SUPPORTING INFORMATION

Oxidant Speciation and Anionic Ligand Effects in the Gold-catalyzed Oxidative Coupling of Arenes and Alkynes

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Contents

1. General information

Equipment: NMR spectra were recorded on AV2 400 or AV2 500 MHz Bruker spectrometers. Chemical shifts are given in ppm. The spectra are calibrated to the residual ^{1}H and ^{13}C signals of the deuterated solvents. Multiplicities are abbreviated as follows: singlet (s), doublet (d), triplet (t), quartet (q), doublet-doublet (dd), doublet-triplet (dt), quintet (quint), sextet (sext), septet (sept), multiplet (m), and broad (br). High-resolution electrospray ionization mass-spectrometry was performed on a Finnigan MAT 900 (Thermo Finnigan, San Jose, CA; USA) double focusing magnetic sector mass spectrometer. Ten spectra were acquired. A mass accuracy ≤ 2 ppm was obtained in the peak matching acquisition mode by using a solution containing 2 µl PEG200, 2µl PP450, and 1.5 mg NaOAc (all obtained from Sigma-Aldrich, CH-Buchs) dissolved in 100 mL MeOH (HPLC Supra grade, Scharlau) as internal standard. GC-MS or GC-FID analysis and the kinetic experiments were performed on a Thermo Scientific ISQ system consisting of a single quadrupole mass spectrometer and a Trace GC Ultra. As stationary phase a Zebron ZB-5MS was used (30 m length, 0.25 mm internal diameter, 0.25 µm film thickness). The separation was performed using the following temperature profile: 5 min 50 °C, 15 °C/min to 250 °C, 10 min 250 °C. GC-FID analyses to measure the reaction order of the reagents were done using the same temperature program. Dodecane was used as an internal standard.

Materials and methods: Unless otherwise stated, starting materials were purchased from Aldrich and/or Fluka. All reagents were used as received. Chloro(triphenylphosphine)gold(I)[1], chlorobis-(triphenylphosphine)gold(I)[2], acetato(triphenylphosphine)gold(I)[3], (methoxycarbonylethynyl)(triphenyl-phosphine)gold(I)[4], pentafluorophenyl(triphenylphosphine)gold(I)[5], dichloro(phenyl)-λ3-iodane[6] were synthesized according to previously reported procedures. Solvents were purchased in HPLC quality, degassed by purging thoroughly with dinitrogen and dried over activated molecular sieves of appropriate size. Alternatively, they were purged with argon and passed through alumina columns in a solvent purification system (Innovative Technology). Unless otherwise stated, reactions were performed under normal conditions without protecting gas, dry solvents and sealed schlenk flasks. Conversion was monitored by thin layer chromatography (TLC) using Merck TLC silica gel 60 F_{254} (Merck) with a silica layer thickness of 0.2 mm and a particle size of 10 – 12 µm supported by aluminium foil. Column chromatography was performed using silica gel 60 M 230 – 400 mesh (Macherey-Nagel) and distilled solvents. Unless otherwise stated, reported yields of pure isolated products after column chromatography are given. For *in situ* relative quantitation by NMR, molar fractions for the corresponding products/intermediates have been determined by integration of ^{1}H and ^{19}F NMR signals.

[1] Y. Li, P. Tang, Y. Chen, B. Yu, *J. Org. Chem.* 2008, **73**, 4323.
[2] N. C. Baenziger, K. M. Dittermore, J. R. Doyle, *Inorg. Chem.* 1974, **13**, 805.
[3] A. Iglesias, K. Muniz, *Chem. Eur. J.* 2009, **15**, 10563.
[4] O. Fujimura, K. Fukunaga, T. Honma, T. Machida, U.S. Patent US 2010/0237770 A1, September 23, 2010.
[5] X. C. Cambeiro, T. C. Boorman, P. Lu, I. Larrosa, *Angew. Chem., Int. Ed.* 2013, **52**, 1781.
[6] A. Podgoršek, J. Iskra, *Molecules* 2010, **15**, 2857.

2. Mechanistic studies with alkynyl-iodonium salts (Scheme 2 in the main text)

Additional pathways to those described in Scheme 2 in the main text can be envisaged from a putative alkynyliodonium intermediate **V**. A regioselective nucleophilic attack of the arene onto the terminal carbon atom of the activated alkyne could produce an alkylidene intermediate (**VIII**). Upon 1,2-migration of the aromatic group, the observed ethynylated products could also be obtained as demonstrated by Nagao *et al.* (Figure S1, path B.3).[7] Alternatively, in the case of aromatic and alkylic ketones, insertion of the carbene into a proximal Csp^2 or Csp^3-H bond could also afford cyclopentenones **IX** and **X** respectively, as previously observed by Stang[8] and Taniguchi[9] (Figure S1, path B.4). However, the reactions of phenyl- or *tert*-butyl alkynyl ketones under the standard reaction conditions delivered the corresponding cross-coupling products in high yield and no C-H insertion products (**IX**, **X**) could be detected, in clear contrast to the above mentioned reports.[8,9]

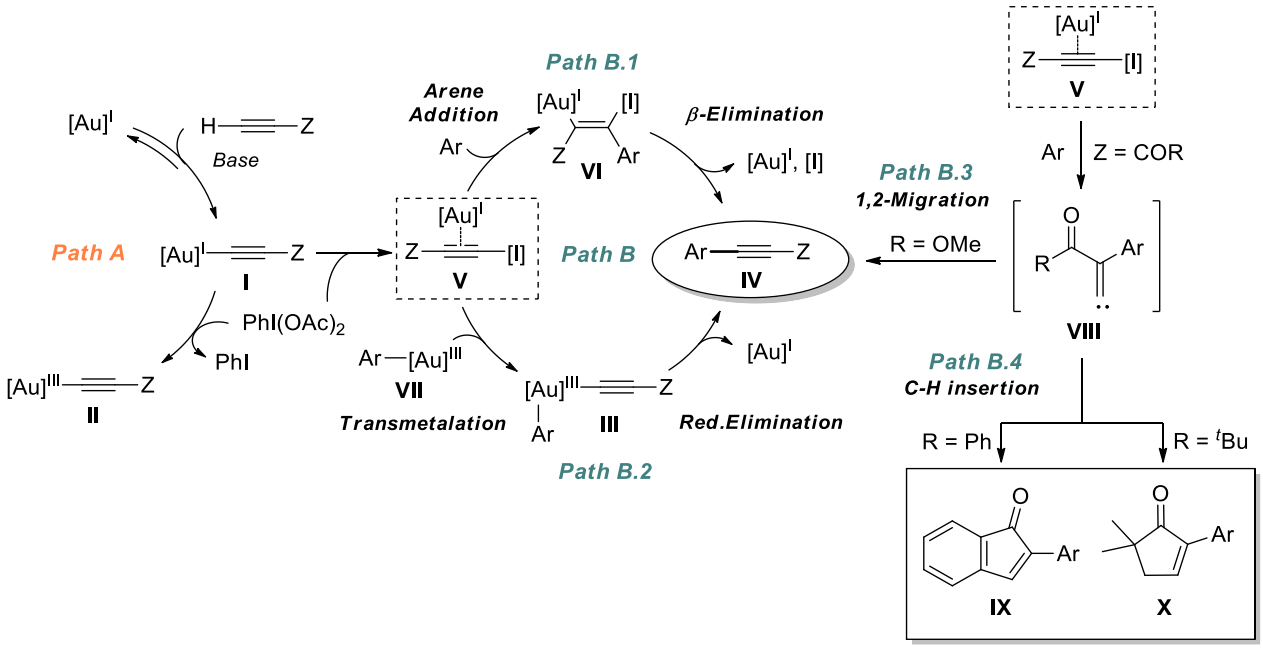
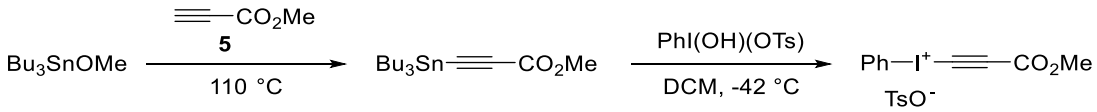


Figure S1. Possible scenarios involving alkynyliodonium intermediates (**V**) – addendum to Scheme 2 in the main text

[7] M. Ochiai, T. Ito, Y. Takaoka, Y. Masaki, M. Kunishima, S. Tani, Y. Nagao, *J. Chem. Soc., Chem. Commun.* 1990, 118.
[8] B. L. Williamson, R. R. Tykwinski, P. J. Stang, *J. Am. Chem. Soc*. 1994, **116**, 93.
[9] T. Kitamura, L. Zheng, H. Taniguchi, *Tetrahedron Lett.* 1993, **34**, 4055.

2.1 Synthesis of alkynyl(phenyl)iodonium tosylate [10,11]



Under dinitrogen atmosphere, a mixture of methoxytributylstannane (4.66 g, 14.5 mmol) and methyl propiolate (2.73 g, 32.5 mmol) was stirred for 3 h at 110 °C. The methanol and the excess of methyl propiolate were distilled off and the crude was dried under vacuum to afford [(carbomethoxy)-ethynyl]tributylstannane in quantitative yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 3.69 (s, 3H), 1.64 - 0.72 (m, 27H).

Under dinitrogen atmosphere, a solution of [(carbomethoxy)ethynyl]tributylstannane (385 mg, 1.03 mmol) in dichloromethane (10 mL) was added dropwise to a stirred suspension of hydroxy{[(4-methylphenyl)-sulfonyl]oxy}phenyl-λ^3-iodane (392 mg, 1.0 mmol, 0.1 M) in dichloromethane at –42 °C. Stirring was maintained at –42 ºC for 45 min monitored by addition of an equal volume of diethyl ether (3 x 20 mL) and stirring at –42 °C for 3 h. The white precipitate was filtered and recrystallized immediately from dichloromethane/pentane and dried to afford the desired product (137 mg, 0.3 mmol) in 30% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.08 (d, J = 7.8 Hz, 2 H), 7.64 -7.53 (m, 3 H), 7.45 (t, J = 7.8 Hz, 2 H), 7.10 (d, J = 7.8 Hz, 2H), 3.77 (s, 3H), 2.33 (s, 3H).

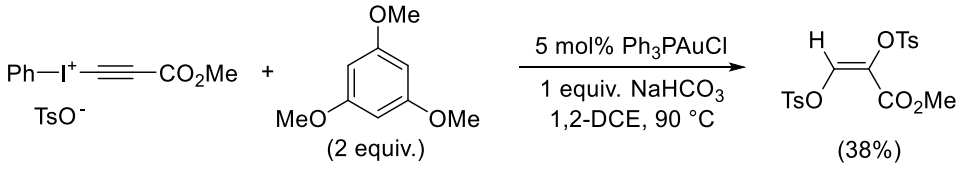
[10] M. W. Logue, K. Teng, *J. Org. Chem* 1982, **47**, 2549.
[11] a) B. L. Williamson, P. J. Stang, A. M. Arif, *J. Am. Chem. Soc.* 1993, **115**, 2590. b) P. J. Stang, M. Boeshar, H. Wingert, T. Kitamura, *J. Am. Chem. Soc.* 1988, **110**, 3272.

2.2 Control experiments: mechanisms B.1, B.2 B.3

Alkynyliodonium salts[12] have been successfully used in metal-catalyzed cross-coupling reactions with organo-copper, -stannanes and -boronic acids[12] and also, as mentioned in the introduction, in reactions with activated arenes.[13] In line with these precedents, several scenarios could be envisaged to justify the formation of the observed cross-coupling products from intermediate **V**. In addition to the proposed arene addition/*β*-elimination already described (Figure S1, path B.1),[14d] transmetalation between alkynyliodonium salt **V** and putative aryl-Au(III) species (**VII**) produced *in situ* within the oxidative reaction media[14] could also deliver intermediate **III**, which would yield the observed products after reductive elimination as shown in Figure S1, path B.2.

Treatment of alkynyl(phenyl)iodonium tosylate with 1,3,5-trimethoxybenzene with or without Ph_3PAuCl, in the presence or absence of base either at 0, 25 or 90 °C, did not furnish the desired Csp^2-Csp cross coupling product. As a representative example, the reaction shown in section 2.2.1, carried out with 5 mol% Ph_3PAuCl and 1 equivalent of $NaHCO_3$ produced (*E*)-methyl 2,3-bis(tosyloxy)acrylate in 38% isolated yield while the arene was recovered intact.

2.2.1 Reactivity of alkynyl(phenyl)iodonium tosylate in presence of Au(I) complexes



To a solution of the alkynyl(phenyl)iodonium tosylate (57.0 mg, 0.125 mmol), $NaHCO_3$ (11.0 mg, 0.125 mmol) and 1,3,5-trimethoxybenzene (42.0 mg, 0.25 mmol) in 1,2-dichloroethane (0.9 mL), chloro(triphenylphosphine)gold(I) (3.0 mg, 0.006 mmol) was added. The mixture was stirred under dinitrogen atmosphere at 90 ºC for 12 h. The reaction mixture was filtered over a pad of Celite and purified by flash column chromatography using hexane:DCM (3:7) to give methyl-1,3-ditosyl-2-propenoate (10.2 mg, 0.024 mmol) in 38% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 7.78 (d, *J* = 8.4 Hz, 2H), 7.72 (d, *J* = 8.4 Hz, 2H), 7.67 (s, 1H), 7.35 (d, *J* = 8.0 Hz, 2H), 7.30 (d, *J* = 7.9 Hz, 2H), 3.71 (s, 3H), 2.45 (s, 3H),

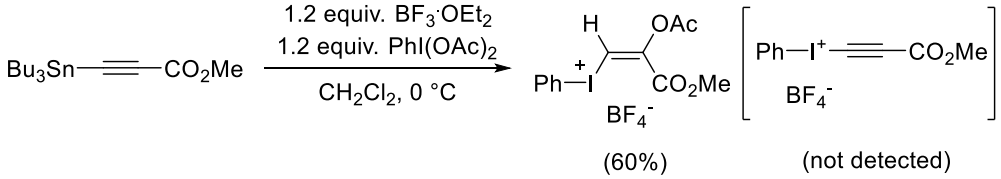
[12] (a) P. J. Stang, T. Kitamura, *J. Am. Chem. Soc.* 1987, **109**, 7561. (b) T. Kitamura, T. Tanaka, H. Taniguchi, P. J. Stang, *J. Chem. Soc., Perkin Trans. 1* 1991, 2892. (c) C. -M. Yu, J. -H. Kweon, P. -S. Ho, S. -C. Kang, G. Y. Lee, *Synlett* 2005, **17**, 2631.

[13] (a) J. P. Brand, J. Charpentier, J. Waser, *Angew. Chem., Int. Ed.* 2009, **48**, 9346. (b) J. P. Brand, J. Waser, *Angew. Chem., Int. Ed.* 2010, **49**, 7304. (c) J. P. Brand, J. Charpentier, J. Waser, J. *Beilstein J. Org. Chem.* 2011, **7**, 565. (d) J. P. Brand, C. Chevalley, R. Scopelliti, J. Waser, *Chem. Eur. J.* 2012, **18**, 5655. (e) Y. Li, J; P. Brand, J. Waser, *Angew. Chem., Int. Ed.* 2013, **52**, 6743. (f) Y. Li, J. Waser, *Beilstein J. Org. Chem.* 2013, **9**, 1763. (g) J. P. Brand, Y. Li, J. Waser, *Israel J. Chem.* 2013, **53**, 901.

[14] (a) M. S. Kharasch, H. S. Isbell, *J. Am. Chem. Soc.* 1931, **53**, 3053. (b) K. S. Liddle, C. Parkin, *J. Chem. Soc. Chem. Commun.* 1972, 26. (c) P. W. J. deGraaf, J. Boersma, G. J. M. Van der Kerk, *J. Organomet. Chem.* 1976, **105**, 399. (d) K. A. Porter, A. Schier, H. Schmidbaur, *Organometallics* 2003, **22**, 4922.

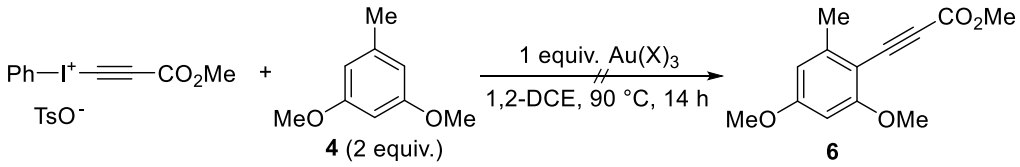
2.44 (s, 3H). ^{13}C NMR (125 MHz, $CDCl_3$): δ = 161.9, 146.8, 145.9, 139.6, 133.4, 131.8, 130.5, 129.9, 128.7, 128.4, 126.7, 52.9, 22.0, 22.0.

2.2.2 Attempt to synthesize [(carbomethoxy)ethynyl]-iodonium tetrafluoroborate



To a solution of [(carbomethoxy)ethynyl]tributylstannane (1.0 g, 2.6 mmol) in dichloromethane (20 mL), $BF_3{\cdot}Et_2O$ (0.39 mL, 3.12 mmol) was added at 0 °C under dinitrogen atmosphere and the mixture was stirred for 15 min. A solution of diacetoxy(phenyl)-λ^3-iodane (1.0 g, 3.2 mmol) in dichloromethane (20 mL) was added at 0 °C and the mixture was stirred for 1 h. After the addition of a saturated aqueous solution of sodium tetrafluoroborate (10 mL), the mixture was stirred for 15 min and then extracted with dichloromethane, washed with water and dried over $MgSO_4$. Further purification by trituration using hexane/diethyl ether gave alkenyl(phenyl)iodonium tetrafluoroborate (675 mg, 1.5 mmol) in 60% isolated yield. ^{1}H NMR (400 MHz, $CDCl_3$): δ = 8.07 (d, J = 7.5 Hz, 2H), 7.76 (s, 1H), 7.67 (t, J = 7.5 Hz, 1H), 7.50 (t, J = 7.5 Hz, 2H), 3.83 (s, 3H), 2.24 (s, 3H). ^{13}C NMR (100 MHz, $CDCl_3$): δ = 167.2, 157.9, 149.5, 136.1, 133.2, 132.6, 110.5, 99.2, 53.9, 19.9. HRMS (ESI): *m/z*: calcd for $C_{12}H_{12}IO_4$: 346.9774 found: 346.9773.

2.2.3 Reactivity of alkynyl(phenyl)iodonium tosylate in presence of Au(III) complexes



General procedure: To a mixture of alkynyl(phenyl)iodonium tosylate (22.1 mg, 0.05 mmol), 3,5-dimethoxytoluene (**4**) (15.2 mg, 0.10 mmol) in 1,2-dichloroethane (0.5 mL), a gold(III) complex (0.05 mmol) was added. The mixture was stirred under dinitrogen atmosphere at 90 ºC for 14 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR and GC-MS. When **4** was pre-stirred with Au(III) to form Ar-Au(III) species in situ, the reaction outcome did not change.

A) Gold(III) acetate

Following the general procedure using gold(III) acetate (18.7 mg, 0.05 mmol), no reactivity to compound **6** was found. Instead, alkynyl iodonium salt decomposed to iodobenzene and the gold(III) acetate to Au(0).

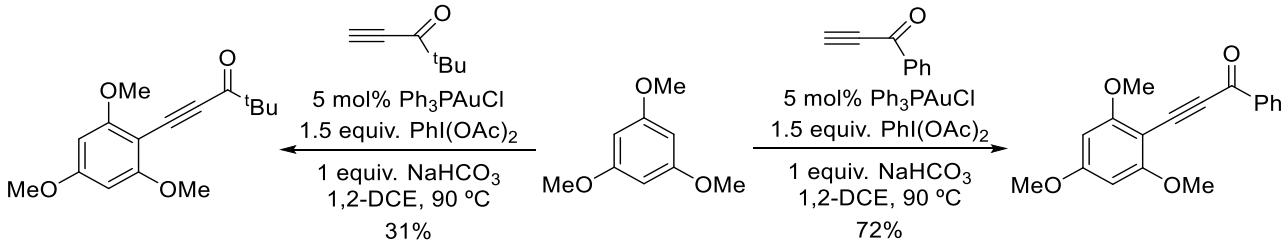
B) Gold(III) chloride

Following the general procedure using gold(III) chloride (15.2 mg, 0.05 mmol), no reactivity to compound **6** was found. Alkynyl iodonium salt decomposed to iodobenzene and the gold(III) chloride showed the formation of Au(0).

C) Trichloro(triphenylphosphine)gold(III)

Following the general procedure using trichloro(triphenylphosphine)gold(III) (28.3 mg, 0.05 mmol), no reactivity to compound **6** was found. Alkynyl iodonium salt decomposed to iodobenzene and the gold(III) chloride showed the formation of Au(0). 2-Chloro-3,5-dimethoxytoluene was found in 51% molar ratio (^{1}H-NMR).

2.3 Control experiments: mechanism B.4

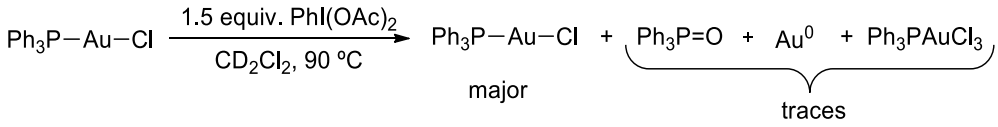


General procedure for the gold-catalyzed ethynylation of arenes: To a solution of 1,3,5-trimethoxybenzene (2 equiv.), diacetoxy(phenyl)-λ3-iodane (1.5 equiv.), $NaHCO_3$ (1.0 equiv.) and the corresponding alkyne (1 equiv.) in anhydrous 1,2-dichloroethane (0,5 M), chloro(triphenylphosphine)-gold(I) (0.05 equiv.) was added. The reaction was stirred at 90 °C for 12 h. The crude was filtered over a pad of Celite and purified by flash column chromatography on silica gel. In case of 4,4-dimethyl-1-pentyn-3-one the coupling product 3-(2,4,6-trimethoxyphenyl)-1-*t*-butyl-2-propyn-1-one was found in 31% isolated yield. Remaining starting materials were recovered. In case of 1-phenyl-2-propyn-1-one the coupling product 3-(2,4,6-trimethoxyphenyl)-1-phenyl-2-propyn-1-one was found in 72% isolated yield. In both reactions, no indication of C-H insertion products (**IX**, **X** in Fig. S1) could be found upon careful spectroscopic analysis of the reaction mixtures. The synthesis and the spectroscopic details of observed cross-coupling products have been already previously reported.[15]

[15] T. de Haro, C. Nevado, *J. Am. Chem. Soc.* 2010, **132**, 1512.

3. Mechanistic investigation with stoichiometric Au(I) and Au(III) complexes

3.1 Oxidation of chloro(triphenylphosphine)gold(I) by $PhI(OAc)_2$



To a solution of diacetoxy(phenyl)-λ3-iodane (19 mg, 0.06 mmol) and dichloromethane-d_2 (0.5 mL), chloro(triphenylphosphine)gold(I) (20 mg, 0.04 mmol) was added. The reaction was performed in a sealed NMR-tube and heated to 90 °C for 3 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S2-3). Trace amounts of $Ph_3P{=}O$, Au^0 and Ph_3PAuCl_3 were found only after prolonged heating.

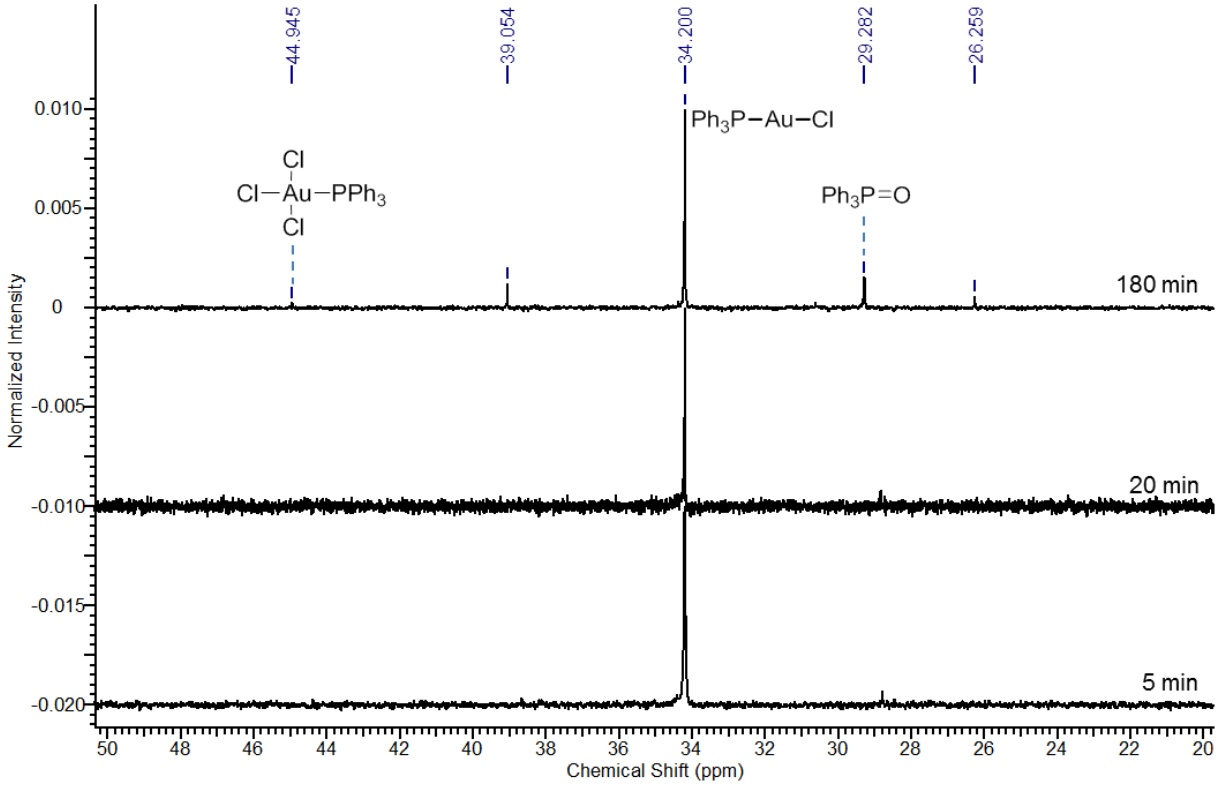


Figure S2. *In situ* ^{31}P-NMR spectrum of the reaction between Ph_3PAuCl and $PhI(OAc)_2$

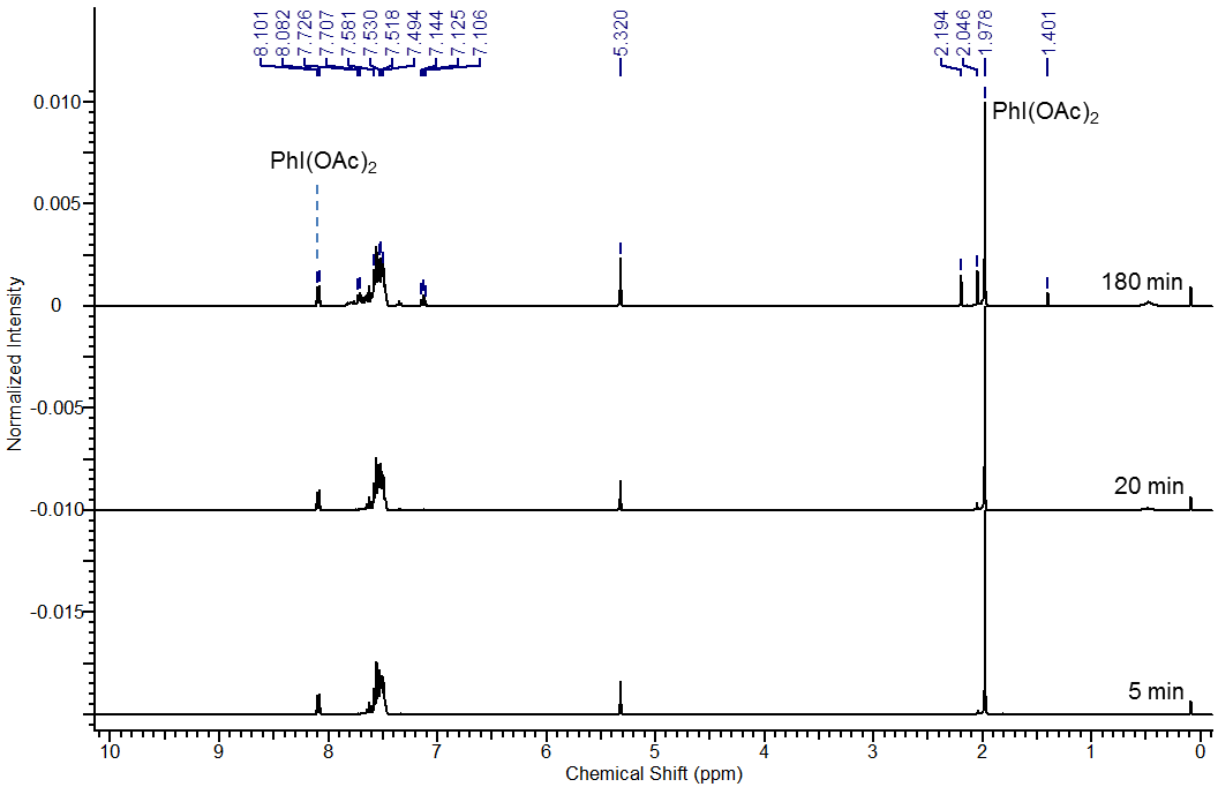
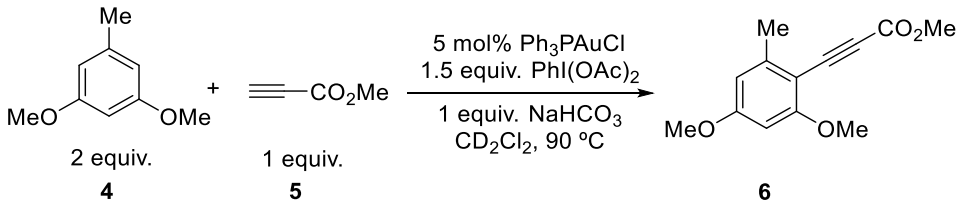


Figure S3. *In situ* ^{1}H-NMR spectrum of the reaction between Ph_3PAuCl and $PhI(OAc)_2$

3.2 Monitoring the reaction mixture by ^{1}H- and ^{31}P-NMR



To a solution of 3,5-dimethoxytoluene (**4**) (12.2 mg, 0.08 mmol), diacetoxy(phenyl)-λ3-iodane (19 mg, 0.06 mmol), $NaHCO_3$ (3 mg, 0.04 mmol) and methyl propiolate (**5**) (3.4 mg, 0.04 mmol) in dichloromethane-d_2 (0.5 mL), chloro(triphenylphosphine)gold(I) (1 mg, 0.002 mmol) was added. The reaction was performed in a sealed NMR-tube and heated to 90 °C for 23 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S4-5). (Methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) was found as an intermediate and a P-containing product with a signal at ca. 31 ppm was found (**7**) (see section 4.3 for identification of this signal).

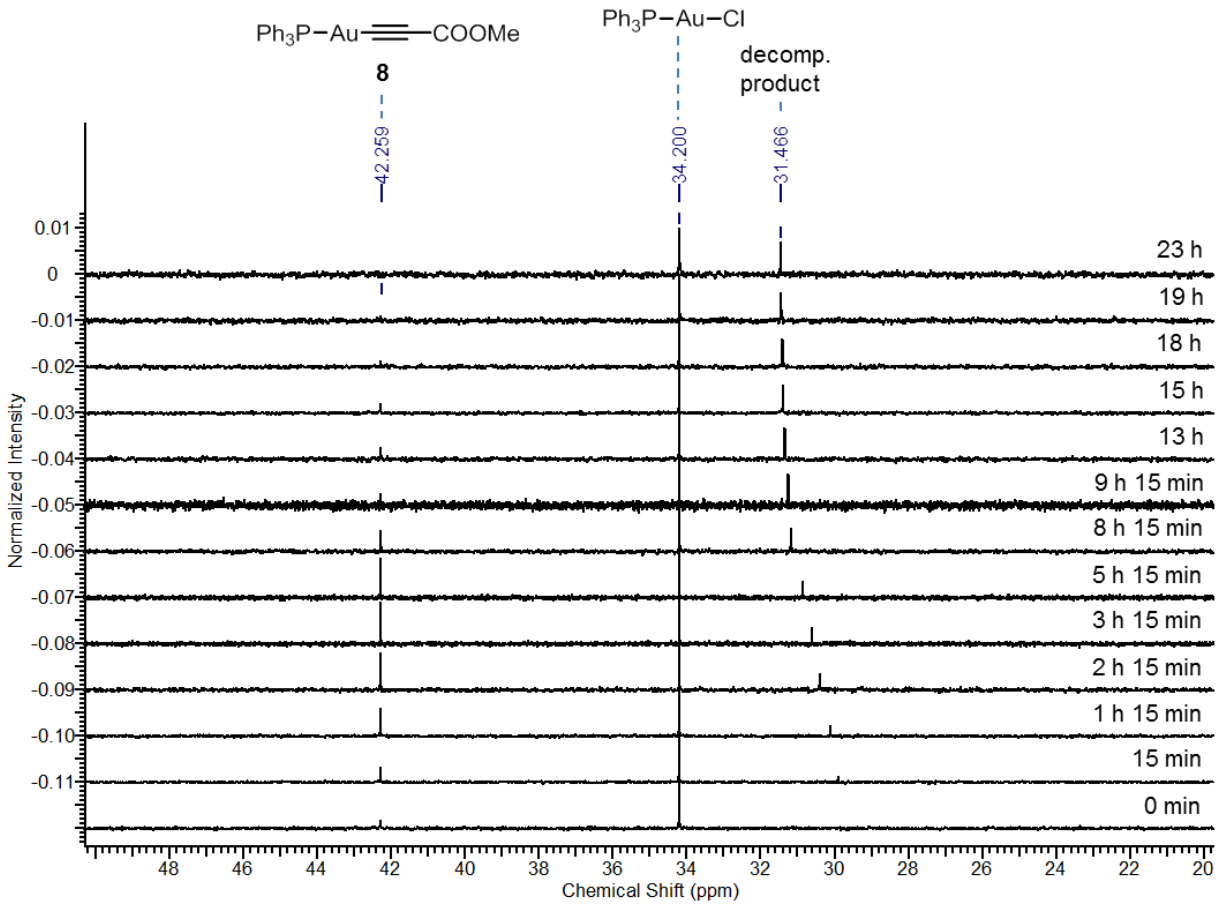


Figure S4. *In situ* ^{31}P-NMR spectrum of the catalytic reaction

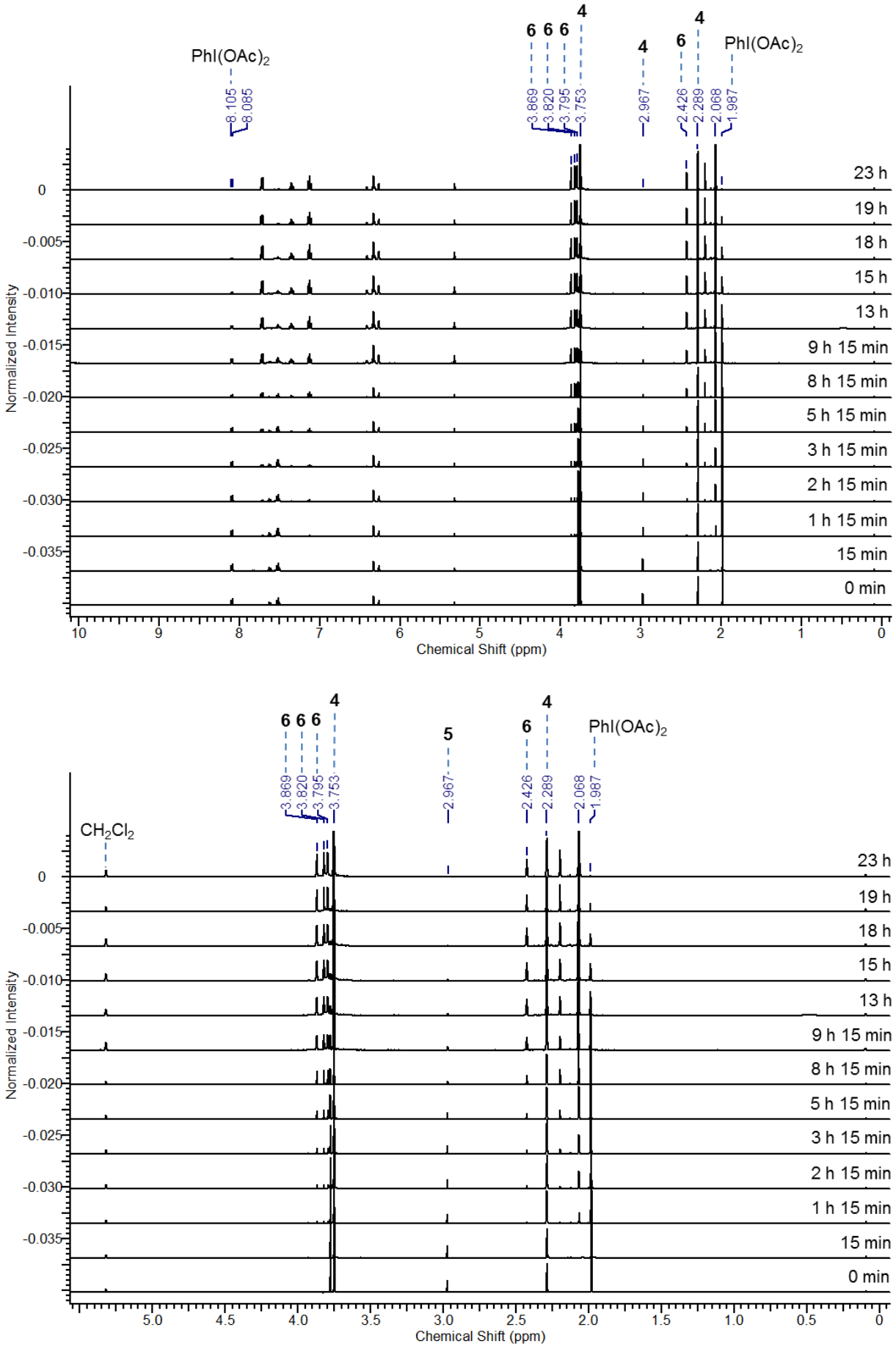
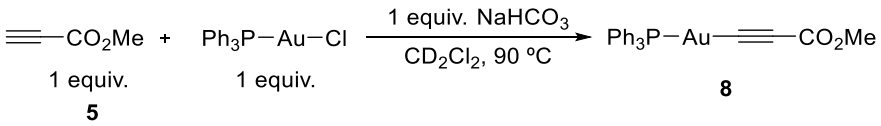


Figure S5. *In situ* ^{1}H-NMR spectrum of the catalytic reaction. Overview (top), close-up (bottom)

3.3 Formation of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (8) (Figure 1 in the main text)

3.3.1 Non oxidative conditions in presence of Ph_3PAuCl (Figures 1b in the main text)



To a solution of methyl propiolate (**5**) (3.4 mg, 0.04 mmol) and $NaHCO_3$ (3 mg, 0.04 mmol) in dichloromethane-d_2 (0.5 mL), chloro(triphenylphosphine)gold(I) (20 mg, 0.04 mmol) was added. The reaction was performed in a sealed NMR-tube and heated to 90 °C for 2 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S6-7). Traces of compound **8** were observed after 2 h.

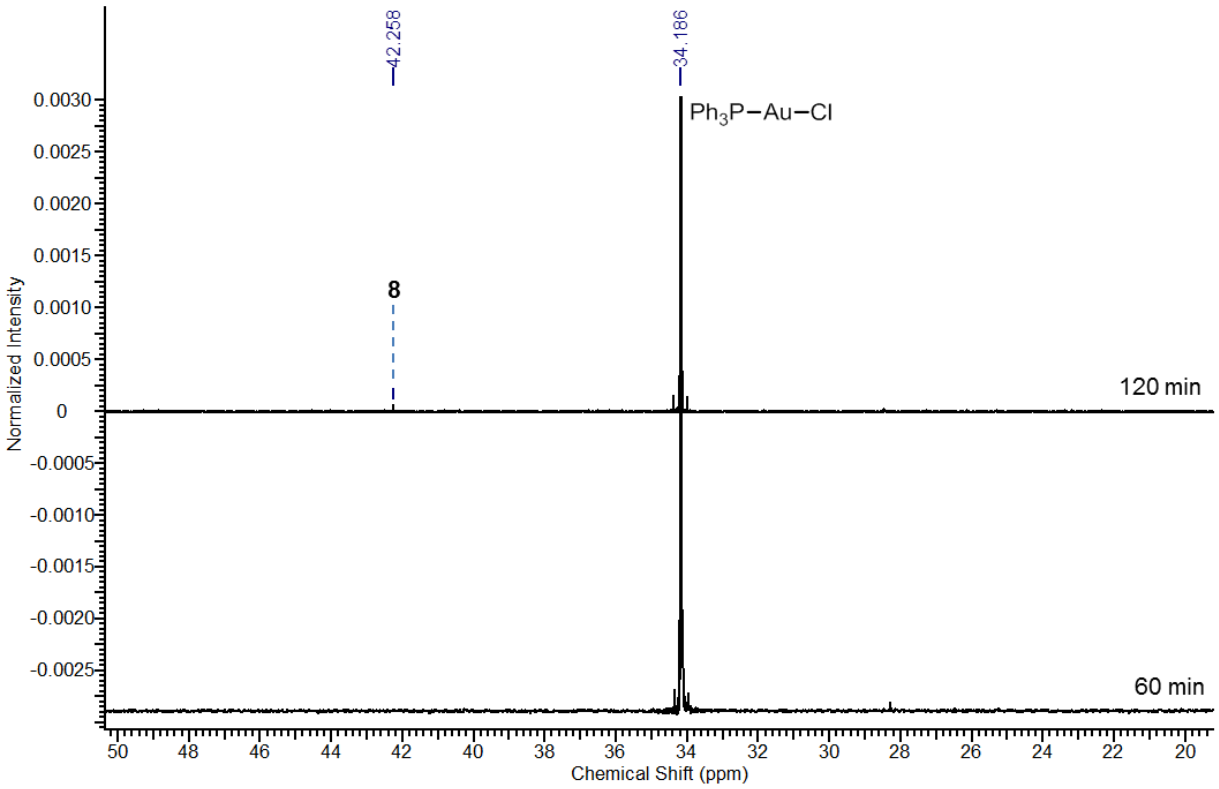


Figure S6. *In situ* ^{31}P-NMR spectrum of the reaction between **5** and Ph_3PAuCl

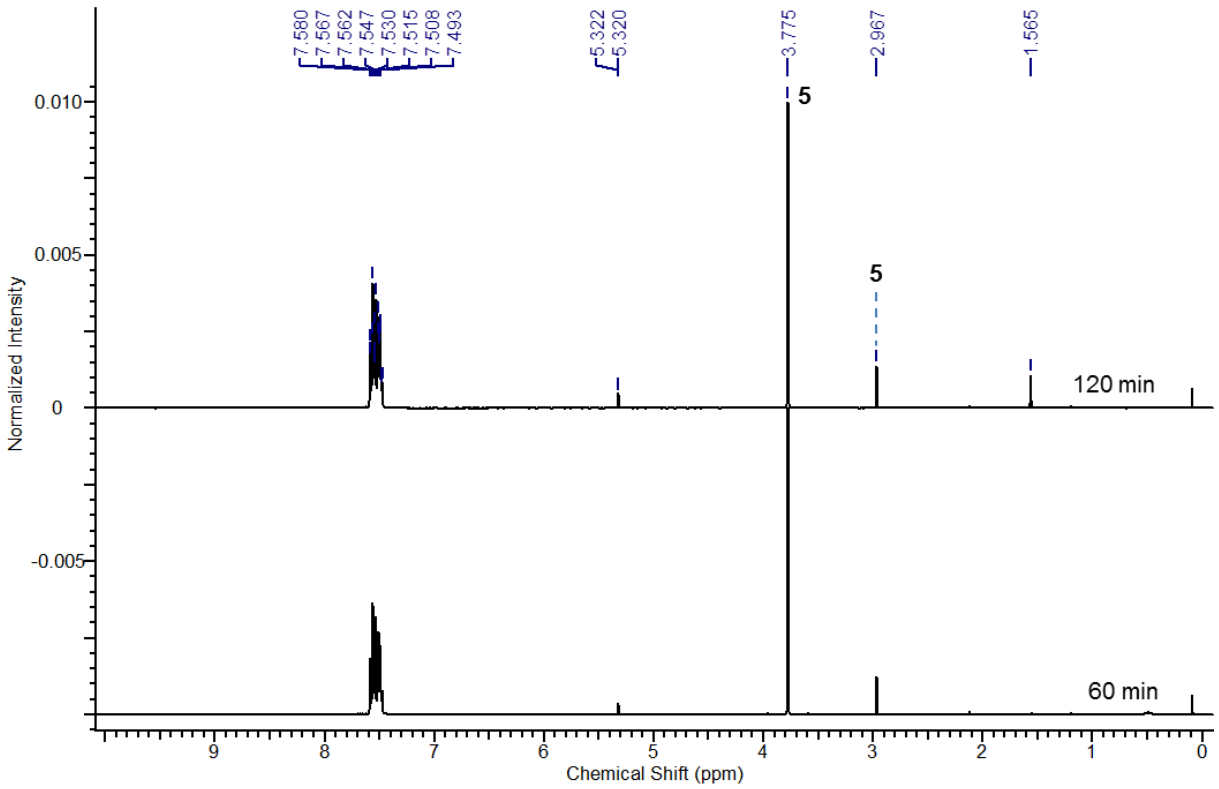
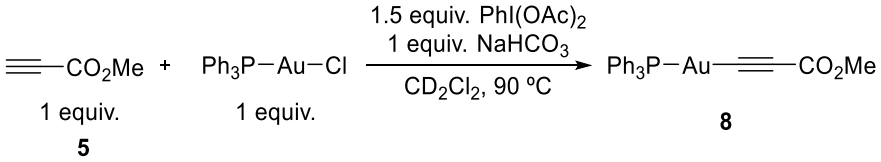


Figure S7. *In situ* ^{1}H-NMR spectrum of the reaction between **5** and Ph_3PAuCl

3.3.2 Oxidative conditions in presence of Ph_3PAuCl (Figure 1c in the main text)



To a solution of diacetoxy(phenyl)-λ3-iodane (19 mg, 0.06 mmol), $NaHCO_3$ (3 mg, 0.04 mmol) and methyl propiolate (**5**) (3.4 mg, 0.04 mmol) in dichloromethane-d_2 (0.5 mL), chloro(triphenyl-phosphine)-gold(I) (20 mg, 0.04 mmol) was added. The reaction was performed in a sealed NMR-tube and heated to 90 °C for 1 h. The reaction was monitored by ^{31}P- and ^{1}H-NMR (Figures S8-9). Compound **8** could be detected already after 5 min by ^{31}P-NMR.

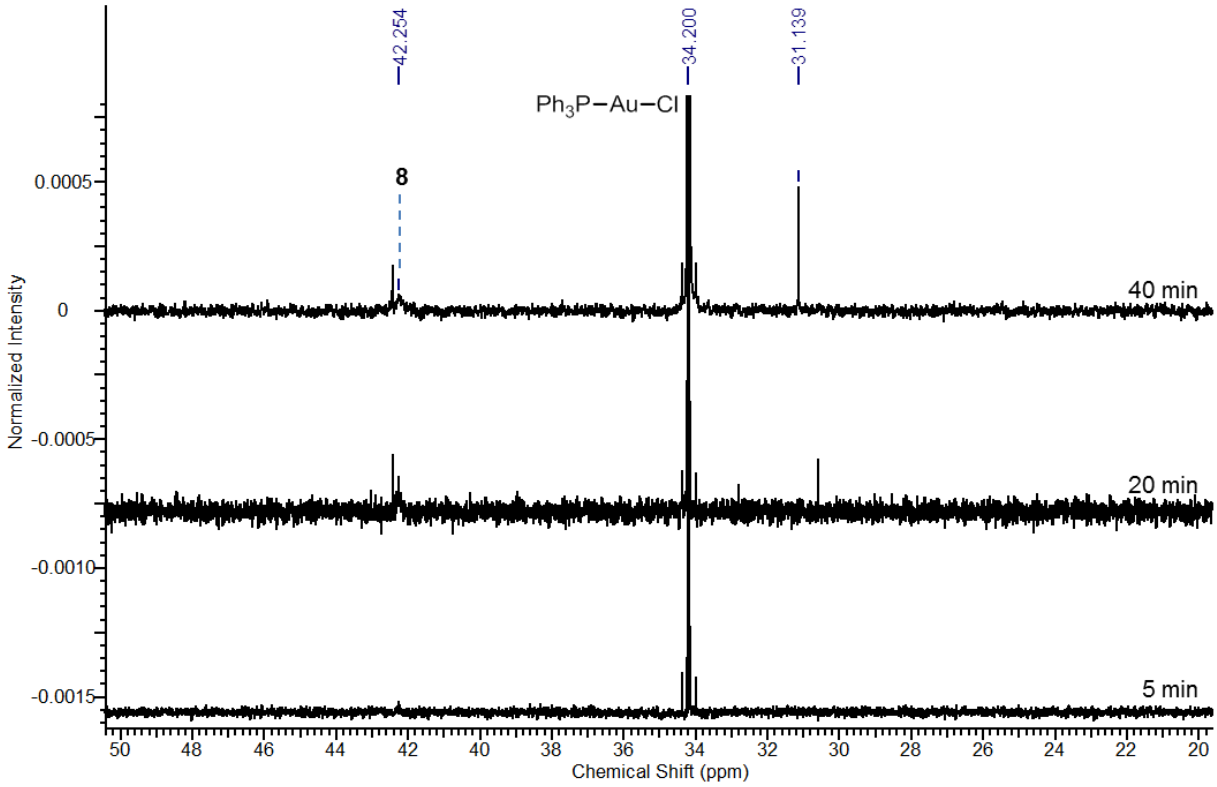


Figure S8. *In situ* ^{31}P-NMR spectrum of the reaction between **5** and Ph_3PAuCl in presence of $PhI(OAc)_2$ at 90 °C

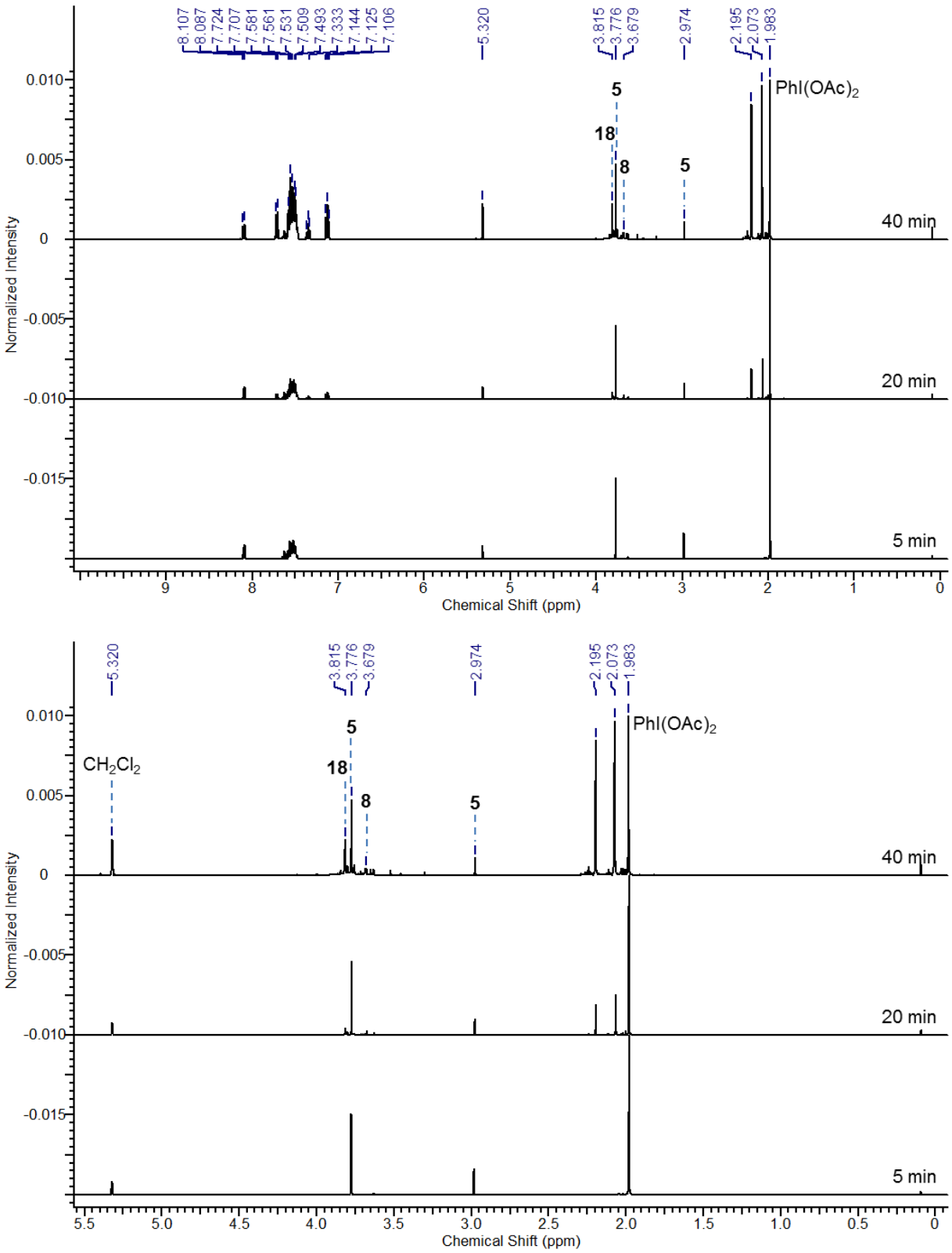
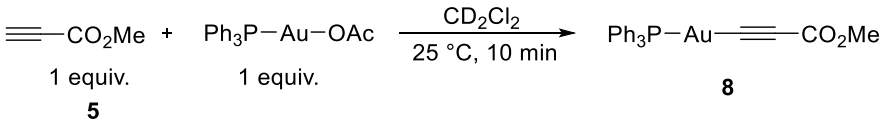


Figure S9. *In situ* ^{1}H-NMR spectrum of the reaction between **8** and Ph_3PAuCl in presence of $PhI(OAc)_2$ at 90 °C; total view (above), close-up (below)

The formation of alkyne homocoupling product **18** was explained by oxidation of **8** followed by an OAc-alkyne ligand exchange reaction on the Au(III)-acetylide intermediate (see section 3.6.1) or by transmetalation between the Au(I) and Au(III)-acetylide species coexisting in the reaction media (see section 3.6.5).

3.3.3 Non oxidative conditions in presence of $Ph_3PAuOAc$ in CD_2Cl_2 (Figure 1d in the main text)



To a mixture of methyl propiolate (**5**) (0.8 mg, 0.01 mmol) and acetato(triphenyl-phosphine)gold(I)[16] (5 mg, 0.01 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C. The reaction was monitored by ^{31}P-NMR (Figure S10). Compound **8** was formed after 10 min in quantitative yield. No formation of Ph_3PAuCl by solvent activation was observed.

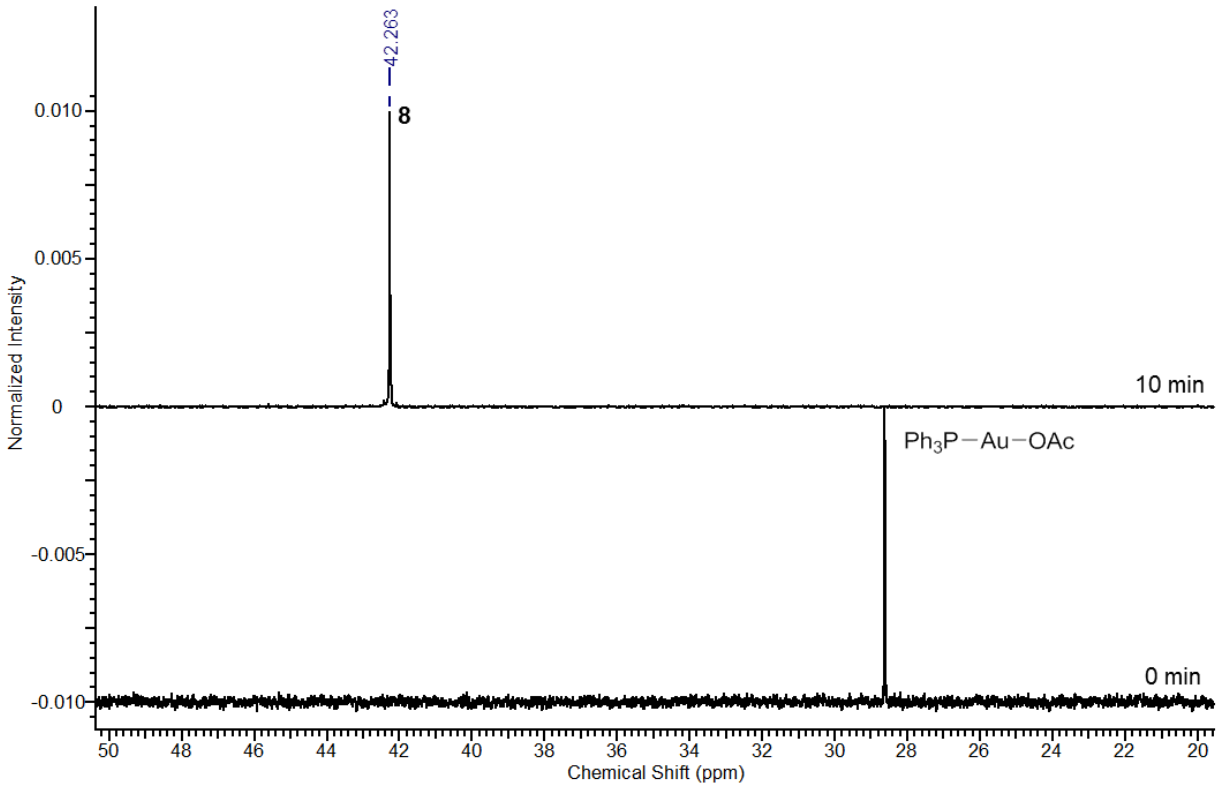
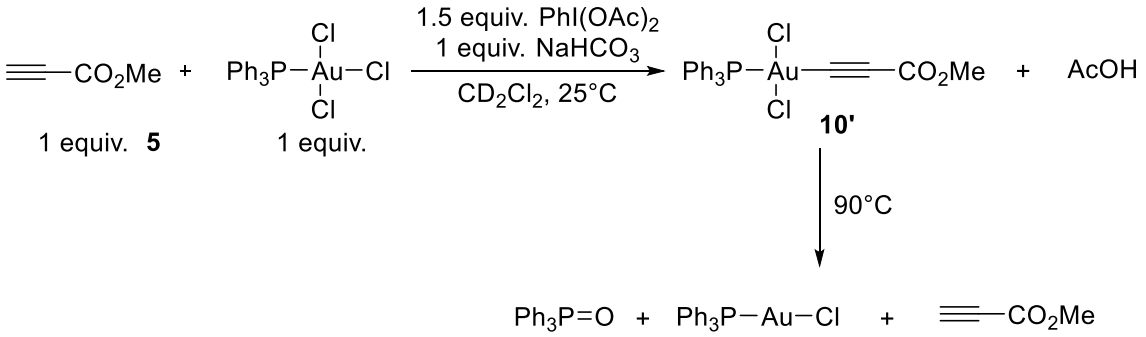


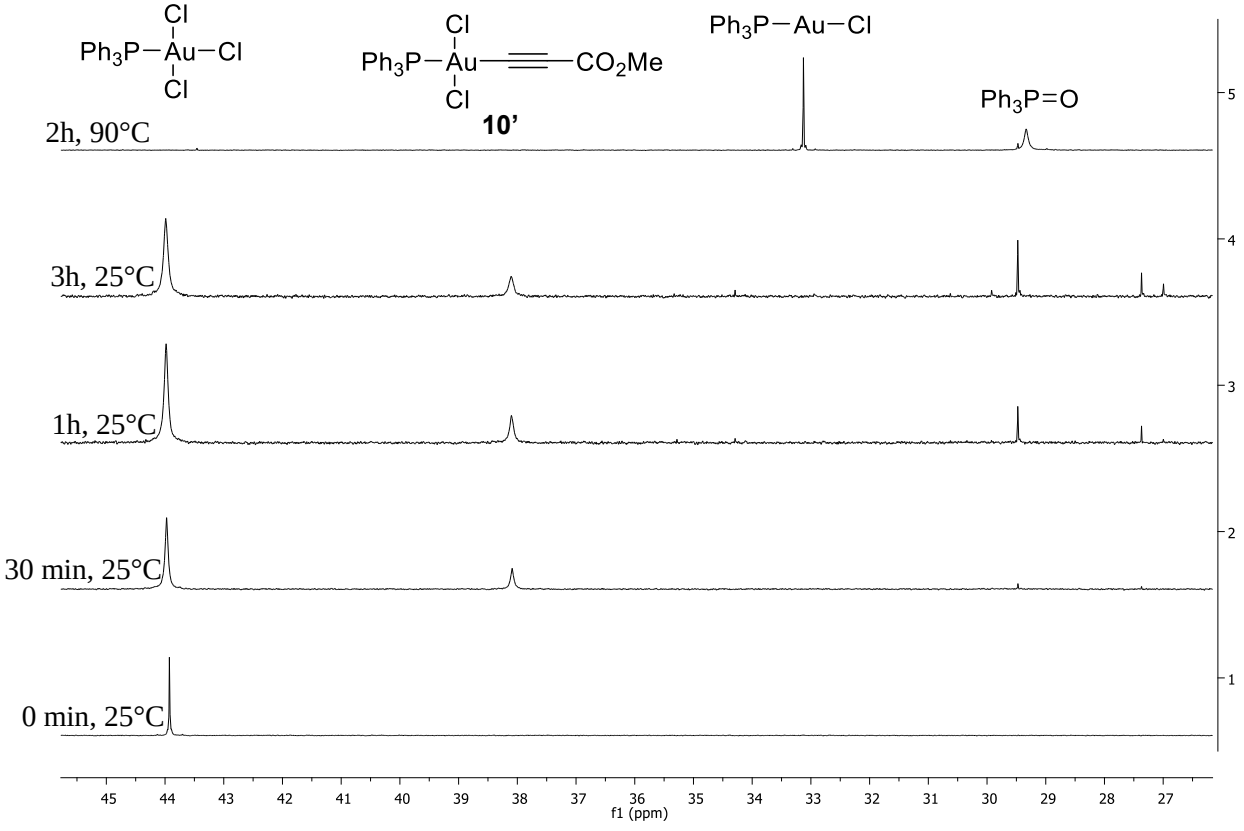
Figure S10. *In situ* ^{31}P-NMR spectrum of the reaction between **5** and $Ph_3PAuOAc$ in CD_2Cl_2

[16] A. Iglesias, K. Muñiz, *Chem. Eur. J.* **2009**, *15*, 10563.

3.3.4 Activation of alkyne with Ph_3PAuCl_3 in presence of $PhI(OAc)_2$.



To a solution of diacetoxy(phenyl)-λ^3-iodane (19 mg, 0.06 mmol), $NaHCO_3$ (3 mg, 0.04 mmol) and methyl propiolate (**5**) (3.4 mg, 0.04 mmol) in dichloromethane-d_2 (0.5 mL), trichloro(triphenyl-phosphine)-gold(III) (22.6 mg, 0.04 mmol) was added. The reaction was stirred in a sealed NMR-tube at 25 °C for 3 hours and then was heated at 90°C for 2 hours. The reaction was monitored by ^{31}P- and ^{1}H-NMR (Figure S11).

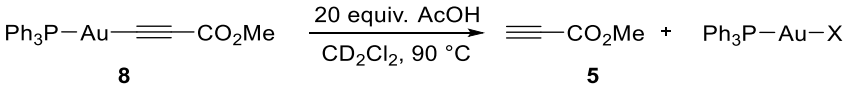


S11. *In situ* ^{31}P-NMR spectrum of the reaction between Ph_3PAuCl_3, $PhI(OAc)_2$ and $NaHCO_3$ at 25°C and 90 °C.

We aimed to clarify here whether $PhI(OAc)_2$ can trigger a Cl/OAc exchange in Au(III) (as we propose is the case with Au(I)) and subsequently, enable the reaction with free alkyne. At room temperature, slow conversion to a new complex (δ 38 ppm) is observed. Based on the chemical shift obtained for compound

10, we hypothesize that this new signal can be adscribed to its *trans*-isomer **10'** (note that, if Cl/OAc exchange were to take place, it would occur with the chloro ligand trans to the Ph_3P ligand. The reaction is slow (as it is the case for Au(I)) and when heated up, oxidation products ($Ph_3P=O$) are clearly observed: we hypothesize that, upon heating, the unreacted Ph_3PAuCl_3 might undergo reductive elimination to form Ph_3PAuCl and Cl_2, the latter responsible for the formation of the oxidation products.

3.3.5 Decomposition of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) under acidic conditions



8 **5**

To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I)[17] (**8**) (5.4 mg, 0.01 mmol) and acetic acid (12.0 mg, 0.20 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was heated in a sealed NMR-tube at 90 °C for 17 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S12-13). Compound **8** evolved to methyl propiolate **5** (12% molar ratio) and Au(0) together with diverse Ph_3PAu complexes.

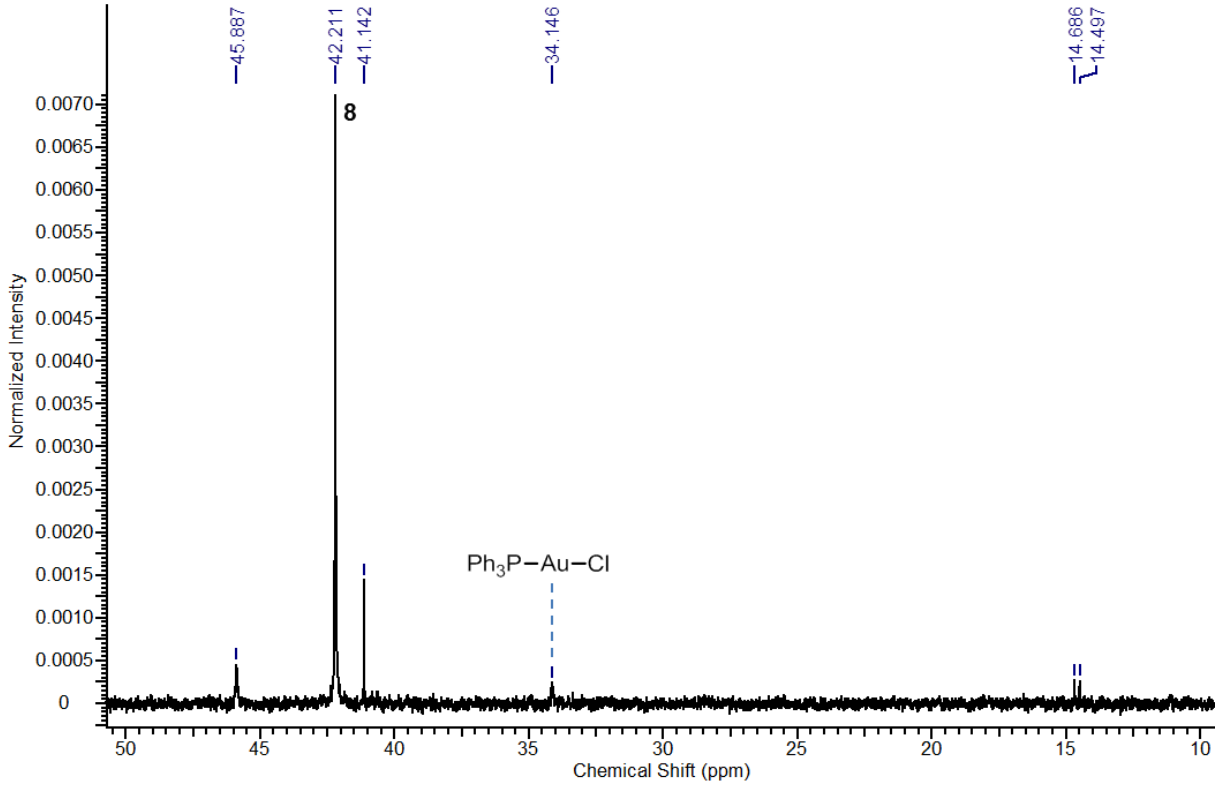


Figure S12. *In situ* ^{31}P-NMR spectrum of the reaction between **8** and AcOH

[17] O. Fujimura, K. Fukunaga, T. Honma, T. Machida, U.S. Patent US 2010/0237770 A1, September 23, 2010.

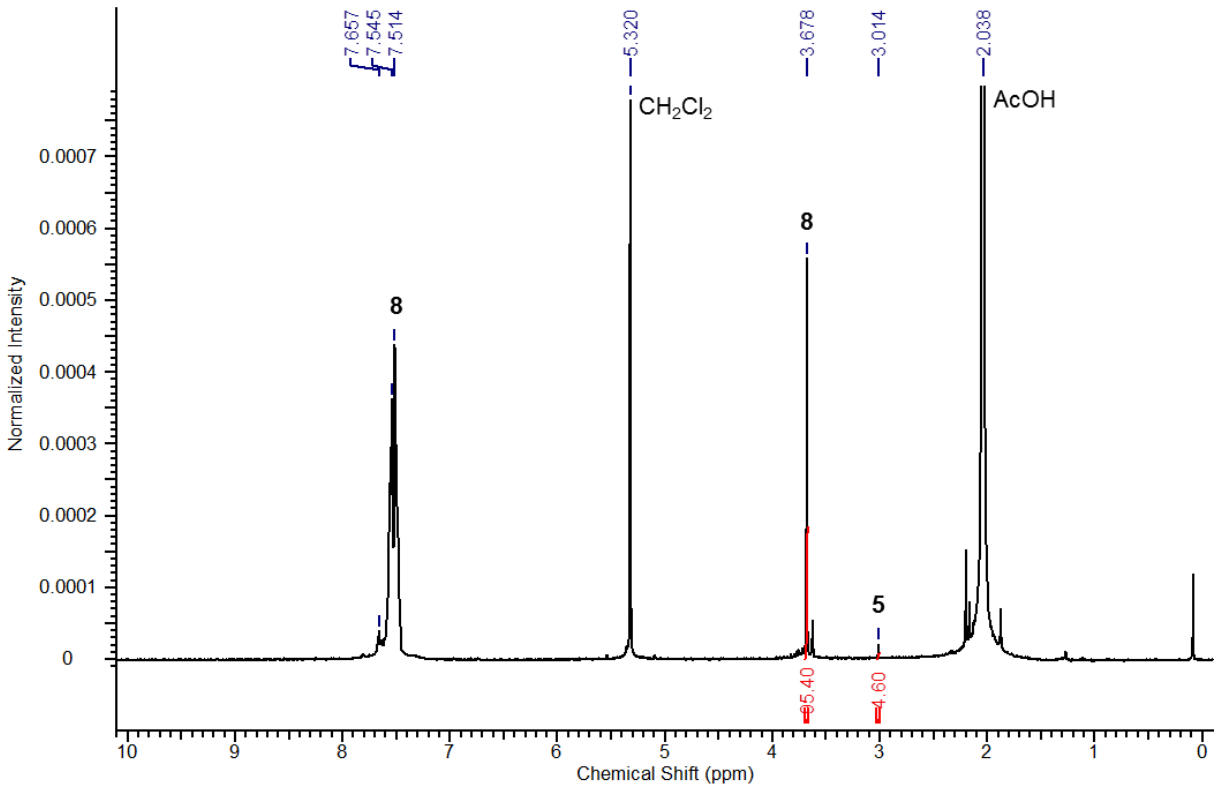
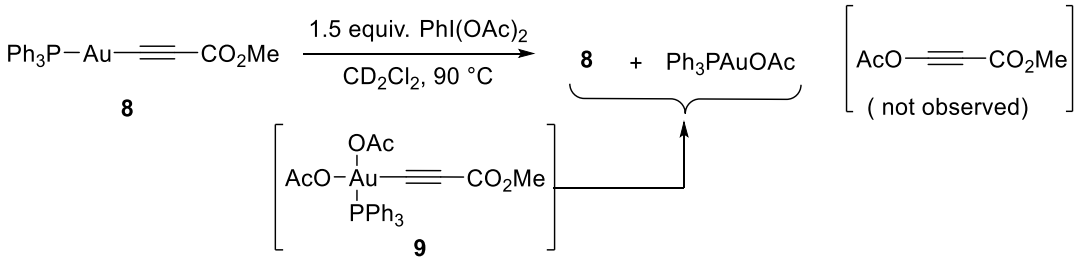


Figure S13. *In situ* ^{1}H-NMR spectrum of the reaction between **8** and AcOH

3.4 Oxidation of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (8) (Equations 2-4 in the main text)

3.4.1 Oxidation of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) by $PhI(OAc)_2$ (equation 2 in the main text)



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (5.4 mg, 0.01 mmol) and diacetoxy(phenyl)-λ^3-iodane (4.8 mg, 0.015 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C for 90 min, at 50 °C for 30 min and at 90 °C for 60 min. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S14-15). $Ph_3PAuOAc$ (^{31}P-NMR, $\delta = 28.51$ ppm) was the main product observed. Trace amounts of Ph_3PAuCl (^{31}P-NMR, $\delta = 34.13$ ppm) and $Ph_3P{=}O$ (^{31}P-NMR, $\delta = 29.48$ ppm) could also be identified in the reaction mixture.

