Electronic Supplementary Material (ESI) for Dalton Transactions.

SUPPORTING INFORMATION

Systematic investigation of the influence of electronic substituents on dinuclear gold(I) amidinates: synthesis, characterisation and photoluminescence studies

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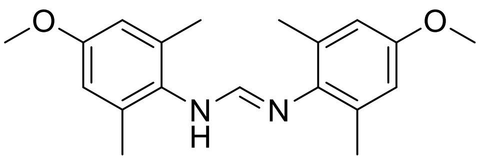
Synthesis and characterization

General procedures

All air- and moisture-sensitive manipulations were performed under dry N_2 or Ar atmosphere using standard Schlenk techniques or in an argon-filled MBraun glovebox, unless otherwise stated. Prior to use, CH_2Cl_2 and MeCN were dried by refluxing over P_2O_5 and CaH_2, respectively, and distilled under a nitrogen atmosphere. Other solvents (THF, Et_2O and toluene) were dried using an MBraun solvent purification system (SPS-800) and degassed. THF was additionally distilled under nitrogen from potassium benzophenone ketyl before storage over 4 Å molecular sieve. C_6D_6 was dried over Na-K alloy and $CDCl_3$ was dried over 4 Å molecular sieves. All deuterated solvents were degassed by freeze-pump-thaw cycles. The Amidine starting Materials 4-methoxy-2,6-dimethylaniline, 4-amino-3,5-dimethylbenzoeacid, 4-amino-3,5-dimethylbenzoeacidmethylester, 2,6-dimethyl-4-(methylthio)aniline and 4-phenyl-2,6-dimethylaniline were prepared according to the literature procedures.[1-11] The Amidine-ligands MeOXylFormH (L^1), MesFormH (L^2), XylFormH (L^4) and the known gold compound [$XylForm_2Au_2$] (**4**) were prepared according to the literature procedures.[1, 3, 4, 12] All other chemicals were obtained from commercial sources and used without further purification. NMR spectra were recorded on Bruker spectrometers (Avance III 300 MHz, Avance 400 MHz or Avance III 400 MHz). Chemical shifts are referenced using signals of the residual protio solvent (^{1}H) or the solvent (^{13}C) and are reported relative to tetramethylsilane (^{1}H, ^{13}C). All NMR spectra were measured at 298 K, unless otherwise specified. The multiplicity of the signals is indicated as s = singlet, d = doublet, t = triplet, m = multiplet and br = broad. Assignments were determined on the basis of unambiguous chemical shifts, coupling patterns and ^{13}C-DEPT experiments or 2D correlations (^{1}H^{1}H COSY, ^{1}H^{13}C HSQC, ^{1}H^{13}C HMBC). Infrared (IR) spectra were recorded in the region 4000–400 cm^{-1} on a Bruker Tensor 37 FTIR spectrometer equipped with a room temperature DLaTGS detector and a diamond attenuated total reflection (ATR) unit. ESI mass spectra were recorded on an LTQ Orbitrap XL Q Exactive mass spectrometer (Thermo Fisher Scientific, San Jose, CA, USA) equipped with a HESI II probe. Elemental analyses were carried out with an elementar Vario Micro Cube. PL measurements were performed with a Horiba Jobin Yvon Fluorolog-322 spectrometer A Hamamatsu R9910 photomultiplier was used as detector for the emission spectral range of about 250- 800 nm.

Synthesis of N,N-(4-methoxy-2,6-dimethylphenyl)formamidine (L^1)



1.42 g of 4-Methoxy-2,6-dimethylanilin (9.40 mmol, 2.00 eq), 0.80 mL triethylorthoformate (0.70 g, 4.70 mmol, 1.00 eq) and 14 µL acetic acid (0.014 g, 0.24 mmol, 0.05 eq) were stirred for 24 hours at 140 °C. The crude product was recrystallized from hot toluene. The product could be obtained as an off white solid at a yield of 62% (0.91 g).

In C_6D_6 (25 °C) this formamidine exists as a mixture of two isomers in a ratio of 2:3. ^{1}H NMR chemical shifts for the two isomers are listed separately.

Isomer 1: ^{1}H NMR (C_6D_6, 400 MHz): δ [ppm] = 6.96 (d, $^3J_{HH}$ = 11.9 Hz, 1 H, NC(*H*)N), 6.83 (s, 2 H, Ar-*H*), 6.48 (s, 2 H, Ar-*H*), 4.95 (d, $^3J_{HH}$ = 11.8 Hz, 1 H, N-*H*), 3.49 (s, 3 H, OMe(*H*)), 3.32 (s, 3 H, OMe(*H*)), 2.33 (s, 6 H, 2,6-Me(*H*)), 1.90 (s, 6 H, 2,6-Me(*H*)).

