

Electronic Supporting information for:

Auriferous alkynylselenolatoalkylidynes

Benjamin J. Frogley,^a Anthony F. Hill^{*a} and Chee S. Onn^a

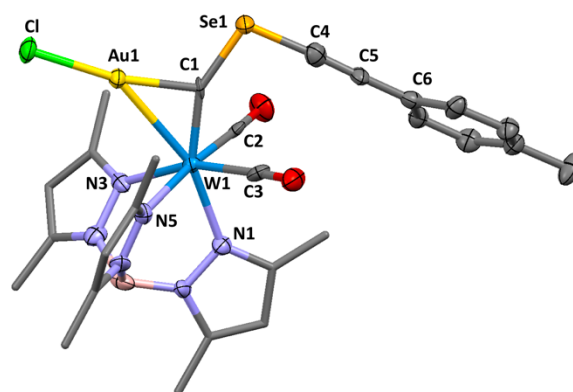


Figure S1. Molecular structure of **3d** in a crystal of **3d**·(CH₂Cl₂)_{0.5} showing 50% thermal probability ellipsoids. Pyrazolyl groups are simplified and hydrogen atoms are not shown for clarity. Selected distances [Å] and angles [°]: W1–C1 1.902(13), W1–Au1 2.8174(7), C1–Au1 1.990(11), Au1–Cl1 2.278(3), C1–Se1 1.890(12), Se1–C4 1.858(15), C4–C5 1.186(19), C5–C21 1.425(19), W1–C1–Se1 151.4(7), W1–C1–Au1 92.7(5), C1–Se1–C4 99.3(6), Se1–C4–C5 176.9(13).

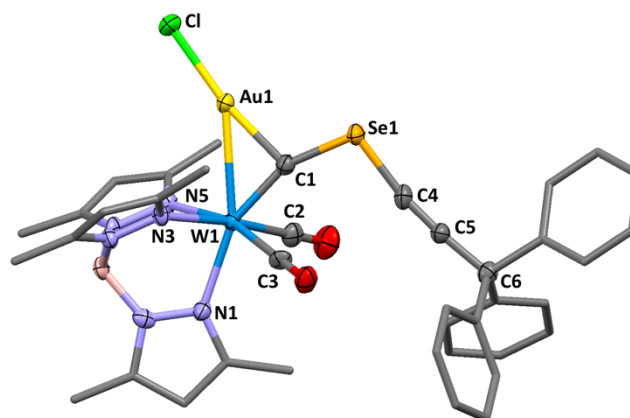
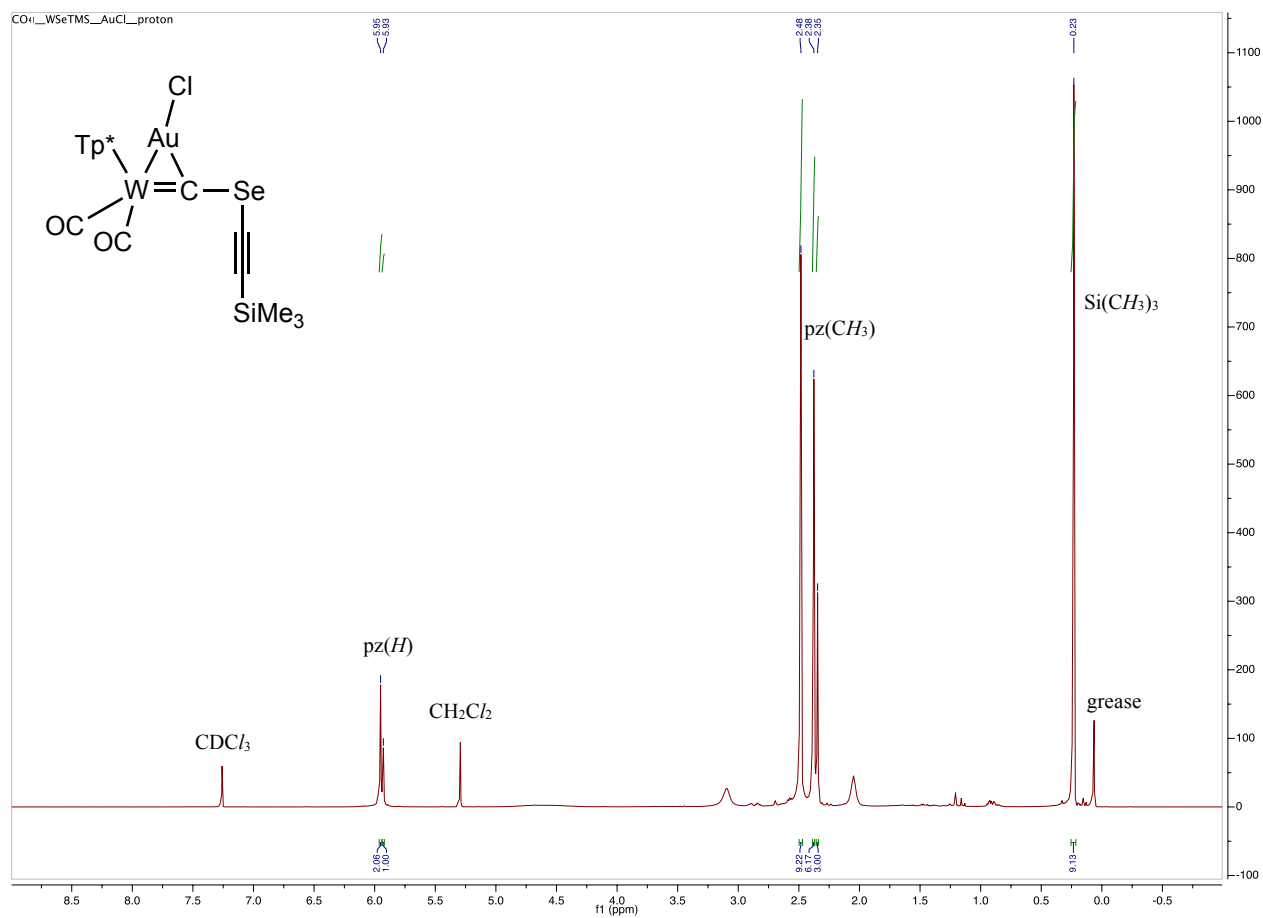
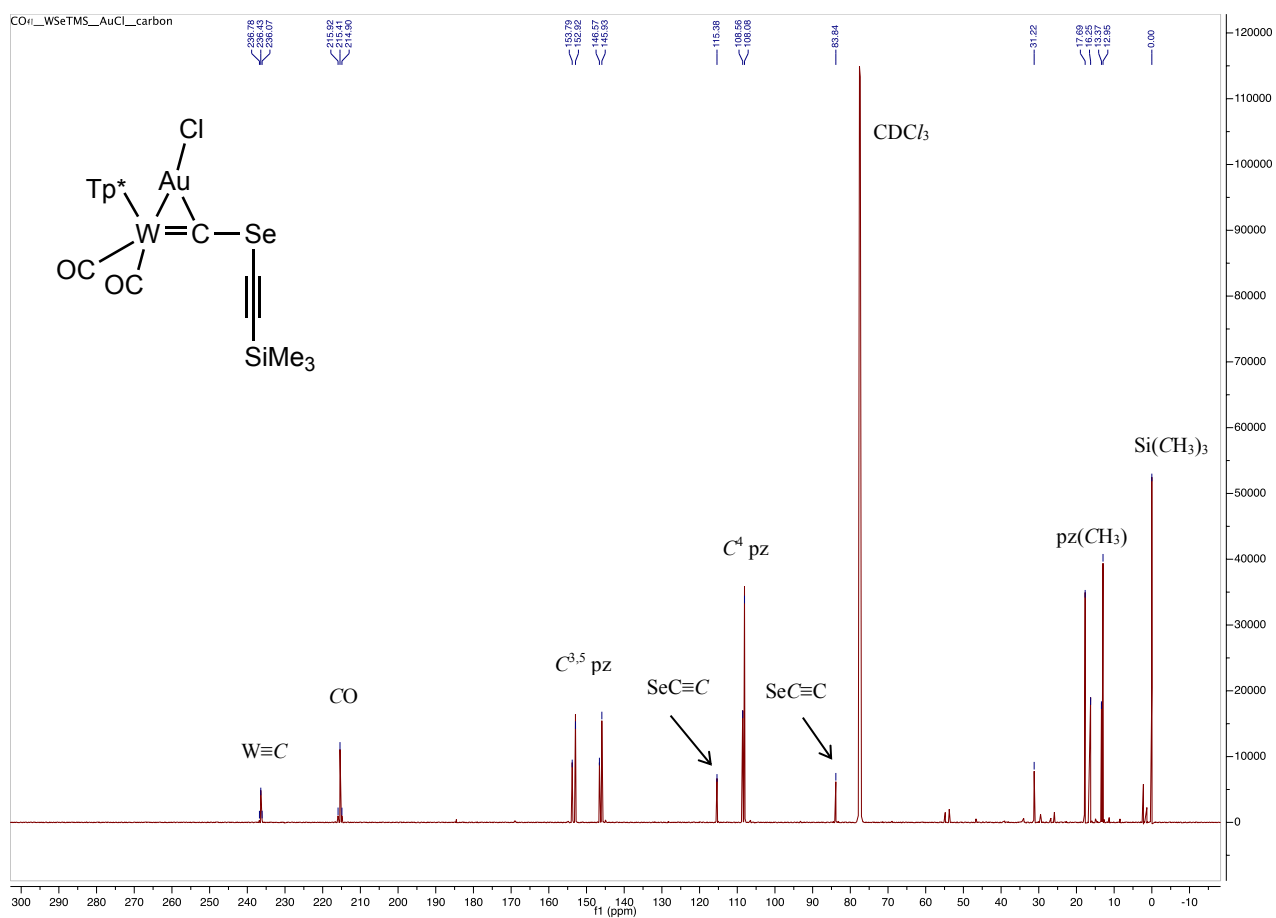


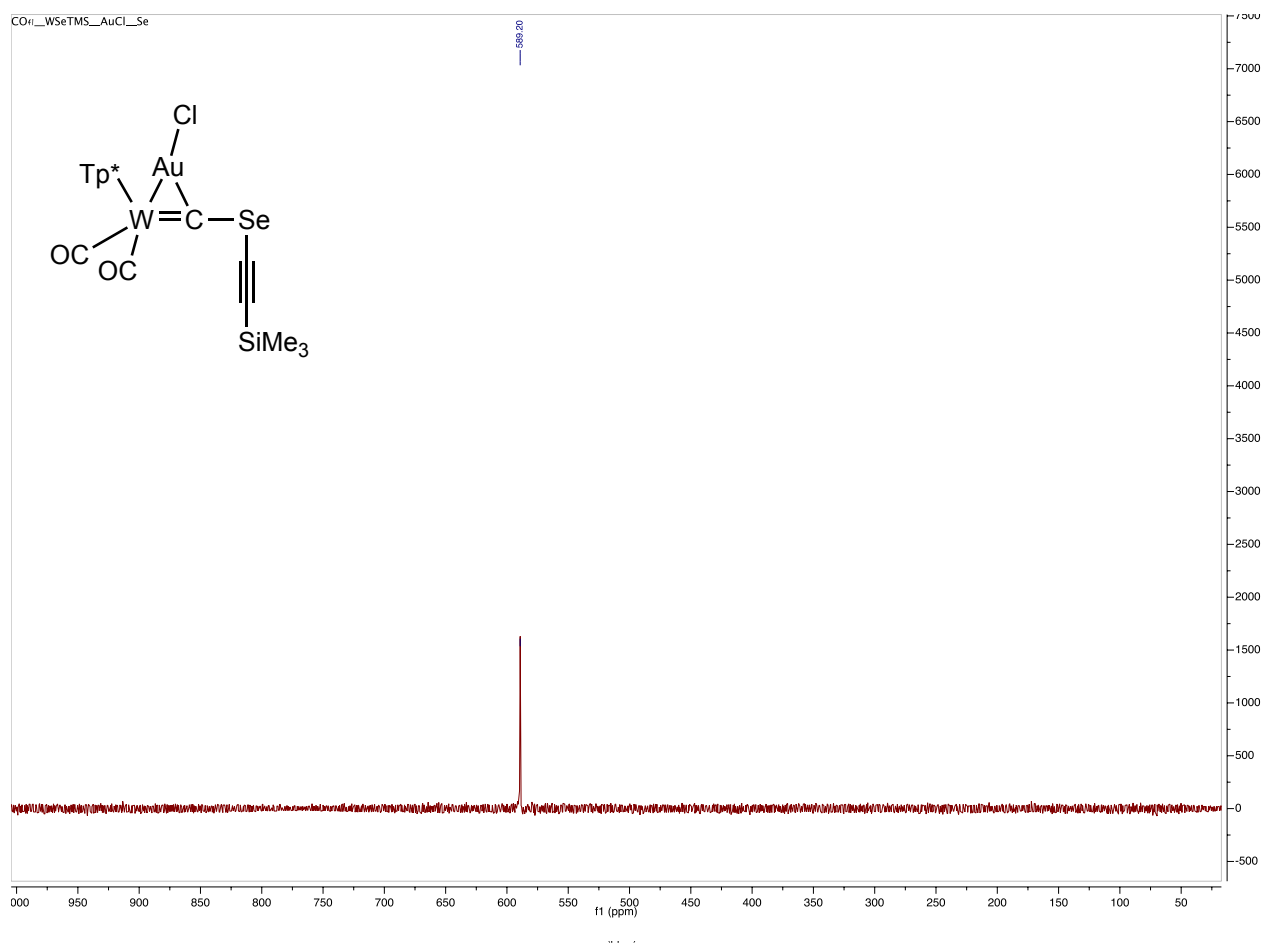
Figure S2. Molecular structure of **3f** showing 50% thermal probability ellipsoids. Pyrazolyl groups and phenyl rings are simplified and hydrogen atoms are not shown for clarity. Selected distances [Å] and angles [°]: W1–C1 1.884(7), W1–Au1 2.7784(4), C1–Au1 2.038(7), Au1–Cl1 2.2776(18), C1–Se1 1.876(7), Se1–C4 1.842(7), C4–C5 1.214(11), C5–C6 1.452(10), W1–C1–Se1 157.1(4), W1–C1–Au1 90.1(3), C1–Au1–Cl1 171.1(2), W1–Au1–Cl1 145.86(5), C1–Se1–C4 102.1(3), Se1–C4–C5 171.2(7), C4–C5–C6 175.1(8).