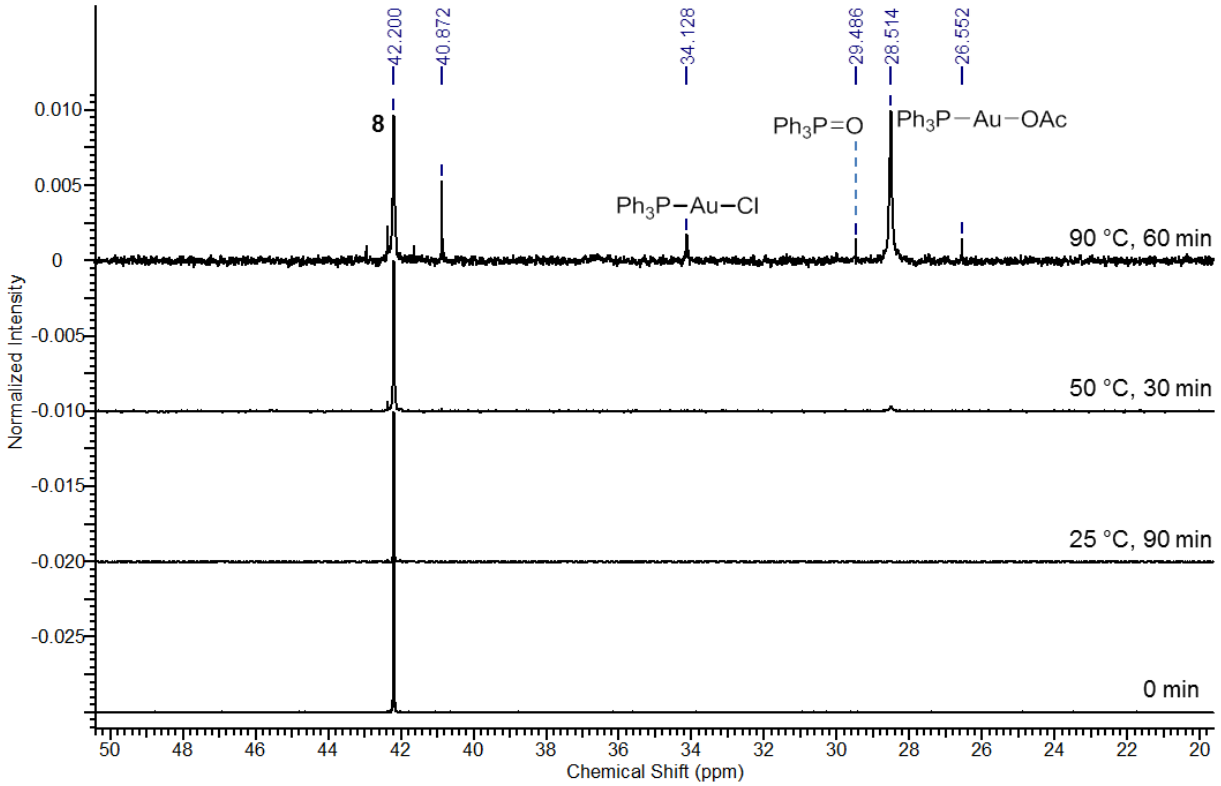


Figure S14. *In situ* ^{31}P-NMR spectrum of the reaction between **8** and $PhI(OAc)_2$

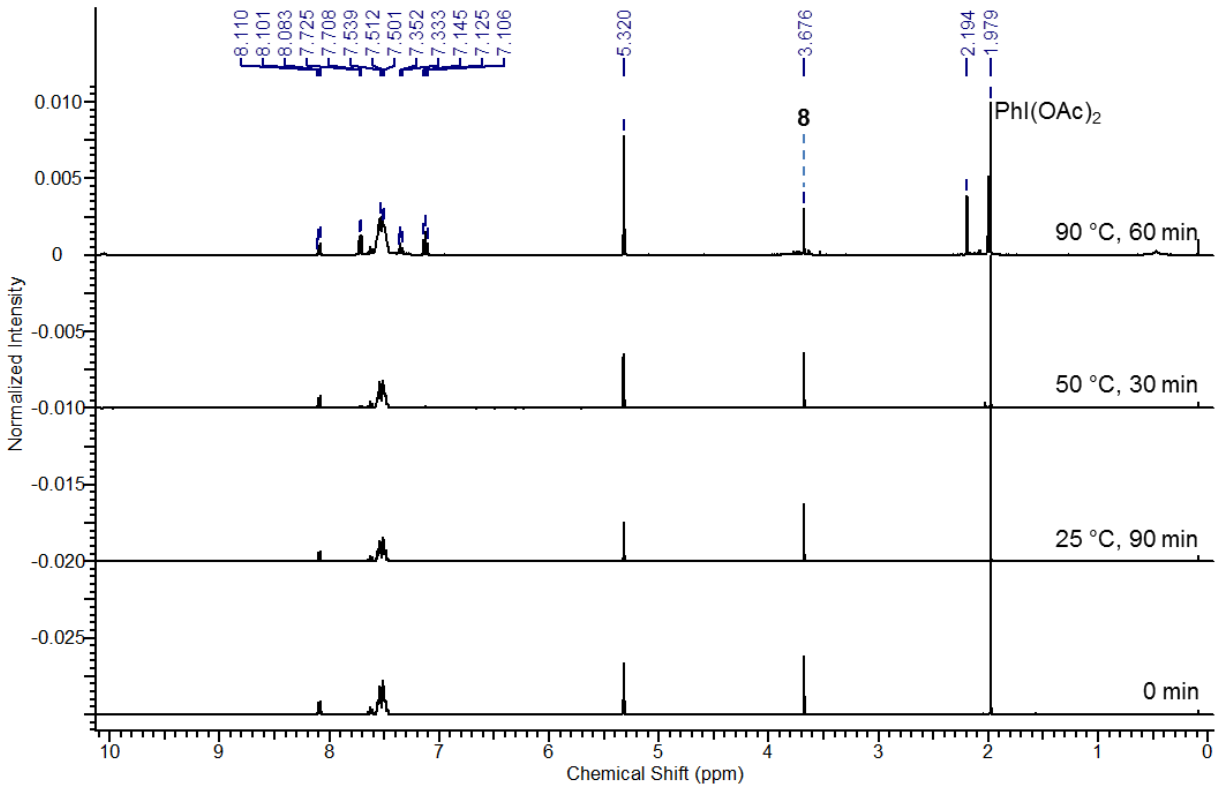
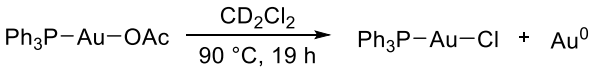


Figure S15. *In situ* ^{1}H-NMR spectrum of the reaction between **8** and $PhI(OAc)_2$

3.4.2 Activation of dichloromethane-d_2 by $Ph_3PAuOAc$



Acetato(triphenylphosphine)gold(I) (10.3 mg, 0.02 mmol) was stirred in dichloromethane-d_2 (0.4 mL). The reaction was performed in a sealed schlenk tube under dinitrogen atmosphere at 90 °C for 19 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR every 15 min (Figures S16-17). After 1h, traces of Ph3PAuCl were observed. Over time, $Ph_3PAuOAc$ was consumed to produce Ph_3PAuCl and Au(0). Analogous results were observed when the reaction was performed in the presence of $NaHCO_3$ (1 equiv.) and/or $PhI(OAc)_2$ (1.5 equiv.).

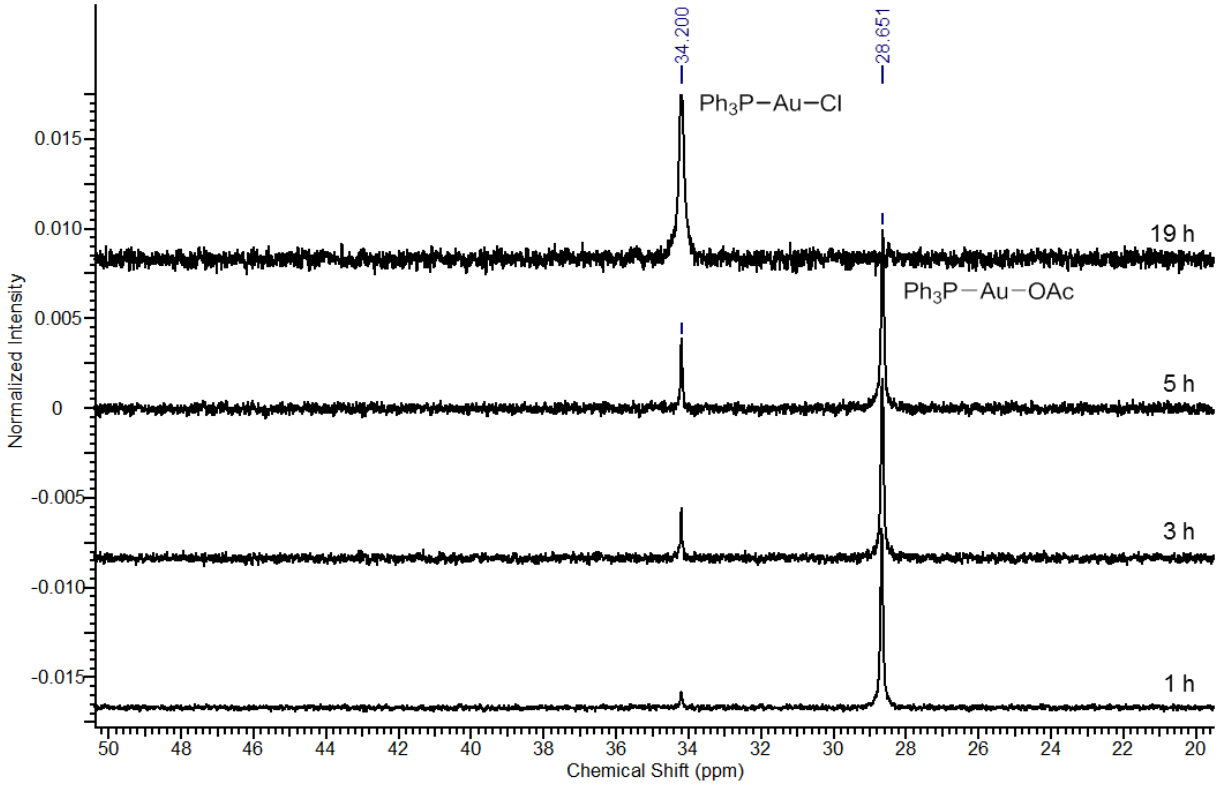


Figure S16. *In situ* ^{31}P-NMR spectrum of the reaction between $Ph_3PAuOAc$ and dichloromethane-d_2

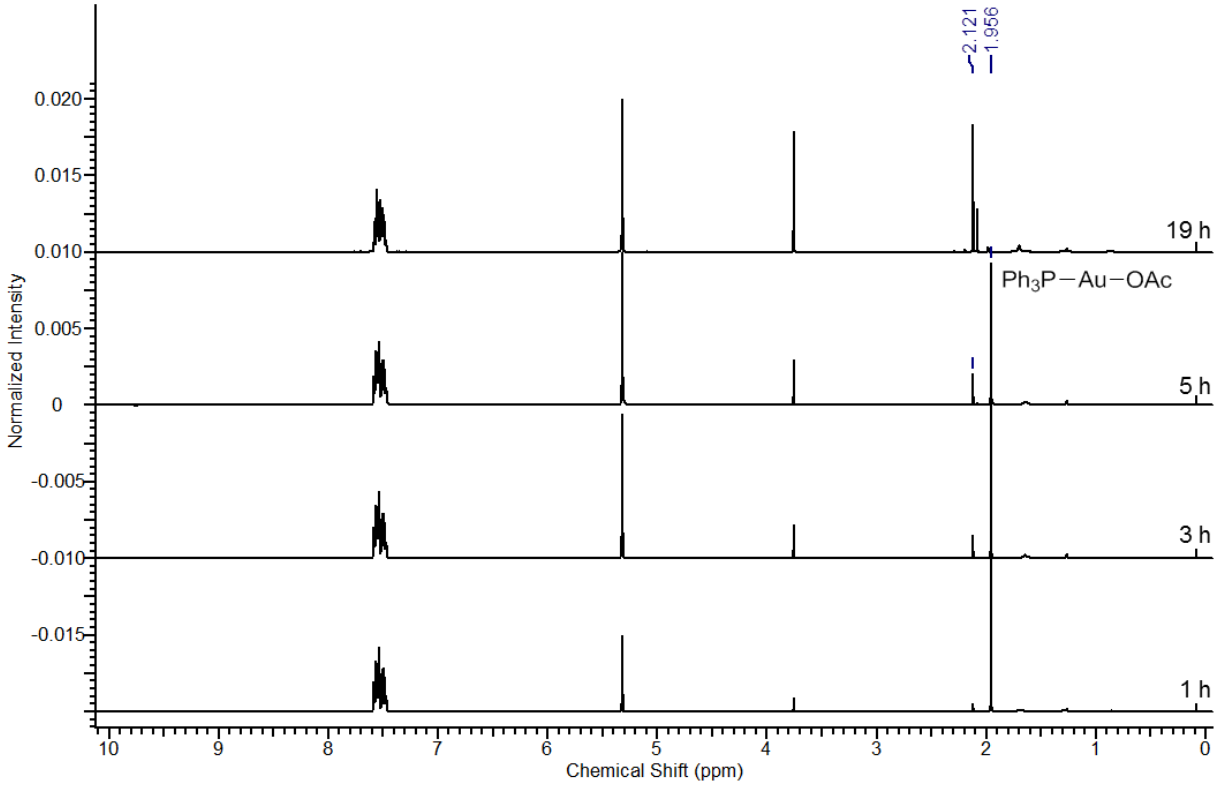
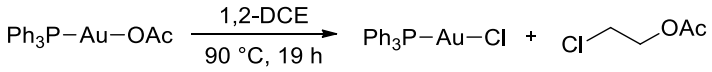


Figure S17. *In situ* ^{1}H-NMR spectrum of the reaction between $Ph_3PAuOAc$ and dichloromethane-d_2

3.4.3 Activation of 1,2-dichloroethane by $Ph_3PAuOAc$



Acetato(triphenylphosphine)gold(I) (5 mg, 0.01 mmol) was stirred in 1,2-dichloroethane (0.2 mL). The reaction was performed in a sealed schlenk tube at 90 °C for 19 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR every 15 min (Figure S18). After 2h, traces of Ph_3PAuCl were observed. Analogous results were observed when the reaction was performed in the presence of $NaHCO_3$ (1 equiv.) and/or $PhI(OAc)_2$ (1.5 equiv.). The solvent was evaporated carefully under reduced pressure to enable complete ^{1}H-NMR analysis of the reaction mixture (Figure S19).[18] ^{1}H NMR (400 MHz, $CDCl_3$): δ = 4.30 (t, J = 5.7 Hz, 2 H), 3.69 (t, J = 5.7 Hz, 2 H), 2.07 (s, 3 H). The formation of 2-chloroethyl-acetate was confirmed by GC-MS analysis.

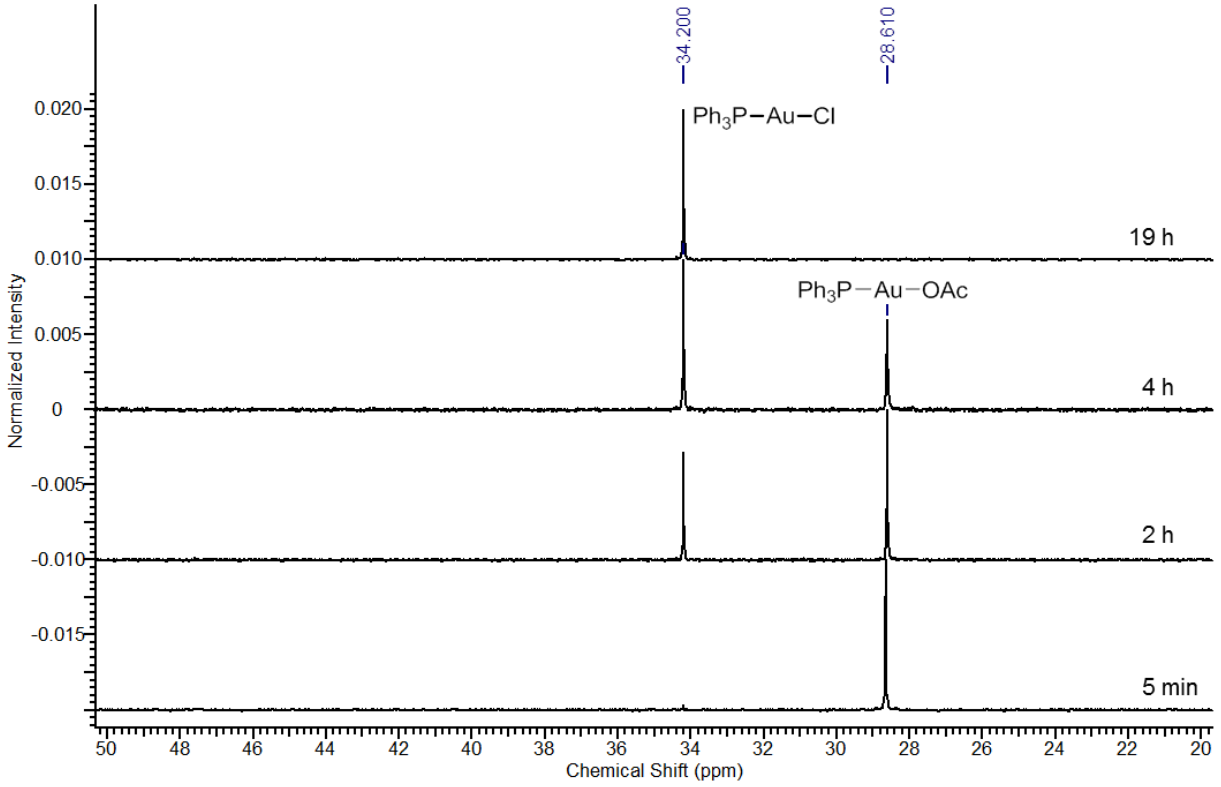


Figure S18. *In situ* ^{31}P-NMR spectrum of the reaction between $Ph_3PAuOAc$ and 1,2-dichloroethane

[18] D. I. Nichols, A. S. Charleston, *J. Chem. Soc. A* 1969, 2581.

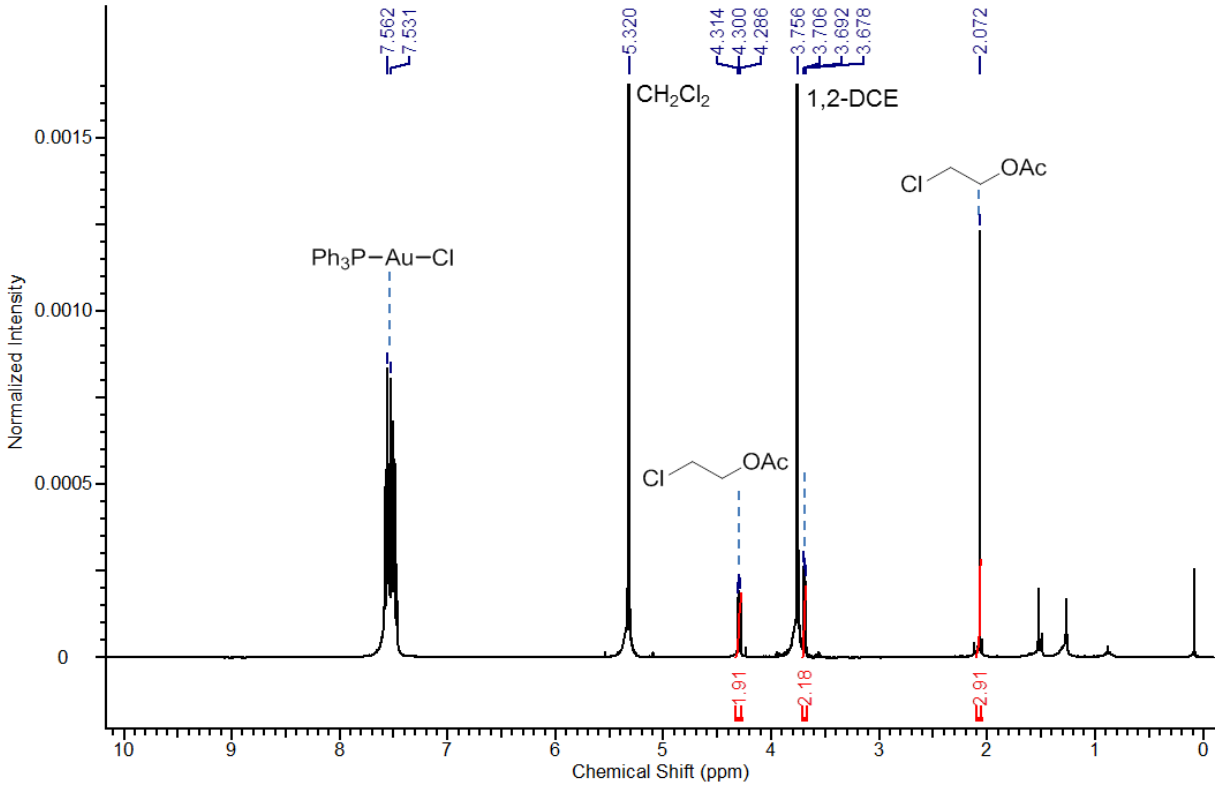
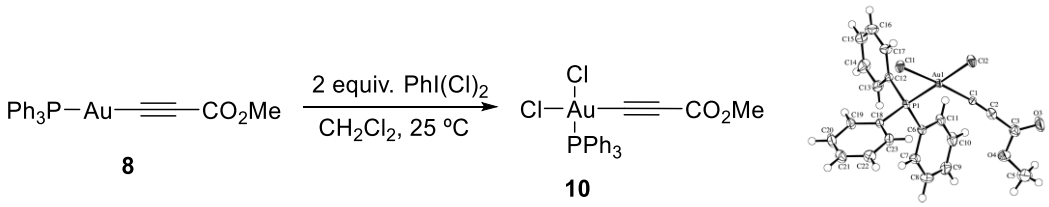


Figure S19. *In situ* ^{1}H-NMR spectrum of the reaction between $Ph_3PAuOAc$ and 1,2-dichloroethane (after evaporation of 1,2-dichloroethane)

3.4.4 Synthesis of *cis*-dichloro(methoxycarbonylethynyl)(triphenylphosphine)gold(III) (**10**) by $PhI(Cl)_2$ (equation 3 in the main text)

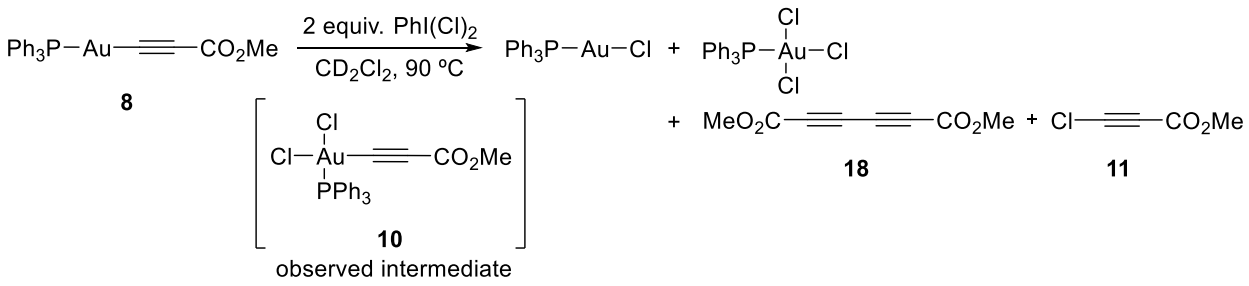


8 **10**

To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (32.5 mg, 0.06 mmol) and dichloro(phenyl)-λ3-iodane (33.0 mg, 0.12 mmol), dichloromethane (1.5 mL) was added. The reaction mixture was stirred in a sealed schlenk flask at 25 °C for 1 h under dinitrogen atmosphere. The solvent was evaporated and the yellow solid was washed three times with 1 mL of ethanol, dried under reduced pressure to afford compound **10** (24.2 mg, 0.044 mmol) in 73% isolated yield. m.p.: 116-118 °C (decomp.). Single crystals suitable for X-ray crystallographic analysis were obtained by recrystallization using dichloromethane/hexane as solvents. ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 7.77 - 7.67 (m, 9H), 7.62 - 7.55 (m, 6H), 3.55 (s, 3H); ^{13}C NMR (126 MHz, CD_2Cl_2): δ = 154.1 (s), 135.5 (d, J = 10.5 Hz), 134.4 (d, J = 3.5 Hz), 129.8 (d, J = 13.1 Hz), 123.8 (d, J = 70.5 Hz), 91.5 (d, J = 2.5 Hz), 87.4 (d, J = 5.5 Hz), 52.7 (s); ^{31}P NMR (162 MHz, CD_2Cl_2): δ = 37.1 (s); FTIR (cm^{-1}): 2172, 1702, 1482, 1435, 1230, 1096, 998, 954, 875, 747, 713; ESI-HRMS (m/z): $[M + Na]^+$ calcd for $C_{22}H_{18}AuCl_2O_2P$, 634.99847; found: 634.99741.

X-Ray diffraction data for complex **10** can be found in section 5. ^{1}H-, ^{13}C-, ^{31}P-NMR traces can be found in section 6.

3.4.5 Oxidation of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) by $PhI(Cl)_2$ at 90 °C (equation 4 in the main text)



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (5.4 mg, 0.01 mmol) and dichloro(phenyl)-λ^3-iodane (5.5 mg, 0.02 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 2 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S20-21). Compound **8** oxidized to the gold(III) complex **10** which at 90 °C decomposed to Ph_3PAuCl and chloro-methyl propiolate **11**.[19] The formation of the homocoupling product of the alkyne (**18**) was explained by Au(I)/Au(III) transmetalation of **8** and **10** and subsequent reductive elimination (see section 3.6.5).

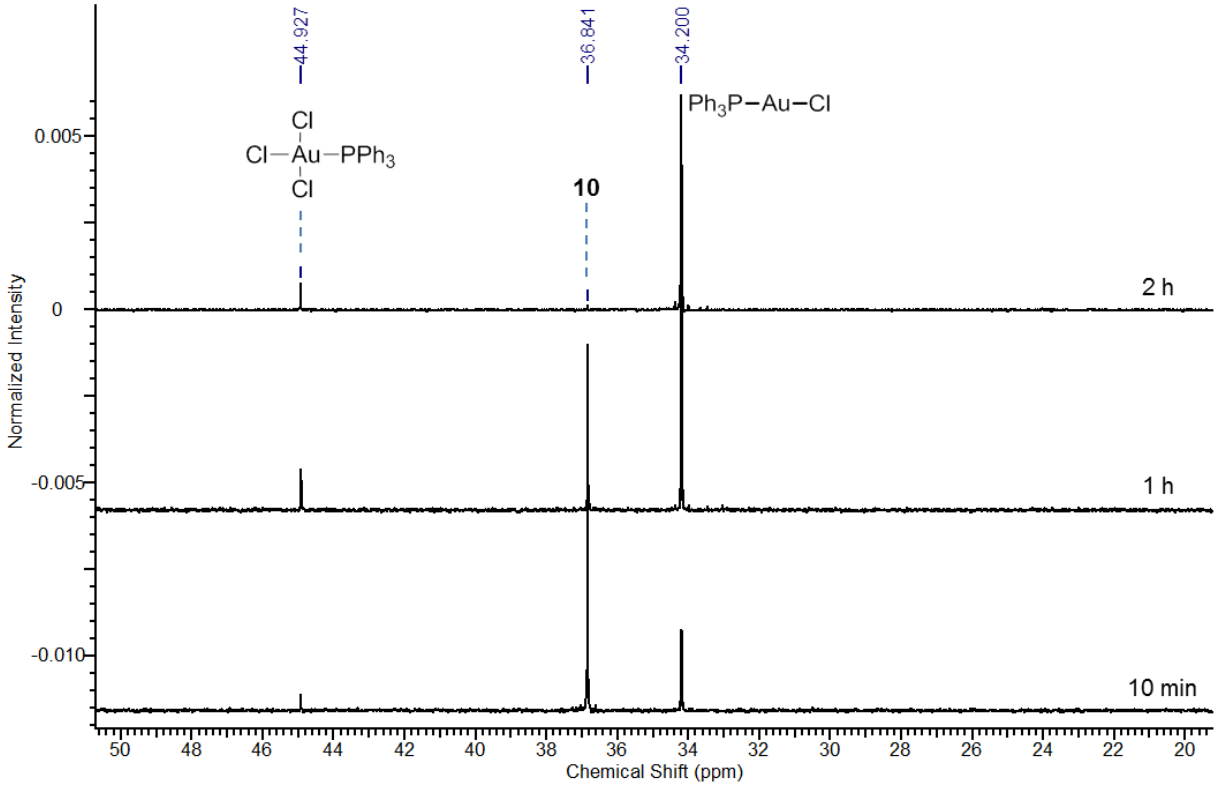


Figure S20. *In situ* ^{31}P-NMR spectrum of the reaction between **8** and $PhI(Cl)_2$ at 90 °C

[21] B. B. Snider, D. M. Roush, D. J. Rodini, D. Gonzalez, D. Spindell, *J. Org. Chem.* 1980, **45**, 2773.

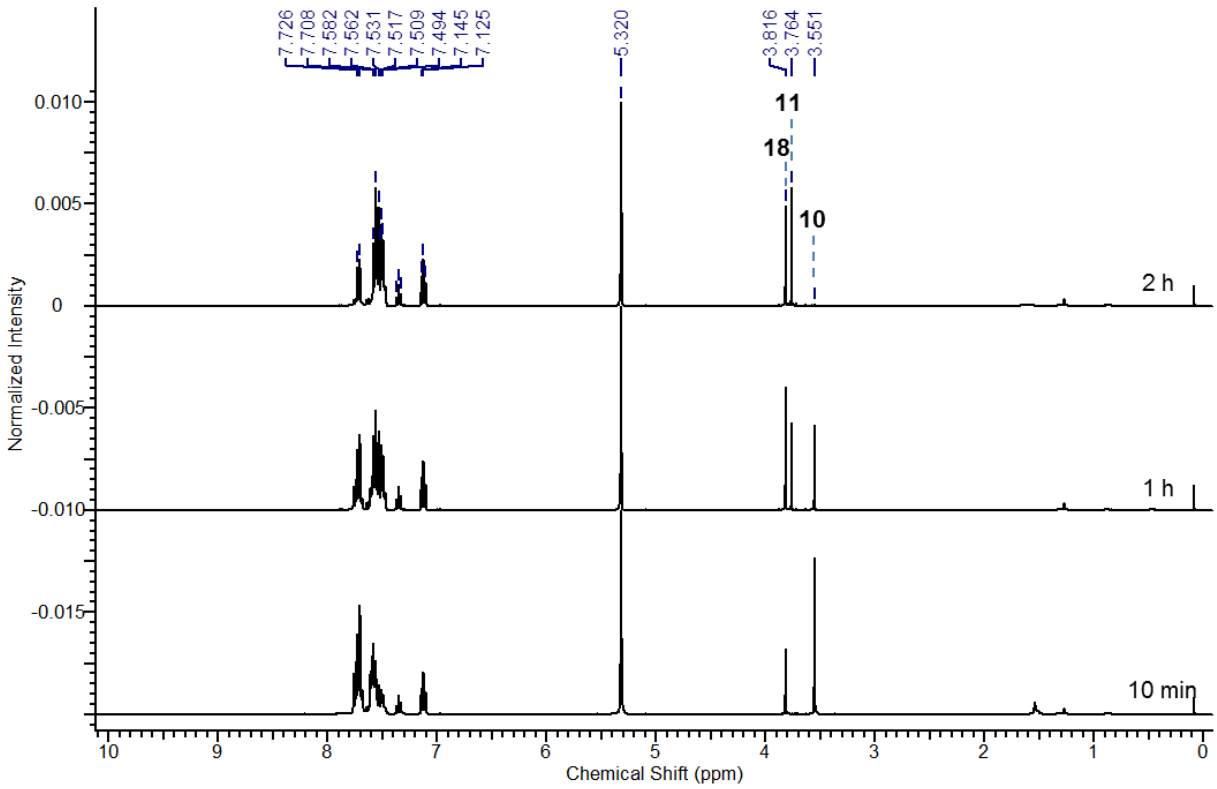
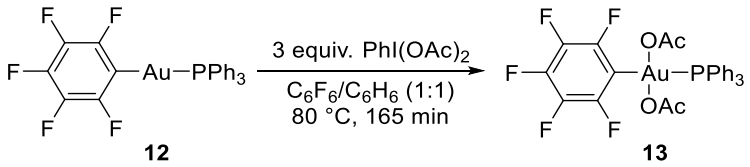


Figure S21. *In situ* ^{1}H-NMR spectrum of the reaction between **8** and $PhI(Cl)_2$ at 90 °C

3.5 Synthesis of *trans*-diacetato(pentafluorophenyl)(triphenylphosphine)gold(III) (13) (Equation 5 in the main text)



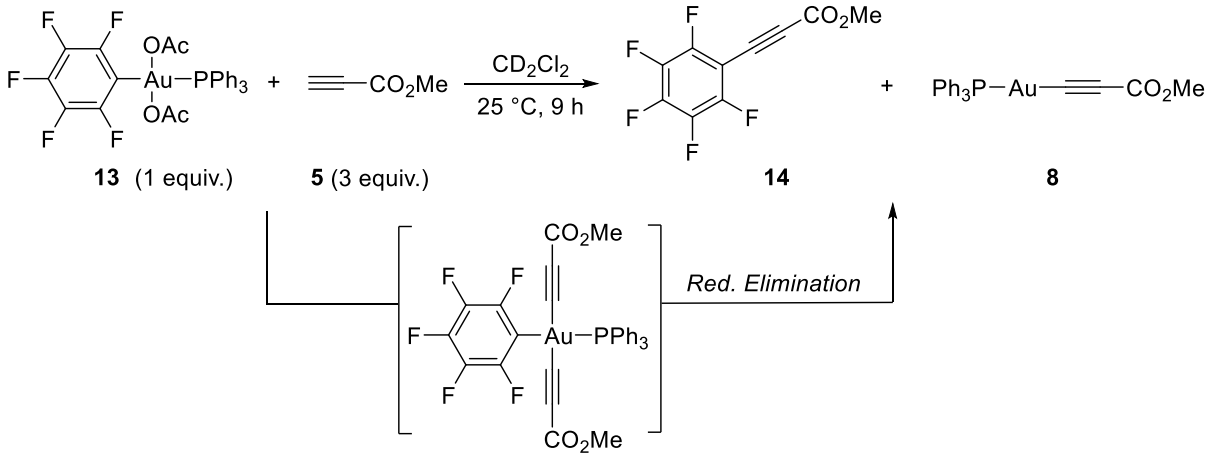
The synthesis of *trans*-diacetato(pentafluorophenyl)(triphenylphosphine)gold(III) (**13**) is reported elsewere.[20] To a mixture of pentafluorophenyl(triphenylphosphine)gold(I) (**12**) (100 mg, 0.16 mmol) and diacetoxy(phenyl)-λ3-iodane (155 mg, 0.48 mmol), a mixture of pentafluorobenzene and benzene (1:1, 3.2 mL) was added. The reaction mixture was stirred under dinitrogen at 80 °C for 165 min. The solvent was evaporated under reduced pressure and the crude was purified by column chromatography (hexane:EtOAc 1:1) to give **13** as a white solid. Isolated yield: 64% (76.2 mg, 0.10 mmol). ^{1}H NMR (500 MHz, CD_2Cl_2): δ = 7.76 - 7.54 (m, 15 H), 1.47 (s, 6 H); ^{13}C NMR (126 MHz, CD_2Cl_2): 174.2 (s), 146.6 (dm, *J* = 235.0 Hz), 140.4 (dm, *J* = 245.0 Hz), 137.6 (dm, *J* = 252.0 Hz), 135.2 (d, *J* = 11.0 Hz), 133.2 (d, *J* = 3.0 Hz), 129.8 (d, *J* = 11.5 Hz), 124.5 (d, *J* = 58.0 Hz), 117.6 (dt, *J* = 155.0, 43.0 Hz), 20.7 (s); ^{31}P-NMR (162 MHz, CD_2Cl_2): δ = 30.28 – 29.80 (m, 1 P); ^{19}F NMR (376 MHz, CD_2Cl_2): δ = -(125.74 - 125.98) (m), -158.20 (t, *J* = 19.8 Hz), -(162.64 - 162.90) (m); ESI-HRMS (m/z): $[M + Na]^+$ calcd for $C_{28}H_{21}AuF_5O_4P$, 767.06608; found: 767.06498.

^{1}H-, ^{13}C-, ^{31}P-, ^{19}F-NMR traces can be found in section 6.

[22] M. Hofer, A. Genoux, R. Kumar, C. Nevado, *Angew. Chem. Int. Ed.* 2017, **56**, 1021.

3.6 Reactivity of gold(III) complexes 10 and 13 (Table 1 in the main text)

3.6.1 Activation of methyl propiolate (**5**) by **13**



To a mixture of *trans*-diacetato(pentafluorophenyl)(triphenylphosphine)gold(III) (**13**) (7.4 mg, 0.010 mmol), methyl propiolate (**5**) (2.5 mg, 0.03 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR tube at 25 °C for 9 h. The reaction was monitored by ^{1}H-, ^{31}P-NMR and ^{19}F-NMR (Figures S22-23). The crude mixture contains compound **14** in 68% molar ratio (^{19}F-NMR). (Methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) was identified by ^{31}P-NMR. The gold(I) complex $Ph_3PAu(C_6F_5)$ (**12**) was observed by ^{19}F-NMR (20% molar ratio). The formation of this minor product can be explained by disproportionation between **8** and **13**.

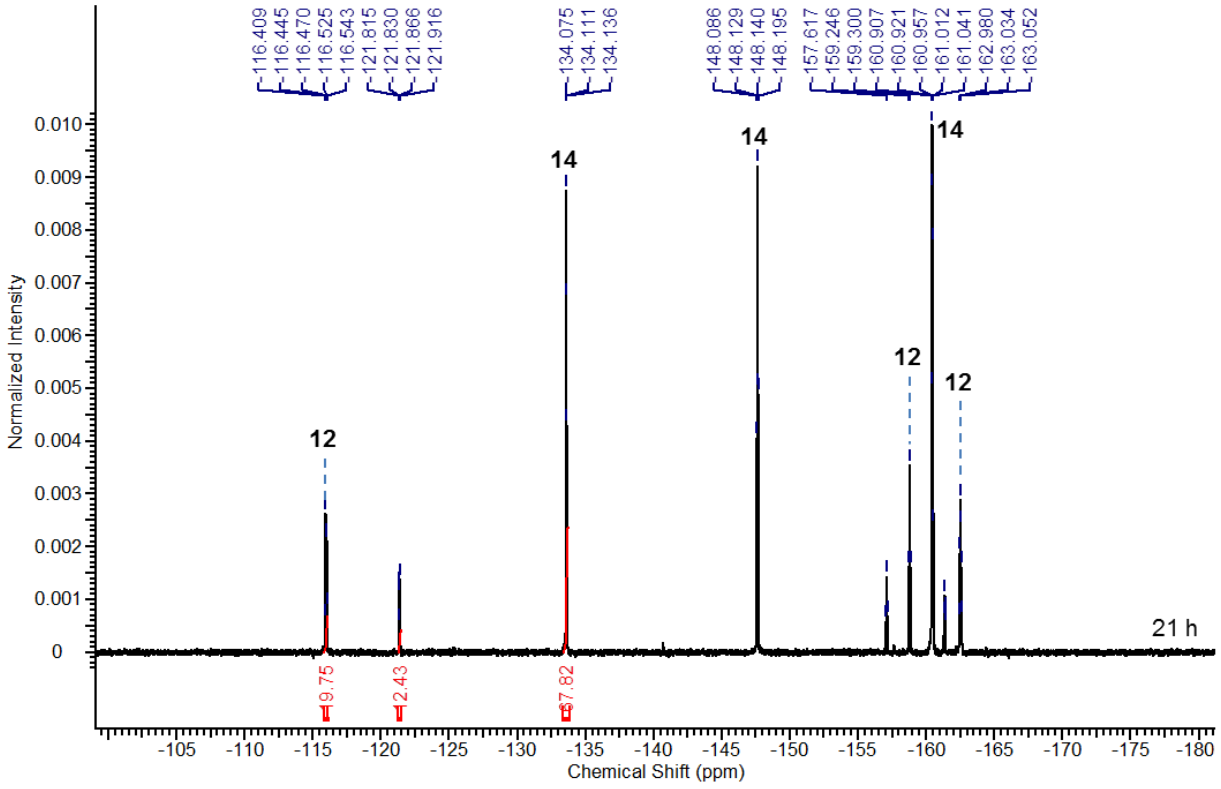


Figure S22. *In situ* ^{19}F-NMR spectrum of the reaction between **13** and **5**

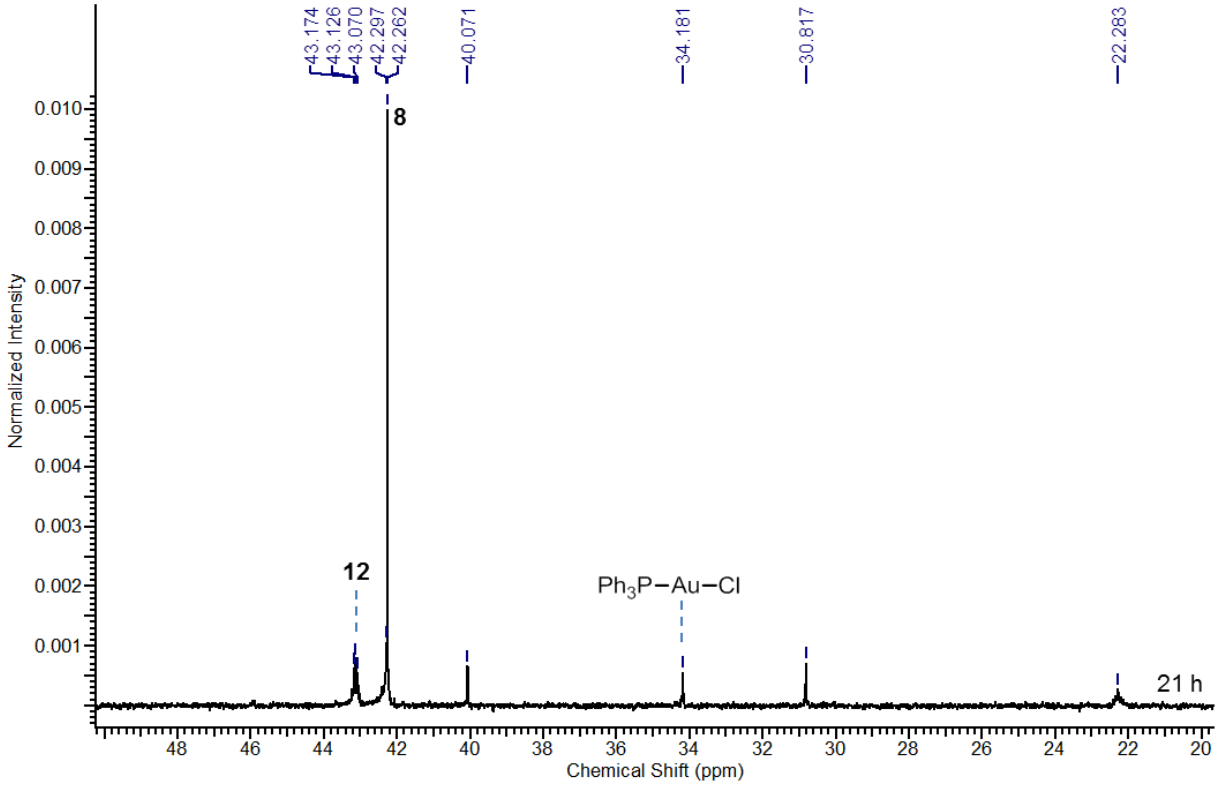
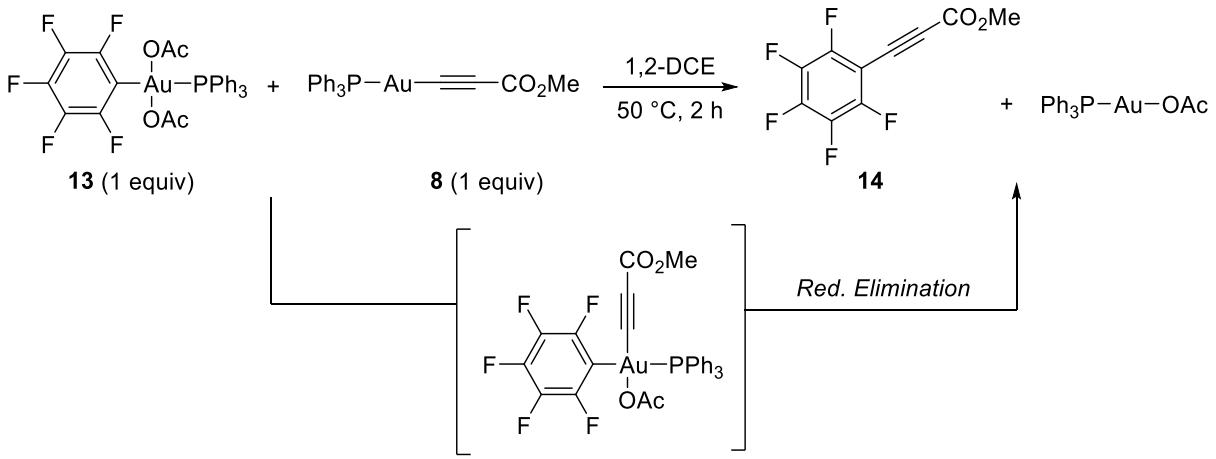


Figure S23. *In situ* ^{31}P-NMR spectrum of the reaction between **13** and **5**

3.6.2 Transmetalation of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) and **13** (Table 1in the main text)



To a mixture of *trans*-diacetato(pentafluorophenyl)(triphenylphosphine)gold(III) (**13**) (7.4 mg, 0.01 mmol) and (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (5.4 mg, 0.01 mmol), 1,2-dichloroethane (0.2 mL) was added. The reaction was performed in a sealed schlenk tube at 50 °C for 2 h. The reaction was monitored by ^{1}H-, ^{31}P-NMR and ^{19}F-NMR (Figures S24-25). The crude mixture contains compound **14** in 62% molar ratio (^{19}F-NMR). $Ph_3PAuOAc$ was identified by ^{31}P-NMR. The formation of the products was explained by a single Au(I)/Au(III) transmetalation monitored by reductive elimination to afford compound **14** and $Ph_3PAuOAc$. The gold(I) complex $Ph_3PAu(C_6F_5)$ (**12**) was observed by ^{19}F-NMR (ca. 10% molar ratio). The formation of this minor product can be explained by disproportionation between **8** and **13**.

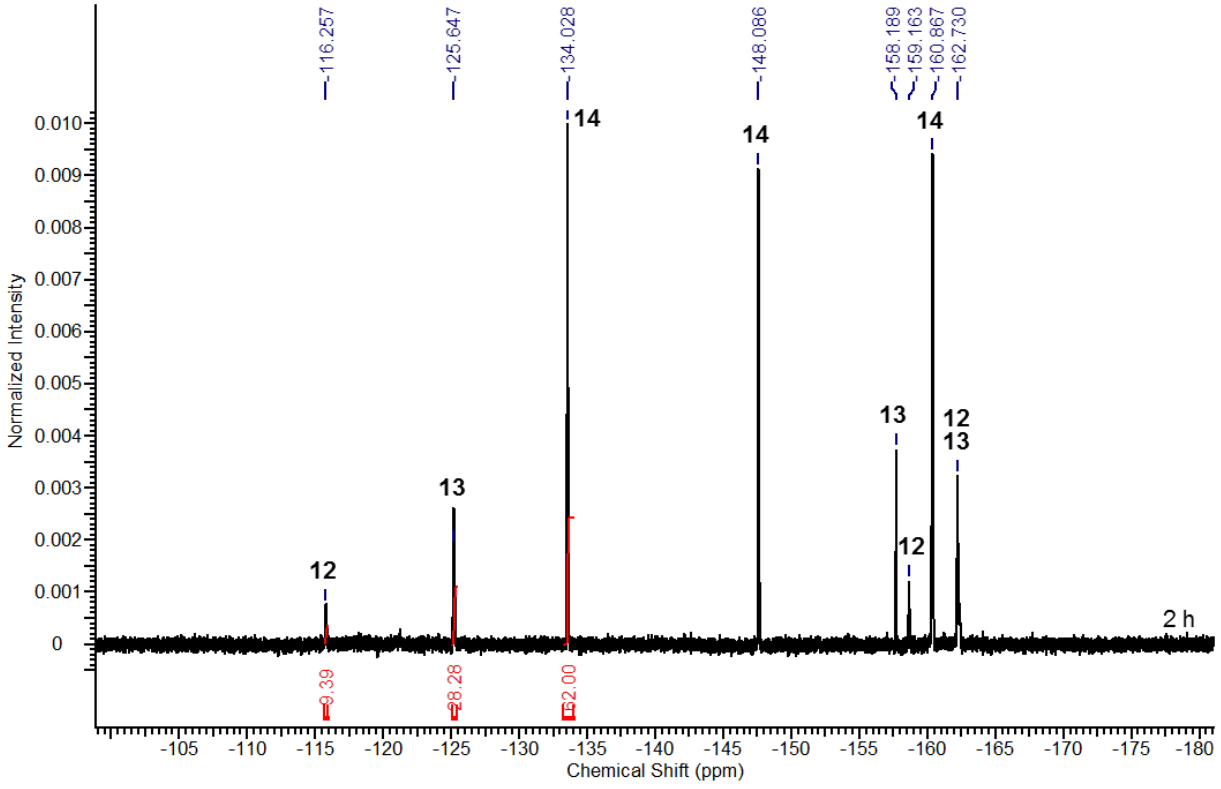


Figure S24. *In situ* ^{19}F-NMR spectrum of the reaction between **13** and **8**

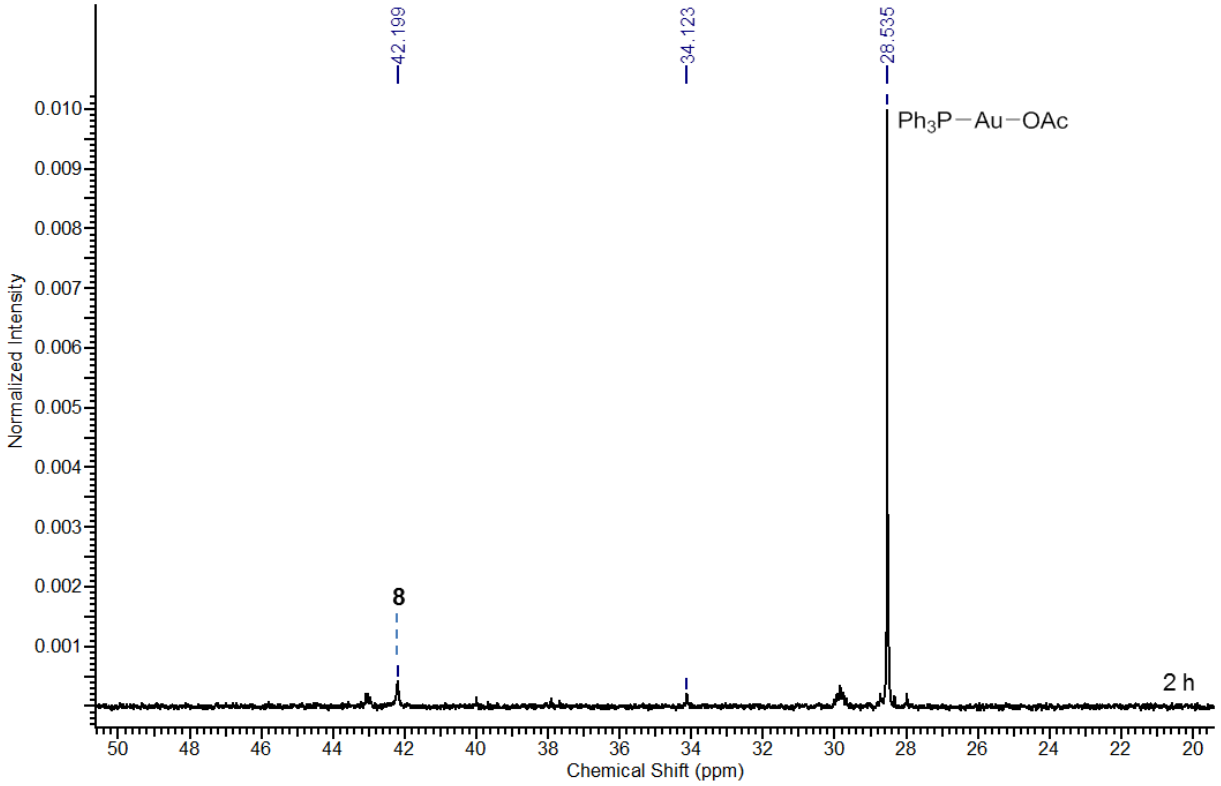
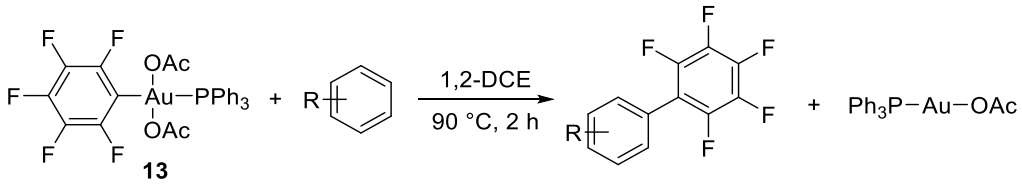


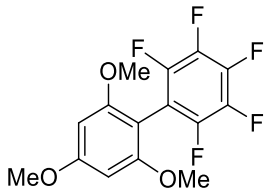
Figure S25. *In situ* ^{31}P-NMR spectrum of the reaction between **13** and **8**

3.6.3 Activation of electron rich arenes by **13** (Table 1 in the main text)



General procedure: To a mixture of *trans*-diacetato(pentafluorophenyl)(triphenylphosphine)-gold(III) (**13**) (28.8 mg, 0.04 mmol) and arene (0.04 mmol), 1,2-dichloroethane (0.8 mL) was added. The reaction was performed in a sealed schlenk tube at 90 °C for 2 h. The reaction was monitored by ^{1}H-, ^{31}P-NMR and ^{19}F-NMR. The solvent was evaporated under reduced pressure and the crude was purified by column chromatography on silica gel using hexane and DCM as solvents.

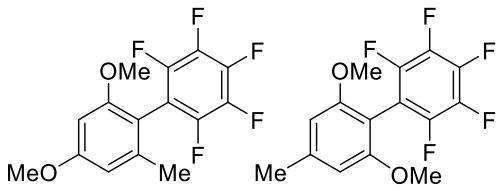
A) 2,3,4,5,6-Pentafluo-2',4',6'-trimethoxybiphenyl (**15**)[21]



Following the general procedure using 1,3,5-trimethoxybenzene (6.7 mg, 0.04 mmol), compound **15** was obtained in 85% isolated yield (11.4 mg, 0.034 mmol). m.p.: 120-121 °C. ^{1}H NMR (300 MHz, CD_2Cl_2): δ = 6.24 (s, 2H), 3.86 (s, 3H), 3.75 (s, 6H). ^{13}C NMR (126 MHz CD_2Cl_2): δ = 163.8 (s), 159.7 (s), 145.5 (dm, *J* = 246.0 Hz), 140.9 (dm, *J* = 250.0 Hz), 138.1 (dm, *J* = 248.0 Hz), 110.0 (td, *J* = 20.0, 4.0 Hz), 96.7 (s), 91.4 (s), 56.5 (s), 56.1 (s). ^{19}F NMR (282 MHz, CD_2Cl_2): δ = -(139.51 - 139.70) (m), -158.17 (t, *J* = 21.0 Hz), -(164.97 - 165.22) (m). FTIR (cm^{-1}): 2954, 1613, 1591, 1528, 1489, 1341, 1230, 1209, 1163, 1130, 1068, 981, 845, 810, 788, 620; EI-HRMS (m/z): calcd for $C_{15}H_{11}O_3F_5$, 334.06284; found: 334.06229.

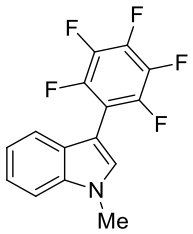
[22] M. Hofer, C. Nevado, *Tetrahedron* 2013, **69**, 5751.

B) 2,3,4,5,6-Pentafluo-2'-methyl-,4',6'dimethoxybiphenyl (**16a**), 2,3,4,5,6-Pentafluo-4'-methyl-,2',6'dimethoxybiphenyl (**16b**)



Following the general procedure using *trans*-diacetato(pentafluorophenyl)(triphenylphosphine)-gold(III) (**13**) (14.9 mg, 0.02 mmol) and 3,5-dimethoxytoluene (**4**) (3.1 mg, 0.02 mmol), a mixture of regioisomers **16a:16b** (0.6:1) was obtained in a combined 74% yield (^{19}F-NMR). The solvent was evaporated under reduced pressure and the crude was purified by column chromatography (hexane:dichloromethane 9:1). Compound **16b** was obtained as a single compound as a white solid. Isolated yield: 38% (2.4 mg, 0.008 mmol). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 6.51 (s, 2 H), 3.75 (s, 6 H), 2.42 (s, 3 H); ^{13}C NMR (126 MHz, CD_2Cl_2): δ = 158.4 (s), 145.2 (dm, *J* = 247.0 Hz), 143.0 (s), 140.8 (dm, *J* = 250.0 Hz), 138.0 (dm, *J* = 248.0 Hz), 109.9 (t, *J* = 20.0 Hz), 105.3 (s), 100.9 (s), 56.4 (s), 22.6 (s); ^{19}F NMR (376 MHz, CD_2Cl_2): δ = -(139.53 - 139.79) (m), -157.99 (t, *J* = 21.0 Hz), -(164.87 - 165.12) (m); FTIR (cm^{-1}): 2363, 2157, 1607, 1580, 1525, 1493, 1457, 1411, 1311, 1130, 1058, 982, 845, 823. EI-HRMS (m/z): calcd for $C_{15}H_{11}O_2F_5$, 318.06792; found: 318.06737.

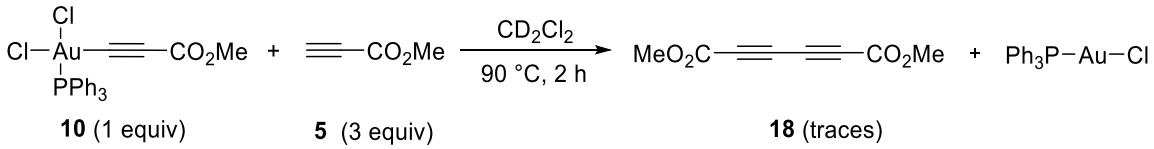
C) 1-Methyl-3-(pentafluorophenyl)-indole (**17**)[22]



Following the general procedure using 1-methylindole (5.2 mg, 0.04 mmol), compound **17** was obtained in 85% isolated yield (10.1 mg, 0.034 mmol). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 7.49 (dm, *J* = 7.6 Hz, 1 H), 7.44 (dm, *J* = 8.3 Hz, 1 H), 7.35 (s, 1 H), 7.31 (tm, *J* = 7.5 Hz, 1 H), 7.20 (tm, *J* = 7.5 Hz, 1 H), 3.89 (s, 3 H); ^{13}C NMR (126 MHz, CD_2Cl_2): δ = 145.0 (dm, *J* = 246.0 Hz), 140.1 (dm, *J* = 251.0 Hz), 138.7 (dm, *J* = 250.0 Hz), 137.6 (s), 130.8 (s), 127.0 (s), 123.0 (s), 121.0 (s), 120.6 (t, *J* = 3.3 Hz), 111.0 (td, *J* = 18.4, 4.0 Hz), 110.4 (s), 100.2 (d, *J* = 2.0 Hz), 33.7 (s) ^{19}F NMR (282 MHz, CD_2Cl_2): δ = -(141.20 - 141.37) (m), -159.22 (t, *J* = 21.0 Hz), -(163.81 - 164.04) (m). EI-HRMS (m/z): calcd for $C_{15}H_{11}O_3F_5$, 297.05769; found: 297.05714.

[23] C. Y, He, S. Fan, X. Zhang, *J. Am. Chem. Soc.*, 2010, **132**, 12850.

3.6.4 Reaction of methyl propiolate (**5**) with *cis*-dichloro(methoxycarbonylethynyl)(triphenylphosphine)-gold(III) (**10**) (Table 1 in the main text)



10 (1 equiv) **5** (3 equiv) **18** (traces)

To a mixture of *cis*-dichloro(methoxycarbonylethynyl)(triphenylphosphine)gold(III) (**10**) (6.1 mg, 0.01 mmol) and methyl propiolate (**5**) (2.5 mg, 0.03 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C for 5 h and at 90 °C for 2 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S26-27). The activation of the alkyne was not observed. The homocoupling product of the alkyne (**18**) was found just in traces (^{1}H-NMR).

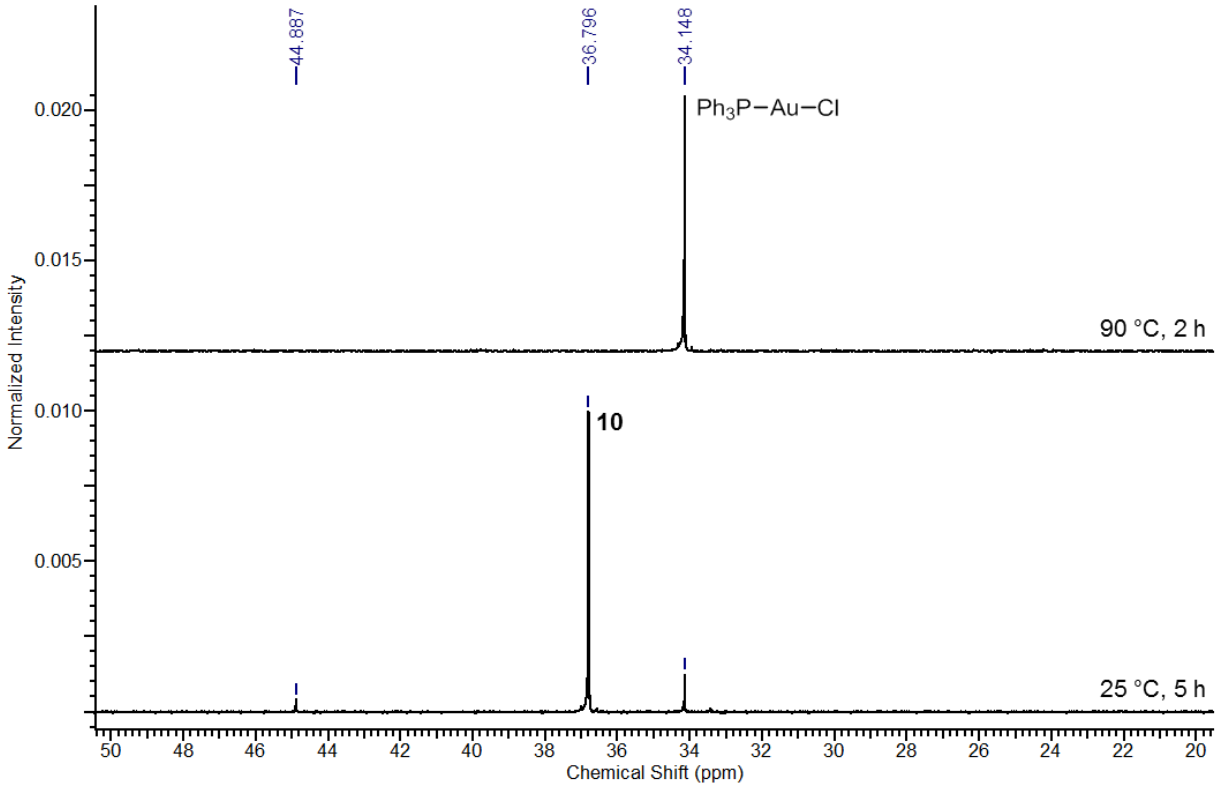


Figure 26. *In situ* ^{31}P-NMR spectrum of the reaction between **10** and **5**

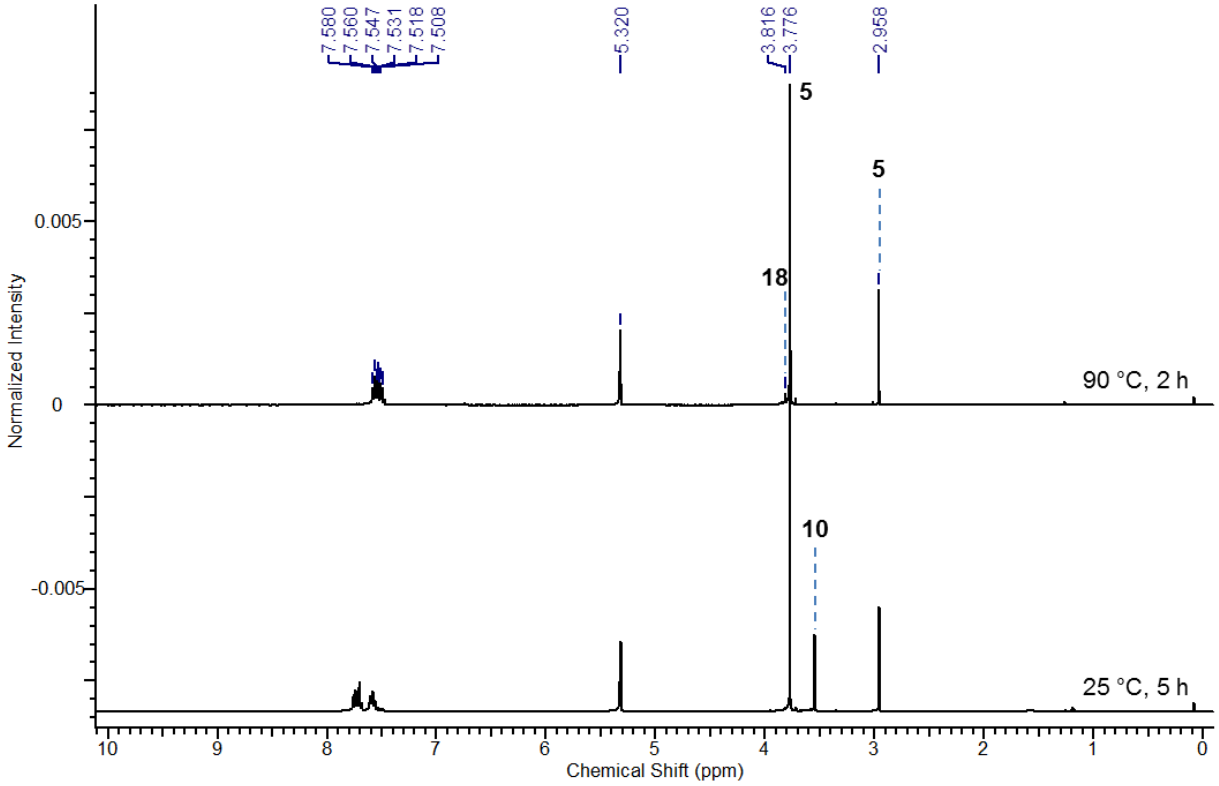
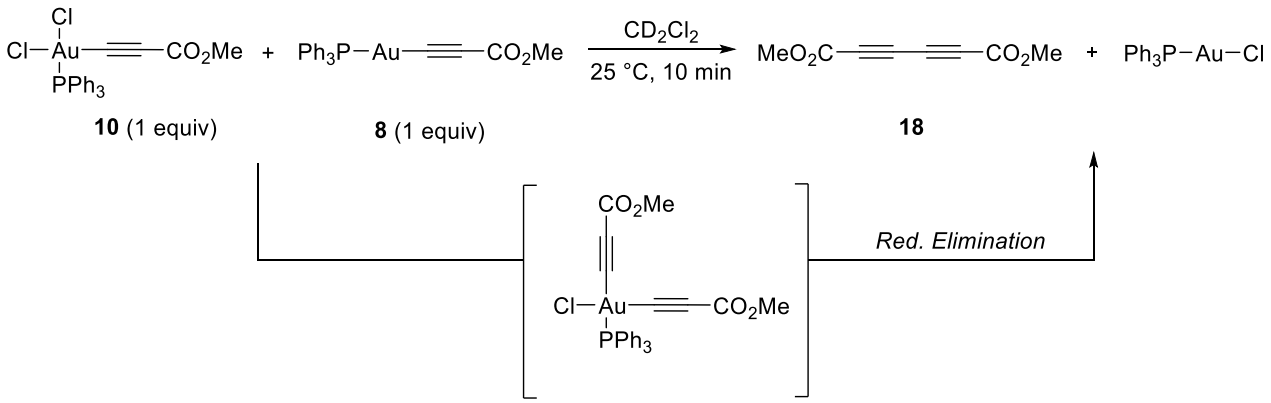


Figure S27. *In situ* ^{1}H-NMR spectrum of the reaction between **10** and **5**

3.6.5 Transmetalation of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) and *cis*-dichloro(methoxycarbonylethynyl)(triphenylphosphine)-gold(III) (**10**) (Table 1 in the main text)



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (5.4 mg, 0.01 mmol) and *cis*-dichloro(methoxycarbonylethynyl)(triphenylphosphine)gold(III) (**10**) (6.1 mg, 0.01 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C for 10 min. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S28-29). Compound **10** and **8** reacted quantitatively to give the homocoupling product **18** and Ph_3PAuCl via Au(I)/Au(III) transmetalation and reductive elimination.

