 9.426013 12.140256 7.799559
C 7.621684 6.860731 8.767816
C 4.050637 10.021562 7.267815
C 7.467390 4.496561 12.129175
H 8.507122 4.386027 12.442874
C 5.665002 4.186927 4.248063
H 5.832371 3.111038 4.171650
C 8.378120 8.017116 5.656784
C 5.509975 13.210806 6.312579
C 7.037346 16.019698 9.716131
H 6.061237 16.197696 10.168961
C 9.900618 10.931932 7.205909
C 4.211764 6.104911 3.992483
H 3.244852 6.526489 3.711357
C 8.468334 7.628503 9.176640
C 5.333309 3.504015 11.566820
H 4.707325 2.619418 11.436367
C 11.769724 9.006251 10.194409
H 12.827908 8.738156 10.188911
C 6.666994 3.366372 11.952303
H 7.083469 2.372051 12.125810
C 9.596426 15.453446 4.878602
H 10.542769 15.106450 4.459441
C 8.592363 14.538097 5.172054
H 8.741008 13.471350 4.994852
C 9.390424 16.815510 5.105703
H 10.178239 17.532469 4.865764
C 7.165014 16.357439 5.922686
H 6.212955 16.702745 6.329137
C 5.233343 6.943111 4.423576
H 5.078547 8.021454 4.491943
C 4.425684 4.728025 3.905098
H 3.623608 4.073666 3.557629
C 8.176535 17.264749 5.626230
H 8.014888 18.330814 5.795769
C 6.786248 15.242243 13.342053
H 5.765770 15.275644 13.728299
C 7.294764 14.053291 12.832202
H 6.681894 13.150421 12.805997
C 8.613029 14.007183 12.347909
C 9.412077 15.161077 12.384433
H 10.436322 15.121193 12.010001
C 8.893133 16.345737 12.895777
H 9.516816 17.240906 12.928437
C 7.583123 16.388201 13.373641
H 7.183045 17.318106 13.782867

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[**4**-I(I)]$^+$
I -2.199888 -0.709502 0.008119

N	-2.183169	-1.127775	2.291181
N	-2.343386	-0.185387	-2.200584
C	0.196992	-4.719212	-0.874448
H	-0.692328	-4.162338	-1.169148
C	0.781116	-5.636860	-1.739146
H	0.340152	-5.811607	-2.722671
C	1.918838	-6.341375	-1.343860
H	2.380249	-7.060503	-2.023846
C	2.472157	-6.124200	-0.081404
H	3.368917	-6.667395	0.222627
C	1.891008	-5.209550	0.791586
H	2.324854	-5.032040	1.776981
C	0.743572	-4.502520	0.400578
C	0.103065	-3.578291	1.284429
C	-0.504594	-2.802435	1.993602
C	-1.275475	-1.958840	2.849101
C	-1.122012	-2.023097	4.238885
H	-0.377873	-2.699395	4.658009
C	-1.933391	-1.239829	5.048520
H	-1.832606	-1.281258	6.134752
C	-2.898731	-0.428594	4.465069
H	-3.575791	0.176977	5.066547
C	-3.011137	-0.397322	3.071663
C	-4.035394	0.384121	2.449303
C	-4.948968	1.013510	1.956272
C	-6.058790	1.719483	1.395528
C	-7.024152	2.272211	2.249867
H	-6.887407	2.188516	3.329211
C	-8.141108	2.919825	1.732009
H	-8.882238	3.348027	2.409159
C	-8.308481	3.028616	0.350816
H	-9.181218	3.541866	-0.056714
C	-7.356530	2.494122	-0.511635
H	-7.478467	2.588149	-1.591912
C	-6.225219	1.836050	-0.007302
C	-5.266261	1.289481	-0.916265
C	-4.456286	0.835610	-1.698263
C	-3.479555	0.401222	-2.648890
C	-3.679225	0.614484	-4.013803
H	-4.604999	1.081763	-4.347670
C	-2.684635	0.241106	-4.912808
H	-2.823442	0.401299	-5.983188
C	-1.506976	-0.313845	-4.436776
H	-0.694838	-0.597007	-5.104948
C	-1.354711	-0.521765	-3.060006
C	0.886904	-1.475302	-2.047025
C	2.085144	-1.908551	-1.398918
C	2.966699	-2.802988	-2.026499
H	2.743381	-3.168128	-3.030294
C	4.117597	-3.217007	-1.365774
H	4.804136	-3.909671	-1.855798
C	4.399883	-2.741747	-0.084324
H	5.310947	-3.061654	0.425482
C	3.527898	-1.850903	0.542284
H	3.755841	-1.472218	1.540374
C	2.372108	-1.433462	-0.107997
H	1.684926	-0.734626	0.371887
C	-0.154547	-1.073989	-2.526570
I	-3.997152	-4.410066	0.874993
N	-2.444017	-6.051076	1.135013
N	-5.606261	-2.733148	0.790112
C	-5.539184	-6.093853	-3.204078
H	-5.938969	-5.906380	-2.206116
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7. Spectroscopic Data

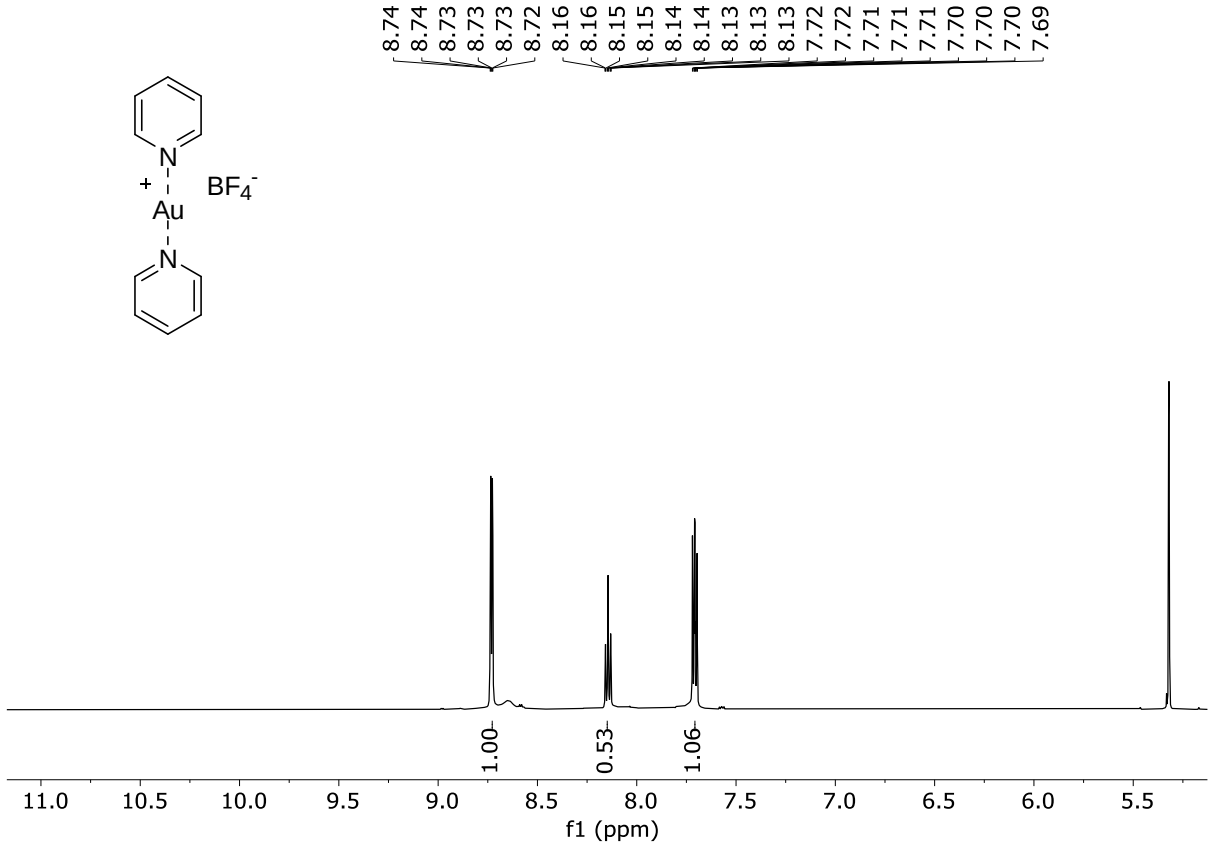

Figure S21. The ^{1}H NMR spectrum of [(**1**-H)$_2$-Au(I)]BF$_4$ acquired at 25 ^{o}C in CD_2Cl_2 at 600 MHz.

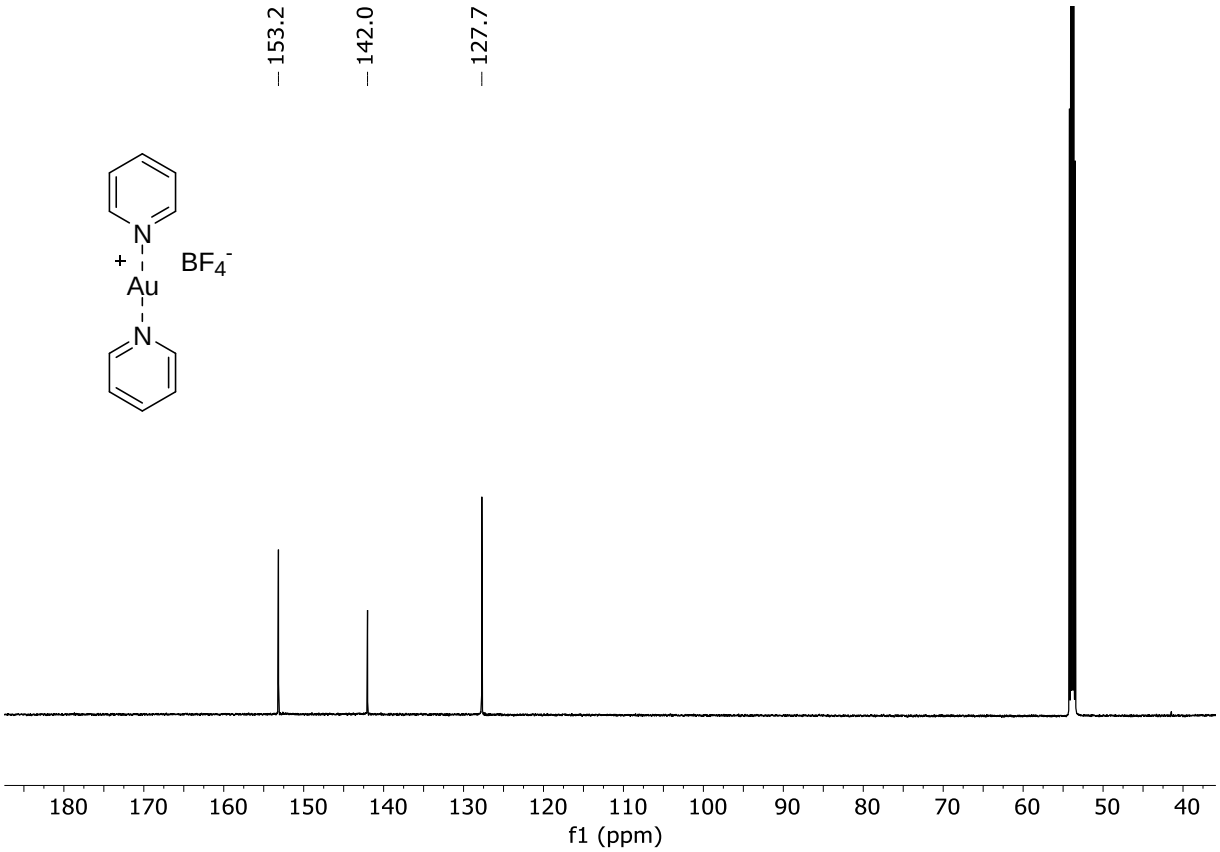

Figure S22. The ^{13}C NMR spectrum of [(**1**-H)$_2$-Au(I)]BF$_4$ acquired at 25 ^{o}C in CD_2Cl_2 at 151 MHz.

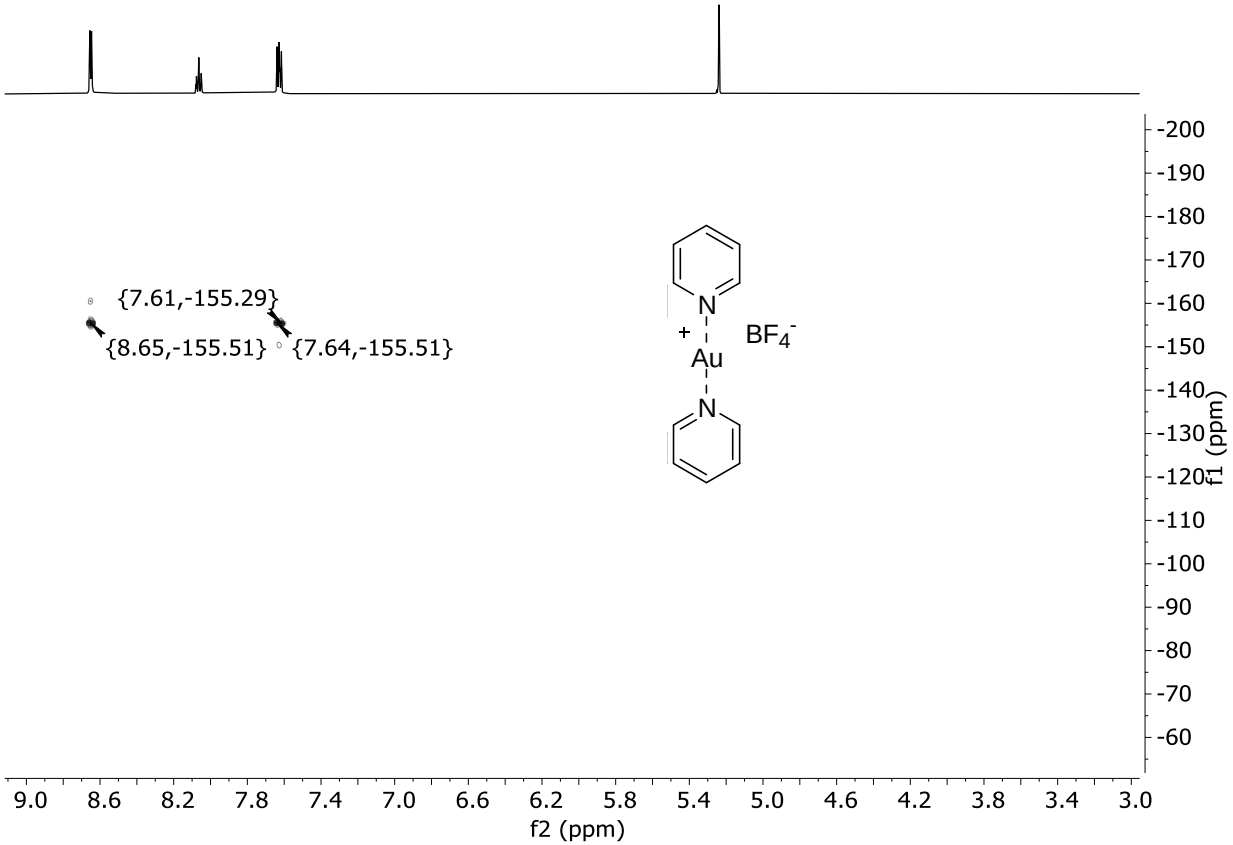

Figure S23. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**1**-H)$_2$-Au(I)]BF_4 acquired at 25 ^{o}C in CD_2Cl_2 at 61 MHz.

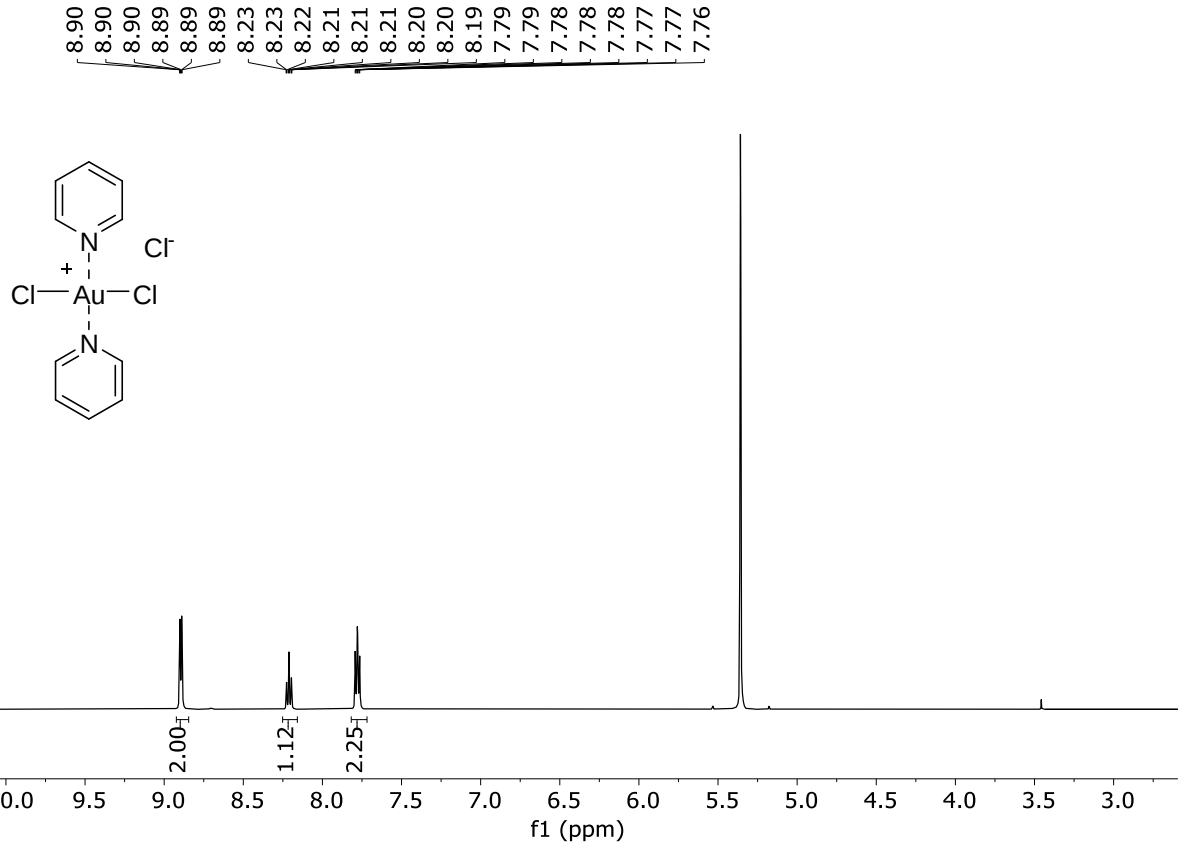

Figure S24. The ^{1}H NMR spectrum of [(**1**-H)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 500 MHz.

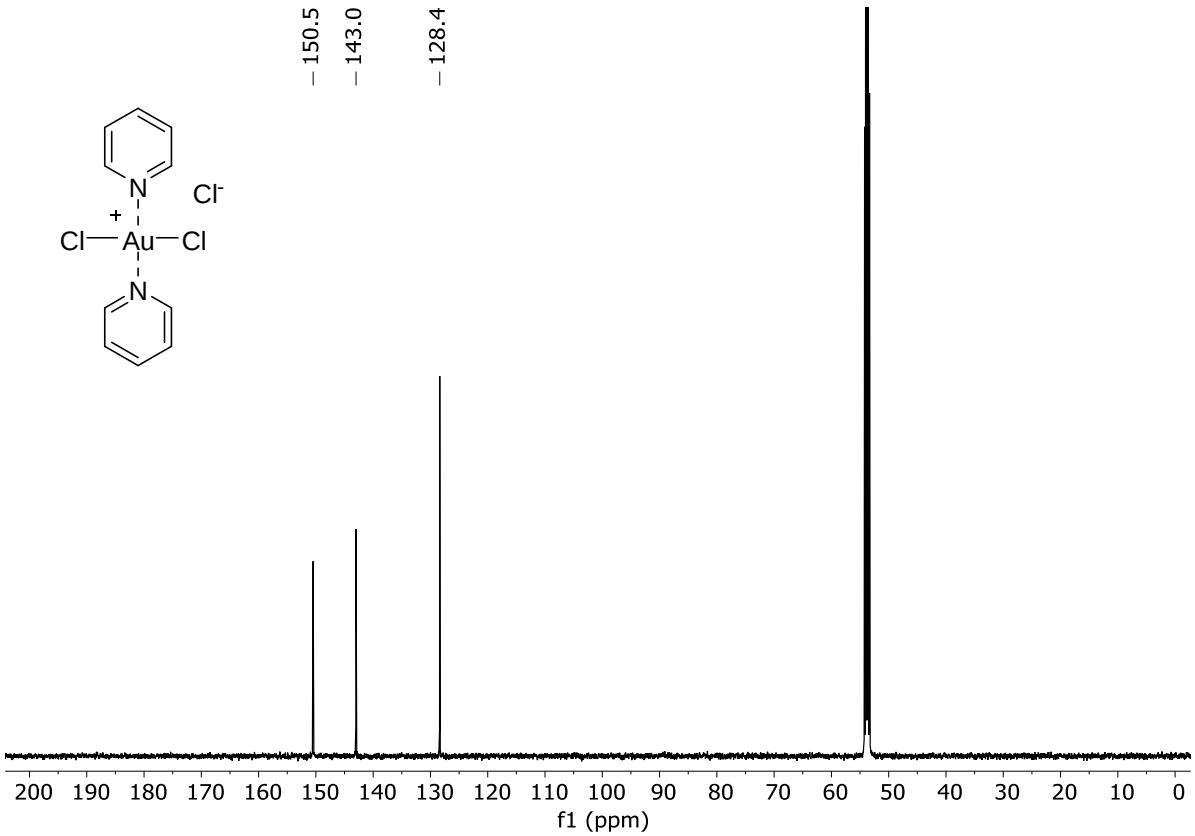

Figure S25. The ^{13}C NMR spectrum of [(**1**-H)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 126 MHz.