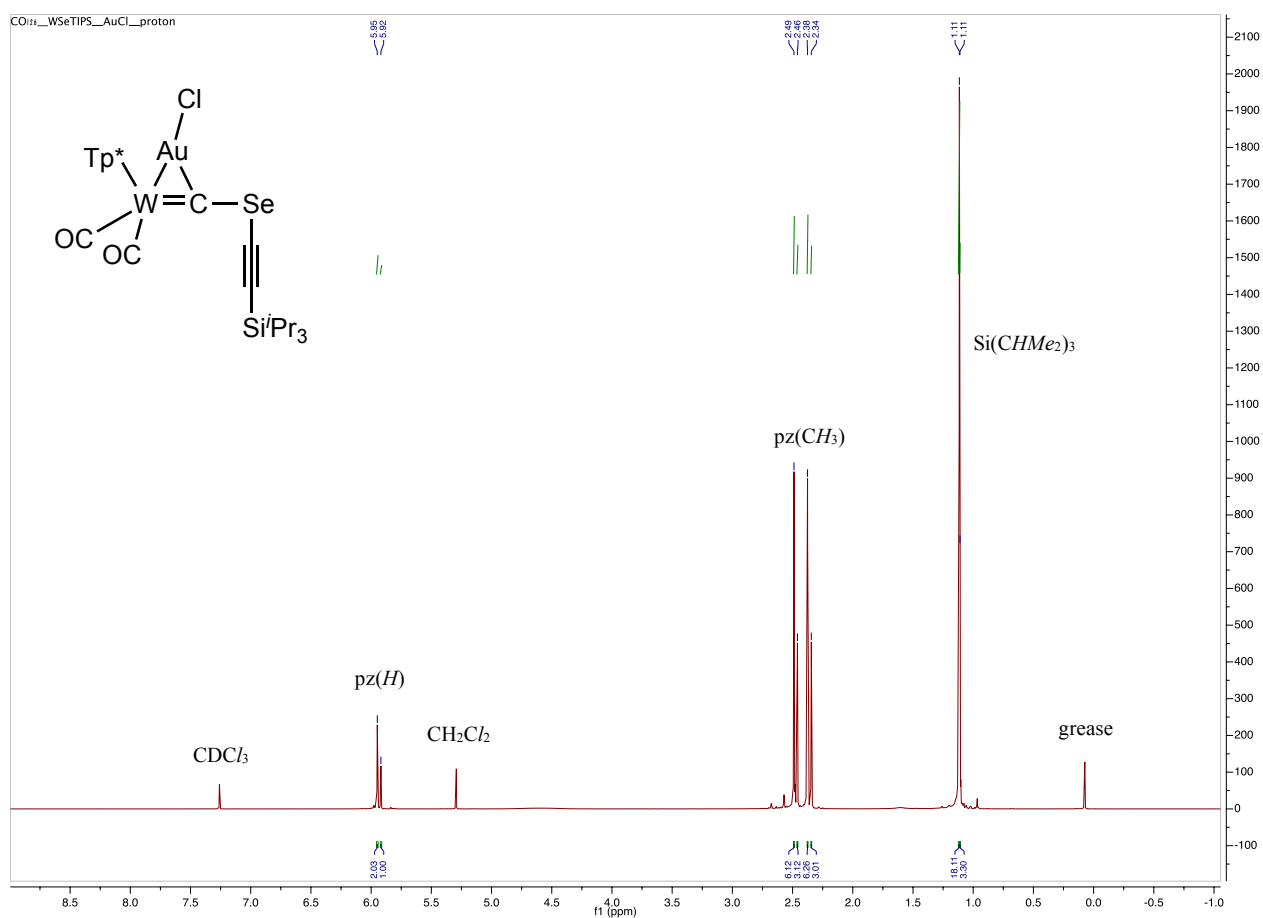
^1H NMR SPECTRUM (600 MHz , CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CSiMe}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3a**).



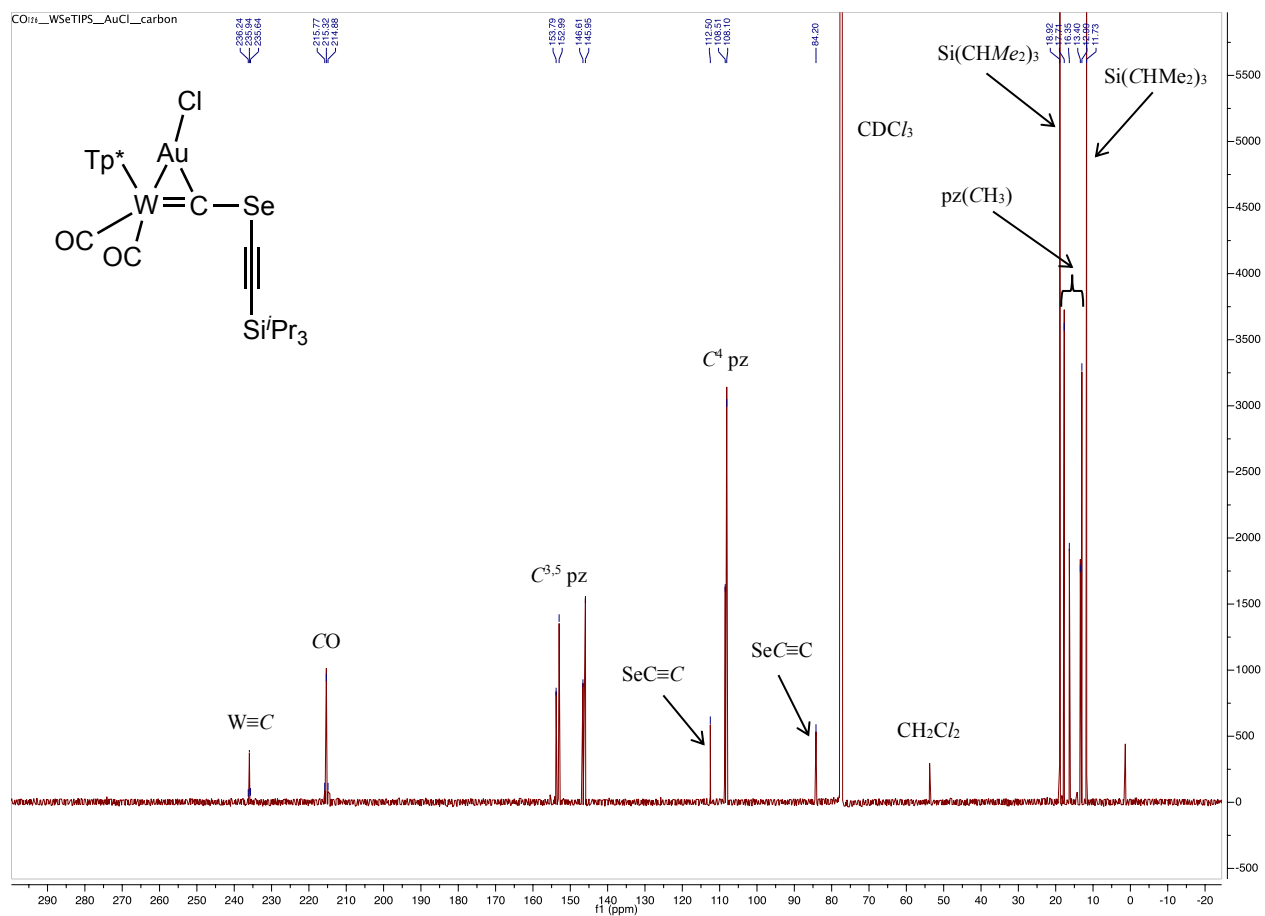
$^{13}\text{C}\{^1\text{H}\}$ NMR SPECTRUM (151 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CSiMe}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3a**).



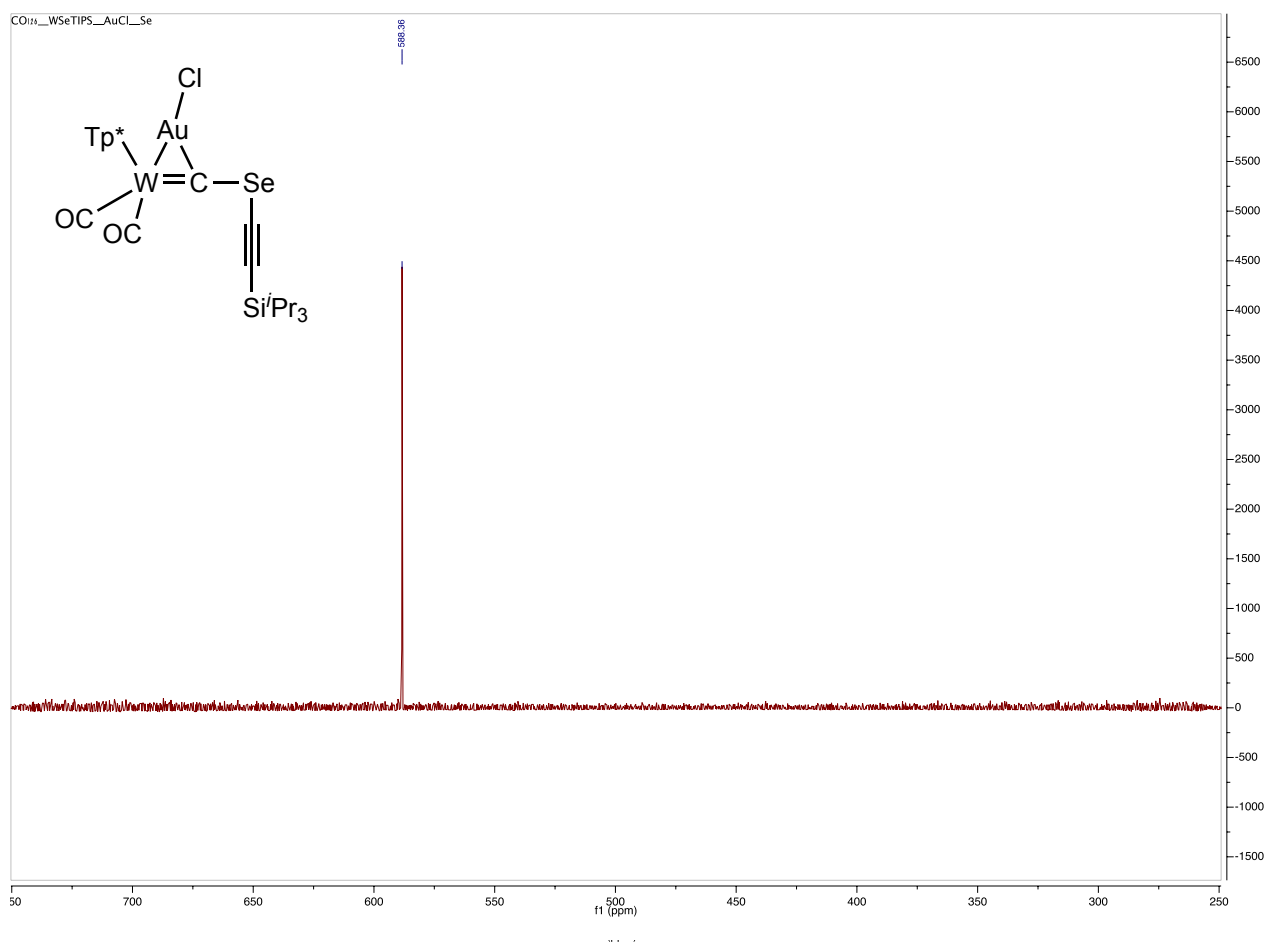
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (76 MHz, CDCl_3 , 25 °C, δ) of $[WAuCl(\mu-CSeC\equiv CSiMe_3)(CO)_2(Tp^*)]$ (**3a**).



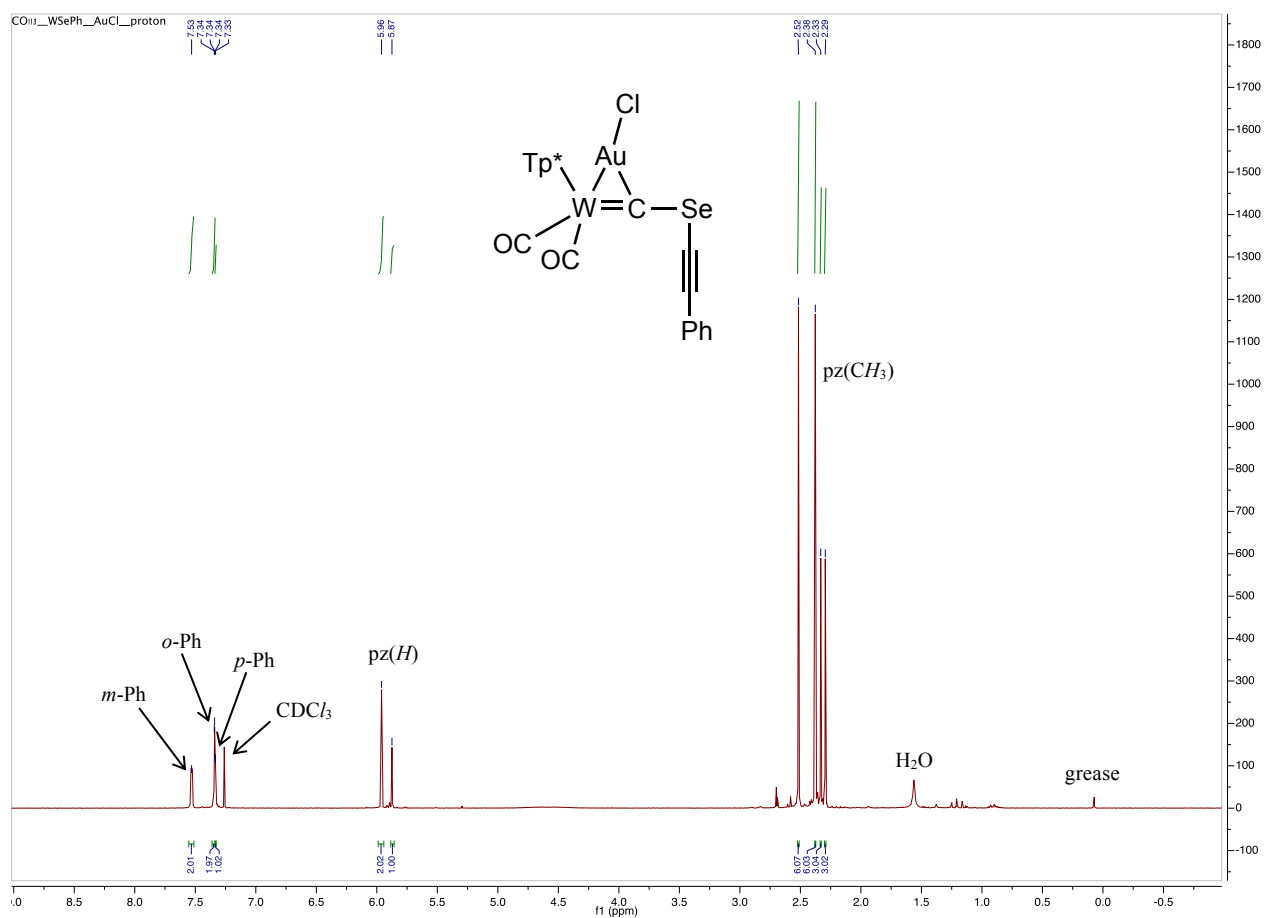
^1H NMR SPECTRUM (700 MHz , CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CSi}^i\text{Pr}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3b**).



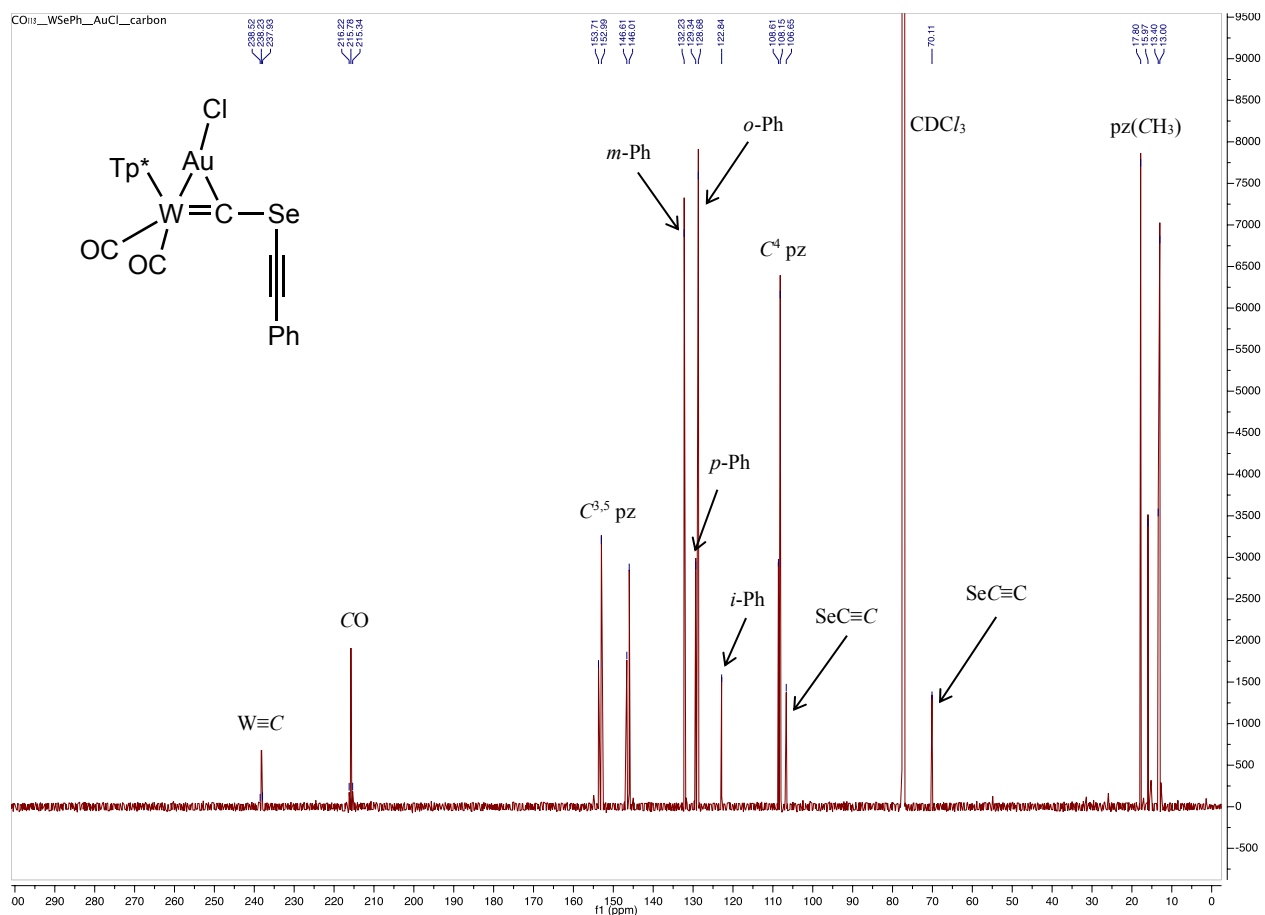
$^{13}\text{C}\{^1\text{H}\}$ NMR SPECTRUM (176 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CSi}^i\text{Pr}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3b**).