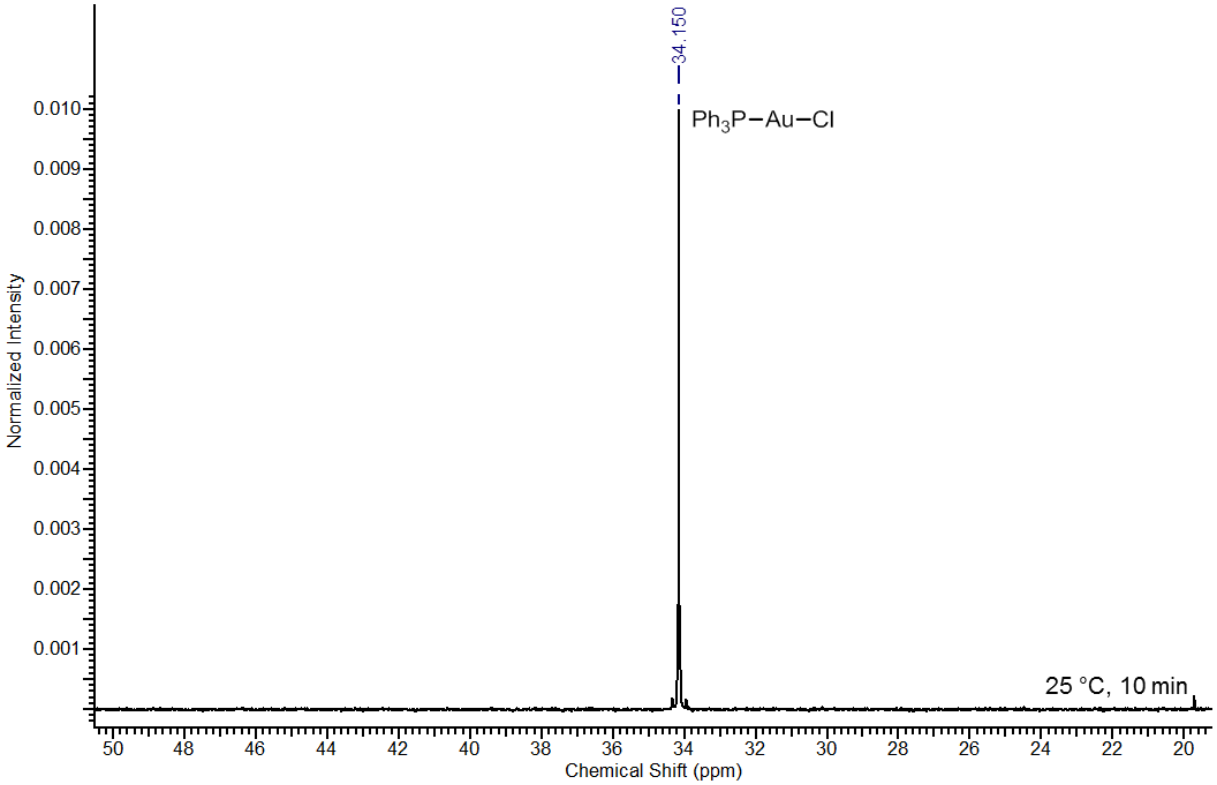


Figure S28. *In situ* ^{31}P-NMR spectrum of the reaction between **10** and **8**

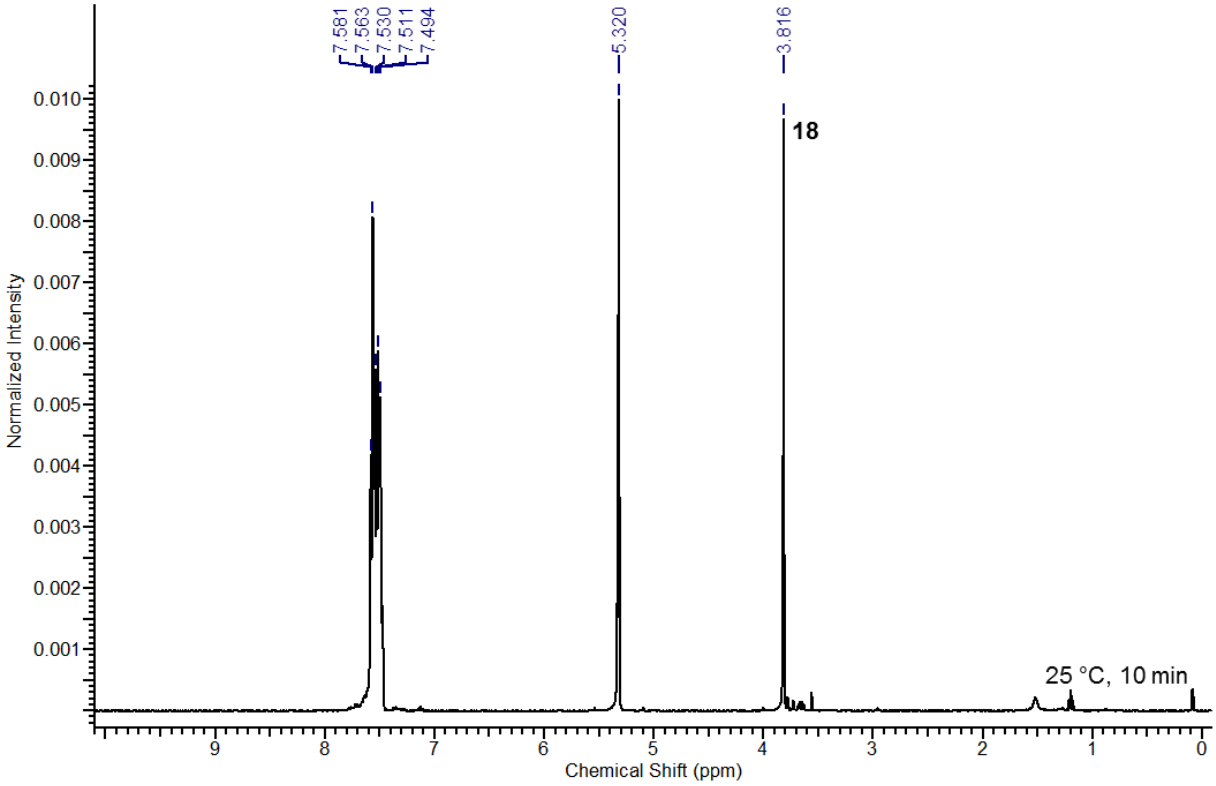
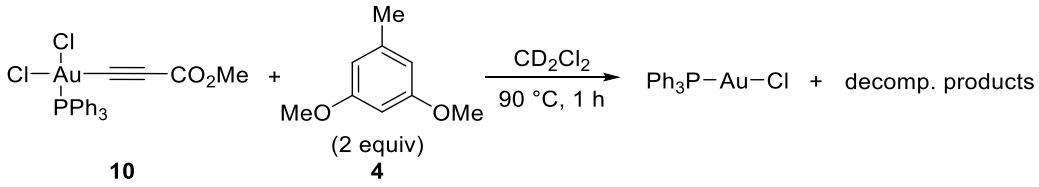


Figure S29. *In situ* ^{1}H-NMR spectrum of the reaction between **10** and **8**

3.6.6 Reactivity of **10** with 3,6-dimethoxytoluene (Table 1 in the main text)



To a mixture of *cis*-dichloro(methoxycarbonylethynyl)(triphenylphosphine)gold(III) (**10**) (6.1 mg, 0.01 mmol) and 3,5-dimethoxytoluene (**4**) (3.0 mg, 0.02 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 1 h. The reaction was monitored by ^{1}H-, ^{31}P-NMR (Figures S30-31). The reaction mixture showed the arene, Ph_3PAuCl and other decomposition products. Cross-coupling products could not be detected.

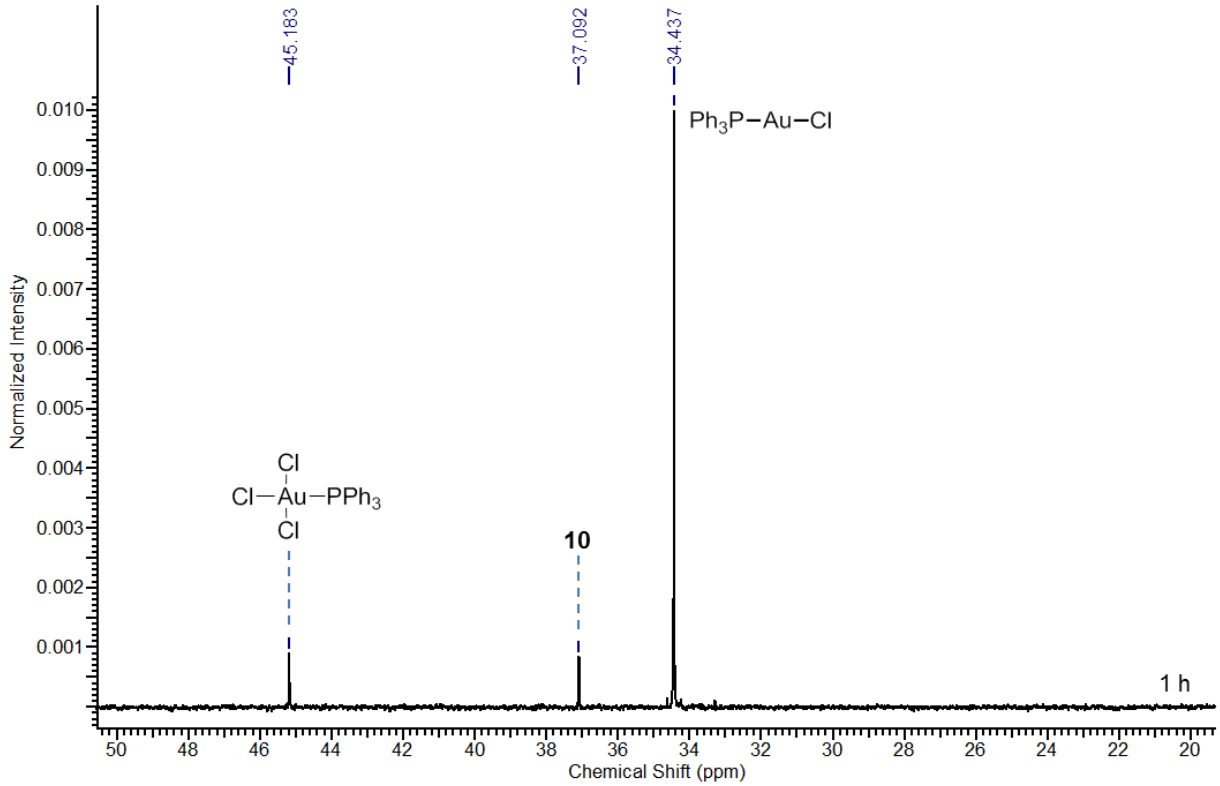


Figure S30. *In situ* ^{31}P-NMR spectrum of the reaction between **10** and 3,5-dimethoxytoluene (**4**)

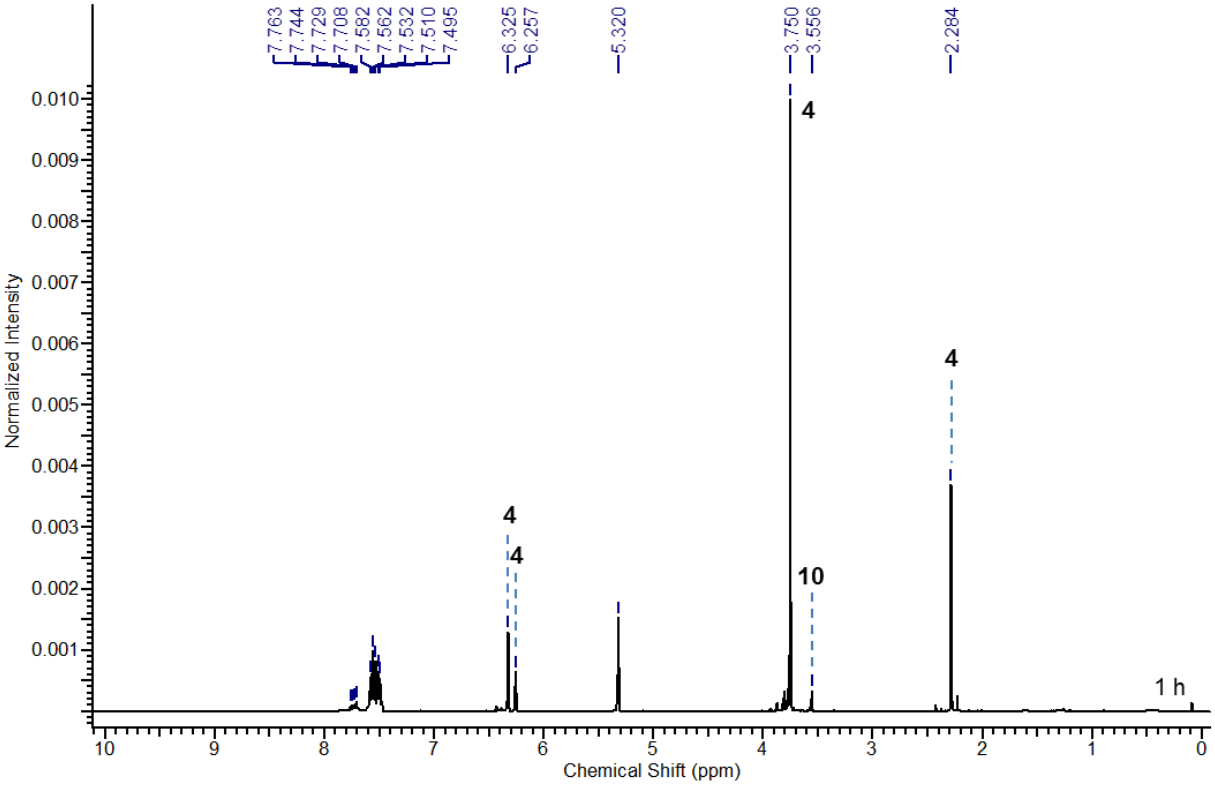
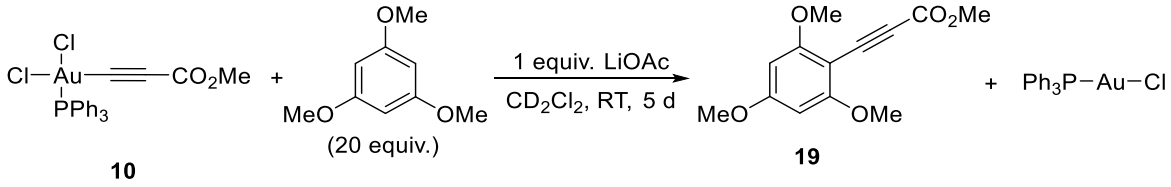


Figure S31. *In situ* ^{1}H-NMR spectrum of the reaction between **10** and 3,5-dimethoxytoluene (**4**)

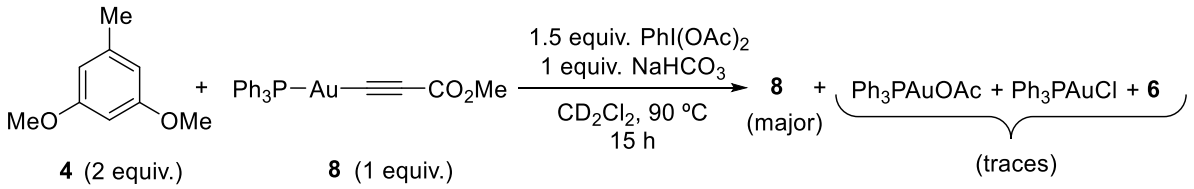
3.6.7 Reactivity of **10** with 1,3,5-trimethoxybenzene in presence of LiOAc (Equation 6 in the main text)



To a mixture of *cis*-dichloro(methoxycarbonylethynyl)(triphenylphosphine)gold(III) (**10**) (36.8 mg, 0.06 mmol), 1,3,5-dimethoxybenzene (201.8 mg, 1.2 mmol) and lithium-acetate (4.0 mg, 0.06 mmol), dichloromethane-d_2 (1.0 mL) was added. The reaction was performed in a sealed schlenk tube at 25 °C for 114 h under dinitrogen atmosphere. The reaction was monitored by ^{1}H-, ^{31}P-NMR. The reaction mixture showed the coupling product **19** and Ph_3PAuCl. The solvent was evaporated under reduced pressure and the crude was purified by column chromatography (hexane:EtOAc 8:2) to give **19** as a white solid. Isolated yield: 61% (9.1 mg, 0.036 mmol). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 6.11 (s, 2 H), 3.88 (s, 6 H), 3.85 (s, 3 H), 3.78 (s, 3H); ^{13}C NMR (126 MHz, CD_2Cl_2): δ = 165.0, 164.8, 155.4, 91.1, 91.0, 88.3, 82.2, 56.7, 56.2, 53.0.

3.7 (Methoxycarbonylethynyl)(triphenylphosphine)gold(I) (8) as reactive intermediate (Equations 7-9 in the main text)

3.7.1 Stoichiometric reaction of **4** with **8** (Equation 7 in the main text)



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (22 mg, 0.04 mmol), diacetoxy(phenyl)-λ3-iodane (19 mg, 0.060 mmol), 3,5-dimethoxytoluene (**4**) (12.2 mg, 0.08 mmol) and $NaHCO_3$ (3.0 mg, 0.04 mmol), dichloromethane-d_2 (0.5 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 15 h and was monitored by ^{1}H-, ^{31}P-NMR (Figures S32-33). The crude mixture contains compound **6** in less than 5% molar ratio (^{1}H-NMR). The formation of $Ph_3PAuOAc$ and Ph_3PAuCl could be confirmed by ^{31}P-NMR.

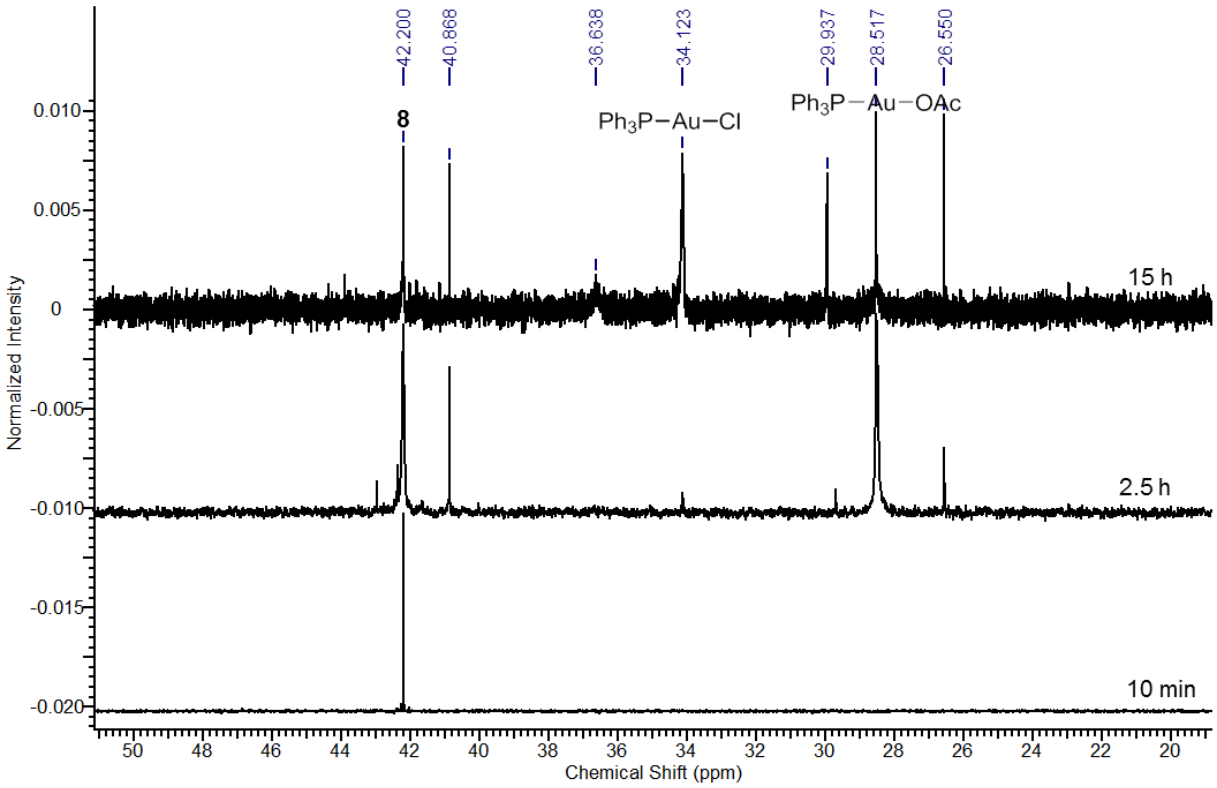


Figure S32. *In situ* ^{31}P-NMR spectrum of the reaction between **4** and **8** in presence of $PhI(OAc)_2$

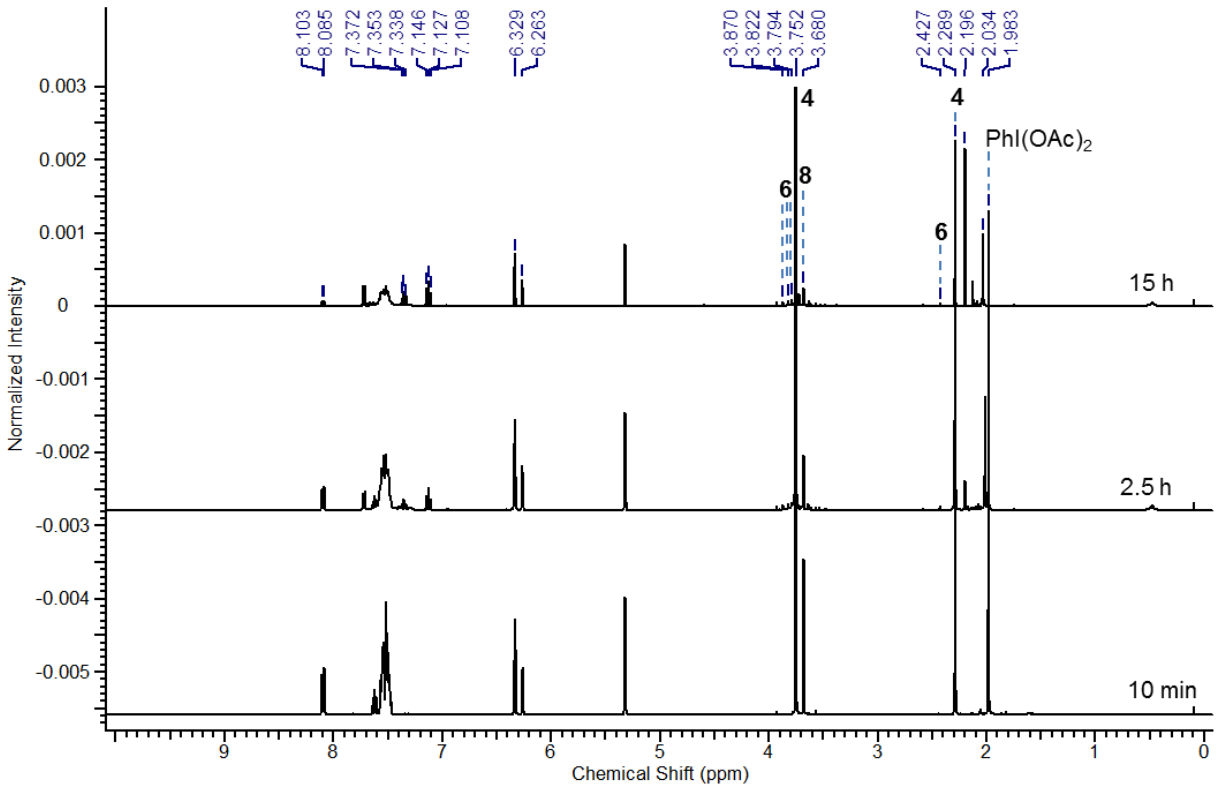
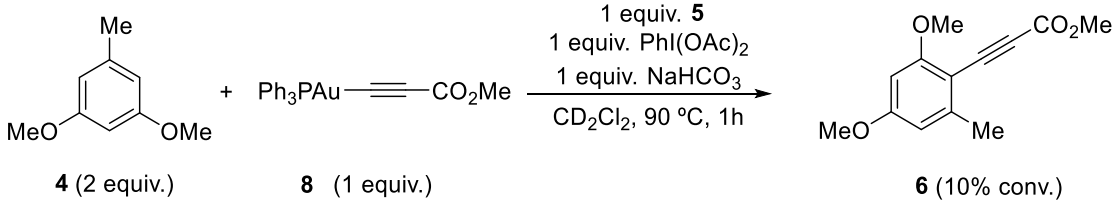


Figure S33. *In situ* ^{1}H-NMR spectrum of the reaction between **4** and **8** in presence of $PhI(OAc)_2$

3.7.2 Stoichiometric reaction of **4** with **8** in presence of additional alkyne (Equation 8 in the main text)



4 (2 equiv.) **8** (1 equiv.) **6** (10% conv.)

To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (22 mg, 0.04 mmol), diacetoxy(phenyl)-λ3-iodane (19 mg, 0.06 mmol), 3,5-dimethoxytoluene (**4**) (12.2 mg, 0.08 mmol), methyl propiolate (**5**) (3.4 mg, 0.04 mmol) and $NaHCO_3$ (3 mg, 0.04 mmol), dichloromethane-d_2 (0.5 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 1 h and was monitored by ^{1}H-, ^{31}P-NMR (Figures S34-35). The crude mixture contains compound **6** in 10% molar ratio after only one hour (^{1}H-NMR).

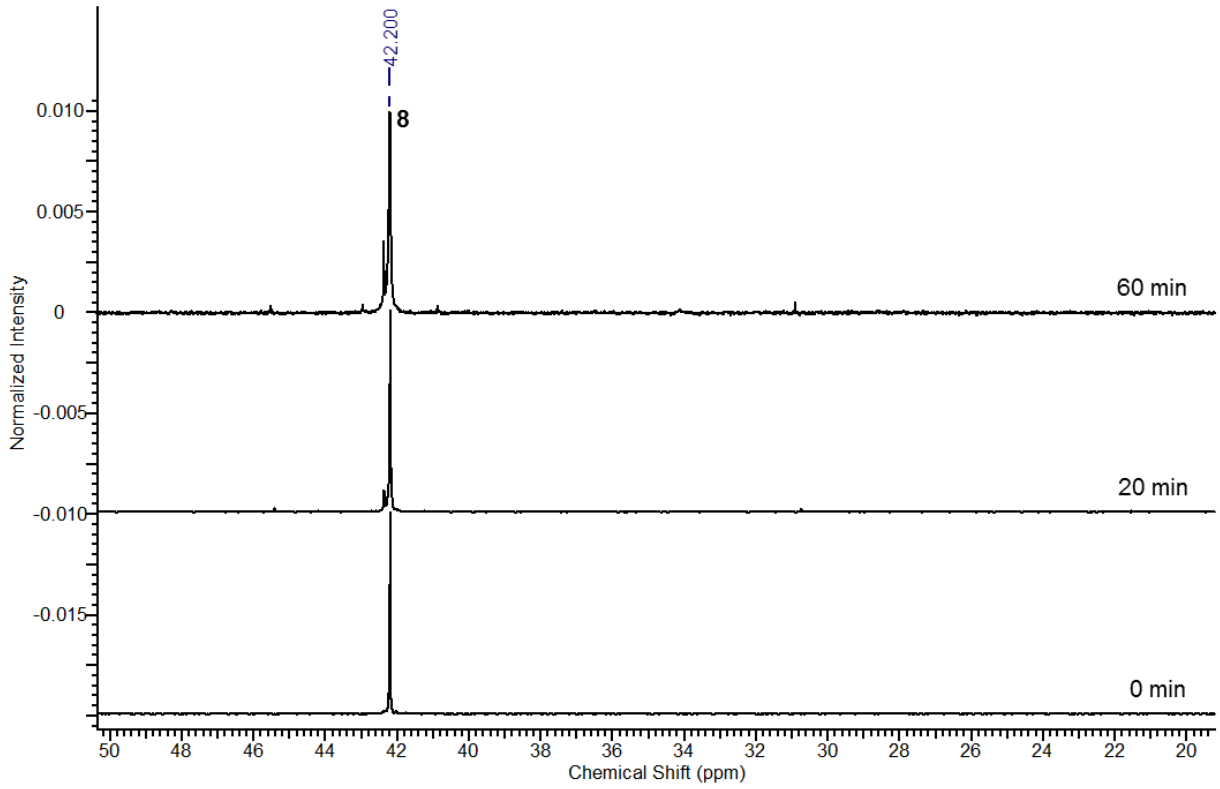


Figure S34. *In situ* ^{31}P-NMR spectrum of the reaction between **4** and **8** in presence of $PhI(OAc)_2$ and **5**

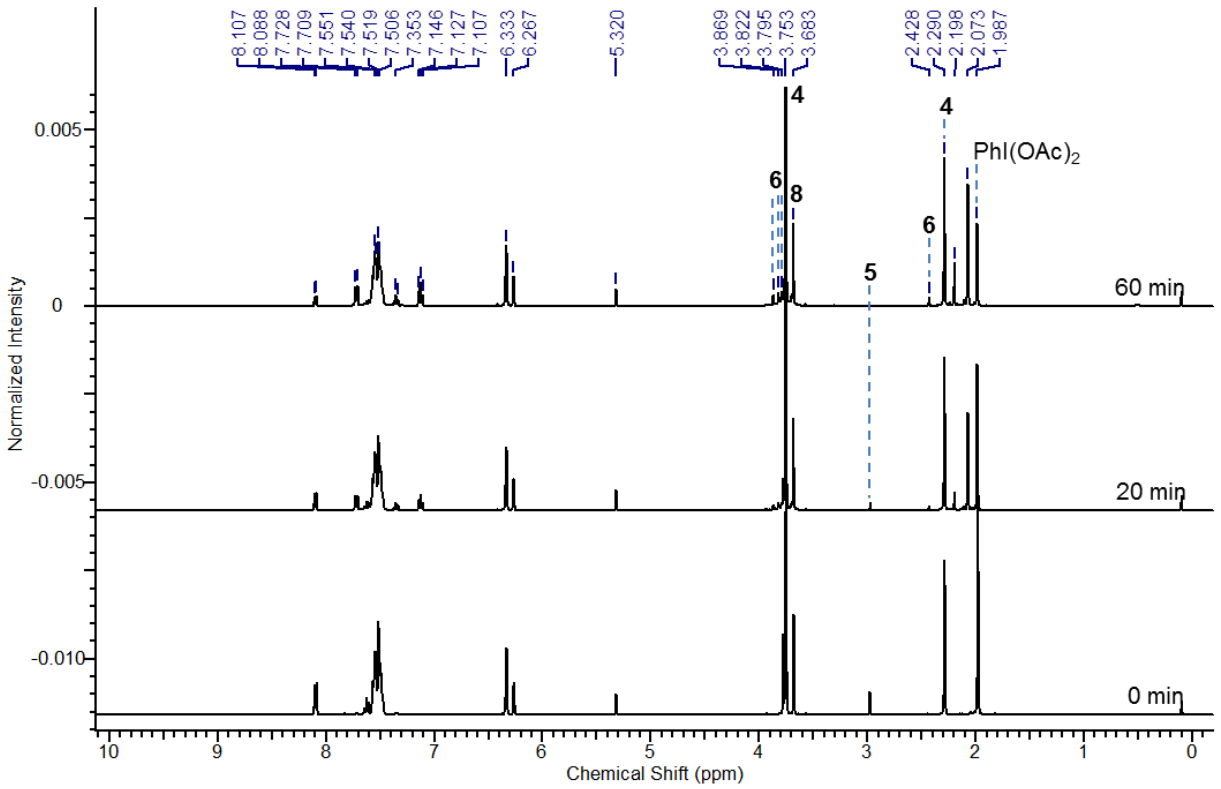
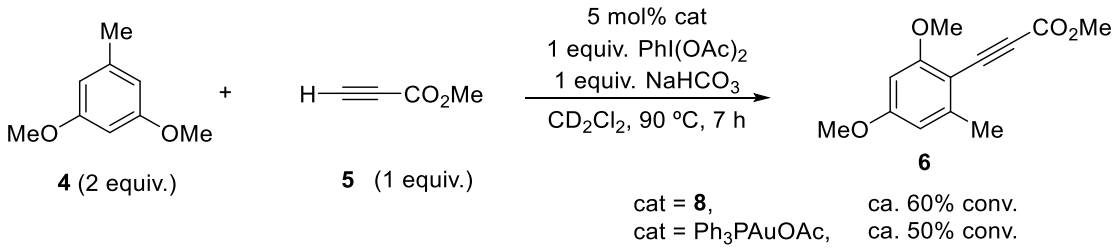


Figure S35. *In situ* ^{1}H-NMR spectrum of the reaction between **4** and **8** in presence of $PhI(OAc)_2$ and **5**

3.7.3 Catalytic reaction in presence of additional alkyne (Equation 9 in the main text)



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (1.1 mg, 0.002 mmol), diacetoxy(phenyl)-λ^3-iodane (19 mg, 0.06 mmol), 3,5-dimethoxytoluene (**4**) (12.2 mg, 0.08 mmol), methyl propiolate (**5**) (3.4 mg, 0.04 mmol) and $NaHCO_3$ (3 mg, 0.04 mmol), dichloromethane-d_2 (0.5 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 7 h and was monitored by ^{1}H-, ^{31}P-NMR (Figures S36-37). The crude mixture contains compound **6** in 63% molar ratio (^{1}H-NMR). Same conditions were applied for $Ph_3PAuOAc$ as catalyst.

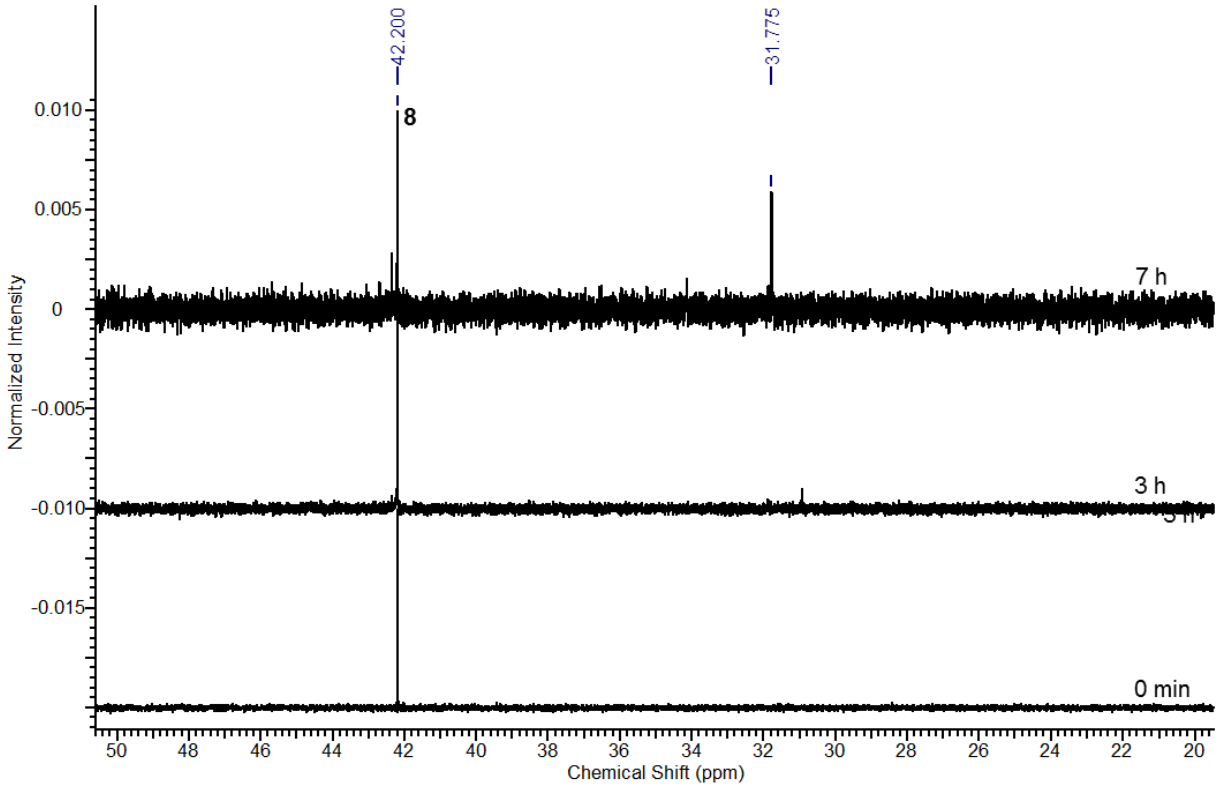


Figure S36. *In situ* ^{31}P-NMR spectrum of the reaction between **4** and **5** catalyzed by **8**

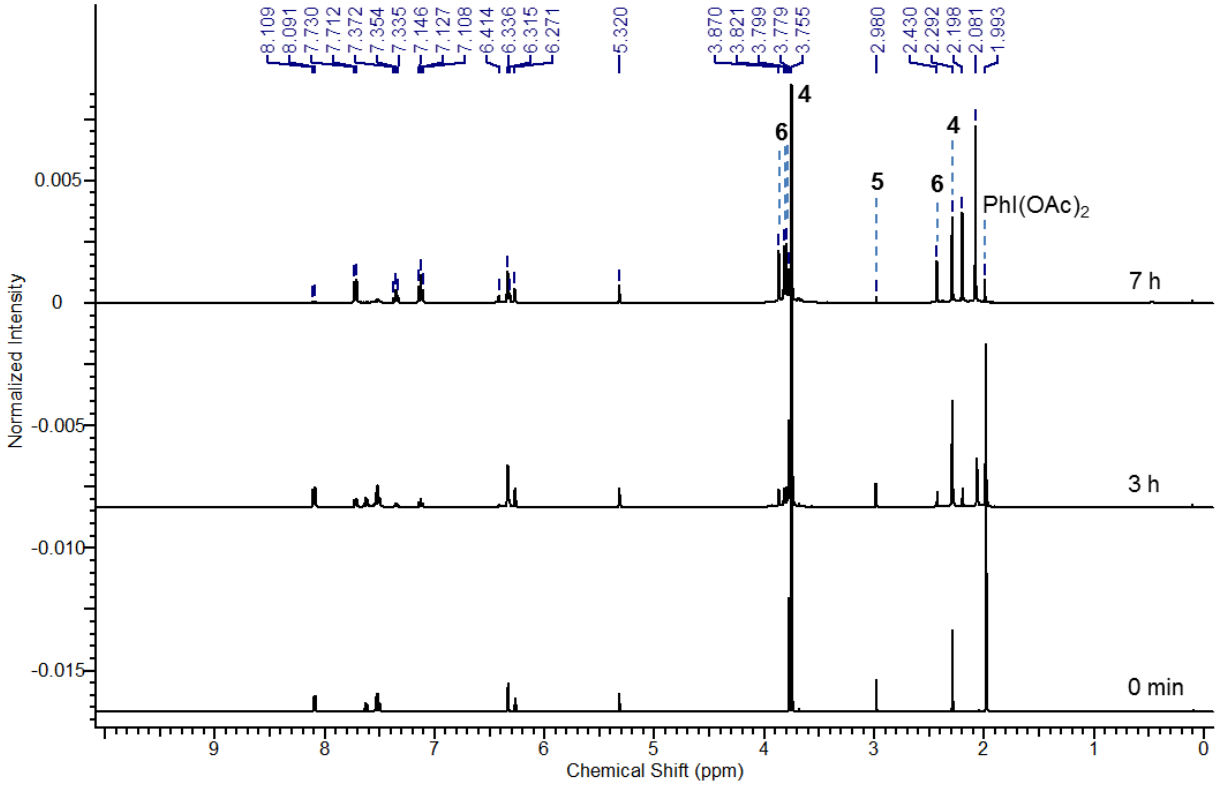
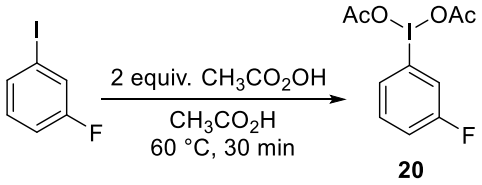


Figure S37. *In situ* ^{1}H-NMR spectrum of the reaction between **4** and **5** catalyzed by **8**

3.8 Formation of a non-symmetric oxidant (Figure 4 in the main text)

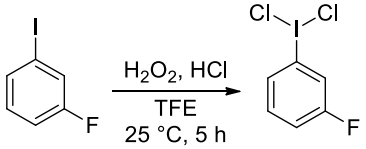
3.8.1 Synthesis of diacetoxy(3-fluorophenyl)-λ3-iodane (**20**)[23]



20

To 1-fluoro-3-iodobenzene (2.22 g, 10 mmol), paracetic acid 39% (3.40 mL, 20 mmol) was added over 30 min at 30 °C and stirred at the same temperature for 60 min. The reaction mixture was cooled down to 0 °C and a white solid precipitated. The solid was filtered off and washed with water and cold ethanol to give **20** as a white solid. Isolated yield: 84% (2.85 g, 8.4 mmol). m.p.: 141-143 °C. ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 7.90 - 7.83 (m, 2 H), 7.57 - 7.49 (m, 1 H), 7.35 - 7.28 (m, 1 H), 1.99 (s, 6 H); ^{13}C NMR (376 MHz, CD_2Cl_2): δ = 177.2 (s), 162.9 (d, *J* = 253.5 Hz), 132.7 (d, *J* = 8.0 Hz), 131.3 (d, *J* = 3.5 Hz), 123.0 (d, *J* = 25.0 Hz), 120.5 (d, *J* = 8.0 Hz), 119.6 (d, *J* = 21.0 Hz), 20.6 (s); ^{19}F NMR (376 MHz, CD_2Cl_2): δ = -(108.37 - 108.50) (m). FTIR (cm^{-1}): 3083, 1587, 1575, 1469, 1419, 1298, 1271, 1210, 1161, 1078, 994, 905, 864, 840, 787; ESI-HRMS (m/z): $[M + Na]^+$ calcd for $C_{10}H_{10}FIO_4$, 362.95055; found: 362.94995.

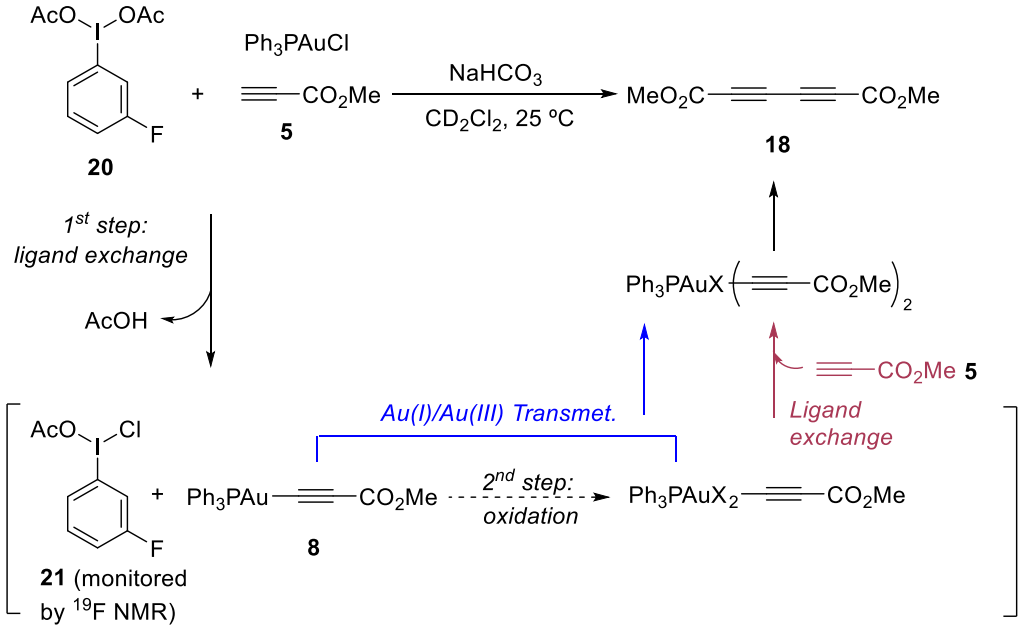
3.8.2 Synthesis of dichloro(3-fluorophenyl)-λ^3-iodane[24]



To 1-fluoro-3-iodobenzene (2.22 g, 10 mmol) and 2,2,2-trifluoroethanol (10.0 mL), hydrogen peroxide 35% (3.89 g, 40 mmol) monitored by HCl 32% (3.93 mL, 40 mmol) was added. The reaction mixture was stirred at 25 °C for 5 h in the dark under dinitrogen atmosphere. A yellow solid precipitated. The solid was filtered off and washed with water, cold ethanol and hexane to give dichloro(3-fluorophenyl)-λ3-iodane as a yellow solid. Isolated yield: 38% (1.1 g, 3.8 mmol). m.p.: 72-73 °C (decomp.). ^{1}H NMR (400 MHz, CD_2Cl_2): δ = 8.05 - 8.01 (m, 1 H), 8.00 - 7.95 (m, 1 H), 7.55 - 7.47 (m, 1 H), 7.37 - 7.31 (m, 1 H); ^{13}C NMR (376 MHz, CD_2Cl_2): δ = 162.6 (d, *J* = 256.0 Hz), 133.1 (d, *J* = 8.0 Hz), 130.2 (d, *J* = 3.5 Hz), 123.9 (d, *J* = 8.5 Hz), 122.0 (d, *J* = 26.0 Hz), 120.3 (d, *J* = 21.0 Hz); ^{19}F NMR (376 MHz, CD_2Cl_2): δ = -(106.34 - 106.50) (m). FTIR (cm^{-1}): 3069, 1640, 1585, 1471, 1421, 1367, 1294, 1263, 1216, 1042, 1011, 997, 925, 865, 845, 797.

[24] J. G. Sharefkin, H. Saltzman, *Org. Synth.* 1963, **43**, 62.
[25] A. Podgoršek, J. Iskra, *Molecules* 2010, **15**, 2857.

3.8.3 Observation of the formation of the non-symmetric oxidant **21** (Figure 4 in the main text)



Chloro(triphenylphosphine)gold(I) (5.0 mg, 0.01 mmol), methyl propiolate (**5**) (0.8 mg, 0.01 mmol), $NaHCO_3$ (1 mg, 0.01 mmol) and diacetoxy(3-fluorophenyl)-λ3-iodane (**20**) (3.4 mg, 0.01 mmol), dichloromethane-d_2 (0.4 mL) was added. The reaction was performed in a sealed NMR tube at 25 °C for 7 h and was monitored by ^{1}H-, ^{31}P- and ^{19}F-NMR (Figures S38-39). The reaction showed the formation of (acetoxy)(chloro)(3-fluorophenyl)-λ^3-iodane (**21**) as an intermediate in low concentration and the formation of the homocoupling product **18**. The formation of **21** was explained by exchange of chloride and acetate ligands of Ph_3PAuCl and **20**. The formation of **18** was explained by in situ oxidation of **8** by **21** monitored by an OAc-alkyne ligand exchange on the Au(III)-acetylide intermediate, which evolves via reductive elimination to give **18** and Ph_3PAuCl (see section 3.6.1) or via Au(I)/Au(III) transmetalation (see section 3.6.5).

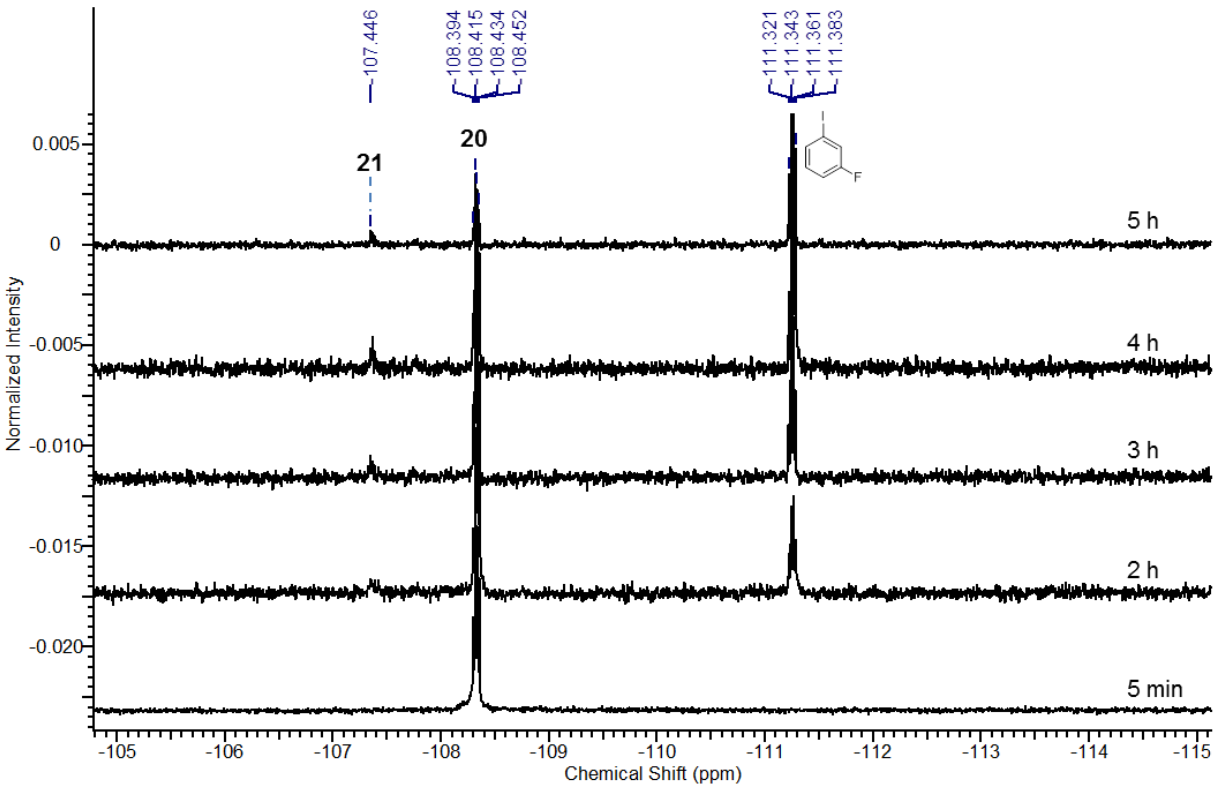


Figure S38. *In situ* ^{19}F-NMR spectrum of the reaction between Ph_3PAuCl and **5** in presence of **20**

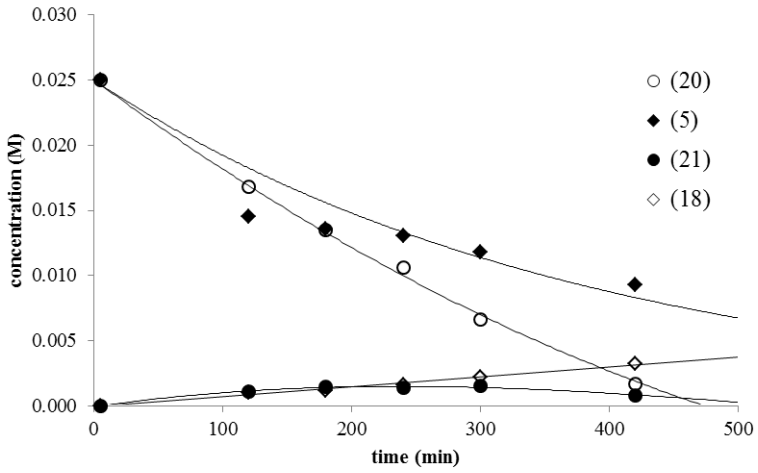
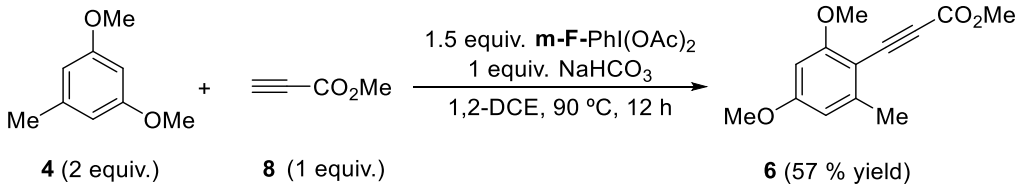


Figure S39. Observed evolution of the concentration of the diacetoxy(3-fluorophenyl)-λ3-iodane (**20**), methyl propiolate (**5**), (acetoxy)(chloro)(3-fluorophenyl)-λ^3-iodane (**21**) and the homocoupling product of the alkyne (**18**) over time

3.8.4 Catalytic reaction in presence of diacetoxy(3-fluorophenyl)-λ3-iodane (**20**) as oxidant

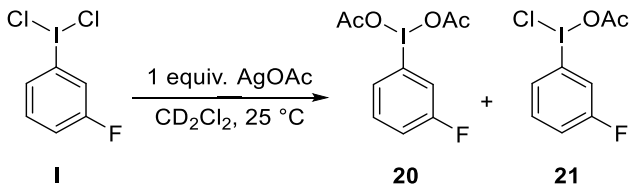


4 (2 equiv.) **8** (1 equiv.) **6** (57 % yield)

To a solution of 3,5-dimethoxytoluene (**4**) (30.4 mg, 0.20 mmol), diacetoxy(3-fluorophenyl)-λ3-iodane (**20**) (51.0 mg, 0.15 mmol), $NaHCO_3$ (8.4 mg, 0.10 mmol) and methyl propiolate (**5**) (8.4 mg, 0.10 mmol) in 1,2-dichloroethane (1.0 mL), chloro(triphenylphosphine)gold(I) (2.47 mg, 0.005 mmol) and dodecane (2.1 mg, 0.0125 mmol) was added. The reaction was performed in a sealed schlenk-tube and heated to 90 °C for 14 h. The reaction mixure was analysed by GC-FID and product **6** was found in 57% yield (dodecane as internal standard).

3.8.5 Synthesis of (acetoxy)(chloro)(3-fluorophenyl)-λ^3-iodane (**21**)

A) Synthesis of **20** with silver-acetate[25]



I **20** **21**

To dichloro(3-fluorophenyl)-λ^3-iodane (5.9 mg, 0.02 mmol) and silver-acetate (3.3 mg, 0.02 mmol), dichloromethane-d_2 (0.4 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C for 1 h and was monitored by ^{1}H- and ^{19}F-NMR (Figures S40-41). The reaction showed a 1:1:2 ratio of **I**:**20**:**21** by ^{19}F-NMR and a ratio of **20**:**21** = 1:2 by ^{1}H-NMR. ^{19}F NMR (376 MHz, CD_2Cl_2): δ = -(107.46 - 107.58) (m). All attempts to separate these compounds were unsuccessful as these species tend to interconvert between each other in solution.

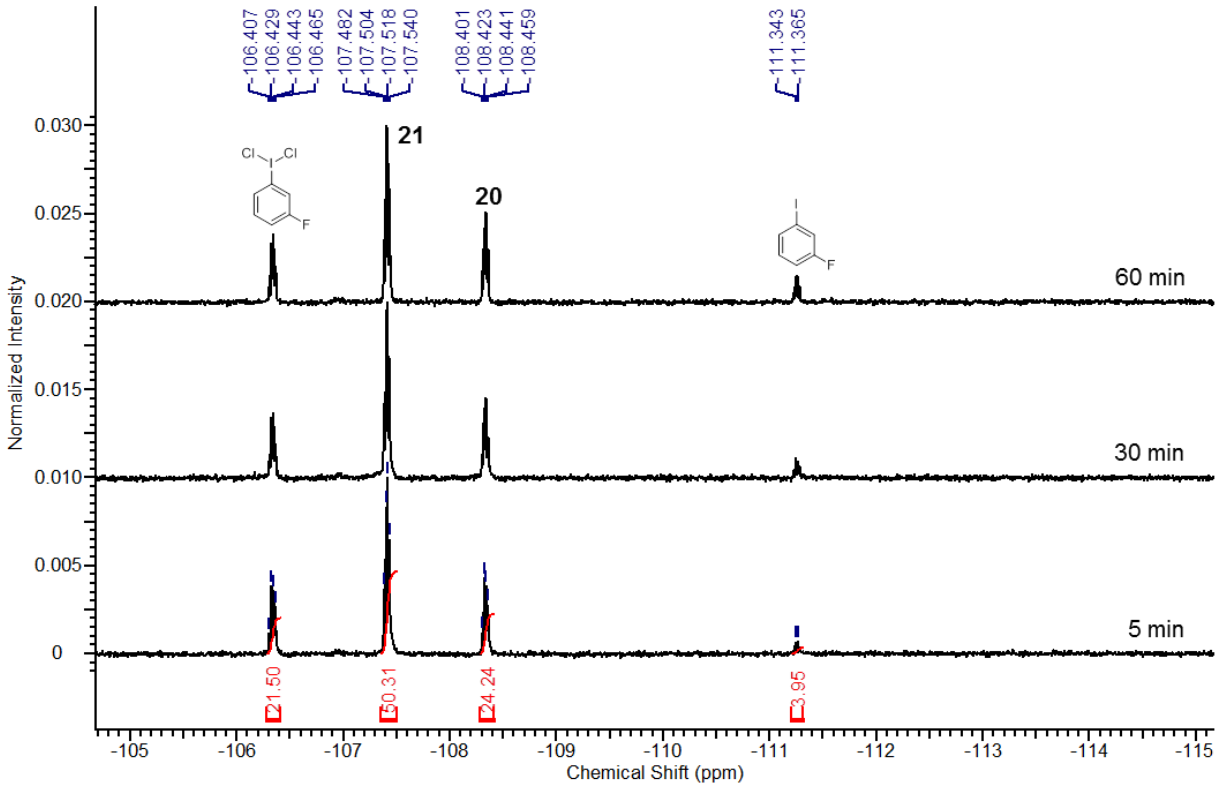


Figure S40. *In situ* ^{19}F-NMR spectrum of the reaction between dichloro(3-fluorophenyl)-λ3-iodane and AgOAc

[25] N. W. Alcock, T. C. Waddington, *J. Chem. Soc.* 1963, 4103.

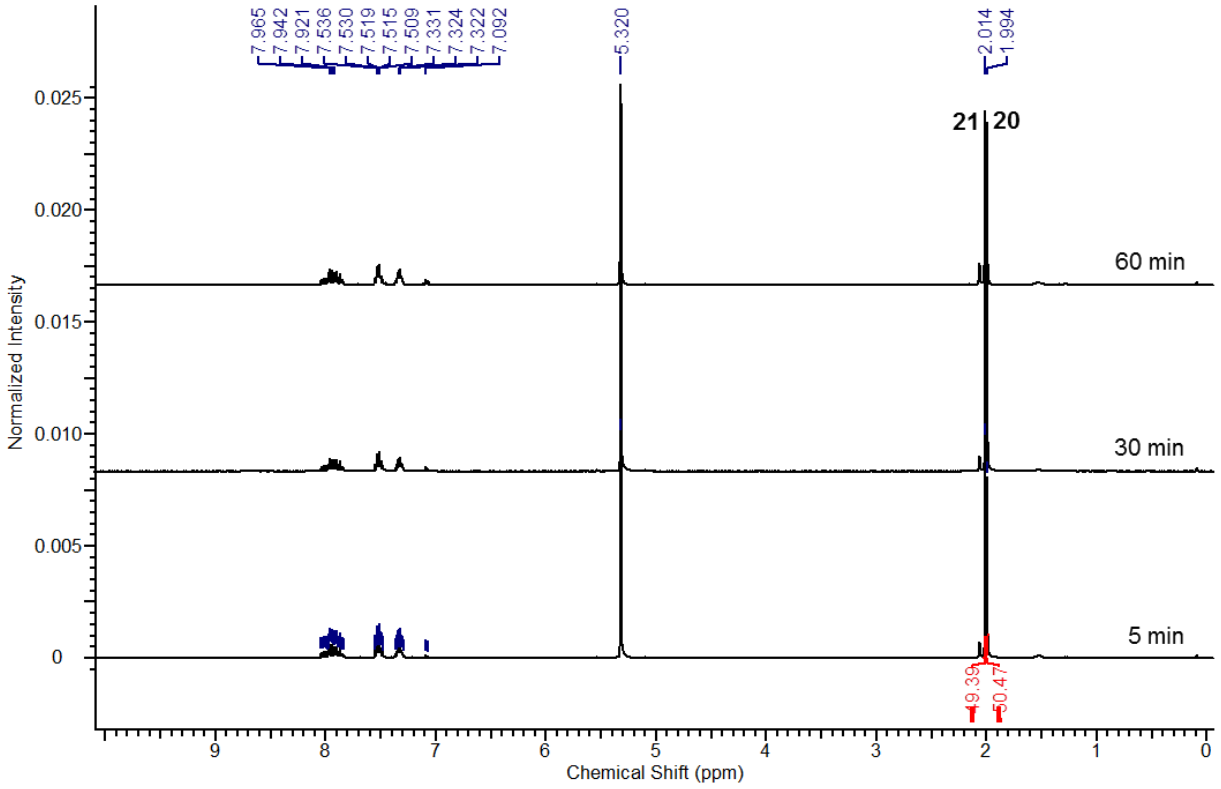
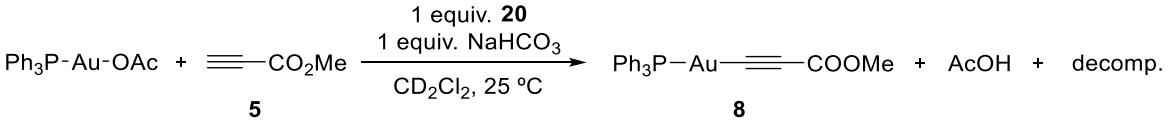


Figure S41. *In situ* ^{1}H-NMR spectrum of the reaction between dichloro(3-fluorophenyl)-λ3-iodane and AgOAc

B) Control experiments

As shown in section 3.8.3, the non-symmetric oxidant **21** was observed in an experiment in which Ph_3PAuCl, alkyne **5** and the *m*-F-containing iodonium diacetate **20** were present in the reaction mixture. Control experiments were designed to investigate whether these three species (Ph_3PAuCl, **5**, **20**) were required to produce **21**.

B1) Control experiment in presence of $Ph_3PAuOAc$



To acetato(triphenylphosphine)gold(I) (5.2 mg, 0.01 mmol), methyl propiolate (**5**) (0.8 mg, 0.01 mmol), $NaHCO_3$ (1 mg, 0.01 mmol) and diacetoxy(3-fluorophenyl)-λ3-iodane (**20**) (3.4 mg, 0.01 mmol), dichloromethane-d_2 (0.4 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C for 7 h and was monitored by ^{1}H-, ^{31}P- and ^{19}F-NMR (Figures S42-43). The reaction showed the fast formation of the gold(I) complex **8** and some decomposition products. The non-symmetric oxidant **21** was not observed thus supporting the idea of a Au-I ligand exchange, which in this case would regenerate **20**. The fact that, in contrast to 3.8.3, no alkyne homocoupling product **18** is detected, also substantiate the idea of a lower redox-potential for **20** compared to **21**.

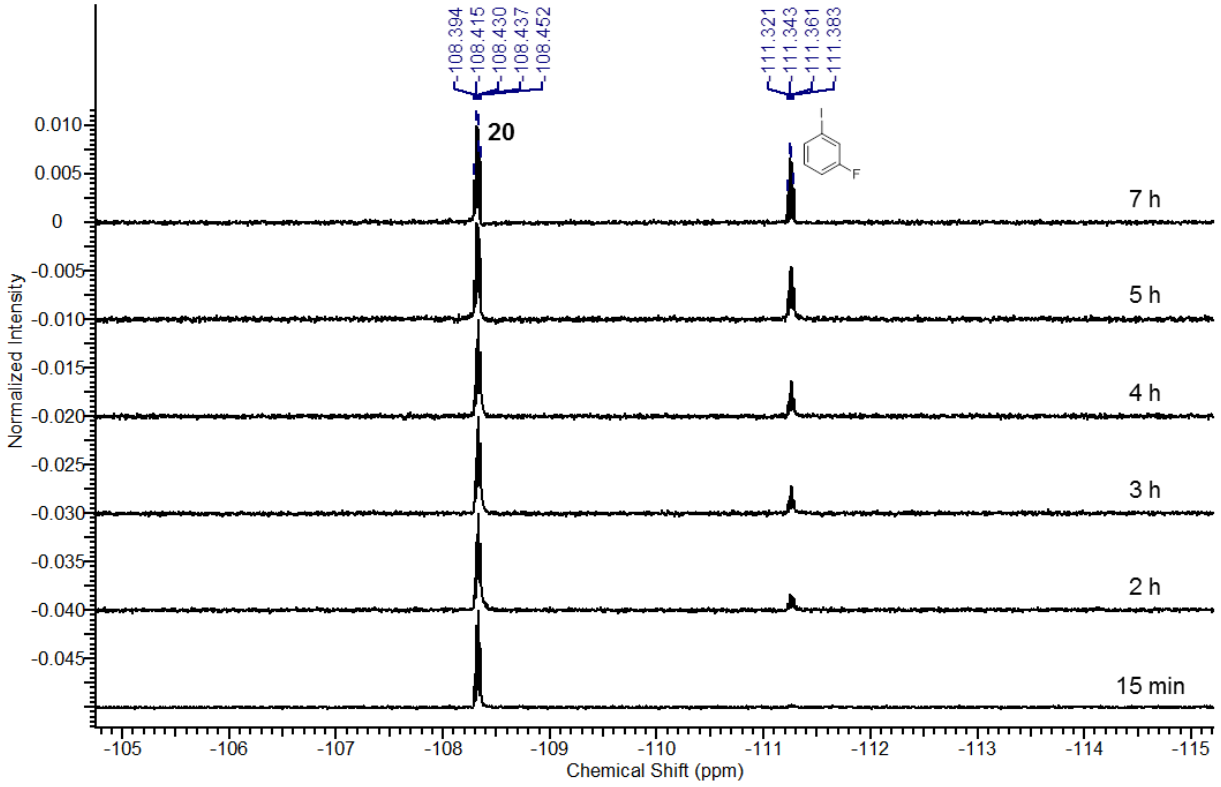


Figure S42. *In situ* ^{19}F-NMR spectrum of the reaction between $Ph_3PAuOAc$ and **5** in presence of **20**

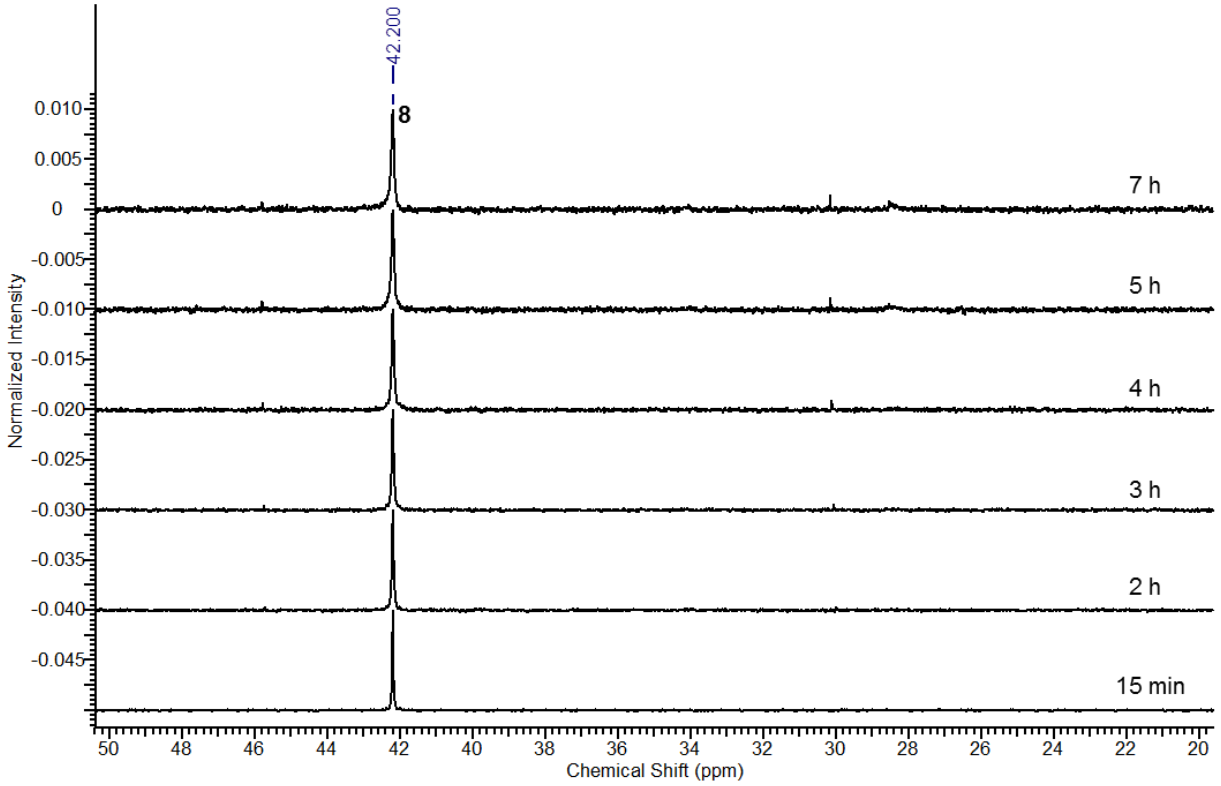
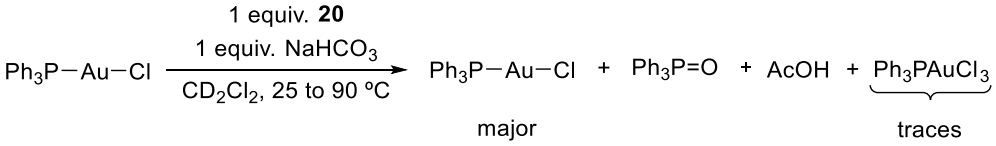


Figure S43. *In situ* ^{31}P-NMR spectrum of the reaction between $Ph_3PAuOAc$ and **5** in presence of **20**

B2) Control experiment in presence of Ph_3PAuCl and oxidant **20**



To chloro(triphenylphosphine)gold(I) (5.0 mg, 0.01 mmol), $NaHCO_3$ (1 mg, 0.01 mmol) and diacetoxy(3-fluorophenyl)-λ^3-iodane (**20**) (3.4 mg, 0.01 mmol), dichloromethane-d_2 (0.4 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C for 5 h and at 90 °C for 45 min and was monitored by ^{1}H-, ^{31}P- and ^{19}F-NMR (Figures S44-45). The reaction showed no reactivity at 25 °C. At 90 °C, trace amounts of $Ph_3P=O$, Au^0 and Ph_3PAuCl_3 were found only after prolonged heating. The formation of Ph_3PAuCl_3 was explained by in situ formation of **21** and subsequent oxidation of Ph_3PAuCl by **21**. The non-symmetric oxidant **21** was not observed.