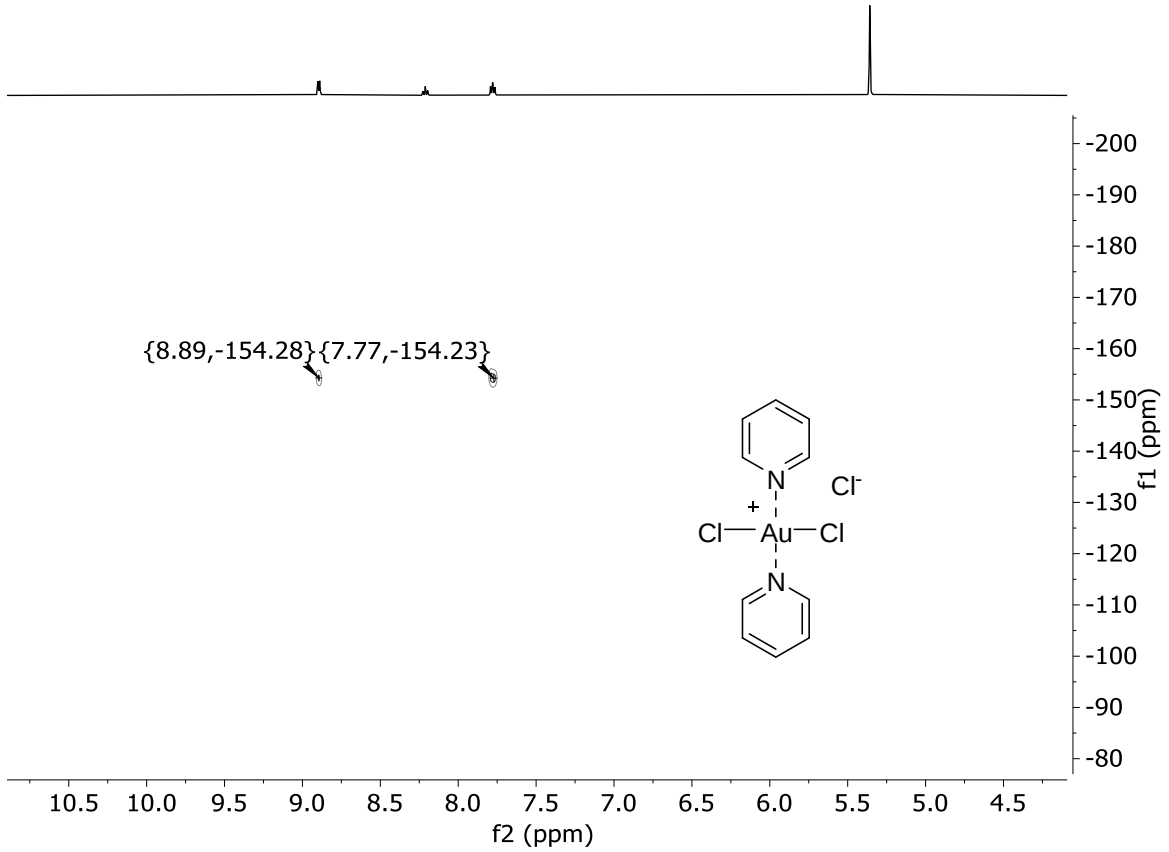

Figure S26. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**1**-H)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 51 MHz

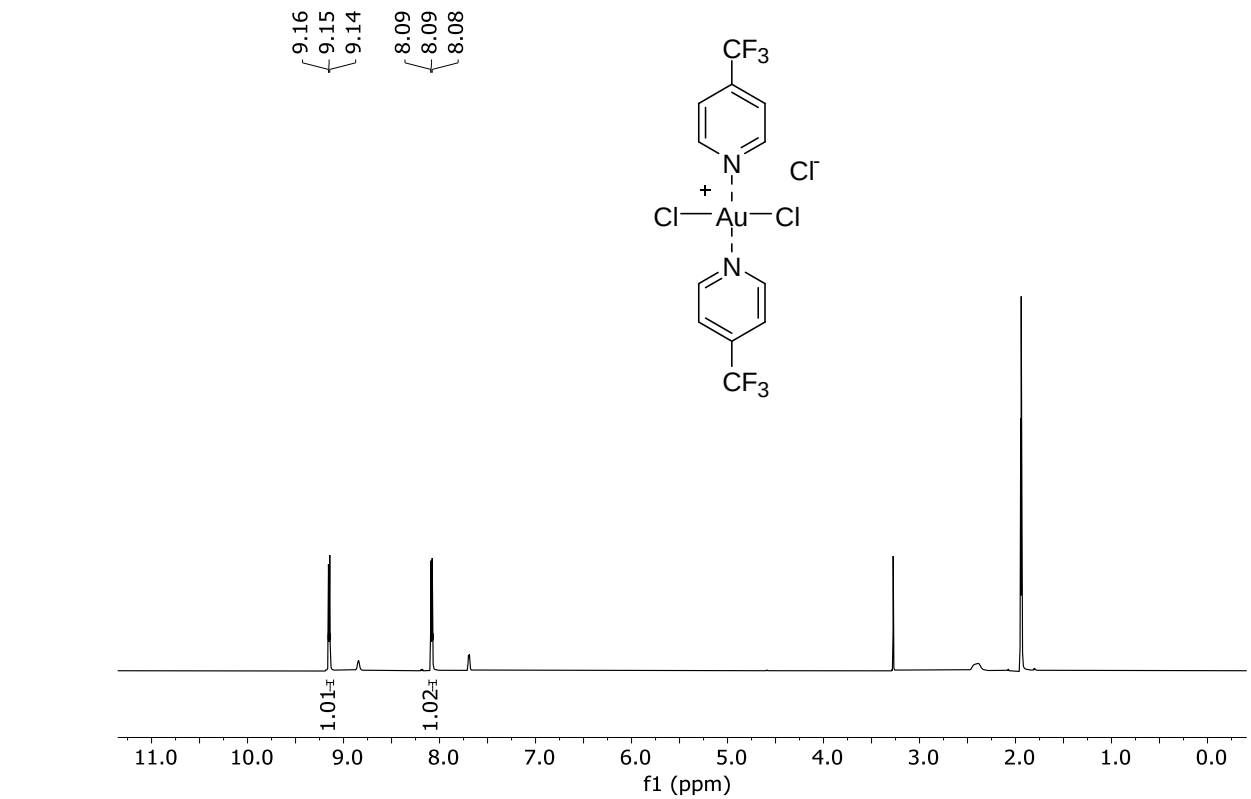

Figure S27. The ^{1}H NMR spectrum of [(**1**-CF_3)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 500 MHz.

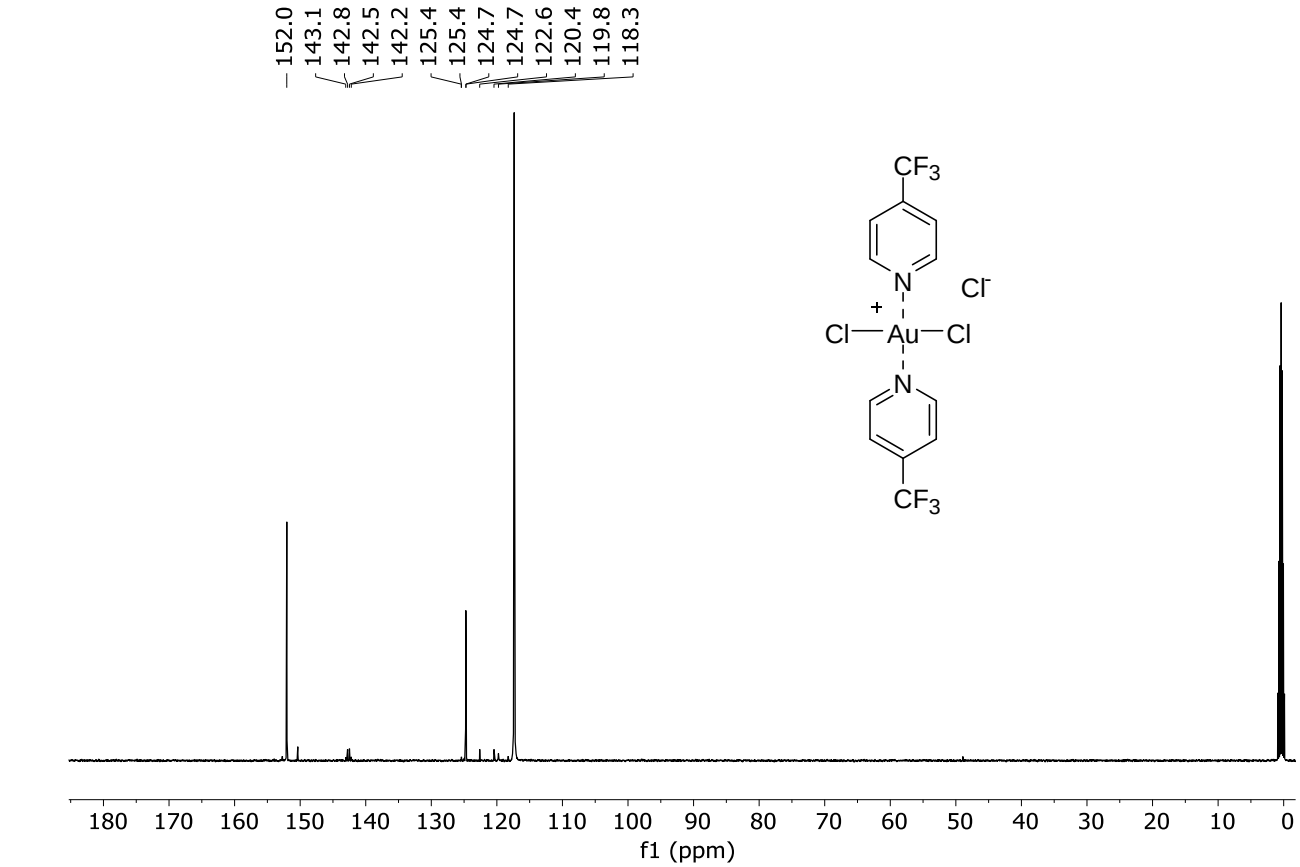

Figure S28. The ^{13}C NMR spectrum of [(**1**-CF_3)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 126 MHz.

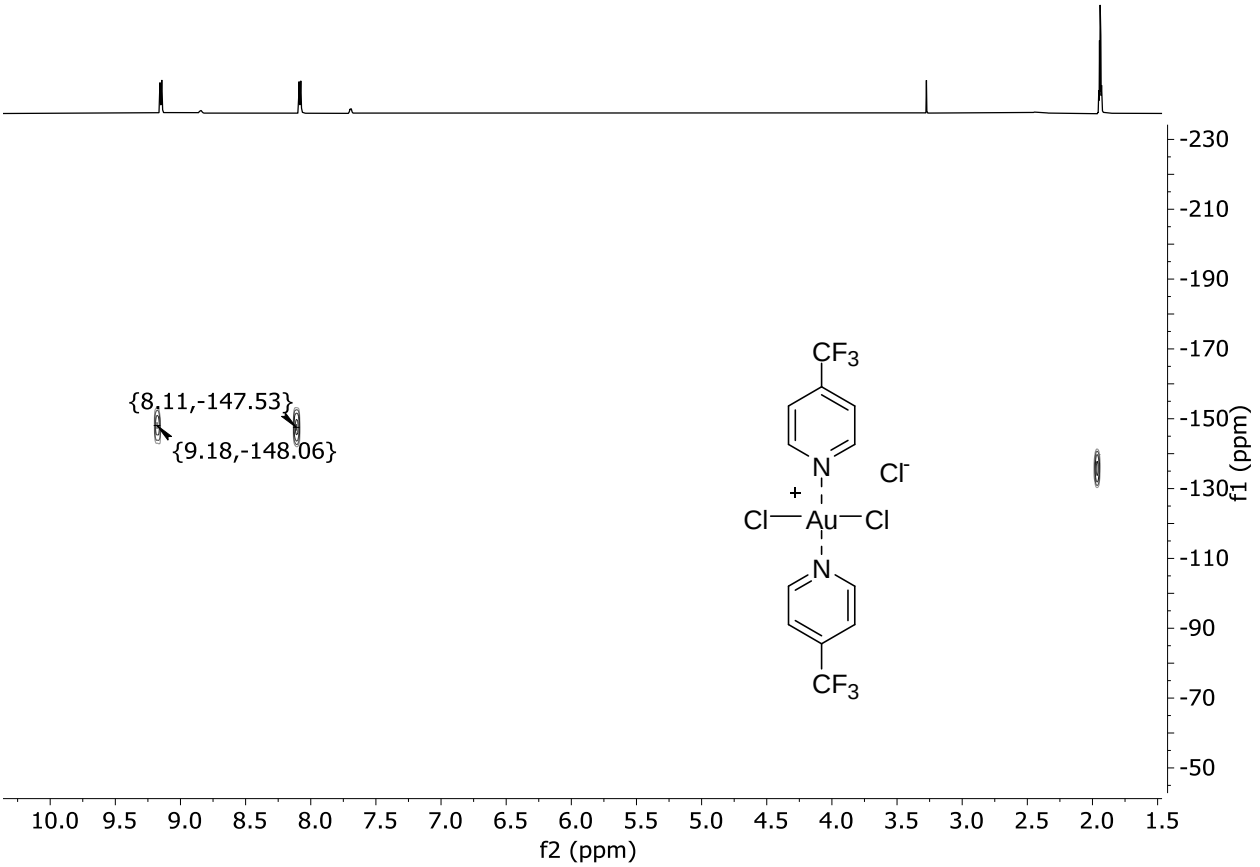

Figure S29. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**1**-CF_3)$_2$-Au(III)]Cl acquired at 25 ºC in CD_2Cl_2 at 51 MHz

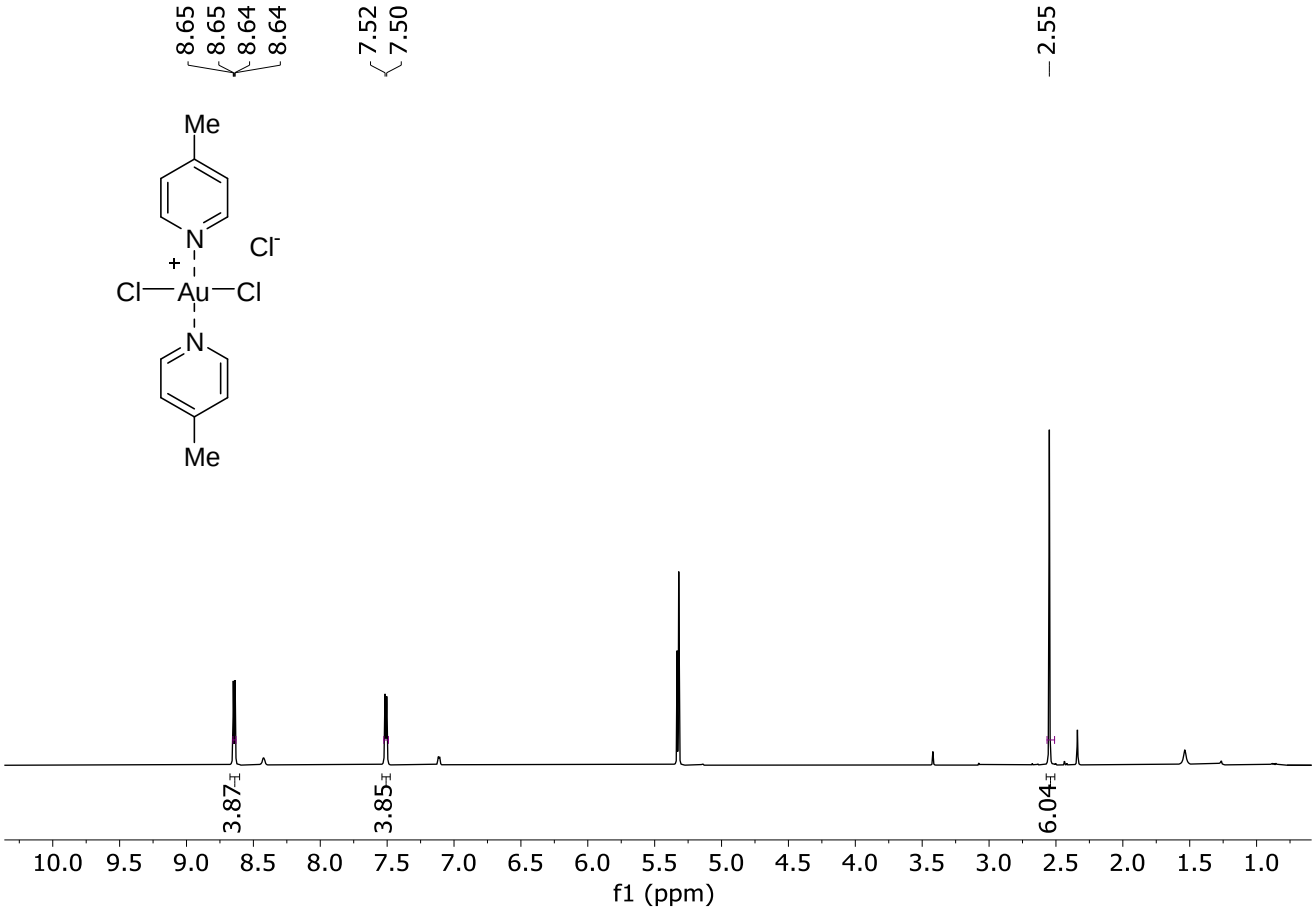

Figure S30. The ^{1}H NMR spectrum of [(**1**-CH_3)$_2$-Au(III)]Cl acquired at 25 ºC in CD_2Cl_2 at 500 MHz.