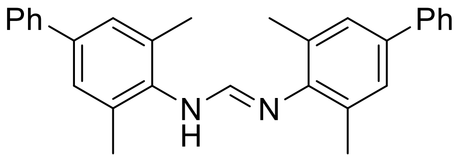
Isomer 2: ^{1}H NMR (C_6D_6, 400 MHz): δ [ppm] = 6.84 (s, 1 H, NC(*H*)N), 6.66 (s, 4 H, Ar-*H*), 3.38 (s, 6 H, OMe(*H*), 2.20 (s, 12 H, 2,6-Me(*H*)).

^{13}C{^{1}H} NMR (C_6D_6, 75 MHz): δ [ppm] = 158.2 (Ar-C^q(OMe)), 156.0 (N-C^q(OMe)), 147.3 (N_2*C*(H)), 140.0 (N-C^q(Ar)), 136.6 (Ar-C^q-2,6-Me), 130.2 (Ar-C^q-2,6-Me), 129.5 (Ar-C^q-2,6-Me), 114.3 (Ar-*C*(H)), 113.8 (Ar-*C*(H)), 113.7 (Ar-*C*(H)), 55.1 (O-*C*(Me)), 54.9 (O-*C*(Me)), 19.1 (2,6-*C*(Me)), 18.9 (2,6-*C*(Me)), 18.6 (2,6- *C*(Me)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3148 (vw), 2940 (w), 2913 (w), 2837 (w), 1640 (m), 1604 (w), 1446 (w), 1477 (m), 1439 (w), 1369 (w), 1310 (w), 1279 (w), 1205 (m), 1147 (w), 1128 (w), 1062 (w), 991 (vw), 900 (vw), 849 (w), 838 (w), 756 (vw), 709 (vw), 654 (w), 612 (vw), 572 (vw), 446 (vw).

MS (ESI$^+$): m/z (%) = 313 ([M+H]$^+$, 100).

Synthesis of N,N-(4-phenyl-2,6-dimethylphenyl)formamidine (L^3)



1.00 g 4-Bromo-2,6-dimethylformamidine (2.44 mmol, 1.00 eq), 1.19 g phenylboronic acid (9.75 mmol, 4.00 eq) and 0.11 g $Pd_2(dba)_3$ (0.12 mmol, 0.05 eq) were put together and 16 mL of THF was added. Through a 2 M solution of 16 mL Na_2CO_3(aq) was bubbled nitrogen gas for 30 min. and then added to the suspension. The resulting biphasic mixture was stirred under nitrogen at 80 °C for 48 hours and then at 60 °C for 24 hours. The reaction was then cooled to room temperature and saturated aqueous ammonium chloride was added. The mixture was extracted with ethyl acetate three times, dried over $MgSO_4$ and concentrated under reduced pressure to give the crude product. Purification by flash column chromatography on silica with 1:1 hexane/ethyl acetate as eluent gave the product as a white solid at a yield of 67% (0,66 g).

In C_6D_6 (25 °C) this formamidine exists as a mixture of two isomers in a ratio of 1:1.

Isomer 1: ^{1}H NMR (C_6D_6, 400 MHz): δ [ppm] = 7.66 (d, $^3J_{HH}$ = 7.2 Hz, 2 H, Ar-*H*), 7.47-7.45 (m, 4 H, Ar-*H*), 7.36-7.31 (m, 2 H, Ar-*H*), 7.25 (s, 2 H, Ar-*H*), 7.17 (bs, 2 H, Ar-*H*), 7.09 (s, 2 H, Ar-*H*), 7.00 (d, J= 12.0 Hz, 1 H, NC(*H*)N), 5.05 (d, $^3J_{HH}$ = 12.5 Hz, 1 H, N-*H*), 2.41 (s, 6 H, 2,6-Me(*H*)), 1.92 (s, 6 H, 2.6-Me(*H*)).

Isomer 2: ^{1}H NMR (C_6D_6, 400 MHz): δ [ppm] = 7.54 (d, $^3J_{HH}$ = 7.3 Hz, 4 H, Ar-*H*), 7.29 (bs, 4 H, Ar-*H*), 7.28-7.26 (m, 4 H, Ar-*H*), 7.21-7.18 (m, 2 H, Ar-*H*), 6.88 (s, 1 H, NC(*H*)N), 2.25 (s, 12 H, 2,6-Me(*H*)).