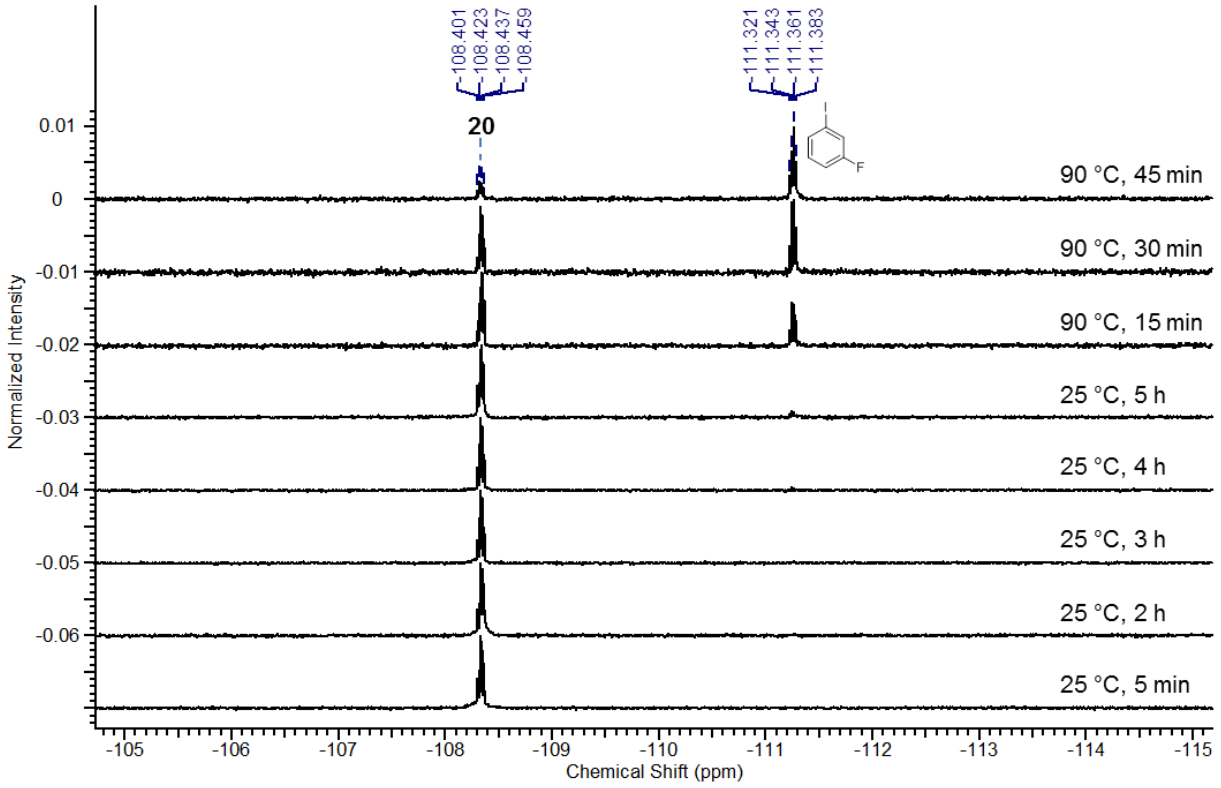


Figure S44. *In situ* ^{19}F-NMR spectrum of the reaction between Ph_3PAuCl and **20**

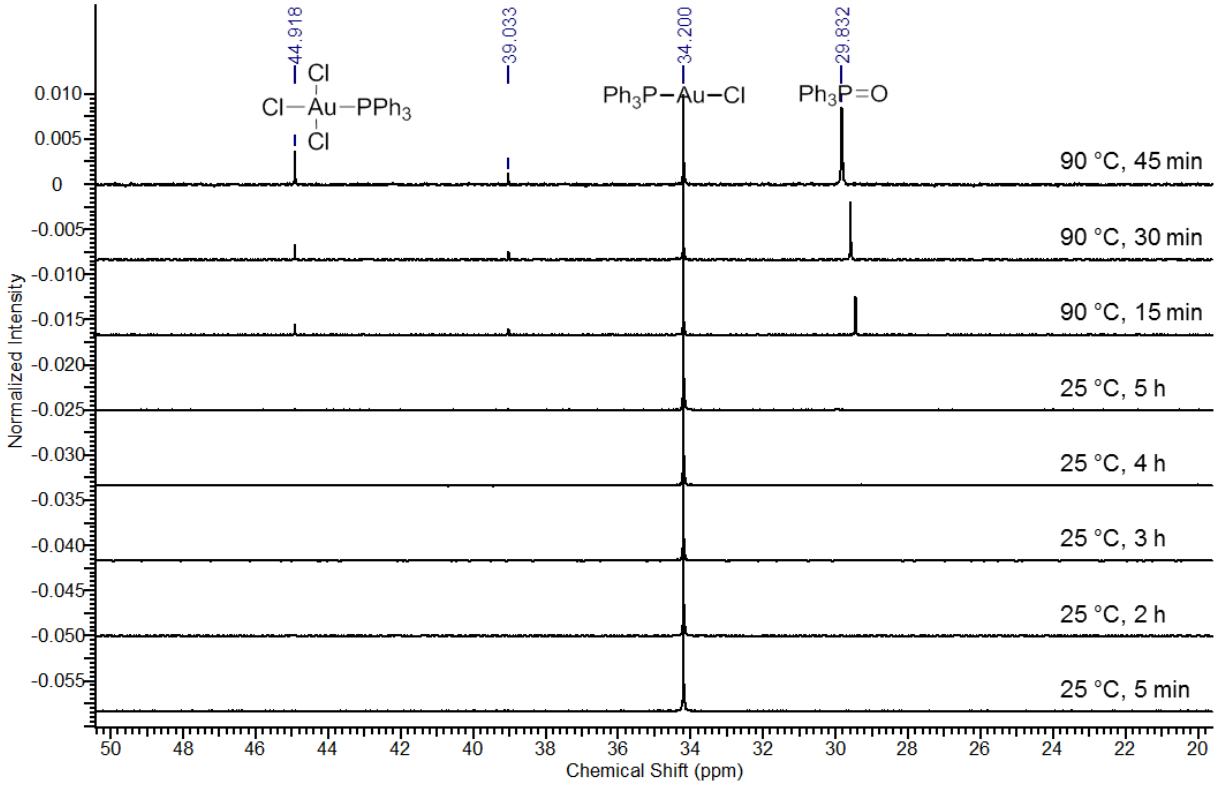
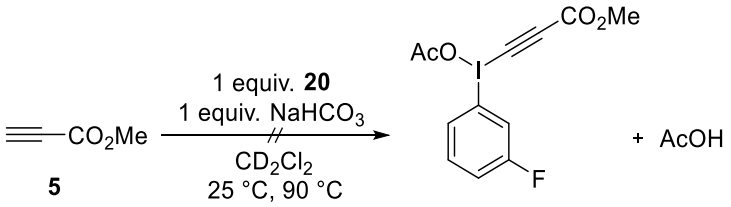


Figure S45. *In situ* ^{1}H-NMR spectrum of the reaction between Ph_3PAuCl and **20**

B3) Control experiment in presence of methyl propiolate **5** and oxidant **20**



To methyl propiolate (**5**) (0.8 mg, 0.01 mmol), $NaHCO_3$ (1 mg, 0.01 mmol) and diacetoxy(3-fluorophenyl)-λ3-iodane (**20**) (3.4 mg, 0.01 mmol), dichloromethane-d_2 (0.4 mL) was added. The reaction was performed in a sealed NMR-tube at 25 °C for 5 h and at 90 °C for 45 min and was monitored by ^{1}H-, ^{31}P- and ^{19}F-NMR (Figure S46). The reaction showed no reactivity at 25 °C and 90 °C.

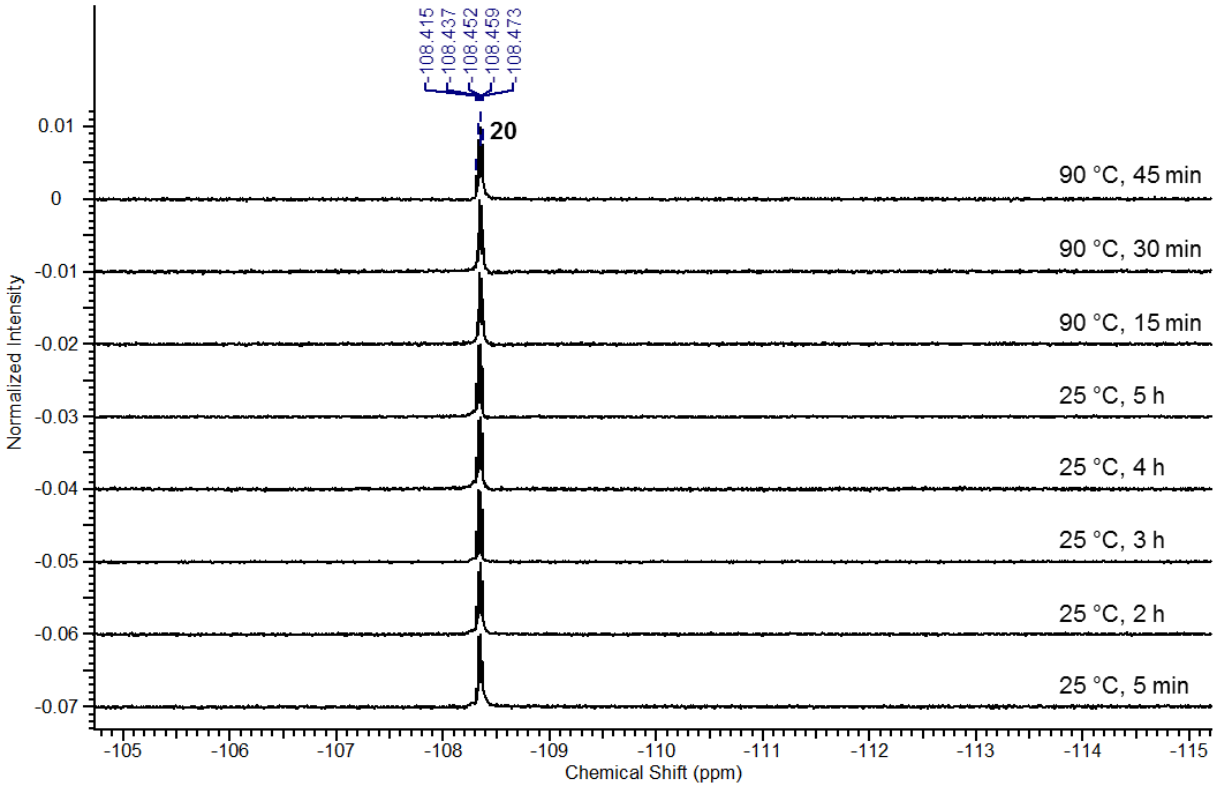


Figure S46. *In situ* ^{19}F-NMR spectrum of the reaction between **5** and **20**

Summary and conclusions of the experiments B1) - B3):

Control experiment B1) showed the fast reaction of $Ph_3PAuOAc$ and methyl propiolate **5** to form gold acetylide **8** and subsequent slow oxidation of **8** by $PhI(OAc)_2$ (Figure S47). As expected, the non-symmetric oxidant **21** was not observed in absence of chloride ligands. Experiment B2) showed the formation of Ph_3PAuCl_3 at 90 °C, but **21** was not observed. However, the formation of Ph_3PAuCl_3 was explained by slow formation of **21** and subsequent oxidation of Ph_3PAuCl by **21**. Therefore, the alkyne is not required for the formation of **21.** No reactivity was found for experiment B3) and the formation of an alkynyliodonium compound was excluded (in line with the results summarized in section 2).

The control experiments suggest a two step mechanism: Ph_3PAuCl is able to exchange the chloride ligand with $PhI(OAc)_2$ to form the non-symmetric oxidant **21** and $Ph_3PAuOAc$ (exp. B2).[26] Once $Ph_3PAuOAc$ is formed, it reacts fast by activation of the alkyne **5** to form the gold(I) intermediate **8** (exp. B1).

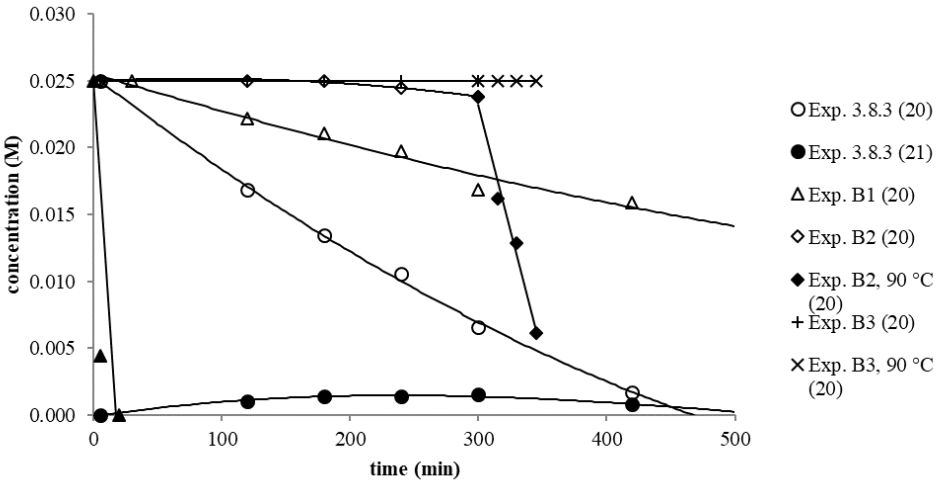


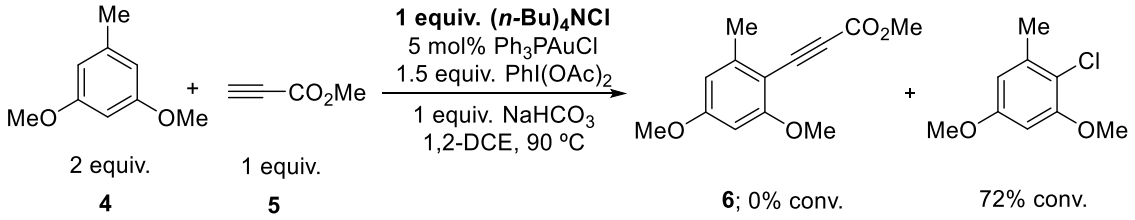
Figure S47. Observed concentrations of diacetoxy(3-fluorophenyl)-λ^3-iodane (**20**) and **21** over time for experiments 3.8.3 and B1 – B3

[26] D.-H. Zhang, L. -Z. Dai, M. Shi, *Eur. J. Org. Chem.* 2010, **28**, 5454.

3.9 Effect of external amounts of chloride

3.9.1 Addition of one equivalent chloride to the standard catalytic reaction

If the transfer of the chloride ligand of Ph_3PAuCl to $PhI(OAc)_2$ to form PhI(Cl)(OAc) represents the initial step of the proposed catalytic cycle, the subsequent formation of **8** and the coupling product would be inhibited in presence of an initial excess of chloride in the reaction mixture as observed in the experiment described below.



To a solution of 3,5-dimethoxytoluene (**4**) (60 mg, 0.40 mmol), diacetoxy(phenyl)-λ3-iodane (96.6 mg, 0.30 mmol), $NaHCO_3$ (16.8 mg, 0.20 mmol), methyl propiolate (**5**) (16.8 mg, 0.20 mmol), tetrabutylammonium chloride (55.6 mg, 0.20 mmol) and 1,2-dichloroethane (2.0 mL), chloro-(triphenylphosphine)gold(I) (4.95 mg, 0.010 mmol) and dodecane (4.3 mg, 0.025 mmol, internal standard) were added. The reaction was heated to 90 °C for 2 h, 4 h, 14 h and was monitored by ^{1}H- and ^{31}P-NMR (Figure S48) and GC, GC-MS. No formation of the coupling product, complete decomposition of $PhI(OAc)_2$ and 2-chloro-3,5-dimethoxytoluene as the main reaction product were found by ^{1}H-NMR already after 2 h at 90°C.

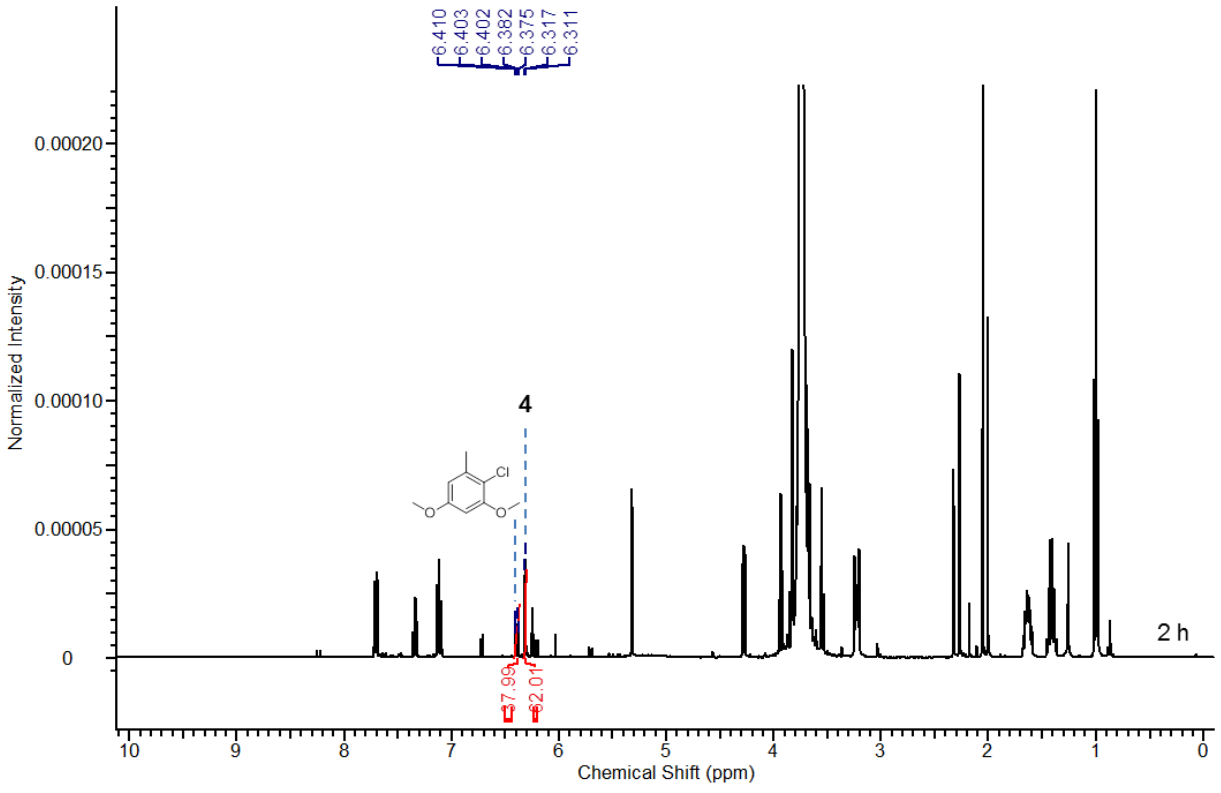
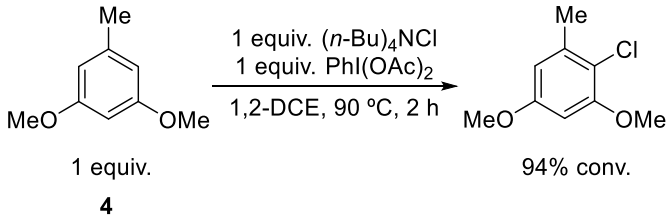


Figure S48. *In situ* ^{1}H-NMR spectrum of the catalytic reaction in presence of 1 equiv. $(n\text{-Bu})_4NCl$

3.9.2 Control experiment

The transfer of the chloride ligand of $(n\text{-Bu})_4NCl$ to $PhI(OAc)_2$ to form PhI(Cl)(OAc) was assumed to be the initial step of the catalytic reaction in experiment in section 3.9.1. Might this be the case, the formation of 2-chloro-3,5-dimethoxytoluene would also be observed in presence of just $(n\text{-Bu})_4NCl$, $PhI(OAc)_2$ and the arene, as it turned out to be the case in the experiment shown below.



1 equiv. **4**

94% conv.

To a mixture of 3,5-dimethoxytoluene (**4**) (60.1 mg, 0.40 mmol), diacetoxy(phenyl)-λ^3-iodane (128.8 mg, 0.40 mmol), tetrabutylammonium chloride (55.6 mg, 0.40 mmol), 1,2-dichloroethane (2.0 mL) was added. The reaction was heated to 90 °C for 2 h and was monitored by ^{1}H-NMR (Figure S49). The crude mixture contains 2-chloro-3,5-dimethoxytoluene in 94% molar ratio by ^{1}H-NMR. For additional control experiments regarding the formation of the chloro-arene see section 4.2.2.

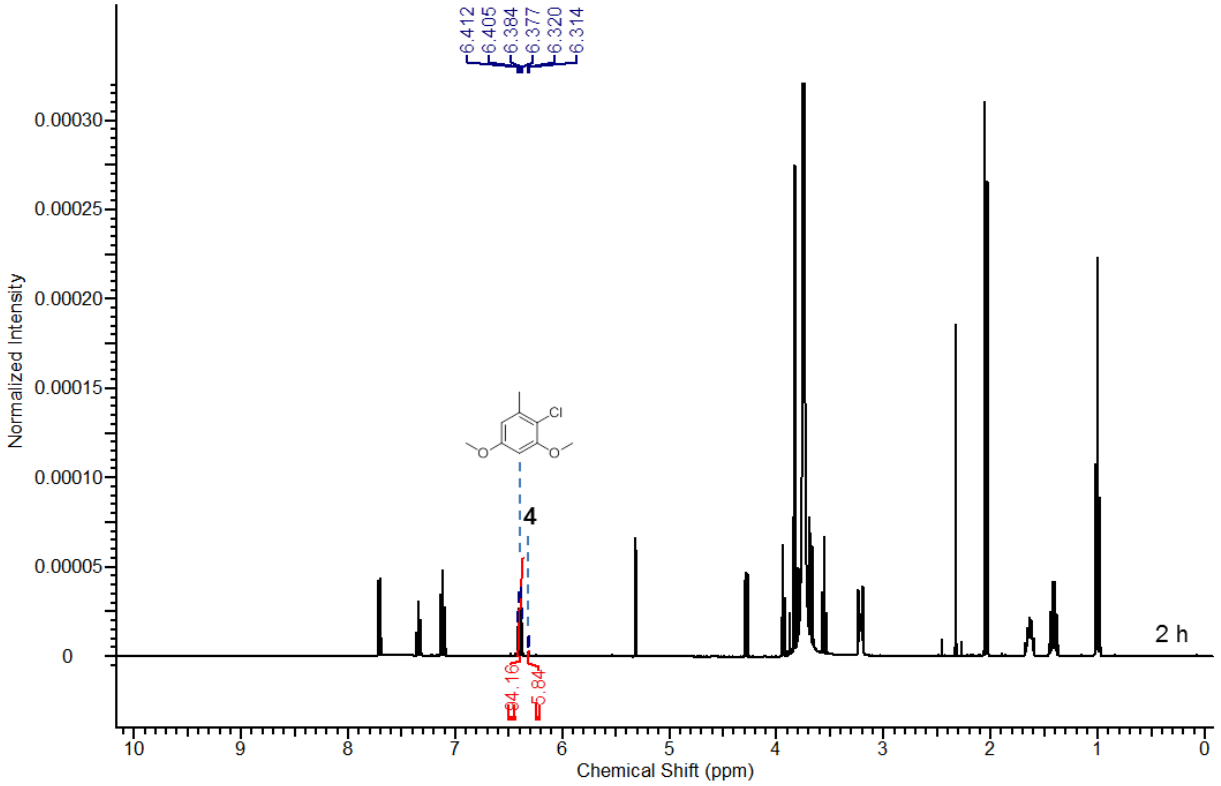
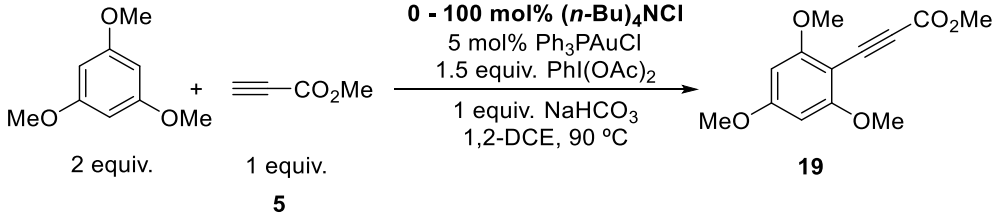


Figure S49. *In situ* ^{1}H-NMR spectrum of the reaction of $(n\text{-Bu})_4NCl$, $PhI(OAc)_2$ and the arene **4**

3.9.3 Effect of Addition of substoichiometric amounts of chloride to the standard catalytic reaction

The inhibition of the catalytic reaction in presence of a substoichiometric initial amount of chloride in the reaction mixture was studied in the experiment described below.



To a solution of 1,3,5-trimethoxybenzene (33.6 mg, 0.20 mmol), diacetoxy(phenyl)-λ3-iodane (48.3 mg, 0.15 mmol), $NaHCO_3$ (8.4 mg, 0.10 mmol), methyl propiolate (**5**) (8.4 mg, 0.10 mmol), tetrabutylammonium chloride (0.0-27.8 mg, 0.0-0.10 mmol) in 1,2-dichloroethane (1.0 mL), chloro(triphenyl-phosphine)gold(I) (2.50 mg, 0.005 mmol) was added. The reaction was heated to 90 °C for 12 h. Dodecane (4.3 mg, 0.025 mmol) was added and the reaction was monitored by GC-FID. The yield of **19** was calculated with dodecane as internal standard (Figure S50). Just low concentrations of (n-Bu)$_4$NCl (2.5 mol%) were tolerated whereas addition of 5-20 mol% (n-Bu)$_4$NCl dramatically reduced the yield of **19**.

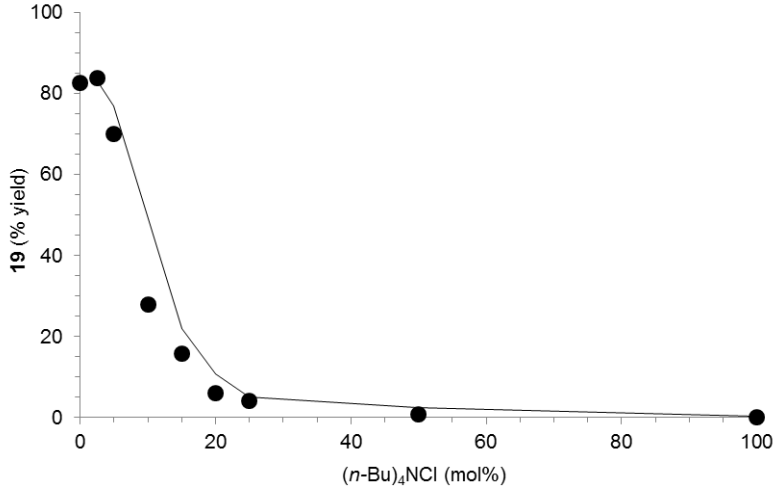
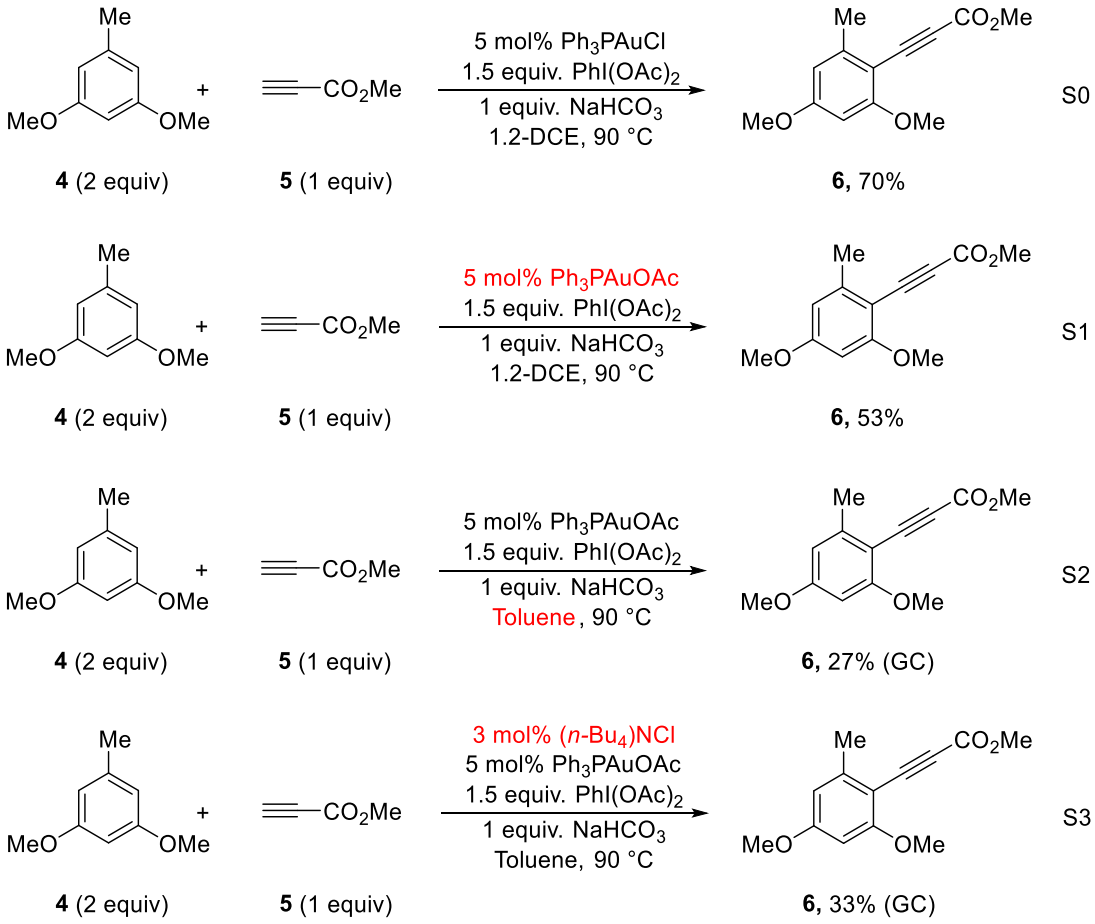


Figure S50. Formation of **19** in presence of (n-Bu)$_4$NCl up to 100 mol%

3.9.4 Effect of Addition of substoichiometric amounts of chloride to the *non*-standard catalytic reaction

The reaction of arene **4** with methyl propiolate **5** has been carried out with $Ph_3PAuOAc$ as catalyst, 1,2-DCE or toluene as solvents in the presence and in the absence of $(n\text{-Bu})_4NCl$ (3 mol%) as external chloride source (equations S1-S3 in the figure below). This reaction delivered the product **6** in 70% yield under the standard conditions (Ph_3PAuCl in 1,2-DCE; equation S0).[27]



As seen in these experiments, toluene is a less suitable solvent for these transformations (S1 vs. S2). This had already been observed in our original communication, in which a large solvent screening revealed 1,2-DCE as the most suitable media in line with a better solubilization of all reagents and stabilization of the different intermediates and transition states.[27]

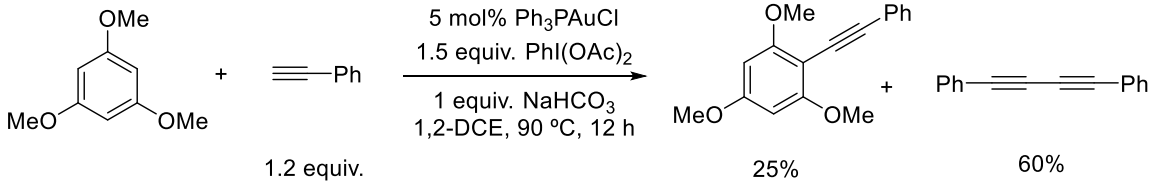
The effect of the reacting ligand of the catalyst is also visible here (S0 vs. S1), with Ph_3PAuCl being preferred over $Ph_3PAuOAc$. Finally, a comparison between S2 and S3 shows that the presence of small amounts of external chloride provides a slight improvement of the reaction outcome in line with the ability to form a more reactive non-symmetric I(III) oxidant.

[27] De Haro, T.; Nevado, C. *J. Am. Chem. Soc.* 2010, **132**, 1512.

4. Side reactions and catalyst decomposition pathways

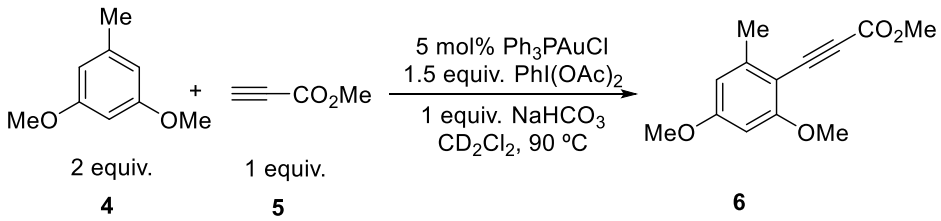
4.1 Formation of alkyne homocoupling products

The cross coupling of 1,3,5-trimethoxybenzene with phenyl acetylene resulted in a 25% yield of the corresponding cross coupling together with alkyne homocoupling product in 60% yield.



After careful monitorization of the standard cross coupling reaction between 3,5-dimethoxytoluene and methyl propiolate, homocoupling of the latter could also be observed as shown in section 4.1.1.

4.1.1 Observation of the alkyne homocoupling product **18** in a catalytic reaction



To a solution of 3,5-dimethoxytoluene (**7**) (12.2 mg, 0.08 mmol), diacetoxy(phenyl)-λ^3-iodane (19 mg, 0.06 mmol), $NaHCO_3$ (3 mg, 0.04 mmol), methyl propiolate (**5**) (3.4 mg, 0.04 mmol) and dichloromethane-d_2 (0.5 mL), chloro(triphenylphosphine)gold(I) (0.002 mmol, 1 mg) was added. The reaction was performed in a sealed NMR-tube and heated to 90 °C for 23 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figure S51-52). The homocoupling product **18** was found as a side product in less than 10% molar ratio (^{1}H-NMR).

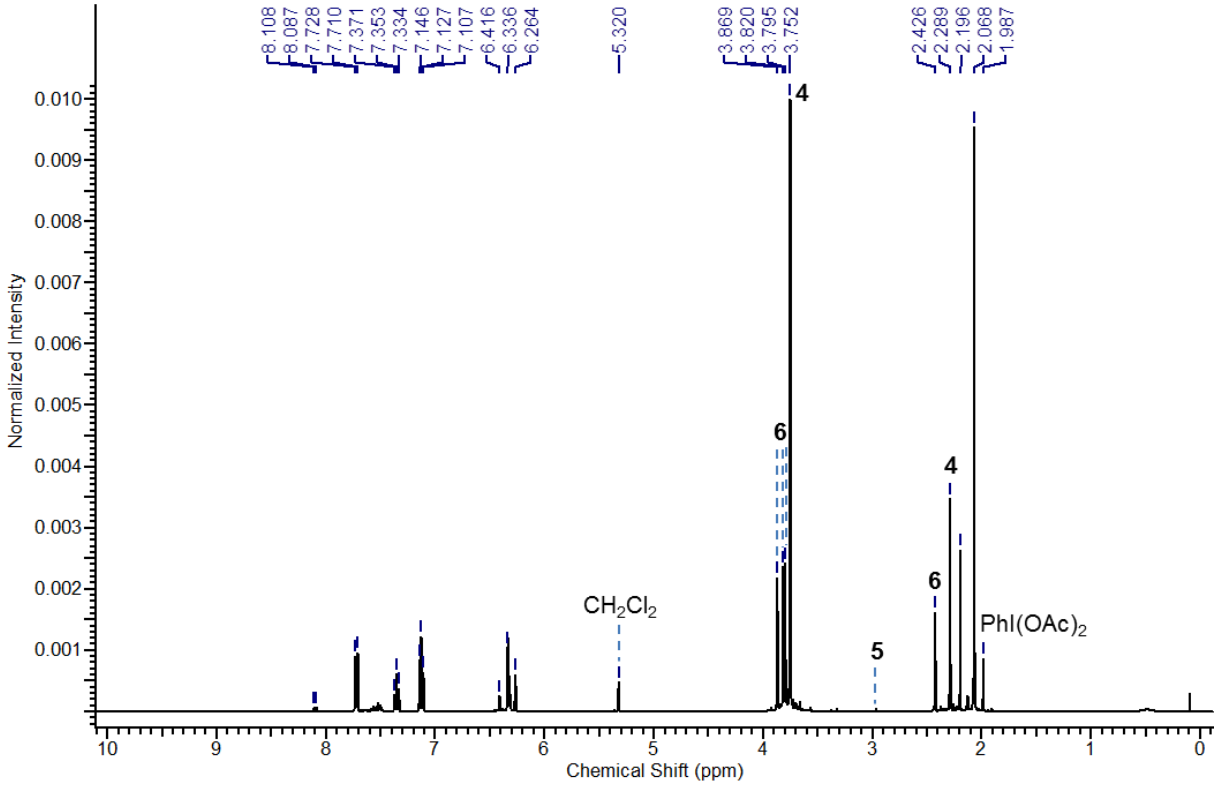


Figure S51. *In situ* ^{1}H-NMR spectrum of the catalytic reaction after 19 h.

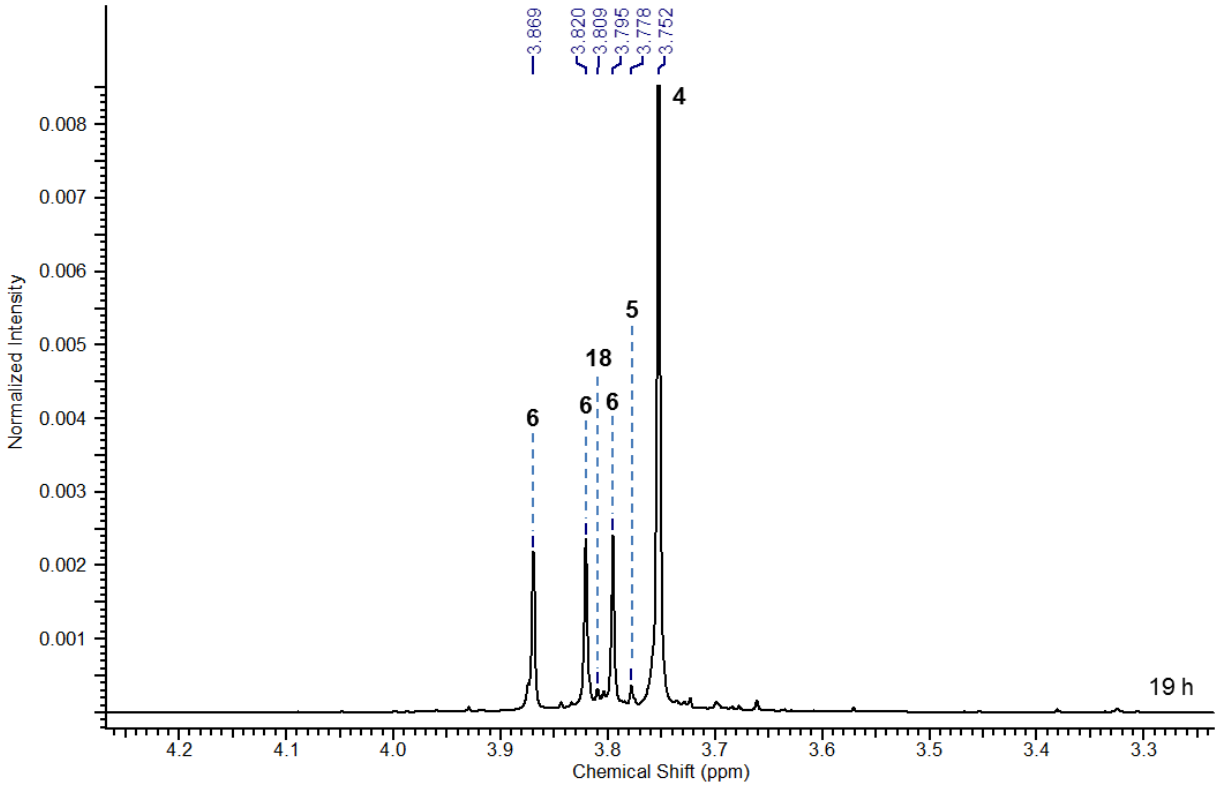
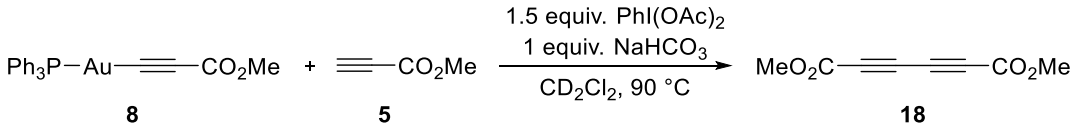


Figure S52. *In situ* ^{1}H-NMR spectrum of the catalytic reaction after 19 h (close-up)

4.1.2 Control experiments to explain the formation of **18**

As shown in equation 2 of the main text, the putative Au(III) complex $Ph_3PAu(C{\equiv}C\text{-}CO_2Me)(OAc)_2$ (**9**), generated upon slow oxidation of **8** with $PhI(OAc)_2$ seems to decompose under the reaction conditions (90 ºC) at higher rate than is able to transmetalate with the gold(I)-acetylide **8** still present in the reaction media (Figures S14-15). Interestingly, when the same reaction was carried out in the presence of free alkyne, homocoupling product **18** was immediately observed, as shown in the following experiment:



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (5.4 mg, 0.018 mmol), methyl propiolate (**5**) (1.5 mg, 0.018 mmol), diacetoxy(phenyl)-λ^3-iodane (8.7 mg, 0.027 mmol) and $NaHCO_3$ (1.5 mg, 0.018 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 1 h. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S53-54). The formation of the homocoupling product **18** was observed.

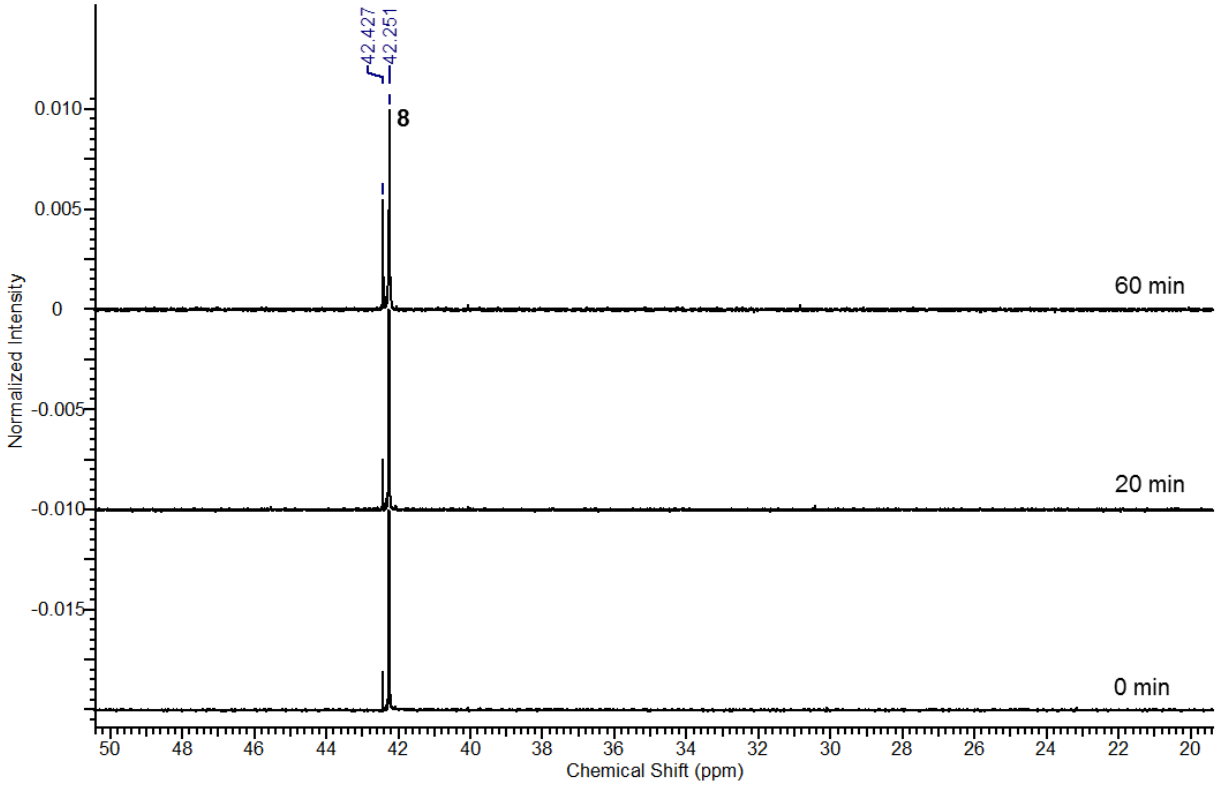


Figure S53. *In situ* ^{31}P-NMR spectrum of the reaction between **8** and **5** in presence of $PhI(OAc)_2$

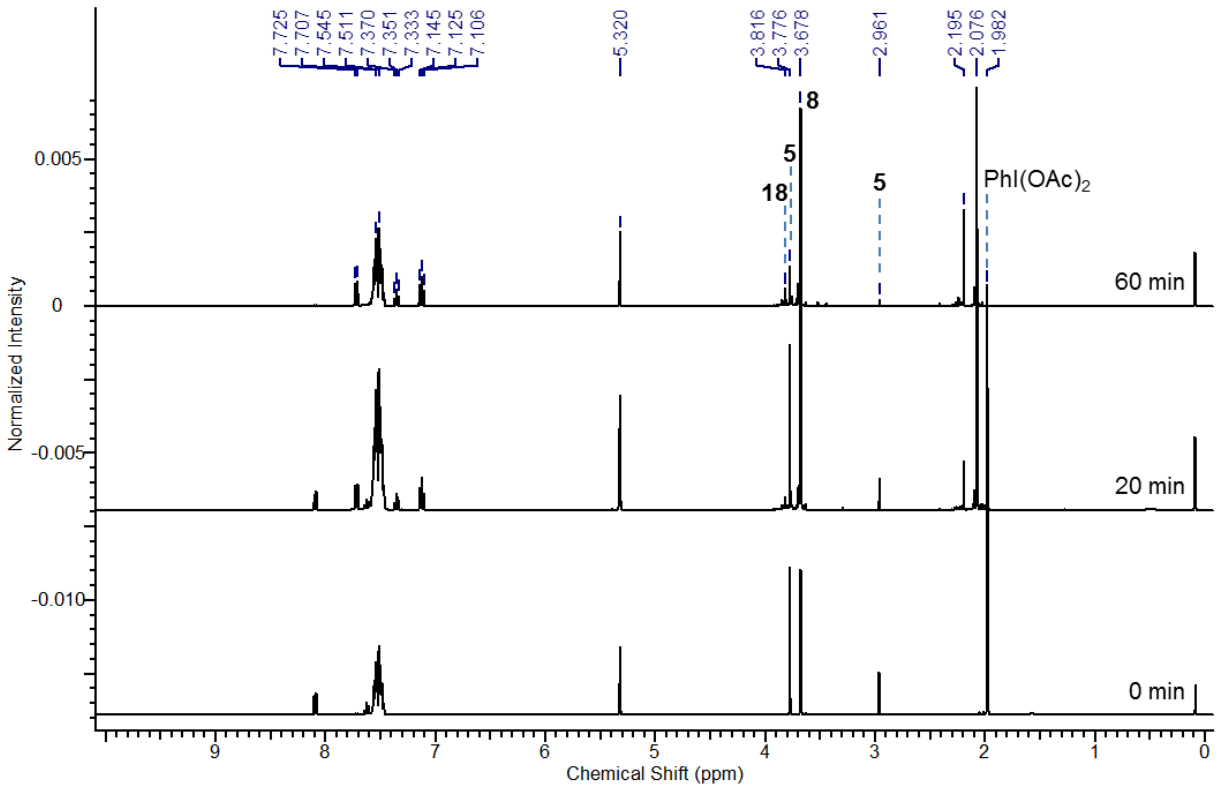
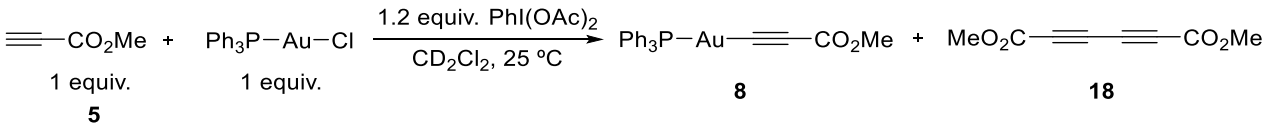


Figure S54. *In situ* ^{1}H-NMR spectrum of the reaction between **8** and **5** in presence of $PhI(OAc)_2$

Along the same lines, the reaction of Ph_3PAuCl with free alkyne in the presence of oxidant, even at room temperature, furnished the corresponding homocoupling product **18**, in line with the results shown in Figure 8 of the main text, which point towards the generation of a more active PhI(OAc)(Cl) oxidant upon gold(I)-I(III) ligand exchange:



To a mixture of diacetoxy(phenyl)-λ^3-iodane (15.5 mg, 0.048 mmol) and methyl propiolate (**5**) (6.7 mg, 0.080 mmol) in dichloromethane-d_2 (0.7 mL), chloro(triphenylphosphine)gold(I) (20 mg, 0.04 mmol) was added. The reaction was performed in a sealed NMR tube at 25 °C. The reaction was monitored by ^{1}H- and ^{31}P-NMR (Figures S55-56). Compound **8** was observed already after 5 min by ^{31}P-NMR. The formation of the alkyne homocoupling product **18** was observed by ^{1}H-NMR.

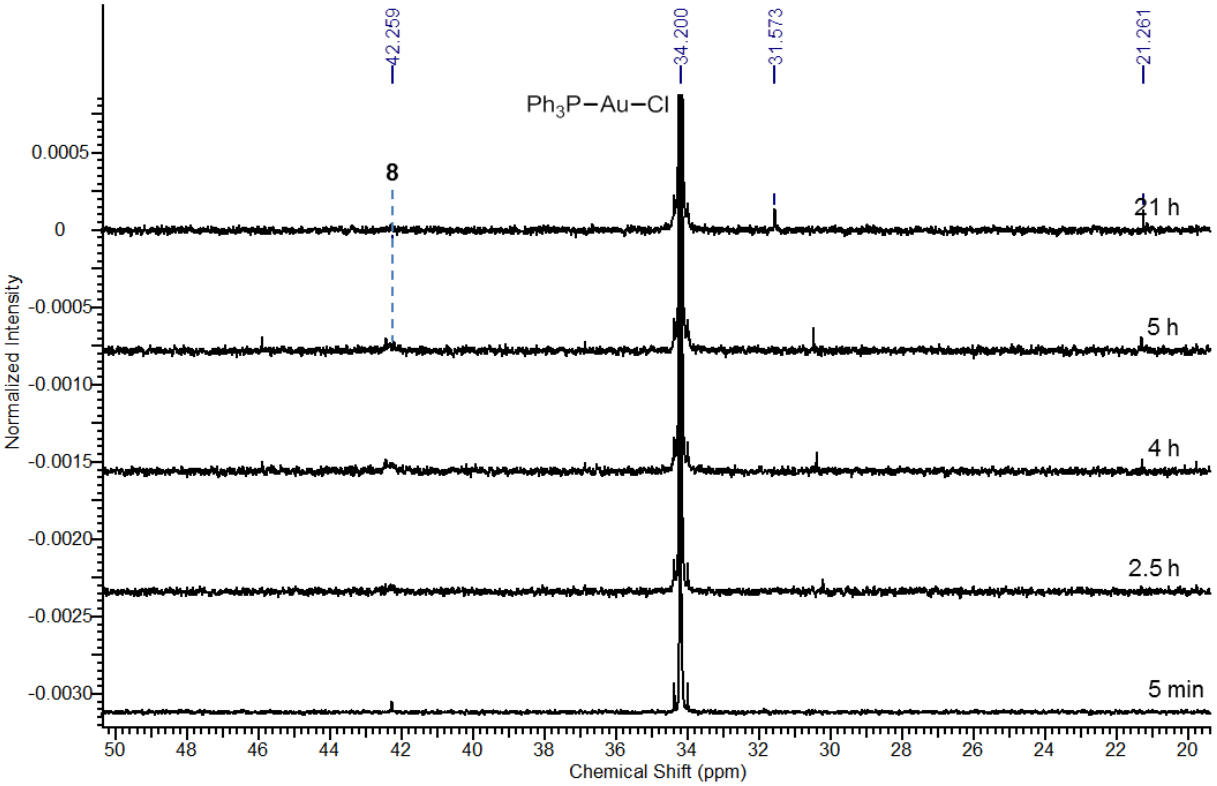


Figure S55. *In situ* ^{31}P-NMR spectrum of the reaction between **5** and Ph_3PAuCl in presence of $PhI(OAc)_2$ at 25 °C

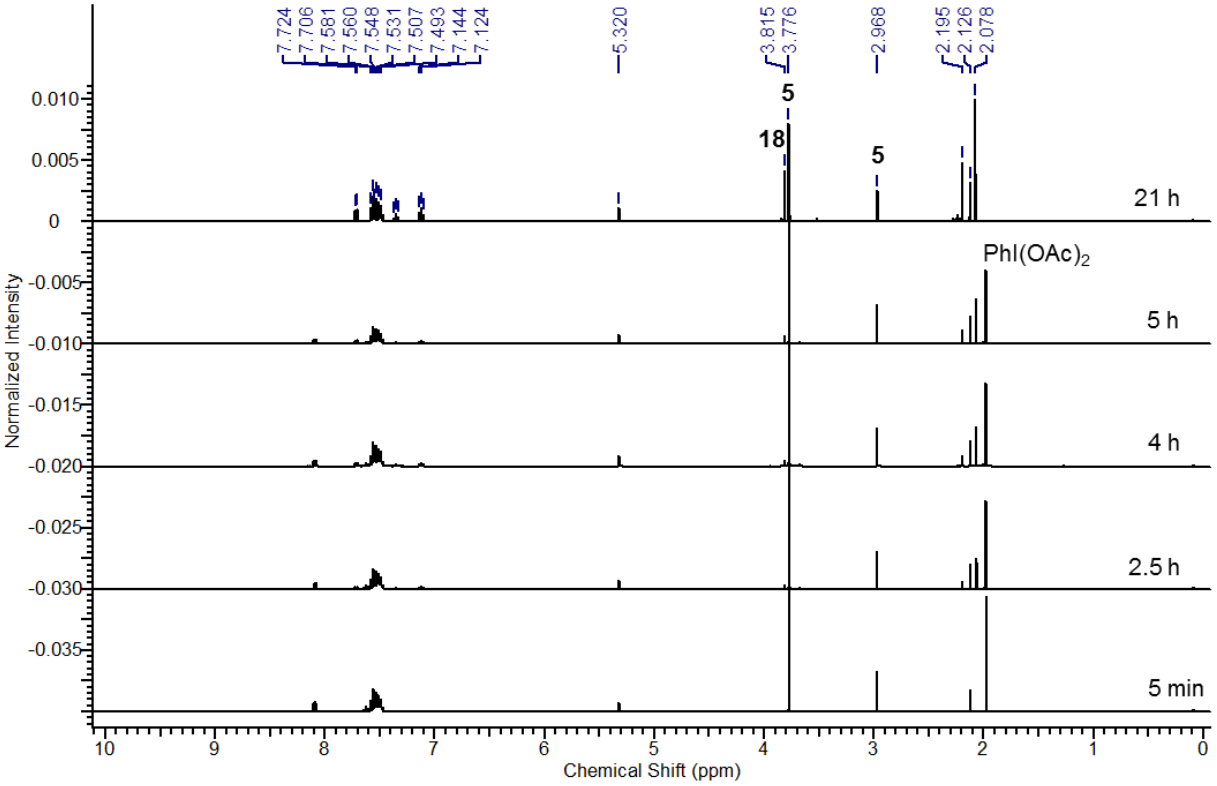
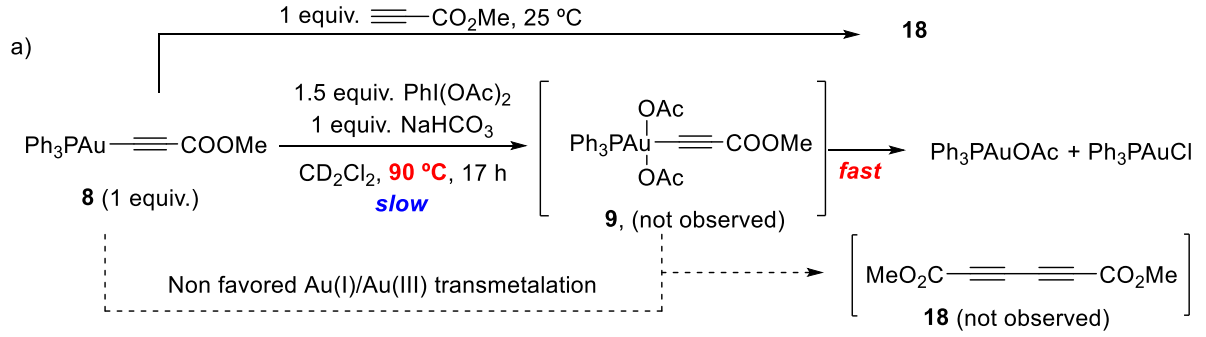
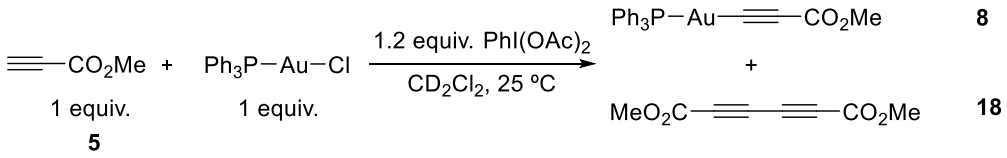


Figure S56. *In situ* ^{1}H-NMR spectrum of the reaction between **5** and Ph_3PAuCl in presence of $PhI(OAc)_2$ at 25 °C

These results, summarized in equation 2, Table 1 and Figure 8 in the manuscript and in Figure S57, indicate that an OAc-alkyne ligand exchange in complex **9** is a much more favorable process compared to the above mentioned Au(I)/Au(III) transmetalation in the presence of OAc anionic ligands on gold. This analysis is confirmed by DFT calculations as the transmetalation product **H´** is disfavored in 1.6 kcal/mol over the sum of the mono-alkynylated Au(I) (**F**) and Au(III) (**H**) complexes (Figure 57c). Meanwhile, the ligand exchange between the free alkyne and acetate in **H** is exergonic in 4.9 kcal/mol, becoming the simplest explanation for the formation of diacetylide complex **H´**. Once a highly reactive Au(III)-diacetylide complex is formed, fast reductive elimination to give homocoupling product **18** will take place.[33]



b) Experimental formation of homocoupling **18** via OAc-Alkyne ligand exchange reaction



c) Computed formation of **H´** by Au(I)/Au(III) transmetalation (upper) or alkynyl / acetate exchange (lower)

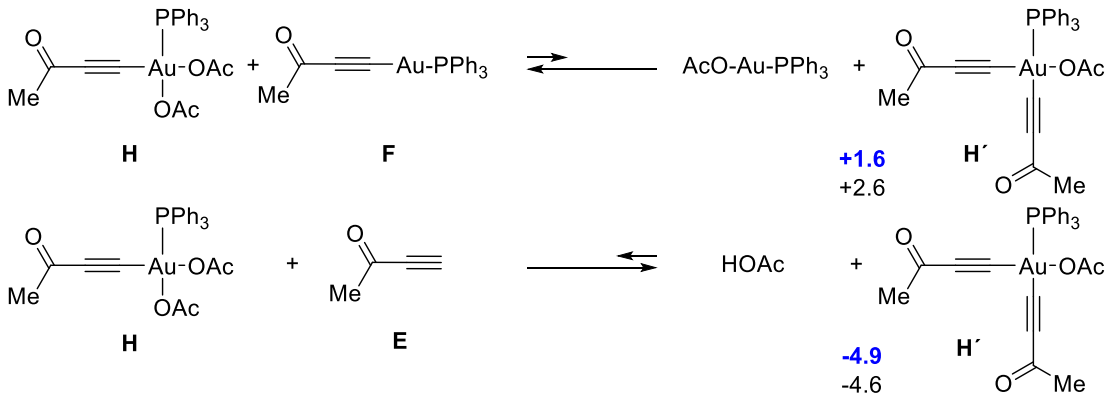
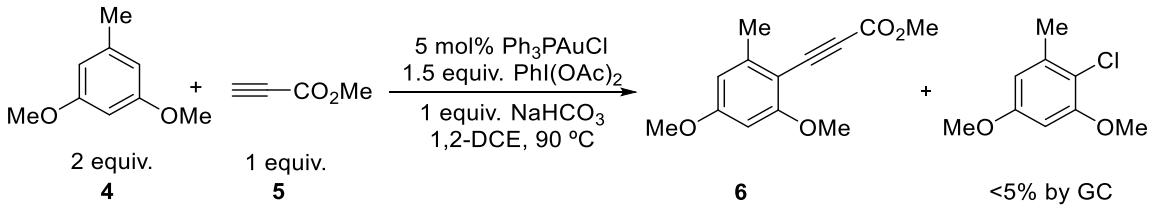


Figure S57. a) and b) Experimental evidence for the formation of homocoupling product **18**. c) Computed Gibbs free energies values (kcal/mol) for the formation of bis-alkynyl complex **H´** via transmetalation vs. ligand exchange reaction calculated with the M06 functional.

4.2 Formation of 2-chloro-3,5-dimethoxytoluene in the reaction mixture

2-Chloro-3,5-dimethoxytoluene was observed in the standard reaction shown in Figure 1a of the main text as a second side product in <5% yield. Control experiments described in the sections herein below revealed that this compound can be produced exclusively by reaction of arene **4** with Ph_3PAuCl and $PhI(OAc)_2$ and does not require the presence of alkyne and $NaHCO_3$. In fact, $PhI(OAc)_2$ is not able to oxidize the arene directly in the absence of Ph_3PAuCl.

4.2.1 Observation of 2-chloro-3,5-dimethoxytoluene in a standard catalytic reaction

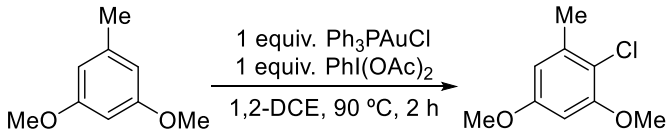


To a solution of 3,5-dimethoxytoluene (**4**) (60.8 mg, 0.40 mmol), diacetoxy(phenyl)-λ^3-iodane (96.6 mg, 0.30 mmol), $NaHCO_3$ (16.8 mg, 0.30 mmol), methyl propiolate (**5**) (16.8 mg, 0.20 mmol) and 1,2-dichloroethane (2.0 mL), chloro(triphenylphosphine)gold(I) (4.95 mg, 0.010 mmol,) and dodecane (4.3 mg, 0.025 mmol, internal standard) was added. The reaction was heated to 90 °C for 2 h and 14 h and was monitored by ^{1}H- and ^{31}P-NMR and GC, GC-MS. 2-Chloro-3,5-dimethoxytoluene was found as a side product in <5% yield (GC).

4.2.2 Control experiments for the formation of 2-chloro-3,5-dimethoxytoluene under the standard reaction conditions

The proposed formation of PhI(Cl)(OAc) and subsequent oxidation of the arene to form 2-chloro-3,5-dimethoxytoluene would be supported, if exclusively Ph_3PAuCl, $PhI(OAc)_2$ and **4** are required to form the chloro-arene in the reaction media (exp. A1). Likewise, if either the chlorogold(I)-complex (exp. A2), or $PhI(OAc)_2$ (exp. A3) would be removed from the raction mixture, the chloro-arene should not be observed anymore. The reaction of $PhI(OAc)_2$ in 1,2-DCE (exp. A4) to form PhI(Cl)(OAc) by activation of the solvent was also investigated. Finally, experiment A5 demonstrated that 2-chloro-3,5-dimethoxy-toluene can be observed in the reaction of **4** with $PhI(Cl)_2$.

A1) Formation of 2-chloro-3,5-dimethoxytoluene in presence of Ph_3PAuCl and $PhI(OAc)_2$

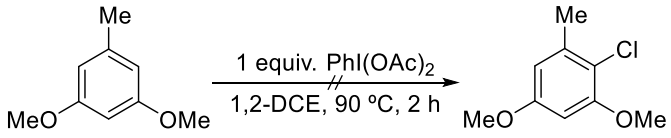


1 equiv.

4

To a mixture of 3,5-dimethoxytoluene (**4**) (6.1 mg, 0.04 mmol), diacetoxy(phenyl)-λ3-iodane (12.9 mg, 0.04 mmol) and 1,2-dichloroethane (0.40 mL), chloro(triphenylphosphine)gold(I) (19.8 mg, 0.04 mmol) was added. The reaction was heated to 90 °C for 2 h and 14 h and was monitored by ^{1}H- and ^{31}P-NMR. The crude mixture contains 2-chloro-3,5-dimethoxytoluene in 20% (2 h, 90 °C) and 55% molar ratio (14 h, 90 °C), respectively (^{1}H-NMR).

A2) Formation of 2-chloro-3,5-dimethoxytoluene in presence of $PhI(OAc)_2$

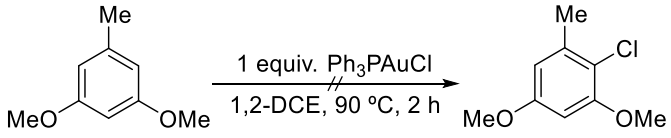


1 equiv.

4

To a mixture of 3,5-dimethoxytoluene (**4**) (60.8 mg, 0.40 mmol) and diacetoxy(phenyl)-λ3-iodane (128.8 mg, 0.40 mmol), 1,2-dichloroethane (2.0 mL) was added. The reaction was heated to 90 °C for 2 h and 14 h and was monitored by ^{1}H-NMR. No reaction was found.

A3) Formation of 2-chloro-3,5-dimethoxytoluene in presence of Ph_3PAuCl

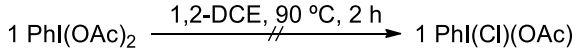


1 equiv.

4

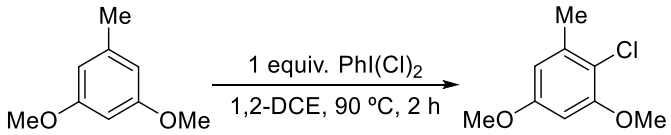
To a mixture of 3,5-dimethoxytoluene (**4**) (6.1 mg, 0.04 mmol) and chloro(triphenyl-phosphine)gold(I) (19.8 mg, 0.04 mmol), 1,2-dichloroethane (0.40 mL), was added. The reaction was heated to 90 °C for 2 h and 14 h and was monitored by ^{1}H- and ^{31}P-NMR. No reaction was found.

A4) Formation of 2-chloro-3,5-dimethoxytoluene in 1,2-DCE



A mixture of diacetoxy(phenyl)-λ^{3}-iodane (128.8 mg, 0.40 mmol) and 1,2-dichloroethane (2.0 mL) was heated to 90 °C for 2 h and 14 h and was monitored by ^{1}H-NMR. No reaction was found.

A5) Formation of 2-chloro-3,5-dimethoxytoluene in presence of $PhI(Cl)_2$



1 equiv.

4

To a mixture of 3,5-dimethoxytoluene (**4**) (60.8 mg, 0.40 mmol) and dichloro(phenyl)-λ^3-iodane (109.9 mg, 0.40 mmol), 1,2-dichloroethane (2.0 mL) was added. The reaction was heated to 90 °C for 2 h and 14 h and was monitored by ^{1}H-NMR. The crude reaction mixture contained 2-chloro-3,5-dimethoxytoluene in 85% molar ratio (90 °C, 2 h) by ^{1}H-NMR.

Summary and conclusions of the experiments A1-A5:

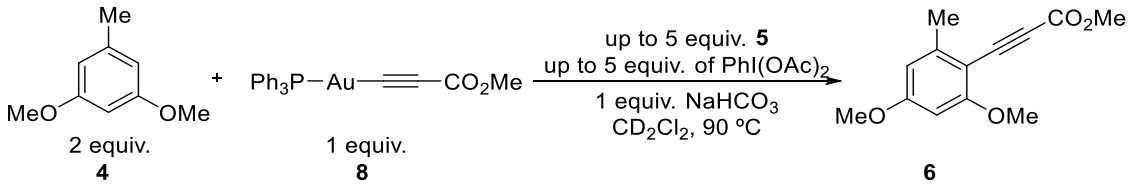
Experiment A1) showed that neither $NaHCO_3$ nor the alkyne were needed to form 2-chloro-3,5-dimethoxytoluene in the catalytic reaction. On the other hand, Ph_3PAuCl and $PhI(OAc)_2$ are required for the formation of the chloro-arene, which was deduced from experiment A2) and A3). Furthemore, experiment A2) showed that the arene is not oxidized in presence of $PhI(OAc)_2$ alone and experiment A4) indicate, that PhI(Cl)(OAc) can not be formed by activation of the solvent.

Based on these experiments, the formation of 2-chloro-3,5-dimethoxytoluene is explained by an initial transfer of the chloride ligand in Ph_3PAuCl to $PhI(OAc)_2$ to form PhI(Cl)(OAc) which subsequently oxidize the arene. This conclusion is confirmed by the results of experiment A5, which showed high conversion to 2-chloro-3,5-dimethoxytoluene in presence of $PhI(Cl)_2$.

4.3 Catalyst decomposition pathways

As discussed in main text of the manuscript, the ^{31}P NMR of a standard alkynylation process shows Ph_3PAuCl (34.2 ppm), Au(I)-acetylide complex **8** (42.3 ppm) and a stable complex (**7**) with a ^{31}P signal at ca. 31 ppm (Figure S2). We first noted that the chemical shift of the latter was displaced towards lower fields during the reaction. A careful revision of the literature showed that the ^{31}P-NMR signals of $[(Ph_3P)_2Au]X$ species appear at ca. 30 ppm in $CDCl_3$,[28] although these can shift depending on the solvent and its acidity, and binding/unbinding events of Ph_3P contribute to broaden the corresponding peaks. A reaction mixture stemming from an aryl-alkynylation reaction in which the signal at 31 ppm was clearly visible was spiked with synthetically prepared $[(Ph_3P)_2Au]Cl$, confirming an increase in the intensity of such peak (Figure S58). We thus propose that the signal initially observed at 31 ppm corresponds to $[(Ph_3P)_2Au]Cl$ (**7**),which is formed in trace amount by slow decomposition of the phosphine-Au species involved in the cross coupling reaction. Additional control experiments also confirmed that $[(Ph_3P)_2Au]Cl$ does not promote the formation of the cross coupling product and also does not react with the alkyne to form Au(I)-acetylide complex **8** (Figure S59-63). These species represent a «dead end» within the catalytic cycle.