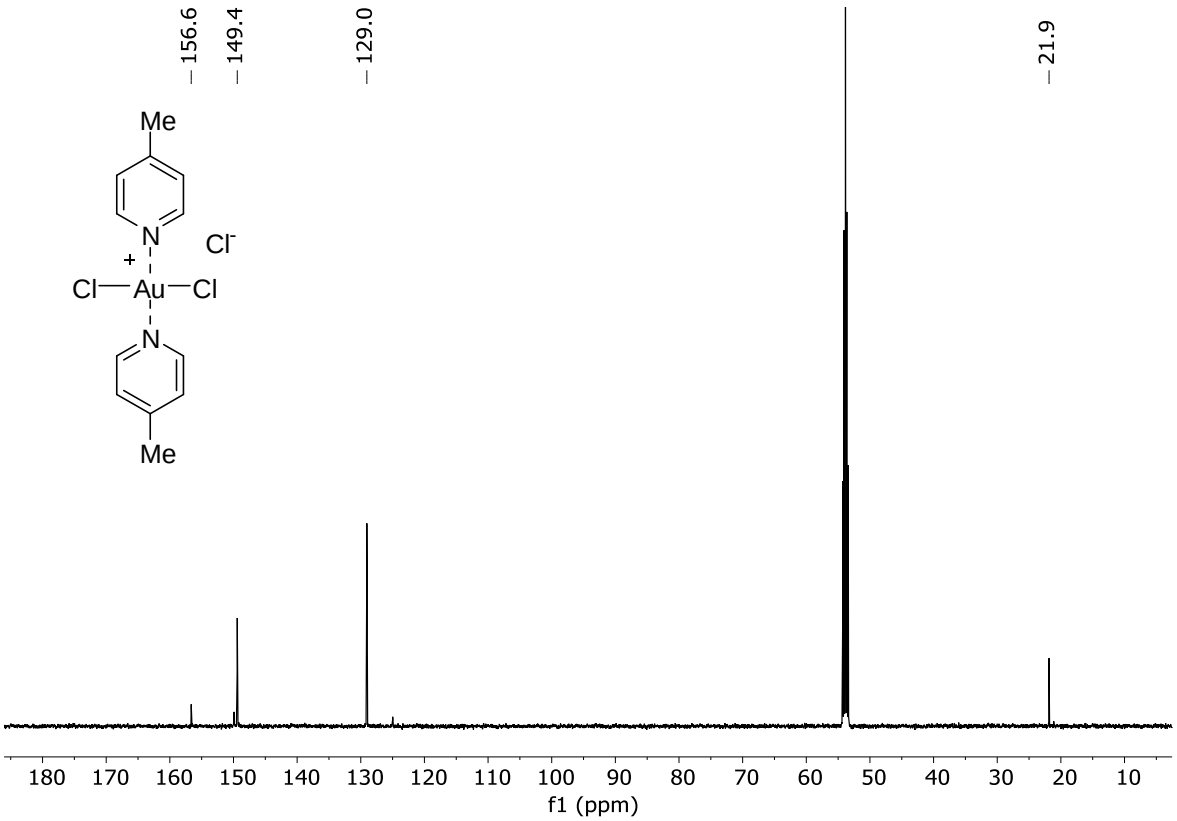

Figure S31. The ^{13}C NMR spectrum of [(**1**-CH_3)$_2$-Au(III)]Cl acquired at 25 ºC in CD_2Cl_2 at 126 MHz.

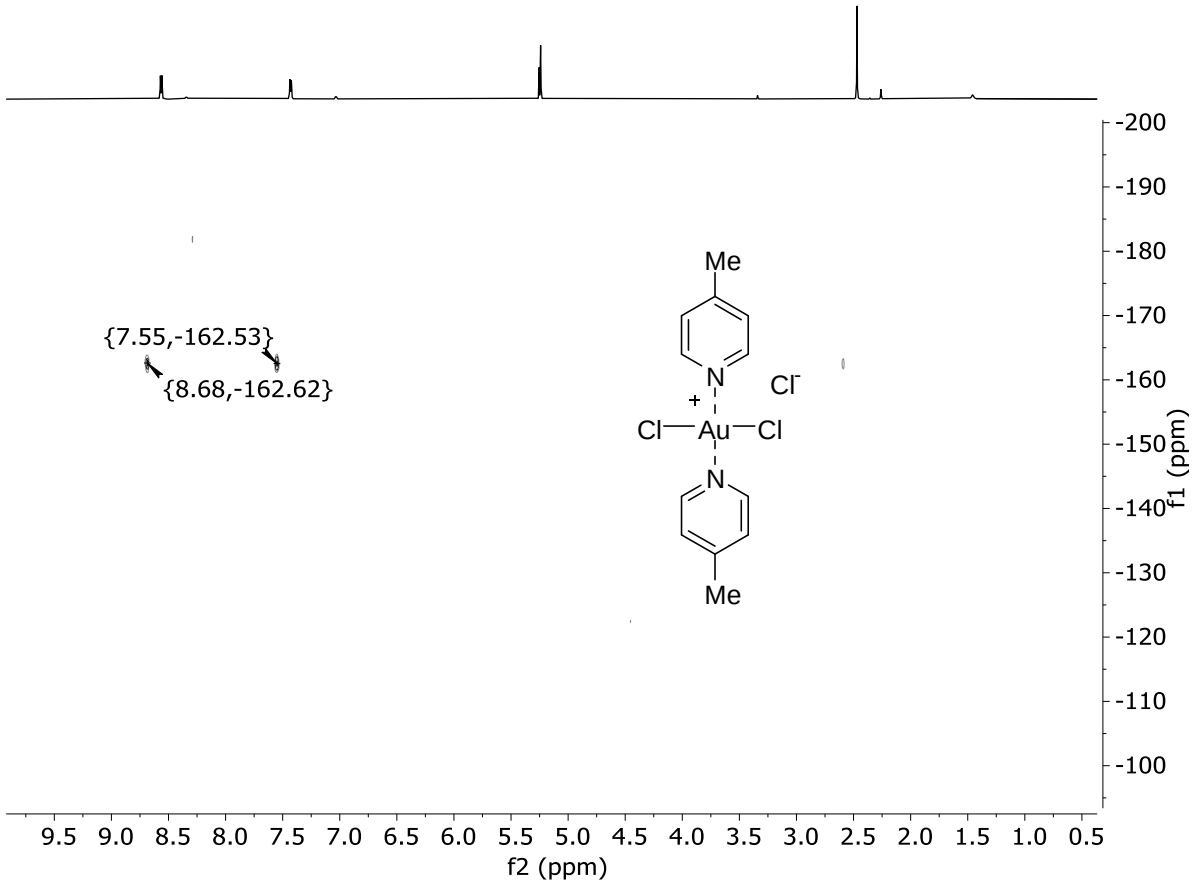

Figure S32. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**1**-CH_3)$_2$-Au(III)]Cl acquired at 25 ºC in CD_2Cl_2 at 51 MHz.

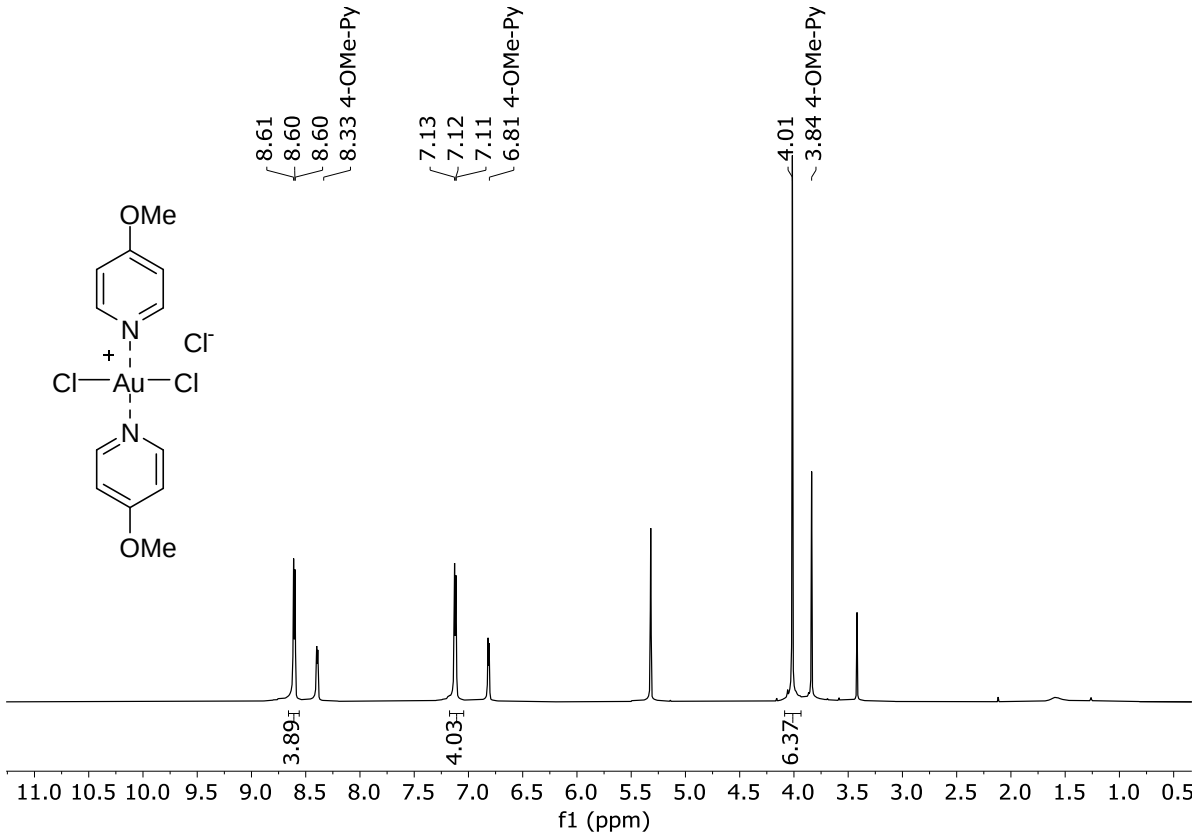

Figure S33. The ^{1}H NMR spectrum of [(**1**-OMe)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 500 MHz.

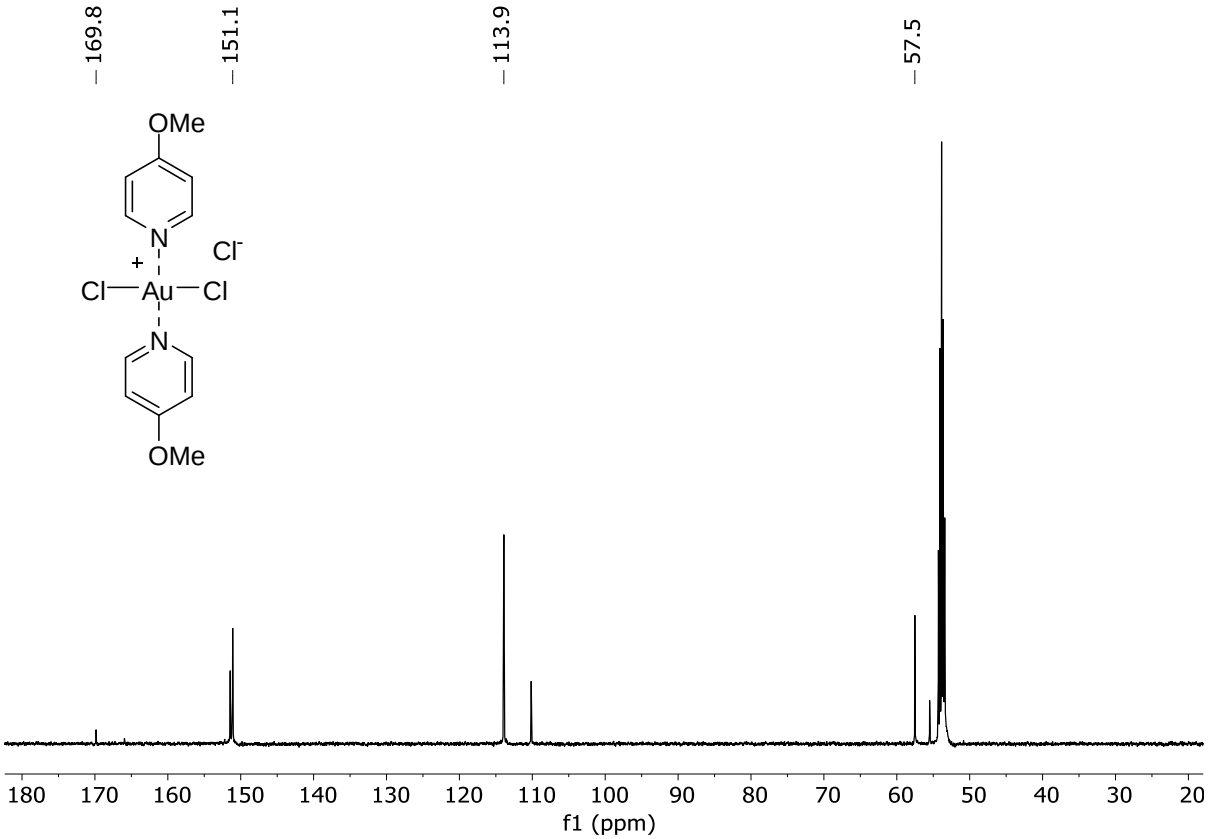

Figure S34. The ^{13}C NMR spectrum of [(**1**-OMe)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 126 MHz.

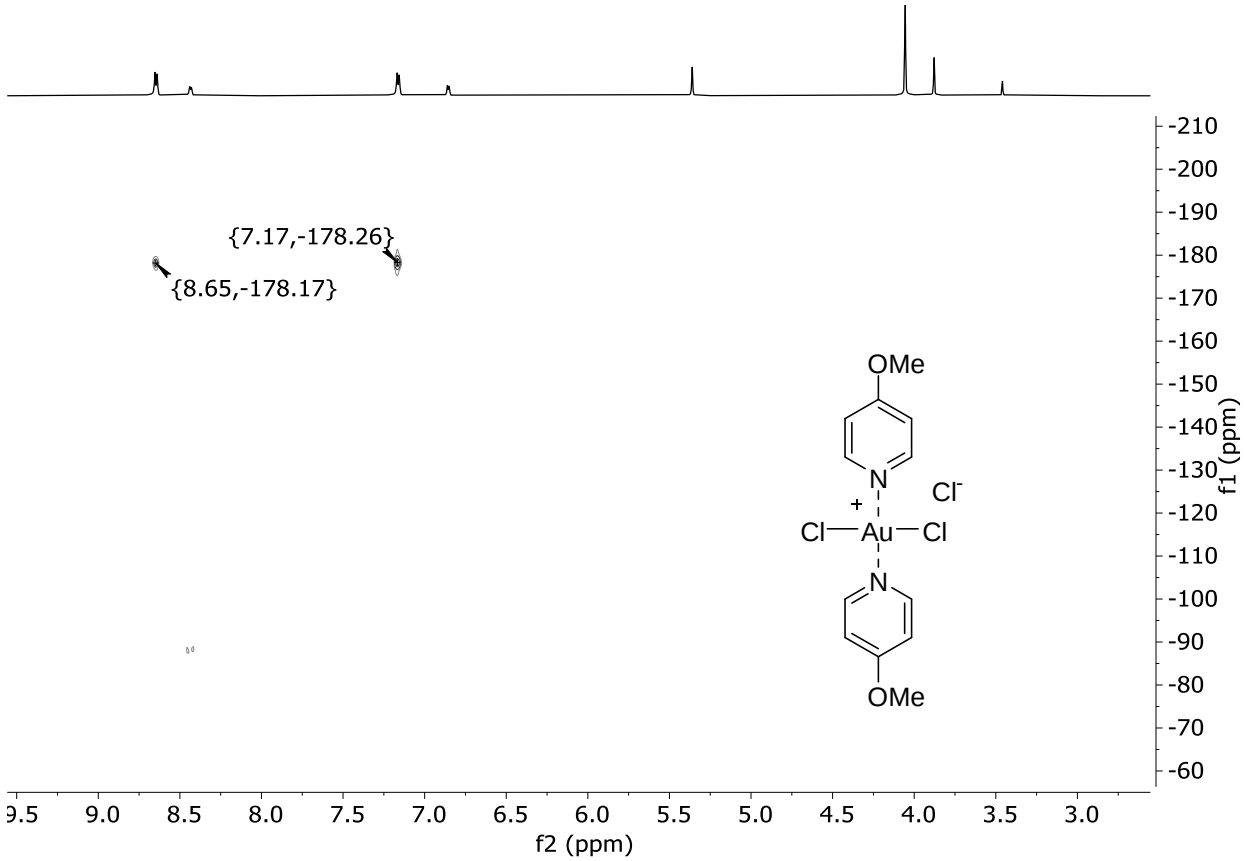

Figure S35. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**1**-OMe)$_2$-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 51 MHz

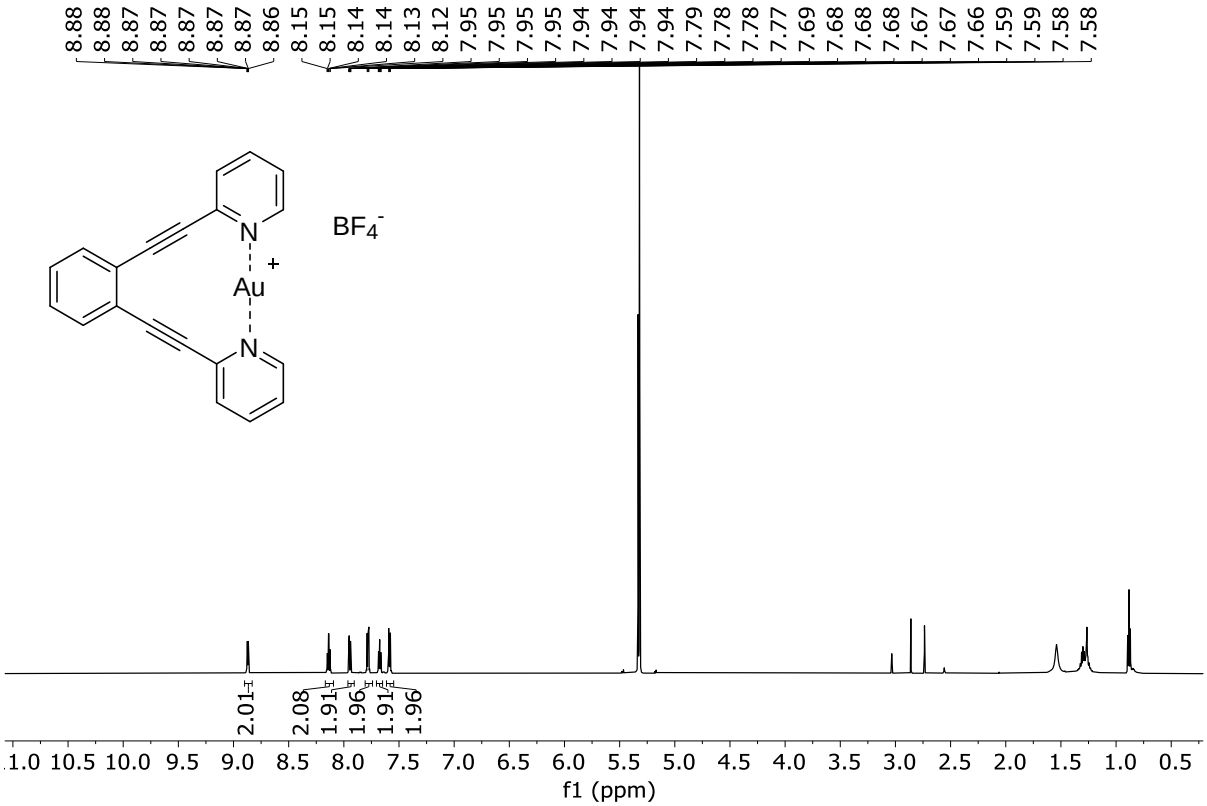

Figure S36. The ^{1}H NMR spectrum of [(**2**-H)-Au(I)]BF_4 acquired at 25 ^{o}C in CD_2Cl_2 at 600 MHz.

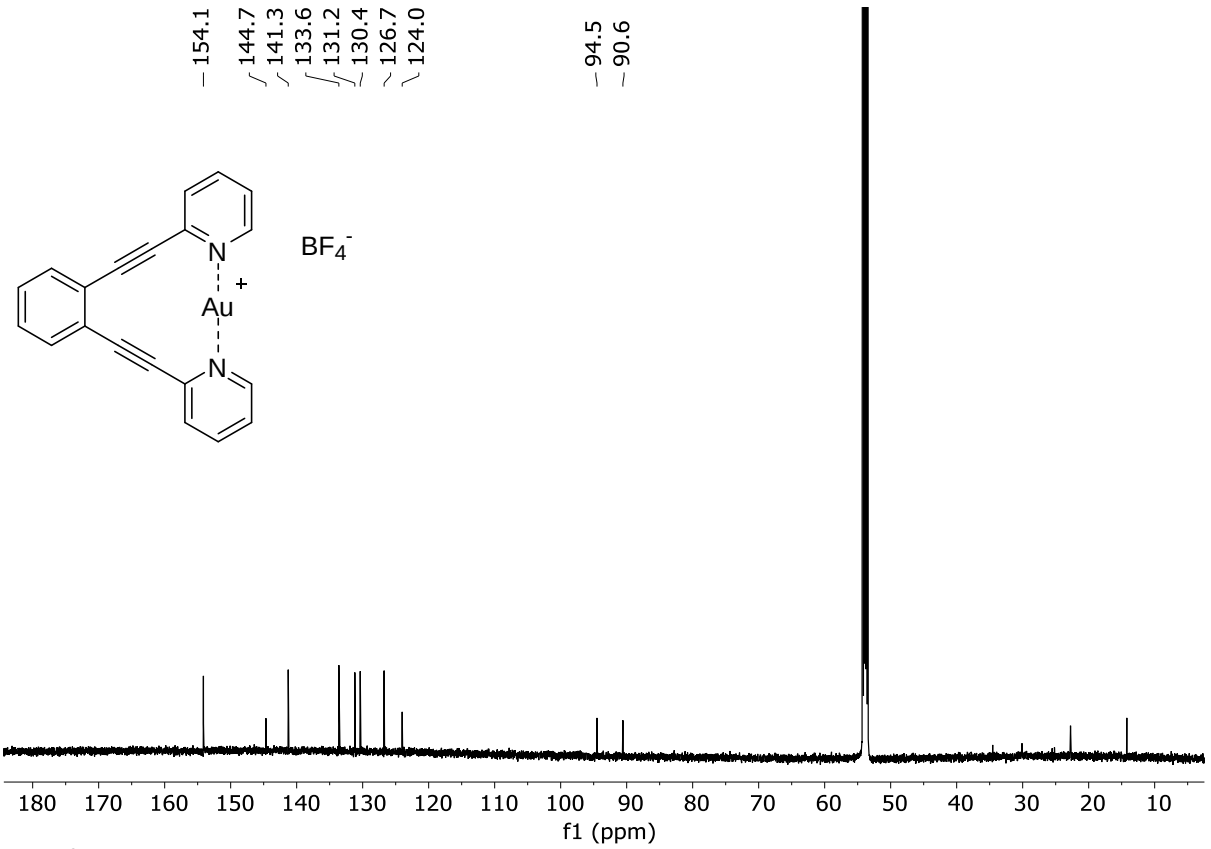

Figure S37. The ^{13}C NMR spectrum of [(**2**-H)-Au(I)]BF_4 acquired at 25 ºC in CD_2Cl_2 at 151 MHz.