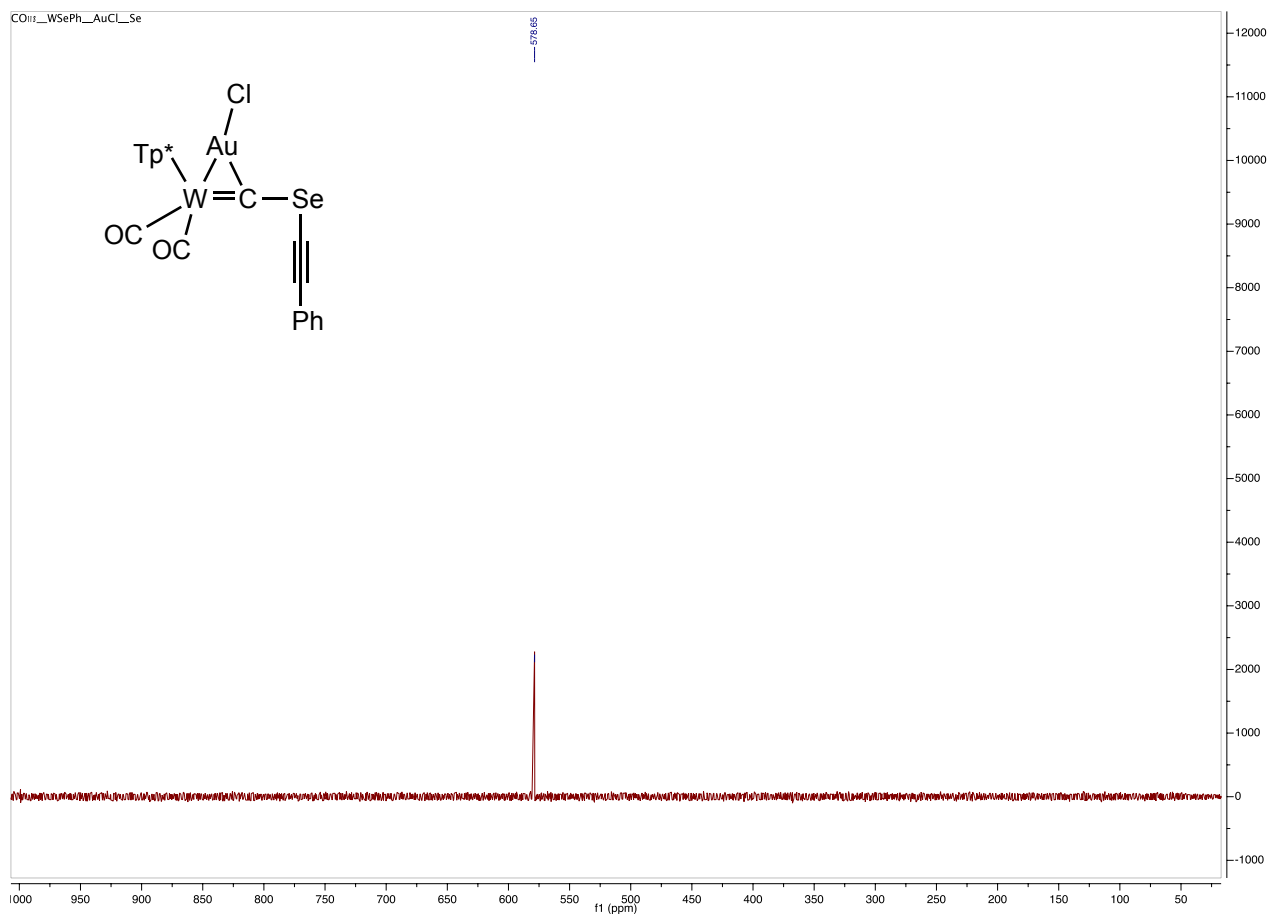
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (76 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CSi}^t\text{Pr}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3b**).



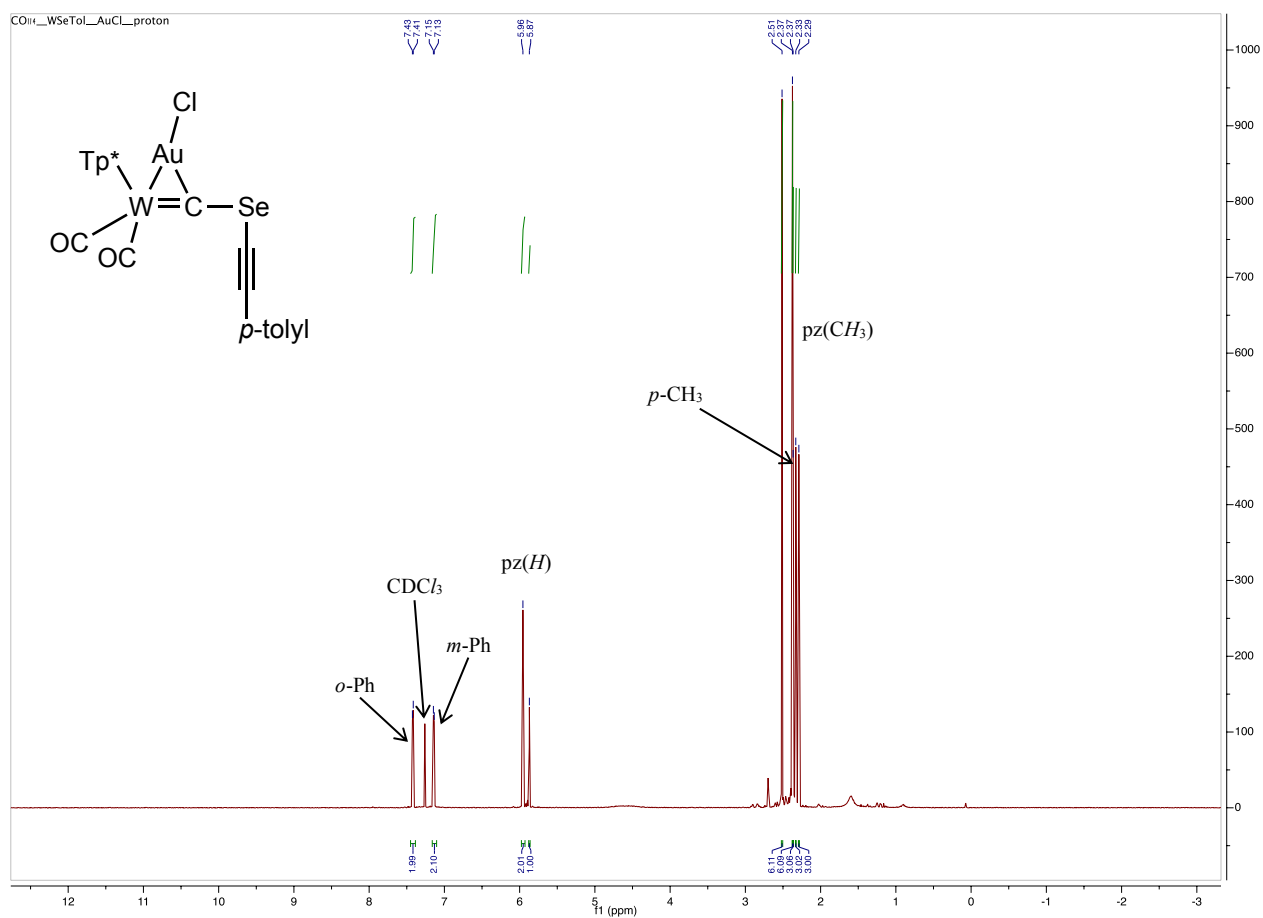
^1H NMR SPECTRUM (700 MHz , CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CPh})(\text{CO})_2(\text{Tp}^*)]$ (**3c**).



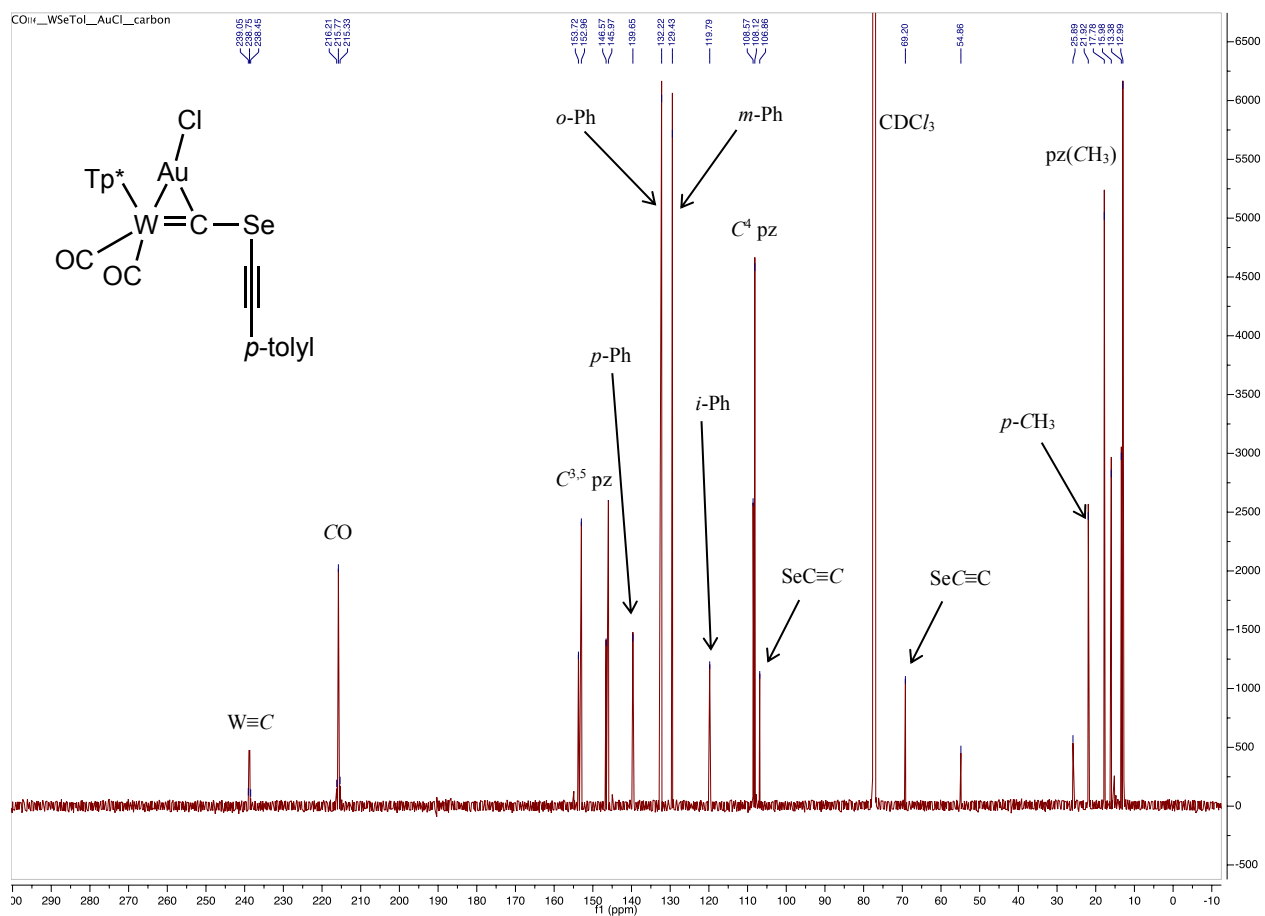
$^{13}C\{^1H\}$ NMR SPECTRUM (176 MHz, $CDCl_3$, 25°C, δ) of $[WAuCl(\mu-CSeC\equiv CPh)(CO)_2(Tp^*)]$ (3c).



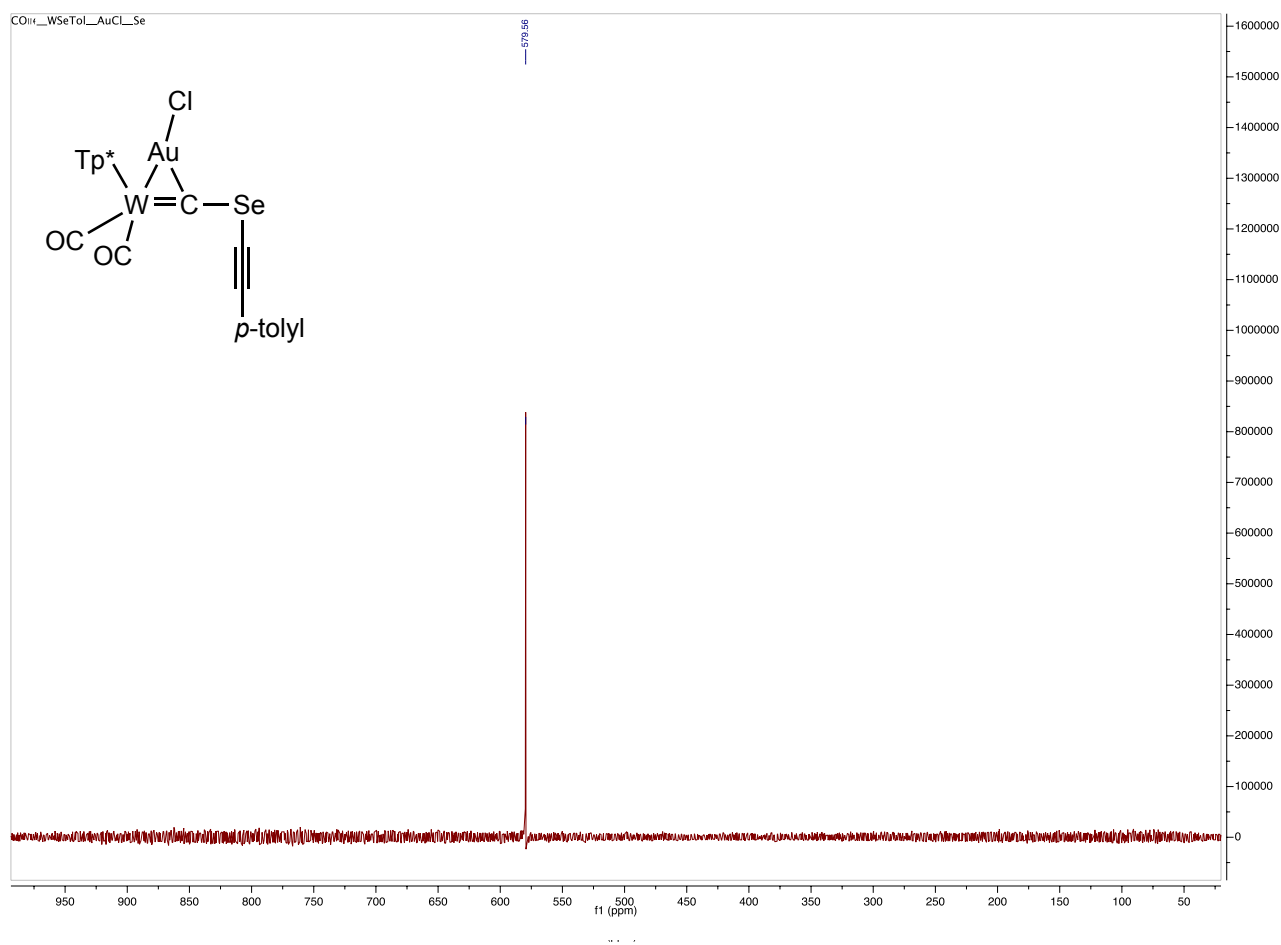
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (76 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CPh})(\text{CO})_2(\text{Tp}^*)]$ (**3c**).