4.3.1 Identification of the decomposition products



To a solution of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (27.1 mg, 0.05 mmol), $NaHCO_3$ (4.1 mg, 0.05 mmol), 3,5-dimethoxytoluene (4) (15.2 mg, 0.10 mmol), methyl propiolate (**5**) (4.2 mg, 0.05 mmol) and diacetoxy(phenyl)-λ3-iodane (16.1 mg, 0.05 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube and heated to 90 °C for 4 h. Diacetoxy(phenyl)-λ3-iodane (16.1 mg, 0.05 mmol) and methyl propiolate (**5**) (4.2 mg, 0.05 mmol) were added and heated to 90 °C for 3 h. This addition of diacetoxy(phenyl)-λ3-iodane and methyl propiolate (**5**) and heating was repeated 5 times to enrich the proportion of the 31 ppm complex. The reaction mixture was spiked with $[(PPh_3)_2Au]Cl$[29] and Au(I)-acetylide (**8**) synthesized independently and monitored by ^{31}P-NMR (Figure S58).

The original reaction mixture showed a signal at 32.4 ppm in ^{31}P-NMR (initially appearing at ca. 31 ppm). The reaction mixture spiked by $[(PPh_3)_2Au]Cl$ showed an increased intensity of the 32.4 ppm signal together with an overall shift of the peaks to a higher fields. Upon addition of **8**, the signal at 42 ppm showed

[28] (a) Harrison, T. J.; Kozak, J. A.; Corbella-Pané, M.; Dake, G. R. *J. Org. Chem.* **2006**, *71*, 4525. (b) Woehrle, G. H.; Brown, L. O.; Hutchison, J. E. *J. Am. Chem. Soc.* **2005**, *127*, 2172. (c) Zhdanko, A.; Ströbele, M.; Maier, M. E. *Chem. Eur. J.* **2012**, *18*, 14732. (d) Kumar, M. Jasinski, J.; Hammond, G.B., Xu, B. *Chem. Eur. J.* **2014**, *20*, 3113.
[29] Baenziger, N. C.; Dittermore, K. M.; Doyle, J. R. *Inorg. Chem.* **1974**, *13*, 805.

an increased intensity. Finally, recording the reaction in MeOD showed an overall shift of the peaks to lower fields.

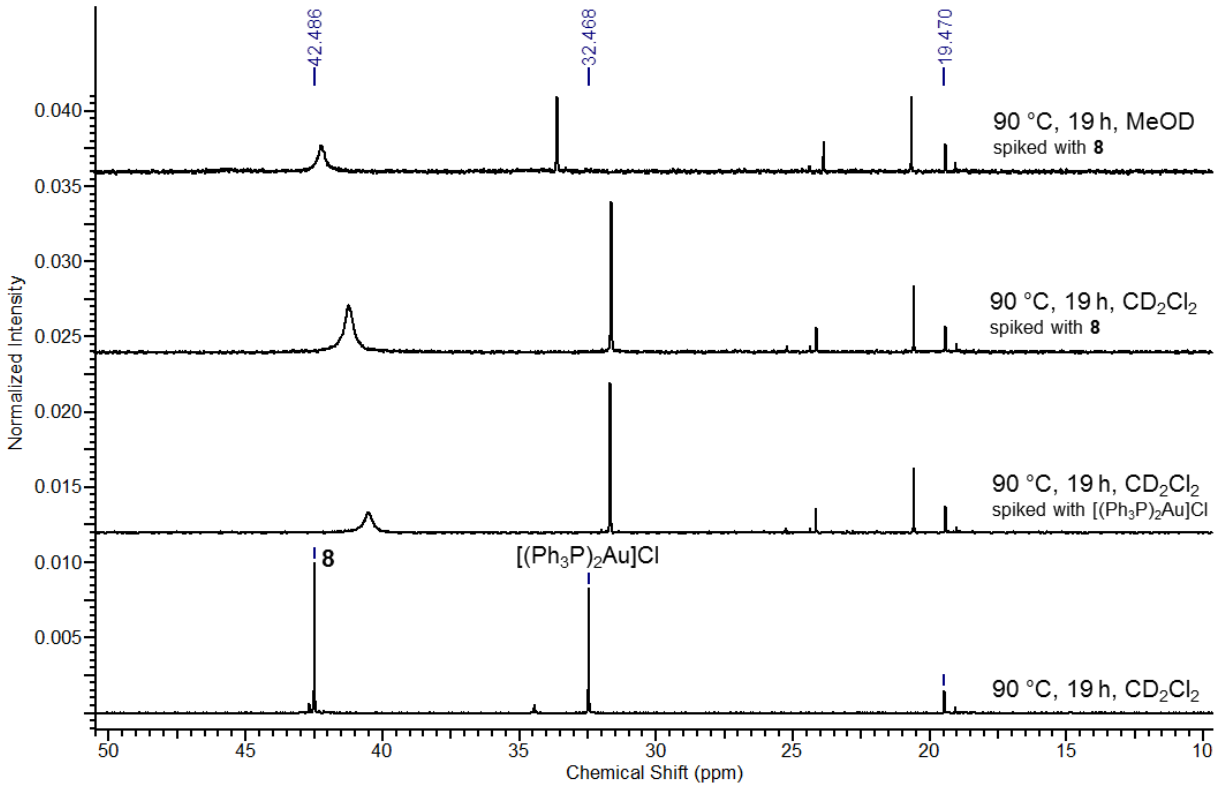
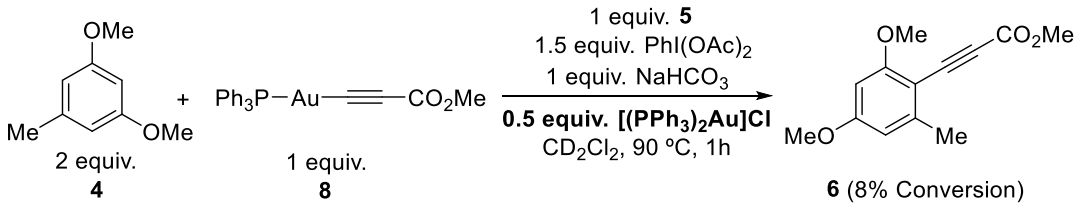


Figure S58. *In situ* ^{31}P-NMR spectrum of the reaction between **4**, **5** and **8** in presence of $PhI(OAc)_2$ spiked with $[(PPh_3)_2Au]Cl$

4.3.2 Reactivity of $[(PPh_3)_2Au]Cl$

A) Stoichiometric reaction in presence of additional alkyne and $[(PPh_3)_2Au]Cl$



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (27 mg, 0.05 mmol), diacetoxy(phenyl)-λ^3-iodane (24 mg, 0.075 mmol), 3,5-dimethoxytoluene (**4**) (15.2 mg, 0.10 mmol), methyl propiolate (**5**) (4.2 mg, 0.05 mmol), $NaHCO_3$ (4.2 mg, 0.05 mmol) and chlorobis-(triphenylphosphine)gold(I) (18.9 mg, 0.025 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 2 h and was monitored by ^{1}H- and ^{31}P-NMR (Figures S59-60). The reaction crude showed the formation of the product **6** in 8% molar ratio (^{1}H-NMR). The 31 ppm peak in ^{31}P-NMR was observed.

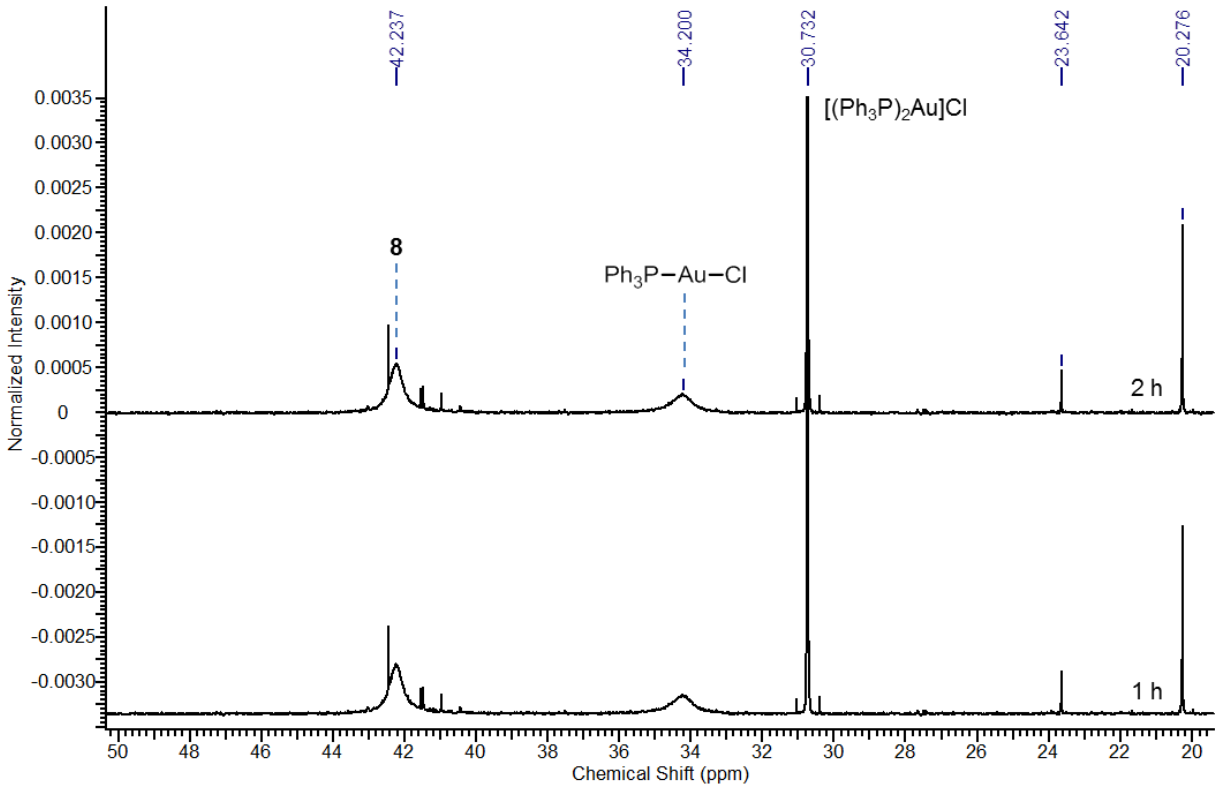


Figure S59. *In situ* ^{31}P-NMR spectrum of the reaction between **4**, **5** and **8** in presence of $PhI(OAc)_2$ and $[(Ph_3P)_2Au]Cl$

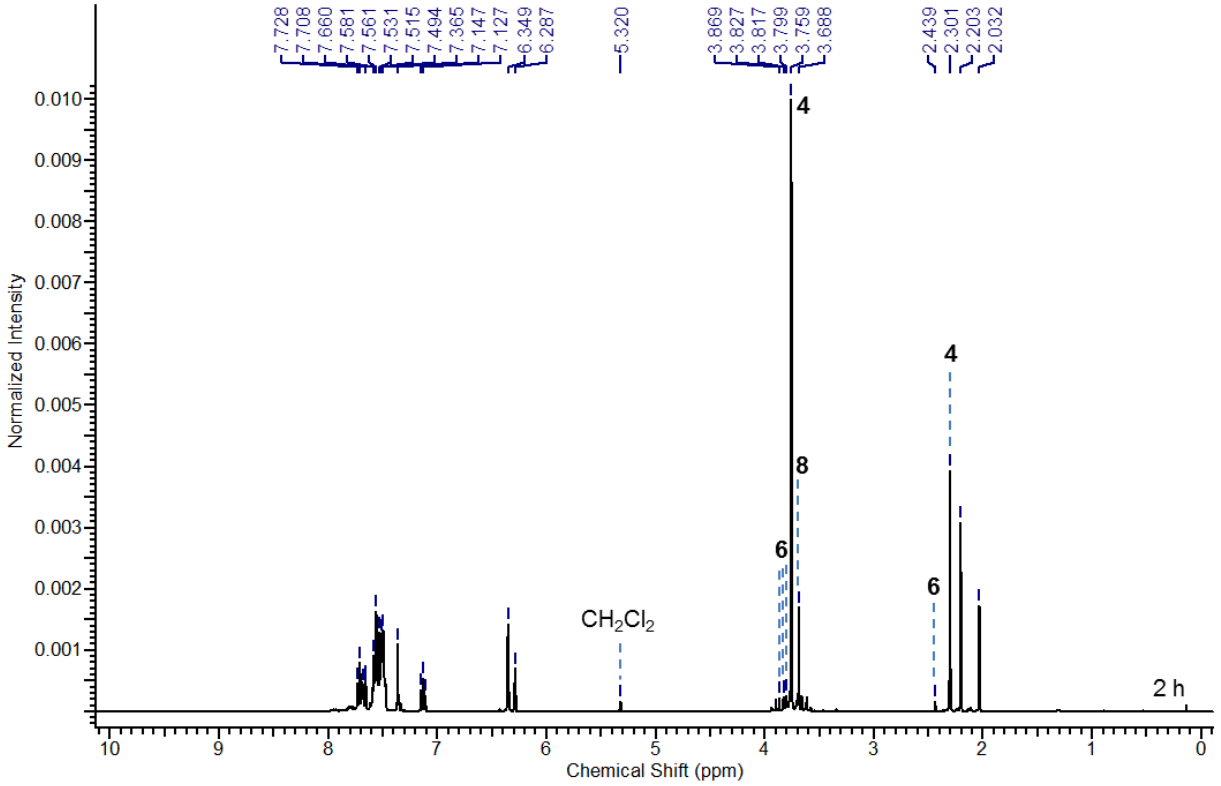
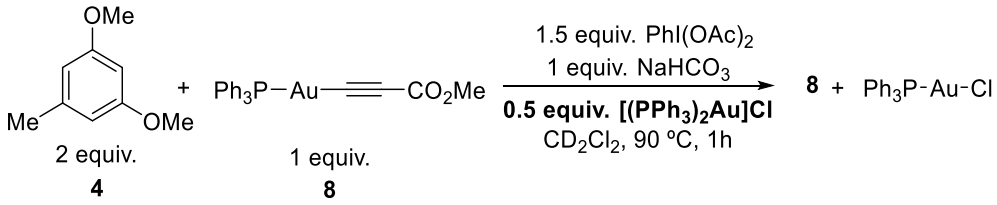


Figure S60. *In situ* ^{1}H-NMR spectrum of the reaction between **8, 4** and **5** in presence of $PhI(OAc)_2$ and $[(Ph_3P)_2Au]Cl$

B) Stoichiometric reaction without additional alkyne



To a mixture of (methoxycarbonylethynyl)(triphenylphosphine)gold(I) (**8**) (27 mg, 0.05 mmol), diacetoxy(phenyl)-λ3-iodane (24 mg, 0.075 mmol), 3,5-dimethoxytoluene (**4**) (15.2 mg, 0.10 mmol), $NaHCO_3$ (4.2 mg, 0.05 mmol) and chlorobis(triphenylphosphine)gold(I) (18.9 mg, 0.025 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube at 90 °C for 2 h and was monitored by ^{1}H- and ^{31}P-NMR (Figure S61-62). The reaction showed no appreciable conversion to **6**.

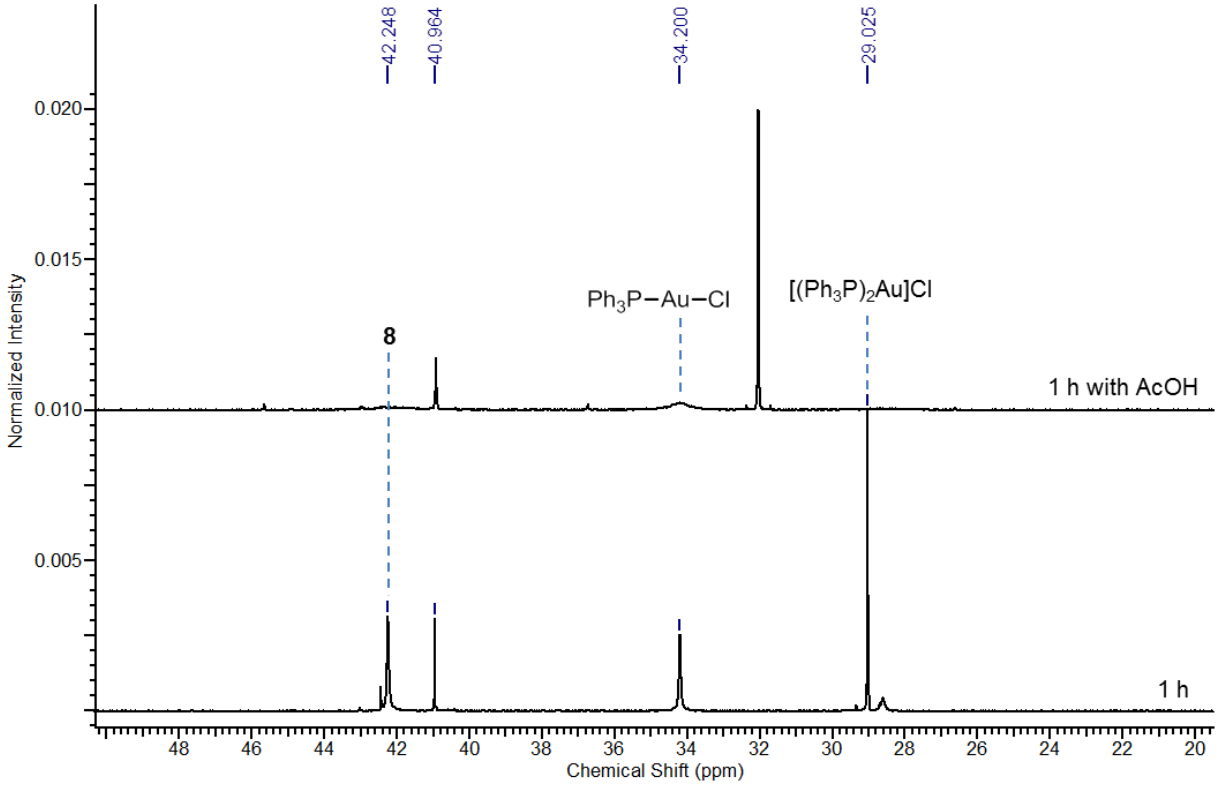


Figure S61. *In situ* ^{31}P-NMR spectrum of the reaction between **4** and **8** in presence of $PhI(OAc)_2$ and $[(Ph_3P)_2Au]Cl$

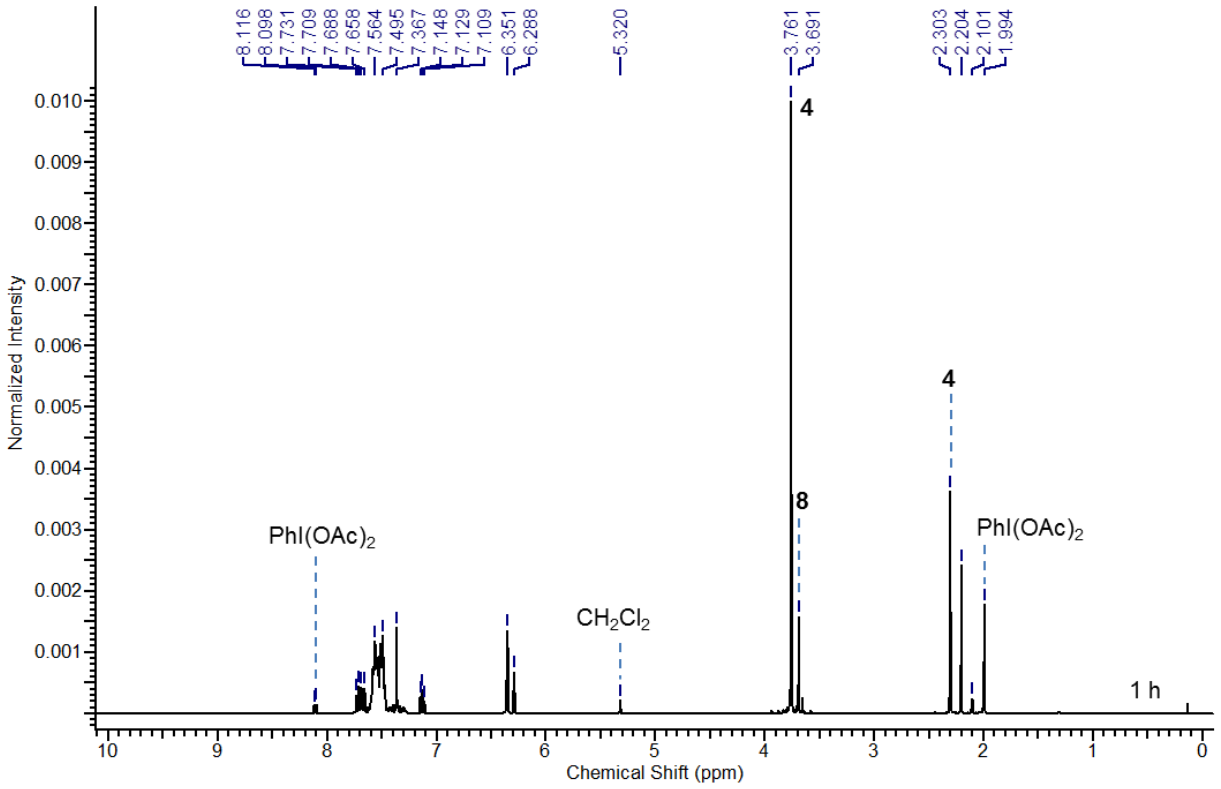
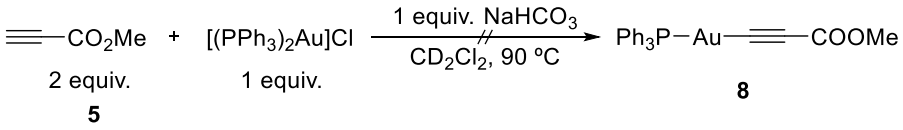


Figure S62. *In situ* ^{1}H-NMR spectrum of the reaction between **4** and **8** in presence of $PhI(OAc)_2$ and $[(Ph_3P)_2Au]Cl$

C) Non oxidative conditions in presence of free alkyne



To methyl propiolate (**5**) (4.2 mg, 0.05 mmol), $NaHCO_3$ (2 mg, 0.025 mmol) and chlorobis-(triphenylphosphine)gold(I) (10 mg, 0.025 mmol), dichloromethane-d_2 (0.3 mL) was added. The reaction was performed in a sealed NMR-tube and heated to 90 °C for 2 h. The reaction was observed directly by ^{1}H- and ^{31}P-NMR (Figure S63). Compound **8** was not observed.

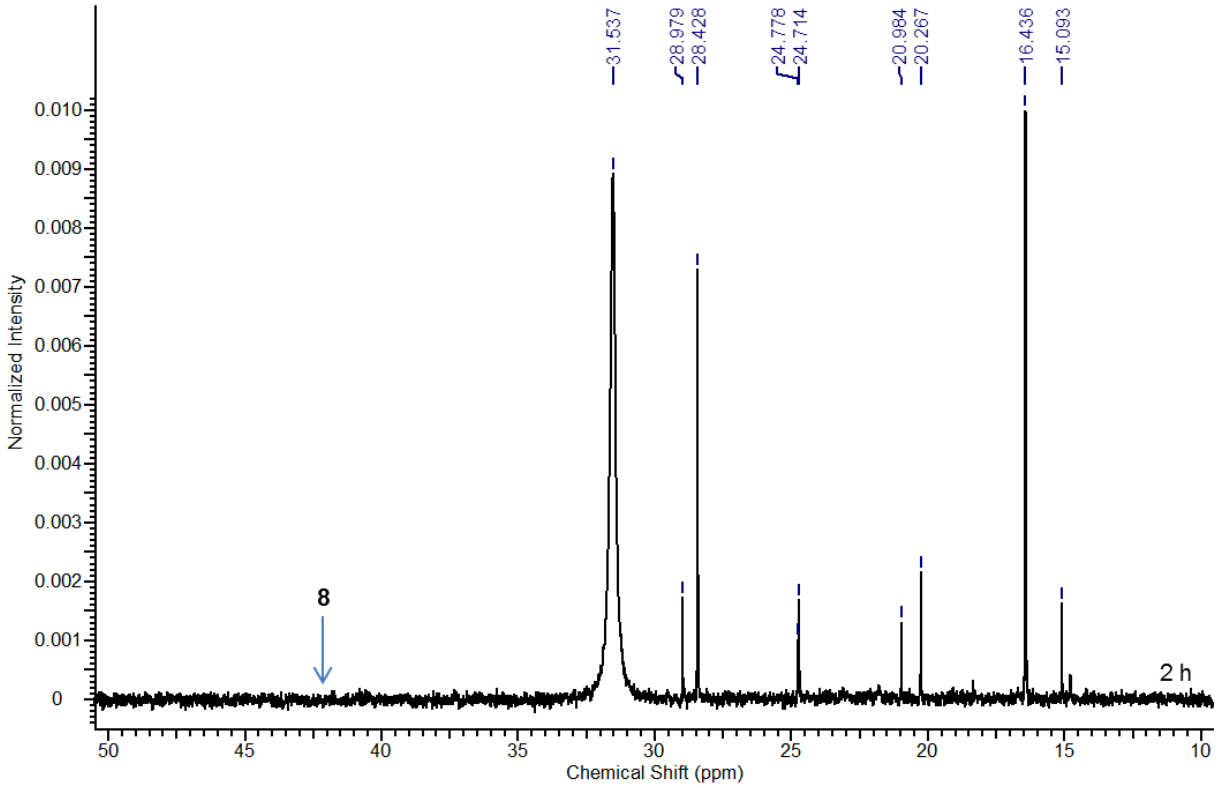
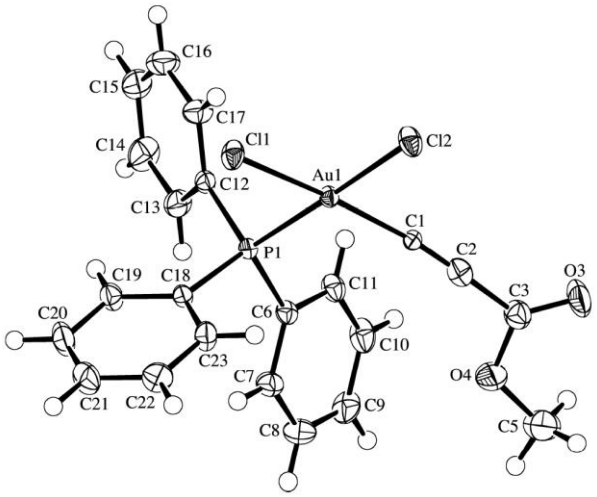


Figure S63. *In situ* ^{31}P-NMR spectrum of the reaction between **5** and $[(Ph_3P)_2Au]Cl$

5. X-Ray diffraction data for complex 10

Table S1. Crystal structure data and refinement details for *cis*-dichloro(methoxycarbonylethynyl)-(triphenylphosphine)gold(III) (**10**) (CCDC 1008765)



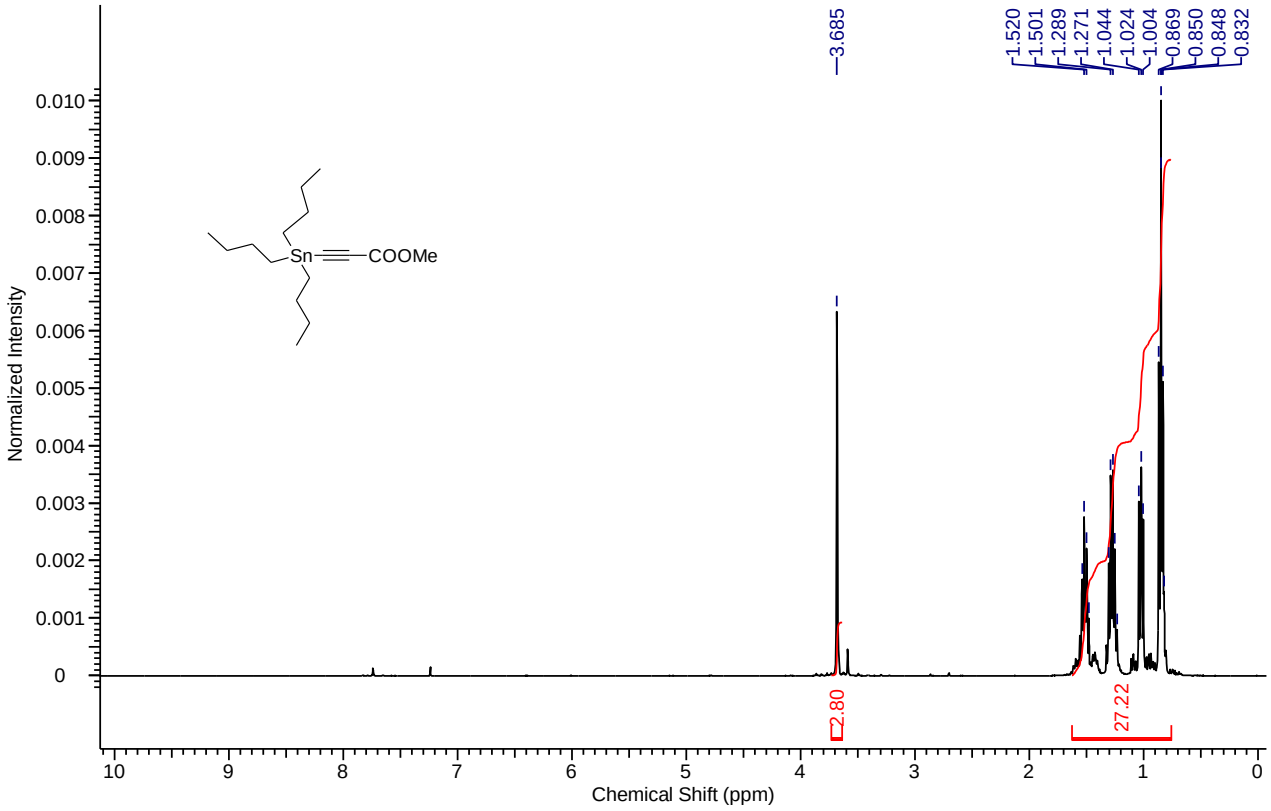
Compound	**10**
Crystallised from	dichloromethane / hexane
Empirical formula	$C_{22.5}H_{19}AuCl_3O_2P$
Formula weight [g mol^{-1}]	655.69
Crystal colour, habit	colorless, prism
Crystal dimensions [mm]	0.18 × 0.22 × 0.33
Temperature [K]	160(1)
Crystal system	monoclinic
Space group	$P2_1/n$ (#14)
Z	4
Reflections for cell determination	14109
2θ range for cell determination [°]	4–61
Unit cell parameters a [Å]	12.59949(18)
b [Å]	10.66900(13)
c [Å]	17.9124(3)
α [°]	90
β [°]	108.3351(15)
γ [°]	90
V [Å^3]	2285.61(5)
F(000)	1260
D_x [g cm^{-3}]	1.905
μ(Mo $K\alpha$) [mm^{-1}]	6.896
Scan type	ω
$2\theta_{(max)}$ [°]	60.9

Transmission factors (min; max)	0.552; 1.000
Total reflections measured	23037
Symmetry independent reflections	6250
R_{int}	0.033
Reflections with $I > 2\sigma(I)$	5692
Reflections used in refinement	6250
Parameters refined	282
Final $R(F)$ [$I > 2\sigma(I)$ reflections]	0.0239
$wR(F^2)$ (all data)	0.0536
Weights:	$w = [\sigma^2(F_o^2) + (0.0197P)^2 + 2.9702P]^{-1}$ where $P = (F_o^2 + 2F_c^2)/3$
Goodness of fit	1.052
Secondary extinction coefficient	0.00076(6)
Final Δ_{max}/σ	0.004
$\Delta\rho$ (max; min) [e Å^{-3}]	1.24; -1.19
$\sigma(d_{(C-C)})$ [Å]	0.004 – 0.005

6. ^{1}H, ^{13}C, ^{31}P, ^{19}F-NMR spectra of starting materials and products

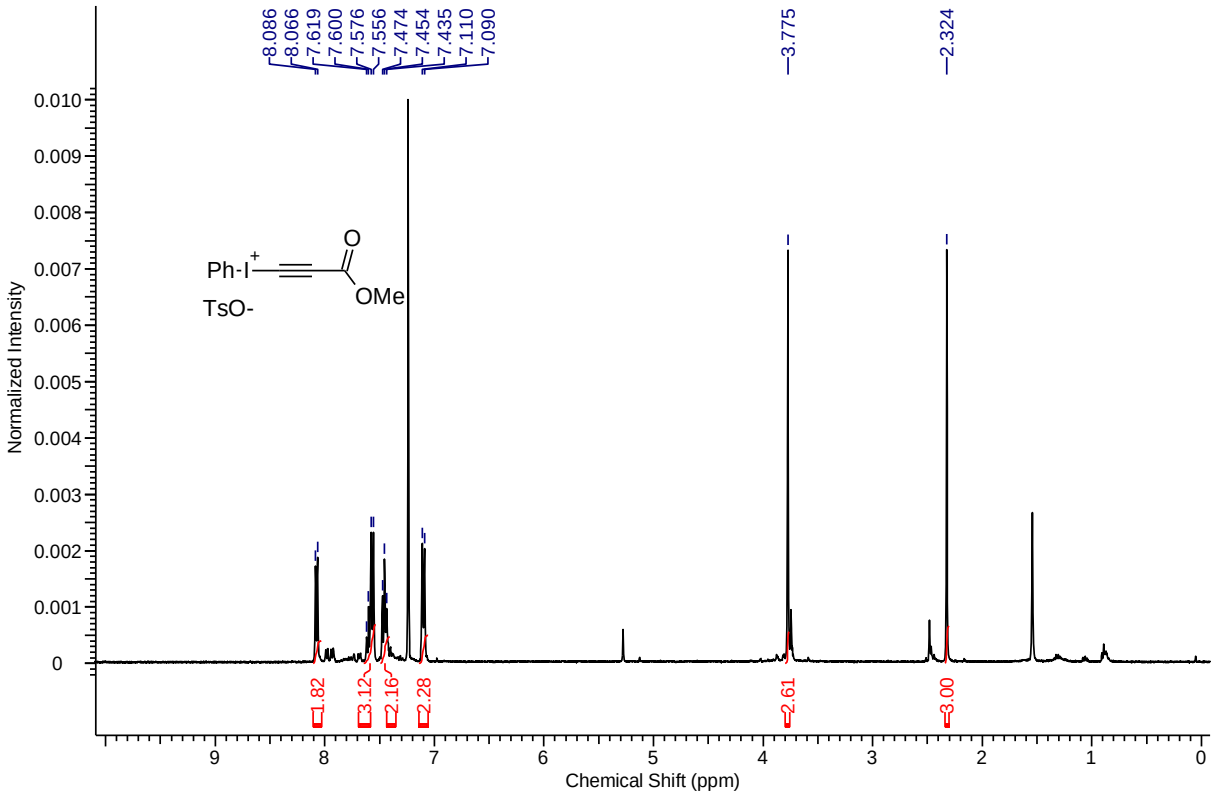
[(Carbomethoxy)ethynyl]tributylstannane

^{1}H-NMR



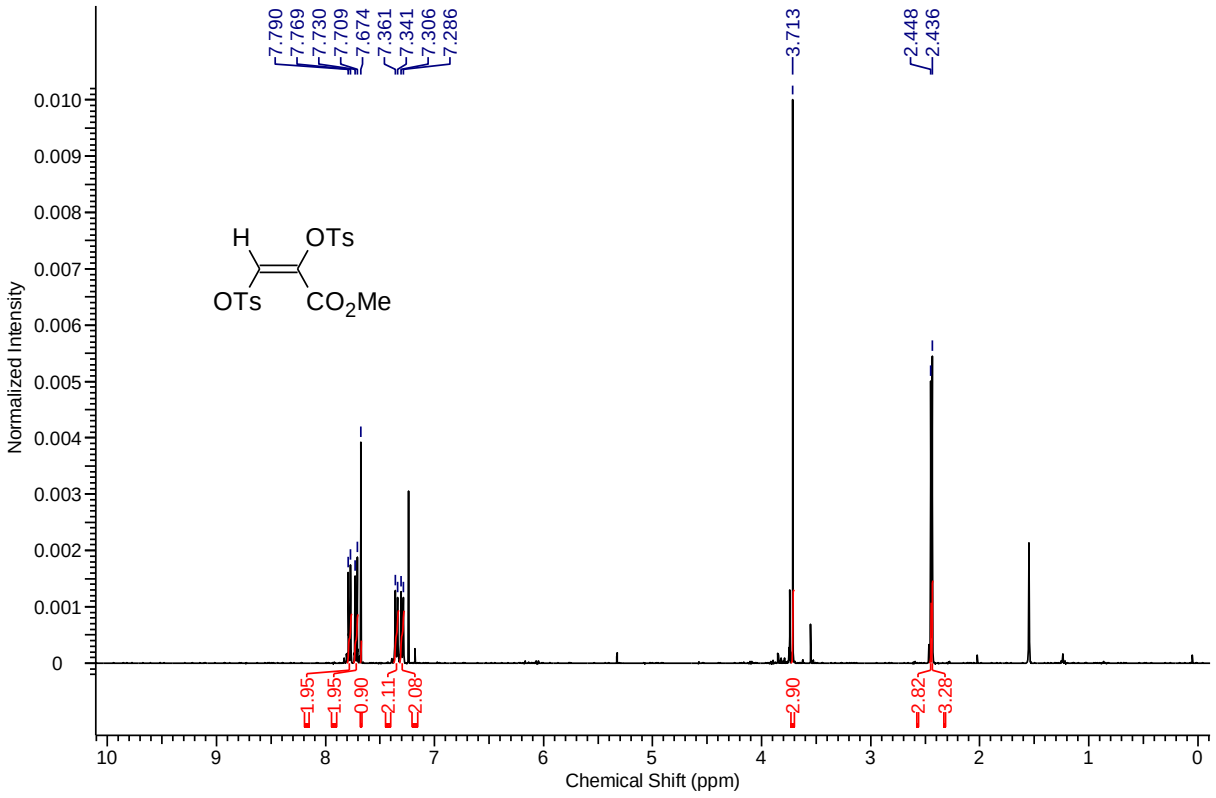
Carbomethoxy[phenyl[[(methyl)sulfonyl]oxy]iodo]acetylene

^{1}H-NMR

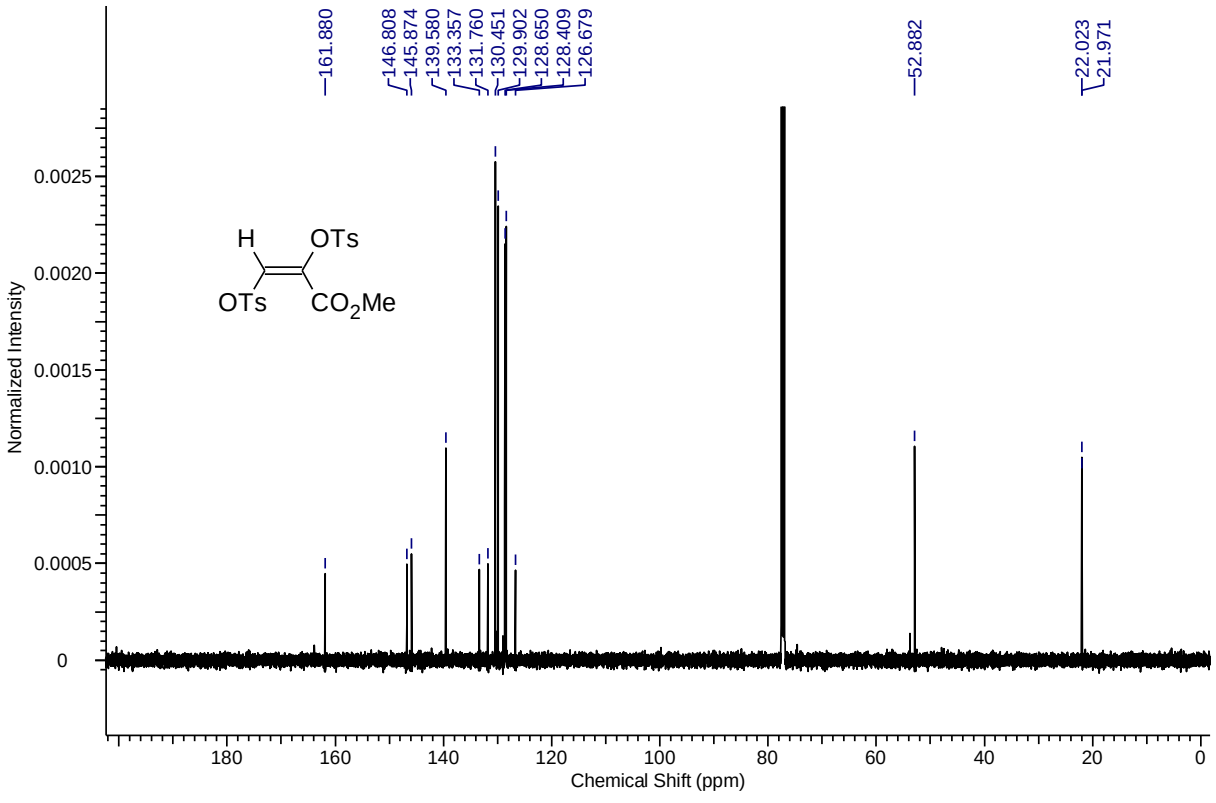


Methyl-1,3-ditosyl-2-propenoate

^{1}H-NMR

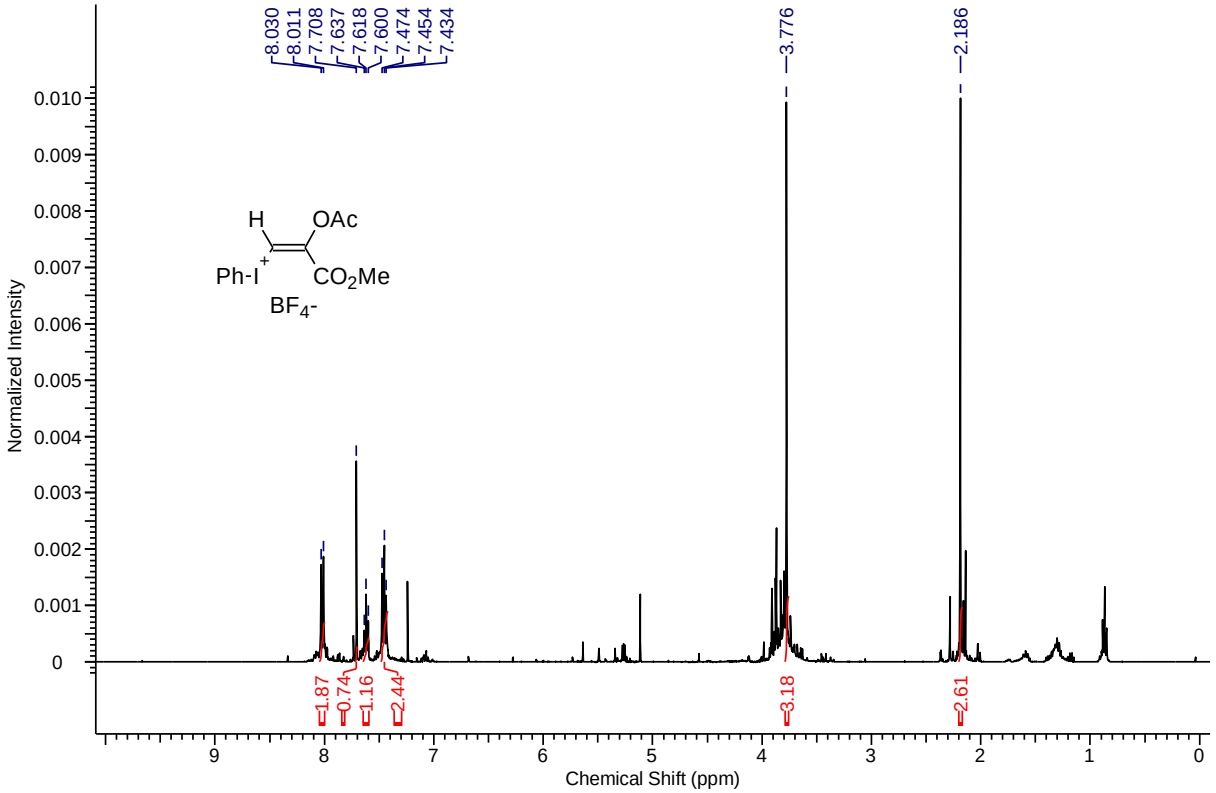


^{13}C-NMR

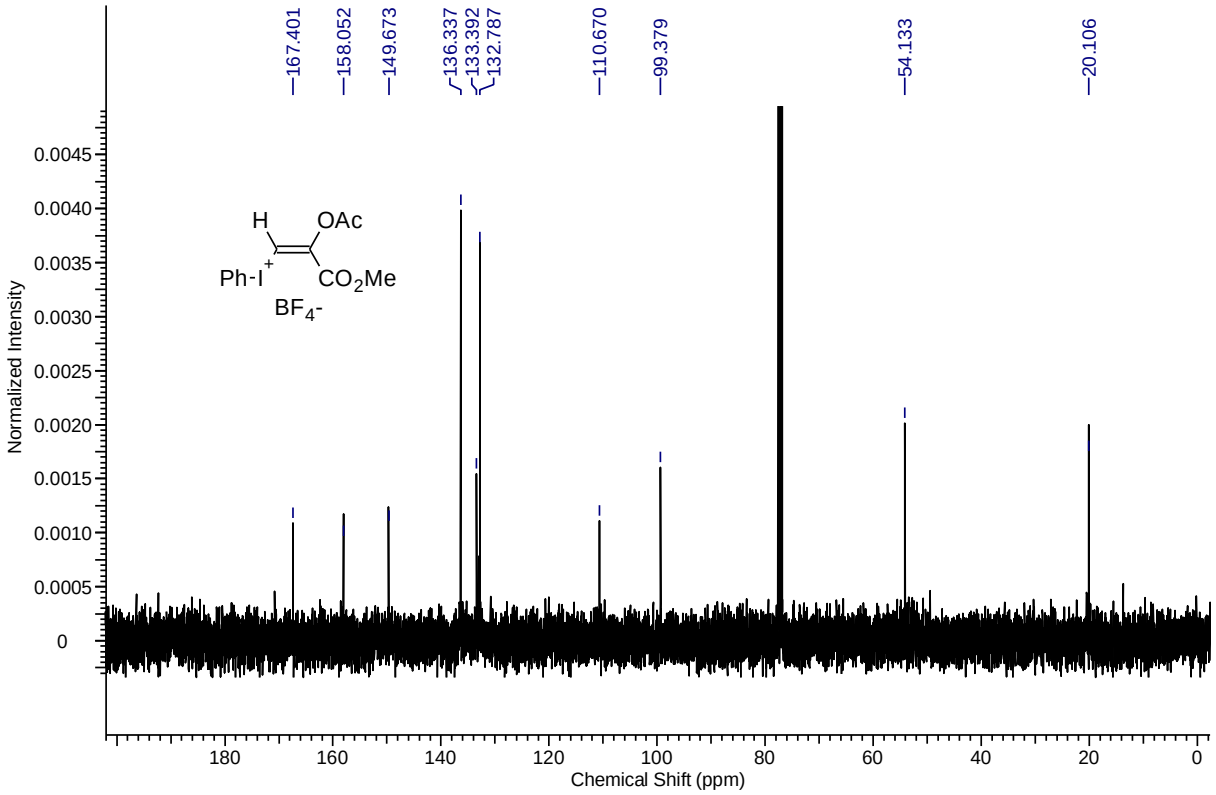


Alkenyl(phenyl)iodonium tetrafluoroborate

^{1}H-NMR

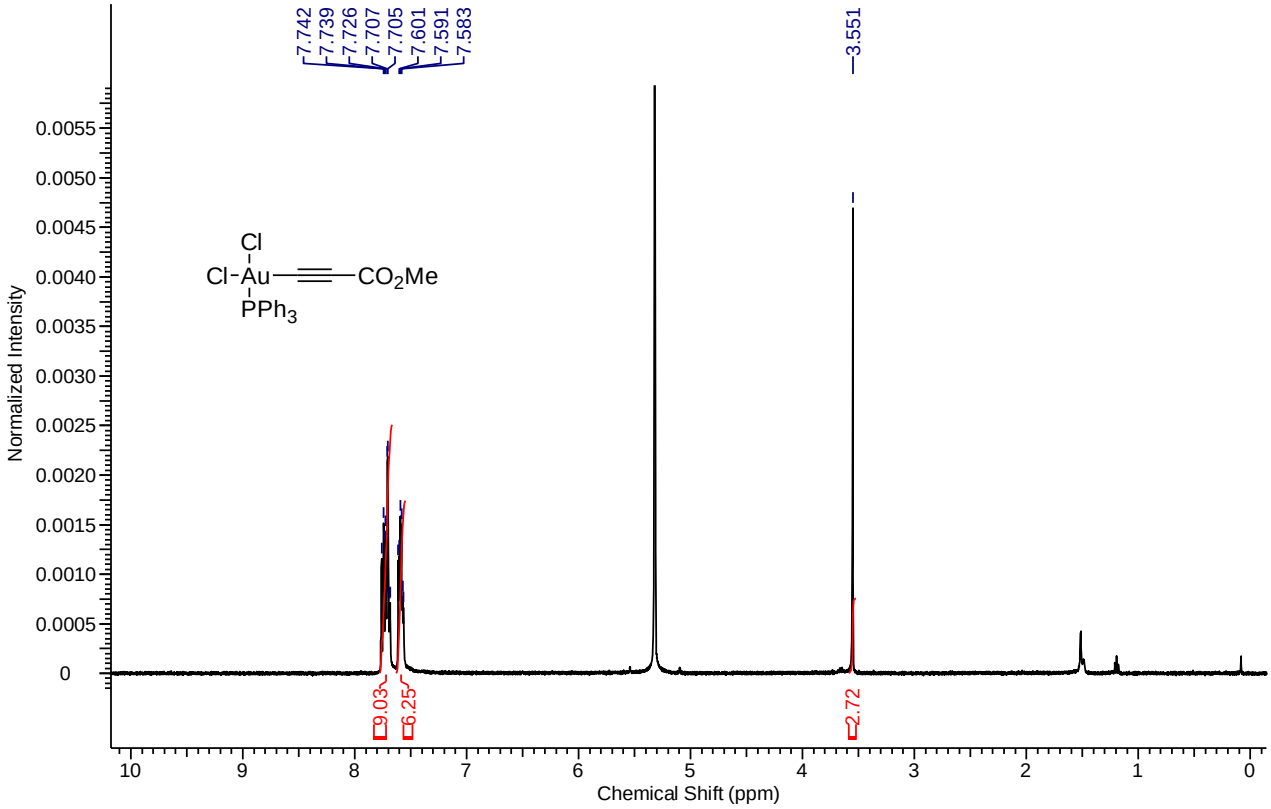


^{13}C-NMR

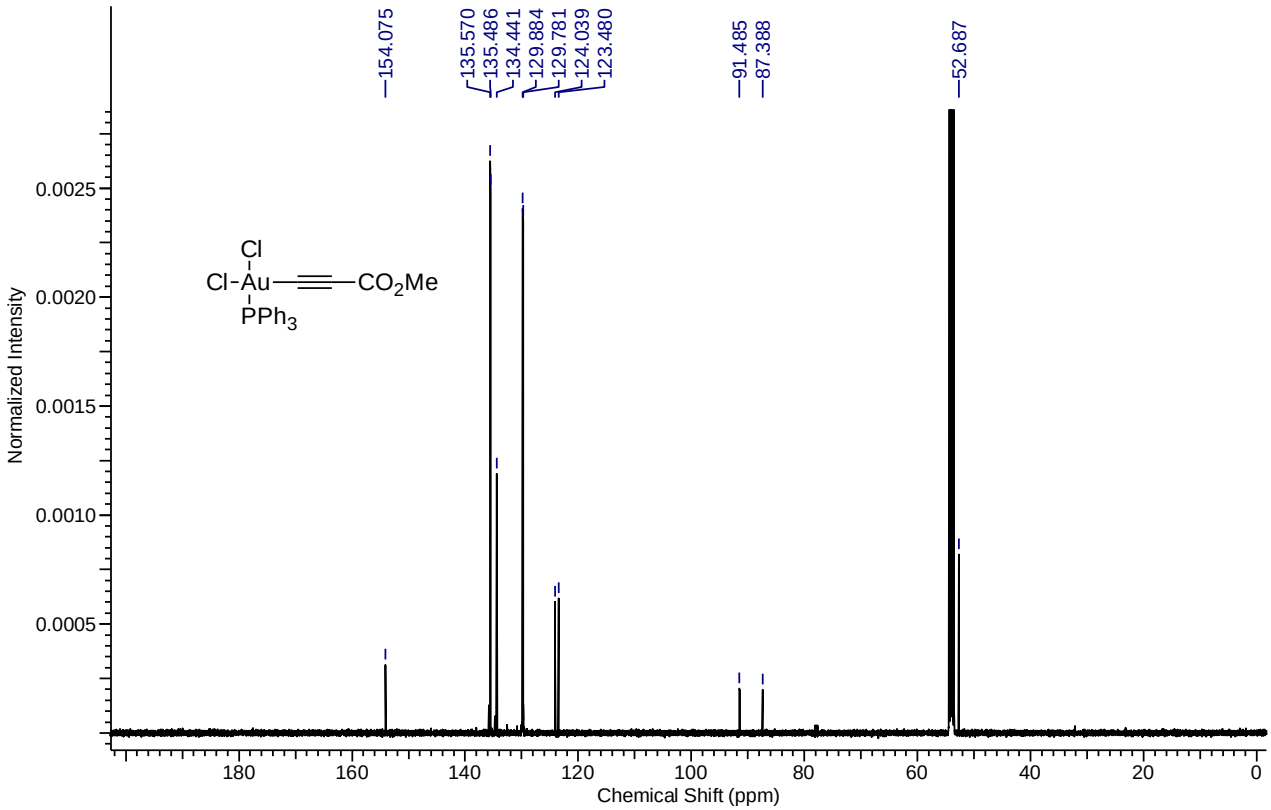


***cis*-Dichloro(triphenylphosphine)gold(III)acetylide (10)**

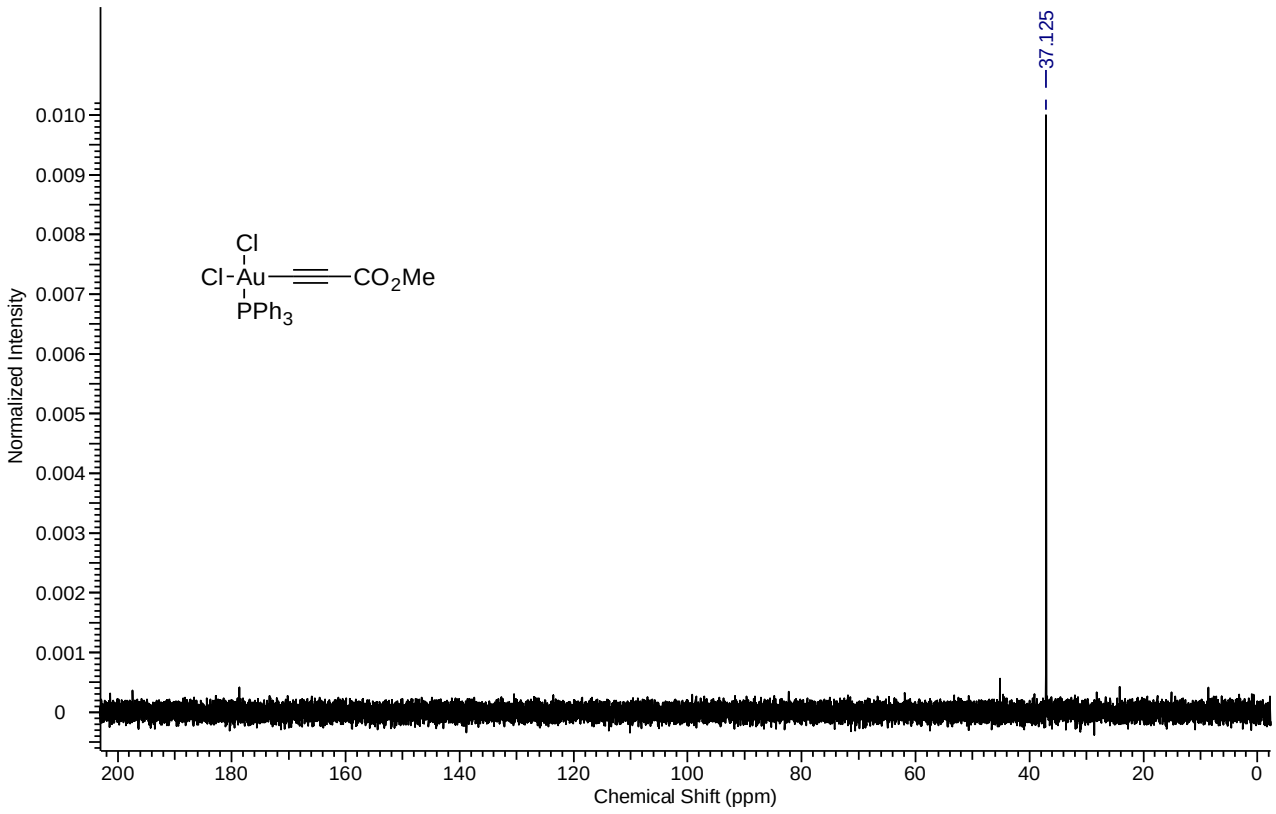
^{1}H-NMR



^{13}C-NMR

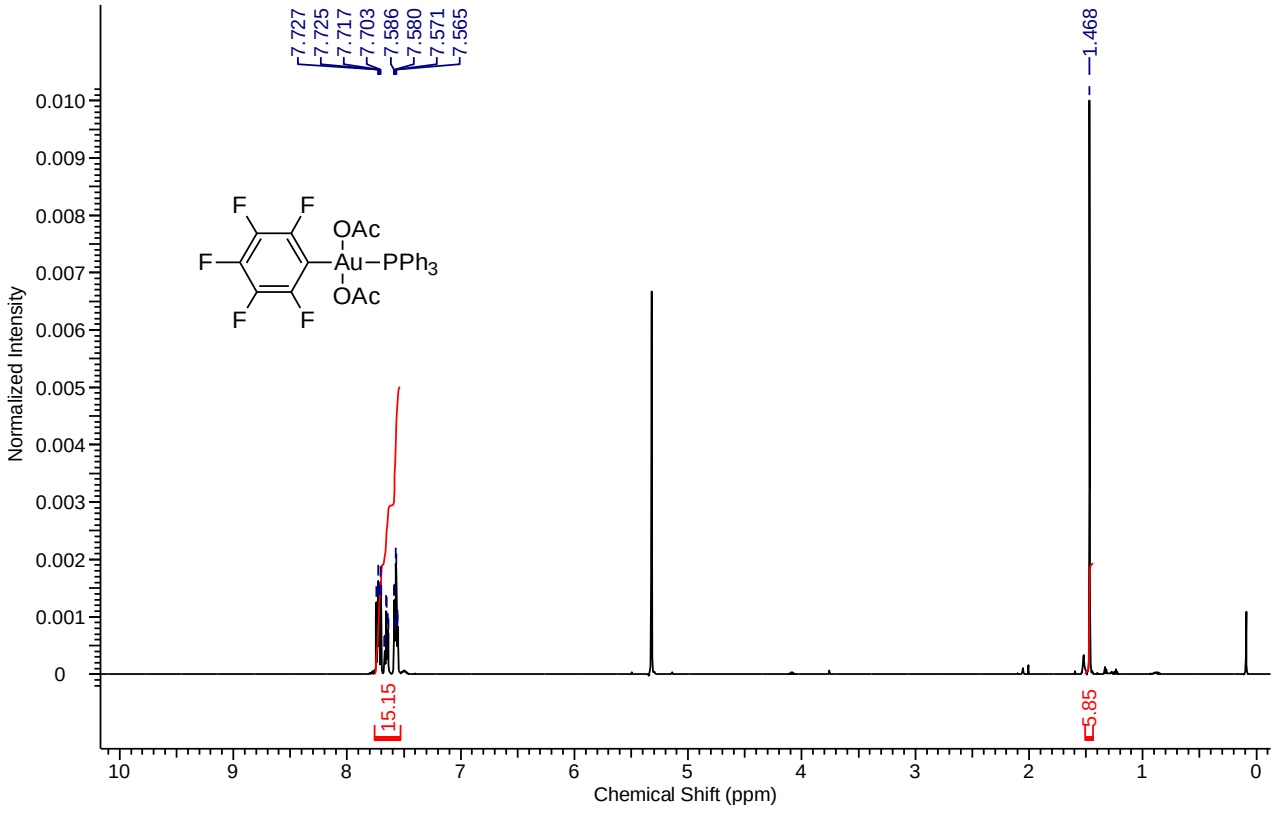


^{31}P-NMR

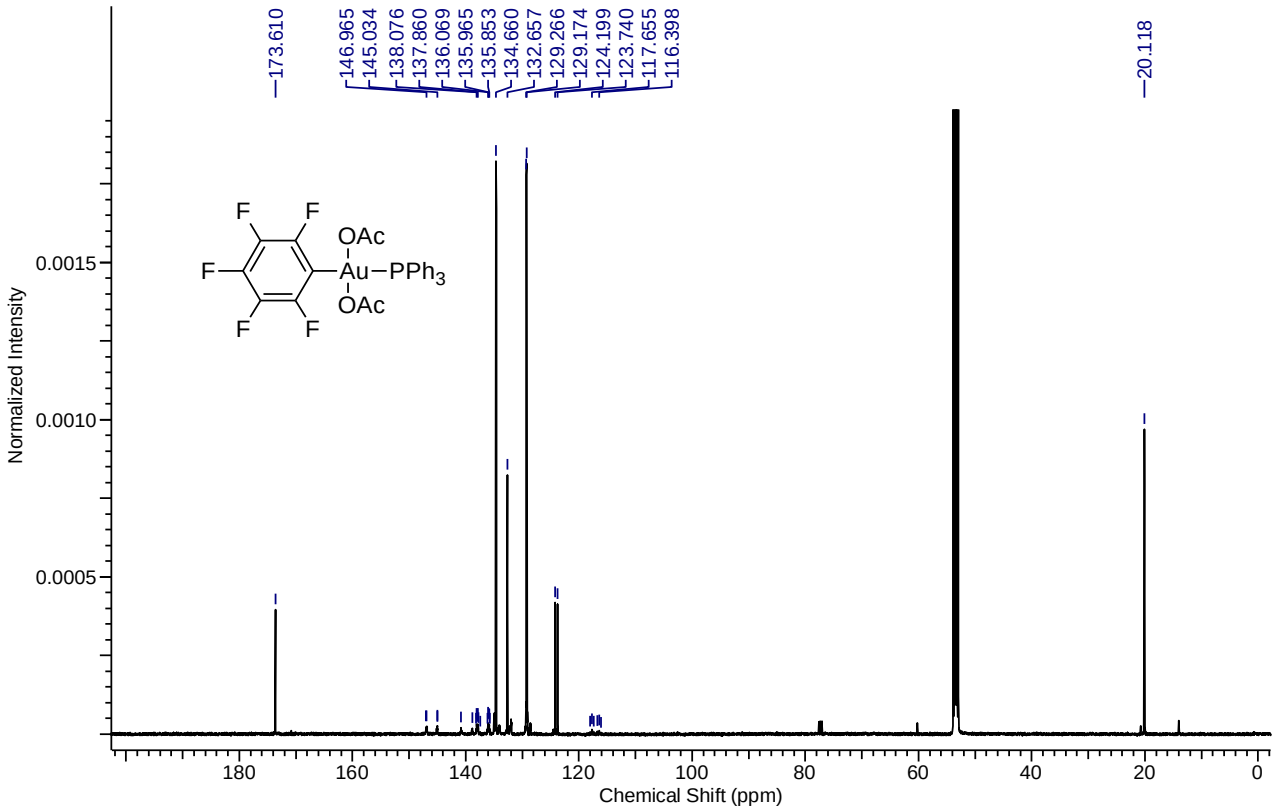


trans-Diacetato(pentafluorophenyl)(triphenylphosphine)gold(III) (13)

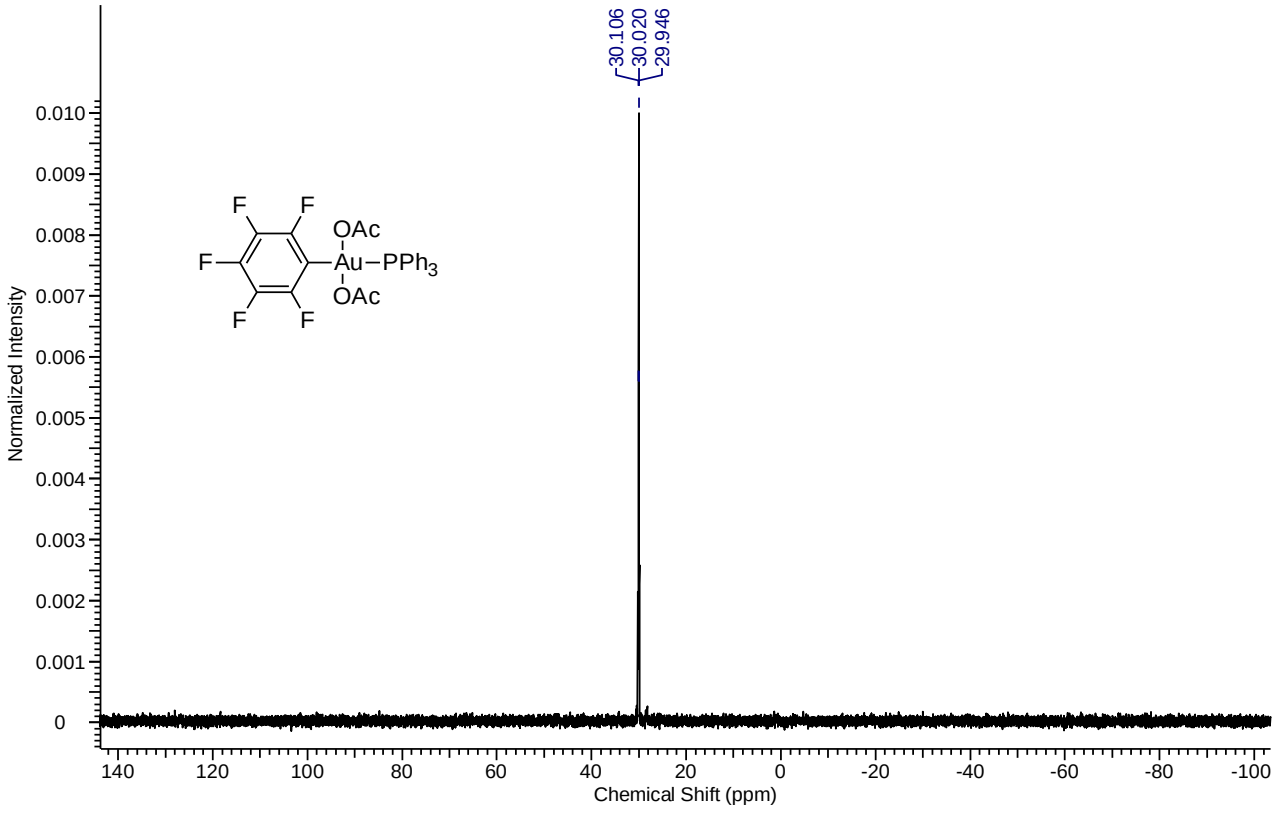
^{1}H-NMR



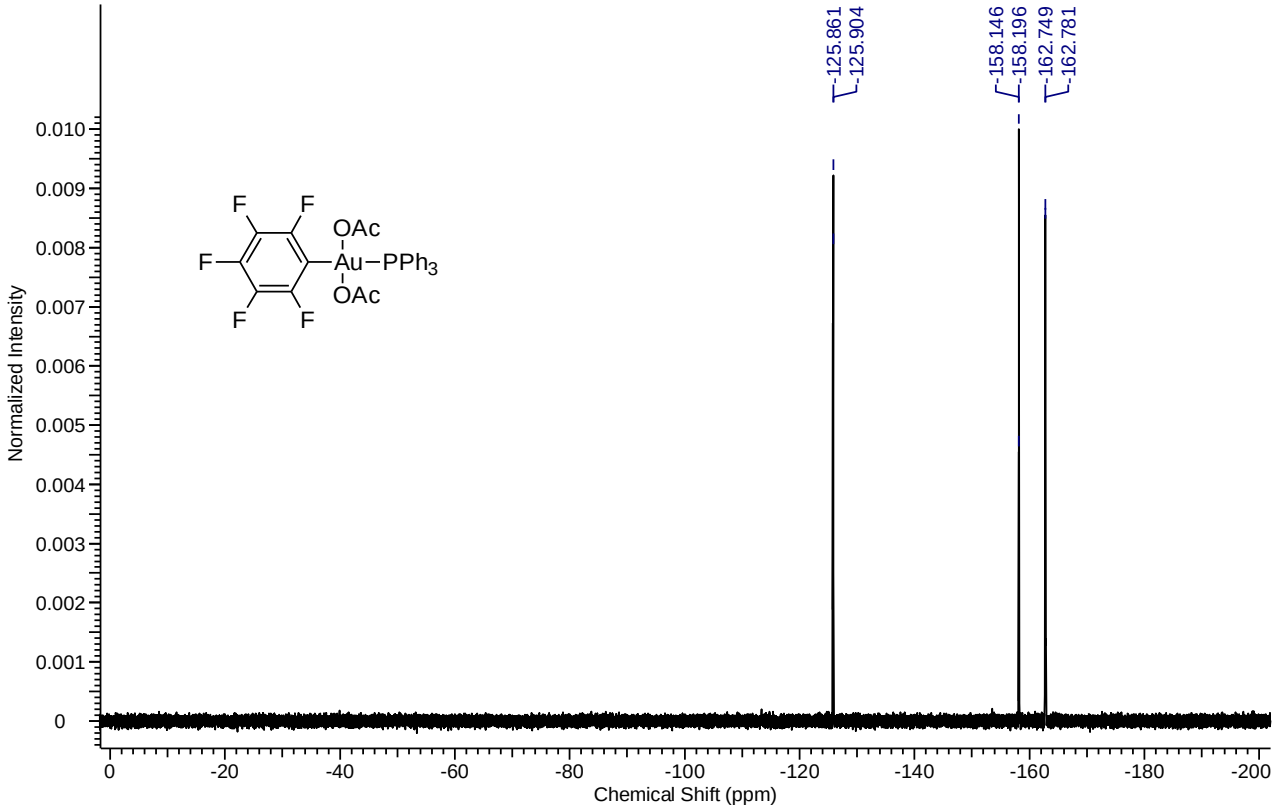
^{13}C-NMR



^{31}P-NMR

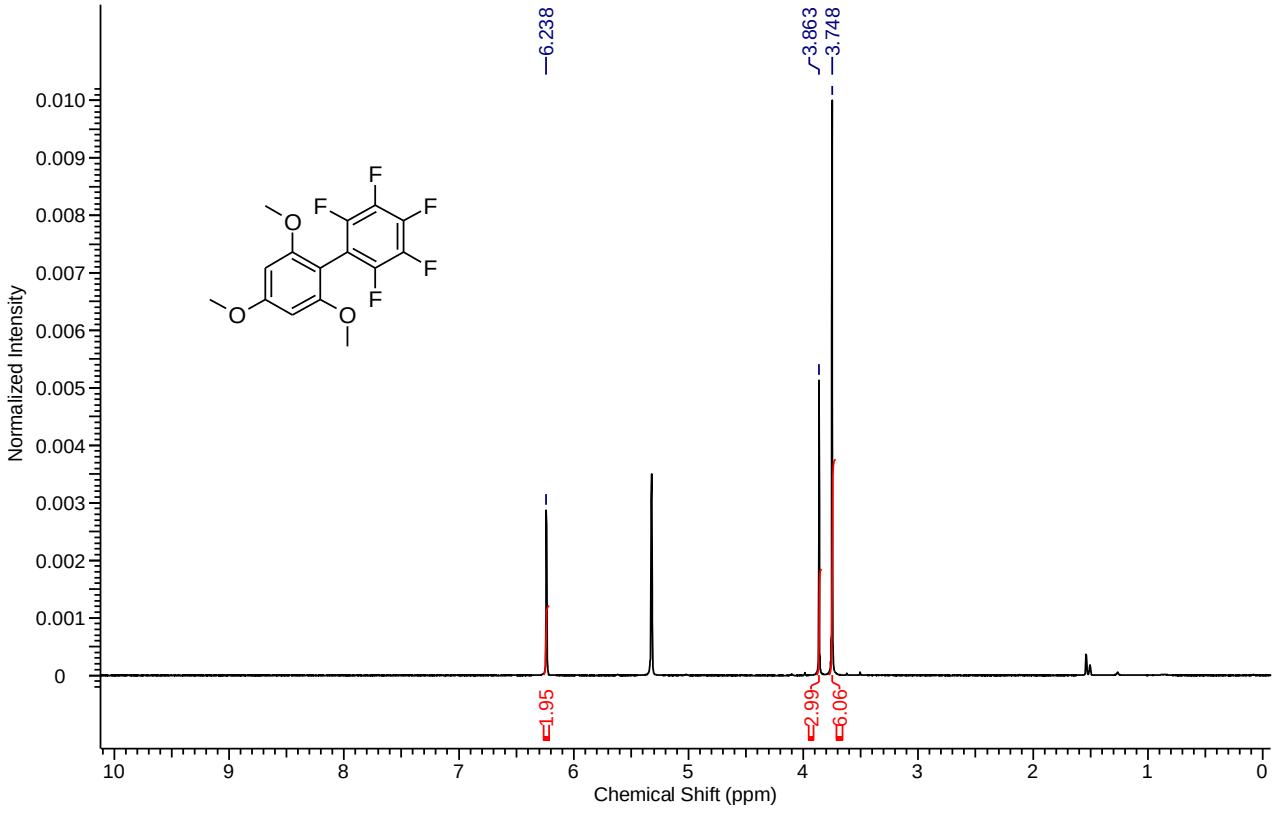


^{19}F-NMR

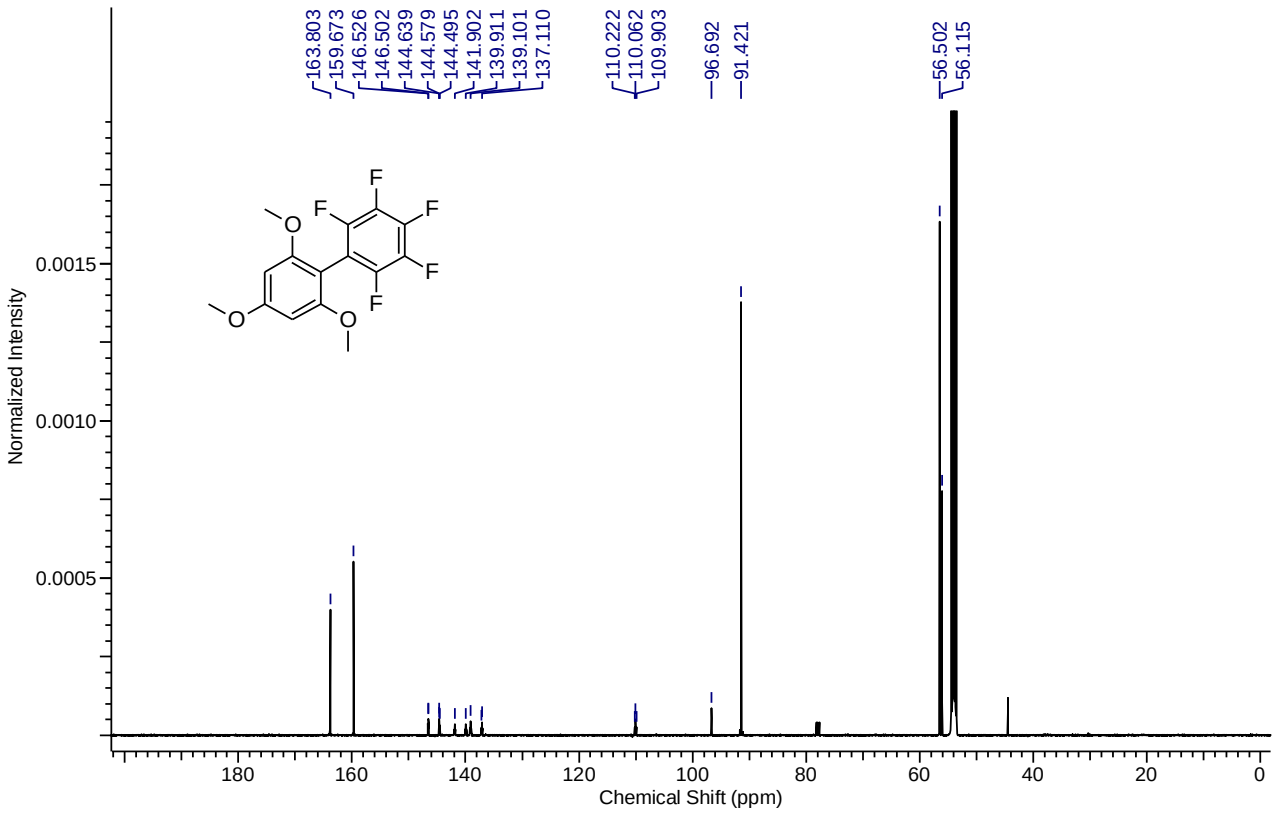


2,3,4,5,6-Pentafluo-2',4',6'-trimethoxybiphenyl (15)