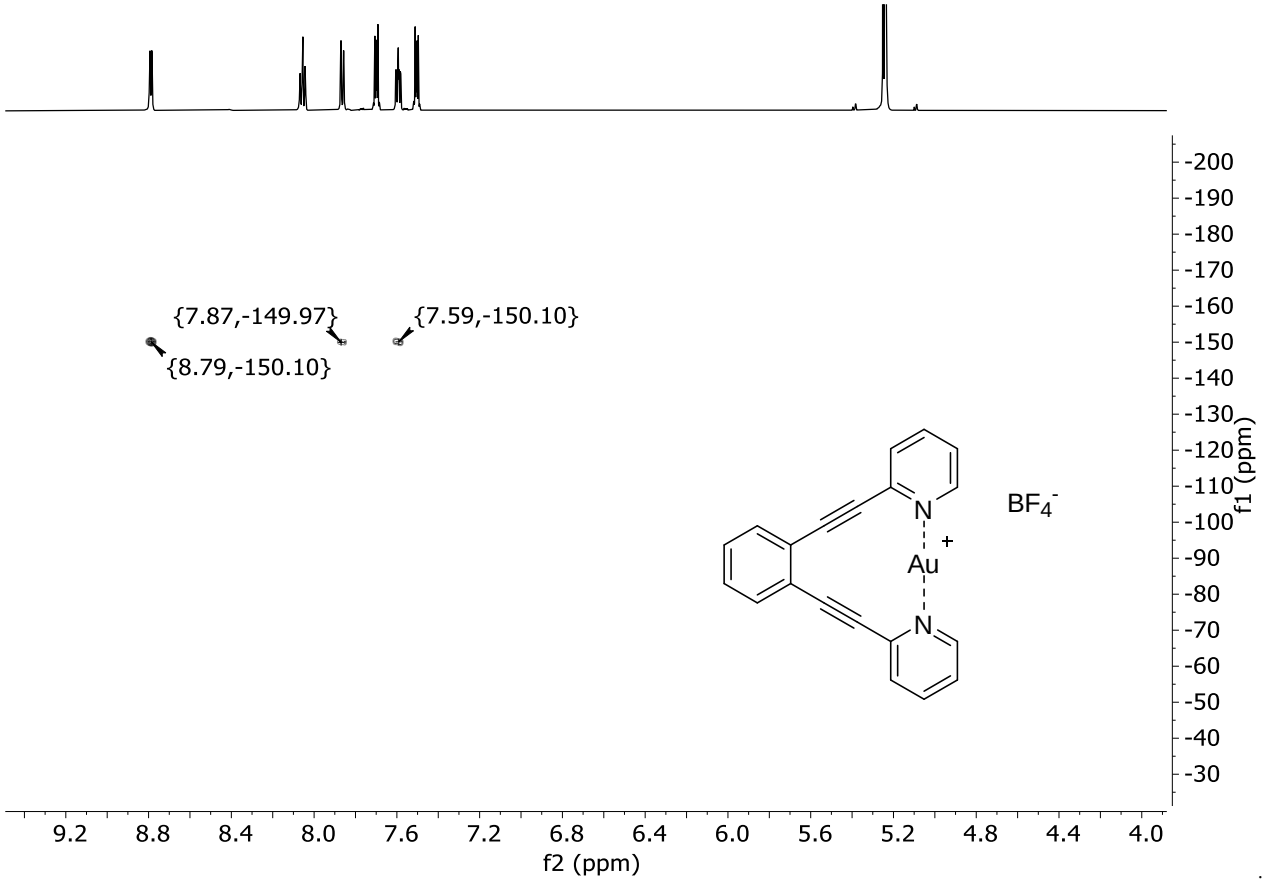

Figure S38. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**2**-H)-Au(I)]BF_4 acquired at 25 ºC in CD_2Cl_2 at 61 MHz.

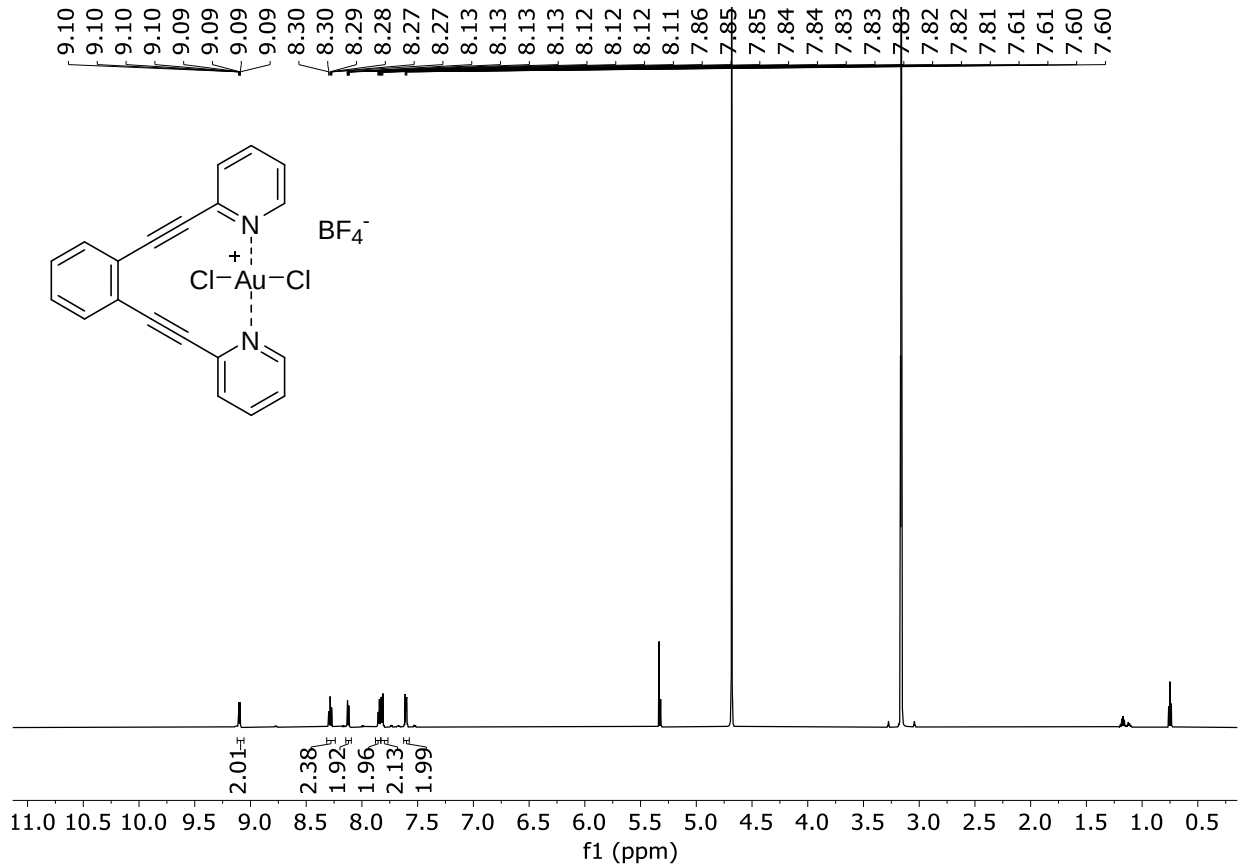

Figure S39. The ^{1}H NMR spectrum of [(**2**-H)-Au(III)]BF_4 acquired at 25 ^{o}C in MeOD at 600 MHz.

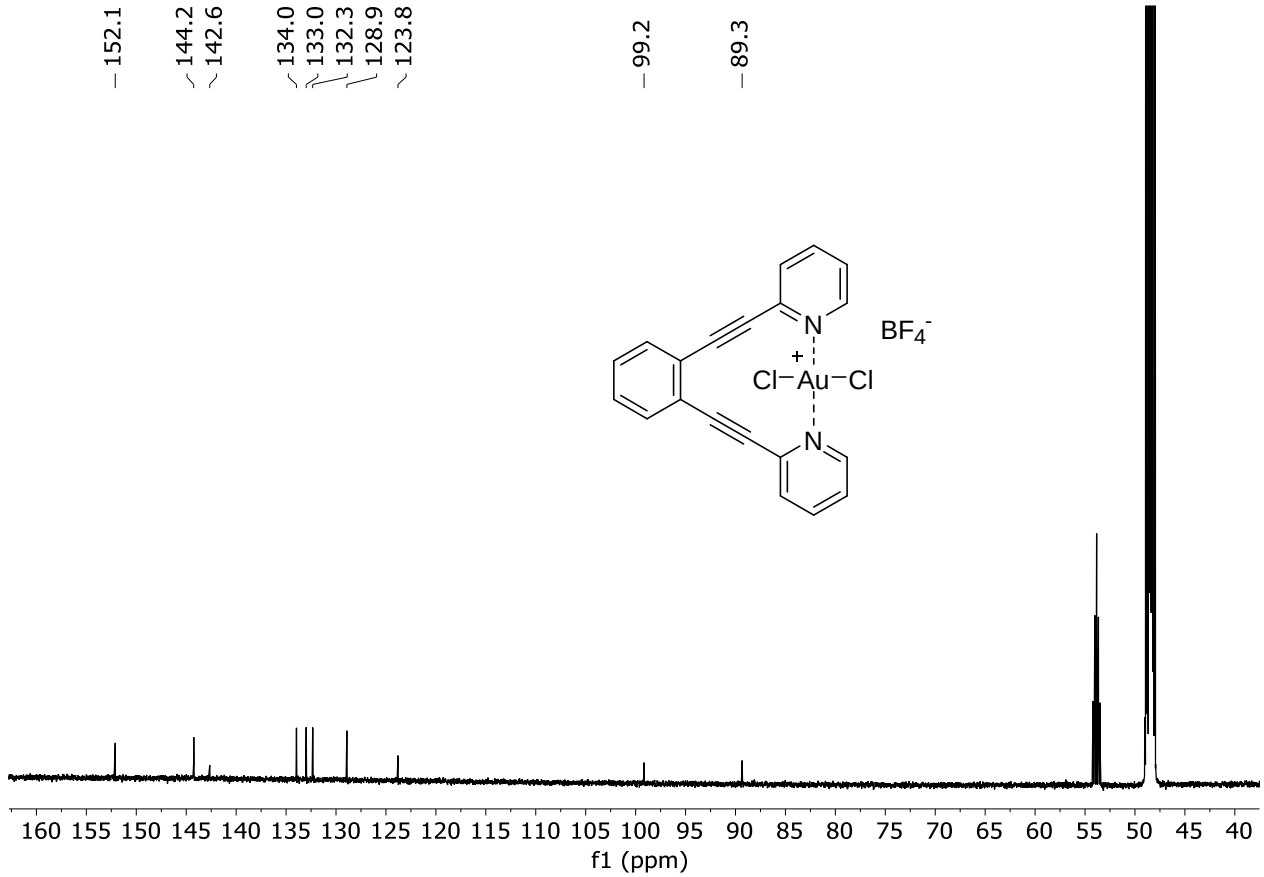

Figure S40. The ^{13}C NMR spectrum of [(**2**-H)-Au(III)]BF_4 acquired at 25 ^{o}C in MeOD at 151 MHz.

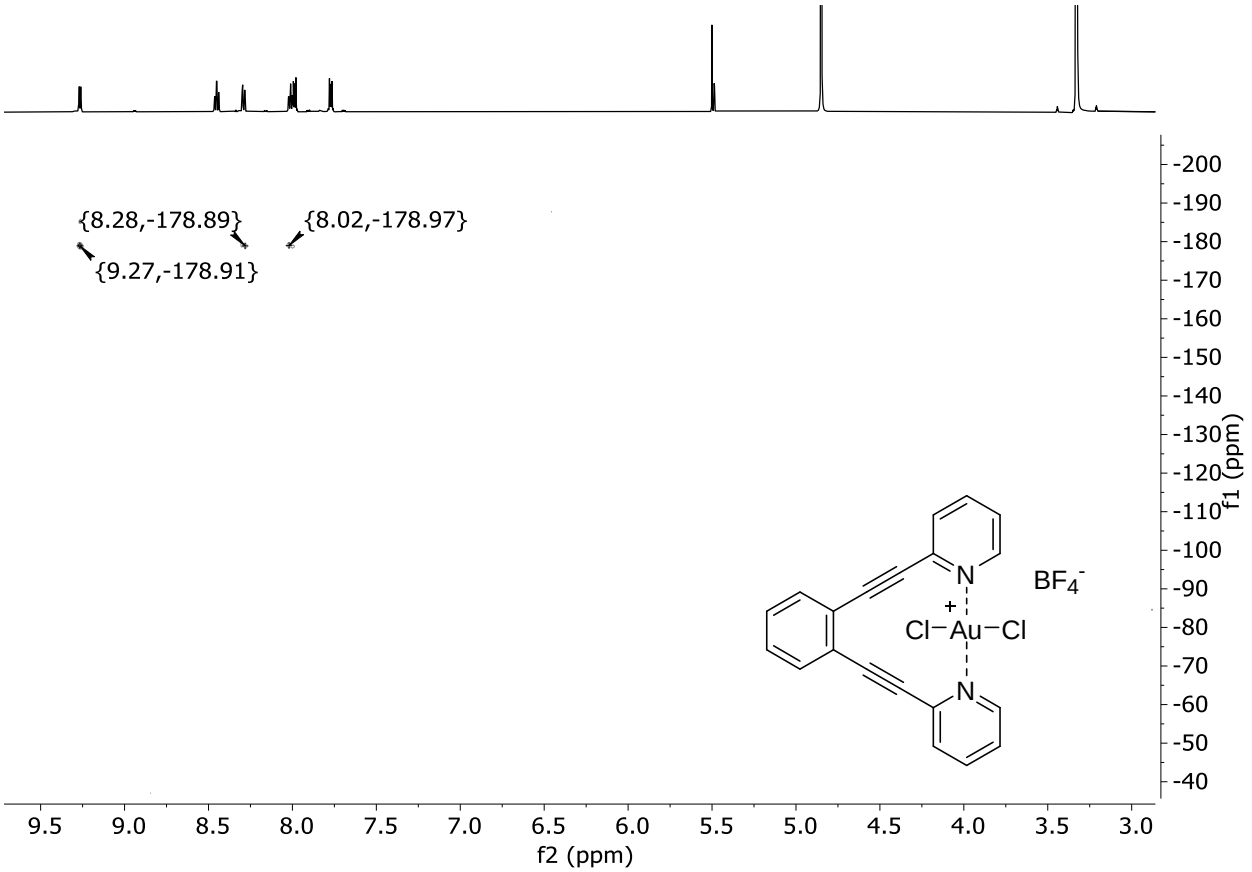

Figure S41. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**2**-H)-Au(III)]BF_4 acquired at 25 °C in MeOD at 61 MHz.

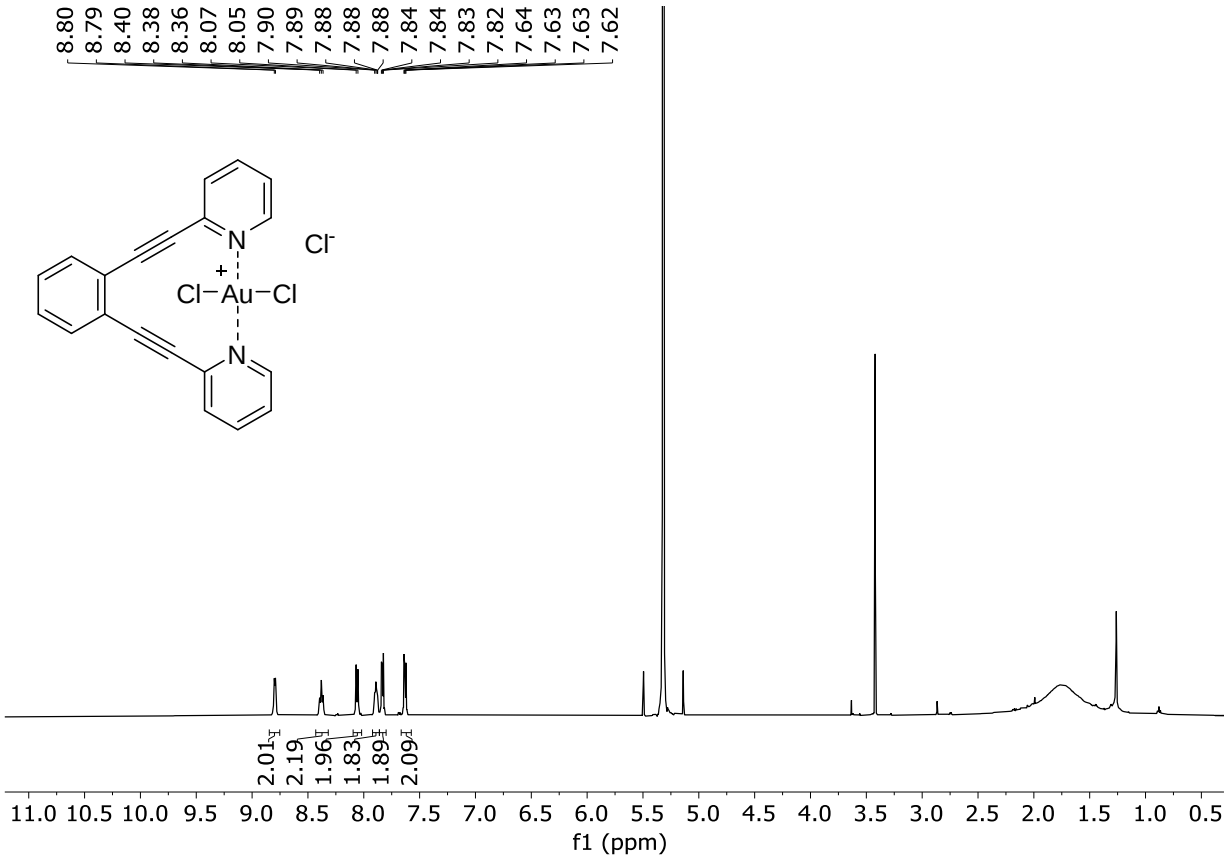

Figure S42. The ^{1}H NMR spectrum of [(**2**-H)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 500 MHz.