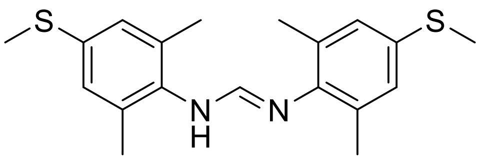
^{13}C{^{1}H} NMR (C_6D_6, 100 MHz): δ [ppm] = 146.1 (C^q), 145.9 (N_2-*C*(H), 142.1 (C^q), 141.8 (C^q), 141.0 (C^q), 139.4 (C^q), 136.3 (C^q), 134.6 (C^q), 129.1 (Ar-*C*(H)), 129.1 (Ar-*C*(H)), 129.0 (Ar-*C*(H)), 128.9 (C^q), 127.7 (Ar-*C*(H)), 127.6 (Ar-*C*(H)), 127.5 (Ar-*C*(H)), 127.4 (Ar-*C*(H)), 127.3 (Ar-*C*(H)), 127.1 (Ar-*C*(H)), 126.9 (Ar-*C*(H)), 19.0 (2,6-*C*(Me)), 18.7 (2,6-*C*(Me)), 18.5 (2,6-*C*(Me)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3261 (w), 3059 (vw), 3030 (vw), 2974 (w), 2912 (w), 2851 (vw), 1629 (m), 1597 (m), 1517 (w), 1469 (w), 1435 (w), 1376 (w), 1280 (vw), 1255 (vw), 1231 (w), 1207 (vw), 1176 (w), 1130 (w), 1078 (vw), 1034 (vw), 984 (vw), 910 (vw), 879 (w), 868 (w), 762 (w), 754 (w), 694 (w), 618 (vw), 532 (vw), 491 (vw).

MS (EI, 70 eV): m/z (%) = 404 ([M]$^+$, 25), 208 ([PhMe$_2$PhNCH]$^+$, 17), 197 ([PhMe$_2$PhNH$_2$]$^+$, 100), 165 ([Ph-PhNH]$^+$, 12).

EA Calcd (%) for [$C_{29}H_{28}N_2$] (404.56 g mol^{-1}): C 86.10, H 6.98, N 6.92; found C 86.24, H 6.93, N 6.91.

Synthesis of N,N-(4-methylthio-2,6-dimethylphenyl)formamidine (L^5)



2.50 g of 4-Methylthio-2,6-dimethylanilin (15.00 mmol, 2.00 eq), 1.24 mL triethylorthoformate (1.11 g, 7.50 mmol, 1.00 eq) and 20 µL acetic acid (0.023 g, 0.38 mmol, 0.05 eq) were stirred for 24 hours at 140 °C. The crude product was washed with n-pentane and dried in vacuum. The product was obtained as a colourless solid at a yield of 81% (2.08 g).

^{1}H NMR ($CDCl_3$, 400 MHz): δ [ppm] = 7.23 (bs, 1 H, N_2C-*H*), 6.97 (bs, 4 H, Ar-*H*), 6.36 (bs, 1 H, N-*H*), 2.46 (s, 6 H; SMe(*H*)), 2.23 (s, 12 H, 2,6-Me(*H*)).

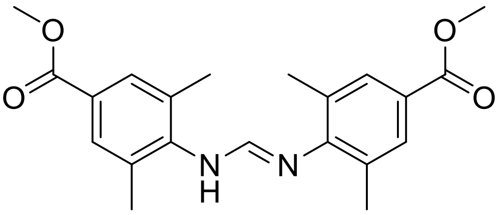
^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ [ppm] = 147.2, 143.2, 136.5, 134.9, 133.7, 131.5, 129.5, 128.3, 127.8, 127.1, 126.8, 18.8, 18.1, 17.0, 16.1.

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3233 (vw), 3138 (vw), 2976 (w), 2914 (w), 2852 (vw), 1635 (m), 1586 (w), 1544 (vw), 1508 (w), 1469 (w), 1430 (w), 1371 (vw), 1297 (vw), 1250 (vw), 1201 (w), 1146 (vw), 987 (vw), 951 (vw), 889 (vw), 844 (w), 657 (vw).

MS (EI, 70 eV): m/z (%) = 344 ($[M]^+$, 22), 167 ($[MeSMe_2PhNH_2]^+$, 100), 152 ($[MeSMe_2Ph]^+$, 55), 131 ($[Me_2PhNCH]^+$, 16), 121 ($[Me_2PhNH_2]^+$, 54), 106 ($[Me_2Ph]^+$, 31), 91 ($[PhN]^+$, 18), 77 ($[Ph]^+$, 18).

EA Calcd (%) for [$C_{19}H_{24}N_2S_2$] (344.54 g mol^{-1}): C 66.24, H 7.02, N 8.13, S 18.61; found C 66.16, H 6.95, N 8.14, S 17.75.