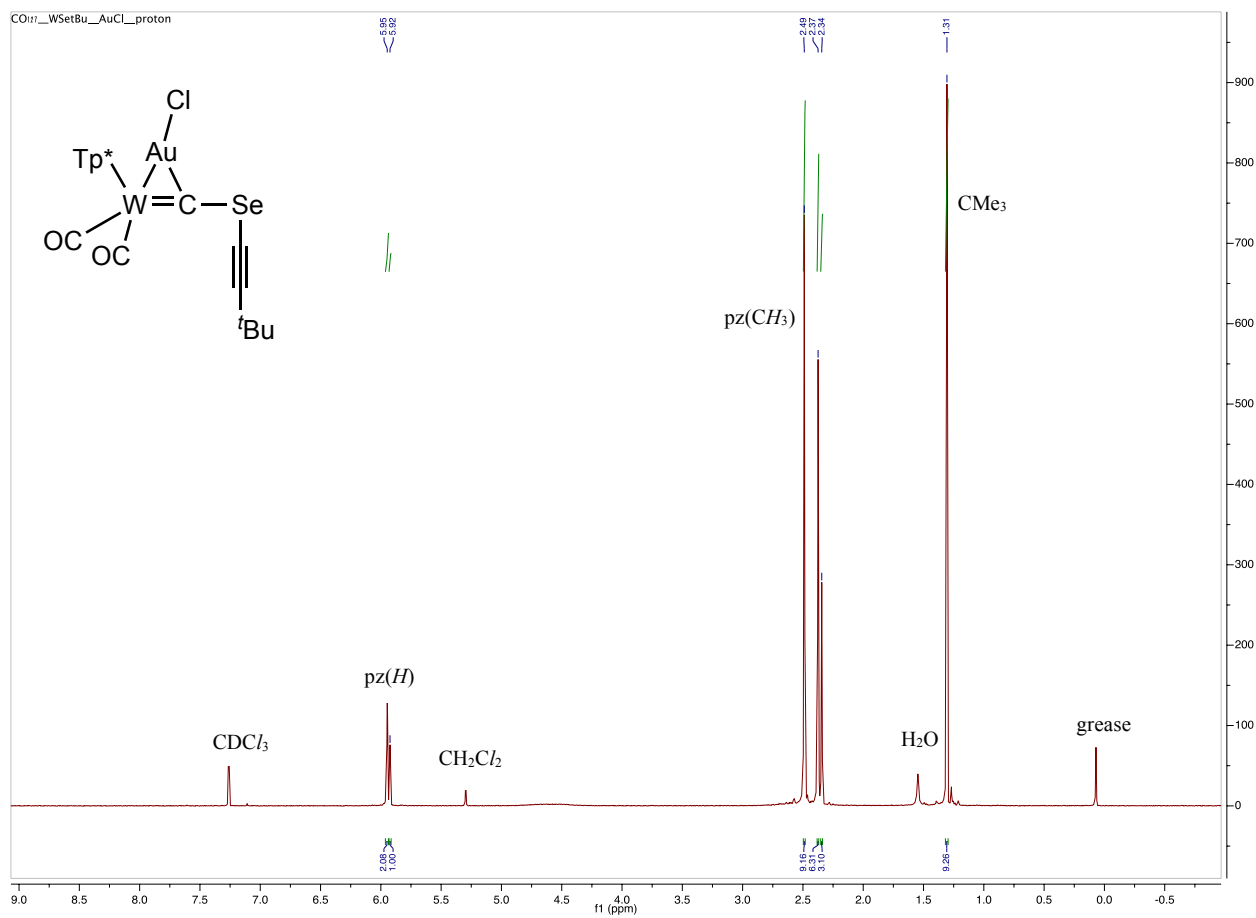
^1H NMR SPECTRUM (700 MHz , CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{Cp-tol})(\text{CO})_2(\text{Tp}^*)]$ (**3d**).



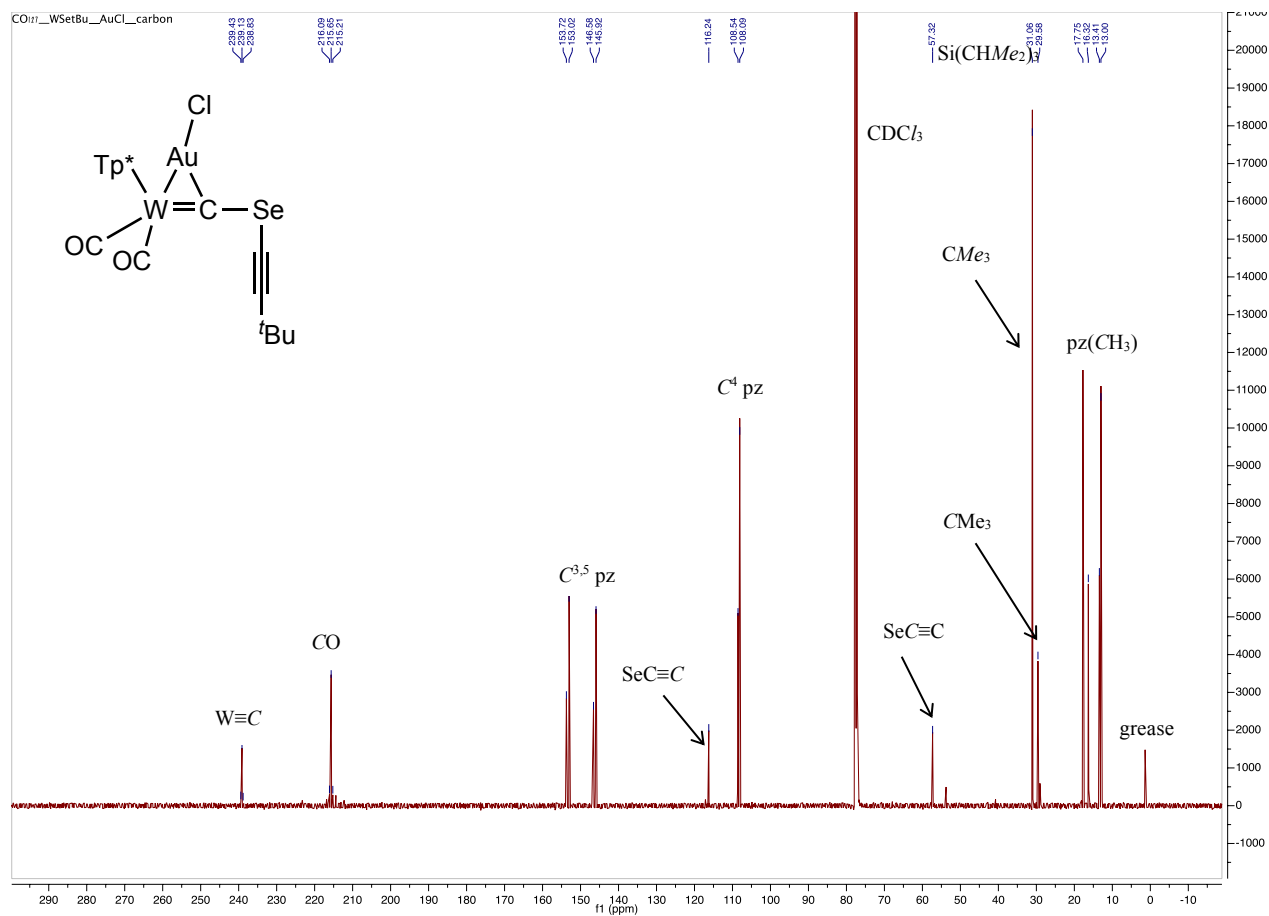
$^{13}\text{C}\{^1\text{H}\}$ NMR SPECTRUM (176 MHz, CDCl_3 , 25°C, δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{Cp-tol})(\text{CO})_2(\text{Tp}^*)]$ (**3d**).



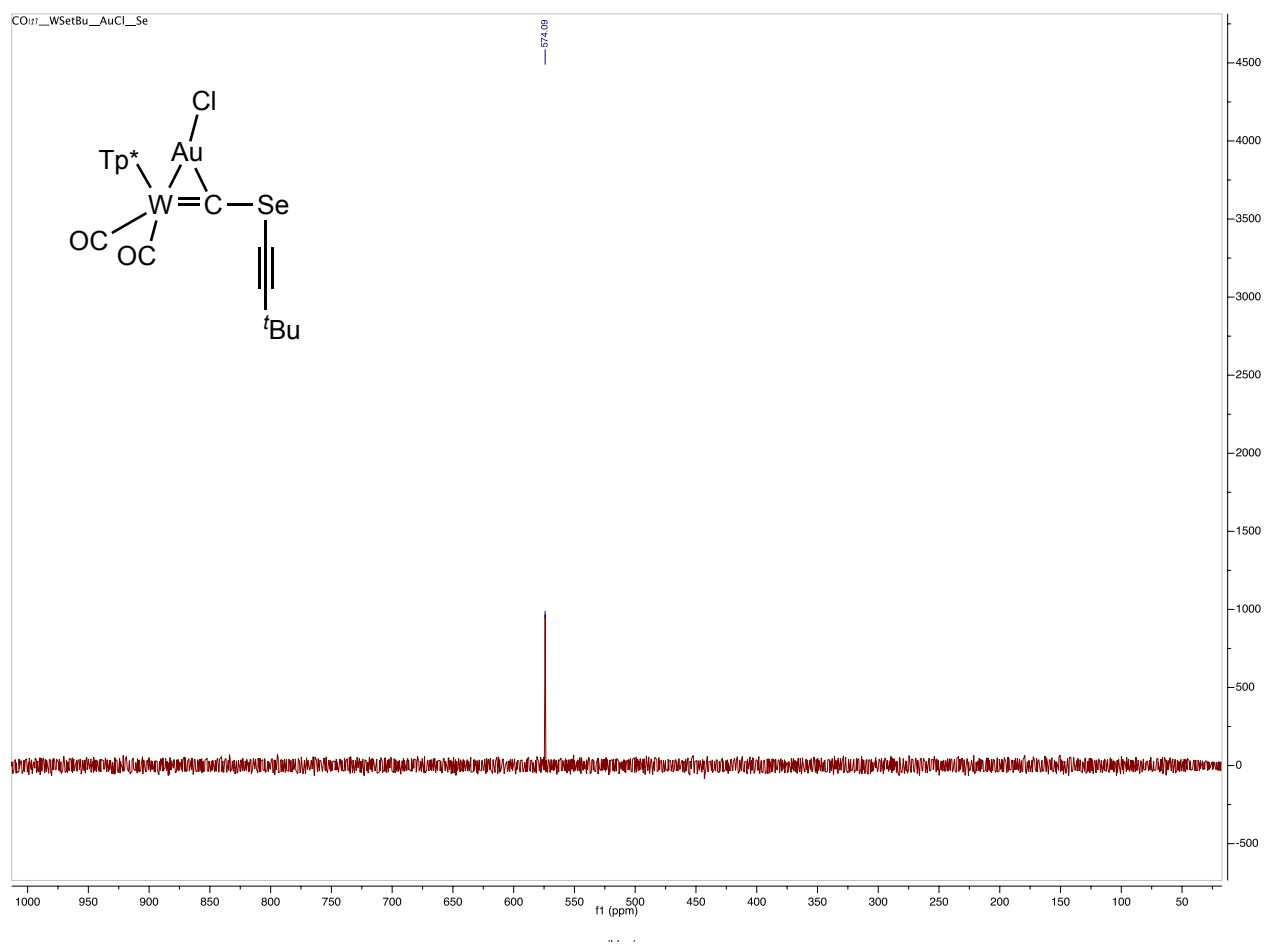
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (76 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{Cp-tol})(\text{CO})_2(\text{Tp}^*)]$ (**3d**).



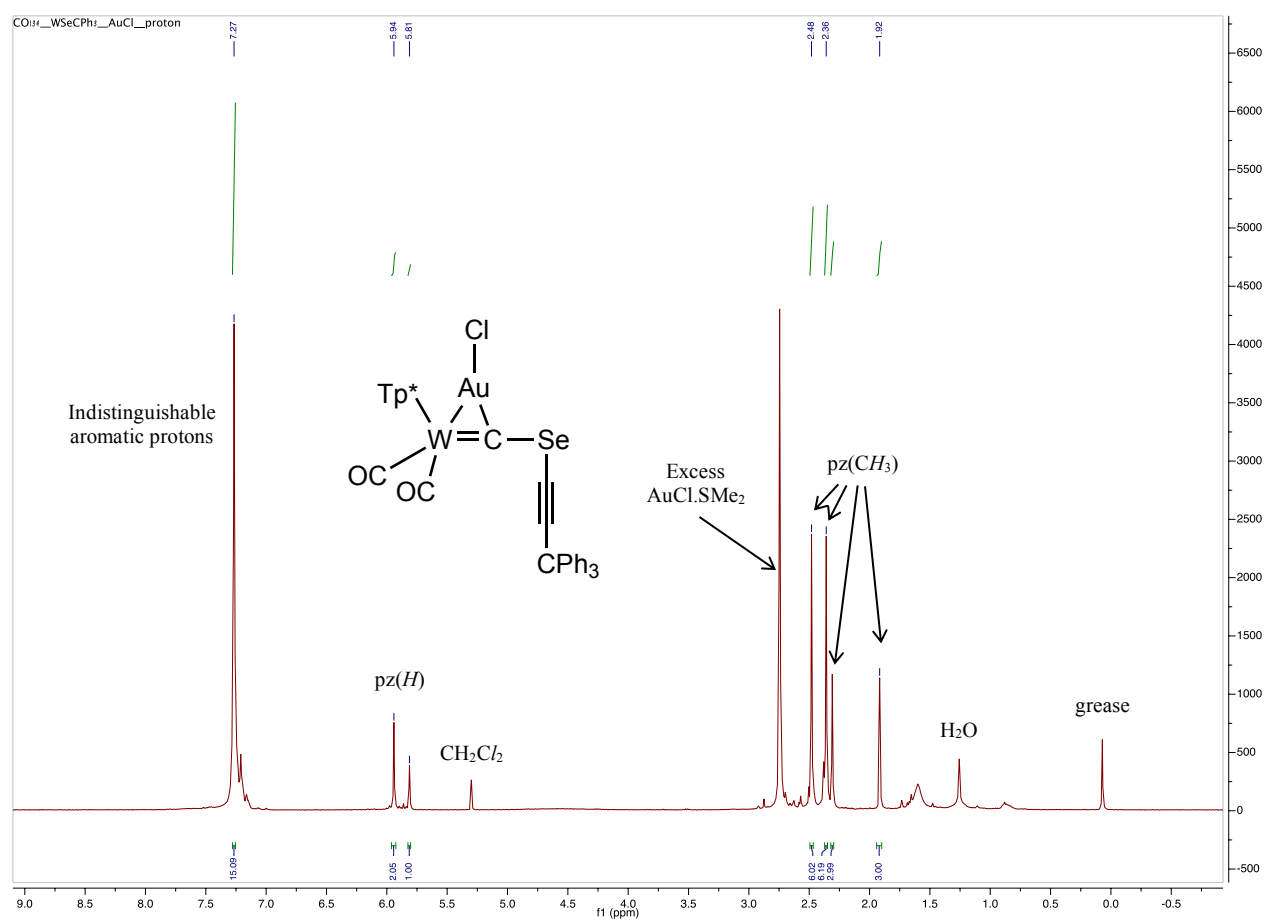
^1H NMR SPECTRUM (700 MHz , CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{C}^t\text{Bu})(\text{CO})_2(\text{Tp}^*)]$ (**3e**).