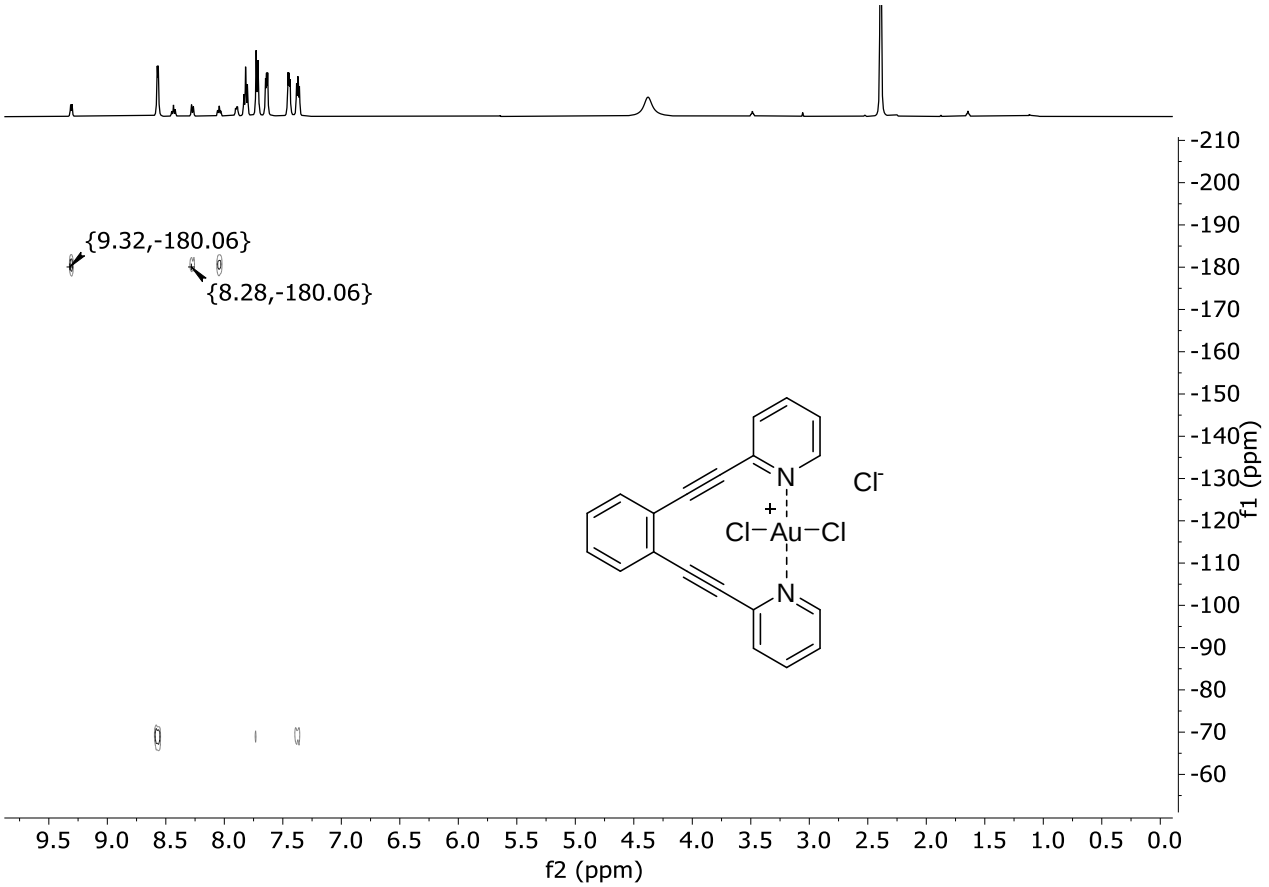

Figure S43. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**2**-H)-Au(III)]Cl acquired at 25 °C in DMSO-d_6 at 51 MHz. The spectrum was acquired in DMSO because of too low solubility in DCM, even if the complex is not stable in for long in DMSO, which is seen by the cross peaks for free ligand at approximately -68 ppm,

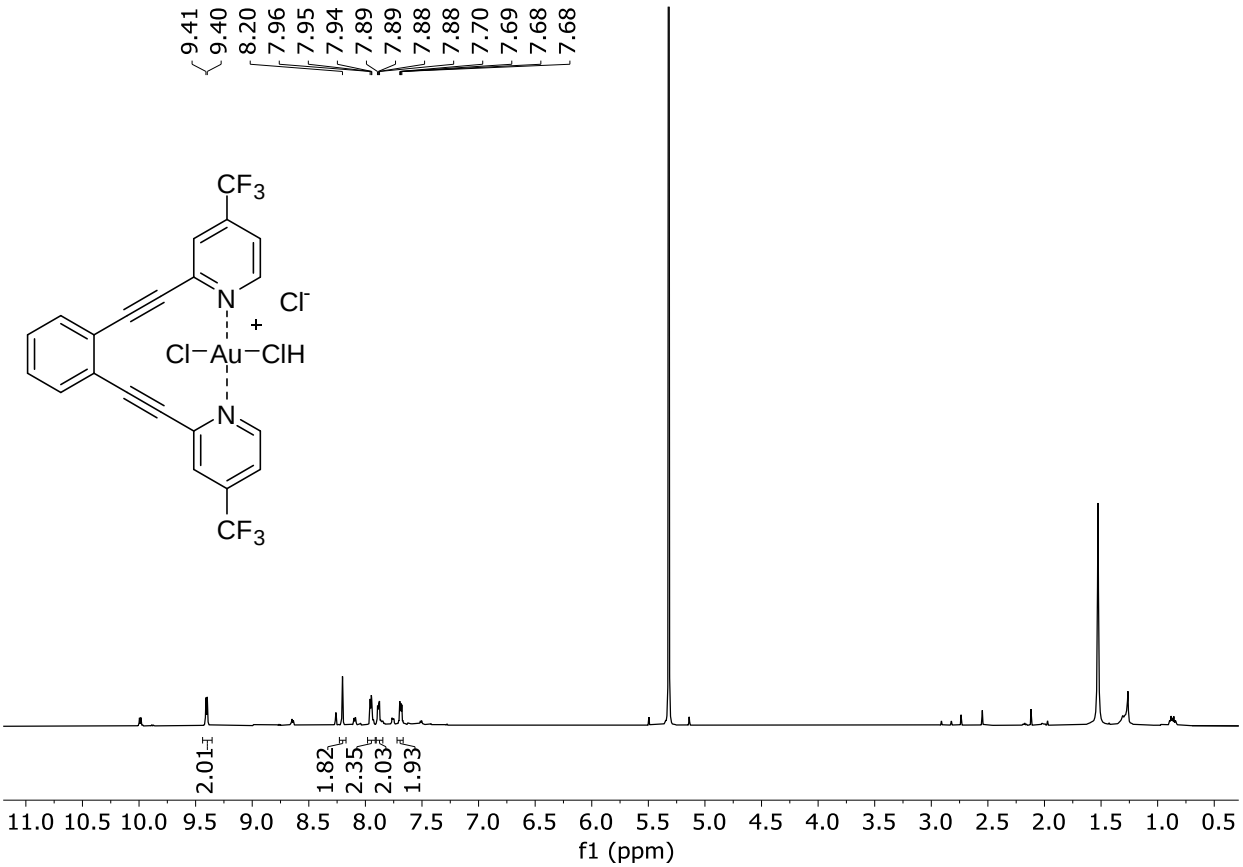

Figure S44. The ^{1}H NMR spectrum of [(**2**-CF_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 500 MHz.

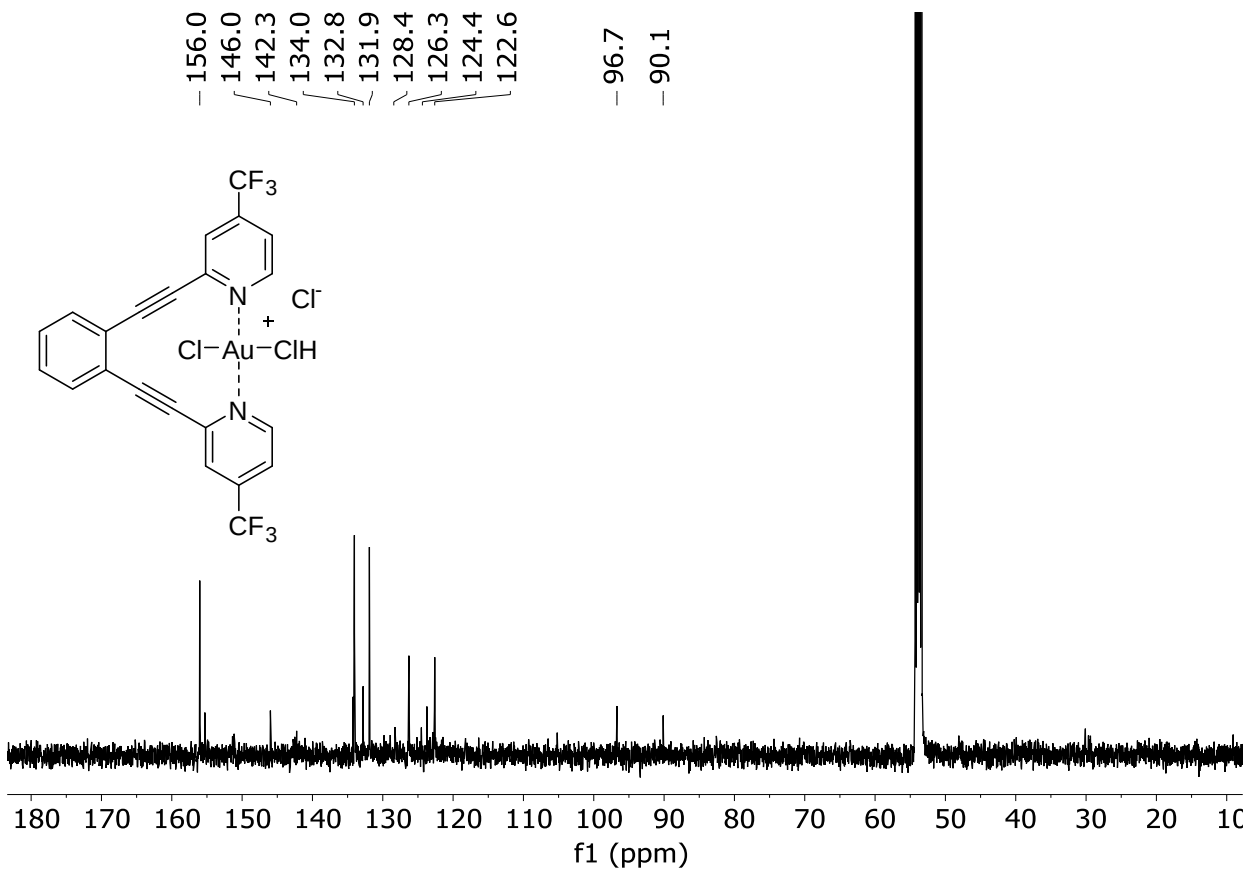

Figure S45. The ^{13}C NMR spectrum of [(**2**-CF_3)-Au(III)]Cl acquired at 25 ºC in CD_2Cl_2 at 126 MHz.

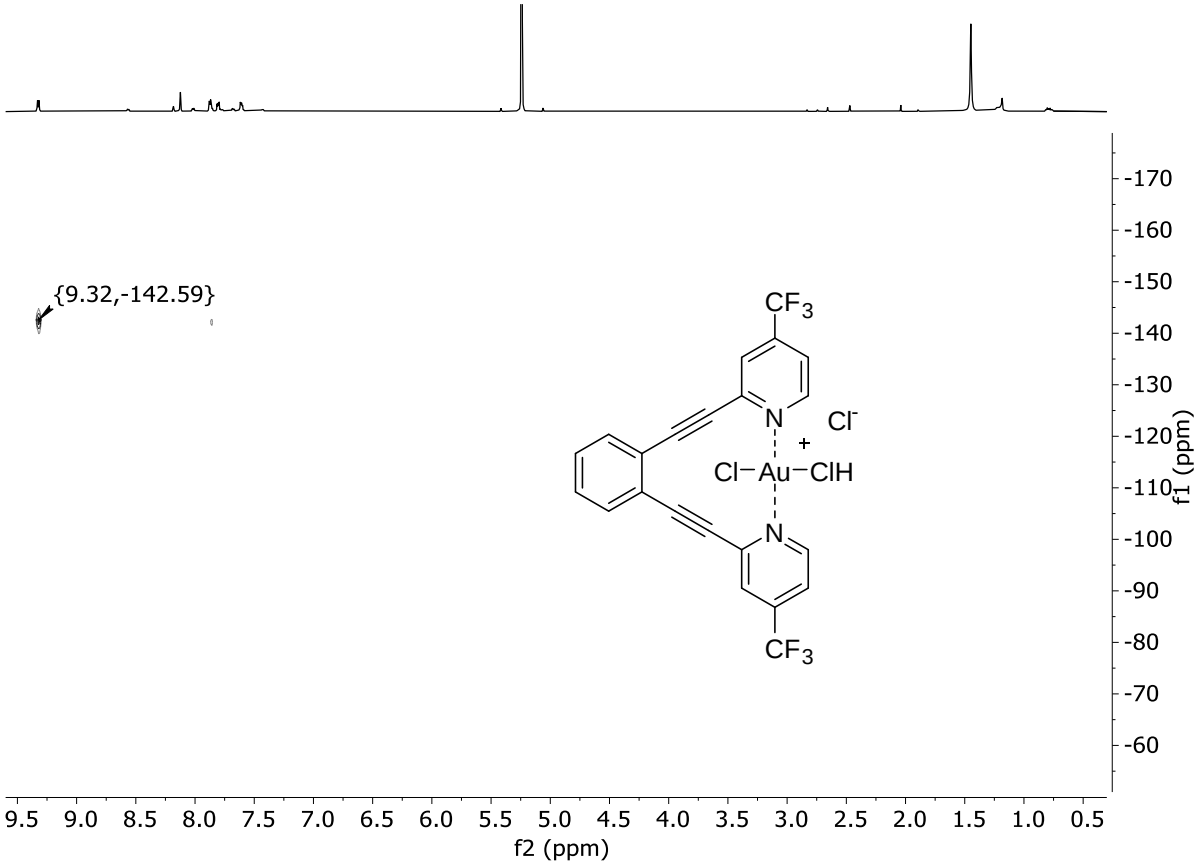

Figure S46. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**2**-CF_3)-Au(III)]Cl acquired at 25 ºC in CD_2Cl_2 at 51 MHz

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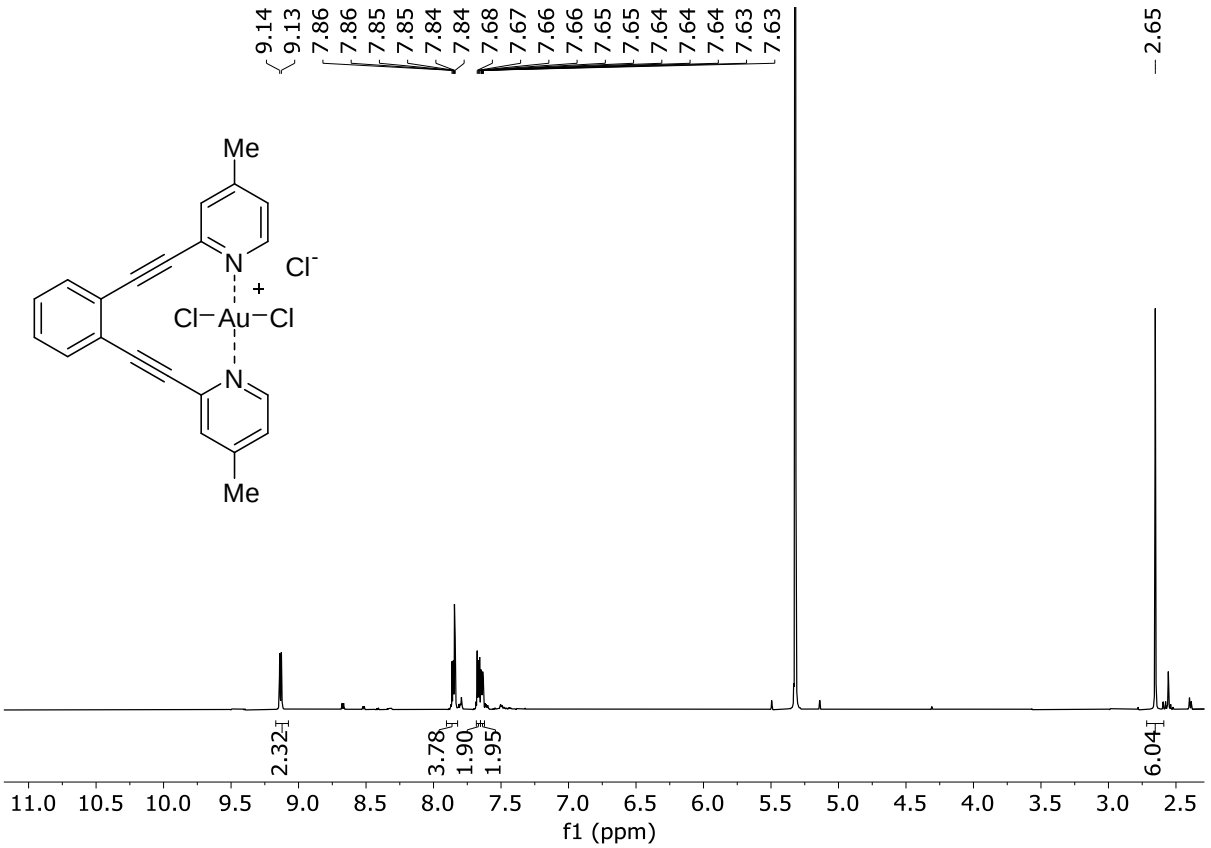

Figure S47. The ^{1}H NMR spectrum of [(**2**-CH_3)-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 500 MHz.

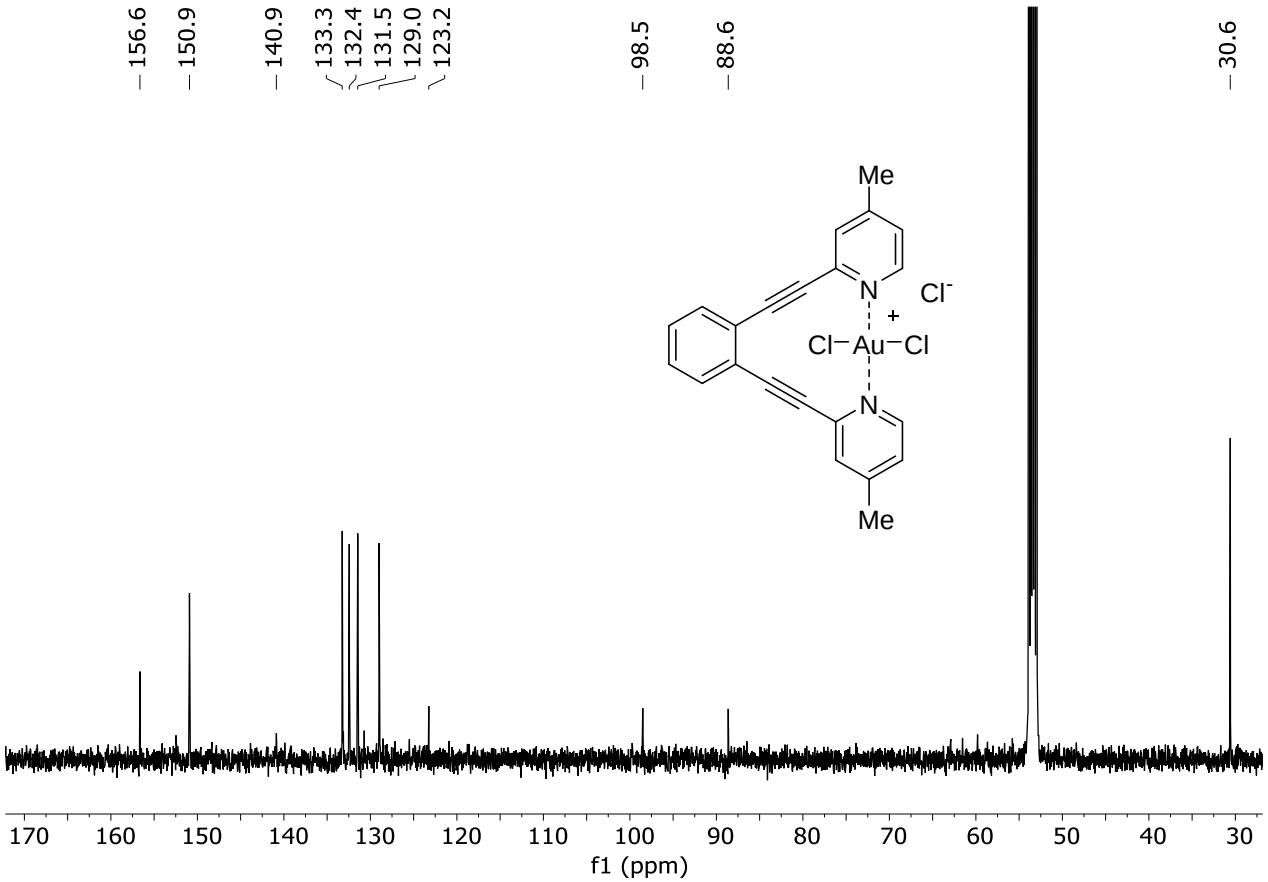

Figure S48. The ^{13}C NMR spectrum of [(**2**-CH_3)-Au(III)]Cl acquired at 25 ^{o}C in CD_2Cl_2 at 126 MHz.