Synthesis of N,N-(4-methylester-2,6-dimethylphenyl)formamidine (L^6)



1.00 g of methyl-4-amino-3,5-dimethylbenzoate (5.58 mmol, 2.00 eq), 0.46 mL triethylorthoformate (0.41 g, 2.79 mmol, 1.00 eq) and 8 µL acetic acid (0.008 g, 0.14 mmol, 0.05 eq) were stirred for 24 hours at 140 °C. The crude product was recrystallized in acetonitrile two times and then washed with n-hexane. After drying in vacuum, the product could be obtained as light brown solid at a yield of 30% (0.31 g).

In C_6D_6 (25 °C) this formamidine exists as a mixture of two isomers in a ratio of 2:3. ^{1}H NMR chemical shifts for the two isomers are listed separately.

Isomer 1: ^{1}H NMR (C_6D_6, 400 MHz): δ [ppm] = 8.11(s, 2 H, Ar-*H*), 7.78 (s, 2 H, Ar-*H*), 6.70 (d, $^3J_{HH}$ = 11.7 Hz, 1 H, NC(*H*)N), 4.86 (d, $^3J_{HH}$ = 11.4 Hz, 1 H, N-*H*), 3.61 (s, 3 H, CO_2Me(*H*)), 3.56 (s, 3 H, CO_2Me(*H*)), 2.17 (s, 6 H, 2,6-Me(*H*)), 1.71 (s, 6 H, 2,6-Me(*H*)).

Isomer 2: ^{1}H NMR (C_6D_6, 400 MHz): δ [ppm] = 7.98 (s, 4 H, Ar-*H*), 6.50 (s, 1 H, NC(*H*)N), 3.57 (s, 6 H, CO_2Me(*H*)), 2.01 (s, 12 H, 2,6-Me(*H*)).

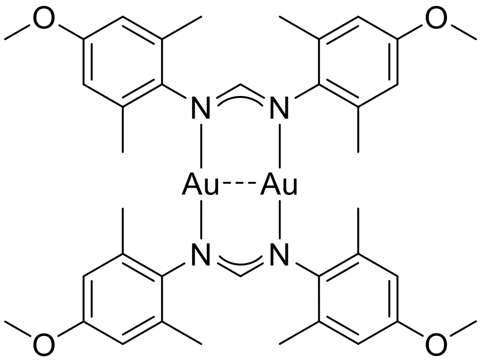
^{13}C{^{1}H} NMR (C_6D_6, 100 MHz): δ [ppm] = 166.8 (ArC-C^q(O_2Me)), 150.9 (Ar-C^q(CO_2Me)), 144.4 (N_2-*C*(H)), 140.7 (N-C^q(Ar), 133.5 (Ar-C^q-2,6-Me), 130.5 (Ar-*C*(H)), 130.4 (Ar-*C*(H)), 130.1 (Ar-*C*(H)), 51.7 (O-*C*(Me)), 51.5 (O-*C*(Me)), 18.65 (2,6-*C*(Me)), 18.4 (2,6-*C*(Me)), 18,0 (2,6-*C*(Me)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3415 (vw), 3222 (vw), 2980 (vw), 2955 (vw), 2914 (vw), 2846 (vw), 1787 (vw), 1720 (s), 1640 (m), 1594 (m), 1511 (w), 1478 (w), 1456 (w), 1430 (m), 1381 (w), 1310 (m), 1265 (vw), 1226 (m), 1194 (m), 1141 (w), 1106 (w), 1012 (w), 947 (vw), 921 (vw), 900 (w), 881 (vw), 794 (vw), 767 (w), 664 (vw), 620 (vw), 585 (vw), 547 (vw).

MS (EI, 70 eV): m/z (%) = 368 ($[M]^+$, 12), 353 ($[M-Me]^+$, 11), 190 ($[MeO_2CXylNCH]^+$, 14), 179 ($[MeO_2CXylNH_2]^+$, 100), 158 ($OCXylNCH]^+$, 18), 148 ($OCXylNH_2]^+$, 48).

EA Calcd (%) for [$C_{31}H_{24}N_2O_4$] (368.43 g mol^{-1}): C 68.46, H 6.57, N 7.60; found C 67.86, H 6.52, N 7.57.

Synthesis of MeOXylForm$_2$Au$_2$ (1)



0.10 g N,N-(4-Methoxy-2,6-dimethylphenyl) formamidine (0.33 mmol, 1.05 eq) and 0.06 g K(BTSA) (0.31 mmol, 1.00 eq) were dissolved in 6 mL of THF and stirred overnight. The solution was added slowly to a suspension of 0.10 g Au(tht)Cl (0.31 mmol, 1.00 eq) in 6 mL of THF at -88 °C. The reaction mixture was stirred at room temperature overnight. The solvent was removed under reduced pressure and the crude product was solved in DCM and filtrated afterwards. Again, the solvent was removed under reduced pressure and 10 mL of THF were added. Crystals suitable for X-ray studies were obtained by slow evaporation of the solvent. The product was obtained as a red crystalline solid in 43% yield (0,07 g).