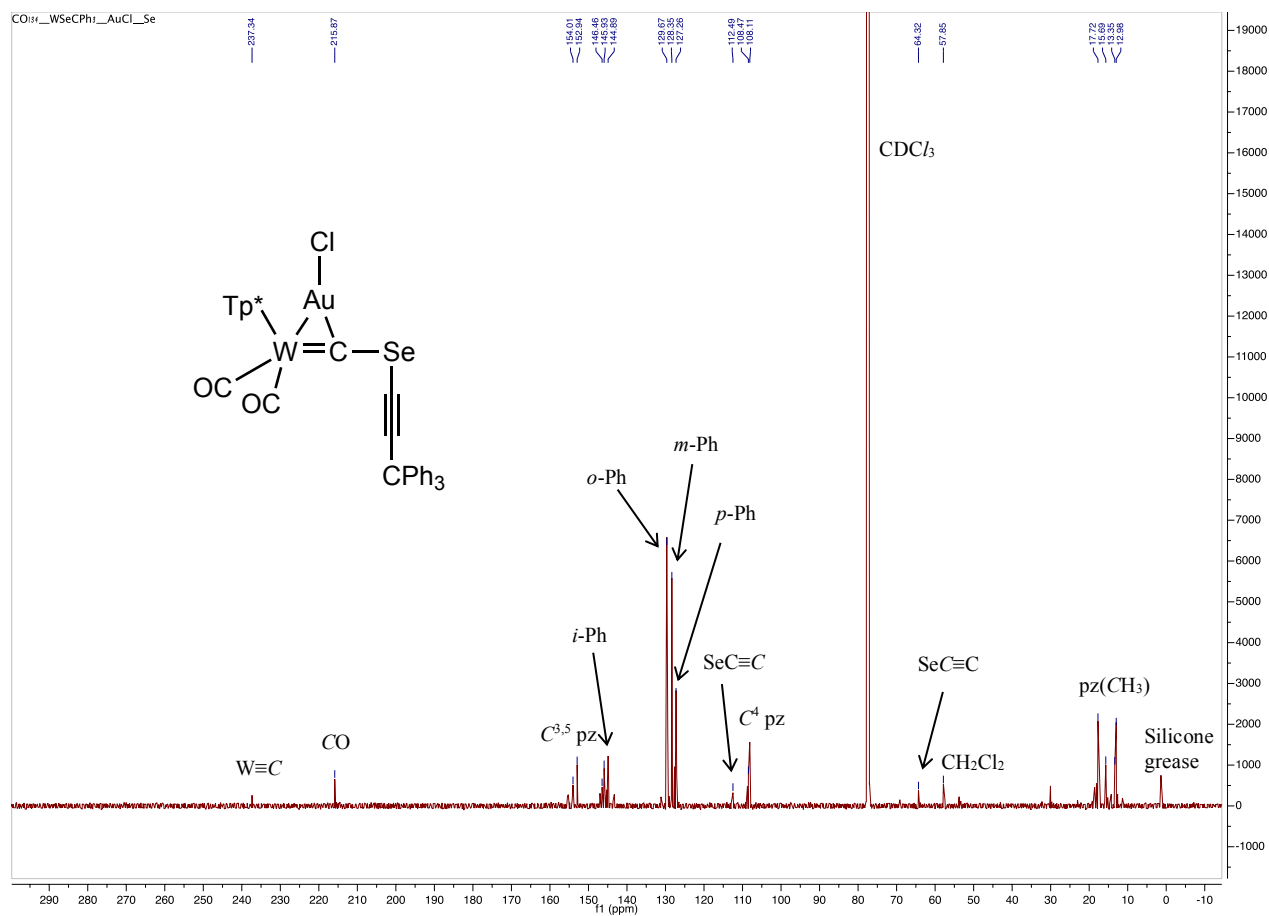
$^{13}C\{^1H\}$ NMR SPECTRUM (176 MHz, $CDCl_3$, 25°C, δ) of $[WAuCl(\mu-CSeC\equiv tBu)(CO)_2(Tp^*)]$ (3e).



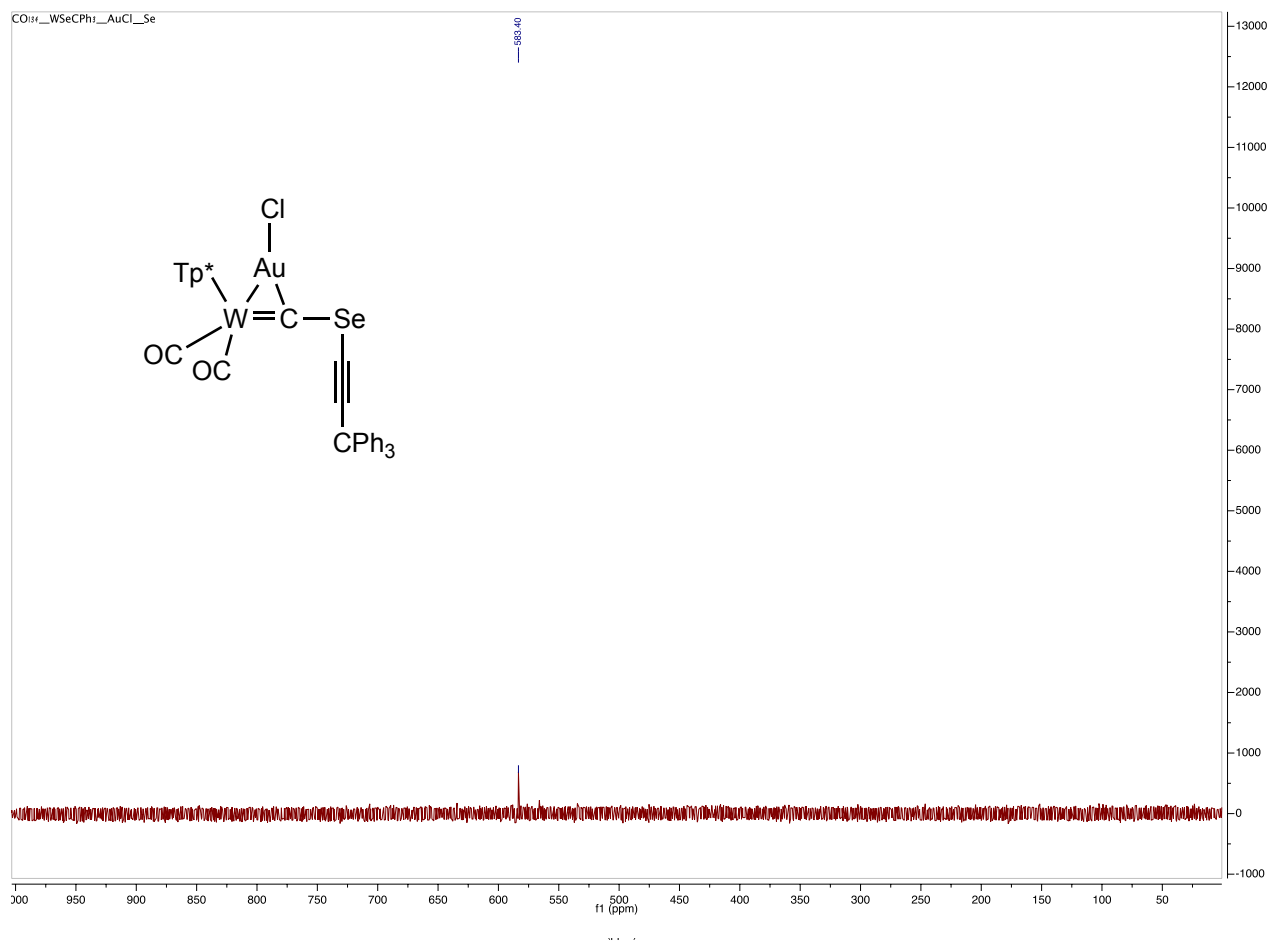
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (76 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{C}^t\text{Bu})(\text{CO})_2(\text{Tp}^*)]$ (**3e**).



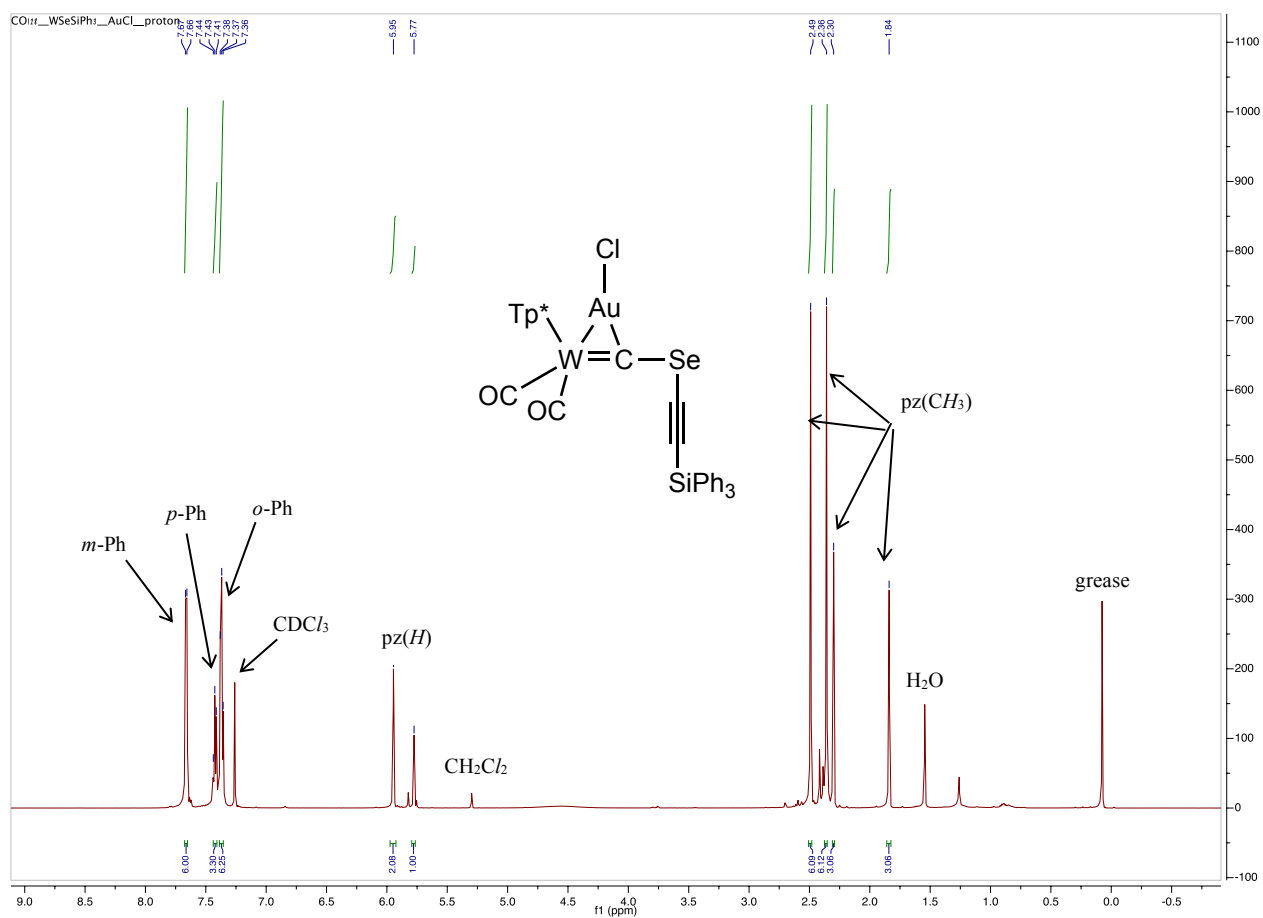
^1H NMR SPECTRUM (400 MHz, CDCl_3 , 25°C, δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3f**).



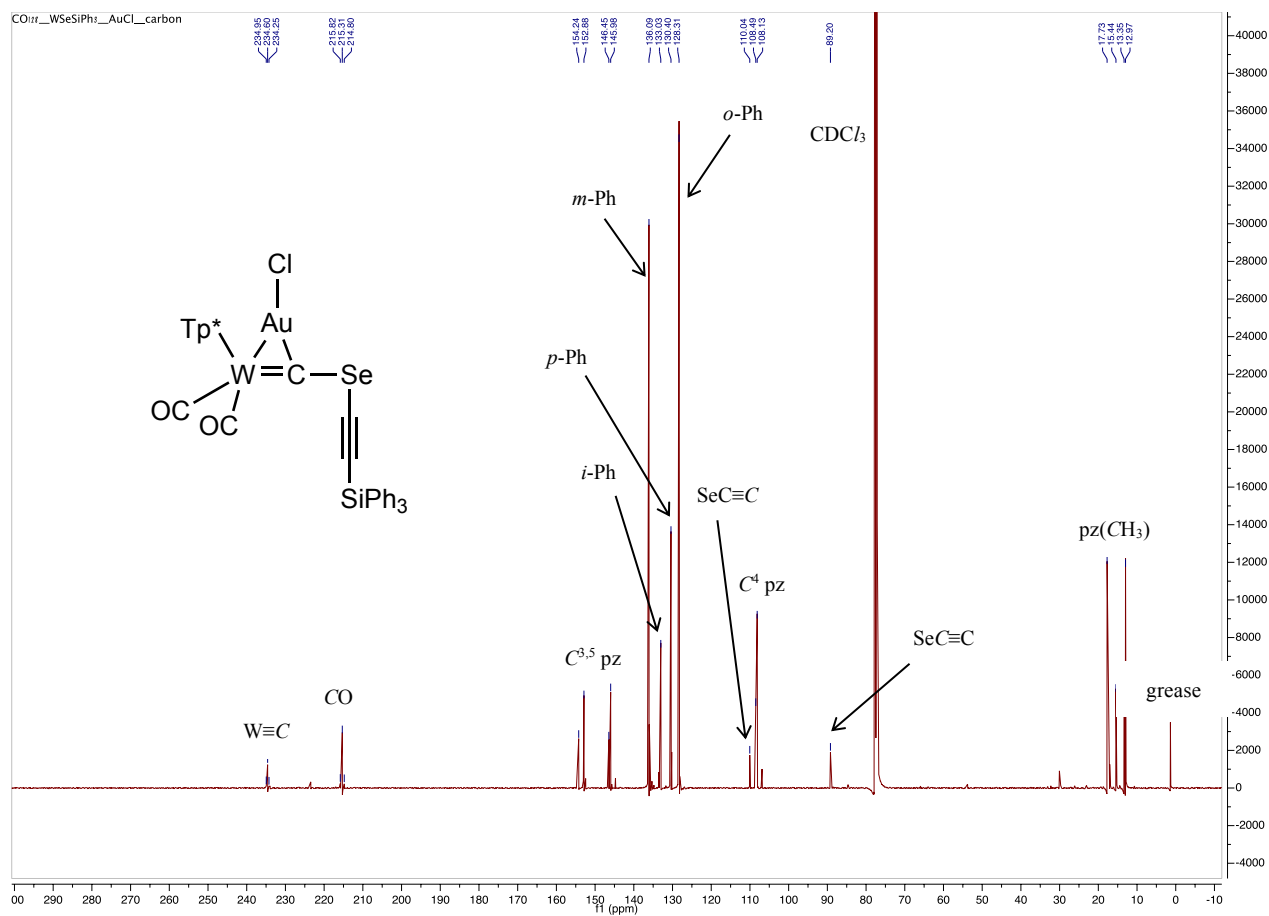
$^{13}\text{C}\{^1\text{H}\}$ NMR SPECTRUM (176 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CCPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3f**).