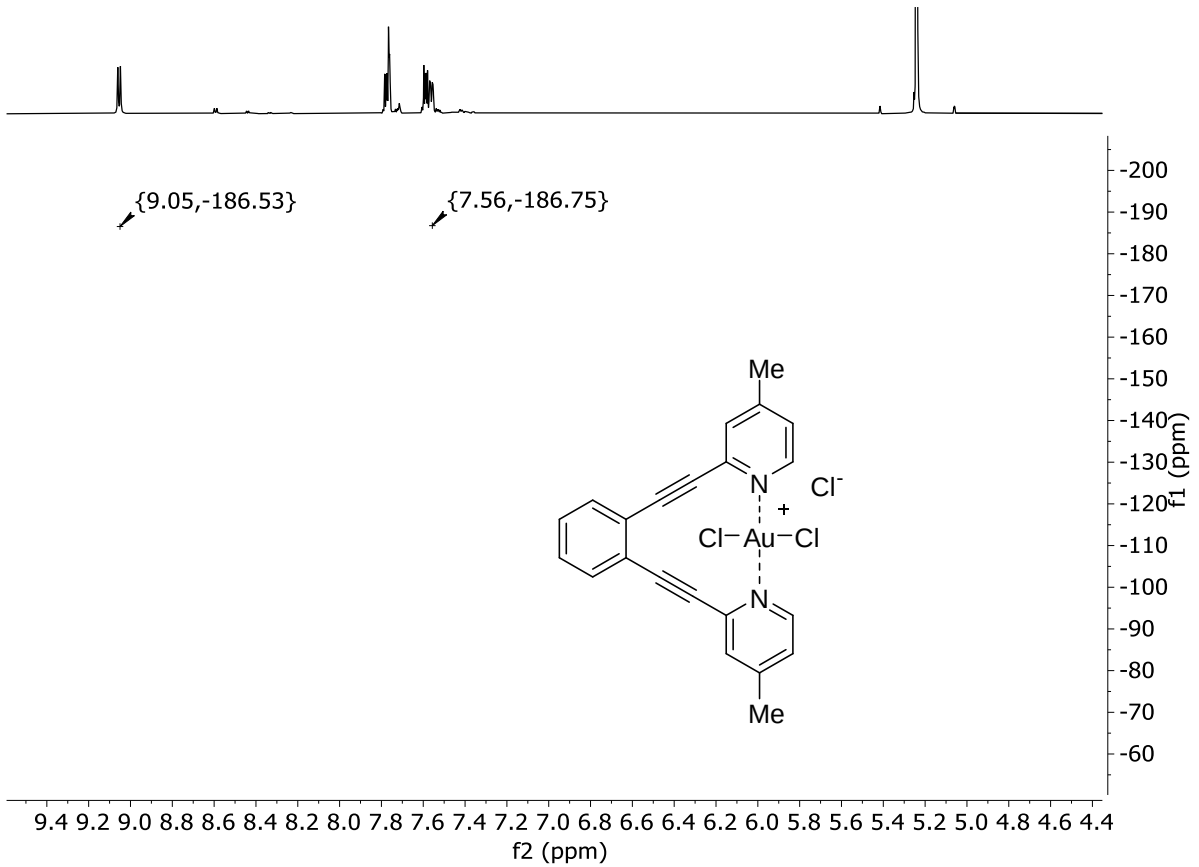

Figure S49. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**2**-CH_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 51 MHz

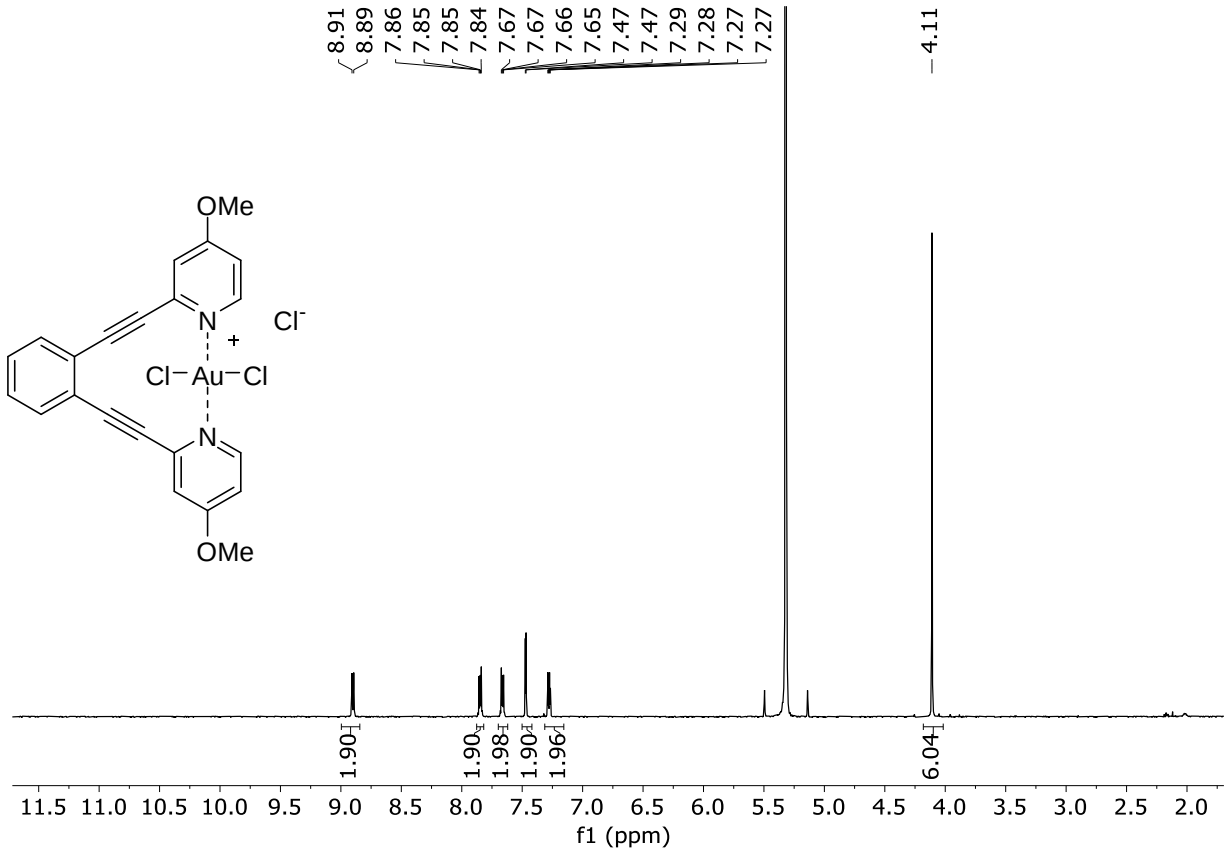

Figure S50. The ^{1}H NMR spectrum of [(**2**-OCH_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 500 MHz.

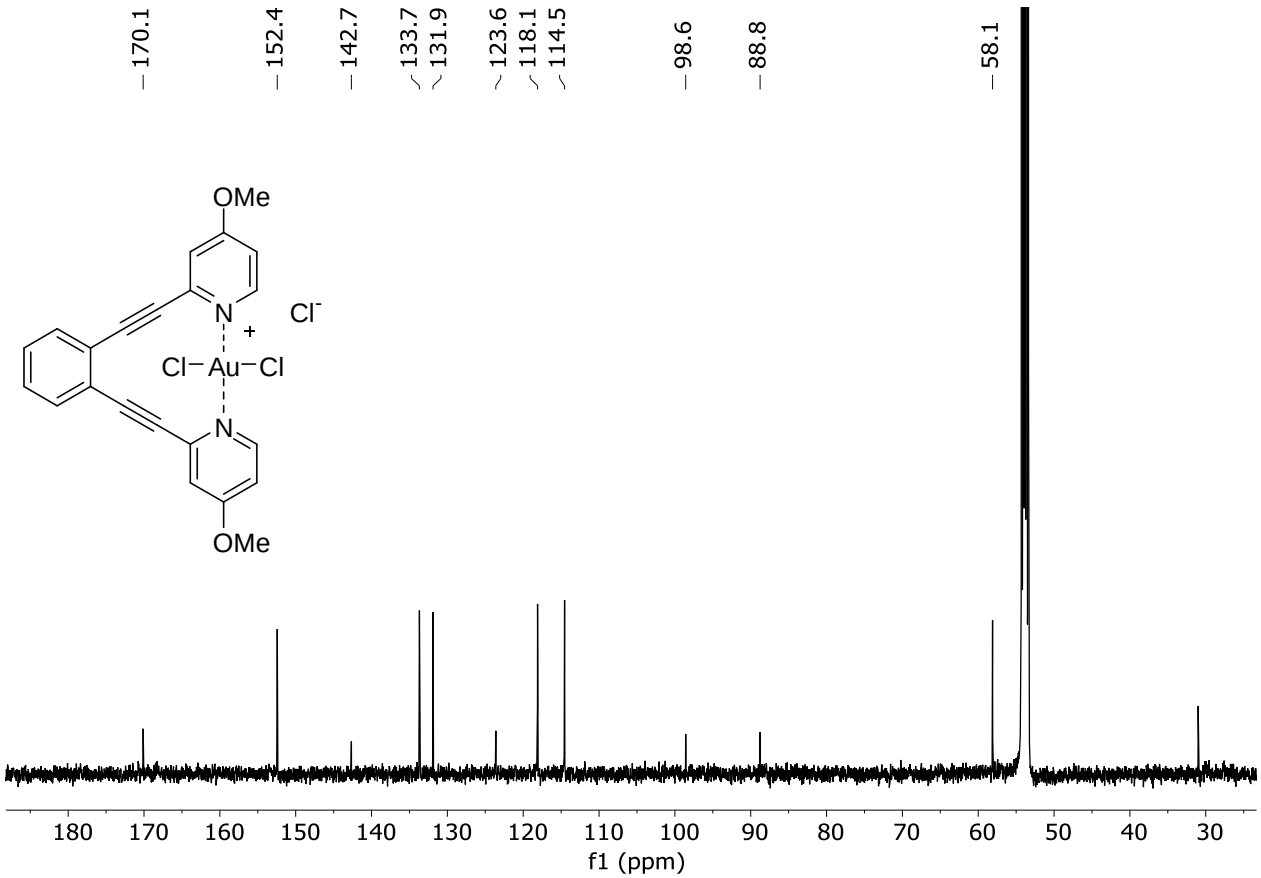

Figure S51. The ^{13}C NMR spectrum of [(**2**-OCH_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 126 MHz.

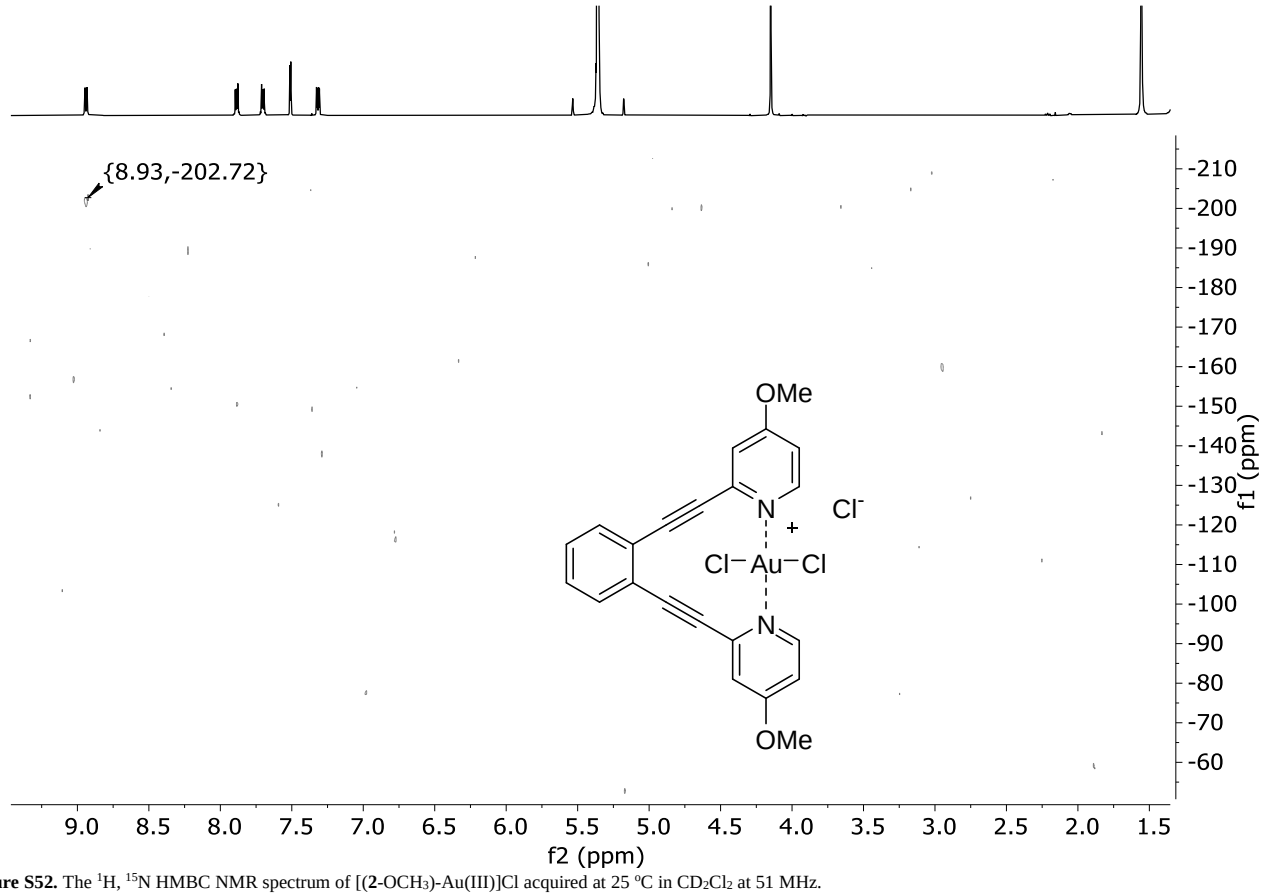

Figure S52. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**2**-OCH_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 51 MHz.

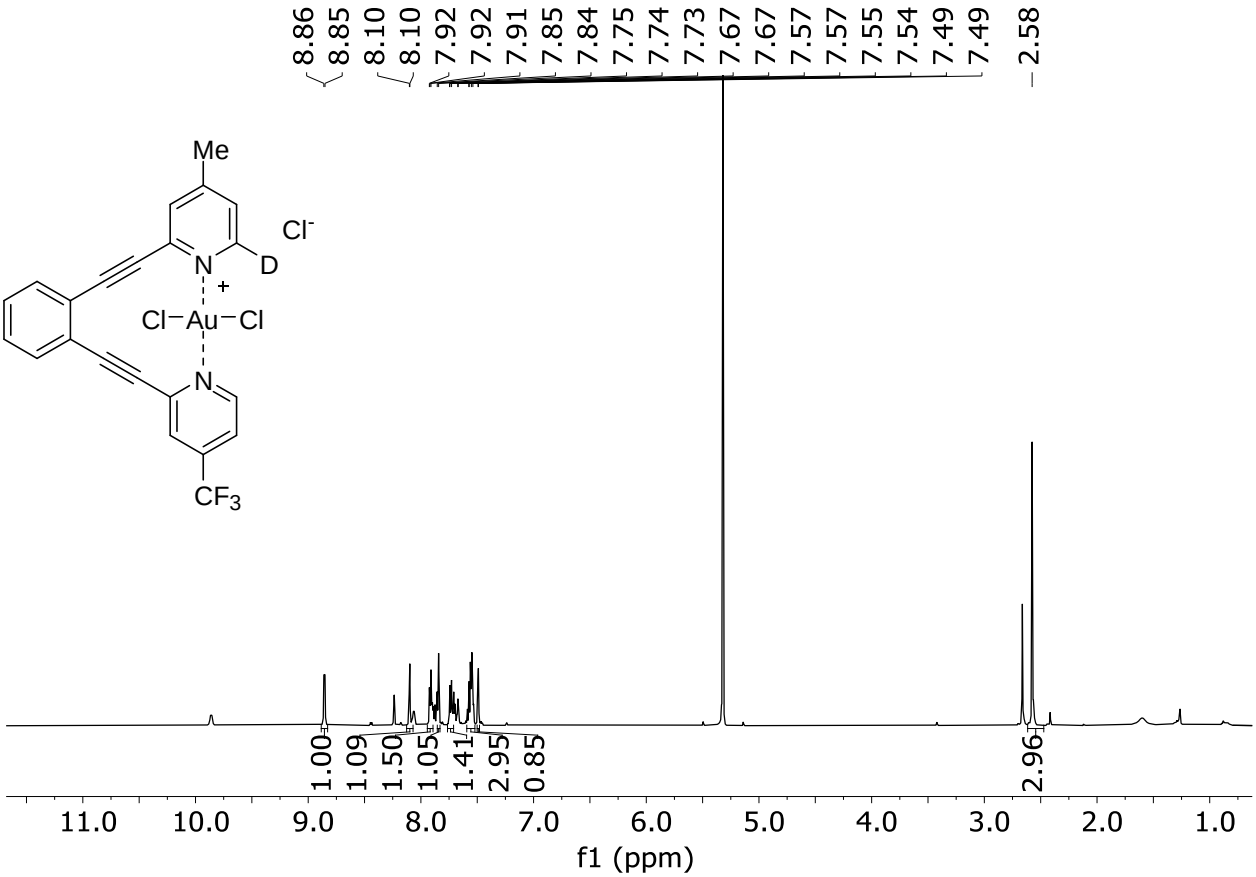

Figure S53. The ^{1}H NMR spectrum of [(**2**-CH_3/CF_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 500 MHz. Contains 25% impurify corresponding to the H^+ complex of ligand **2**-CH_3/CF_3.

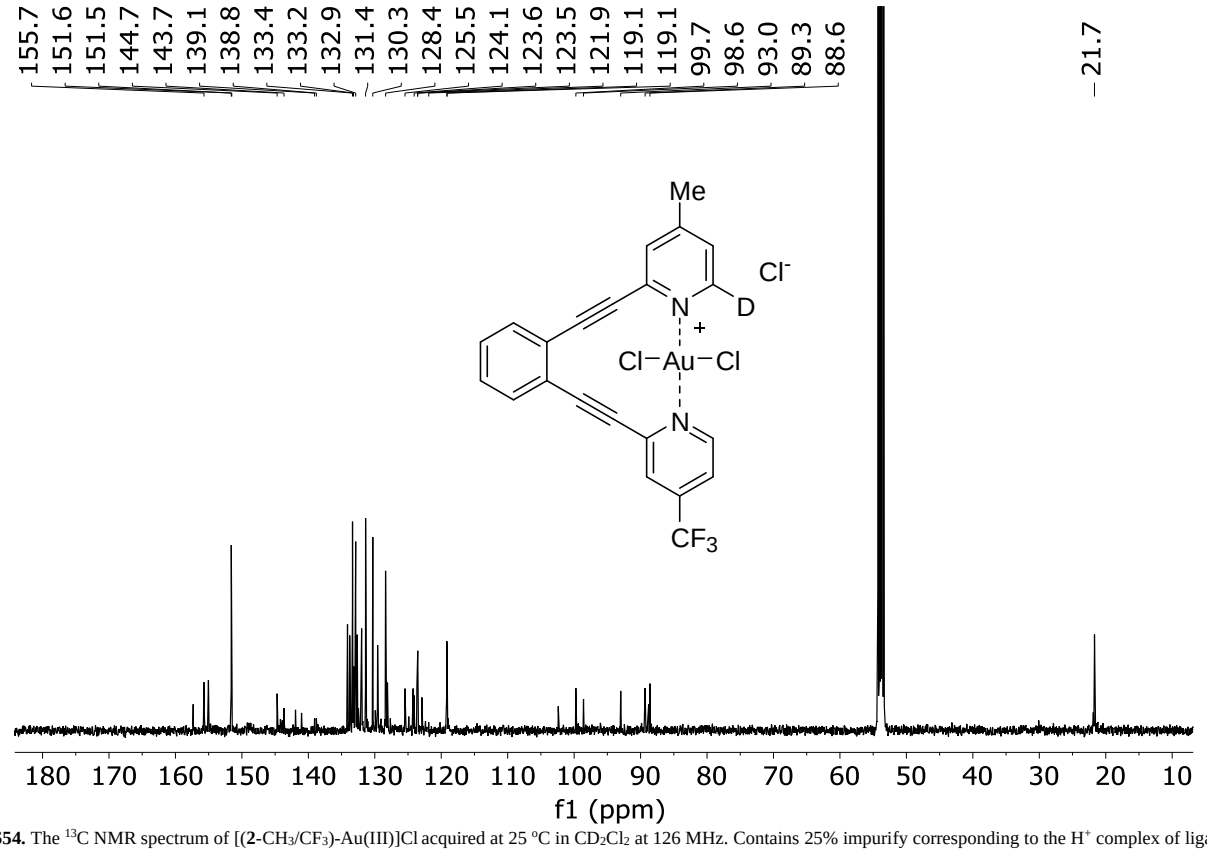

Figure S54. The ^{13}C NMR spectrum of [(**2**-CH_3/CF_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 126 MHz. Contains 25% impurify corresponding to the H^+ complex of ligand **2**-CH_3/CF_3.