^{1}H NMR (THF-d$_8$, 300 MHz): δ [ppm] = 7.42 (s, 2 H, N$_2$C-*H*), 6.47 (s, 8 H, Ar-*H*), 3.59 (s, 12 H, O-Me(*H*)), 2.35 (s, 24 H, 2,6-Me(*H*)).

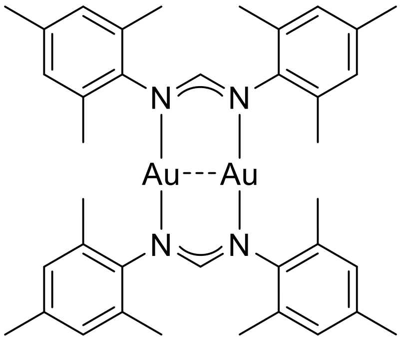
^{13}C{^{1}H} NMR (THF-d$_8$, 75 MHz): δ [ppm] = 171.2 (N$_2$-*C*(H)), 158.0 (N-*C*^{q}(Ar)), 142.0 ((Ar)*C*^{q}-O), 134.8 (*C*^{q}-2,6-Me), 114.1 ((Ar-*C*(H)), 55.6 (OMe(*C*)), 19.6 (2,6-Me(*C*)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3009 (vw), 2969 (vw), 2936 (w), 2905 (vw), 2835 (vw), 1641 (vw), 1631 (vw), 1608 (w), 1575 (w), 1480 (w), 1464 (w), 1432 (w), 1425 (w), 1375 (vw), 1345 (vw), 1318 (w), 1281 (w), 1238 (vw), 1230 (w), 1205 (w), 1188 (w), 1149 (w), 1063 (w), 1029 (vw), 996 (vw), 854 (w), 834 (vw), 820 (vw), 615 (vw), 573 (vw), 468 (vw), 453 (vw).

MS (ESI$^+$): m/z (%) = 1016 ([M]$^+$, 100)

EA Calcd (%) for [$C_{38}H_{46}Au_2N_4O_4$] (1016.74 g mol^{-1}): C 44.89, H 4.56, N 5.51; found C 44.54, H 4.52, N 5.61.

Synthesis of MesForm$_2$Au$_2$ (2)



0.09 g N,N-(2,4,6-Trimethylphenyl)formamidine (0.31 mmol, 1.00 eq) and 0.06 g K(BTSA) (0.31 mmol, 1.00 eq) were dissolved in 6 mL of THF and stirred overnight. The solution was added slowly to a suspension of 0.10 g Au(tht)Cl (0.31 mmol, 1.00 eq) in 6 mL of THF at -88 °C. The reaction mixture was stirred at room temperature overnight. The solvent was removed at reduced pressure and the crude product was solved in DCM and filtrated afterwards. The solvent was removed under reduced pressure and 10 mL of THF were added. Crystals suitable for x-ray analysis could be obtained by slow evaporation of the solvent. The product could be obtained as an orange crystalline solid in 40% (0.06 g) yield.

^{1}H NMR (THF-*d*$_8$, 300 MHz): δ [ppm] = 7.43 (s, 2 H, N$_2$C-H), 6.75 (s, 8 H, Ar-H), 2.38 (s, 24 H, 2,6-Me(H)), 2.16 (s, 12 H, 4-Me(H)).

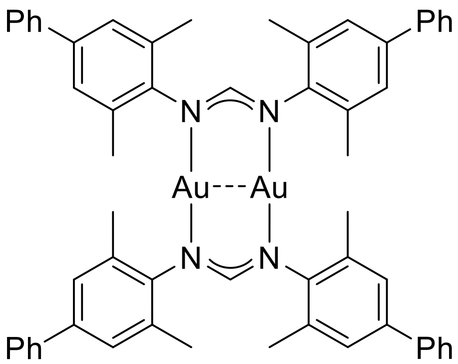
^{13}C{^{1}H} NMR (THF-d$_8$, 75 MHz): δ [ppm] = 170.4 (N$_2$-C(H)), 146,2 (N-C^q(Ar)), 135.2 ((Ar)C^q-4-Me), 133.5 ((Ar)C^q-2,6-Me), 129.6 (Ar-C(H)), 20.9 (4-Me(C)), 19.2 (2,6-Me(C)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3008 (vw), 2964 (w), 2938 (w), 2908 (w), 2846 (vw), 1724 (vw), 1611 (w), 1573 (m), 1477 (w), 1431 (w), 1371 (vw), 1343 (w), 1299 (vw), 1235 (w), 1209 (w), 1149 (vw), 1032 (vw), 1007 (vw), 984 (vw), 848 (w), 626 (vw), 567 (vw), 481 (vw), 440 (vw).