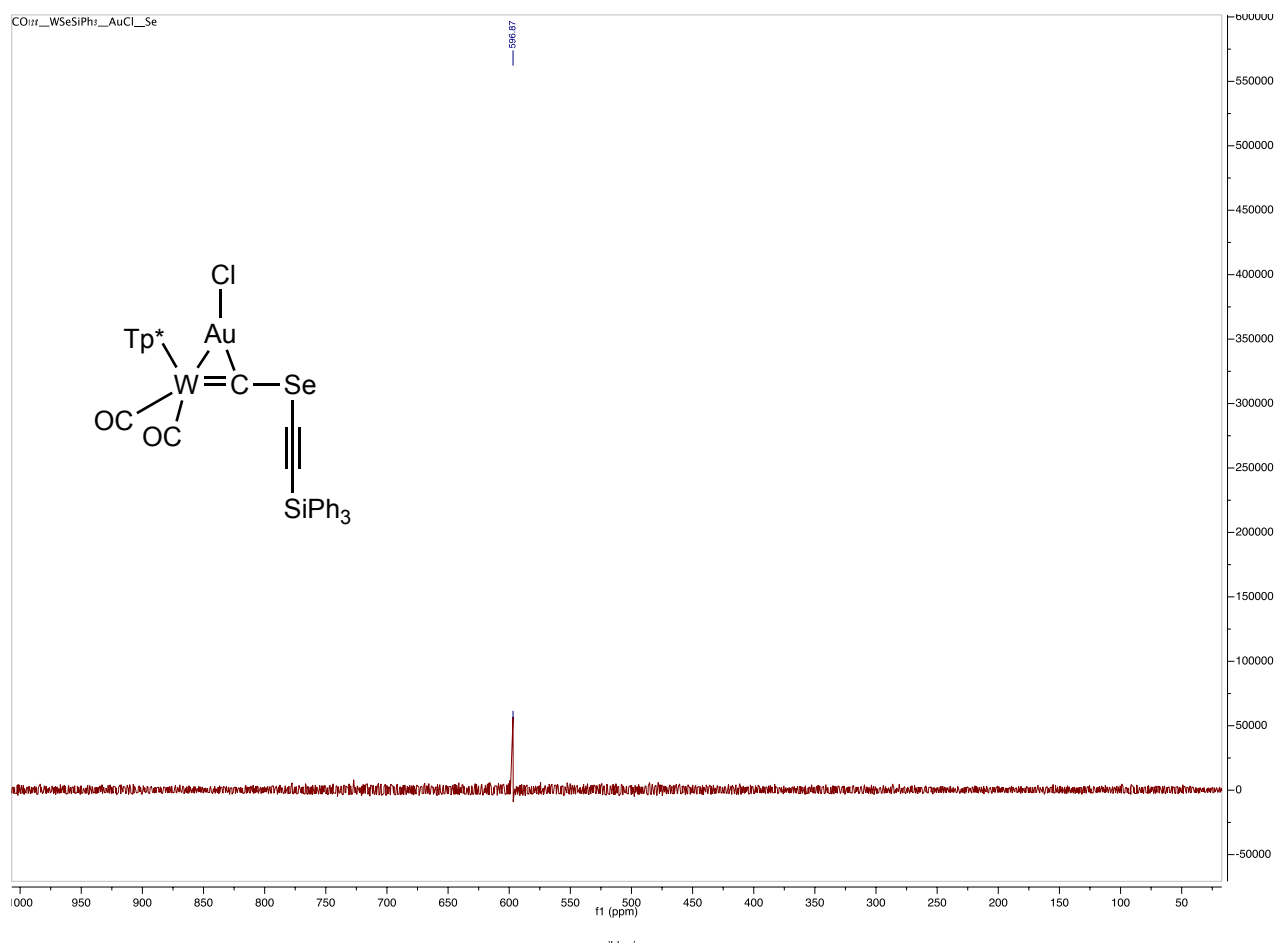


$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (134 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3f**).

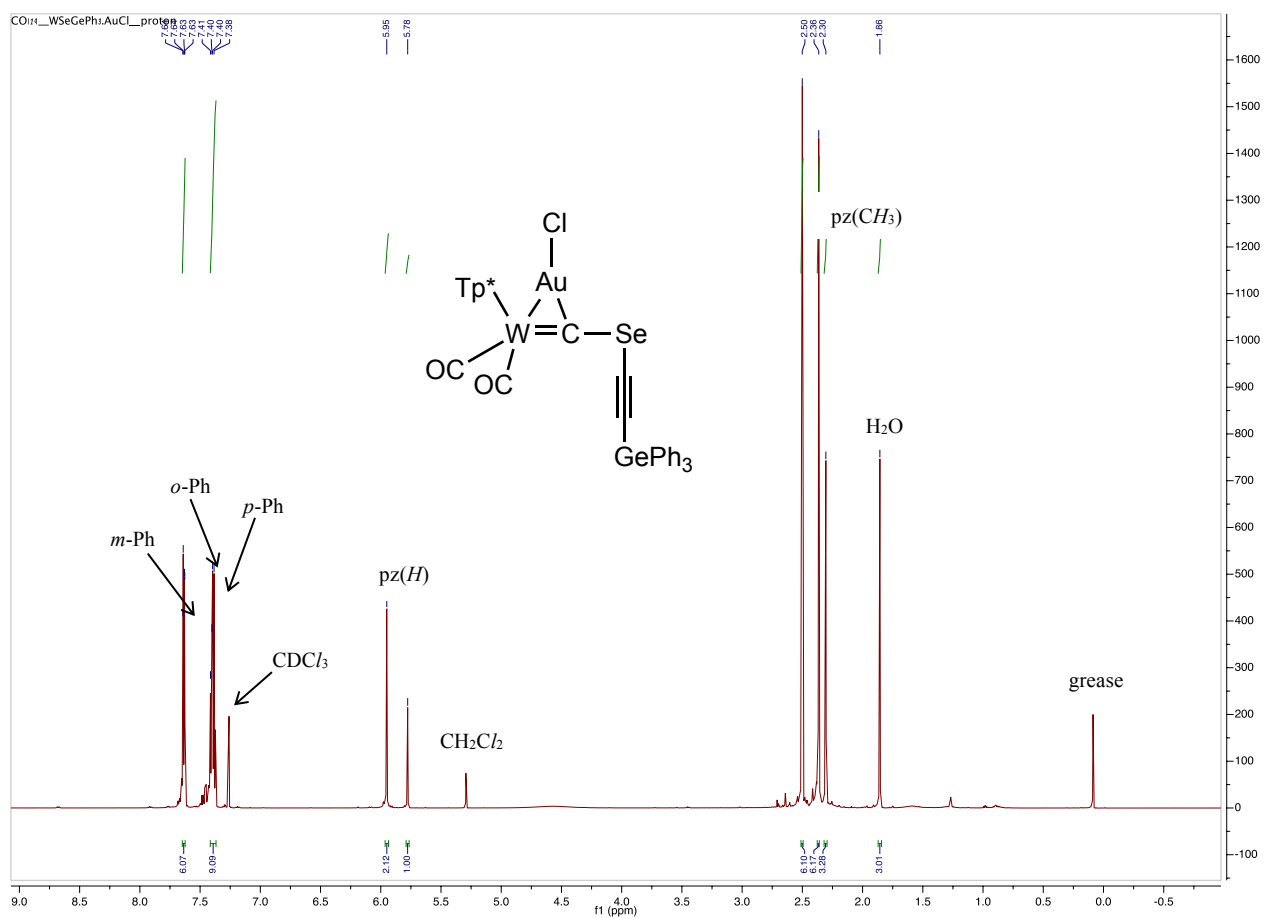


^1H NMR SPECTRUM (400 MHz, CDCl_3 , 25°C, δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CSiPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3g**).

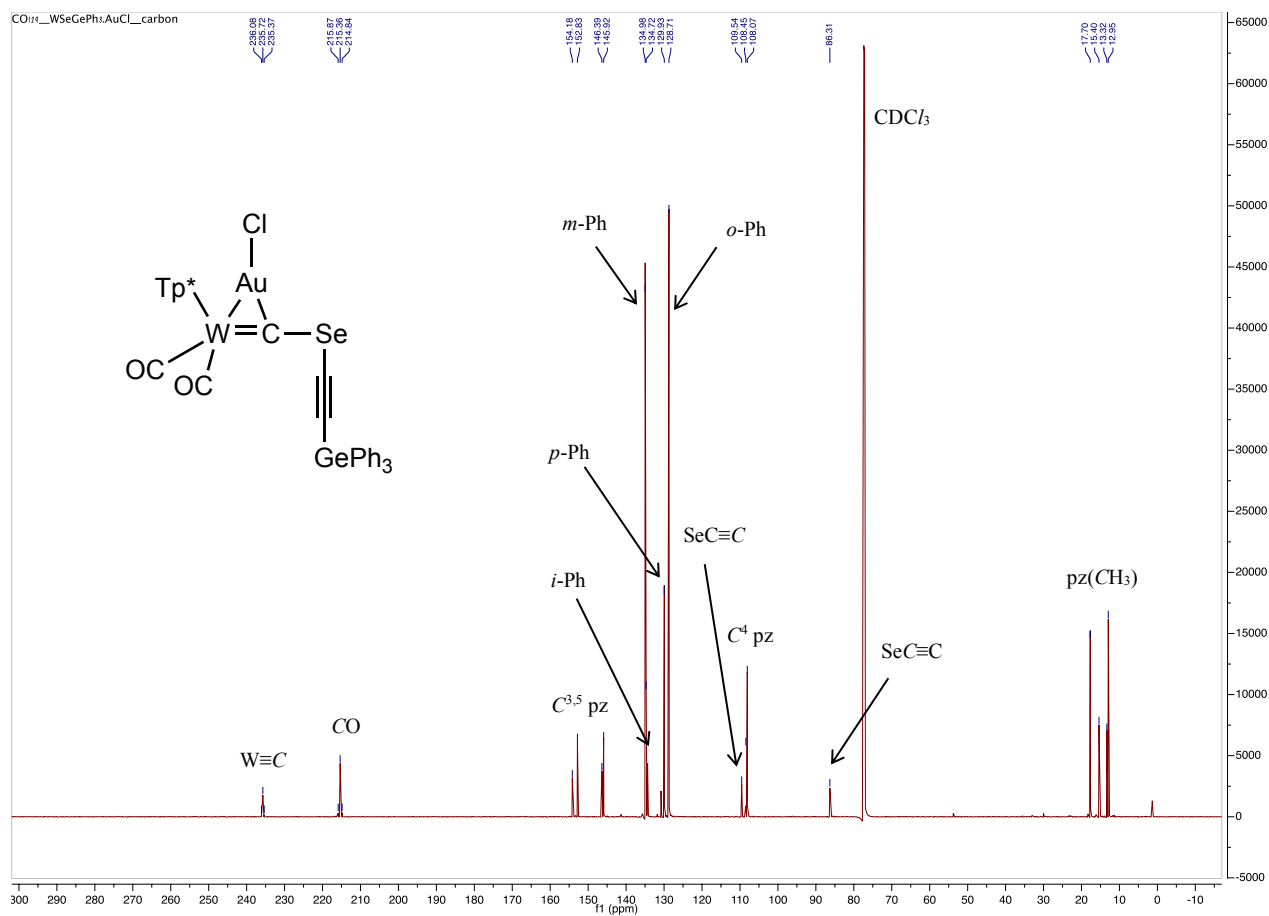




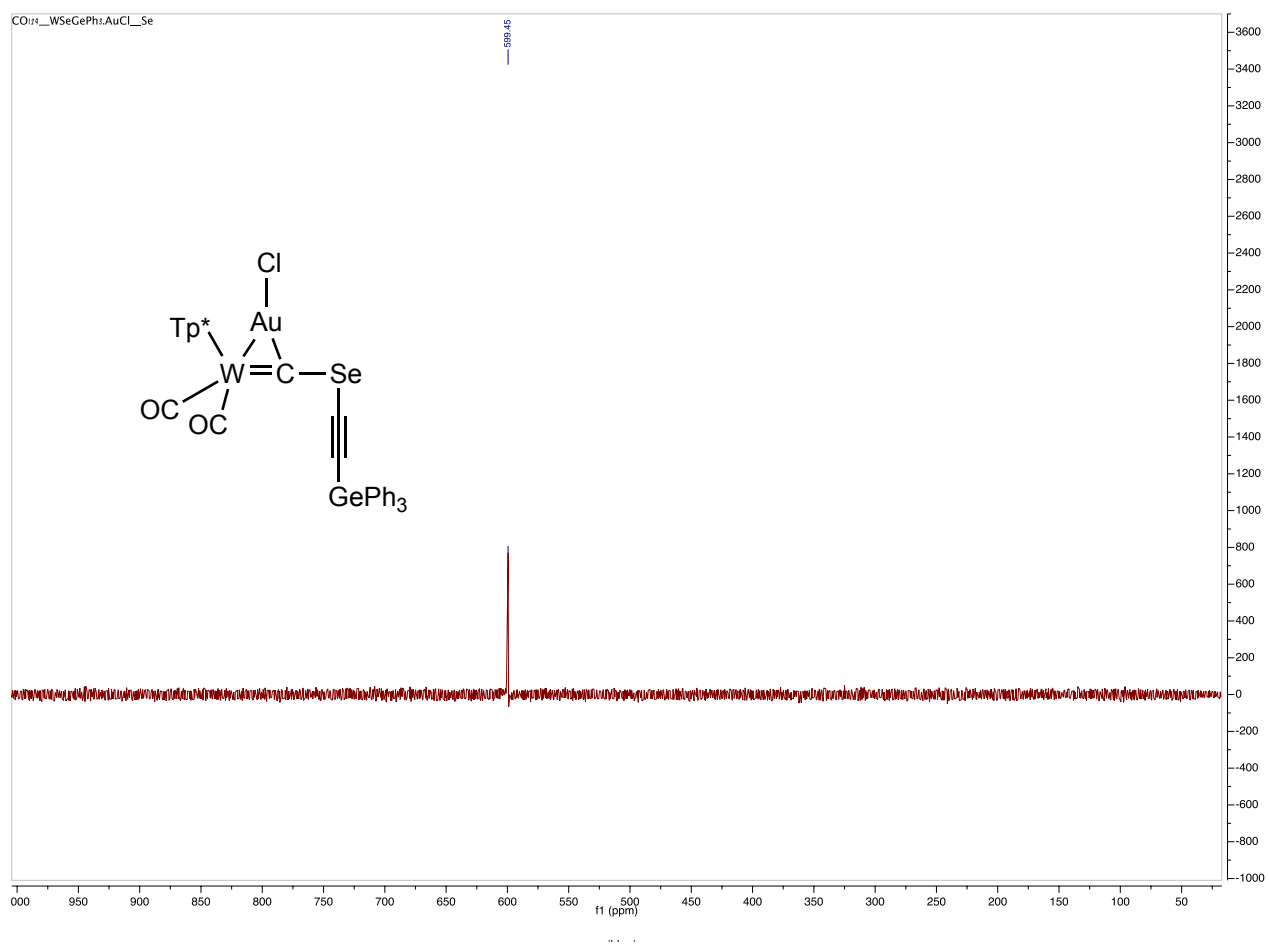
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (134 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CSiPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3g**).