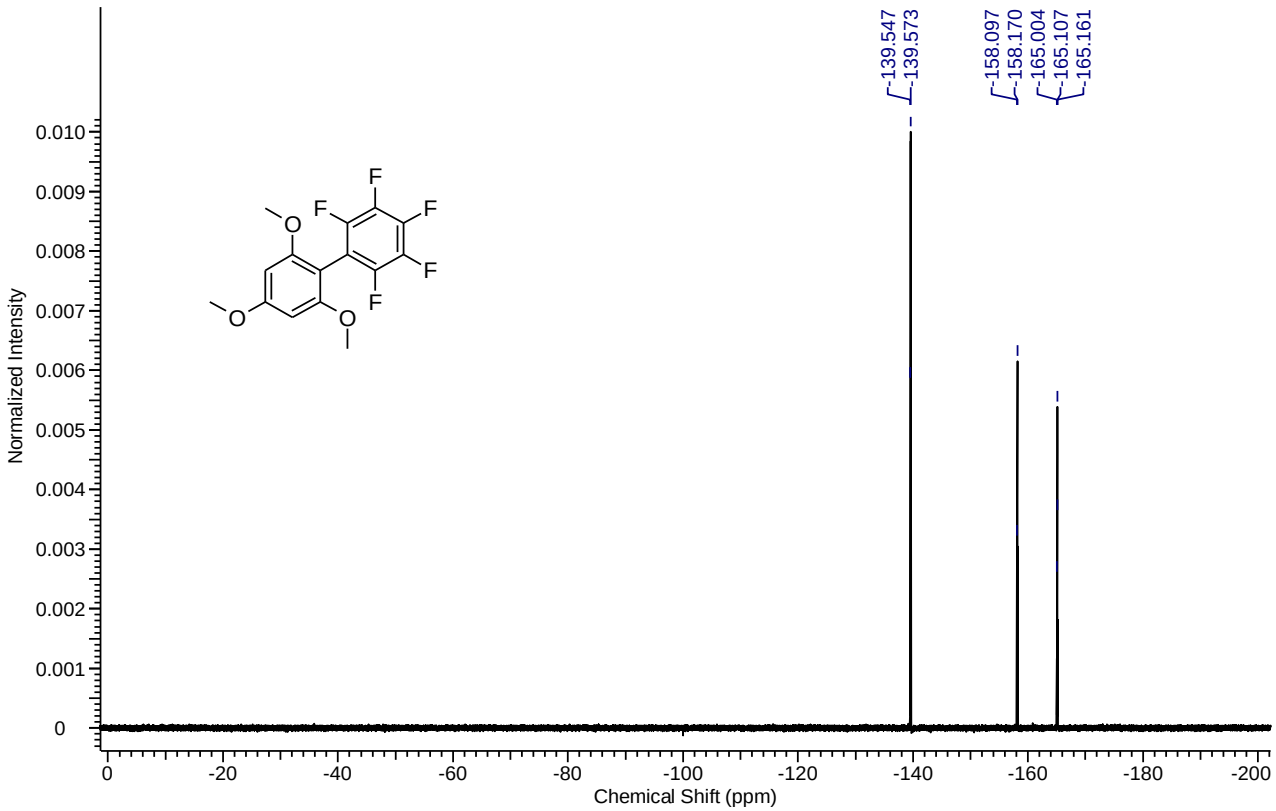
^{1}H-NMR



^{13}C-NMR

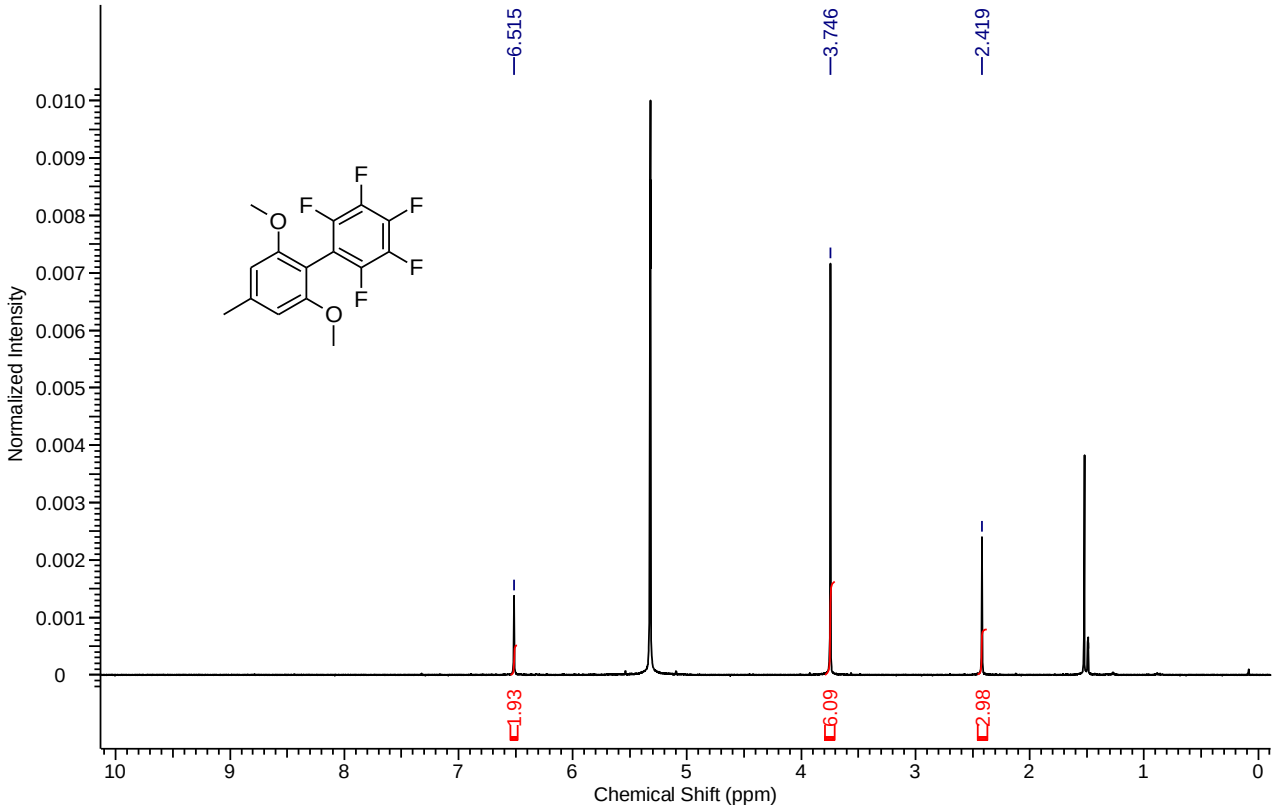

163.803
159.673
146.526
146.502
144.639
144.579
144.495
141.902
139.911
139.101
137.110
110.222
110.062
109.903
96.692
91.421
56.502
56.115
F
F
F
F
F
O
O
O
Normalized Intensity
0.0015
0.0010
0.0005
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

^{19}F-NMR

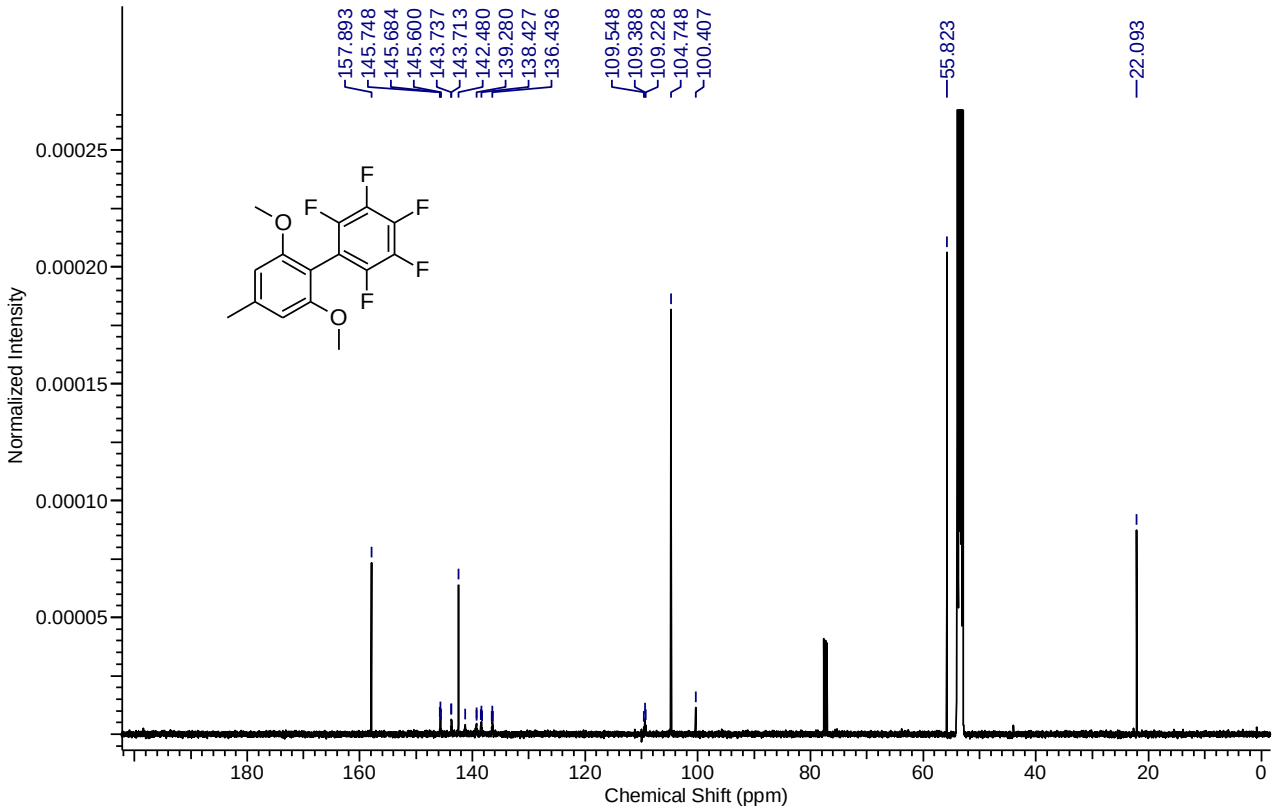

-139.547
-139.573
-158.097
-158.170
-165.004
-165.107
-165.161
F
F
F
F
F
O
O
O
Normalized Intensity
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
Chemical Shift (ppm)

2,3,4,5,6-Pentafluo-4'-methyl-,2',6'dimethoxybiphenyl (16b)

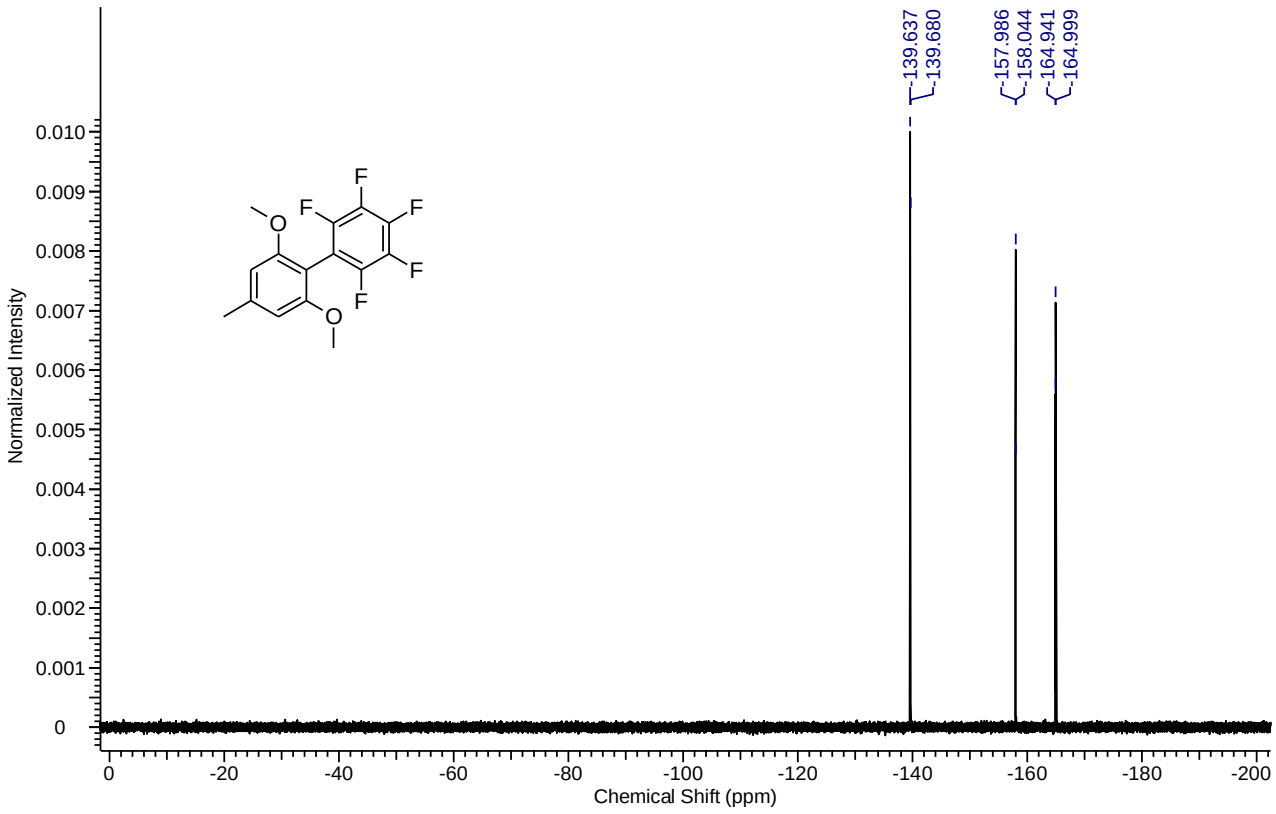
^{1}H-NMR



^{13}C-NMR

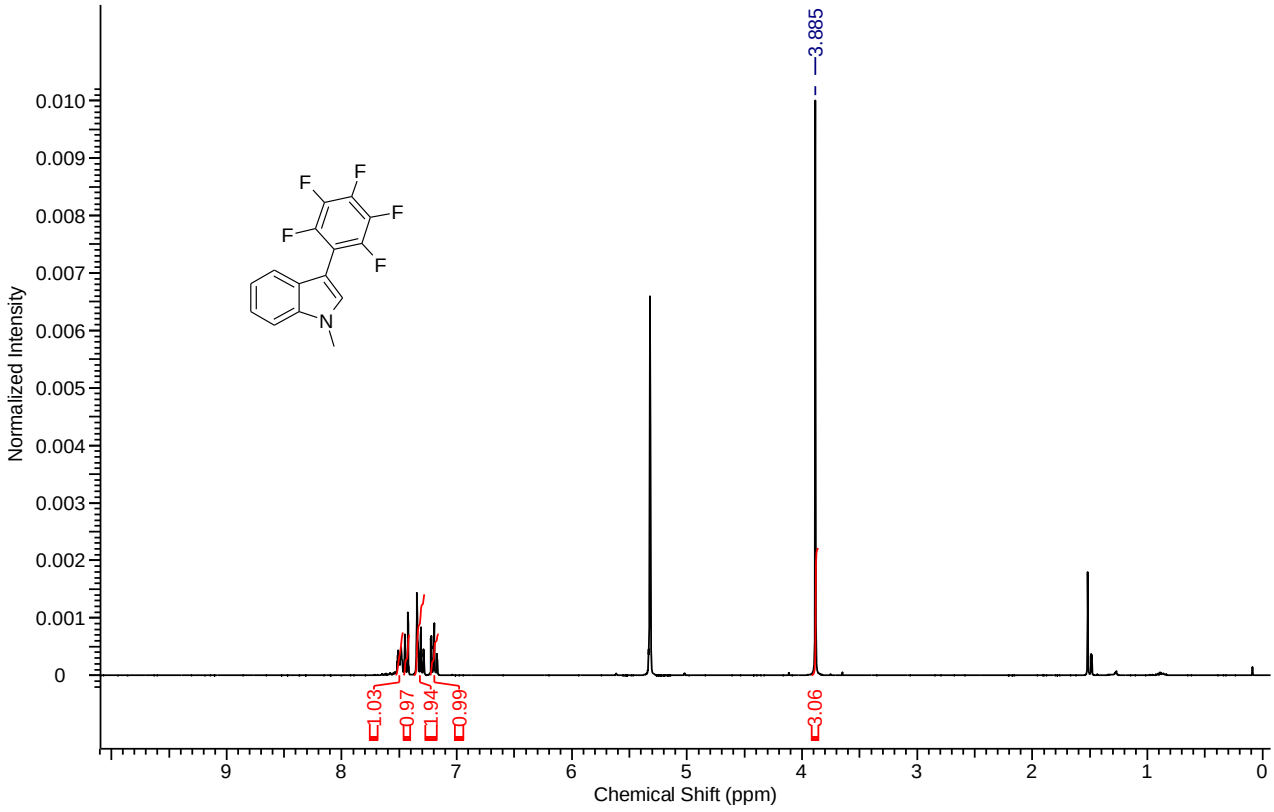


^{19}F-NMR

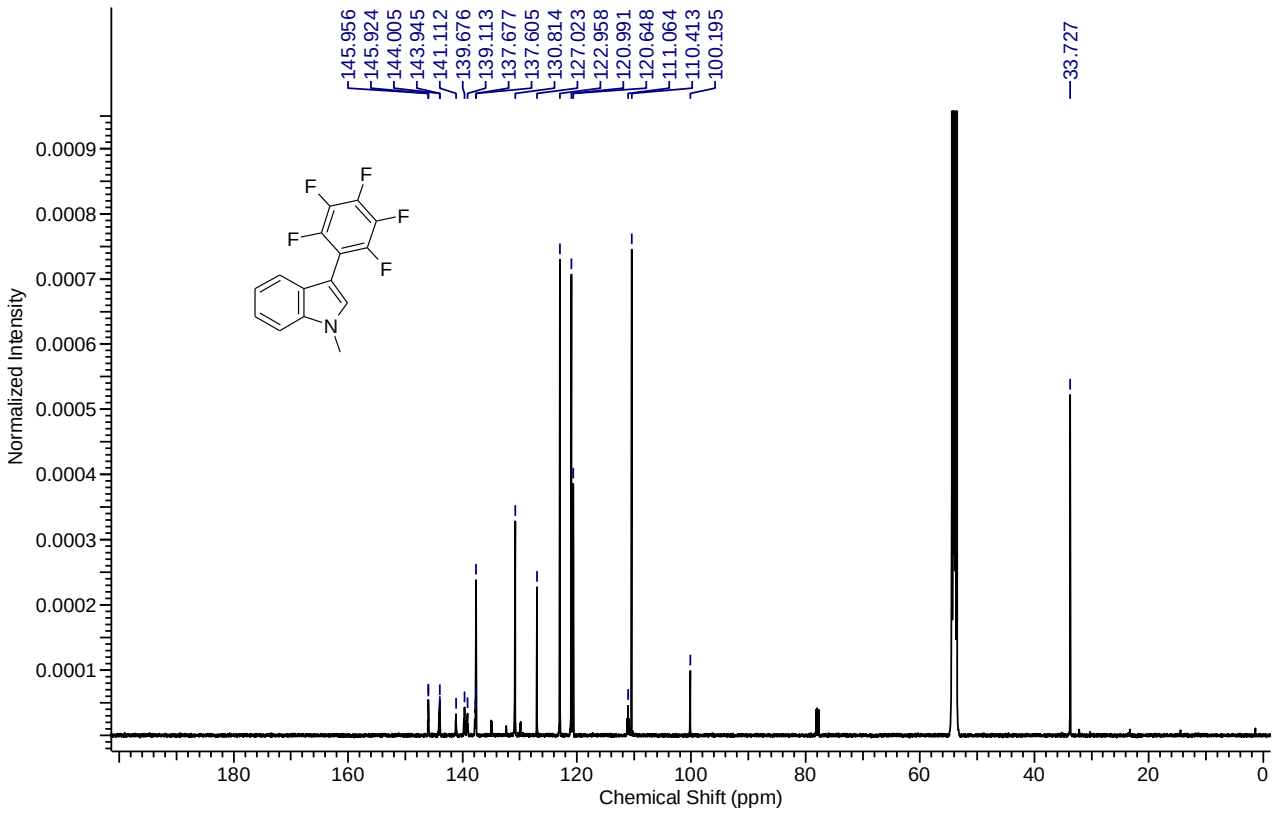


1-Methyl-3-(pentafluorophenyl)-indole (17)

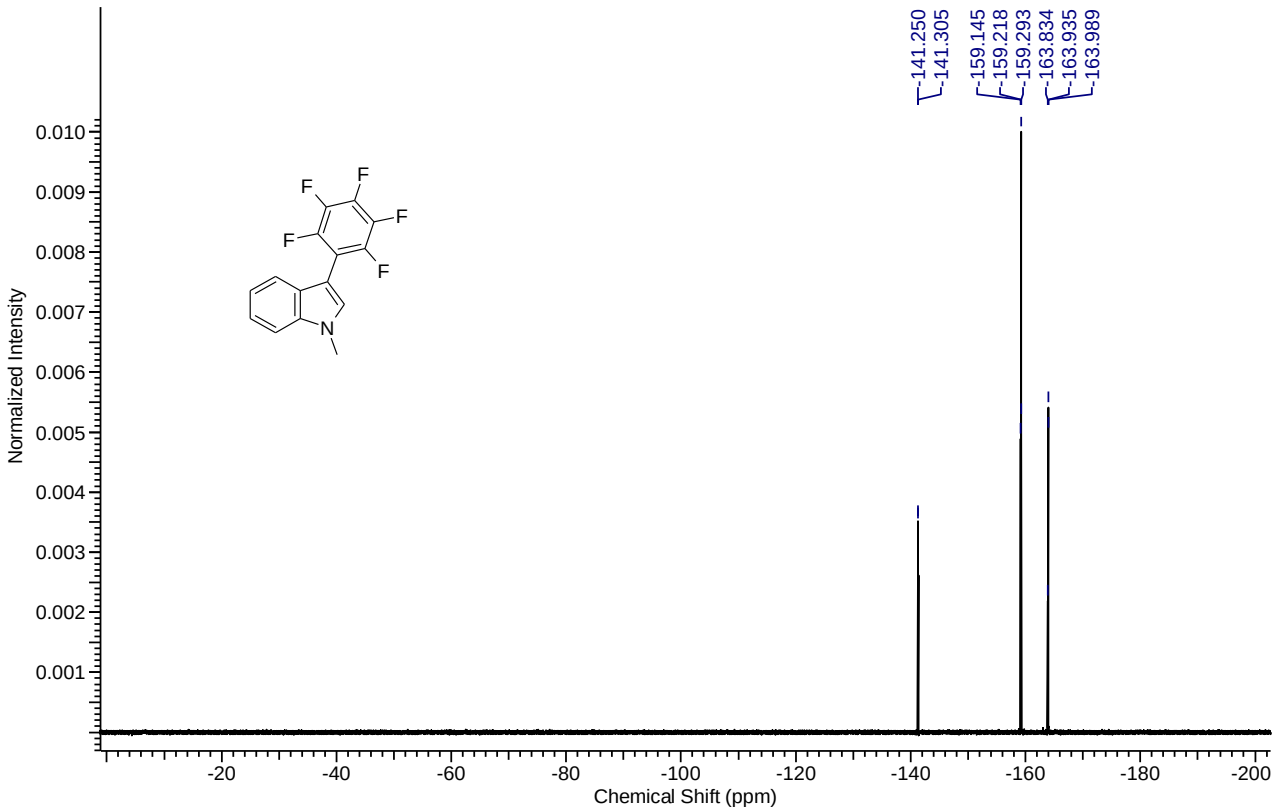
^{1}H-NMR



^{13}C-NMR

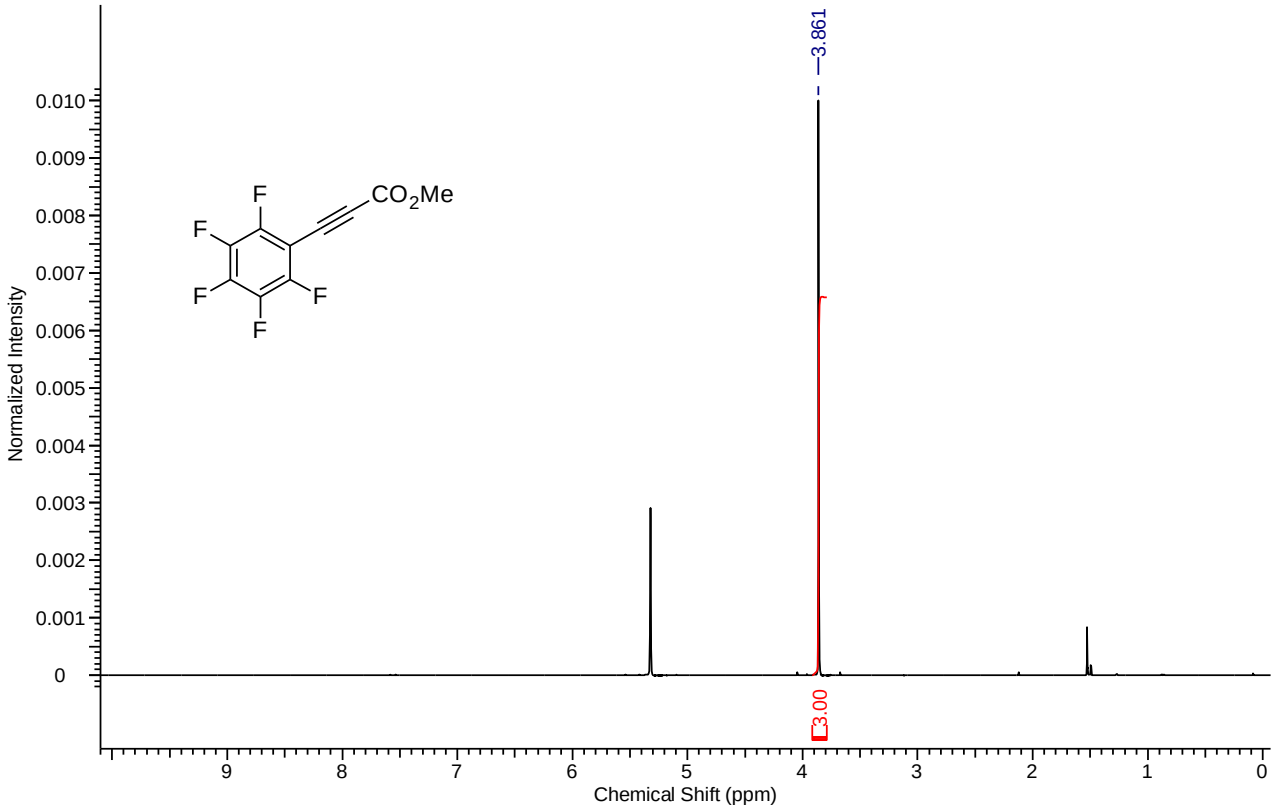

145.956
145.924
144.005
143.945
141.112
139.676
139.113
137.677
137.605
130.814
127.023
122.958
120.991
120.648
111.064
110.413
100.195
33.727
F
F
F
F
F
N
Normalized Intensity
0.0009
0.0008
0.0007
0.0006
0.0005
0.0004
0.0003
0.0002
0.0001
180
160
140
120
100
80
60
40
20
0
Chemical Shift (ppm)

^{19}F-NMR

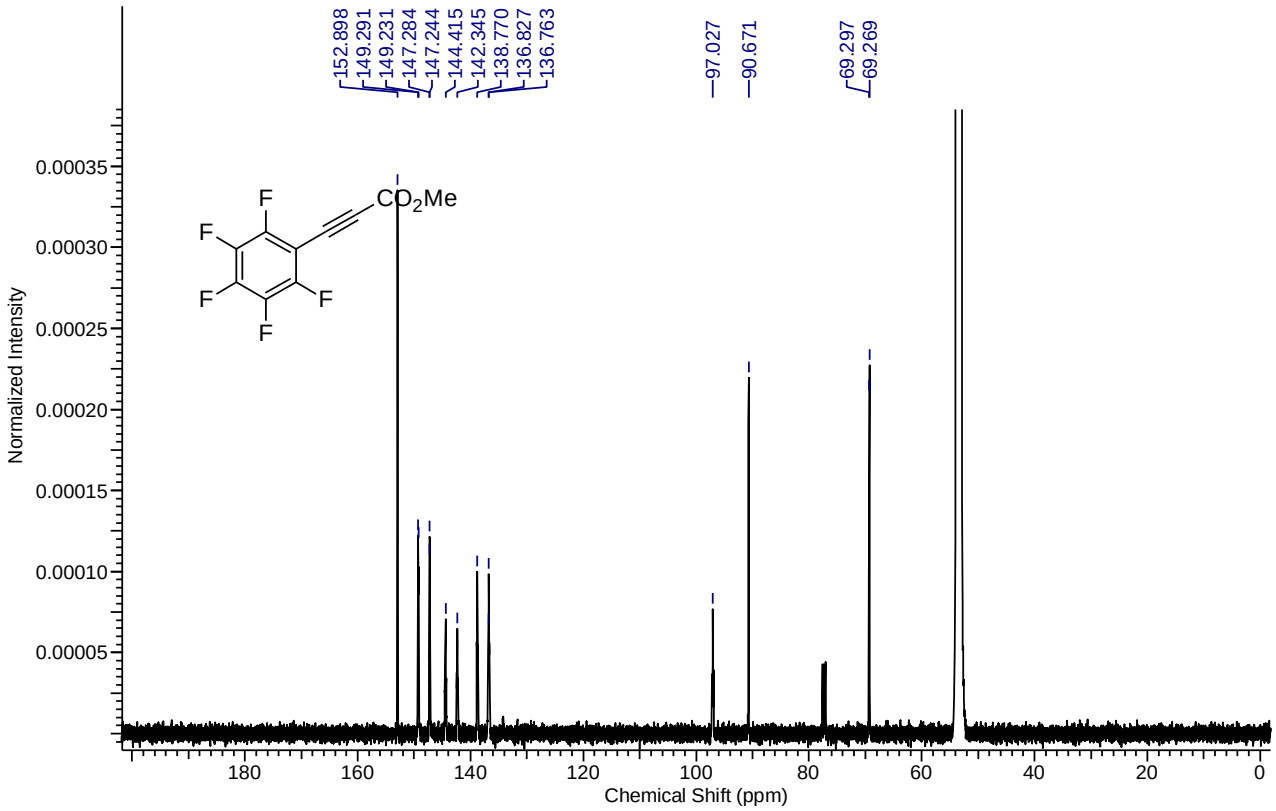

141.250
141.305
159.145
159.218
159.293
163.834
163.935
163.989
F
F
F
F
F
N
Normalized Intensity
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
Chemical Shift (ppm)

3-(2,3,4,5,6-Pentafluorophenyl)-2-propynoic acid methyl ester (14)

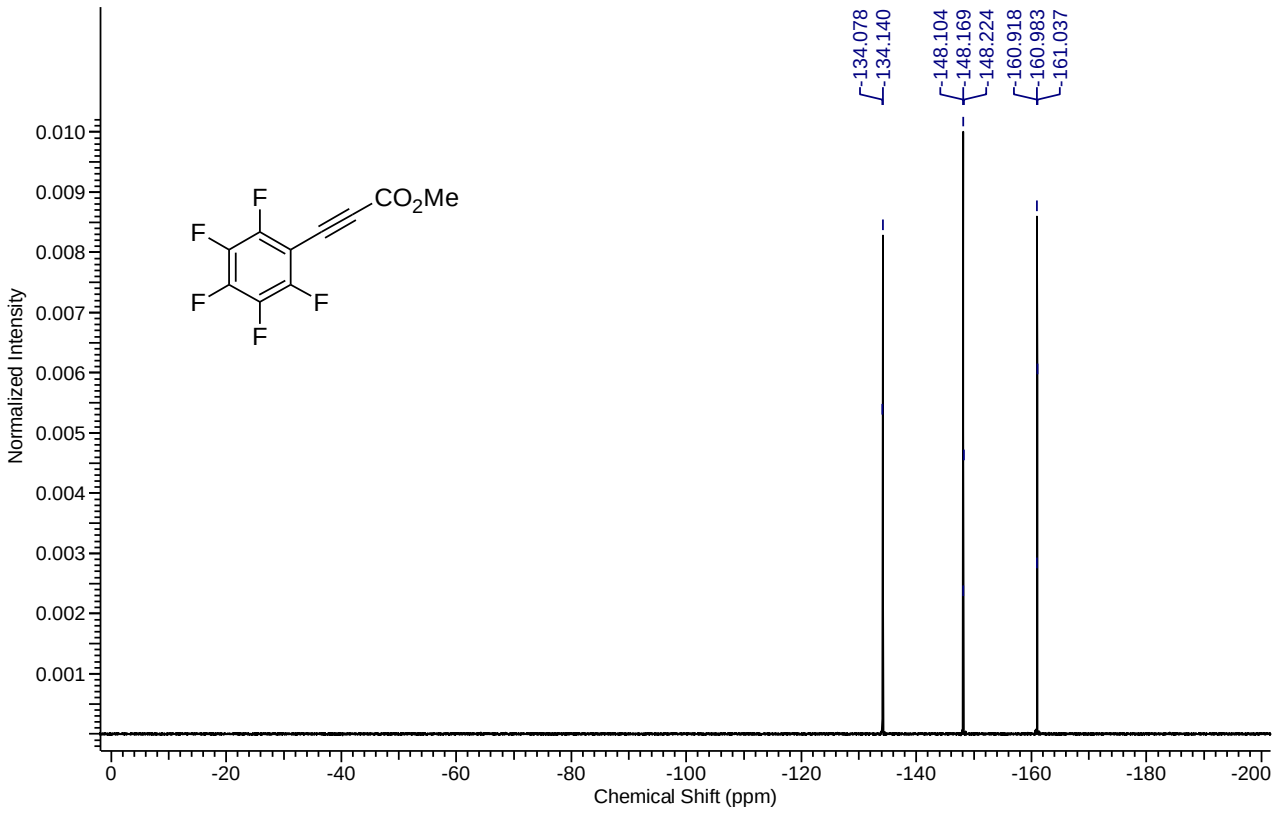
^{1}H-NMR



^{13}C-NMR

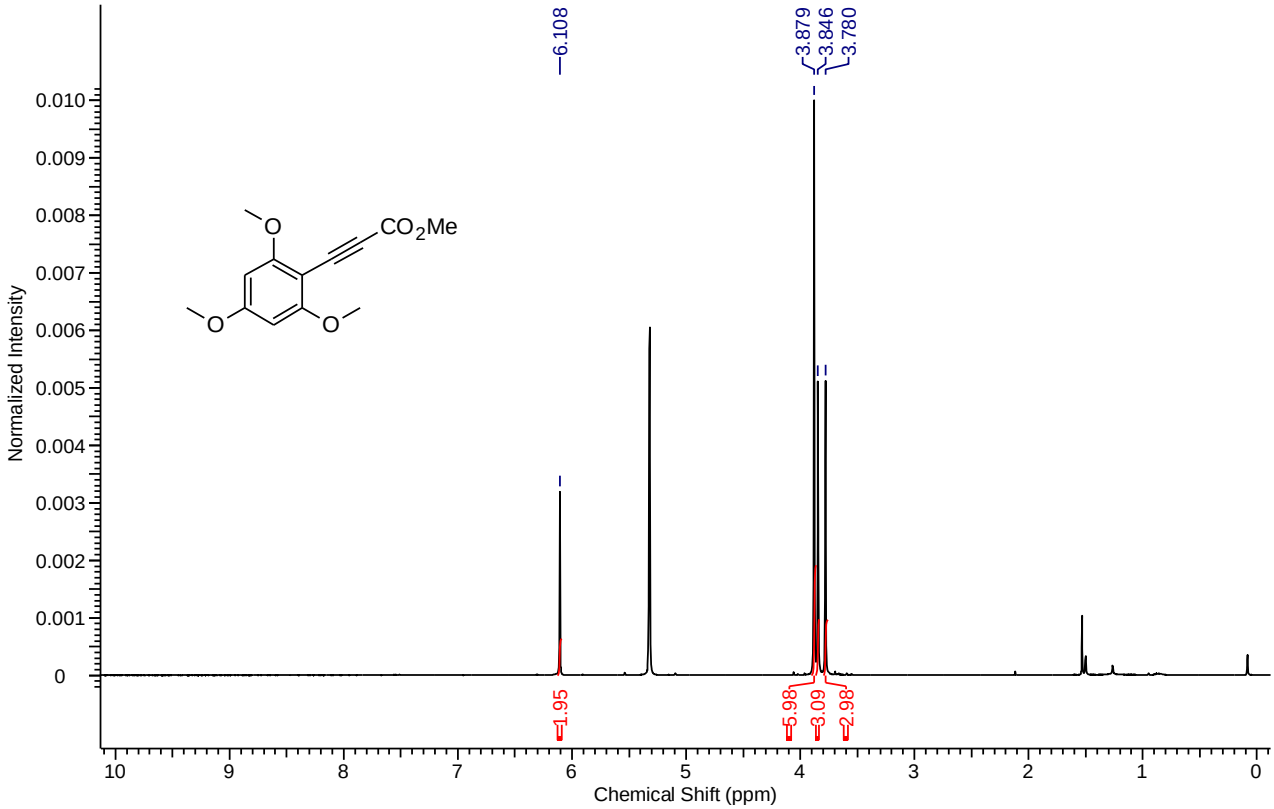


^{19}F-NMR

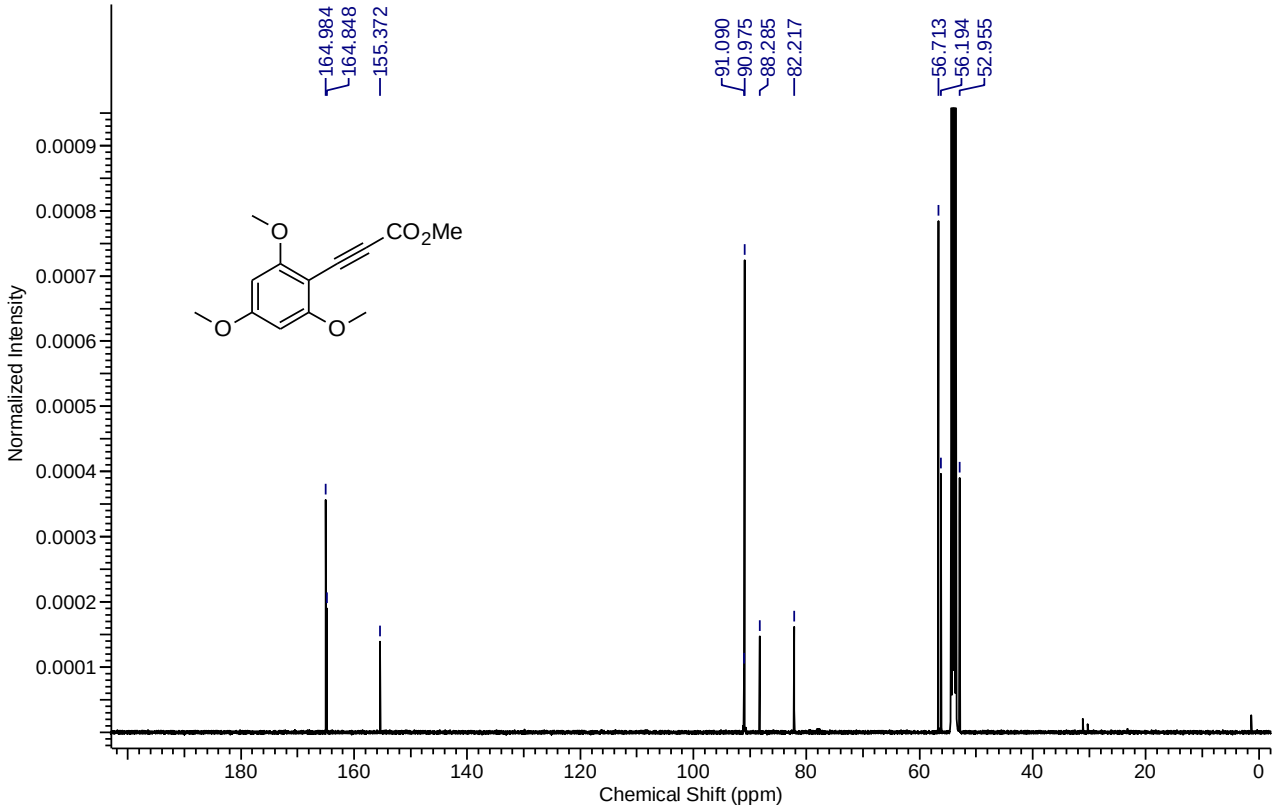


Methyl-3-(2,4,6-trimethoxyphenyl)-propiolate (19)

^{1}H-NMR

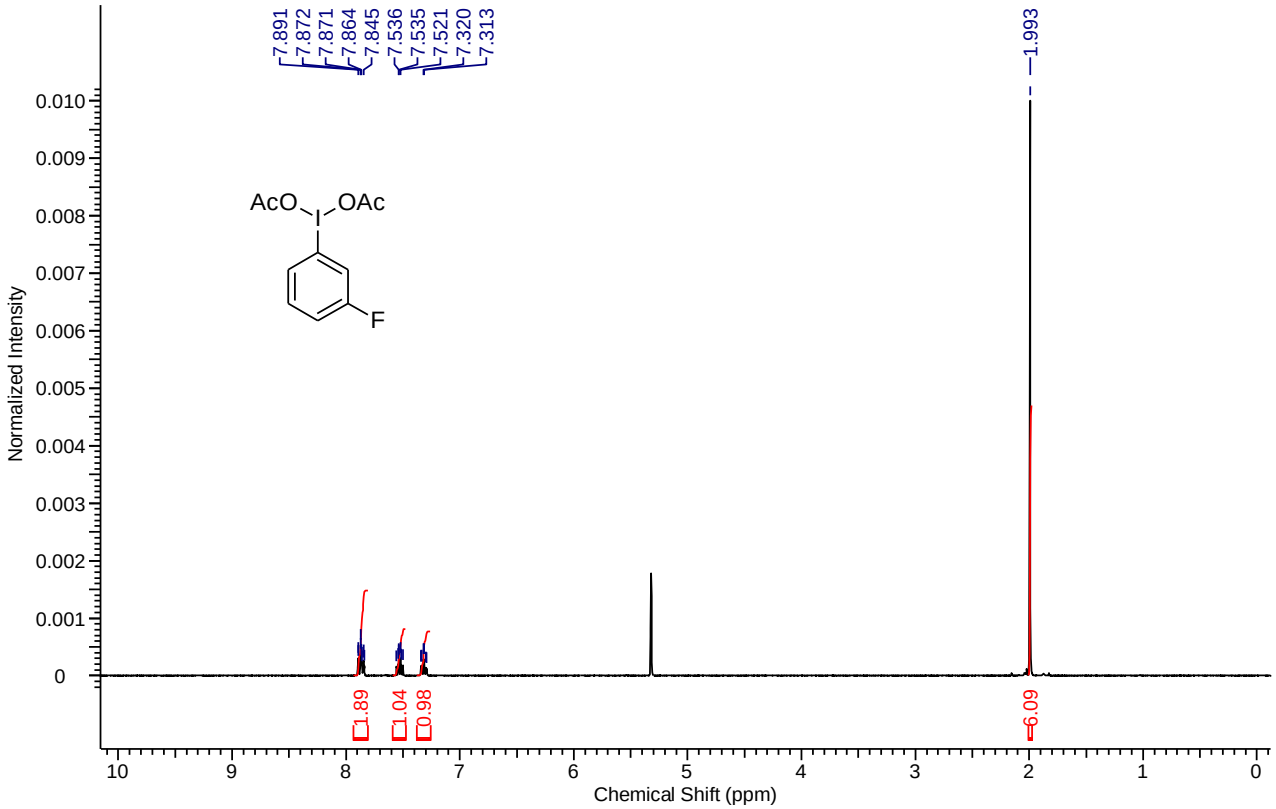


^{13}C-NMR

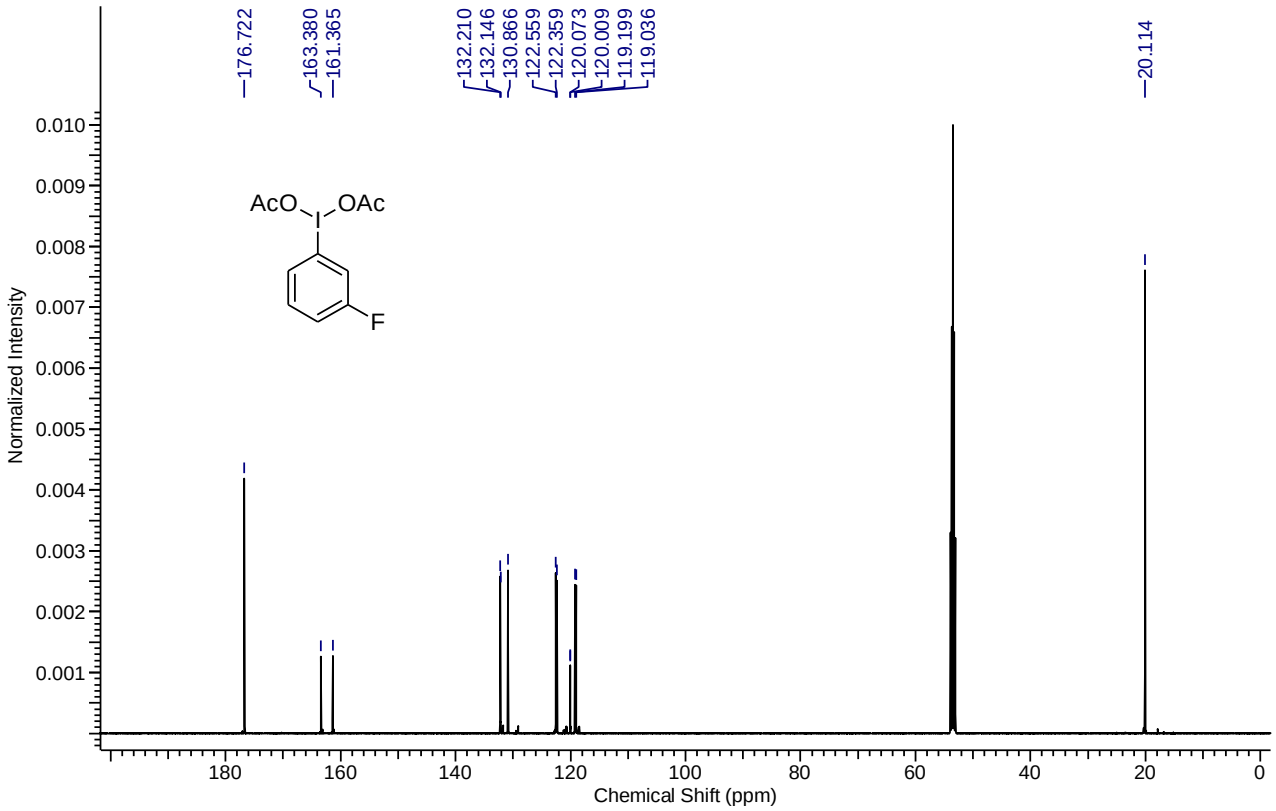


Diacetoxy(3-fluorophenyl)-λ3-iodane (20)

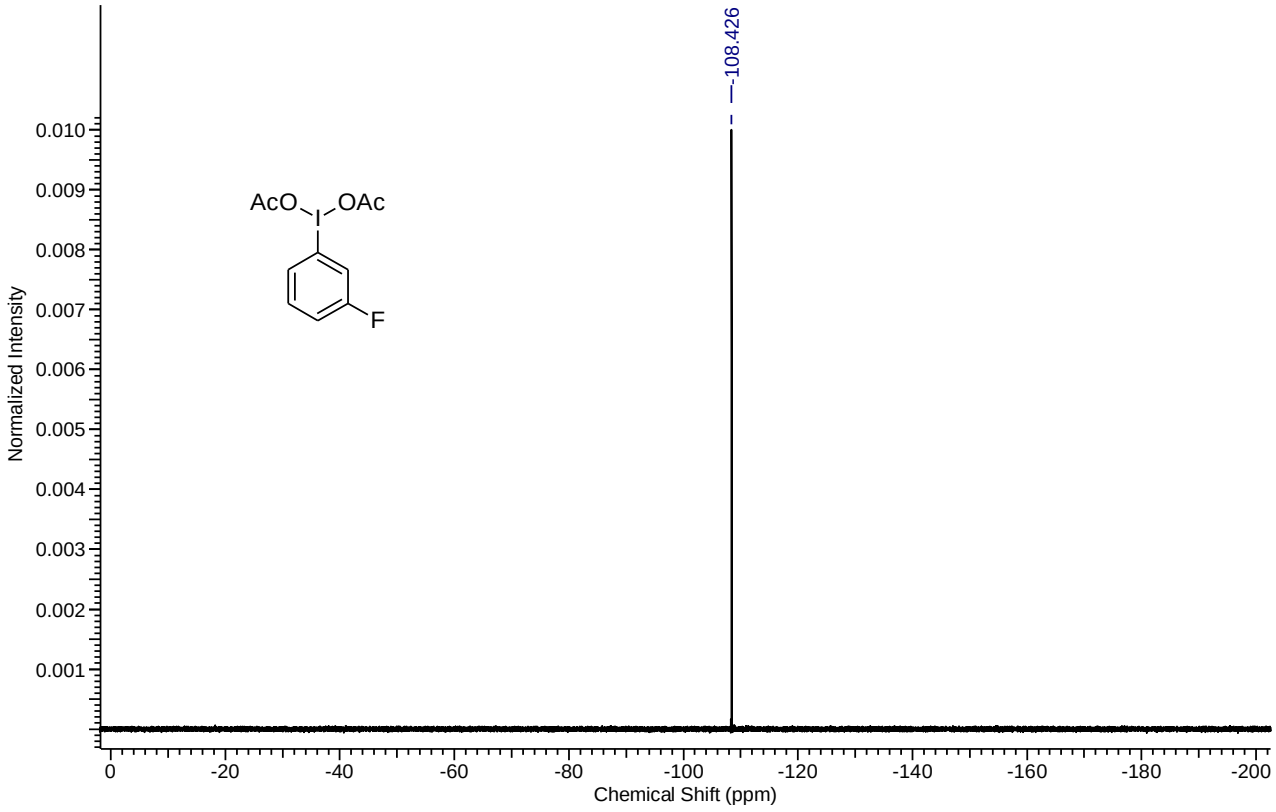
^{1}H-NMR



^{13}C-NMR

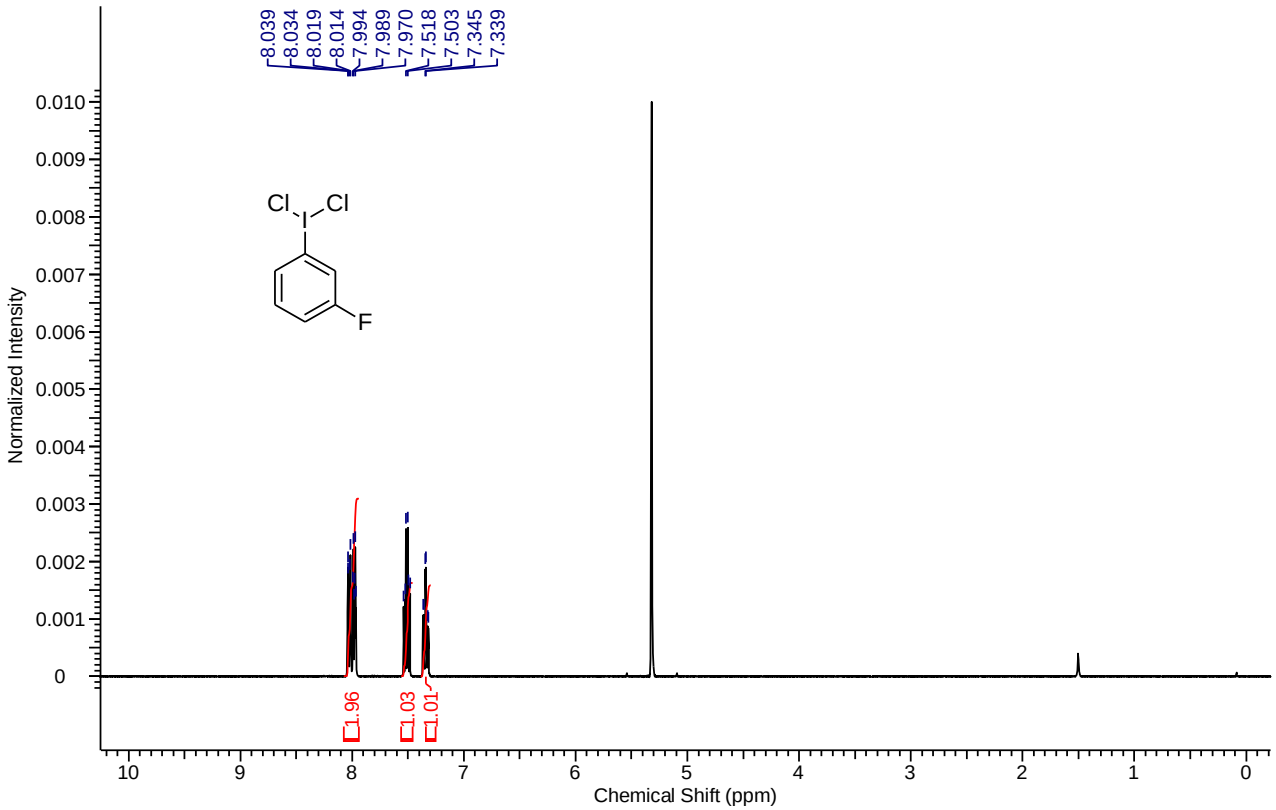


^{19}F-NMR

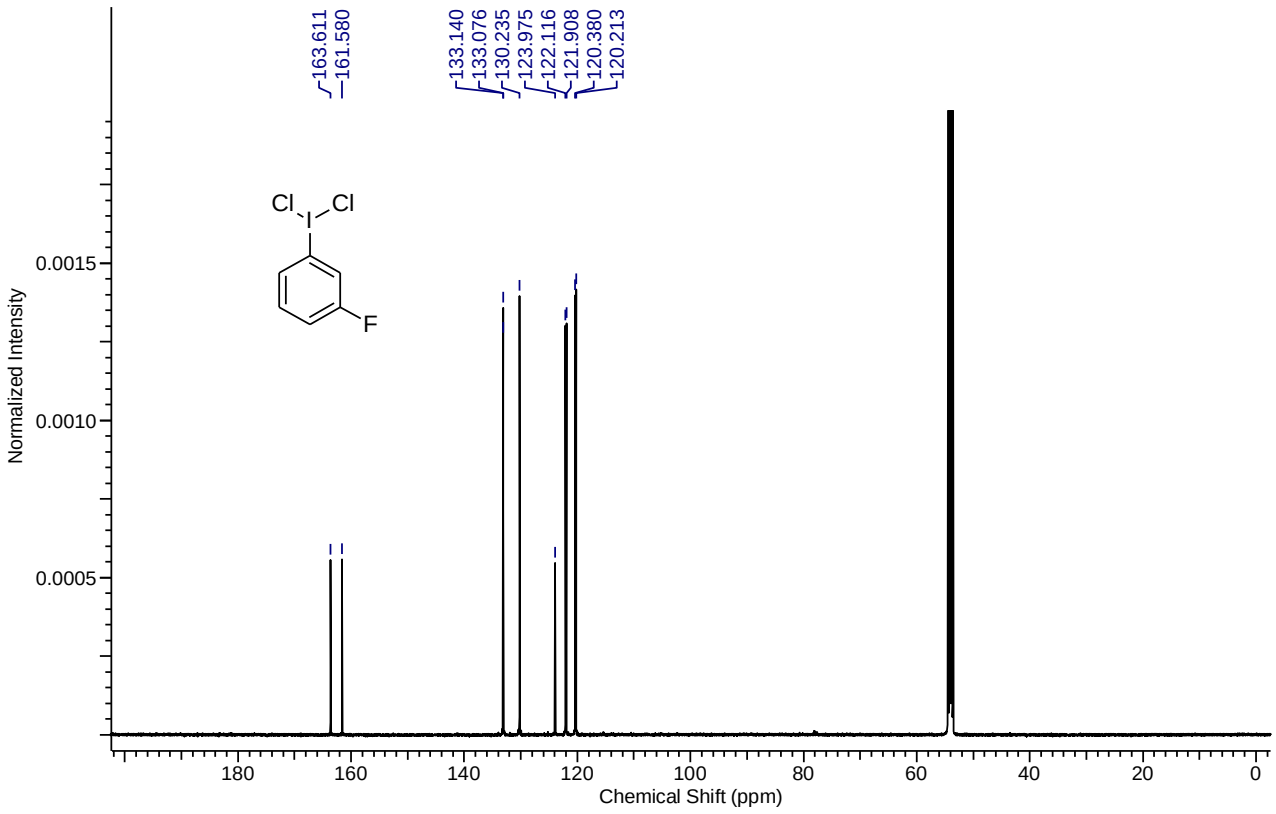


Dichloro(3-fluorophenyl)-λ3-iodane

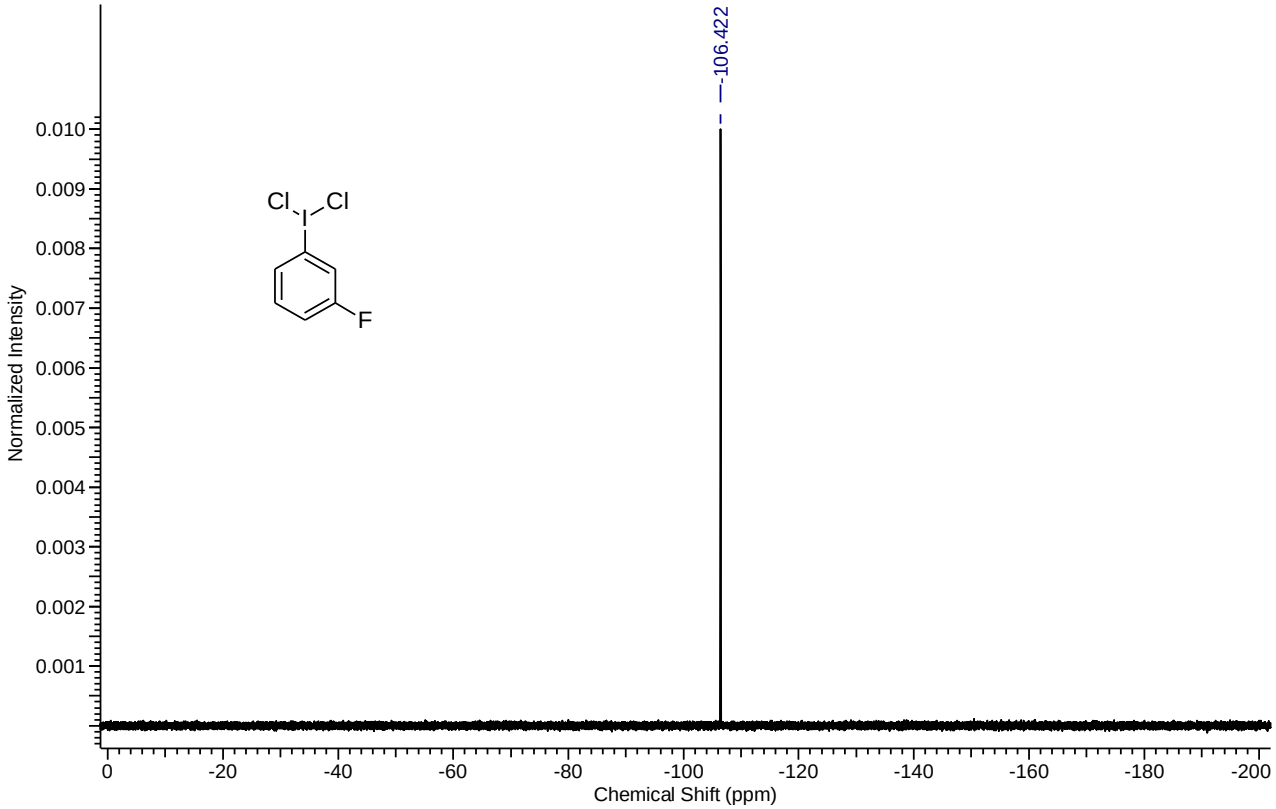
^{1}H-NMR



^{13}C-NMR



^{19}F-NMR


-106.422
Cl
I
Cl
F
Normalized Intensity
0.010
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
-20
-40
-60
-80
-100
-120
-140
-160
-180
-200
Chemical Shift (ppm)

7. Computational studies

7.1 General remarks and energies of intermediates and transition states

All reported structures were optimized at DFT level by using the B3LYP[30] hybrid functional as implemented in Gaussian 09.[31] Optimizations were carried out by using the standard 6-31G(d) basis set for C, H, O, Cl and P. The LANL2DZ basis set, which includes the relativistic effective core potential (ECP) of Hay and Wadt and employs a split-valence (double-ζ) basis set was used for I and Au.[32] Reported energy values correspond to Gibbs Free (G) energies, and include single point refinement of the previous structures by means of the Truhlar´s last generation M06 functional,[33] and the 6-311+G(d,p) basis set for C, H, O, Cl and P, and SDD basis set for I and Au, in a solvent model[34] (IEFPCM, solvent = dichloromethane). The critical stationary points were characterized by frequency calculations in order to verify that they have the right number of imaginary frequencies, and the intrinsic reaction coordinates (IRC)[35] were followed to verify the energy profiles connecting those transition structures to the correct associated local minima.

[30] (a) Lee, C.; Yang, W.; Parr, R. G. *Phys. Rev. B* **1988**, *37*, 785–789. (b) Becke, A. D. *J. Chem. Phys*. **1993**, *98*, 5648–5652. (c) Kohn, W.; Becke, A. D.; Parr, R. G. *J. Phys. Chem*. **1996**, *100*, 12974–12980.