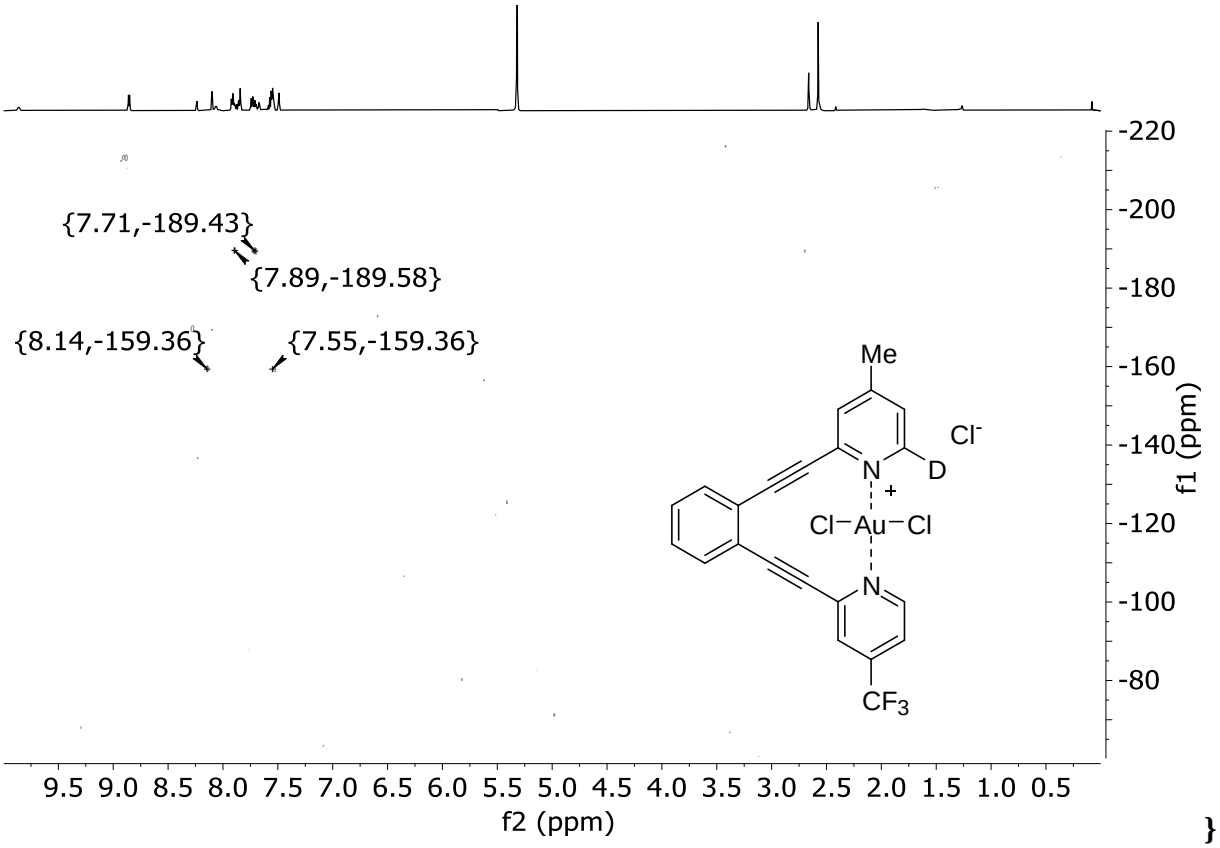

Figure S55. The ^{1}H, ^{15}N HMBC NMR spectrum of [(**2**-CH_3/CF_3)-Au(III)]Cl acquired at 25 °C in CD_2Cl_2 at 51 MHz.

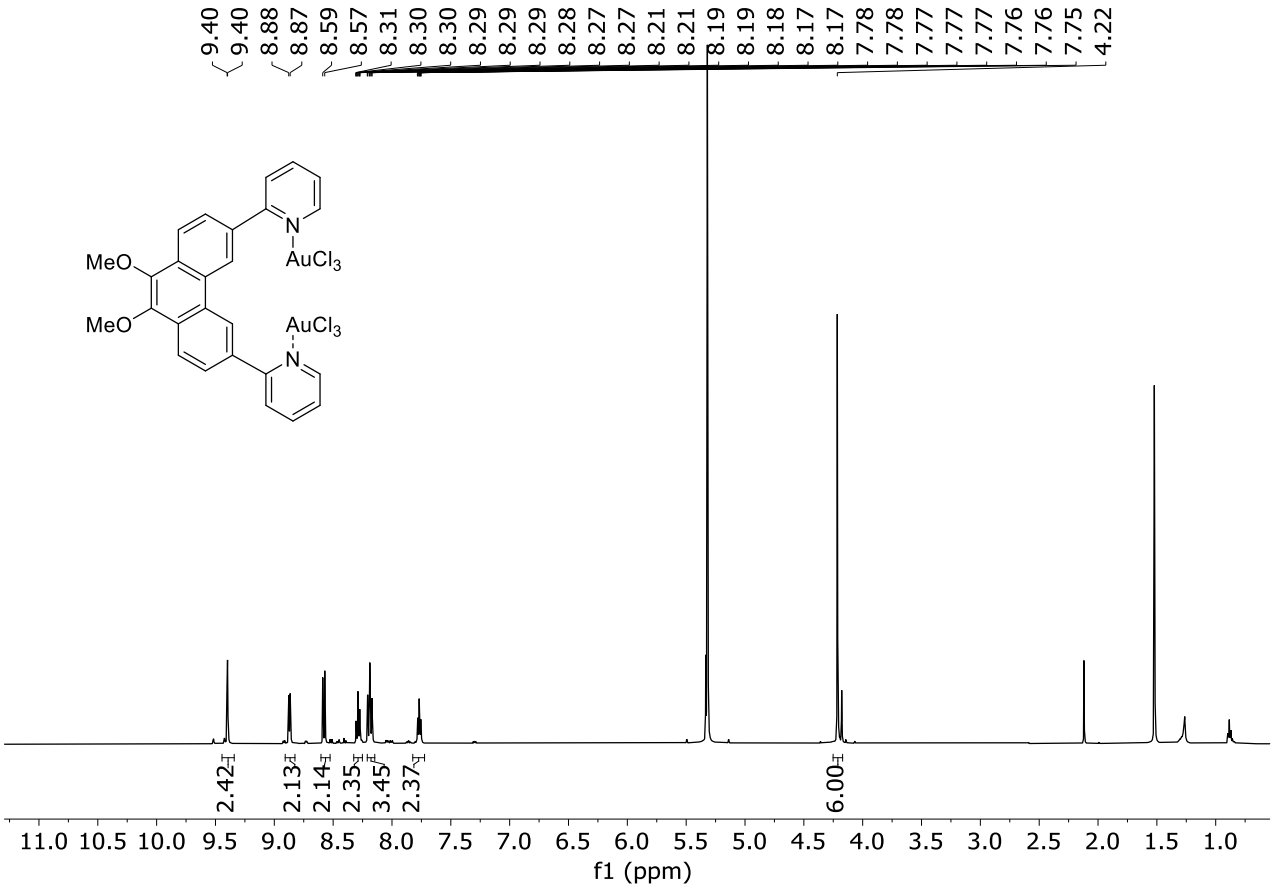

Figure S56. The ^{1}H NMR spectrum of [**3**-$Au(III)_2$] acquired at 25 °C in CD_2Cl_2 at 500 MHz.

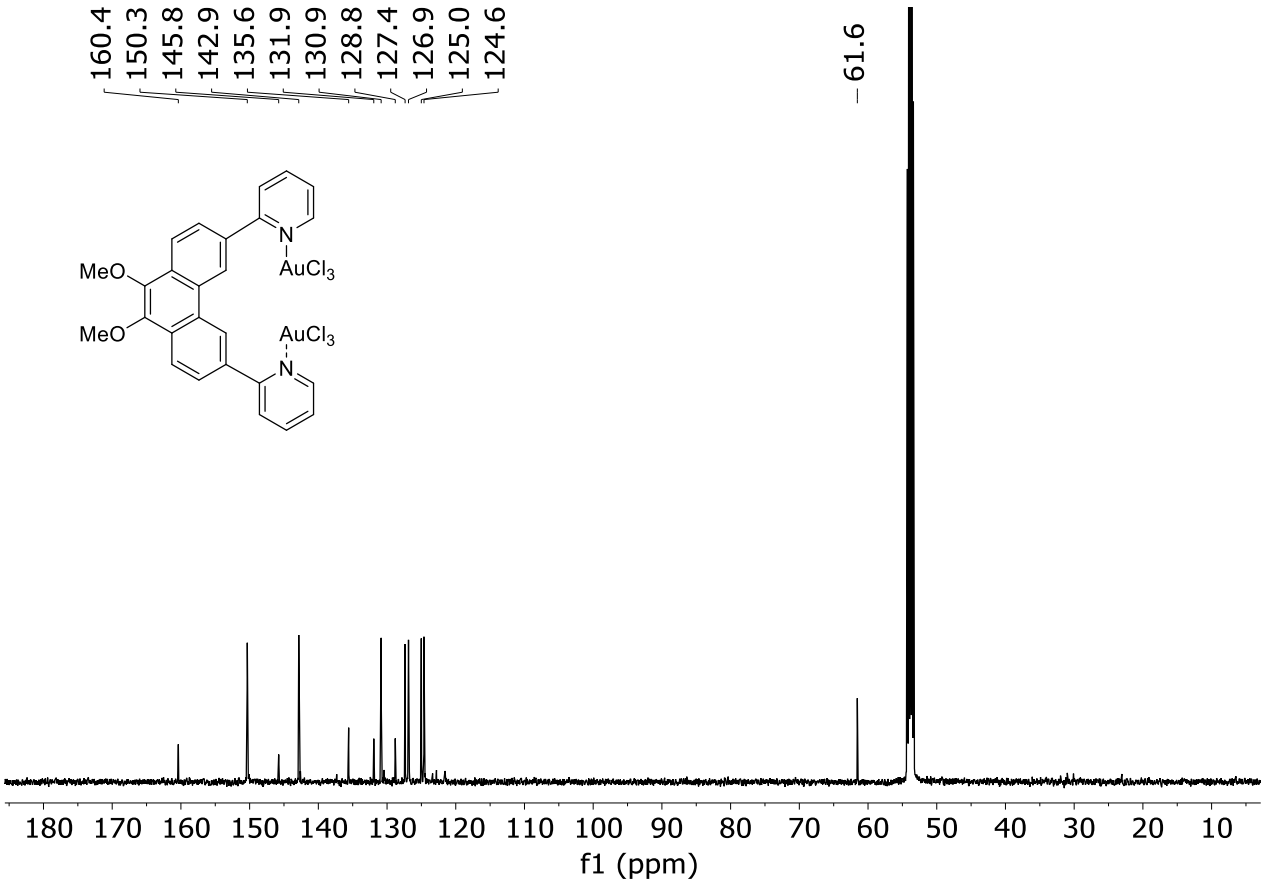

Figure S57. The ^{13}C NMR spectrum of [**3**-Au(III)$_2$] acquired at 25 ^{o}C in CD_2Cl_2 at 126 MHz.

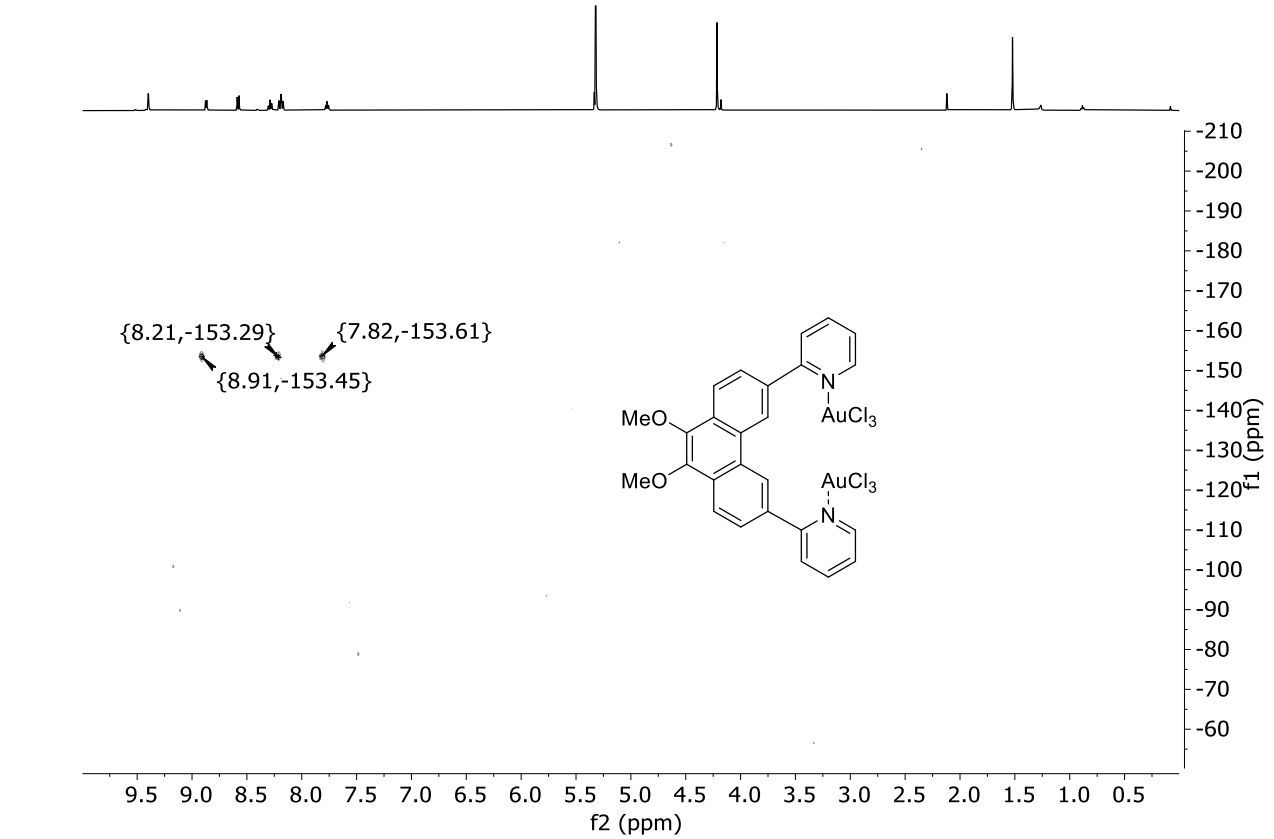

Figure S58. The ^{1}H, ^{15}N HMBC NMR spectrum of [**3**-Au(III)$_2$] acquired at 25 ^{o}C in CD_2Cl_2 at 51 MHz..

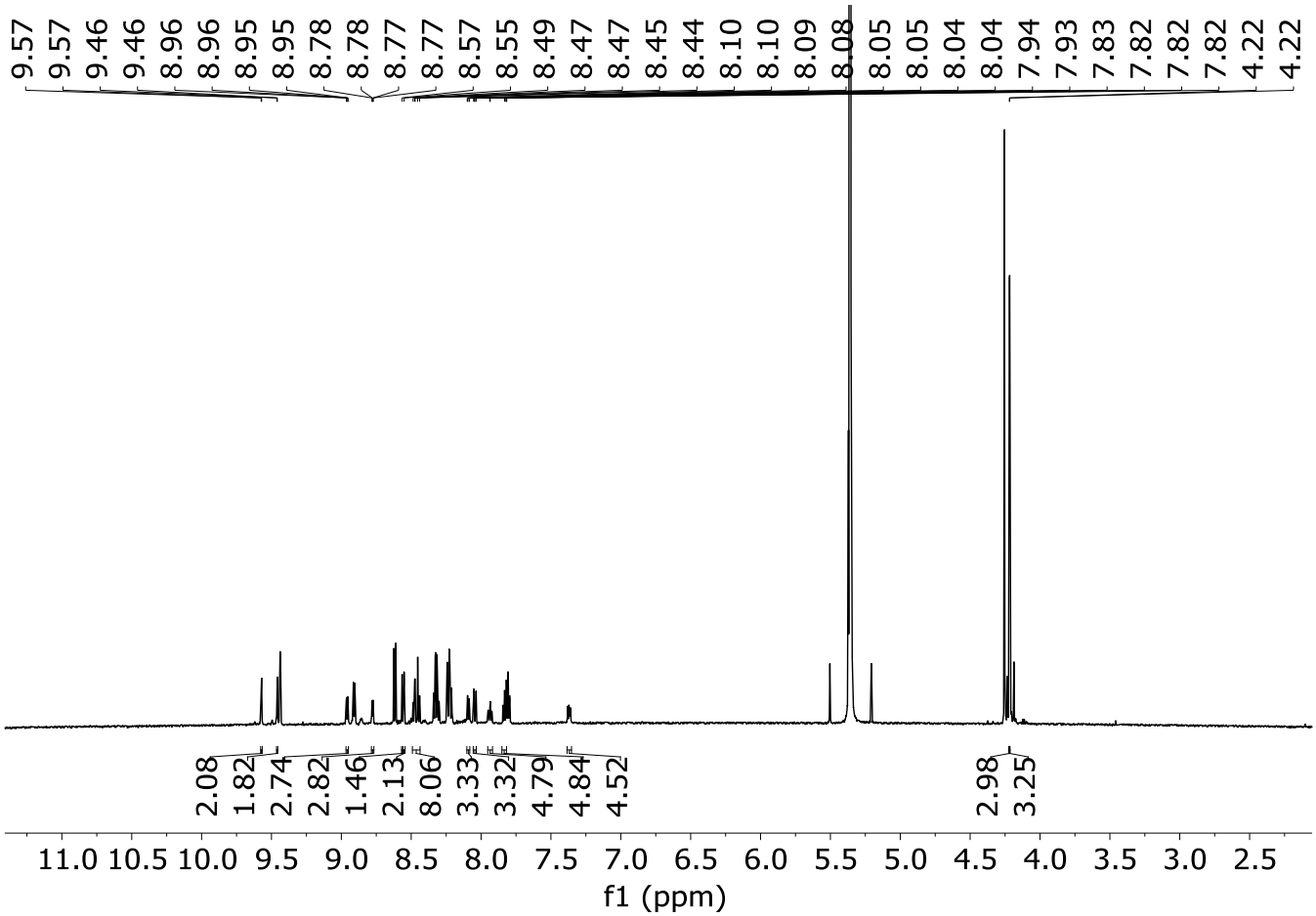

Figure S59. The ^{1}H NMR spectrum of as 4:3 mixture of [**3**-Au(III)$_2$] and [**3**-Au(III)]$_2$Cl$_2$ acquired at 25 ^{o}C in CD_2Cl_2 at 500 MHz. The selected peaks represent the ^{1}H chemical shift of [**3**-Au(III)]$_2$Cl$_2$.