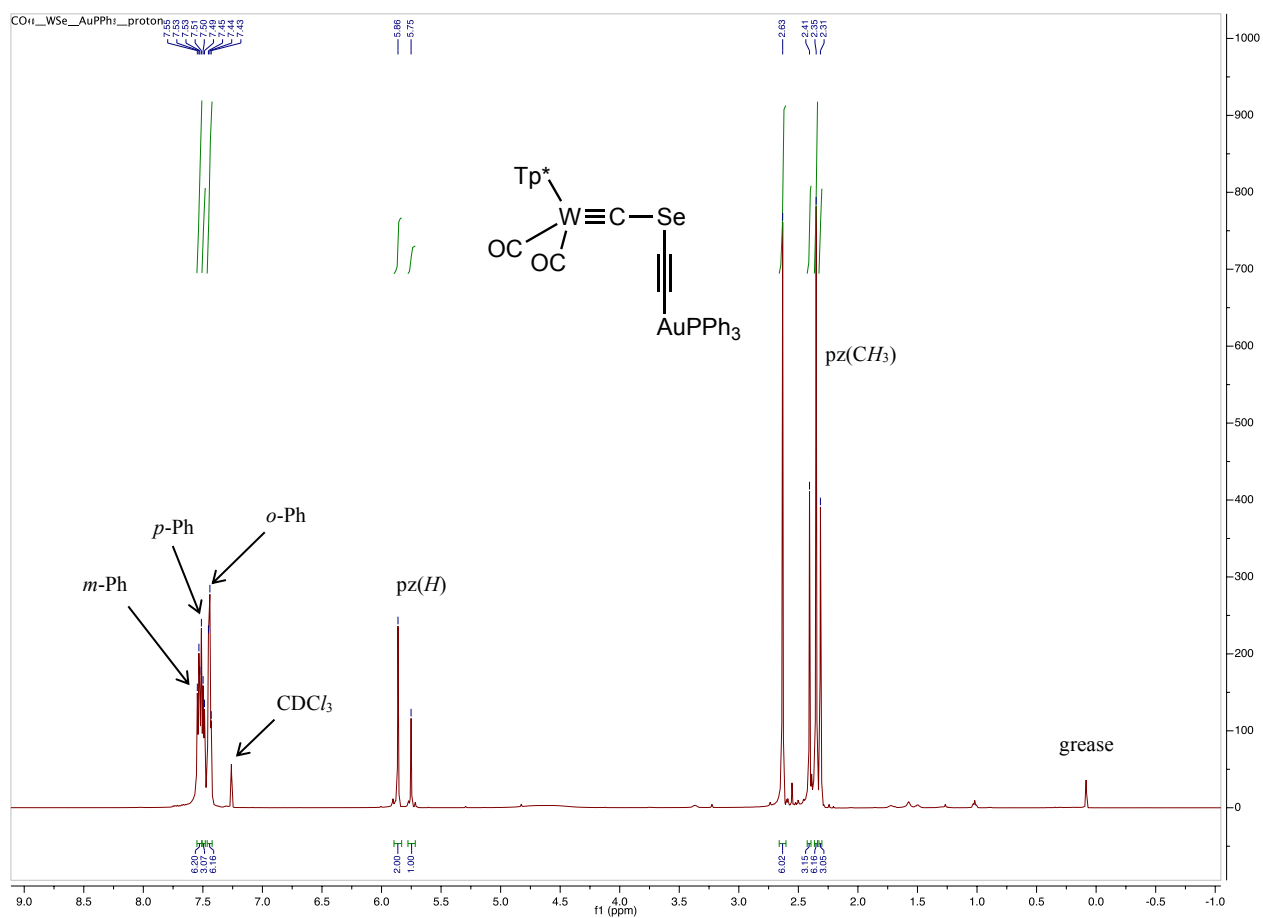
^1H NMR SPECTRUM (600 MHz, CDCl_3 , 25°C, δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CGePh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3h**).



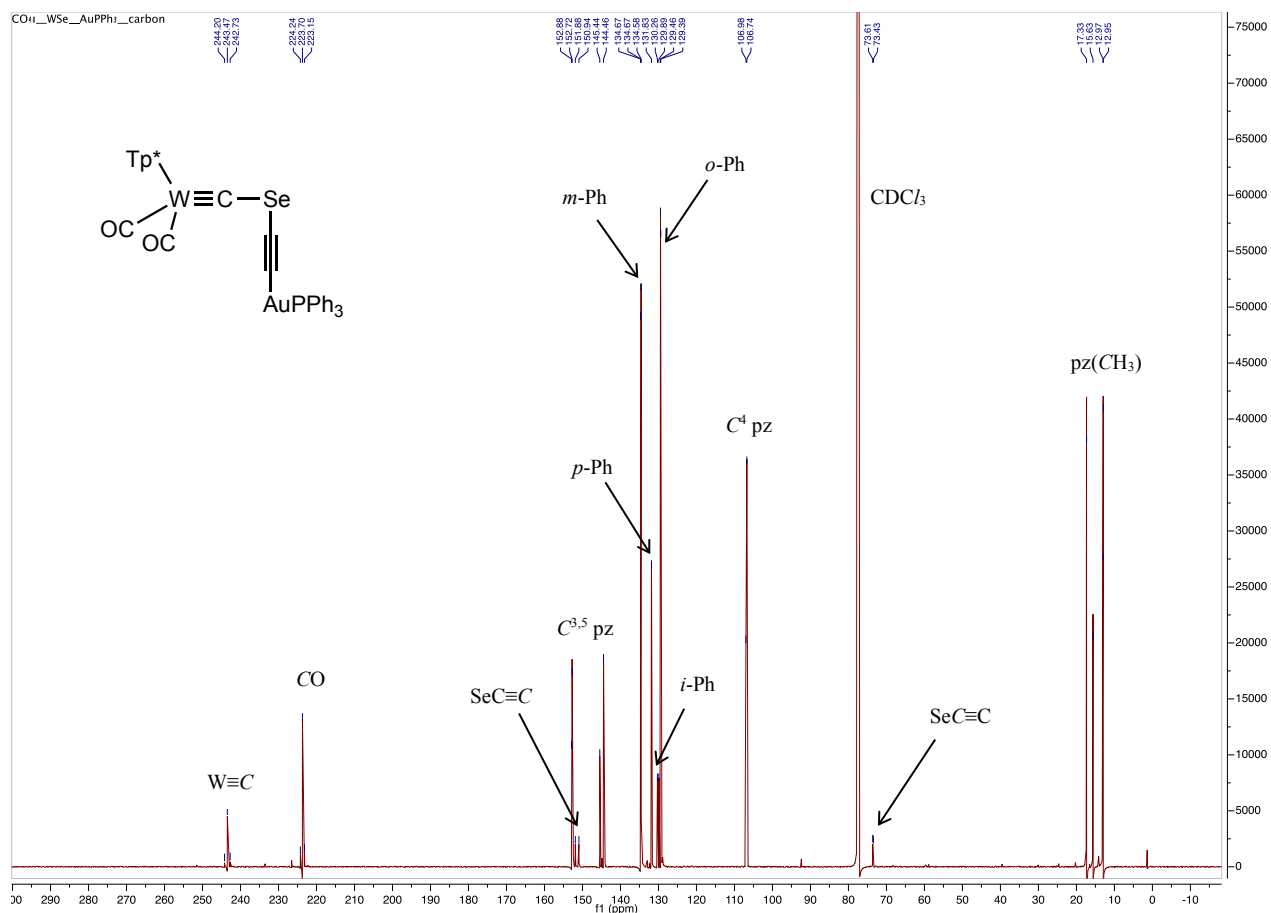
$^{13}\text{C}\{^1\text{H}\}$ NMR SPECTRUM (151 MHz, CDCl_3 , 25°C, δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CGePh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3h**).



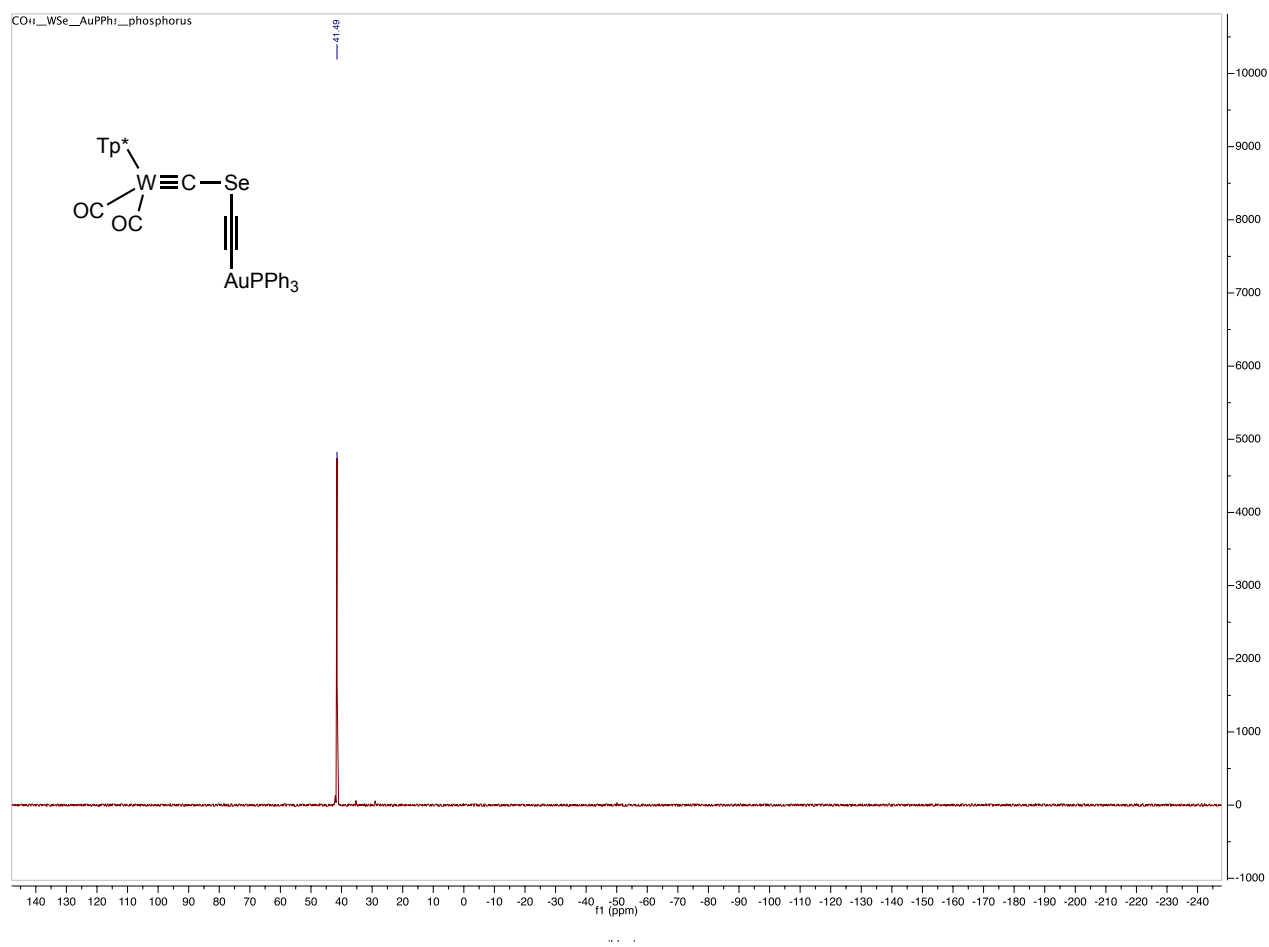
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (134 MHz, CDCl_3 , 25°C , δ) of $[\text{WAuCl}(\mu\text{-CSeC}\equiv\text{CGePh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**3h**).



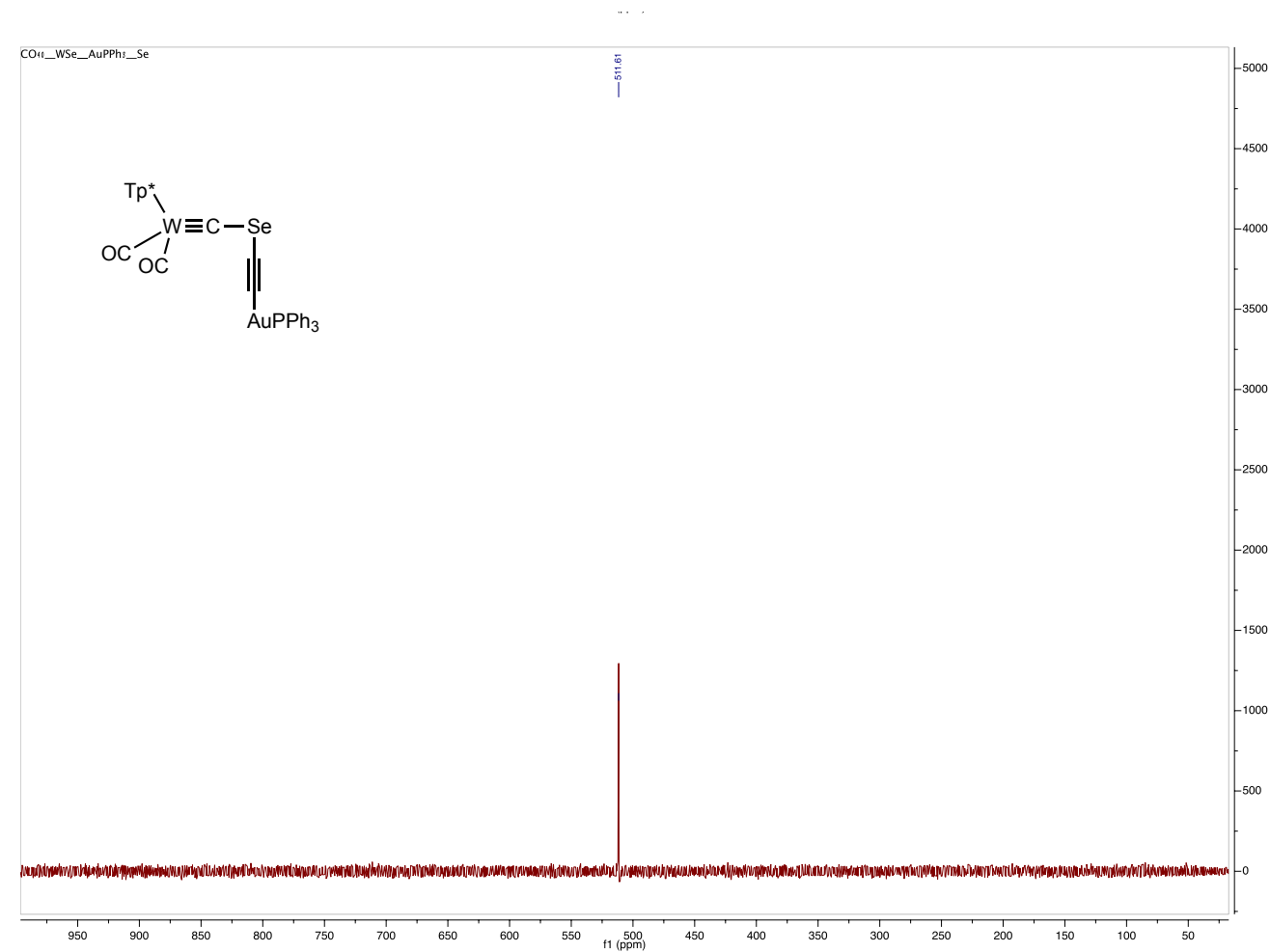
^1H NMR SPECTRUM (600 MHz , CDCl_3 , 25°C , δ) of $[\text{W}(\equiv\text{CSeC}\equiv\text{CAuPPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**4a**).