MS (ESI$^+$): m/z (%) = 987 ([M+H+2 H$_2$O]$^+$, 12), 952 ([M]$^+$, 100).

EA Calcd (%) for [C$_{38}$H$_{46}$Au$_2$N$_4$] (952.75 g mol^{-1}): C 47.91, H 4.87, N 5.88; found C 47.56, H 4,85, N 5.97.

Synthesis of PhXylForm₂Au₂ (3)



0.13 g N,N-(4-Phenyl-2,6-dimethylphenyl)formamidine (0.31 mmol, 1.00 eq) and 0.06 g K(BTSA) (0.31 mmol, 1.00 eq) were dissolved in 6 mL of THF and stirred overnight. The solution was added slowly to a suspension of 0.10 g Au(tht)Cl (0.31 mmol, 1.00 eq) in 6 mL of THF at -88 °C. The reaction mixture was stirred at room temperature overnight. The solvent was removed at reduced pressure and the crude product was dissolved in DCM and filtrated afterwards. The solvent was removed under reduced pressure and 15 mL of THF were added. After slow evaporation the product could be obtained as colourless crystals in 75% (0,14 g) yield. These crystals were suitable for X-ray analysis.

^{1}H NMR (THF-d_8, 400 MHz): δ [ppm] = 7.66 (s, 2 H, N_2C-*H*), 7.50-7.47 (m, 8 H, *o*Ph-*H*), 7,35-7,31 (m, 8 H, *m*Ph-*H*), 7.26 (s, 8 H, Ar-*H*), 7.24-7.20 (m, 4 H, *p*Ph-*H*).

^{13}C{^{1}H} NMR (THF-d_8, 100 MHz): δ [ppm] = 170.3 (N_2-*C*(H)), 147.9 (N-C^q(Ar), 142.2 ((Ph)C^q-PhN), 139.3 (Ph-C^q(PhN)), 134.3 ((Ar)C^q-2,6-Me), 129.5 (Ar-*C*(H)), 127.8 (Ar-*C*(H)), 19.5 (2,6-Me(*C*)).

^{1}H NMR ($CDCl_3$, 400 MHz): δ [ppm] = 7.53 (s, 2 H, N_2C-*H*), 7.51-7.48 (m, 8 H, *o*Ph-*H*), 7.41-7.36 (m, 8 H, *m*Ph-*H*), 7.31-7.26 (m, 4 H, *p*Ph-*H*), 7.23 (s, 8 H, Ar-*H*), 2.56 (s, 24 H, 2,6-Me(*H*)).

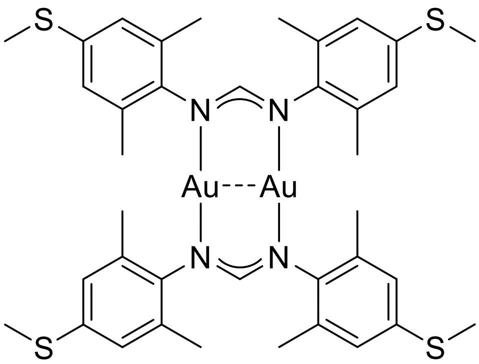
^{13}C{^{1}H} NMR ($CDCl_3$, 100 MHz): δ [ppm] = 168.3 (N_2-*C*(H)), 146.7 (N-C^q(Ar)), 141.2 ((Ph)C^q-PhN), 138.4 (Ph-C^q(PhN), 133.6 ((Ar)C^q-2,6-Me), 128.7 (Ar-*C*(H)), 127.2 (Ar-*C*(H)), 127.1 (Ar-*C*(H)), 127.0 (Ar-*C*(H)), 19.4 (2,6-Me(*C*)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3058 (vw), 3027 (vw), 2964 (vw), 2931 (vw), 2849 (vw), 1602 (w), 1569 (m), 1470 (m), 1434 (w), 1373 (vw), 1337 (w), 1231 (w), 1195 (vw), 1179 (w), 1077 (vw), 1029 (vw), 984 (vw), 871 (w), 759 (w), 694 (w), 656 (vw), 569 (vw), 537 (vw), 506 (vw), 470 (vw), 442 (vw).

MS (ESI$^+$): m/z (%) = 1200,37 ($[M+H]^+$, 9), 891 ($[M-4-Ph]^+$, 49).

EA Calcd (%) for [$C_{58}H_{54}Au_2N_4$] (1203.05 g mol^{-1}): C 57.91, H 4.69, N 4.66; found C 57.85, H 4.39, N 4.64.