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Table S2. Energies of the structures involved in the computational study

	B3LYP/6-311+G**[a]	Correction to G (B3LYP)[a]	M06/6-311+G** Single Point energy [a]	relative **G** B3LYP/M0[b]	Frequency
Structures in Figure 3 and Figure S64					
Ph_3PAuCl	-1632.074810	0.222896	-1631.966098		
Alkyne	-229.984496	0.036688	-229.889844		
$Ph_3PAu(CCCOMe)$	-1401.231510	0.272843	-1401.032003		
HCl	-460.803806	-0.011178	-460.795533		
$PhI(OAc)_2$	-699.914468	0.144004	-699.689421		
$Ph_3PAuOAc$	-1400.330134	0.268305	-1400.166236		
PhI(Cl)(OAc)	-931.644729	0.098613	-931.468853		
AcOH	-229.097068	0.034713	-229.037016		
TS_3	-2332.842651	0.388046	-2332.485468		-130.6
TS_3'	-2101.103749	0.436295	-2100.694277		-84.7
PhI	-243.030831	0.058373	-242.903412		
H	-1858.152141	0.362215	-1857.851418		
Structures in Figure 5 and Figure S69					
SUM (0)	-2561.973774	0.403588	-2561.545363	0	
TS_1	-2331.970752	0.386648	-2331.641580	21.1	-35.7
INT_1	-2561.959359	0.403606	-2561.524933	12.8	
TS_2	-1630.294192	0.317654	-1630.048273	25.7	-267.2
INT_2	-2561.973307	0.406169	-2561.537872	6.3	
TS_3	-2332.842651	0.388046	-2332.485468	26.4	-130.6
INT_3	-2332.870209	0.389175	-2332.516369	7.7	
INT_4	-1861.201042	0.273193	-1861.001510	16.2	
$Ph(OMe)_3$	-575.840674	0.160641	-576.600410		
INT_5	-2437.068867	0.456295	-2436.651222	-0.7	
TS_4	-2665.677049	0.494821	-2665.220291	7.2	-60.9
INT_6	-2436.619185	0.441299	-2436.208326	-22.0	
TS_5	-2436.607758	0.441119	-2436.197515	-15.4	-362.3
Final	-804.644185	0.197821	-804.315555	-81.0	
Structures in Figure S57 and Figure S65					
H	-1858.152141	0.362215	-1857.851418		
$Ph_3PAu(CCCOMe$	-1401.231510	0.272843	-1401.032003		
Alkyne	-229.984496	0.036688	-229.889844		
H'	-1859.047843	0.365194	-1858.713063		
$Ph_3PAuOAc$	-1400.330134	0.268305	-1400.166236		
AcOH	-229.097068	0.034713	-229.037016		
Structures in Figure S66					
H	-1858.152141	0.362215	-1857.851418	0	
TS-S1	-1858.122338	0.361418	-1857.823214	17.2	-353.3
H´	-1859.047843	0.365194	-1858.713063	0	
TS-S2	-1859.024903	0.364227	-1858.692233	12.5	-420.7
TS-S3	-1859.008622	0.364807	-1858.675919	23.7	-326.5
S1	-1859.946143	0.369447	-1859.576824	0	
TS-S4	-1859.917729	0.367061	-1859.551143	14.6	-435.5
S2	-2205.783431	0.491686	-2205.271152	0	
TS-S5	-2205.761106	0.491078	-2205.264280	3.9	-365.0
TS-S6	-2205.742277	0.490875	-2205.245811	15.4	-438.8
S3	-2204.887929	0.490292	-2204.424035	0	
TS-S7	-2204.867308	0.488895	-2204.405729	10.6	-364.9

[a] Energy units: Hartrees. [b] Energy units: kcal/mol

Table S2. Continued

	B3LYP/6-311+G**[a]	Correction to G (B3LYP)[a]	M06/6-311+G** Single Point energy [a]	relative **G** B3LYP/M0[b]	Frequency
Structures in Figure S67					
S4	-700.793947	0.146512	-700.543341		
S4+$Ph_3PAu(CCCOMe)$	2102.025457	0.419355	-2101.575344		
TS-S8	-2101.996003	0.437988	-2101.555968	23.9	-158.5
S5	-1163.370192	0.053918	-1163.245207		
S5+$Ph_3PAu(CCCOMe)$	-2564.601702	0.326761	-2564.277210		
TS-S9	-2564.569435	0.343262	-2564.263043	19.2	-118.6
S4+Ph_3PAuCl	-2332.868757	0.369408	-2332.509439		
TS-S10	-2332.842651	0.388046	-2332.485468	26.7	-420.1
Structures in Figure S68					
Alkyne+Ph_3PAuCl	-1862.059306	0.259584	-1861.855942	0	
TS-S11	-1862.015018	0.272371	-1861.801337	42.3	-63.7
$Ph_3PAu(CCCOMe)$+HCl	-1862.035316	0.261665	-1861.827536	19.1	
Structures in Figure S69					
INT_{5A}	-2089.886068	0.318841	-2089.641883	-17.9	
INT_{5B}	-2665.685643	0.498828	-2665.232221	0.5	
TS_{4A}	-2665.677749	0.495138	-2665.218200	7.0	-466.9

[a] Energy units: Hartrees. [b] Energy units: kcal/mol

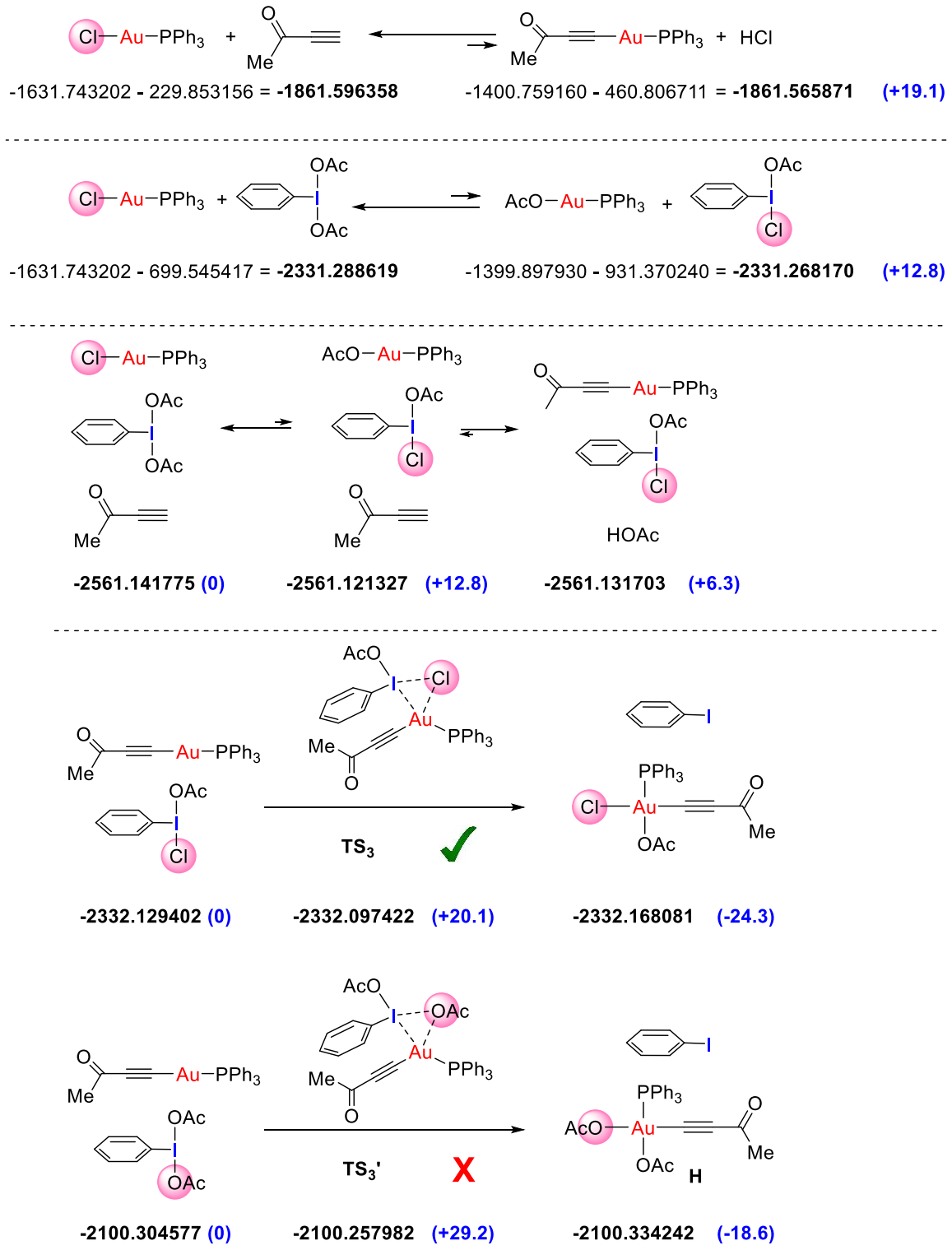
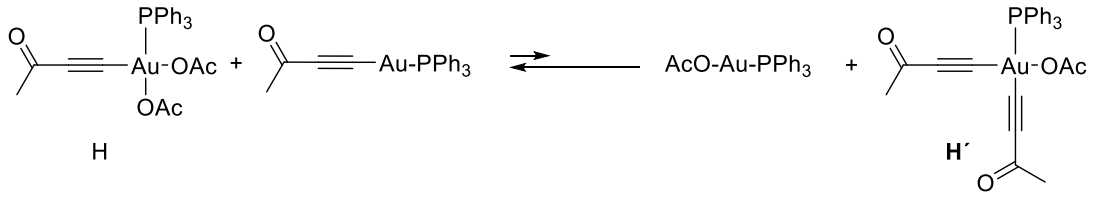
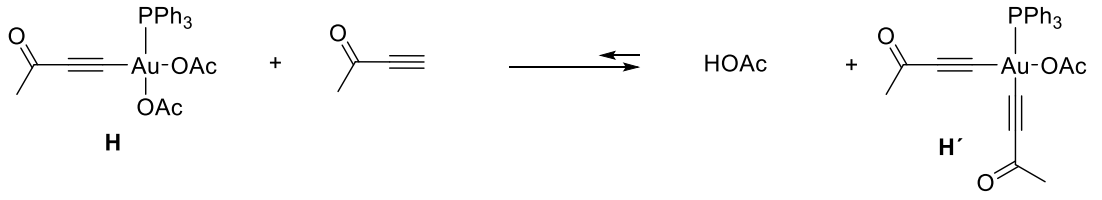


Figure S64. Absolute energies correspond to M06 functional hartrees (in brackets: kcal/mol) for the structures in the figure 3 of the main text.



-1857.489203 - 1400.759162 = **-3258.248365** -1399.897931 - 1858.347869 = **-3258.245800** **(+1.6)**



-1857.489203 - 229.853156 = **-2087.342359** -229.002303 - 1858.347869 = **-2087.350172** **(- 4.9)**

Figure S65. Absolute energies correspond to M06 functional in hartrees (in brackets: kcal/mol)

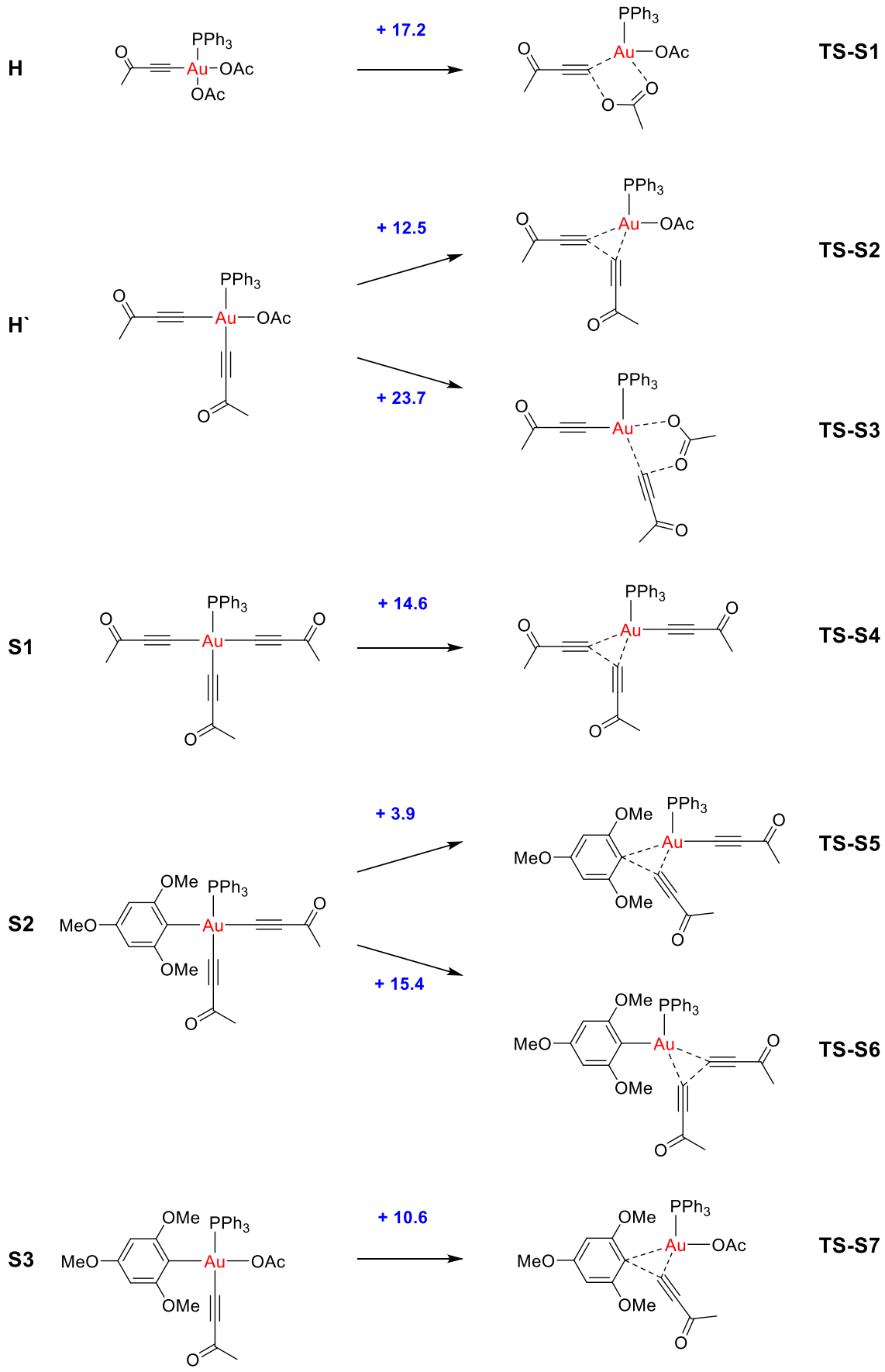


Figure S66. Transition states for some selected reductive elimination processes, not shown in the main text. M06 functional energy (kcal/mol).

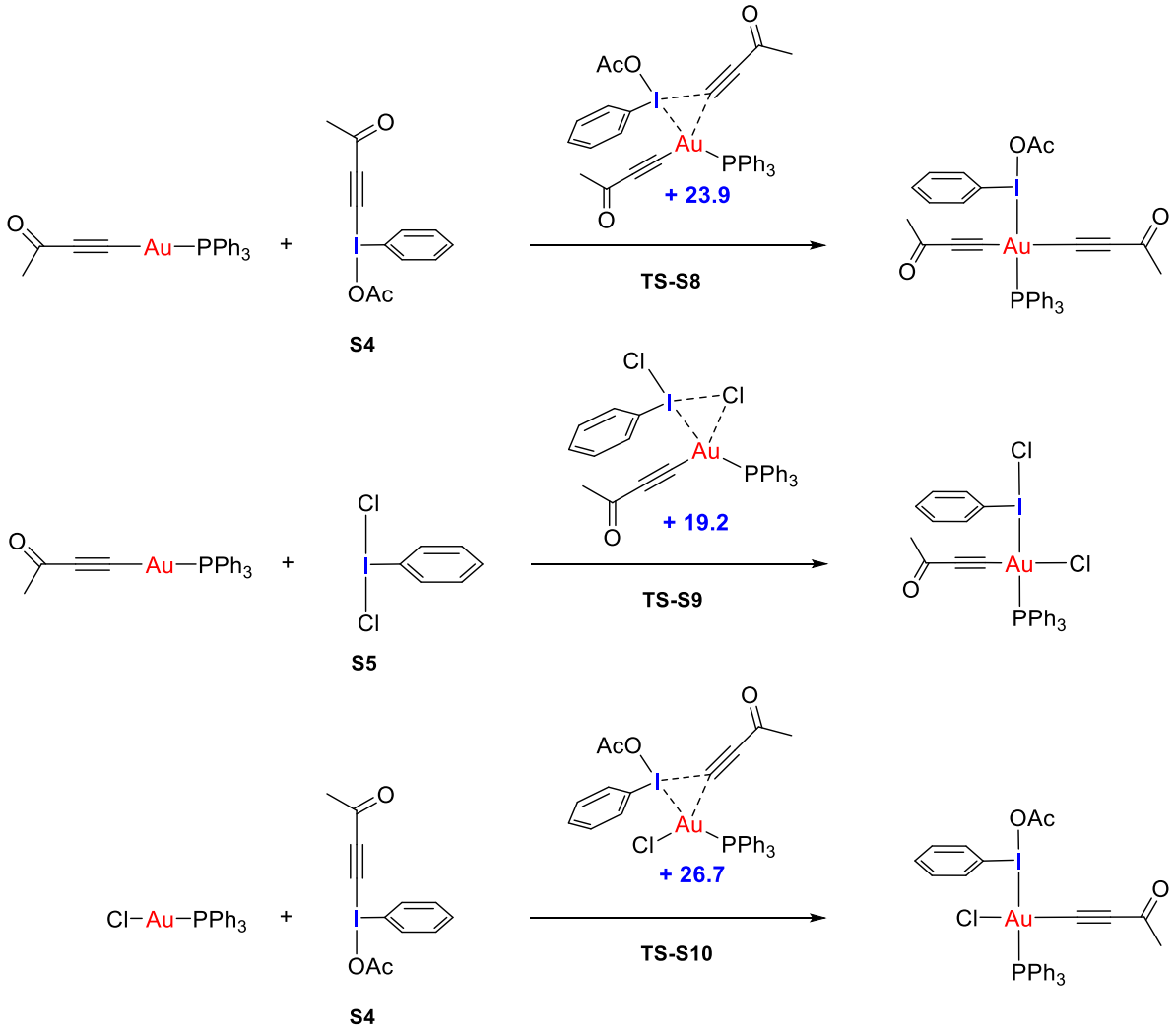


Figure S67. Alternative oxidation processes of the alkynylgold (I) complex. M06 functional energy (kcal/mol).

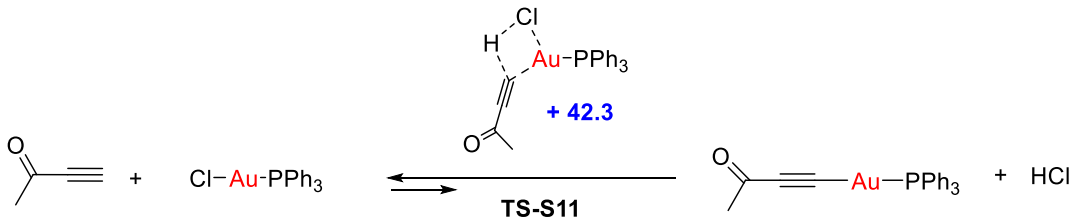


Figure S68. Alkynylgold(I) complex formation by deprotonation of alkyne with Cl-Au-PPh_3. M06 functional energy (kcal/mol).

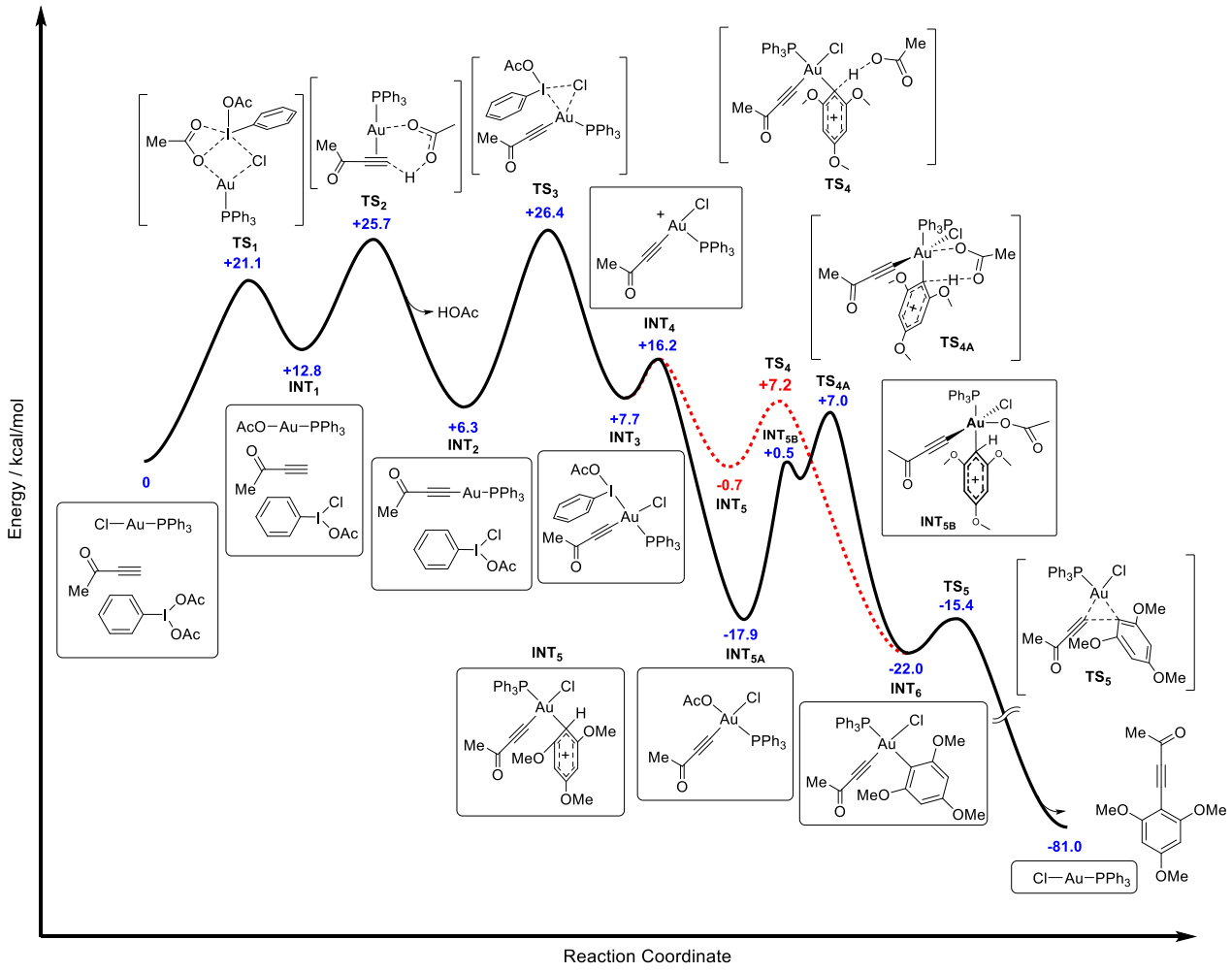


Figure S69. Comparative reaction profile between an associative and dissociative mechanism for the acetate/aryl ligand exchange

7.2 Cartesian coordinates

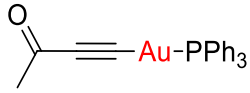
Cl−Au−PPh_3

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.197453	-3.169889	-2.902994
2	1	0	0.473084	-4.344457	-2.352054
3	1	0	3.792753	-1.766349	-3.272224
4	1	0	2.884013	-0.044847	-1.750817
5	1	0	-0.447371	-2.621530	-0.834543
6	1	0	2.631149	-1.132050	5.172865
7	1	0	3.814465	-1.947030	3.145586
8	1	0	0.508512	0.142259	4.939543
9	1	0	-0.426900	0.594778	2.694794
10	1	0	2.890711	-1.490385	0.899682
11	1	0	2.608379	5.052568	-1.616830
12	1	0	0.451360	4.235801	-2.546939
13	1	0	3.835789	3.679873	0.051215
14	1	0	2.920794	1.504610	0.785473
15	1	0	-0.473861	2.062979	-1.810665
16	6	0	1.006253	-3.408709	-2.214116
17	6	0	2.871071	-1.959495	-2.731193
18	6	0	2.359917	-0.987807	-1.869142
19	6	0	0.488882	-2.439965	-1.354964
20	1	0	2.595016	-3.921898	-3.578238
21	6	0	1.166880	-1.224375	-1.169887
22	6	0	2.892672	-1.381105	3.048170
23	6	0	1.035516	-0.206683	4.056675
24	6	0	0.509400	0.052285	2.791611
25	6	0	2.372926	-1.120906	1.778979
26	6	0	2.227041	-0.923479	4.186569
27	6	0	1.178891	-0.397112	1.642074
28	6	0	0.997381	3.635085	-1.825862
29	6	0	2.898421	3.322374	-0.364922
30	6	0	2.383800	2.092334	0.047733
31	6	0	0.476890	2.408641	-1.414521
32	6	0	2.208113	4.093347	-1.301951
33	6	0	1.170503	1.624133	-0.479288
34	15	0	0.461013	0.001135	0.000425
35	79	0	-1.850651	-0.000510	0.006465
36	17	0	-4.201396	-0.001947	0.001072

Standard orientation:

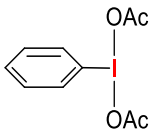
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.191304	-0.168337	-0.000363
2	6	0	-0.994001	0.004729	0.000413
3	6	0	0.452323	0.201597	0.000062
4	8	0	0.933508	1.320713	-0.000076
5	6	0	1.287917	-1.060407	-0.000059
6	1	0	2.345963	-0.794738	-0.000885
7	1	0	1.052340	-1.668427	-0.880454
8	1	0	1.053614	-1.667640	0.881232
9	1	0	-3.249590	-0.300398	0.000406



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.802743	-2.929960	-3.149466
2	1	0	-1.062775	-2.409351	-4.314595
3	1	0	-4.414584	-3.266597	-1.756749
4	1	0	-3.507950	-1.731044	-0.045851
5	1	0	-0.145043	-0.877885	-2.601567
6	1	0	-3.216266	5.165646	-1.166230
7	1	0	-4.421740	3.137593	-1.945851
8	1	0	-1.082368	4.932161	0.089219
9	1	0	-0.157512	2.685900	0.556753
10	1	0	-3.507918	0.890240	-1.473500
11	1	0	-3.181752	-1.592420	5.074263
12	1	0	-1.035137	-2.534189	4.244219
13	1	0	-4.413972	0.073984	3.703632
14	1	0	-3.514443	0.794768	1.518006
15	1	0	-0.125206	-1.811042	2.060271
16	6	0	-1.603213	-2.254905	-3.385529
17	6	0	-3.486085	-2.736443	-1.947681
18	6	0	-2.976176	-1.866487	-0.982355
19	6	0	-1.087373	-1.388326	-2.422363
20	1	0	-3.199526	-3.610912	-3.896760
21	6	0	-1.774531	-1.181112	-1.215517
22	6	0	-3.494543	3.039983	-1.388699
23	6	0	-1.618821	4.049123	-0.244590
24	6	0	-1.098809	2.783161	0.022925
25	6	0	-2.980701	1.770342	-1.119364
26	6	0	-2.816606	4.179027	-0.950735

27	6	0	-1.780383	1.632857	-0.406219
28	6	0	-1.583187	-1.813689	3.644562
29	6	0	-3.481137	-0.347444	3.340537
30	6	0	-2.975284	0.057320	2.104111
31	6	0	-1.071660	-1.409549	2.411808
32	6	0	-2.788160	-1.283365	4.110340
33	6	0	-1.768136	-0.475930	1.627570
34	15	0	-1.057537	-0.005806	0.000539
35	79	0	1.313039	0.013366	-0.002739
36	6	0	3.306275	0.056869	-0.004774
37	6	0	4.529633	0.122491	-0.003551
38	6	0	5.974248	0.168807	-0.001947
39	8	0	6.599102	1.220993	0.010080
40	6	0	6.677953	-1.179157	-0.015781
41	1	0	7.758717	-1.025137	-0.014646
42	1	0	6.381687	-1.751427	-0.901820
43	1	0	6.382567	-1.768707	0.859184



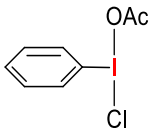
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.476252	1.260286	-0.076071
2	6	0	1.475982	1.506165	0.857864
3	6	0	0.514518	3.523649	-0.843559
4	6	0	1.526452	3.802664	0.077268
5	6	0	2.003330	2.799701	0.921825
6	6	0	-0.023555	2.238156	-0.930278
7	1	0	2.786592	3.016292	1.641971
8	1	0	1.941648	4.804257	0.137090
9	1	0	-0.819172	2.017419	-1.631421
10	1	0	1.842027	0.712613	1.499129
11	1	0	0.140134	4.302833	-1.500584
12	53	0	-0.357656	-0.718131	-0.204481
13	8	0	-2.200708	0.404336	0.225930
14	8	0	1.609561	-1.485188	-0.794825
15	6	0	-3.205717	-0.449359	0.246310
16	6	0	2.470857	-1.765004	0.174492
17	8	0	-3.069181	-1.654346	0.055009
18	8	0	2.325020	-1.482400	1.355431
19	6	0	3.698433	-2.486129	-0.359805
20	1	0	3.399761	-3.424057	-0.836414
21	1	0	4.391457	-2.685569	0.457763
22	1	0	4.185010	-1.873590	-1.124168
23	6	0	-4.543141	0.204940	0.536477
24	1	0	-4.521846	0.657294	1.532245
25	1	0	-5.335015	-0.542274	0.485445
26	1	0	-4.732802	1.006066	-0.183065

AcO-Au-PPh_3

Standard orientation:

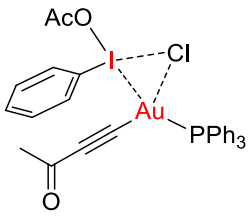
Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.448200	-0.498663	0.341093
2	8	0	-3.733589	0.924918	-0.756566
3	6	0	-4.193040	0.011984	-0.066487
4	8	0	-3.480907	-0.858231	0.606522
5	6	0	-5.694734	-0.185204	0.094304
6	1	0	-5.994778	0.133092	1.098614
7	1	0	-5.955971	-1.242042	-0.004298
8	1	0	-6.233219	0.410221	-0.644311
9	6	0	0.927898	1.784108	-0.423396
10	6	0	1.119027	4.494489	-1.100127
11	6	0	-0.073539	3.802558	-1.317003
12	6	0	1.341759	-0.077096	2.721616
13	6	0	2.427632	-0.368401	-2.283785
14	6	0	2.152242	-0.252228	3.842484
15	6	0	2.605547	-2.472542	-3.466616
16	6	0	1.680674	-3.044065	-2.589916
17	6	0	3.198470	-0.679974	1.286476
18	6	0	1.502178	-0.937970	-1.396797
19	6	0	4.004568	-0.858479	2.412334
20	6	0	-0.176599	2.452294	-0.978850
21	6	0	2.122168	2.487446	-0.197772
22	6	0	2.215749	3.836801	-0.538512
23	6	0	1.126855	-2.280867	-1.563018
24	6	0	2.975496	-1.135562	-3.313596
25	6	0	1.861307	-0.282243	1.433585
26	6	0	3.484405	-0.643111	3.689444
27	15	0	0.760459	0.004748	-0.007076
28	1	0	-0.933667	4.312493	-1.739781
29	1	0	-1.119895	1.931916	-1.126891
30	1	0	2.972390	1.988108	0.256685
31	1	0	0.301396	0.211213	2.843105
32	1	0	4.112724	-0.786708	4.563658
33	1	0	0.391971	-2.722253	-0.895613
34	1	0	3.686705	-0.684461	-3.999363
35	1	0	1.380808	-4.080591	-2.711449
36	1	0	2.711677	0.673833	-2.181110
37	1	0	1.191820	5.547119	-1.357972
38	1	0	3.607793	-0.860544	0.297529
39	1	0	5.037418	-1.171237	2.289830
40	1	0	3.029572	-3.065210	-4.271930
41	1	0	1.740336	-0.092227	4.834395
42	1	0	3.141421	4.375278	-0.357153



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-2.379106	-3.478287	-1.106695
2	1	0	-2.394921	0.969361	1.119211
3	1	0	-0.330411	-2.077074	-1.130691
4	1	0	-4.425088	-2.677430	0.057290
5	1	0	-4.424921	-0.457960	1.179770
6	53	0	0.520309	0.749489	-0.037541
7	6	0	-1.229309	-1.725968	-0.641769
8	6	0	-3.534530	-0.815551	0.671900
9	6	0	-3.531981	-2.060309	0.041856
10	6	0	-2.384578	-2.512171	-0.611163
11	6	0	-2.391518	-0.010681	0.657367
12	6	0	-1.269516	-0.494171	-0.000362
13	1	0	3.419645	-2.918108	-0.595460
14	1	0	4.712535	-1.999809	0.233686
15	1	0	3.398636	-2.781451	1.163539
16	6	0	3.652688	-2.253037	0.240549
17	8	0	3.319317	0.139627	0.066672
18	6	0	2.830552	-0.982018	0.134466
19	8	0	1.528685	-1.208078	0.125912
20	17	0	-0.987507	2.904051	-0.201690

TS_3

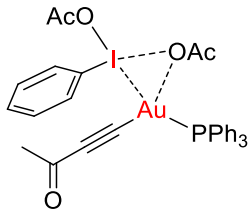


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-6.654292	2.350001	-2.019969
2	1	0	-3.071268	-3.300953	-3.780407
3	6	0	2.674853	3.910272	-0.438650
4	6	0	-3.645170	1.413800	-0.716637
5	6	0	-5.012380	3.691423	-1.622181
6	6	0	-3.702808	3.802413	-1.151319
7	6	0	-2.931505	-1.908795	-2.147642
8	6	0	-4.182339	0.578146	2.276006
9	6	0	-3.496887	-2.983341	-2.833156

10	6	0	-3.795410	-0.522854	4.396837
11	6	0	-2.796868	-1.302628	3.807137
12	6	0	-4.561602	-2.181823	-0.378076
13	6	0	-3.182918	-0.202929	1.678480
14	6	0	-5.121423	-3.260333	-1.064812
15	6	0	2.382323	5.171567	-1.228804
16	6	0	0.932452	1.898424	-0.482025
17	6	0	1.693342	2.861369	-0.486953
18	6	0	-3.018484	2.670530	-0.706666
19	6	0	-4.960729	1.309764	-1.196499
20	6	0	-5.638314	2.443520	-1.646915
21	6	0	-2.484397	-1.142368	2.458225
22	6	0	-4.484270	0.417530	3.630530
23	6	0	-3.467755	-1.489963	-0.920080
24	6	0	-4.592631	-3.659930	-2.293537
25	79	0	-0.187260	0.245097	-0.336681
26	8	0	3.712281	3.789894	0.213819
27	15	0	-2.703563	-0.039601	-0.090899
28	1	0	-3.206920	4.768664	-1.139517
29	1	0	2.228770	4.926512	-2.285433
30	1	0	-1.991037	2.758339	-0.365510
31	1	0	-5.453440	0.343119	-1.225132
32	1	0	-2.061341	-1.403867	-2.556264
33	1	0	-5.026628	-4.502654	-2.824064
34	1	0	-1.698274	-1.741781	2.006492
35	1	0	-5.258953	1.029412	4.084033
36	1	0	-2.254554	-2.033584	4.400066
37	1	0	-4.723920	1.311742	1.688030
38	1	0	-5.540698	4.572199	-1.976016
39	1	0	-4.972050	-1.881873	0.581014
40	1	0	-5.967841	-3.790014	-0.636856
41	1	0	-4.032058	-0.645727	5.449948
42	1	0	3.212006	5.873073	-1.123954
43	1	0	1.455407	5.632503	-0.870063
44	6	0	3.071059	-0.443838	1.529314
45	6	0	3.478815	0.852141	1.833827
46	6	0	2.917691	-1.048434	3.835199
47	6	0	3.339124	0.238209	4.178777
48	6	0	3.616962	1.178960	3.185528
49	6	0	2.780354	-1.406949	2.493234
50	53	0	2.883443	-1.012439	-0.523280
51	1	0	3.933854	2.183348	3.448520
52	1	0	3.445087	0.509477	5.225034
53	1	0	2.437155	-2.395643	2.211652
54	1	0	3.670005	1.605320	1.076238
55	1	0	2.694452	-1.778758	4.606945
56	1	0	7.232248	-1.342938	-2.957483
57	1	0	7.271504	0.004450	-1.781534
58	1	0	7.467461	-1.653876	-1.207585
59	8	0	5.064113	-0.874522	-0.547572
60	6	0	5.457227	-1.138607	-1.781777
61	8	0	4.684175	-1.429730	-2.685106
62	6	0	6.961869	-1.030848	-1.949172
63	17	0	0.136721	-2.392800	-0.101844

TS_3‘



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-6.184986	3.267929	1.251027
2	1	0	-4.696844	-1.553027	-3.721973
3	6	0	3.012006	3.565199	-2.284973
4	6	0	-3.171941	1.765017	0.713027
5	6	0	-4.273015	4.257985	1.386027
6	6	0	-2.890010	4.115026	1.263027
7	6	0	-3.695865	-0.840998	-1.958973
8	6	0	-2.600885	-0.161966	3.125027
9	6	0	-4.697845	-1.538027	-2.635973
10	6	0	-1.699829	-2.063940	4.321027
11	6	0	-1.238814	-2.598926	3.115027
12	6	0	-4.661845	-1.530026	0.156027
13	6	0	-2.141869	-0.695953	1.913027
14	6	0	-5.658824	-2.226056	-0.526973
15	6	0	2.630977	4.531187	-3.389973
16	6	0	1.151056	1.838144	-1.476973
17	6	0	1.996033	2.646169	-1.847973
18	6	0	-2.341974	2.878042	0.922027
19	6	0	-4.561946	1.918977	0.834027
20	6	0	-5.106982	3.159961	1.167027
21	6	0	-1.450833	-1.921932	1.915027
22	6	0	-2.378865	-0.844959	4.324027
23	6	0	-3.678866	-0.822998	-0.555973
24	6	0	-5.680824	-2.227056	-1.923973
25	79	0	-0.187904	0.485105	-0.900973
26	8	0	4.140006	3.563232	-1.790973
27	15	0	-2.377894	0.155041	0.295027
28	1	0	-2.236035	4.967045	1.421027
29	1	0	2.311994	3.975178	-4.278973
30	1	0	-1.266971	2.776073	0.802027
31	1	0	-5.220921	1.074957	0.659027
32	1	0	-2.903879	-0.352975	-2.517973
33	1	0	-6.454808	-2.773079	-2.454973
34	1	0	-1.073821	-2.329921	0.980027
35	1	0	-2.738877	-0.421970	5.257027
36	1	0	-0.708786	-3.546910	3.108027
37	1	0	-3.130913	0.785018	3.138027
38	1	0	-4.701043	5.223972	1.641027
39	1	0	-4.641844	-1.545026	1.241027
40	1	0	-6.413808	-2.772078	0.031027
41	1	0	-1.529814	-2.593935	5.254027
42	1	0	3.484959	5.166212	-3.631973

43	1	0	1.779959	5.146162	-3.076973
44	6	0	3.081094	0.561201	1.263027
45	6	0	3.889065	1.545224	0.700027
46	6	0	3.343066	1.498208	3.455027
47	6	0	4.162037	2.493232	2.913027
48	6	0	4.428036	2.518240	1.543027
49	6	0	2.785095	0.523192	2.627027
50	53	0	2.235139	-0.971824	0.032027
51	1	0	5.042014	3.299258	1.107027
52	1	0	4.585015	3.255245	3.561027
53	1	0	2.139117	-0.243827	3.039027
54	1	0	4.079063	1.604230	-0.363973
55	1	0	3.129067	1.482202	4.519027
56	1	0	5.147235	-4.266739	1.695027
57	1	0	5.056261	-5.136741	0.130027
58	1	0	6.075218	-3.678712	0.313027
59	8	0	3.949173	-2.128774	0.798027
60	6	0	3.967207	-3.293773	0.176027
61	8	0	3.141217	-3.632798	-0.659973
62	6	0	5.139232	-4.160739	0.608027
63	1	0	-1.176768	-4.155924	-2.331973
64	1	0	-0.534785	-3.581905	-3.895973
65	1	0	0.568229	-4.038873	-2.558973
66	8	0	-0.142831	-2.015894	-1.024973
67	6	0	-0.416827	-2.142902	-2.284973
68	8	0	-0.691855	-1.187910	-3.032973
69	6	0	-0.386785	-3.570901	-2.814973

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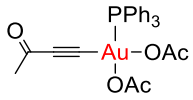
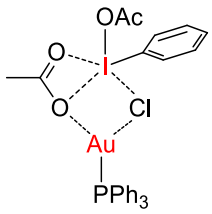


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.390658	1.740969	-0.484041
2	6	0	-0.261515	2.495902	-0.306041
3	6	0	0.732901	5.037130	-0.916041
4	6	0	1.319074	4.286265	0.106959
5	6	0	-2.216989	0.202453	-2.265041
6	6	0	-1.577422	2.086600	2.552959
7	6	0	-3.340950	0.032195	-3.071041
8	6	0	-2.248144	0.877446	4.538959
9	6	0	-2.082866	-0.333516	3.861959
10	6	0	-3.661099	0.682122	-0.367041
11	6	0	-1.407142	0.869639	1.871959
12	6	0	-4.780058	0.501865	-1.181041
13	6	0	5.388735	1.406198	-1.569041
14	6	0	2.230014	0.188474	-0.298041
15	6	0	3.228855	0.881703	-0.390041

16	6	0	0.827365	3.019152	0.412959
17	6	0	-0.848689	3.253767	-1.332041
18	6	0	-0.347980	4.521882	-1.631041
19	6	0	-1.664863	-0.346420	2.532959
20	6	0	-1.998421	2.084503	3.882959
21	6	0	-2.374066	0.536417	-0.909041
22	6	0	-4.621984	0.180901	-2.531041
23	79	0	0.643281	-0.975891	-0.151041
24	8	0	4.540441	2.687004	0.281959
25	15	0	-0.905137	0.845754	0.118959
26	8	0	2.017654	-2.601575	1.890959
27	8	0	-0.992425	-2.256266	0.079959
28	6	0	2.303771	-3.111510	0.806959
29	6	0	-1.345283	-2.876347	-1.028041
30	8	0	1.905669	-2.665601	-0.360041
31	8	0	-0.843331	-2.665232	-2.130041
32	6	0	-2.461052	-3.882603	-0.808041
33	6	0	3.181056	-4.350308	0.695959
34	1	0	2.168985	4.674460	0.657959
35	1	0	5.778967	0.393288	-1.420041
36	1	0	1.298497	2.440260	1.198959
37	1	0	-1.690600	2.864574	-1.892041
38	1	0	-1.227956	0.059680	-2.685041
39	1	0	-5.494952	0.039701	-3.161041
40	1	0	-1.547647	-1.287393	2.006959
41	1	0	-2.127637	3.027474	4.403959
42	1	0	-2.276650	-1.273561	4.369959
43	1	0	-1.384638	3.028644	2.053959
44	1	0	1.121675	6.023219	-1.154041
45	1	0	-3.792157	0.934092	0.678959
46	1	0	-5.773084	0.613637	-0.758041
47	1	0	-2.570145	0.880372	5.575959
48	1	0	6.207569	2.127386	-1.553041
49	1	0	4.897732	1.418086	-2.548041
50	1	0	-3.215890	-0.227776	-4.117041
51	1	0	-0.807114	5.102777	-2.425041
52	1	0	-2.161883	-4.616534	-0.055041
53	1	0	-2.699936	-4.387658	-1.744041
54	1	0	-3.350169	-3.369807	-0.429041
55	1	0	4.102999	-4.102097	0.159959
56	1	0	2.668234	-5.126426	0.121959
57	1	0	3.426141	-4.723252	1.690959

TS_1

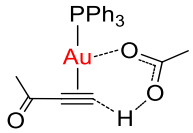


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.773939	-0.181966	-0.489997
2	6	0	-6.252169	3.070799	1.140003
3	6	0	-5.197133	1.979834	1.115003
4	6	0	6.157969	-1.053787	-2.340997
5	6	0	4.611922	0.341162	-3.568997
6	6	0	3.763921	0.378133	-2.462997
7	6	0	5.314967	-1.014815	-1.227997
8	6	0	5.808946	-0.374798	-3.509997
9	6	0	4.112943	-0.293855	-1.279997
10	6	0	3.018062	-3.865892	1.963003
11	6	0	4.767019	-2.568833	3.015003
12	6	0	4.446983	-1.476844	2.207003
13	6	0	2.691026	-2.775902	1.156003
14	6	0	4.055059	-3.763857	2.893003
15	6	0	3.409986	-1.574879	1.267003
16	6	0	5.075831	3.054177	1.653003
17	6	0	2.874831	3.073104	2.653003
18	6	0	2.532869	1.934092	1.926003
19	6	0	4.739870	1.909166	0.927003
20	6	0	4.146812	3.636146	2.517003
21	6	0	3.465889	1.338123	1.062003
22	15	0	2.969939	-0.180893	0.154003
23	6	0	-5.934962	-3.147190	-0.962997
24	6	0	-5.903977	-2.691189	1.413003
25	6	0	-5.040013	-1.614161	1.204003
26	6	0	-5.075998	-2.068162	-1.185997
27	6	0	-6.347951	-3.457204	0.333003
28	6	0	-4.638023	-1.315147	-0.096997
29	53	0	-3.294078	0.338898	-0.427997
30	6	0	-1.162153	2.581969	-0.844997
31	6	0	-0.165191	3.734002	-0.872997
32	8	0	-0.768114	1.425982	-1.223997
33	8	0	-4.961120	1.596842	-0.148997
34	8	0	-4.651118	1.530852	2.102003
35	8	0	-2.337160	2.806930	-0.462997
36	17	0	-1.291009	-1.723035	-0.790997
37	1	0	-5.806200	3.994814	0.762003
38	1	0	-7.090161	2.814771	0.488003
39	1	0	-6.593174	3.217788	2.165003
40	1	0	6.464947	-0.410777	-4.374997
41	1	0	7.083987	-1.618756	-2.293997
42	1	0	4.330905	0.862152	-4.478997

43	1	0	2.823903	0.921102	-2.516997
44	1	0	5.588985	-1.553806	-0.326997
45	1	0	4.302087	-4.610849	3.527003
46	1	0	2.453093	-4.787910	1.873003
47	1	0	5.567016	-2.482807	3.744003
48	1	0	4.996952	-0.546826	2.318003
49	1	0	1.867028	-2.847930	0.452003
50	1	0	4.408782	4.529155	3.077003
51	1	0	6.062817	3.493210	1.538003
52	1	0	2.144816	3.526079	3.317003
53	1	0	1.537883	1.509059	2.020003
54	1	0	5.465884	1.469190	0.251003
55	1	0	-7.016923	-4.296226	0.502003
56	1	0	-6.278942	-3.741202	-1.804997
57	1	0	-6.225969	-2.932200	2.422003
58	1	0	-4.700033	-1.006149	2.035003
59	1	0	-4.748006	-1.830151	-2.191997
60	1	0	-0.664223	4.684986	-0.683997
61	1	0	0.341808	3.761019	-1.841997
62	1	0	0.601814	3.571028	-0.107997

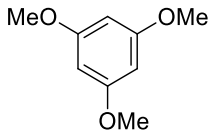
TS_2



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-4.126552	-3.903750	1.224958
2	1	0	-4.483557	-3.873806	-0.500042
3	1	0	-3.365362	-5.116631	0.147958
4	1	0	3.062244	-2.607621	-4.650042
5	1	0	-0.085598	2.755884	-0.430042
6	1	0	3.803651	1.165495	0.583958
7	1	0	4.734292	3.453642	0.591958
8	1	0	0.865044	5.032034	-0.434042
9	1	0	3.269987	5.396412	0.076958
10	1	0	3.498095	-1.659553	0.309958
11	1	0	0.366843	-0.051044	2.792958
12	1	0	1.388012	-1.126884	4.772958
13	1	0	4.508265	-2.740394	2.289958
14	1	0	3.461224	-2.477558	4.527958
15	1	0	0.490220	-2.452025	-1.208042
16	1	0	3.126701	0.848389	-2.099042
17	1	0	3.944890	-0.351482	-4.097042
18	1	0	1.337408	-3.651892	-3.191042
19	6	0	-3.696524	-4.080683	0.233958
20	8	0	-1.390604	-3.575321	-0.215042
21	6	0	-2.514670	-3.157497	0.006958

22	6	0	-2.840893	-1.732548	0.069958
23	6	0	-3.485061	-0.666650	0.110958
24	79	0	-1.240164	-0.009297	0.039958
25	15	0	1.101818	0.103071	-0.007042
26	6	0	1.806552	1.796182	0.033958
27	6	0	2.861145	4.389347	0.063958
28	6	0	0.976380	2.895051	-0.241042
29	6	0	3.162519	2.007395	0.340958
30	6	0	3.686316	3.298477	0.351958
31	6	0	1.512177	4.185135	-0.227042
32	6	0	1.873955	-0.763808	1.418958
33	6	0	3.019148	-1.996628	3.659958
34	6	0	3.040075	-1.530625	1.284958
35	6	0	1.280933	-0.627901	2.683958
36	6	0	1.855029	-1.236811	3.797958
37	6	0	3.608171	-2.143535	2.403958
38	6	0	1.767948	-0.724824	-1.505042
39	6	0	1.259148	-1.995904	-1.827042
40	6	0	2.736856	-0.137672	-2.330042
41	6	0	3.198963	-0.816600	-3.460042
42	6	0	1.734254	-2.669830	-2.951042
43	6	0	2.702162	-2.082678	-3.770042
44	1	0	-3.982237	0.453272	0.110958
45	8	0	-4.370445	1.781211	0.068958
46	6	0	-3.395571	2.581365	-0.070042
47	6	0	-3.732803	4.058312	-0.244042
48	1	0	-3.692842	4.307318	-1.311042
49	1	0	-2.996901	4.680427	0.269958
50	1	0	-4.738836	4.270154	0.123958
51	8	0	-2.168521	2.263557	-0.101042

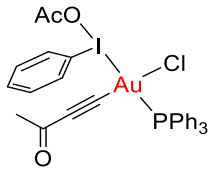


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.005740	-1.373124	1.675178
2	6	0	-2.974627	-2.284244	4.142178
3	6	0	-1.128671	-1.933015	2.616178
4	6	0	-3.375754	-1.267294	1.984178
5	6	0	-3.853697	-1.726353	3.210178
6	6	0	-1.615615	-2.384075	3.844178
7	6	0	-2.344003	0.741834	-0.279822
8	6	0	-3.873290	3.052644	-0.735822
9	6	0	-2.575117	1.658806	0.758178
10	6	0	-2.877035	1.001768	-1.551822
11	6	0	-3.635178	2.153674	-1.776822
12	6	0	-3.338259	2.804711	0.531178
13	6	0	-1.902666	-1.970111	-1.255822
14	6	0	-2.671453	-3.687206	-3.326822

15	6	0	-1.236671	-1.931028	-2.491822
16	6	0	-2.947553	-2.883241	-1.059822
17	6	0	-3.327447	-3.738288	-2.095822
18	6	0	-1.626565	-2.782077	-3.523822
19	15	0	-1.387812	-0.800047	0.051178
20	6	0	1.212830	2.084276	1.273178
21	6	0	0.134673	3.351142	-1.044822
22	6	0	0.534683	3.273192	1.407178
23	6	0	1.412908	1.456301	-0.046822
24	6	0	0.791823	2.146224	-1.187822
25	6	0	0.013604	3.905127	0.251178
26	8	0	1.793912	1.423348	2.268178
27	8	0	0.987899	1.528248	-2.347822
28	8	0	-0.591539	5.060052	0.491178
29	6	0	1.816842	1.991351	3.588178
30	6	0	-1.130637	5.850985	-0.583822
31	6	0	0.579821	2.158197	-3.575822
32	79	0	1.087177	-0.704740	-0.002822
33	6	0	3.091189	-0.805491	-0.084822
34	6	0	4.305181	-0.740340	-0.160822
35	6	0	5.757168	-0.635160	-0.254822
36	8	0	6.286032	0.461906	-0.329822
37	6	0	6.531329	-1.933064	-0.253822
38	17	0	1.009475	-3.109749	0.072178
39	1	0	-0.075657	-2.041884	2.387178
40	1	0	-4.066809	-0.822380	1.276178
41	1	0	-4.912707	-1.645485	3.438178
42	1	0	-0.929561	-2.818990	4.564178
43	1	0	-3.350583	-2.639291	5.097178
44	1	0	-2.189093	1.466854	1.754178
45	1	0	-2.732947	0.291786	-2.359822
46	1	0	-4.063200	2.329621	-2.758822
47	1	0	-3.529345	3.493687	1.349178
48	1	0	-4.491399	3.929568	-0.903822
49	1	0	-0.400755	-1.252924	-2.641822
50	1	0	-3.453545	-2.944304	-0.102822
51	1	0	-4.130358	-4.450388	-1.934822
52	1	0	-1.101569	-2.753011	-4.473822
53	1	0	-2.966370	-4.359243	-4.126822
54	1	0	0.401621	3.773175	2.357178
55	1	0	-0.291390	3.859089	-1.895822
56	1	0	2.309721	2.968412	3.576178
57	1	0	2.391929	1.292422	4.192178
58	1	0	0.801831	2.082225	3.987178
59	1	0	-0.339673	6.140083	-1.281822
60	1	0	-1.540748	6.738934	-0.105822
61	1	0	-1.923570	5.303887	-1.100822
62	1	0	1.077701	3.125259	-3.692822
63	1	0	-0.507194	2.280062	-3.599822
64	1	0	0.897905	1.481237	-4.366822
65	1	0	7.598303	-1.720931	-0.326822
66	1	0	6.213407	-2.560103	-1.093822
67	1	0	6.320399	-2.497090	0.661178
68	1	0	2.489920	1.365435	-0.235822

INT_3

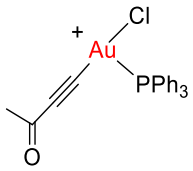


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.380023	3.718115	-1.057053
2	1	0	2.205031	2.069100	4.320947
3	6	0	-0.349980	4.174087	0.151947
4	6	0	3.157035	1.136104	-1.020053
5	6	0	3.994025	3.260108	-2.645053
6	6	0	2.976029	2.407103	-3.080053
7	6	0	2.392036	1.024100	2.453947
8	6	0	4.520048	-1.616889	-1.591053
9	6	0	2.771034	1.333102	3.759947
10	6	0	5.018060	-3.974887	-1.386053
11	6	0	4.068060	-4.088891	-0.369053
12	6	0	4.219043	-0.563891	2.304947
13	6	0	3.567049	-1.722894	-0.565053
14	6	0	4.587042	-0.254889	3.615947
15	6	0	-0.032983	4.941089	-1.118053
16	6	0	-0.197967	1.515088	-0.017053
17	6	0	-0.256973	2.733088	0.060947
18	6	0	2.553034	1.354101	-2.269053
19	6	0	4.178031	1.996109	-0.589053
20	6	0	4.591026	3.054111	-1.400053
21	6	0	3.337055	-2.972895	0.036947
22	6	0	5.240054	-2.739886	-1.997053
23	6	0	3.119040	0.075104	1.712947
24	6	0	3.867037	0.692108	4.343947
25	79	0	-0.017957	-0.461911	-0.087053
26	8	0	-0.670982	4.735086	1.190947
27	15	0	2.588042	-0.281899	-0.007053
28	1	0	2.505028	2.565101	-4.045053
29	1	0	0.957018	4.664093	-1.496053
30	1	0	1.748037	0.707097	-2.602053
31	1	0	4.646032	1.842111	0.377947
32	1	0	1.536033	1.524096	2.010947
33	1	0	4.155036	0.928109	5.364947
34	1	0	2.579056	-3.077899	0.803947
35	1	0	5.977053	-2.646882	-2.790053
36	1	0	3.881065	-5.048892	0.100947
37	1	0	4.704044	-0.659888	-2.068053
38	1	0	4.318021	4.084110	-3.274053
39	1	0	4.785047	-1.302888	1.748947
40	1	0	5.439044	-0.757885	4.064947
41	1	0	5.580064	-4.848884	-1.706053
42	1	0	-0.074989	6.013088	-0.916053
43	1	0	-0.757982	4.683085	-1.898053

44	6	0	-3.602965	1.063071	0.001947
45	6	0	-3.329969	1.887073	1.087947
46	6	0	-4.858973	2.797065	-1.074053
47	6	0	-4.587977	3.646067	0.000947
48	6	0	-3.825975	3.193070	1.077947
49	6	0	-4.362967	1.492068	-1.083053
50	53	0	-2.883955	-0.963925	-0.006053
51	1	0	-3.594978	3.854071	1.906947
52	1	0	-4.970982	4.662065	-0.001053
53	1	0	-4.584963	0.823067	-1.907053
54	1	0	-2.726967	1.538076	1.917947
55	1	0	-5.458975	3.145062	-1.910053
56	1	0	-7.400947	-2.566947	-0.772053
57	1	0	-6.927939	-4.110945	0.005947
58	1	0	-7.332946	-2.673947	0.987947
59	8	0	-5.241953	-1.301937	0.013947
60	6	0	-5.396947	-2.592937	0.043947
61	8	0	-4.482943	-3.419933	0.062947
62	6	0	-6.864945	-3.023944	0.063947
63	17	0	-0.050945	-2.867911	-0.182053

INT_4

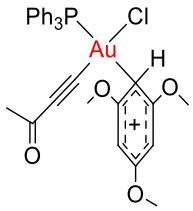


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.682844	-0.481012	-0.157810
2	6	0	0.525585	1.923175	-0.404410
3	6	0	2.246299	3.988359	-1.153555
4	6	0	2.680277	3.017982	-0.241664
5	6	0	-2.192290	0.578800	-2.155623
6	6	0	-0.281513	1.641675	2.712169
7	6	0	-3.387568	0.711627	-2.850328
8	6	0	-1.231437	0.589003	4.671929
9	6	0	-1.767428	-0.433970	3.881896
10	6	0	-3.358509	1.095556	-0.068559
11	6	0	-0.825791	0.612361	1.913764
12	6	0	-4.548544	1.229414	-0.781414
13	6	0	5.770518	-1.437777	-0.563109
14	6	0	2.109811	-1.183559	-0.386315
15	6	0	3.299086	-0.912076	-0.305998
16	6	0	1.828331	1.986692	0.133152
17	6	0	0.095465	2.898392	-1.333698
18	6	0	0.958284	3.928809	-1.693414
19	6	0	-1.564427	-0.435071	2.505390
20	6	0	-0.495700	1.623570	4.086944

21	6	0	-2.174846	0.781598	-0.761078
22	6	0	-4.564956	1.034831	-2.165168
23	79	0	0.184941	-1.603614	-0.390881
24	15	0	-0.624344	0.659144	0.132885
25	1	0	3.688531	3.034999	0.154659
26	1	0	5.688728	-2.365057	0.015567
27	1	0	2.191338	1.222832	0.808628
28	1	0	-0.902810	2.864924	-1.750607
29	1	0	-1.286068	0.299263	-2.685002
30	1	0	-5.497842	1.128552	-2.711003
31	1	0	-1.959543	-1.241942	1.895357
32	1	0	-0.086470	2.418613	4.701759
33	1	0	-2.333087	-1.238893	4.338636
34	1	0	0.280395	2.452575	2.264768
35	1	0	2.919310	4.786810	-1.450686
36	1	0	-3.352030	1.240812	1.004805
37	1	0	-5.462091	1.481051	-0.254467
38	1	0	-1.384779	0.577853	5.746286
39	1	0	6.745209	-0.977357	-0.396301
40	1	0	5.657250	-1.708872	-1.618318
41	1	0	-3.407512	0.549517	-3.922917
42	1	0	0.624759	4.683776	-2.397186
43	17	0	-1.959861	-2.592055	-0.381820
44	8	0	4.891024	0.637948	0.291834

INT_5

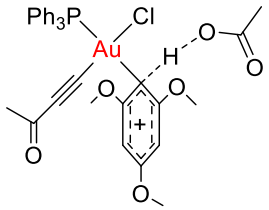


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	0.777030	-3.002218	0.467620
2	1	0	3.038744	4.685369	-1.984412
3	1	0	0.770091	2.790586	4.059734
4	1	0	6.355034	-3.259290	-1.138192
5	1	0	4.951960	1.877099	3.632772
6	1	0	4.487046	0.693990	1.521025
7	1	0	1.979895	4.159548	-4.169387
8	1	0	3.731114	-0.101907	-2.384996
9	1	0	5.203933	-3.360098	1.062462
10	1	0	5.605468	-1.628502	-2.856768
11	1	0	3.309035	-1.861915	1.541015
12	1	0	3.098566	2.922391	4.916809
13	1	0	0.289130	1.621678	1.941718
14	1	0	3.035866	3.012206	-0.166680
15	1	0	0.878515	0.272030	-2.710997

16	1	0	0.907427	1.946189	-4.528461
17	15	0	2.009200	0.252158	-0.012275
18	6	0	2.890979	2.407282	3.983971
19	6	0	2.353030	1.067885	1.583588
20	6	0	5.104612	-1.676721	-1.895056
21	6	0	3.813715	-1.796864	0.584265
22	6	0	2.569731	3.719523	-2.144517
23	6	0	2.568928	2.774889	-1.116652
24	6	0	1.359517	1.232846	-2.551029
25	6	0	3.932424	1.819082	3.264801
26	6	0	3.393815	-0.863940	-0.383416
27	6	0	3.670420	1.149736	2.069170
28	6	0	4.882252	-2.646191	0.311056
29	6	0	5.526457	-2.590110	-0.927694
30	6	0	1.581669	2.332081	3.503304
31	6	0	4.041540	-0.814510	-1.629712
32	6	0	1.308379	1.665482	2.310157
33	6	0	1.371260	2.178494	-3.574836
34	6	0	1.974511	3.423120	-3.371663
35	6	0	1.965138	1.524922	-1.318048
36	79	0	-0.210330	-0.854673	0.119888
37	6	0	-1.087999	0.910972	-0.141214
38	6	0	-1.690885	1.963578	-0.263012
39	6	0	-2.437418	3.203249	-0.394437
40	8	0	-3.574636	3.300198	0.047503
41	6	0	-1.734598	4.343804	-1.093604
42	1	0	-0.821706	4.610844	-0.549528
43	1	0	-2.400589	5.205746	-1.151716
44	1	0	-1.424541	4.035584	-2.098083
45	6	0	-2.240179	-1.881524	0.289999
46	6	0	-2.979327	-1.188869	1.338718
47	6	0	-2.829217	-1.852936	-1.046776
48	6	0	-3.911117	-1.052725	-1.331555
49	1	0	-4.348334	-0.976945	-2.317437
50	6	0	-4.064945	-0.384330	1.053381
51	1	0	-4.569180	0.173712	1.827057
52	6	0	-4.507530	-0.301297	-0.287595
53	8	0	-2.214636	-2.654358	-1.920703
54	8	0	-2.493973	-1.405682	2.562984
55	8	0	-5.527504	0.450621	-0.673281
56	6	0	-2.708497	-2.733725	-3.264102
57	1	0	-3.745850	-3.082686	-3.275552
58	1	0	-2.069016	-3.457531	-3.766851
59	1	0	-2.636008	-1.761561	-3.762923
60	6	0	-3.124447	-0.788148	3.693163
61	1	0	-4.167745	-1.108375	3.777341
62	1	0	-3.070475	0.302823	3.619070
63	1	0	-2.563202	-1.129447	4.561533
64	6	0	-6.186672	1.331343	0.259887
65	1	0	-6.655622	0.756435	1.063984
66	1	0	-6.955673	1.834680	-0.323943
67	1	0	-5.469602	2.059523	0.644714
68	1	0	-1.823008	-2.842259	0.584860

TS_4

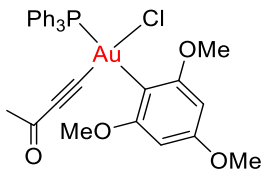


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	5.103065	3.761941	-1.273010
2	1	0	1.678034	2.025003	4.474990
3	1	0	5.448910	-4.852065	-1.104010
4	1	0	5.502000	0.125934	3.939990
5	1	0	4.834987	-0.595054	1.679990
6	1	0	4.163981	-0.900042	-2.179010
7	1	0	4.085912	-4.736040	0.972990
8	1	0	5.472945	-2.927065	-2.678010
9	1	0	2.754948	-2.724016	1.471990
10	1	0	3.927023	1.430962	5.353990
11	1	0	1.007021	1.327015	2.207990
12	1	0	4.358034	2.028955	0.318990
13	1	0	1.609007	0.510004	-2.643010
14	1	0	2.378038	2.232990	-4.233010
15	1	0	-0.589916	4.779044	1.827990
16	1	0	-0.364892	6.116040	0.657990
17	1	0	4.122067	3.869959	-3.554010
18	1	0	-4.231964	2.153110	-1.568010
19	1	0	-4.432996	0.384113	2.351990
20	1	0	-3.494974	1.572096	-3.644010
21	1	0	-1.795977	1.439066	-4.170010
22	1	0	-2.232956	2.601074	-2.880010
23	1	0	-4.129039	-1.999892	2.809990
24	1	0	-3.194017	-0.803909	3.783990
25	1	0	-2.571047	-2.458920	3.559990
26	1	0	-6.576980	1.237152	2.067990
27	1	0	-6.873949	2.973157	1.773990
28	1	0	-5.426958	2.465131	2.686990
29	1	0	0.949087	4.945016	0.986990
30	17	0	0.050946	-2.821968	-0.212010
31	15	0	2.383994	-0.178010	0.083990
32	79	0	-0.115010	-0.418965	-0.107010
33	8	0	-1.226919	4.637055	-1.221010
34	8	0	-2.154992	0.582072	-2.374010
35	8	0	-2.399026	-1.307923	1.909990
36	8	0	-5.417963	2.192131	0.612990
37	6	0	-3.134032	-1.651910	3.093990
38	6	0	3.633018	1.120968	4.355990
39	6	0	2.869003	0.309982	1.782990
40	6	0	4.879945	-2.883055	-1.769010
41	6	0	3.349948	-2.760027	0.566990
42	6	0	4.345052	3.045955	-1.575010

43	6	0	3.924035	2.066962	-0.674010
44	6	0	2.381019	1.210990	-2.341010
45	6	0	4.518004	0.386952	3.562990
46	6	0	3.371967	-1.663028	-0.314010
47	6	0	4.140997	-0.020041	2.282990
48	6	0	4.102927	-3.898041	0.283990
49	6	0	4.866926	-3.962055	-0.885010
50	6	0	2.370024	1.454991	3.862990
51	6	0	4.136966	-1.735041	-1.488010
52	6	0	1.986016	1.052997	2.583990
53	6	0	2.813037	2.186983	-3.239010
54	6	0	3.793054	3.105965	-2.857010
55	6	0	2.940018	1.141980	-1.054010
56	6	0	-0.266974	1.558038	-0.034010
57	6	0	-0.422953	2.766041	-0.098010
58	6	0	-0.645927	4.189045	-0.237010
59	6	0	-0.132911	5.072036	0.876990
60	6	0	-2.296010	-0.433925	-0.263010
61	6	0	-2.912010	-0.418914	1.061990
62	6	0	-2.783992	0.587084	-1.193010
63	6	0	-3.830977	1.422102	-0.879010
64	6	0	-3.959995	0.430105	1.383990
65	6	0	-4.411978	1.336113	0.407990
66	6	0	-2.450973	1.623078	-3.319010
67	6	0	-6.107963	2.205144	1.871990
68	1	0	-5.938084	-4.500859	-0.992010
69	1	0	-5.000080	-4.286876	-2.502010
70	1	0	-4.357098	-5.279888	-1.195010
71	6	0	-4.938082	-4.375878	-1.414010
72	8	0	-3.226052	-2.721908	-1.471010
73	8	0	-4.650051	-2.703883	0.286990
74	6	0	-4.227060	-3.155890	-0.801010
75	1	0	-2.525029	-1.485921	-0.741010

INT_6



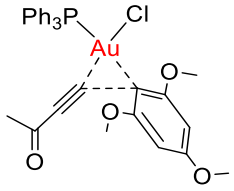
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	17	0	-0.449000	-2.778087	-0.289806
2	1	0	5.156964	3.511407	-1.132023
3	1	0	1.671370	1.789214	4.508110
4	1	0	4.983969	-4.839373	-1.754115
5	1	0	5.198300	-0.594560	3.888763
6	1	0	4.461466	-1.092529	1.585795
7	1	0	3.937138	4.103070	-3.215286

8	1	0	4.031769	-0.674444	-2.185507
9	1	0	3.434342	-4.992793	0.185165
10	1	0	5.267696	-2.672058	-2.939609
11	1	0	2.170245	-3.010402	0.924072
12	1	0	3.806705	0.844489	5.363107
13	1	0	0.931028	1.303049	2.202244
14	1	0	4.359169	1.653635	0.288437
15	1	0	1.095216	0.976808	-2.445850
16	1	0	1.907122	2.825854	-3.866736
17	15	0	2.074230	-0.238778	0.009991
18	6	0	3.484359	0.631739	4.347900
19	6	0	2.646910	0.074265	1.729125
20	6	0	4.596909	-2.745805	-2.088606
21	6	0	2.860942	-2.925498	0.093192
22	6	0	4.275323	2.949353	-1.426107
23	6	0	3.826194	1.899763	-0.624431
24	6	0	1.995466	1.514779	-2.165176
25	6	0	4.265597	-0.176703	3.521089
26	6	0	3.026791	-1.695115	-0.566289
27	6	0	3.851490	-0.456018	2.217667
28	6	0	3.570968	-4.047140	-0.330683
29	6	0	4.438192	-3.960837	-1.422172
30	6	0	2.285316	1.162450	3.867939
31	6	0	3.896556	-1.615354	-1.663866
32	6	0	1.863766	0.885133	2.567729
33	6	0	2.451980	2.561635	-2.965770
34	6	0	3.590255	3.280362	-2.596937
35	6	0	2.683528	1.172673	-0.990790
36	79	0	-0.459347	-0.384014	-0.084214
37	6	0	-0.612792	1.587170	0.080810
38	6	0	-0.716471	2.801582	0.138251
39	6	0	-0.829094	4.242930	0.210136
40	8	0	-0.748513	4.950856	-0.783201
41	6	0	-1.055326	4.821174	1.596393
42	1	0	-1.972551	4.410186	2.032230
43	1	0	-1.128152	5.908078	1.528453
44	1	0	-0.230121	4.543469	2.261791
45	6	0	-2.520201	-0.403171	-0.156448
46	6	0	-3.259741	-0.591442	1.005661
47	6	0	-3.173254	-0.255556	-1.383219
48	6	0	-4.567276	-0.320737	-1.451432
49	1	0	-5.109392	-0.223150	-2.382445
50	6	0	-4.663366	-0.661403	0.959555
51	1	0	-5.234461	-0.815833	1.863013
52	6	0	-5.299834	-0.527049	-0.277111
53	8	0	-2.373522	-0.056312	-2.472830
54	8	0	-2.545379	-0.696801	2.168393
55	8	0	-6.656232	-0.579680	-0.445430
56	6	0	-2.988633	0.081198	-3.743870
57	1	0	-3.553519	-0.818634	-4.017474
58	1	0	-2.175209	0.224966	-4.456580
59	1	0	-3.656178	0.951357	-3.777201
60	6	0	-3.233746	-1.022534	3.363184
61	1	0	-3.771269	-1.974807	3.272627
62	1	0	-3.941528	-0.235093	3.654797
63	1	0	-2.467777	-1.115706	4.134670
64	6	0	-7.469313	-0.798354	0.693354

65	1	0	-7.243874	-1.758459	1.176101
66	1	0	-8.498778	-0.813911	0.331101
67	1	0	-7.361546	0.007025	1.432152

TS_5

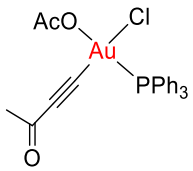


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.942885	-0.151488	-1.450771
2	6	0	-4.462210	-0.686768	-3.740794
3	6	0	-2.314203	-0.559106	-2.637244
4	6	0	-4.339177	-0.025305	-1.417011
5	6	0	-5.093950	-0.292076	-2.559963
6	6	0	-3.072690	-0.818983	-3.778130
7	6	0	-2.963322	-0.003721	1.489981
8	6	0	-4.590704	-0.402138	3.735844
9	6	0	-3.056772	-1.276773	2.076923
10	6	0	-3.687926	1.066868	2.039087
11	6	0	-4.498309	0.864989	3.157087
12	6	0	-3.871109	-1.468670	3.193633
13	6	0	-1.566191	2.021625	-0.062717
14	6	0	-0.943277	4.757342	-0.108644
15	6	0	-0.711608	2.574300	0.906575
16	6	0	-2.098149	2.853009	-1.058314
17	6	0	-1.786653	4.214565	-1.078441
18	6	0	-0.407169	3.934162	0.884972
19	15	0	-1.898121	0.215405	0.008884
20	6	0	2.256817	0.723377	1.358784
21	6	0	3.106711	1.959932	-1.016586
22	6	0	3.128906	1.805971	1.419978
23	6	0	1.824625	0.213354	0.113342
24	6	0	2.235207	0.864929	-1.064537
25	6	0	3.553797	2.413665	0.229891
26	8	0	1.761017	0.091043	2.453373
27	8	0	1.744623	0.352463	-2.226553
28	8	0	4.401889	3.465793	0.393808
29	6	0	2.345026	0.360888	3.723838
30	6	0	4.901308	4.126307	-0.759233
31	6	0	2.215158	0.873921	-3.461470
32	79	0	0.195385	-1.123547	0.020447
33	6	0	2.124297	-1.714473	0.038649
34	6	0	3.123049	-2.427881	0.071782
35	6	0	4.280144	-3.279667	0.103837
36	8	0	4.872820	-3.538366	1.146126