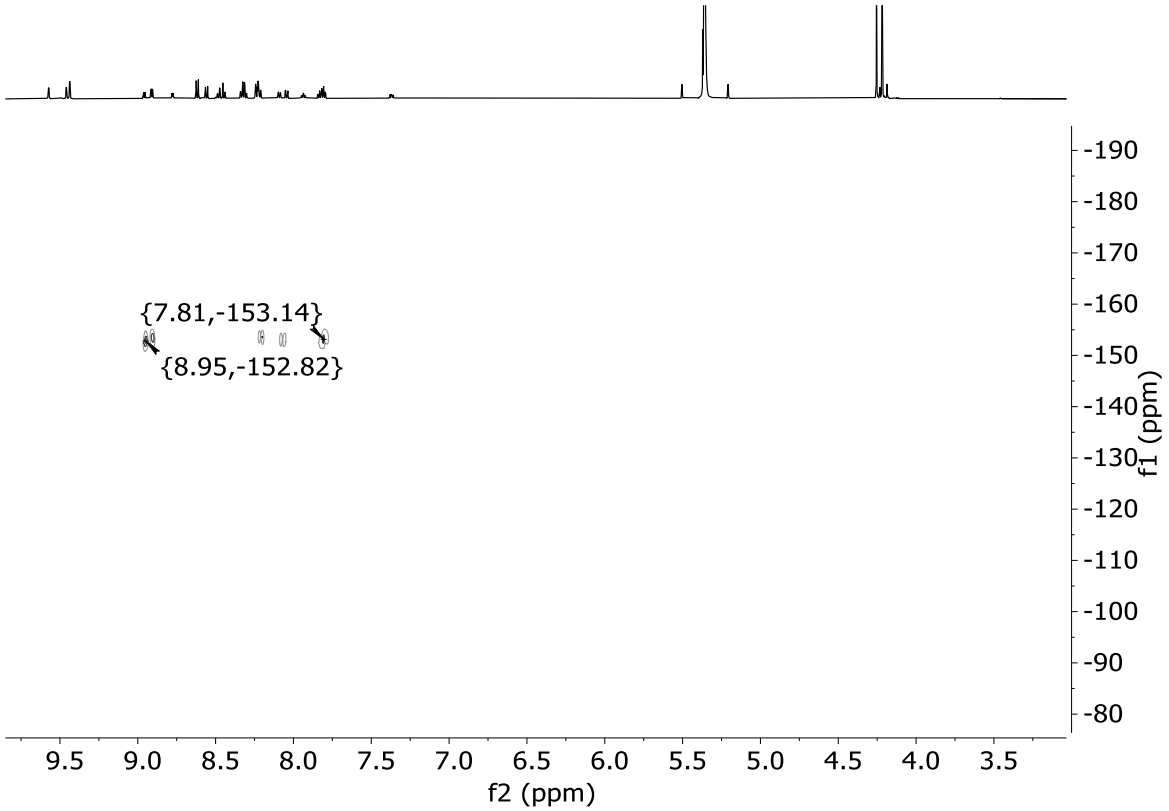

Figure S60. The ^{1}H, ^{15}N NMR spectrum of as 4:3 mixture of [**3**-Au(III)$_2$] and [**3**-Au(III)]$_2$Cl$_2$ acquired at 25 ^{o}C in CD_2Cl_2 at 500 MHz. The selected peaks represent the cross peaks of [**3**-Au(III)]$_2$Cl$_2$.

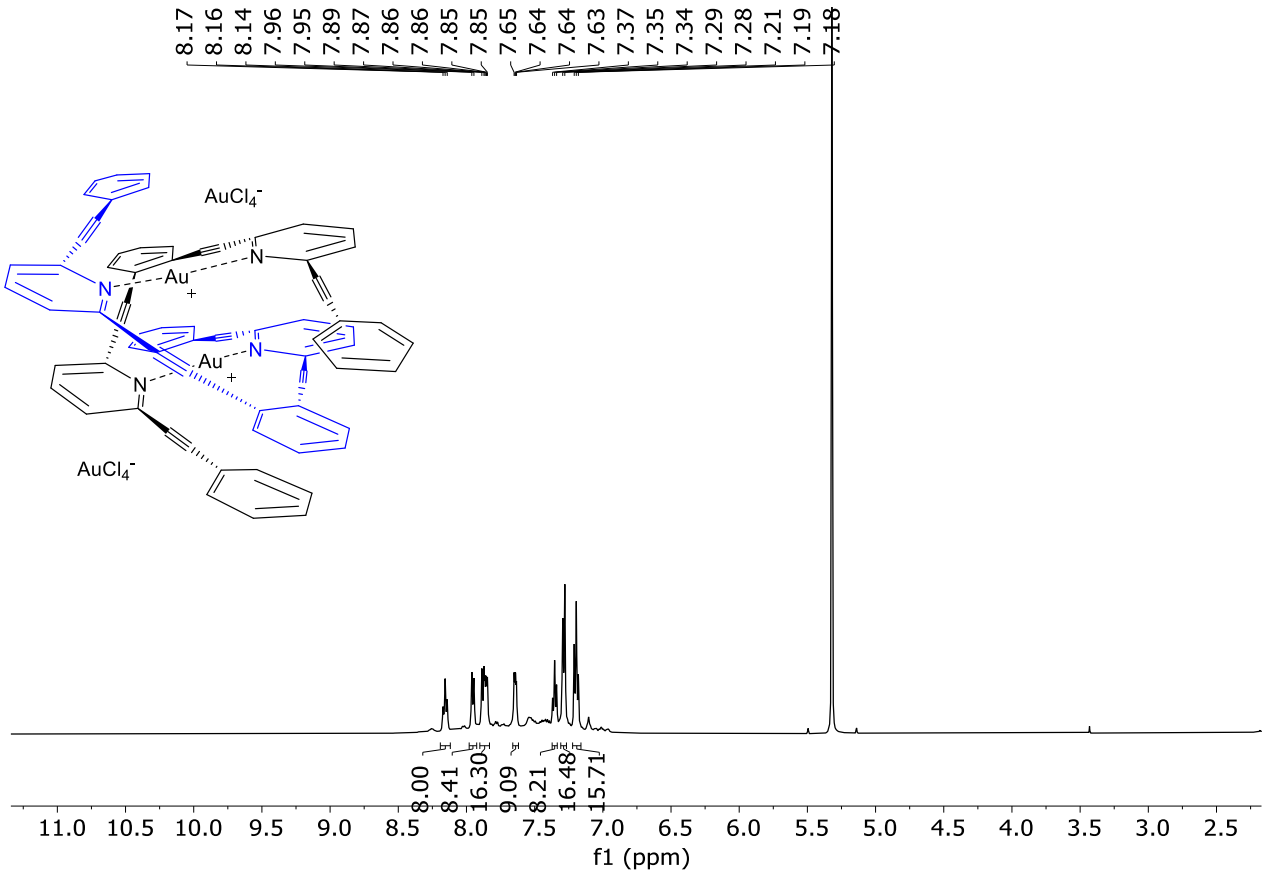

Figure S61. The ^{1}H NMR spectrum of [**4**-Au(I)]$_2$(AuCl$_4$)$_2$ acquired at 25 °C in CD_2Cl_2 at 500 MHz.

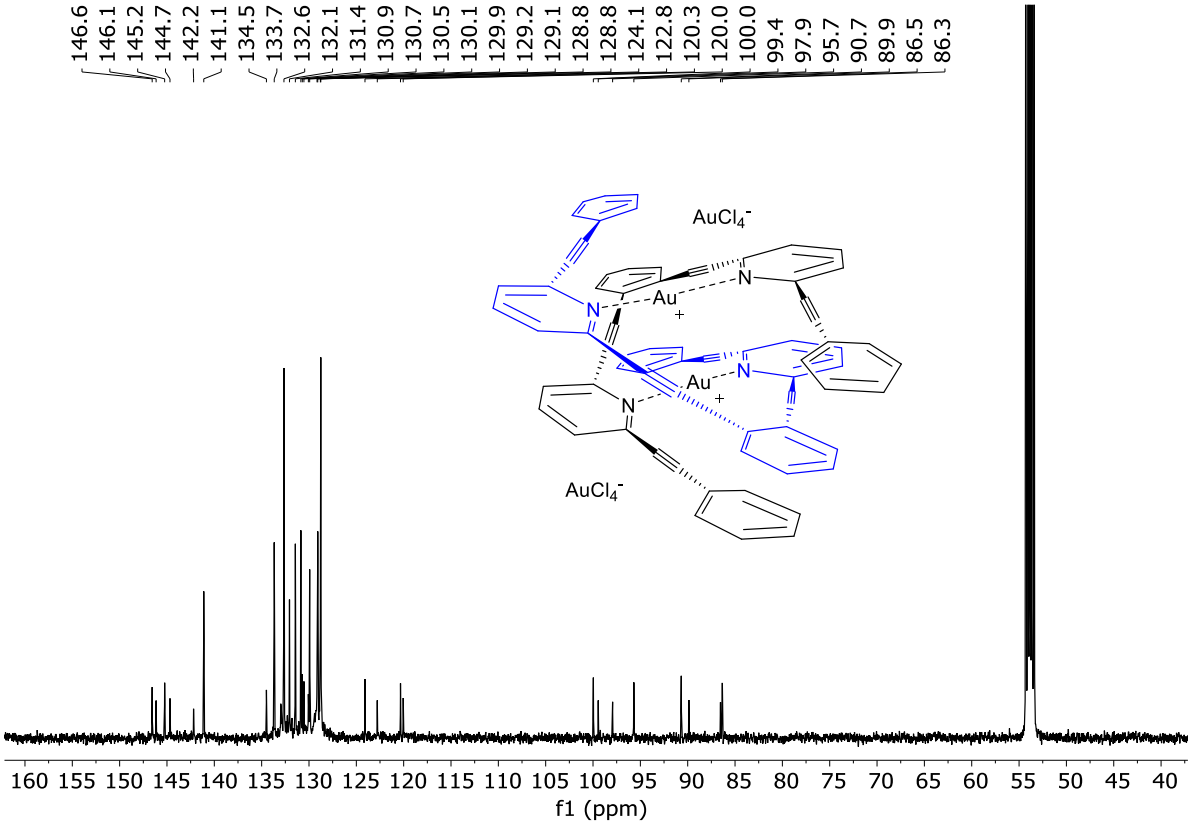

Figure S62. The ^{1}H NMR spectrum of [**4**-Au(I)]$_2$(AuCl$_4$)$_2$ acquired at 25 °C in CD_2Cl_2 at 126 MHz.

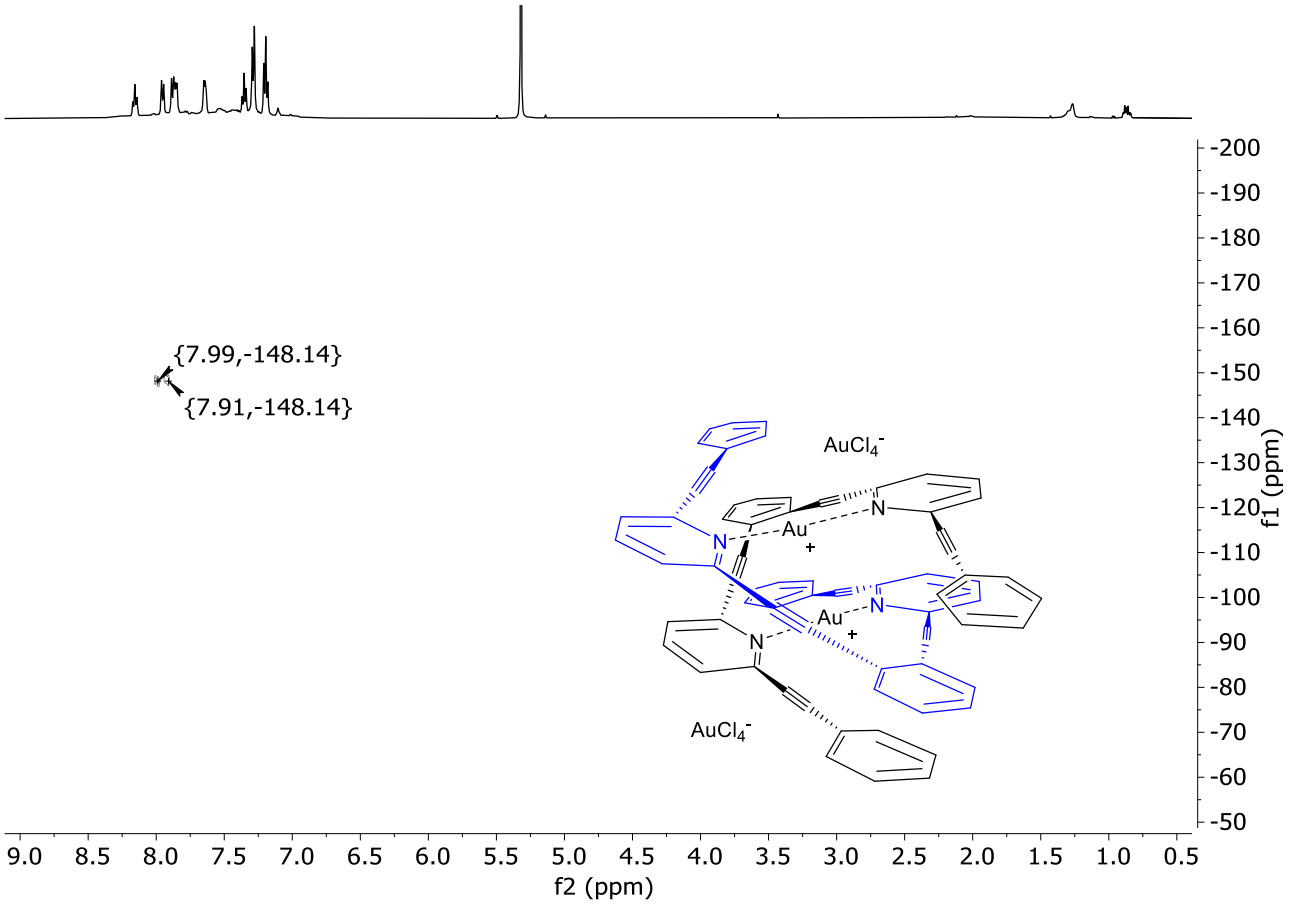

Figure S63. The ^{1}H, ^{15}N HMBC NMR spectrum of [**4**-Au(I)]$_2$(AuCl$_4$)$_2$ acquired at 25 ^{o}C in CD_2Cl_2 at 51 MHz..

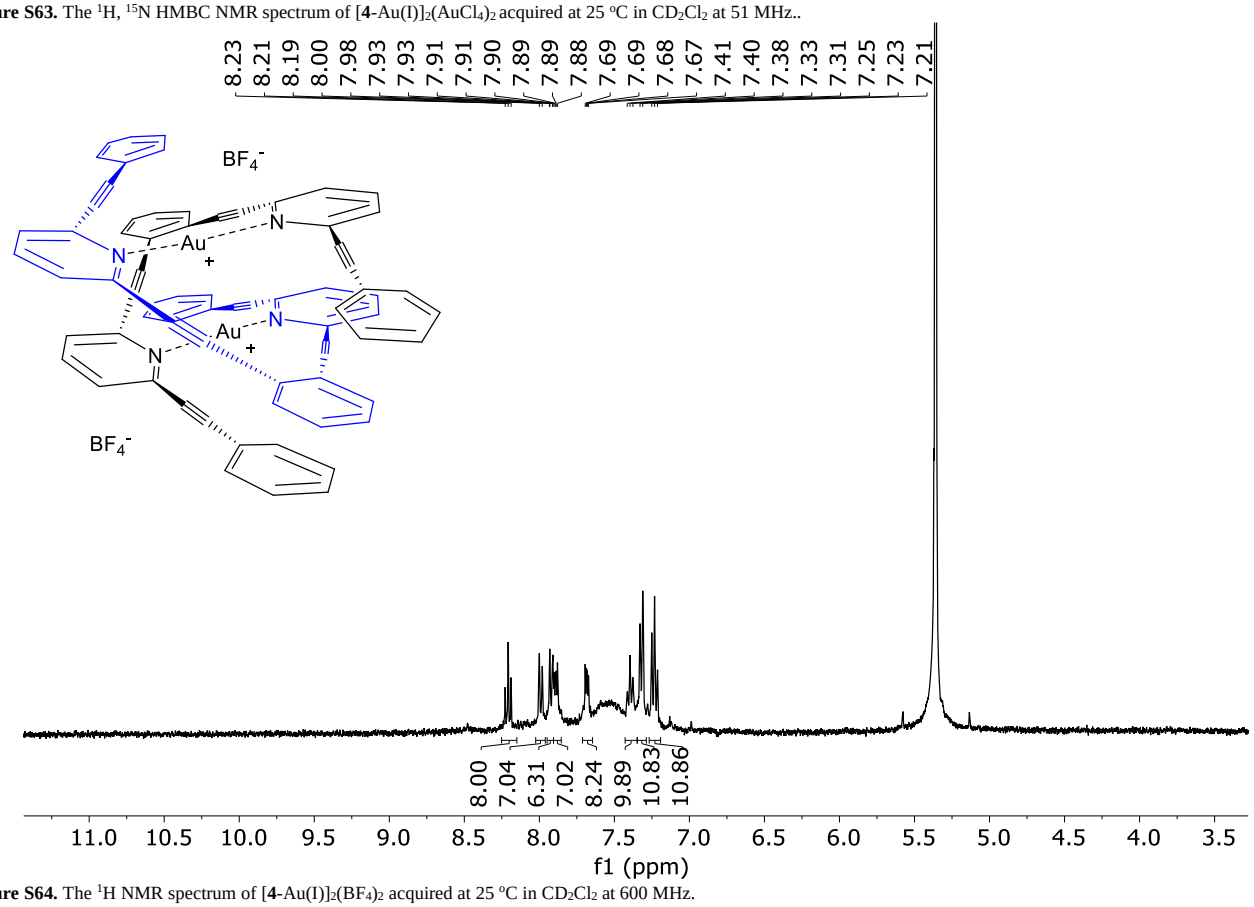

Figure S64. The ^{1}H NMR spectrum of [**4**-Au(I)]$_2$(BF$_4$)$_2$ acquired at 25 ^{o}C in CD_2Cl_2 at 600 MHz.

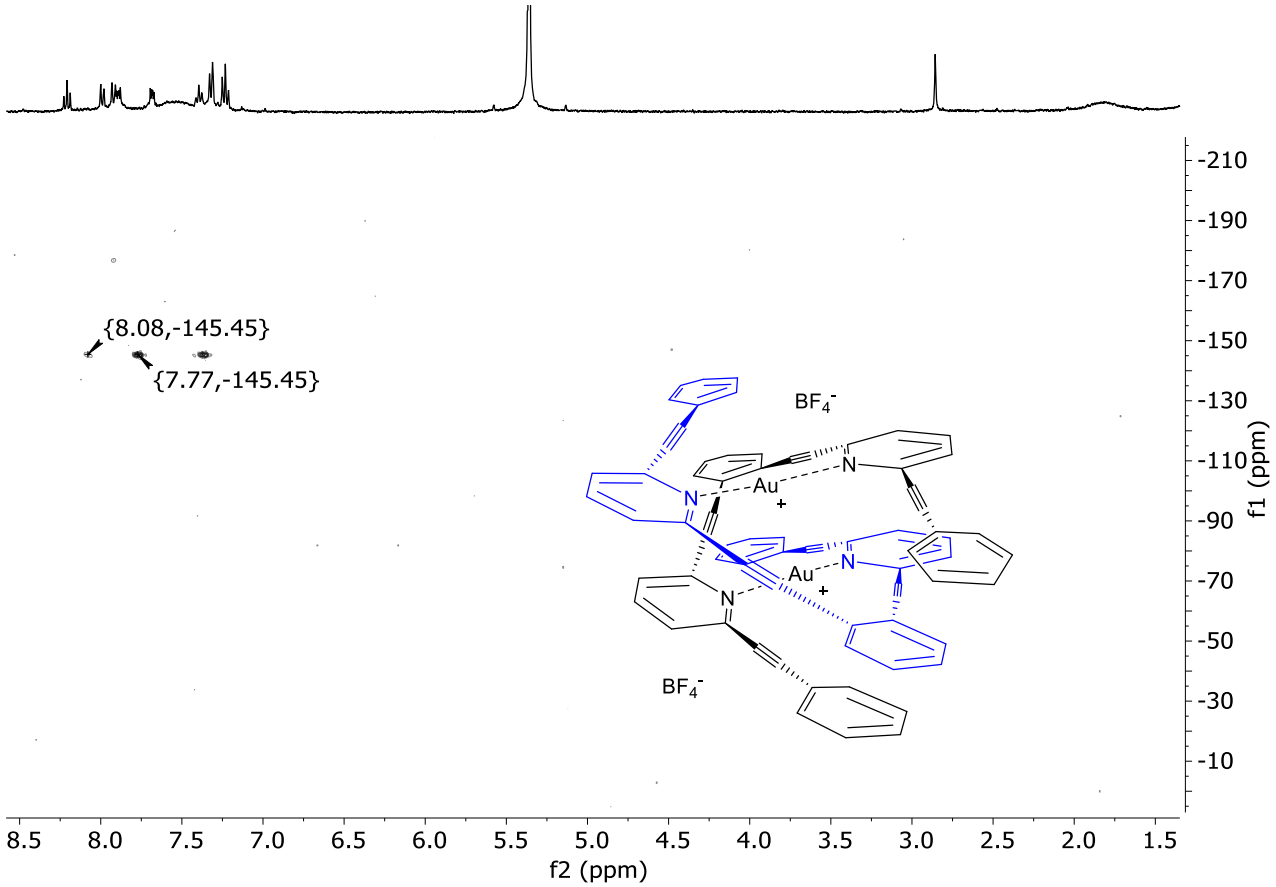

Figure S65. The ^{1}H, ^{15}N HMBC NMR spectrum of [**4**-Au(I)]$_2$(BF$_4$)$_2$ acquired at 25 ^{o}C in CD_2Cl_2 at 61 MHz.

8. References

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