Synthesis of MeSXylForm$_2$Au$_2$ (5)



0,21 g N,N-(4-Methylthio-2,6-dimethylphenyl) formamidine (0.62 mmol, 1.00 eq) and 0.12 g K(BTSA) (0.62 mmol, 1.00 eq) were dissolved in 6 mL of THF and stirred overnight. The solution was added slowly to a suspension of 0.20 g Au(tht)Cl (0.62 mmol, 1.00 eq) in 6 mL of THF at -88 °C. The reaction mixture was stirred at room temperature overnight. The solvent was removed at reduced pressure and the crude product was dissolved in DCM and filtrated afterwards. The solvent was removed under reduced pressure and 10 mL of THF were added. The Product could be obtained by slow evaporation of the solvent as colourless crystals that were suitable for X-ray analysis in a 45% yield (0,15 g).

^{1}H NMR (THF-d$_8$, 400 MHz): δ [ppm] = 7.51 (s, 2 H, N$_2$C-*H*), 6.92 (s, 8 H, Ar-*H*), 2.40 (s, 24 H, 2,6-Me(*H*)), 2.35 (s, 12 H, SMe(*H*)).

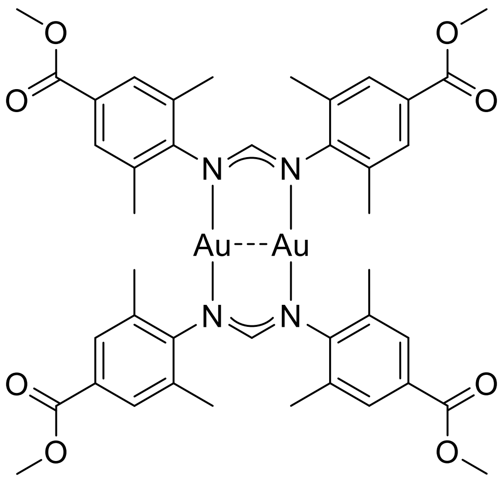
^{13}C{^{1}H} NMR (THF-d$_8$, 100 MHz): δ [ppm] = 170.4 (N$_2$-*C*(H)), 146.1 (N-*C*^{q}(Ar)), 135.9 ((Ar)*C*^{q}-S), 134.5 (*C*^{q}-2,6-Me), 127.9 (Ar-*C*(H)), 19.3 (2,6-Me(*C*)), 16.6 (SMe(*C*)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 2973 (vw), 2941 (vw), 2911 (w), 2848 (vw), 1594 (m), 1565 (m), 1469 (w), 1427 (w), 1372 (vw), 1333 (w), 1227 (w), 1199 (w), 1026 (vw), 994 (vw), 969 (vw), 947 (vw), 893 (vw), 847 (vw), 800 (vw), 623 (vw), 578 (vw), 497 (vw), 439 (vw).

MS (ESI$^+$): m/z (%) = 1112 ([M+OMe]$^+$,42), 1080 ([M]$^+$, 70), 891 ([M-4 SMe, 40), 849 (,100), 835 (,25), 809 (,38).

EA Calcd (%) for [$C_{38}H_{46}Au_2N_4S_4$] (1080.99 g mol^{-1}): C 42.22, H 4.29, N 5.18, S 11.86; found C 42.38, H 4.19, N 5.11, S 11.47.

Synthesis of $MeO_2CXylForm_2Au_2$ (6)



0,12 g N,N-(4-Methylester-2,6-dimethylphenyl) formamidine (0.31 mmol, 1.00 eq) and 0.06 g K(BTSA) (0.31 mmol, 1.00 eq) were dissolved in 6 mL of THF and stirred overnight. The solution was added slowly to a suspension of 0.10 g Au(tht)Cl (0.31 mmol, 1.00 eq) in 6 mL of THF at -88 °C. The reaction mixture was stirred at room temperature overnight. The solvent was removed at reduced pressure and the crude product was dissolved in DCM and filtrated afterwards. The solvent was removed under reduced pressure and 10 mL Then, toluene was added. After slow evaporation of the solvent the product could be obtained as colourless crystals in 68% (0,12 g) yield. These crystals were suitable for X-ray analysis.

^{1}H NMR (THF-d_8, 400 MHz): δ [ppm] = 7.67 (s, 8 H, Ar-*H*), 7.66 (s, 2 H, N_2C-*H*), 3.77 (s, 12 H, CO_2Me(*H*)), 2.49 (s, 24 H, 2,6-Me(*H*)).

^{13}C{^{1}H} NMR (THF-d_8, 100 MHz): δ [ppm] = 169.5 (N_2-*C*(H)), 166.8 (Ar-*C*(O_2)), 152.1 (N-C^q(Ar)), 134.3 (C^q-2,6-Me), 130.5 (Ar-*C*(H)), 128.2 ((Ar)C^q-CO_2Me), 52.0 (O-Me(*C*)), 19.3 (2,6-Me(*C*)).