37	6	0	4.721400	-3.849100	-1.235388
38	1	0	-1.235981	-0.686111	-2.660276
39	1	0	-4.836801	0.269482	-0.498551
40	1	0	-6.175469	-0.198536	-2.524519
41	1	0	-2.579466	-1.141219	-4.690355
42	1	0	-5.052492	-0.900723	-4.627188
43	1	0	-2.500351	-2.109058	1.654788
44	1	0	-3.614820	2.057388	1.601926
45	1	0	-5.053715	1.699335	3.575965
46	1	0	-3.937159	-2.455948	3.641217
47	1	0	-5.219390	-0.556473	4.608272
48	1	0	-0.284462	1.939753	1.677044
49	1	0	-2.756294	2.441017	-1.815988
50	1	0	-2.207361	4.849379	-1.853119
51	1	0	0.257262	4.347485	1.637934
52	1	0	-0.702094	5.816344	-0.126982
53	1	0	3.490888	2.205479	2.358041
54	1	0	3.417234	2.450951	-1.926726
55	1	0	3.425596	0.181958	3.707490
56	1	0	1.871116	-0.331673	4.419661
57	1	0	2.148083	1.390897	4.046275
58	1	0	5.466328	3.441211	-1.403559
59	1	0	5.569304	4.906682	-0.392001
60	1	0	4.094276	4.587966	-1.342463
61	1	0	3.303934	0.777352	-3.549394
62	1	0	1.931087	1.926029	-3.589224
63	1	0	1.736877	0.276081	-4.238071
64	1	0	3.932787	-4.487283	-1.649072
65	1	0	5.633390	-4.432198	-1.094327
66	1	0	4.898105	-3.044992	-1.958076
67	17	0	-1.099272	-3.217485	-0.209475

INT_{5A}

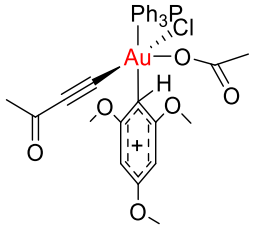


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	4.736712	-0.459386	-0.239131
2	6	0	0.818300	2.099158	-0.658357
3	6	0	2.722746	3.864437	-1.702915
4	6	0	3.040317	3.070239	-0.598808
5	6	0	-2.099135	0.573308	-2.173618
6	6	0	-0.295680	2.660012	2.266786
7	6	0	-3.241151	0.823050	-2.934143
8	6	0	-1.293850	2.137432	4.407938
9	6	0	-1.735735	0.911079	3.905598

10	6	0	-2.957795	2.032722	-0.428589
11	6	0	-0.736185	1.426817	1.761360
12	6	0	-4.096924	2.273323	-1.196267
13	6	0	5.657224	-1.501032	-0.837444
14	6	0	2.140924	-1.044477	-0.094256
15	6	0	3.331927	-0.802925	-0.173448
16	6	0	2.094194	2.191876	-0.074706
17	6	0	0.506312	2.896433	-1.772336
18	6	0	1.457757	3.777577	-2.286200
19	6	0	-1.461747	0.548931	2.587681
20	6	0	-0.577523	3.010270	3.587988
21	6	0	-1.952128	1.184218	-0.918223
22	6	0	-4.237842	1.671927	-2.448730
23	79	0	0.208933	-1.401091	0.101898
24	8	0	5.144799	0.619533	0.175061
25	15	0	-0.413311	0.941876	0.028486
26	8	0	-1.932941	-2.396694	-1.699979
27	6	0	-2.424100	-2.318449	-0.579419
28	8	0	-1.812827	-1.785786	0.462630
29	6	0	-3.812633	-2.835303	-0.246907
30	1	0	4.029800	3.098625	-0.156119
31	1	0	5.595907	-2.429419	-0.259155
32	1	0	2.365825	1.568198	0.767482
33	1	0	-0.471019	2.832902	-2.236100
34	1	0	-1.353044	-0.124376	-2.536707
35	1	0	-5.128265	1.857738	-3.042214
36	1	0	-1.811376	-0.402319	2.197443
37	1	0	-0.231999	3.964353	3.974449
38	1	0	-2.291360	0.228860	4.541706
39	1	0	0.267165	3.340673	1.638025
40	1	0	3.463847	4.544280	-2.113136
41	1	0	-2.853688	2.500475	0.544578
42	1	0	-4.874101	2.927759	-0.813153
43	1	0	-1.505789	2.411085	5.437358
44	1	0	6.682237	-1.126528	-0.840868
45	1	0	5.339352	-1.742094	-1.857831
46	1	0	-3.355552	0.338116	-3.898372
47	1	0	1.207875	4.391680	-3.146155
48	1	0	-4.333415	-3.111928	-1.163979
49	1	0	-4.383325	-2.080283	0.300684
50	1	0	-3.722224	-3.713629	0.399762
51	17	0	0.727114	-3.727054	0.432959

INT_{5B}

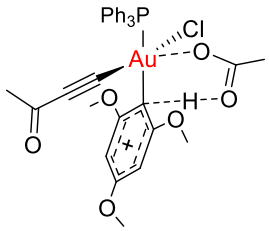


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.331466	-1.900773	-2.988814
2	6	0	-6.081426	0.173021	2.560746
3	6	0	-3.335155	1.593864	-3.015276
4	6	0	-4.611394	-0.003340	0.675321
5	6	0	-4.100401	-1.233275	1.127038
6	6	0	-4.194688	0.590096	-0.529590
7	6	0	-3.185456	-0.015614	-1.260773
8	6	0	-3.125872	-1.862334	0.352177
9	6	0	-2.499813	-1.197591	-0.768603
10	6	0	-0.705946	4.995189	0.369210
11	6	0	-1.554676	4.002007	-0.401075
12	6	0	-1.178598	2.614272	-0.288537
13	6	0	-0.876319	1.432882	-0.227005
14	6	0	2.354685	1.676948	-0.547731
15	6	0	3.024137	3.954519	-2.029281
16	6	0	2.372453	2.883110	-2.644456
17	6	0	0.992954	0.967594	2.934726
18	6	0	3.866193	-1.063904	-1.198136
19	6	0	1.134353	1.334557	4.273146
20	6	0	5.123036	-3.025969	-0.546603
21	6	0	4.440523	-3.061094	0.670628
22	6	0	3.382716	0.590391	2.792968
23	6	0	3.186963	-1.087926	0.029625
24	6	0	3.517168	0.958514	4.131755
25	6	0	2.027099	1.746242	-1.913595
26	6	0	3.004482	2.755082	0.072194
27	6	0	3.338137	3.889112	-0.670795
28	6	0	3.469847	-2.103671	0.958608
29	6	0	4.832937	-2.027870	-1.478354
30	6	0	2.116391	0.593824	2.182363
31	6	0	2.394173	1.329775	4.873677
32	6	0	-3.107895	-3.815753	1.724617
33	1	0	0.334383	4.935497	0.030994
34	1	0	-5.284871	0.061214	3.304866
35	1	0	-6.802608	0.913237	2.908148
36	1	0	-6.588702	-0.788157	2.418433
37	1	0	-2.595948	-4.775481	1.671533
38	1	0	-2.773562	-3.274249	2.615335
39	1	0	-4.192214	-3.975134	1.762163
40	1	0	-3.150403	2.464408	-2.378296

41	1	0	-2.836201	1.721885	-3.975586
42	1	0	-4.411171	1.461631	-3.178274
43	1	0	-4.514781	-1.720452	1.996537
44	1	0	-4.669833	1.510307	-0.839039
45	1	0	3.283590	4.838526	-2.605046
46	1	0	-1.093717	6.003929	0.216387
47	1	0	-0.710463	4.749043	1.436818
48	1	0	2.120186	2.933295	-3.699682
49	1	0	1.509643	0.909273	-2.381784
50	1	0	3.249009	2.719562	1.127811
51	1	0	0.011462	0.968137	2.472761
52	1	0	2.501075	1.609994	5.917606
53	1	0	2.926766	-2.154750	1.893882
54	1	0	5.355379	-1.999194	-2.429776
55	1	0	4.652540	-3.841890	1.394742
56	1	0	3.638397	-0.304355	-1.934085
57	1	0	4.259734	0.293519	2.227729
58	1	0	4.499656	0.949998	4.594409
59	1	0	5.874621	-3.777520	-0.770743
60	1	0	0.256987	1.617043	4.847284
61	1	0	3.843460	4.718710	-0.184562
62	8	0	-5.573131	0.678752	1.329693
63	8	0	-2.732538	-3.119025	0.540103
64	8	0	-2.764553	0.406516	-2.451702
65	8	0	-2.507353	4.362245	-1.086247
66	79	0	-0.385565	-0.491010	-0.031256
67	15	0	1.923483	0.172527	0.409907
68	8	0	0.820685	-0.996808	-2.216305
69	8	0	-0.774204	-2.459470	-2.869669
70	1	0	-1.979131	-1.815266	-1.526685
71	17	0	0.190861	-2.639579	0.968374
72	6	0	1.232090	-2.298523	-4.167793
73	1	0	0.767017	-3.083499	-4.766847
74	1	0	2.199111	-2.647376	-3.790021
75	1	0	1.427147	-1.425007	-4.800038

TS_{4A}



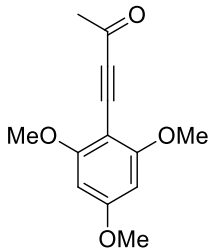
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.866880	-2.834928	2.317962
2	6	0	6.905067	0.674750	-1.868038
3	6	0	2.990084	1.005959	3.132962
4	6	0	4.977045	0.265853	-0.496038

5	6	0	4.379002	-0.540115	-1.480038
6	6	0	4.355058	0.506886	0.741962
7	6	0	3.114028	-0.053048	0.991962
8	6	0	3.128972	-1.096049	-1.226038
9	6	0	2.434982	-0.913012	0.032962
10	6	0	0.455298	5.012094	0.069962
11	6	0	1.296241	3.949049	0.742962
12	6	0	0.973168	2.577066	0.422962
13	6	0	0.698106	1.412081	0.188962
14	6	0	-2.419905	1.202247	1.258962
15	6	0	-2.851825	2.701270	3.581962
16	6	0	-2.124889	1.509231	3.642962
17	6	0	-1.491877	1.727197	-2.500038
18	6	0	-4.001051	-1.536669	0.988962
19	6	0	-1.802836	2.500214	-3.621038
20	6	0	-5.247142	-3.235602	-0.202038
21	6	0	-4.609122	-2.871636	-1.391038
22	6	0	-3.857894	1.407324	-2.074038
23	6	0	-3.362031	-1.162703	-0.203038
24	6	0	-4.160853	2.185340	-3.191038
25	6	0	-1.895929	0.760219	2.487962
26	6	0	-3.147841	2.399286	1.198962
27	6	0	-3.358802	3.145297	2.359962
28	6	0	-3.665068	-1.846687	-1.394038
29	6	0	-4.940106	-2.568619	0.984962
30	6	0	-2.515906	1.177252	-1.715038
31	6	0	-3.134824	2.731285	-3.966038
32	6	0	3.123915	-2.166049	-3.373038
33	1	0	-0.595709	4.880150	0.347962
34	1	0	6.348088	1.070780	-2.722038
35	1	0	7.828097	1.239701	-1.740038
36	1	0	7.141010	-0.381263	-2.032038
37	1	0	2.422881	-2.813011	-3.899038
38	1	0	3.292964	-1.256058	-3.957038
39	1	0	4.070887	-2.694099	-3.225038
40	1	0	3.019138	2.019957	2.722962
41	1	0	2.290082	0.963996	3.966962
42	1	0	3.984068	0.700906	3.476962
43	1	0	4.881992	-0.718142	-2.418038
44	1	0	4.874091	1.122858	1.461962
45	1	0	-3.016794	3.284279	4.482962
46	1	0	0.798351	6.003075	0.371962
47	1	0	0.514292	4.910091	-1.018038
48	1	0	-1.722907	1.164210	4.590962
49	1	0	-1.308977	-0.153812	2.542962
50	1	0	-3.545822	2.755307	0.254962
51	1	0	-0.453886	1.559142	-2.238038
52	1	0	-3.374792	3.331298	-4.839038
53	1	0	-3.173053	-1.576713	-2.322038
54	1	0	-5.433121	-2.845592	1.911962
55	1	0	-4.841150	-3.388624	-2.316038
56	1	0	-3.779024	-1.020681	1.915962
57	1	0	-4.663917	0.975367	-1.490038
58	1	0	-5.198844	2.358395	-3.458038
59	1	0	-5.980184	-4.036563	-0.202038
60	1	0	-1.001814	2.916171	-4.224038
61	1	0	-3.920752	4.073327	2.304962

62	8	0	6.174076	0.853789	-0.649038
63	8	0	2.499931	-1.868015	-2.122038
64	8	0	2.475036	0.089986	2.159962
65	8	0	2.200256	4.227001	1.525962
66	79	0	0.273005	-0.489897	-0.191038
67	15	0	-2.121960	0.181231	-0.231038
68	8	0	0.033929	-1.907884	2.212962
69	8	0	1.912871	-2.999984	1.593962
70	1	0	2.129927	-1.941996	0.662962
71	17	0	-0.350113	-2.690863	-1.057038
72	6	0	0.640822	-3.915916	3.378962
73	1	0	1.579809	-4.168966	3.878962
74	1	0	0.274774	-4.825897	2.890962
75	1	0	-0.099161	-3.591877	4.112962

Final Product



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.541853	1.360412	-0.000107
2	6	0	2.028047	-1.029058	-0.000066
3	6	0	1.932308	1.412554	0.000308
4	6	0	-0.144434	0.114257	-0.000393
5	6	0	0.629345	-1.070783	-0.000462
6	6	0	2.664077	0.217746	0.000293
7	8	0	-0.253935	2.453706	-0.000177
8	8	0	-0.081349	-2.226357	-0.000894
9	8	0	4.015264	0.375308	0.000632
10	6	0	0.350085	3.740321	0.000357
11	6	0	4.840067	-0.781503	0.001237
12	6	0	0.616953	-3.462719	-0.000667
13	6	0	-1.556210	0.062782	-0.000805
14	6	0	-2.773910	0.028537	-0.000323
15	6	0	-4.215529	-0.036603	-0.000095
16	8	0	-4.914264	0.968324	0.000083
17	6	0	-4.808724	-1.435471	0.000226
18	1	0	2.478098	2.345822	0.000603
19	1	0	2.603440	-1.942162	-0.000133
20	1	0	0.965113	3.894724	0.895116
21	1	0	-0.474884	4.452980	0.000312
22	1	0	0.965635	3.895231	-0.893950
23	1	0	4.674317	-1.394330	0.895760
24	1	0	5.867416	-0.415599	0.001930

25	1	0	4.675563	-1.394380	-0.893490
26	1	0	1.241339	-3.573710	0.894418
27	1	0	1.241873	-3.573754	-0.895367
28	1	0	-0.150987	-4.236932	-0.000886
29	1	0	-4.471090	-1.989881	0.882655
30	1	0	-4.467240	-1.992388	-0.879088
31	1	0	-5.897883	-1.366302	-0.002045

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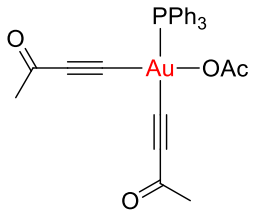
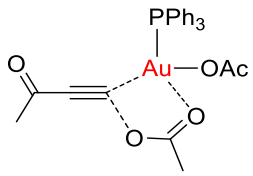


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	1.007815	-0.184447	0.048678
2	6	0	2.998154	-0.350380	0.179910
3	6	0	4.204738	-0.463144	0.301282
4	6	0	5.642417	-0.623919	0.400446
5	8	0	6.232361	-0.540823	1.466705
6	6	0	6.360787	-0.902650	-0.907126
7	1	0	7.430944	-1.004423	-0.718399
8	1	0	6.179927	-0.089320	-1.618452
9	1	0	5.969504	-1.818215	-1.364005
10	8	0	1.361308	-2.565924	-1.735633
11	6	0	1.074678	-2.991284	-0.622365
12	8	0	0.758805	-2.230437	0.408488
13	6	0	1.042429	-4.472722	-0.285557
14	1	0	1.231308	-5.060486	-1.183977
15	1	0	0.072182	-4.741422	0.141878
16	1	0	1.804834	-4.694044	0.467422
17	6	0	-2.208057	-1.429188	-0.886707
18	6	0	-3.415514	-3.439541	-2.410722
19	6	0	-2.251788	-2.819619	-2.869479
20	6	0	-1.355823	-1.185356	2.602618
21	6	0	-3.127882	1.439014	-1.666669
22	6	0	-1.752211	-1.347507	3.929494
23	6	0	-3.338684	3.848587	-1.588999
24	6	0	-2.434740	3.896505	-0.525643
25	6	0	-3.033258	0.551807	2.327815
26	6	0	-2.221330	1.480000	-0.595192
27	6	0	-3.421282	0.380725	3.657752
28	6	0	-1.644666	-1.817270	-2.112144
29	6	0	-3.375036	-2.058335	-0.425332
30	6	0	-3.974159	-3.060616	-1.188068
31	6	0	-1.878934	2.719439	-0.027366
32	6	0	-3.684507	2.621199	-2.156156

33	6	0	-1.997483	-0.229738	1.793952
34	6	0	-2.781206	-0.565366	4.459244
35	15	0	-1.457612	-0.051652	0.051418
36	1	0	-1.803241	-3.122716	-3.810345
37	1	0	-0.717008	-1.372746	-2.456223
38	1	0	-3.811843	-1.770061	0.525209
39	1	0	-0.559883	-1.799312	2.191650
40	1	0	-3.081511	-0.691579	5.495337
41	1	0	-1.166639	2.778753	0.786155
42	1	0	-4.385631	2.579131	-2.984430
43	1	0	-2.129875	4.843669	-0.094134
44	1	0	-3.399043	0.492109	-2.119190
45	1	0	-3.882068	-4.223156	-3.000629
46	1	0	-3.529143	1.295641	1.713914
47	1	0	-4.221026	0.991619	4.065734
48	1	0	-3.767168	4.767220	-1.979296
49	1	0	-1.250658	-2.083129	4.551039
50	1	0	-4.874793	-3.546534	-0.824662
51	6	0	1.255250	1.765661	-0.143363
52	6	0	1.388992	2.973011	-0.226903
53	6	0	1.475562	4.418010	-0.295996
54	8	0	0.593050	5.127723	0.169995
55	6	0	2.707835	4.987043	-0.965923
56	1	0	2.650075	6.076710	-0.973979
57	1	0	2.790476	4.605609	-1.989668
58	1	0	3.607163	4.662217	-0.431088

TS-S1

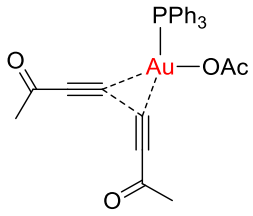


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	3.864732	1.963954	-0.479943
2	6	0	-0.146926	2.386216	-0.302943
3	6	0	0.956113	4.893320	-0.871943
4	6	0	1.432513	4.154932	0.211057
5	6	0	-1.989909	-0.052286	-2.322943
6	6	0	-1.743117	2.151514	2.411057
7	6	0	-3.027017	-0.184443	-3.246943
8	6	0	-2.720001	1.065308	4.339057
9	6	0	-2.565011	-0.176819	3.718057
10	6	0	-3.548123	0.914981	-0.729943
11	6	0	-1.581131	0.904381	1.787057
12	6	0	-4.578236	0.776818	-1.658943
13	6	0	4.356872	2.135554	-1.913943
14	6	0	2.392977	-0.193850	0.006057

15	6	0	3.025827	0.851635	-0.236943
16	6	0	0.891492	2.899372	0.492057
17	6	0	-0.612322	3.129594	-1.401943
18	6	0	-0.063305	4.380148	-1.678943
19	6	0	-1.998083	-0.265280	2.447057
20	6	0	-2.311056	2.226975	3.683057
21	6	0	-2.247457	0.503923	-1.060943
22	6	0	-4.318680	0.230607	-2.917943
23	79	0	0.594195	-1.154388	0.088057
24	8	0	4.167402	2.787708	0.392057
25	15	0	-0.867241	0.768801	0.104057
26	8	0	1.705723	-2.965292	0.316057
27	8	0	-1.223758	-2.325910	0.258057
28	6	0	2.937921	-2.722294	0.490057
29	6	0	-1.433300	-2.992740	-0.849943
30	8	0	3.448863	-1.563709	0.466057
31	8	0	-0.773183	-2.849277	-1.880943
32	6	0	-2.590101	-3.976800	-0.760943
33	6	0	3.857965	-3.898043	0.724057
34	1	0	2.254810	4.520264	0.814057
35	1	0	4.401102	1.188517	-2.457943
36	1	0	1.287027	2.328050	1.324057
37	1	0	-1.403639	2.739238	-2.031943
38	1	0	-0.999207	-0.418092	-2.569943
39	1	0	-5.123770	0.120262	-3.638943
40	1	0	-1.888867	-1.230369	1.961057
41	1	0	-2.430269	3.195073	4.160057
42	1	0	-2.882747	-1.082561	4.225057
43	1	0	-1.423379	3.059254	1.912057
44	1	0	1.383905	5.866972	-1.093943
45	1	0	-3.755779	1.338150	0.248057
46	1	0	-5.583978	1.094636	-1.397943
47	1	0	-3.157951	1.126664	5.332057
48	1	0	5.341257	2.608753	-1.894943
49	1	0	3.669415	2.804113	-2.444943
50	1	0	-2.823377	-0.626609	-4.216943
51	1	0	-0.432839	4.952449	-2.524943
52	1	0	-2.391698	-4.711961	0.024057
53	1	0	-2.724514	-4.484691	-1.716943
54	1	0	-3.508671	-3.448053	-0.487943
55	1	0	4.855241	-3.559854	1.002057
56	1	0	3.911487	-4.486086	-0.196943
57	1	0	3.437445	-4.537701	1.503057

TS-S2

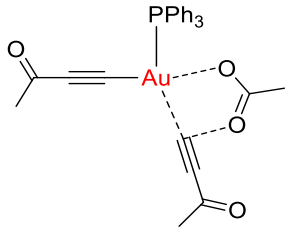


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.867087	-0.486076	0.114991
2	6	0	2.895087	-0.483975	0.231991
3	6	0	4.066103	-0.814917	0.372991
4	6	0	5.451123	-1.214848	0.515991
5	8	0	6.059115	-1.045818	1.562991
6	6	0	6.081155	-1.851817	-0.707009
7	1	0	7.121168	-2.100765	-0.487009
8	1	0	6.031121	-1.167819	-1.561009
9	1	0	5.530200	-2.754844	-0.989009
10	8	0	0.842203	-2.809078	-1.638009
11	6	0	0.427224	-3.242098	-0.560009
12	8	0	0.223188	-2.502108	0.498991
13	6	0	0.103298	-4.713114	-0.351009
14	1	0	0.260325	-5.267107	-1.277009
15	1	0	-0.933697	-4.825166	-0.022009
16	1	0	0.740318	-5.123083	0.437991
17	6	0	-2.519897	-0.808245	-1.109009
18	6	0	-4.073825	-2.247322	-2.937009
19	6	0	-2.708834	-2.071254	-3.168009
20	6	0	-1.929880	-1.153216	2.456991
21	6	0	-2.623053	2.325750	-1.445009
22	6	0	-2.496871	-1.328244	3.718991
23	6	0	-1.998168	4.641781	-1.117009
24	6	0	-1.108149	4.261825	-0.109009
25	6	0	-3.123985	0.951725	2.231991
26	6	0	-1.736034	1.937794	-0.430009
27	6	0	-3.683975	0.765697	3.495991
28	6	0	-1.928870	-1.355216	-2.258009
29	6	0	-3.892887	-0.997313	-0.875009
30	6	0	-4.663852	-1.713352	-1.789009
31	6	0	-0.976082	2.916832	0.232991
32	6	0	-2.754120	3.673743	-1.782009
33	6	0	-2.245937	-0.007231	1.704991
34	6	0	-3.371919	-0.372287	4.240991
35	15	0	-1.500946	0.183806	0.039991
36	1	0	-2.241813	-2.501231	-4.048009
37	1	0	-0.859874	-1.265162	-2.422009
38	1	0	-4.353908	-0.592336	0.019991
39	1	0	-1.246843	-1.895182	2.053991
40	1	0	-3.804912	-0.512309	5.226991
41	1	0	-0.269068	2.636867	1.006991

42	1	0	-3.444135	3.964709	-2.568009
43	1	0	-0.492186	4.998856	0.394991
44	1	0	-3.210016	1.580721	-1.972009
45	1	0	-4.676797	-2.809352	-3.645009
46	1	0	-3.362029	1.844713	1.662991
47	1	0	-4.360013	1.513663	3.898991
48	1	0	-2.097220	5.688776	-1.389009
49	1	0	-2.246827	-2.212231	4.298991
50	1	0	-5.723845	-1.857405	-1.602009
51	6	0	1.984005	1.157979	-0.061009
52	6	0	2.323947	2.330996	-0.181009
53	6	0	2.692878	3.721015	-0.313009
54	8	0	2.236835	4.569992	0.443991
55	6	0	3.656861	4.057063	-1.432009
56	1	0	3.818807	5.136071	-1.460009
57	1	0	3.260878	3.710043	-2.393009
58	1	0	4.611886	3.542110	-1.273009

TS-S3

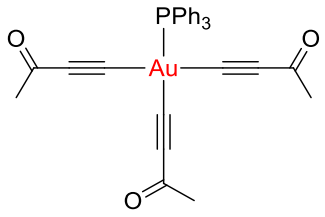


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-4.572915	0.352574	-0.112095
2	6	0	-1.370368	-2.106178	-0.076595
3	6	0	-3.669730	-3.693098	-0.220280
4	6	0	-3.562885	-2.713549	0.766701
5	6	0	1.213116	-1.219202	-2.518351
6	6	0	0.426205	-2.488435	2.491461
7	6	0	2.050702	-1.745360	-3.502444
8	6	0	2.045029	-1.901488	4.190352
9	6	0	2.482468	-0.832164	3.404392
10	6	0	2.222573	-2.703896	-0.881902
11	6	0	0.859947	-1.411483	1.702160
12	6	0	3.056744	-3.221778	-1.871457
13	6	0	-5.249106	0.328812	-1.479649
14	6	0	-2.151611	1.442002	-0.018234
15	6	0	-3.257659	0.871033	-0.075160
16	6	0	-2.421478	-1.913188	0.835318
17	6	0	-1.491021	-3.085674	-1.078113
18	6	0	-2.636139	-3.877200	-1.143104
19	6	0	1.896782	-0.581255	2.163952
20	6	0	1.019590	-2.728817	3.730955
21	6	0	1.293558	-1.702023	-1.203529

22	6	0	2.969783	-2.746038	-3.181765
23	79	0	-0.120479	1.309628	-0.166396
24	8	0	-5.151992	-0.097708	0.884138
25	15	0	0.125149	-1.083134	0.055112
26	8	0	-0.098655	3.446457	-0.148011
27	6	0	-1.248004	3.909475	0.120776
28	8	0	-2.283228	3.199937	0.290558
29	6	0	-1.391750	5.409992	0.227585
30	1	0	-4.377164	-2.528698	1.456649
31	1	0	-4.861301	1.098188	-2.152284
32	1	0	-2.362335	-1.141620	1.594441
33	1	0	-0.693259	-3.235667	-1.796820
34	1	0	0.533370	-0.411134	-2.765912
35	1	0	3.623558	-3.148306	-3.950495
36	1	0	2.245738	0.243311	1.549264
37	1	0	0.676482	-3.562076	4.336685
38	1	0	3.280517	-0.186949	3.758211
39	1	0	-0.373625	-3.133501	2.145937
40	1	0	-4.562333	-4.309797	-0.277123
41	1	0	2.295821	-3.075687	0.135488
42	1	0	3.775723	-3.995960	-1.617770
43	1	0	2.502405	-2.088346	5.158601
44	1	0	-6.325923	0.451691	-1.343052
45	1	0	-5.075390	-0.649828	-1.941835
46	1	0	1.991634	-1.358893	-4.514884
47	1	0	-2.719488	-4.637211	-1.914619
48	1	0	-2.378887	5.678674	0.601193
49	1	0	-1.242306	5.844927	-0.765088
50	1	0	-0.611927	5.802851	0.883619
51	6	0	1.977087	1.351778	-0.255678
52	6	0	3.169855	1.376292	-0.307338
53	6	0	4.698987	1.407650	-0.372776
54	8	0	5.265972	1.446438	-1.459737
55	6	0	5.521814	1.389873	0.918488
56	1	0	5.009382	1.982649	1.685938
57	1	0	6.512375	1.818263	0.727022
58	1	0	5.631291	0.356602	1.267828

S1

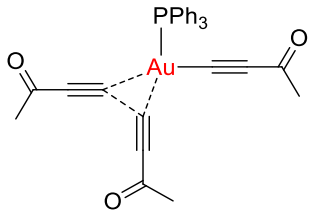


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-1.039795	-0.141844	0.002998
2	6	0	-0.577557	-2.102048	0.029066
3	6	0	-2.982338	-0.618353	0.060641

4	6	0	-1.582469	1.795681	0.030851
5	6	0	-1.912869	2.967843	0.095356
6	6	0	-4.161647	-0.917825	0.113750
7	6	0	-0.262959	-3.277207	0.114021
8	6	0	0.208946	-4.632059	0.294873
9	6	0	-5.565788	-1.272914	0.146893
10	6	0	-2.225644	4.375930	0.212463
11	8	0	1.211381	-4.857067	0.963578
12	8	0	-1.443593	5.157799	0.741080
13	8	0	-6.173437	-1.420062	1.196024
14	6	0	-3.561489	4.821871	-0.344003
15	1	0	-3.669890	5.900260	-0.216518
16	1	0	-4.374254	4.299305	0.172493
17	1	0	-3.635827	4.557959	-1.404760
18	6	0	-0.589538	-5.734330	-0.367159
19	1	0	-0.659768	-5.555638	-1.445762
20	1	0	-1.613315	-5.738542	0.023269
21	1	0	-0.113386	-6.697355	-0.175652
22	6	0	-6.230221	-1.449960	-1.207018
23	1	0	-6.149471	-0.527065	-1.791796
24	1	0	-7.280155	-1.710726	-1.062919
25	1	0	-5.723341	-2.236607	-1.776783
26	15	0	1.392977	0.323856	-0.035226
27	6	0	2.179545	-0.725978	-1.311110
28	6	0	3.377747	-2.224507	-3.350231
29	6	0	1.516088	-0.916574	-2.533390
30	6	0	3.447220	-1.292724	-1.117715
31	6	0	4.040139	-2.041474	-2.135781
32	6	0	2.115832	-1.659247	-3.548789
33	1	0	0.528989	-0.491268	-2.690672
34	1	0	3.966602	-1.161275	-0.174589
35	1	0	5.018268	-2.484505	-1.974811
36	1	0	1.593788	-1.803530	-4.489807
37	1	0	3.840696	-2.810402	-4.138761
38	6	0	2.162438	-0.104723	1.576427
39	6	0	3.295357	-0.780854	4.049715
40	6	0	2.749824	0.884440	2.380919
41	6	0	2.150335	-1.440364	2.020033
42	6	0	2.720236	-1.769758	3.248660
43	6	0	3.309765	0.543871	3.613079
44	1	0	2.777508	1.916419	2.051468
45	1	0	1.708119	-2.227326	1.420639
46	1	0	2.707064	-2.805566	3.573346
47	1	0	3.759096	1.318437	4.227334
48	1	0	3.732386	-1.042547	5.008982
49	6	0	1.898186	2.040119	-0.432938
50	6	0	2.671786	4.668503	-1.024145
51	6	0	2.847232	2.290362	-1.438003
52	6	0	1.341142	3.120939	0.271613
53	6	0	1.725988	4.427800	-0.026134
54	6	0	3.231590	3.600033	-1.726485
55	1	0	3.285659	1.470639	-1.995057
56	1	0	0.588572	2.958070	1.031923
57	1	0	1.253591	5.245673	0.506952
58	1	0	3.966082	3.781937	-2.505514
59	1	0	2.966024	5.687214	-1.259682

TS-S4

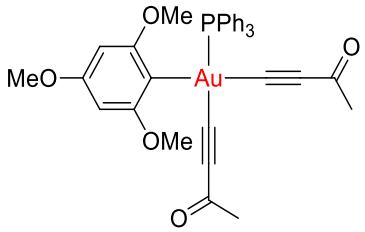


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-0.734030	0.734892	-0.059075
2	6	0	-2.226113	-0.641018	0.012925
3	6	0	-2.729006	1.147012	0.004925
4	6	0	0.274076	2.504831	-0.069075
5	6	0	0.942137	3.527791	-0.045075
6	6	0	-3.801970	1.741076	0.048925
7	6	0	-2.833177	-1.706982	0.095925
8	6	0	-3.541252	-2.960940	0.196925
9	6	0	-5.071929	2.427152	0.088925
10	6	0	1.813206	4.679739	-0.000075
11	8	0	-3.656287	-3.541933	1.267925
12	8	0	3.015199	4.560667	0.217925
13	8	0	-5.635914	2.672186	1.145925
14	6	0	1.171288	6.032777	-0.232075
15	1	0	1.932335	6.813732	-0.185075
16	1	0	0.399299	6.214824	0.522925
17	1	0	0.673289	6.050807	-1.208075
18	6	0	-4.107285	-3.512906	-1.098075
19	1	0	-3.297296	-3.684954	-1.816075
20	1	0	-4.797242	-2.793864	-1.552075
21	1	0	-4.627342	-4.449874	-0.892075
22	6	0	-5.650905	2.826187	-1.257075
23	1	0	-4.962865	3.496146	-1.782075
24	1	0	-6.608875	3.324245	-1.101075
25	1	0	-5.787958	1.942195	-1.890075
26	15	0	1.280882	-0.731229	-0.024075
27	6	0	0.931787	-2.310208	-0.889075
28	6	0	0.406645	-4.677177	-2.294075
29	6	0	0.271789	-2.268168	-2.128075
30	6	0	1.316712	-3.548231	-0.356075
31	6	0	1.051642	-4.726215	-1.057075
32	6	0	0.018719	-3.446153	-2.830075
33	1	0	-0.048154	-1.316149	-2.543075
34	1	0	1.816710	-3.595261	0.605925
35	1	0	1.347584	-5.681233	-0.633075
36	1	0	-0.485279	-3.403123	-3.791075
37	1	0	0.201589	-5.595164	-2.837075
38	6	0	1.633855	-1.167250	1.720925
39	6	0	2.091814	-1.862278	4.394925
40	6	0	2.941853	-1.200329	2.226925
41	6	0	0.554836	-1.483185	2.564925

42	6	0	0.787815	-1.833199	3.893925
43	6	0	3.164833	-1.545342	3.560925
44	1	0	3.780868	-0.949379	1.586925
45	1	0	-0.463162	-1.464124	2.187925
46	1	0	-0.052199	-2.077149	4.537925
47	1	0	4.179832	-1.563403	3.946925
48	1	0	2.269798	-2.127288	5.432925
49	6	0	2.837920	-0.094323	-0.746075
50	6	0	5.203982	0.936535	-1.835075
51	6	0	3.547876	-0.824365	-1.713075
52	6	0	3.324995	1.155648	-0.328075
53	6	0	4.501026	1.667578	-0.874075
54	6	0	4.726907	-0.308436	-2.251075
55	1	0	3.184818	-1.790343	-2.046075
56	1	0	2.785031	1.749681	0.397925
57	1	0	4.838085	2.648557	-0.555075
58	1	0	5.269873	-0.880469	-2.997075
59	1	0	6.118006	1.338480	-2.263075

S2

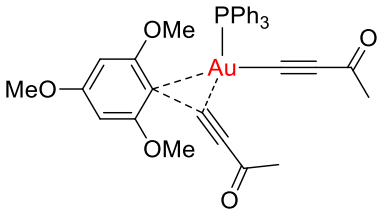


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	0.508118	2.038021	-0.133082
2	1	0	1.893152	5.178006	-1.607082
3	1	0	1.477167	6.530011	-0.507082
4	1	0	-5.542943	-3.560913	-0.127082
5	1	0	-1.503919	-1.318957	4.741918
6	1	0	-4.723856	4.404078	-2.552082
7	1	0	-4.750889	1.410078	4.021918
8	1	0	-4.195889	1.442072	1.615918
9	1	0	-4.528955	-4.699924	-2.090082
10	1	0	-4.030902	0.181070	-2.207082
11	1	0	-3.157852	4.810061	-0.644082
12	1	0	-5.140882	2.077082	-3.323082
13	1	0	-2.059872	2.942049	0.467918
14	1	0	-3.407904	0.034064	5.596918
15	1	0	-0.941918	-1.292963	2.335918
16	1	0	-4.488921	-1.533925	0.812918
17	1	0	-1.397923	-1.766958	-2.183082
18	1	0	-2.448946	-3.794947	-3.109082
19	6	0	1.660155	5.456009	-0.573082
20	8	0	-0.575847	5.282033	0.287918

21	6	0	0.435147	4.700022	-0.096082
22	6	0	0.515131	3.259021	-0.121082
23	1	0	2.530152	5.183999	0.033918
24	15	0	-2.090904	0.022049	0.025918
25	6	0	-3.165904	0.042061	4.537918
26	6	0	-2.534903	0.073054	1.806918
27	6	0	-4.469880	2.265075	-2.490082
28	6	0	-2.741875	2.733056	-0.346082
29	6	0	-4.640939	-3.162923	-0.583082
30	6	0	-4.047926	-2.016929	-0.053082
31	6	0	-2.315928	-2.140948	-1.744082
32	6	0	-3.919895	0.815069	3.654918
33	6	0	-2.973889	1.415059	-0.778082
34	6	0	-3.608895	0.832066	2.293918
35	6	0	-3.371863	3.802063	-0.983082
36	6	0	-4.236865	3.570073	-2.054082
37	6	0	-2.095912	-0.716951	4.058918
38	6	0	-3.841891	1.190068	-1.859082
39	6	0	-1.776912	-0.700954	2.701918
40	6	0	-2.910940	-3.288942	-2.268082
41	6	0	-4.072946	-3.799929	-1.688082
42	6	0	-2.879921	-1.496942	-0.633082
43	79	0	0.437096	0.024022	-0.117082
44	6	0	0.491074	-1.987979	-0.087082
45	6	0	0.504061	-3.209979	-0.126082
46	6	0	0.481045	-4.651979	-0.204082
47	8	0	0.080039	-5.238974	-1.201082
48	6	0	0.981037	-5.396984	1.020918
49	1	0	2.025040	-5.133995	1.219918
50	1	0	0.892025	-6.471983	0.853918
51	1	0	0.402040	-5.105978	1.904918
52	6	0	2.508096	0.007999	-0.163082
53	6	0	3.239096	0.048991	1.018918
54	6	0	3.178095	-0.044008	-1.388082
55	6	0	4.574095	-0.055023	-1.434082
56	1	0	5.126095	-0.095029	-2.364082
57	6	0	4.646096	0.038976	0.998918
58	1	0	5.208096	0.068970	1.919918
59	6	0	5.297096	-0.013031	-0.236082
60	8	0	2.387095	-0.079999	-2.503082
61	8	0	2.511097	0.095999	2.178918
62	8	0	6.657095	-0.028046	-0.381082
63	6	0	3.013094	-0.156006	-3.773082
64	1	0	3.646104	0.718987	-3.966082
65	1	0	2.204094	-0.181997	-4.505082
66	1	0	3.618084	-1.067013	-3.871082
67	6	0	3.201098	0.189992	3.411918
68	1	0	3.823108	1.092985	3.461918
69	1	0	3.832088	-0.691015	3.594918
70	1	0	2.432098	0.244000	4.183918
71	6	0	7.459096	0.007946	0.785918
72	1	0	7.291106	0.924947	1.366918
73	1	0	8.495096	-0.012066	0.442918
74	1	0	7.277086	-0.862052	1.430918

TS-S5

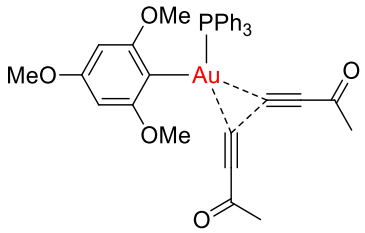


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-2.836201	-1.182823	-1.239093
2	6	0	-4.929207	-1.261674	-3.106093
3	6	0	-3.698123	-0.081762	-1.390093
4	6	0	-3.035282	-2.323809	-2.034093
5	6	0	-4.076284	-2.357735	-2.963093
6	6	0	-4.738126	-0.126688	-2.316093
7	6	0	-0.578307	-2.676983	-0.152093
8	6	0	0.851523	-5.069084	-0.469093
9	6	0	0.337683	-2.823048	-1.207093
10	6	0	-0.765382	-3.738970	0.744907
11	6	0	-0.051467	-4.928020	0.584907
12	6	0	1.043598	-4.015098	-1.366093
13	6	0	-2.295198	-1.144861	1.643907
14	6	0	-3.444204	-1.221780	4.198907
15	6	0	-1.551170	-0.749914	2.767907
16	6	0	-3.620229	-1.573767	1.810907
17	6	0	-4.190231	-1.610727	3.084907
18	6	0	-2.124173	-0.794873	4.037907
19	15	0	-1.481194	-1.083919	-0.001093
20	6	0	2.587869	-0.193208	-1.395093
21	6	0	3.811809	-1.046294	0.980907
22	6	0	3.768817	-0.923291	-1.457093
23	6	0	2.010895	0.171833	-0.153093
24	6	0	2.627862	-0.301210	1.022907
25	6	0	4.377788	-1.341334	-0.266093
26	8	0	1.903899	0.224841	-2.494093
27	8	0	2.004885	0.032834	2.189907
28	8	0	5.525737	-2.054416	-0.427093
29	6	0	2.546895	0.167795	-3.764093
30	6	0	6.221706	-2.500465	0.726907
31	6	0	2.664867	-0.230213	3.420907
32	79	0	0.034951	0.954974	-0.081093
33	6	0	1.719030	2.068854	-0.103093
33	6	0	1.719030	2.068854	-0.103093
34	6	0	2.465099	3.045801	-0.140093
35	6	0	3.330180	4.185740	-0.180093
36	8	0	3.761213	4.651709	-1.232093
37	6	0	3.685223	4.796715	1.168907
38	1	0	-3.562059	0.816229	-0.800093
39	1	0	-2.382343	-3.183855	-1.932093

40	1	0	-4.219347	-3.245725	-3.573093
41	1	0	-5.387065	0.738358	-2.411093
42	1	0	-5.738209	-1.293617	-3.831093
43	1	0	0.498741	-2.004059	-1.901093
44	1	0	-1.467375	-3.638920	1.565907
45	1	0	-0.205524	-5.744009	1.284907
46	1	0	1.750591	-4.116148	-2.184093
47	1	0	1.406458	-5.995124	-0.591093
48	1	0	-0.528146	-0.404986	2.643907
49	1	0	-4.208250	-1.868725	0.948907
50	1	0	-5.218254	-1.937654	3.203907
51	1	0	-1.543151	-0.482914	4.901907
52	1	0	-3.891205	-1.245748	5.187907
53	1	0	4.236798	-1.194324	-2.394093
54	1	0	4.272784	-1.398327	1.891907
55	1	0	3.500933	0.705728	-3.747093
56	1	0	1.865929	0.654844	-4.462093
57	1	0	2.715821	-0.868217	-4.084093
58	1	0	6.533765	-1.660487	1.359907
59	1	0	7.107669	-3.021528	0.359907
60	1	0	5.615656	-3.196422	1.320907
61	1	0	3.651900	0.245717	3.454907
62	1	0	2.772790	-1.307221	3.599907
63	1	0	2.030897	0.200832	4.196907
64	1	0	4.135170	4.046683	1.827907
65	1	0	2.781249	5.164779	1.666907
66	1	0	4.382282	5.622665	1.013907
67	6	0	-1.563958	2.241087	-0.012093
68	6	0	-2.557907	2.956158	-0.028093
69	6	0	-3.786854	3.706245	-0.110093
70	8	0	-4.797889	3.221316	-0.612093
71	6	0	-3.770754	5.116244	0.447907
72	1	0	-3.475755	5.100223	1.502907
73	1	0	-4.759722	5.565314	0.341907
74	1	0	-3.025711	5.719191	-0.082093

TS-S6



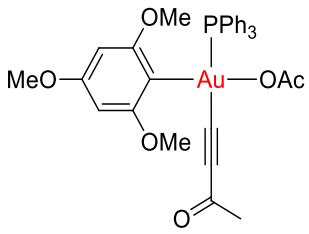
Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	0.323091	0.838964	0.000021
2	6	0	0.833359	2.798894	-0.042979
3	6	0	0.776528	4.028902	-0.060979

4	6	0	0.737724	5.464907	-0.066979
5	8	0	0.808813	6.116897	-1.103979
6	6	0	0.594815	6.127927	1.294021
7	1	0	0.596963	7.211926	1.166021
8	1	0	1.415774	5.828814	1.955021
9	1	0	-0.338228	5.812054	1.774021
10	6	0	0.196663	-2.287019	1.719021
11	6	0	-0.210470	-3.258963	4.318021
12	6	0	0.328704	-1.986037	4.124021
13	6	0	-1.946367	-2.508726	-0.871979
14	6	0	2.790513	-3.380374	0.235021
15	6	0	-2.810458	-3.167607	-1.744979
16	6	0	4.838555	-3.077654	-1.017979
17	6	0	4.313712	-1.926583	-1.605979
18	6	0	-0.058465	-3.220984	-2.213979
19	6	0	2.252671	-2.225300	-0.355979
20	6	0	-0.930554	-3.872865	-3.087979
21	6	0	0.525771	-1.498064	2.832021
22	6	0	-0.349512	-3.564944	1.921021
23	6	0	-0.551578	-4.045917	3.216021
24	6	0	3.024770	-1.502406	-1.277979
25	6	0	4.075455	-3.804550	-0.099979
26	6	0	-0.559371	-2.534915	-1.096979
27	6	0	-2.305551	-3.849676	-2.854979
28	15	0	0.560753	-1.632069	0.045021
29	1	0	0.591789	-1.368073	4.978021
30	1	0	0.926908	-0.500119	2.687021
31	1	0	-0.621596	-4.179907	1.071021
32	1	0	-2.352294	-1.970670	-0.021979
33	1	0	-2.981621	-4.360584	-3.533979
34	1	0	2.637895	-0.594353	-1.724979
35	1	0	4.483333	-4.698606	0.363021
36	1	0	4.908794	-1.329664	-2.288979
37	1	0	2.212436	-3.943295	0.961021
38	1	0	-0.368522	-3.634942	5.324021
39	1	0	1.009531	-3.250130	-2.401979
40	1	0	-0.529626	-4.400920	-3.947979
41	1	0	5.845510	-3.403792	-1.264979
42	1	0	-3.879454	-3.140461	-1.558979
43	1	0	-0.976713	-5.034858	3.362021
44	6	0	2.238199	1.628702	-0.112979
45	6	0	3.456210	1.705535	-0.274979
46	6	0	4.876220	1.779340	-0.500979
47	8	0	5.392151	1.280270	-1.496979
48	6	0	5.692318	2.498229	0.557021
49	1	0	6.750312	2.450084	0.292021
50	1	0	5.529256	2.044251	1.540021
51	1	0	5.375461	3.545272	0.629021
52	6	0	-1.771916	0.788251	0.038021
53	6	0	-4.588915	0.794636	0.028021
54	6	0	-2.501913	0.811350	1.233021
55	6	0	-2.493917	0.782349	-1.155979
56	6	0	-3.899916	0.785542	-1.186979
57	6	0	-3.900914	0.804542	1.247021
58	1	0	-4.434917	0.782615	-2.124979
59	1	0	-4.481912	0.820622	2.159021
60	8	0	-5.954915	0.794823	0.133021

61	8	0	-1.732920	0.761245	-2.299979
62	8	0	-1.751909	0.841248	2.385021
63	6	0	-2.428902	0.889340	3.629021
64	1	0	-3.051779	1.787426	3.717021
65	1	0	-1.651899	0.915234	4.396021
66	1	0	-3.057024	0.002426	3.786021
67	6	0	-6.720911	0.828928	-1.056979
68	1	0	-6.511787	1.727899	-1.650979
69	1	0	-7.766909	0.841071	-0.744979
70	1	0	-6.544032	-0.058096	-1.681979
71	6	0	-2.382916	0.788334	-3.557979
72	1	0	-2.994792	1.691418	-3.679979
73	1	0	-3.014037	-0.097579	-3.708979
74	1	0	-1.589915	0.793226	-4.306979

S3

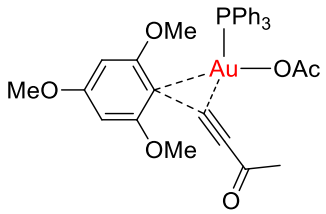


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	2.347966	0.905975	1.203048
2	6	0	2.923950	2.132983	-1.250952
3	6	0	3.344953	1.880989	1.135048
4	6	0	1.635971	0.526966	0.058048
5	6	0	1.928963	1.145970	-1.155952
6	6	0	3.628945	2.482993	-0.095952
7	1	0	3.913949	2.191996	2.002048
8	1	0	3.138943	2.605986	-2.196952
9	8	0	1.978975	0.291970	2.367048
10	8	0	1.180969	0.734959	-2.226952
11	8	0	4.620932	3.423006	-0.064952
12	6	0	2.825973	0.420982	3.501048
13	1	0	3.849977	0.106996	3.269048
14	1	0	2.407982	-0.240024	4.261048
15	1	0	2.838959	1.448982	3.884048
16	6	0	4.996924	4.048011	-1.279952
17	1	0	5.353934	3.319016	-2.017952
18	1	0	5.809915	4.731022	-1.028952
19	1	0	4.167916	4.623000	-1.715952
20	6	0	1.474962	1.257963	-3.511952
21	1	0	1.295947	2.340961	-3.558952
22	1	0	0.797968	0.751954	-4.201952
23	1	0	2.509964	1.048977	-3.805952
24	79	0	0.263992	-0.990053	0.115048

25	6	0	1.837008	-2.219032	0.158048
26	6	0	2.790019	-2.976019	0.223048
27	6	0	3.902031	-3.900004	0.263048
28	8	0	4.566034	-4.083995	1.274048
29	6	0	4.195041	-4.629000	-1.036952
30	1	0	5.047050	-5.297988	-0.894952
31	1	0	4.411031	-3.908997	-1.833952
32	1	0	3.316049	-5.200012	-1.354952
33	8	0	-0.754981	-3.019067	-1.929952
34	6	0	-1.261977	-3.310073	-0.849952
35	8	0	-1.133986	-2.616072	0.256048
36	6	0	-2.124960	-4.554085	-0.671952
37	1	0	-2.267953	-5.050087	-1.632952
38	1	0	-3.094964	-4.284098	-0.243952
39	1	0	-1.638951	-5.240079	0.027048
40	6	0	-2.860024	0.170905	-1.196952
41	6	0	-4.647017	-0.304119	-3.294952
42	6	0	-3.307012	-0.670101	-3.422952
43	6	0	-2.710010	-0.871093	2.329048
44	6	0	-1.676063	3.069921	-1.116952
45	6	0	-3.429008	-1.002103	3.517048
46	6	0	-0.522089	5.007936	-0.239952
47	6	0	-0.089079	4.253942	0.854048
48	6	0	-3.193042	1.508900	2.321048
49	6	0	-1.248053	2.309927	-0.019952
50	6	0	-3.911040	1.364891	3.509048
51	6	0	-2.410016	-0.435089	-2.378952
52	6	0	-4.213029	0.527887	-1.066952
53	6	0	-5.100025	0.292875	-2.114952
54	6	0	-0.444061	2.910938	0.964048
55	6	0	-1.313081	4.414926	-1.222952
56	6	0	-2.588027	0.391909	1.723048
57	6	0	-4.029023	0.110889	4.109048
58	15	0	-1.663029	0.530921	0.141048
59	1	0	-2.955006	-1.155096	-4.327952
60	1	0	-1.380011	-0.765075	-2.467952
61	1	0	-4.572035	0.980882	-0.147952
62	1	0	-2.252998	-1.740087	1.866048
63	1	0	-4.585022	0.001882	5.037048
64	1	0	-0.095053	2.331942	1.812048
65	1	0	-1.654089	4.995921	-2.074952
66	1	0	0.534915	4.706951	1.618048
67	1	0	-2.292057	2.616913	-1.885952
68	1	0	-5.343015	-0.494129	-4.107952
69	1	0	-3.097055	2.490902	1.870048
70	1	0	-4.374052	2.235884	3.965048
71	1	0	-0.241103	6.053940	-0.323952
72	1	0	-3.515995	-1.980104	3.982048
73	1	0	-6.145029	0.567861	-2.007952

TS-S7

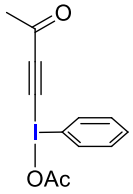


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	-3.427057	-0.292913	-0.301941
2	6	0	-5.925050	-1.464928	-0.791941
3	6	0	-3.603052	-1.149914	-1.399941
4	6	0	-4.508059	-0.036919	0.553059
5	6	0	-5.751055	-0.622927	0.307059
6	6	0	-4.849049	-1.727921	-1.642941
7	6	0	-1.815067	1.258097	1.591059
8	6	0	-1.795073	2.261097	4.208059
9	6	0	-1.762061	0.374097	2.685059
10	6	0	-1.837075	2.641097	1.818059
11	6	0	-1.825078	3.138097	3.124059
12	6	0	-1.765064	0.881097	3.984059
13	6	0	-1.890071	1.928096	-1.275941
14	6	0	-2.031083	4.048096	-3.109941
15	6	0	-0.810072	2.202103	-2.125941
16	6	0	-3.050075	2.718089	-1.365941
17	6	0	-3.116081	3.773089	-2.272941
18	6	0	-0.883078	3.260102	-3.036941
19	15	0	-1.791062	0.520097	-0.091941
20	6	0	2.274938	0.531121	1.392059
21	6	0	3.523929	1.929128	-0.701941
22	6	0	3.208932	1.521127	1.683059
23	6	0	1.953940	0.210119	0.049059
24	6	0	2.579935	0.934123	-0.980941
25	6	0	3.830928	2.211130	0.635059
26	8	0	1.630942	-0.198883	2.330059
27	8	0	2.211937	0.598121	-2.251941
28	8	0	4.726922	3.160135	1.023059
29	6	0	1.991941	-0.041881	3.696059
30	6	0	5.422918	3.892140	0.026059
31	6	0	2.963934	1.109125	-3.343941
32	79	0	0.225947	-0.955891	-0.294941
33	6	0	2.089951	-1.703880	-0.266941
34	6	0	3.011956	-2.515875	-0.295941
35	6	0	4.081961	-3.472868	-0.346941
36	8	0	4.572964	-3.964865	0.663059
37	6	0	4.568964	-3.845865	-1.738941
38	1	0	-2.760051	-1.393909	-2.036941
39	1	0	-4.380063	0.610082	1.414059

40	1	0	-6.581057	-0.420931	0.978059
41	1	0	-4.976045	-2.391922	-2.492941
42	1	0	-6.893048	-1.919933	-0.979941
43	1	0	-1.713055	-0.696903	2.508059
44	1	0	-1.863079	3.334097	0.984059
45	1	0	-1.841084	4.212097	3.289059
46	1	0	-1.738060	0.193097	4.825059
47	1	0	-1.792075	2.649097	5.222059
48	1	0	0.079931	1.583108	-2.089941
49	1	0	-3.905074	2.499084	-0.733941
50	1	0	-4.018085	4.376084	-2.332941
51	1	0	-0.042080	3.461107	-3.694941
52	1	0	-2.086088	4.867095	-3.820941
53	1	0	3.474930	1.783128	2.699059
54	1	0	3.995926	2.475131	-1.504941
55	1	0	3.057942	-0.243874	3.850059
56	1	0	1.398945	-0.775884	4.242059
57	1	0	1.748935	0.964118	4.059059
58	1	0	6.020922	3.233143	-0.614941
59	1	0	6.086914	4.571144	0.562059
60	1	0	4.735914	4.478136	-0.598941
61	1	0	4.026936	0.860131	-3.248941
62	1	0	2.854928	2.197124	-3.438941
63	1	0	2.556937	0.630123	-4.235941
64	1	0	4.902958	-2.953863	-2.281941
65	1	0	3.753966	-4.289870	-2.319941
66	1	0	5.392968	-4.556861	-1.651941
67	8	0	-1.481044	-2.578901	1.459059
68	6	0	-1.548041	-3.145902	0.359059
69	8	0	-1.002043	-2.708898	-0.734941
70	6	0	-2.337033	-4.437906	0.190059
71	1	0	-3.267034	-4.221912	-0.346941
72	1	0	-2.580030	-4.861908	1.166059
73	1	0	-1.770029	-5.157903	-0.405941

S4



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-0.727429	3.989827	-1.594430
2	1	0	1.925409	1.037663	1.420895
3	1	0	-0.974584	1.523626	-1.736917
4	1	0	0.823715	4.992597	0.069977
5	1	0	2.141276	3.526341	1.583426
6	53	0	0.253241	-0.972954	-0.290367

7	6	0	-0.291539	1.965895	-1.020991
8	6	0	1.464443	3.091274	0.853806
9	6	0	0.721917	3.913265	0.005279
10	6	0	-0.152033	3.354121	-0.928714
11	6	0	1.347118	1.698894	0.782402
12	6	0	0.466980	1.186984	-0.157892
13	1	0	5.106373	-0.774086	-0.744592
14	1	0	5.337433	-1.444556	0.899706
15	1	0	4.734283	-2.467080	-0.438659
16	6	0	4.713698	-1.467358	0.005847
17	8	0	2.939602	-0.841449	1.515919
18	6	0	3.280055	-1.089770	0.358461
19	8	0	2.490868	-1.056124	-0.688533
20	6	0	-1.859264	-0.693951	-0.034626
21	6	0	-3.068628	-0.702268	0.112371
22	6	0	-4.512004	-0.696211	0.297481
23	8	0	-5.171340	-1.711437	0.146000
24	6	0	-5.122684	0.632873	0.690033
25	1	0	-6.202837	0.518267	0.790529
26	1	0	-4.893962	1.393275	-0.064783
27	1	0	-4.692827	0.980289	1.636496

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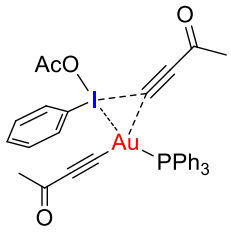

Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	79	0	-0.089996	0.573018	-0.339995
2	53	0	2.795992	-1.107002	-0.436995
3	6	0	3.116000	-0.028005	1.397005
4	6	0	3.545009	1.338993	3.745005
5	6	0	3.561009	1.285992	1.321005
6	6	0	2.872995	-0.687003	2.598005
7	6	0	3.094000	0.016996	3.784005
8	6	0	3.775014	1.968991	2.521005
9	1	0	3.720012	1.799991	0.383005
10	1	0	2.513988	-1.709000	2.621005
11	1	0	2.909997	-0.473003	4.735005
12	1	0	4.104021	3.001989	2.471005
13	1	0	3.711013	1.878991	4.672005
14	6	0	0.368990	-1.519986	0.022005
15	6	0	-0.100018	-2.623982	0.324005
16	6	0	-0.710027	-3.865978	0.725005
17	8	0	-1.236028	-3.984974	1.829005

18	6	0	-0.682034	-4.997978	-0.281995
19	1	0	-1.282033	-4.723974	-1.157995
20	1	0	-1.092041	-5.899975	0.176005
21	1	0	0.338964	-5.183985	-0.632995
22	15	0	-2.570999	0.190035	-0.101995
23	6	0	0.879016	2.341011	-0.607995
24	6	0	1.599023	3.336006	-0.655995
25	6	0	2.527031	4.436000	-0.647995
26	8	0	3.609030	4.358992	-0.067995
27	6	0	2.114039	5.694002	-1.387995
28	1	0	1.915038	5.464004	-2.439995
29	1	0	2.906044	6.441997	-1.311995
30	1	0	1.184042	6.091009	-0.965995
31	6	0	-3.558989	1.526042	-0.892995
32	6	0	-5.025975	3.610052	-2.063995
33	6	0	-4.902991	1.334051	-1.252995
34	6	0	-2.954981	2.770037	-1.132995
35	6	0	-3.689974	3.807042	-1.711995
36	6	0	-5.630984	2.371056	-1.835995
37	1	0	-5.378997	0.373054	-1.082995
38	1	0	-1.909980	2.922030	-0.877995
39	1	0	-3.212967	4.766039	-1.893995
40	1	0	-6.668985	2.211063	-2.112995
41	1	0	-5.593970	4.415056	-2.520995
42	6	0	-3.230009	-1.354961	-0.847995
43	6	0	-4.207025	-3.647954	-2.139995
44	6	0	-2.759012	-1.710964	-2.123995
45	6	0	-4.184015	-2.169954	-0.221995
46	6	0	-4.667023	-3.310951	-0.865995
47	6	0	-3.252020	-2.843961	-2.768995
48	1	0	-2.003008	-1.099969	-2.608995
49	1	0	-4.544013	-1.919952	0.771005
50	1	0	-5.404027	-3.935946	-0.368995
51	1	0	-2.885021	-3.102963	-3.757995
52	1	0	-4.587031	-4.533951	-2.639995
53	6	0	-3.088999	0.173038	1.661005
54	6	0	-3.731999	0.186043	4.393005
55	6	0	-2.636006	-0.860965	2.503005
56	6	0	-3.855992	1.214044	2.206005
57	6	0	-4.172992	1.219046	3.565005
58	6	0	-2.967006	-0.851963	3.857005
59	1	0	-2.038012	-1.680969	2.119005
60	1	0	-4.206986	2.021046	1.573005
61	1	0	-4.767986	2.031050	3.974005
62	1	0	-2.620011	-1.662965	4.492005
63	1	0	-3.982999	0.190044	5.450005
64	8	0	5.038993	-0.985018	-0.548995
65	6	0	5.396989	-1.612020	-1.643995
66	8	0	4.606985	-2.168015	-2.405995
67	6	0	6.896989	-1.578031	-1.890995
68	1	0	7.215996	-0.544033	-2.052995
69	1	0	7.136985	-2.182032	-2.765995
70	1	0	7.428987	-1.953034	-1.012995

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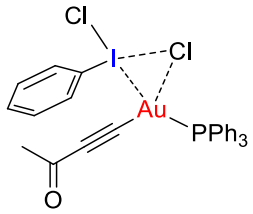
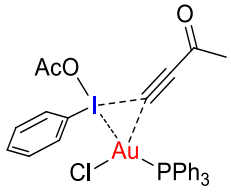


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	3.946998	1.425176	-0.007924
2	1	0	3.318759	5.815142	-1.973924
3	1	0	1.569775	5.519046	-1.716924
4	1	0	2.404820	4.690092	-3.026924
5	1	0	4.315986	1.655196	4.258076
6	1	0	2.882184	-1.979882	2.457076
7	1	0	3.484113	-0.675849	4.481076
8	1	0	4.534929	2.692208	1.989076
9	15	0	-2.426923	-0.009172	0.118076
10	79	0	-0.070942	0.330957	-0.617924
11	6	0	1.166974	1.878024	-0.876924
12	6	0	1.915921	2.845065	-0.985924
13	6	0	2.865862	3.922117	-1.068924
14	8	0	3.908862	3.915174	-0.415924
15	6	0	2.524800	5.066098	-2.004924
16	17	0	0.031204	-2.335038	-1.171924
17	53	0	2.884158	-1.498882	-0.611924
18	6	0	3.392095	-0.350854	1.120076
19	6	0	4.056017	1.087182	3.370076
20	6	0	3.855024	0.953171	0.960076
21	6	0	3.245129	-0.962862	2.367076
22	6	0	3.586089	-0.223844	3.499076
23	6	0	4.188985	1.671189	2.109076
24	17	0	5.411195	-2.174744	-1.038924
25	6	0	-3.338010	1.586778	0.204076
26	6	0	-4.664145	4.051706	0.388076
27	6	0	-2.618075	2.761818	0.471076
28	6	0	-4.728014	1.660702	0.019076
29	6	0	-5.385081	2.888666	0.111076
30	6	0	-3.281141	3.985781	0.569076
31	1	0	-1.539072	2.719876	0.586076
32	1	0	-5.294965	0.762671	-0.202924
33	1	0	-6.460084	2.935608	-0.038924
34	1	0	-2.714191	4.888812	0.775076
35	1	0	-5.177197	5.006678	0.456076
36	6	0	-3.437865	-1.083227	-0.969924
37	6	0	-4.970780	-2.636311	-2.727924
38	6	0	-3.198867	-1.034214	-2.352924
39	6	0	-4.438818	-1.932282	-0.473924
40	6	0	-5.202776	-2.702324	-1.351924

41	6	0	-3.967825	-1.802256	-3.225924
42	1	0	-2.402901	-0.407171	-2.740924
43	1	0	-4.618815	-1.995292	0.594076
44	1	0	-5.975740	-3.356366	-0.959924
45	1	0	-3.772828	-1.760246	-4.293924
46	1	0	-5.562747	-3.241343	-3.407924
47	6	0	-2.559883	-0.743179	1.799076
48	6	0	-2.659819	-1.921185	4.342076
49	6	0	-1.880817	-1.950142	2.049076
50	6	0	-3.277917	-0.130219	2.835076
51	6	0	-3.325884	-0.719221	4.101076
52	6	0	-1.939785	-2.535145	3.313076
53	1	0	-1.307791	-2.423111	1.256076
54	1	0	-3.800968	0.802753	2.658076
55	1	0	-3.884911	-0.235252	4.897076
56	1	0	-1.418734	-3.470117	3.495076
57	1	0	-2.698794	-2.377187	5.327076

TS-S10

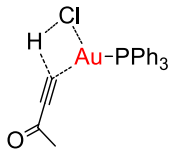


Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	1	0	-6.653943	2.350095	-2.019942
2	1	0	-3.071013	-3.300949	-3.779942
3	6	0	2.675076	3.909980	-0.438942
4	6	0	-3.644955	1.414058	-0.716942
5	6	0	-5.011926	3.691075	-1.621942
6	6	0	-3.702925	3.802058	-1.150942
7	6	0	-2.931996	-1.908951	-2.147942
8	6	0	-4.181965	0.578064	2.276058
9	6	0	-3.497009	-2.982944	-2.832942
10	6	0	-3.794979	-0.522940	4.397058
11	6	0	-2.796988	-1.302953	3.807058
12	6	0	-4.561999	-2.181931	-0.377942
13	6	0	-3.182975	-0.202948	1.678058
14	6	0	-5.121012	-3.259924	-1.064942
15	6	0	2.382092	5.171983	-1.228942
16	6	0	0.932051	1.898001	-0.481942
17	6	0	1.693063	2.860992	-0.486942
18	6	0	-3.017939	2.671050	-0.706942
19	6	0	-4.960956	1.310074	-1.195942
20	6	0	-5.637942	2.444082	-1.646942
21	6	0	-2.483986	-1.141957	2.458058
22	6	0	-4.483967	0.418068	3.631058
23	6	0	-3.467991	-1.489944	-0.919942
24	6	0	-4.593017	-3.659930	-2.293942

25	79	0	-0.186969	0.245015	-0.336942
26	8	0	3.712075	3.789967	0.214058
27	15	0	-2.703973	-0.039954	-0.090942
28	1	0	-3.206913	4.769052	-1.139942
29	1	0	2.229089	4.926985	-2.284942
30	1	0	-1.990938	2.758037	-0.365942
31	1	0	-5.452968	0.343080	-1.224942
32	1	0	-2.060989	-1.403962	-2.555942
33	1	0	-5.027028	-4.502925	-2.823942
34	1	0	-1.697994	-1.741966	2.006058
35	1	0	-5.258959	1.029078	4.084058
36	1	0	-2.254997	-2.033959	4.400058
37	1	0	-4.723956	1.312071	1.688058
38	1	0	-5.540916	4.572081	-1.975942
39	1	0	-4.971995	-1.881926	0.581058
40	1	0	-5.968019	-3.789913	-0.636942
41	1	0	-4.031980	-0.645937	5.450058
42	1	0	3.212101	5.872973	-1.123942
43	1	0	1.455098	5.632995	-0.869942
44	6	0	3.071022	-0.444025	1.529058
45	6	0	3.479038	0.851970	1.834058
46	6	0	2.918015	-1.048023	3.835058
47	6	0	3.339031	0.237971	4.179058
48	6	0	3.617043	1.178968	3.186058
49	6	0	2.780011	-1.407022	2.493058
50	53	0	2.883015	-1.012023	-0.522942
51	1	0	3.934055	2.182964	3.449058
52	1	0	3.445034	0.508970	5.225058
53	1	0	2.436998	-2.396017	2.212058
54	1	0	3.670048	1.604967	1.076058
55	1	0	2.694006	-1.779021	4.607058
56	1	0	7.232011	-1.343077	-2.956942
57	1	0	7.272028	0.003923	-1.781942
58	1	0	7.467007	-1.654080	-1.207942
59	8	0	5.064017	-0.875050	-0.547942
60	6	0	5.457014	-1.139055	-1.781942
61	8	0	4.684010	-1.430045	-2.684942
62	6	0	6.962015	-1.031073	-1.948942
63	17	0	0.136998	-2.392989	-0.101942

TS-S11



Standard orientation:

Center Number	Atomic Number	Atomic Type	Coordinates (Angstroms) X	Y	Z
1	6	0	1.731361	-3.313720	-3.329888
2	1	0	-0.094118	-4.194517	-2.584866

3	1	0	3.500779	-2.200512	-3.859432
4	1	0	3.183317	-0.493144	-2.103510
5	1	0	-0.430329	-2.479892	-0.839231
6	1	0	2.623699	-2.629635	4.916796
7	1	0	3.737296	-3.296337	2.797161
8	1	0	0.810478	-0.927697	4.880270
9	1	0	0.120051	0.106589	2.743229
10	1	0	3.045067	-2.277609	0.656028
11	1	0	4.671977	4.215271	-0.717728
12	1	0	2.230216	4.523211	-1.097107
13	1	0	5.540412	2.007938	0.025697
14	1	0	3.989301	0.118586	0.373539
15	1	0	0.672799	2.656369	-0.756305
16	6	0	0.628310	-3.391400	-2.474739
17	6	0	2.647989	-2.270749	-3.191046
18	6	0	2.471323	-1.306485	-2.195732
19	6	0	0.442042	-2.428319	-1.485117
20	1	0	1.869926	-4.060059	-4.106792
21	6	0	1.368636	-1.383305	-1.332764
22	6	0	2.952280	-2.546494	2.787687
23	6	0	1.306729	-1.216047	3.959202
24	6	0	0.916163	-0.633937	2.752954
25	6	0	2.566466	-1.965358	1.578896
26	6	0	2.325192	-2.172514	3.977594
27	6	0	1.548205	-1.000190	1.555190
28	6	0	2.622152	3.554691	-0.801716
29	6	0	4.479671	2.140056	-0.164678
30	6	0	3.604821	1.072336	0.022253
31	6	0	1.737585	2.488055	-0.623918
32	6	0	3.988797	3.381625	-0.581651
33	6	0	2.229962	1.236159	-0.224554
34	15	0	1.065850	-0.155850	-0.000852
35	79	0	-1.171939	0.455607	-0.028596
36	6	0	-3.305194	1.038540	-0.056526
37	6	0	-3.941922	-0.017955	-0.006968
38	6	0	-4.681495	-1.269630	0.049874
39	8	0	-4.094545	-2.339609	0.034514
40	6	0	-6.185655	-1.140642	0.145308
41	1	0	-6.638493	-2.119739	-0.025534
42	1	0	-6.566532	-0.407887	-0.573756
43	1	0	-6.456850	-0.784934	1.146884
44	17	0	-1.899180	3.645116	-0.057033
45	1	0	-2.891671	2.210391	-0.067976