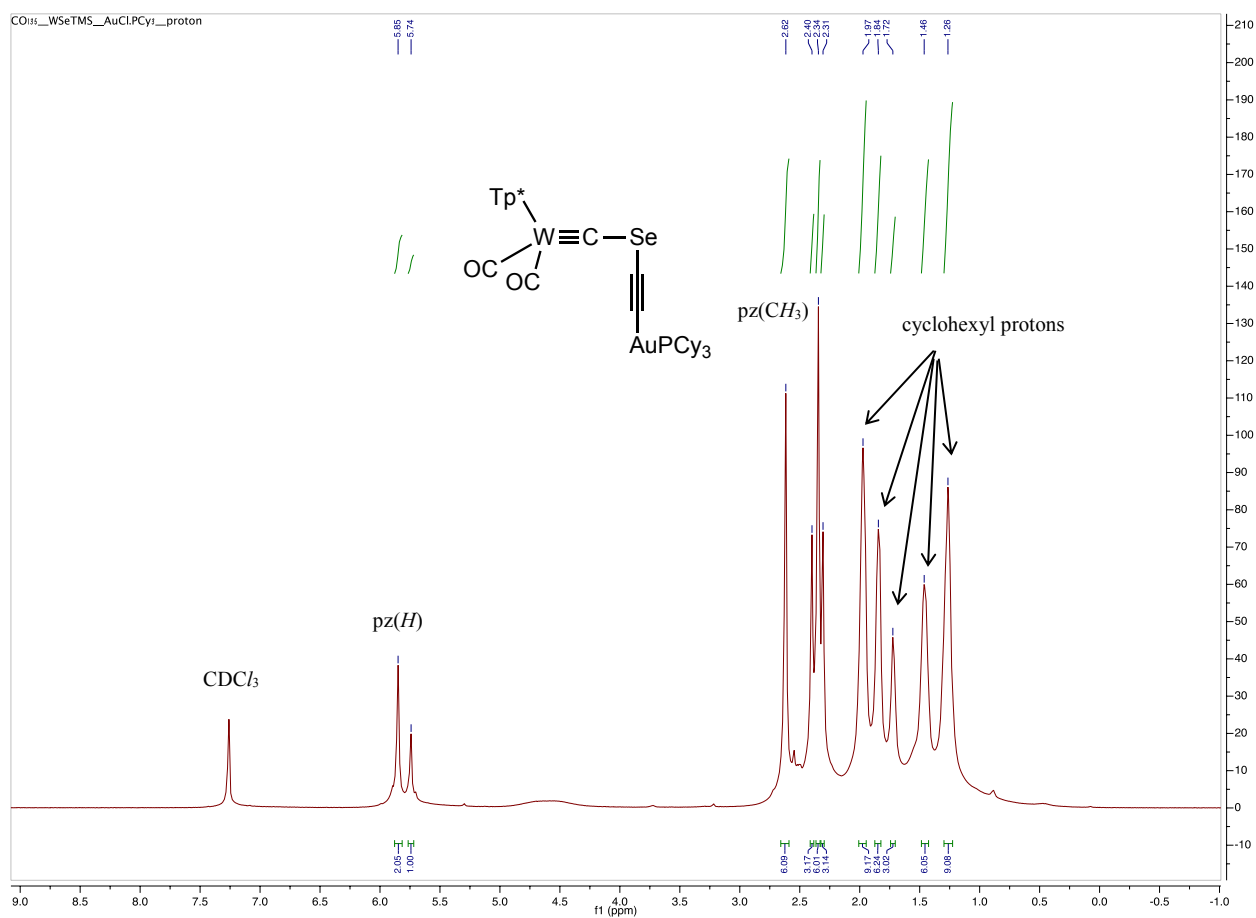
$^{13}\text{C}\{^1\text{H}\}$ NMR SPECTRUM (151 MHz, CDCl_3 , 25°C, δ) of $[\text{W}(\equiv\text{CSeC}\equiv\text{CAuPPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**4a**).



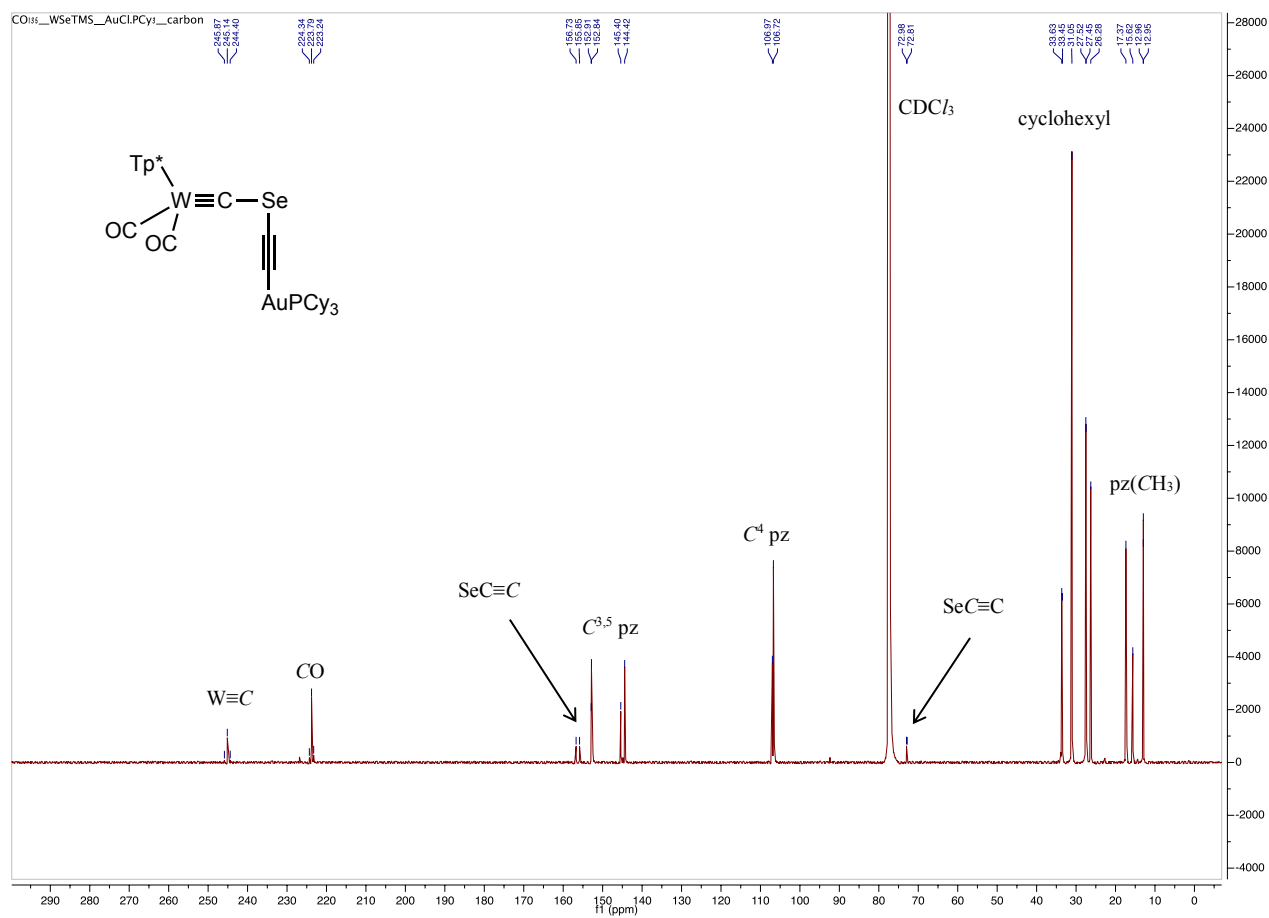
$^{31}P\{^1H\}$ NMR SPECTRUM (162 MHz, C_6D_6 , 25 °C, δ) of $[W(=CSeC\equiv CAuPPh_3)(CO)_2(Tp^*)]$ (**4a**).



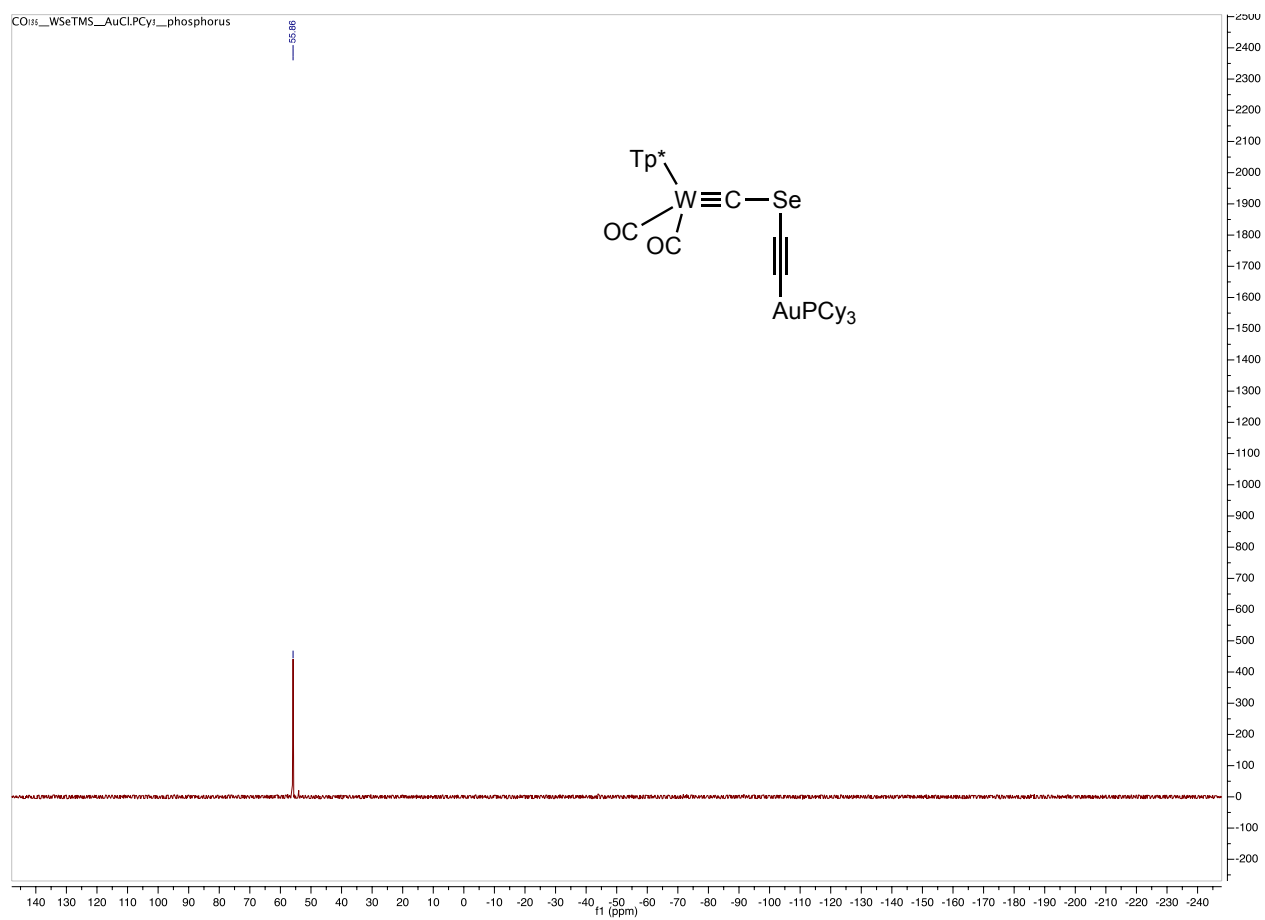
$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (76 MHz, CDCl_3 , 25 °C, δ) of $[\text{W}(\equiv\text{CSeC}\equiv\text{CAuPPh}_3)(\text{CO})_2(\text{Tp}^*)]$ (**4a**).



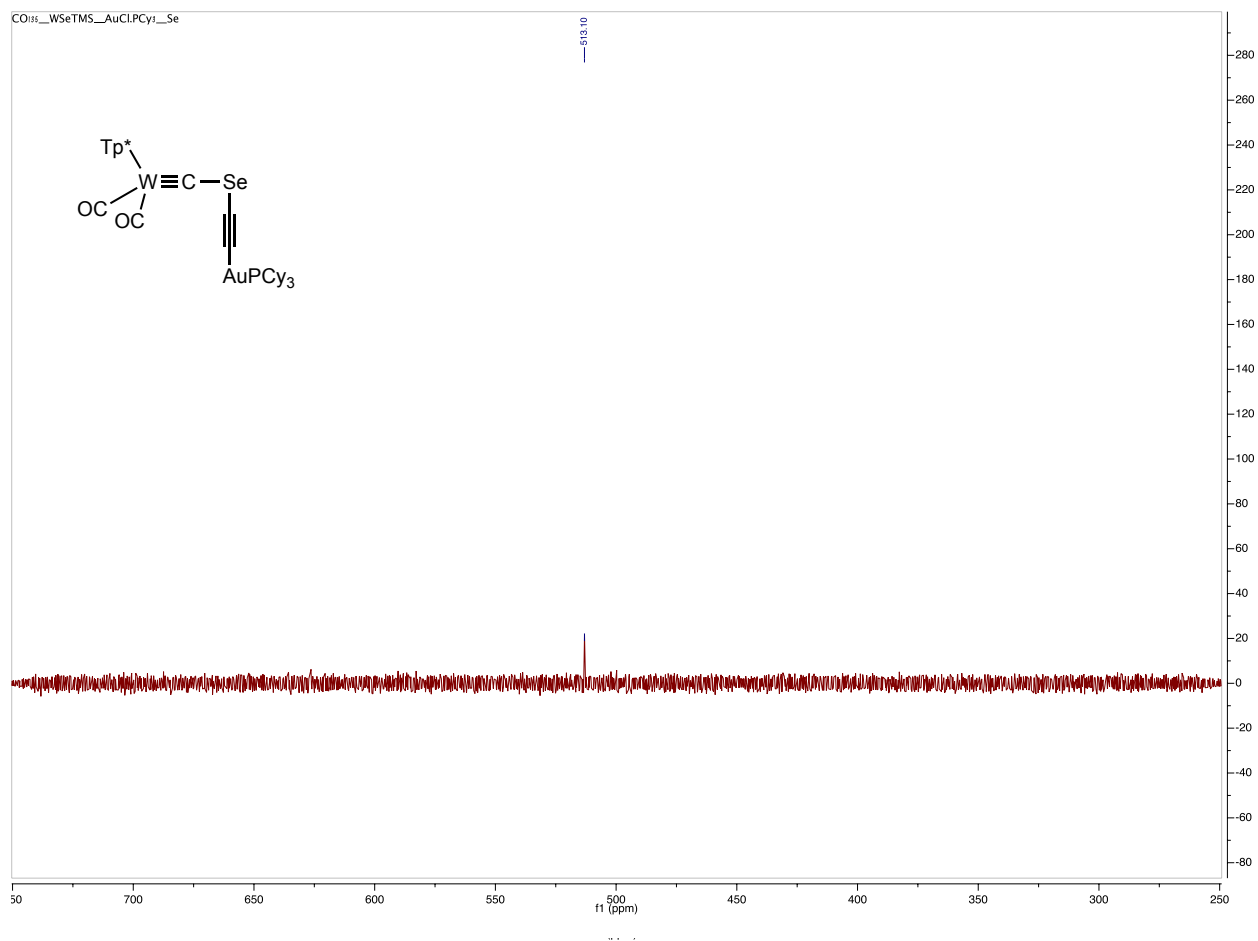
^1H NMR SPECTRUM (600 MHz, CDCl_3 , 25°C, δ) of $[\text{W}(=\text{CSeC}\equiv\text{CAuPCy}_3)(\text{CO})_2(\text{Tp}^*)]$ (**4b**).



$^{13}\text{C}\{^1\text{H}\}$ NMR SPECTRUM (151 MHz, CDCl_3 , 25 °C, δ) of $[\text{W}(\equiv\text{CSeC}\equiv\text{CAuPCy}_3)(\text{CO})_2(\text{Tp}^*)]$ (4b).



$^{31}P\{^1H\}$ NMR SPECTRUM (162 MHz, C_6D_6 , 25 °C, δ) of $[W(\equiv CSeC\equiv CAuPCy_3)(CO)_2(Tp^*)]$ (4b).



$^{77}\text{Se}\{^1\text{H}\}$ NMR SPECTRUM (76 MHz, CDCl_3 , 25°C , δ) of $[\text{W}(\equiv\text{CSeC}\equiv\text{CAuPCy}_3)(\text{CO})_2(\text{Tp}^*)]$ (**4b**).



Dalton Transactions

ARTICLE