^{1}H NMR ($CDCl_3$, 400 MHz): δ [ppm] = 7.69 (s, 8 H, Ar-*H*), 7.38 (s, 2 H, N_2C-*H*), 3.85 (s, 12 H, CO_2Me(*H*)), 2.48 (s, 24 H, 2,6-Me(*H*)).

^{13}C{^{1}H} NMR ($CDCl_3$, 75 MHz): δ [ppm] = 167.1 (N_2*C*(H)), 166.9 (Ar-*C*(O_2)), 150.9 (N-C^q(Ar)), 133.4 (C^q-2,6-Me), 129.9 (Ar-*C*(H)), 127.1 ((Ar)C^q-CO_2Me), 52.1 (O-Me(*C*)), 19.1 (2,6-Me(*C*)).

IR (ATR): ($\tilde{\vartheta}$) [cm^{-1}] = 3024 (vw), 2945 (vw), 2837 (vw), 1784 (vw), 1715 (m), 1603 (w), 1564 (m), 1472 (m), 1431 (m), 1377 (vw), 1352 (m), 1310 (m), 1223 (m), 1181 (m), 1109 (w), 1013 (w), 983 (vw), 899 (vw), 879 (vw), 819 (vw), 761 (w), 729 (w), 694 (vw), 569 (vw), 546 (vw), 490 (vw), 454 (vw).

MS (ESI^+): m/z (%) = 1128. ($[M]^+$, 57), 891 ($[M\text{-}4\ CO_2Me]^+$,100).

EA Calcd (%) for [$C_{42}H_{48}Au_2N_4O_8$ 0.5 C_7H_8] (1174.85 g mol^{-1}): C 46.52, H 4.29, N 4.77; found C 46.93, H 4.09, N 4.53.

NMR Spectra

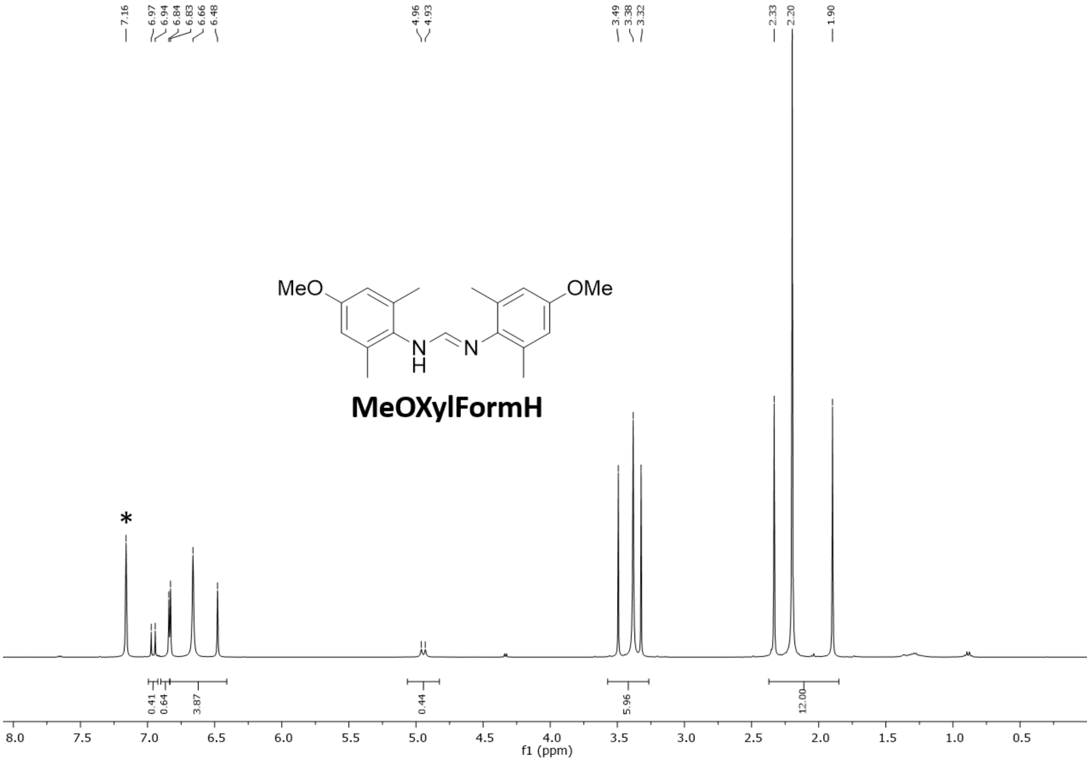


Figure S1: ^{1}H NMR spectrum of **MeOXylFormH** (**L^{1}**) in C_6D_6: *, residual protio solvent signal.

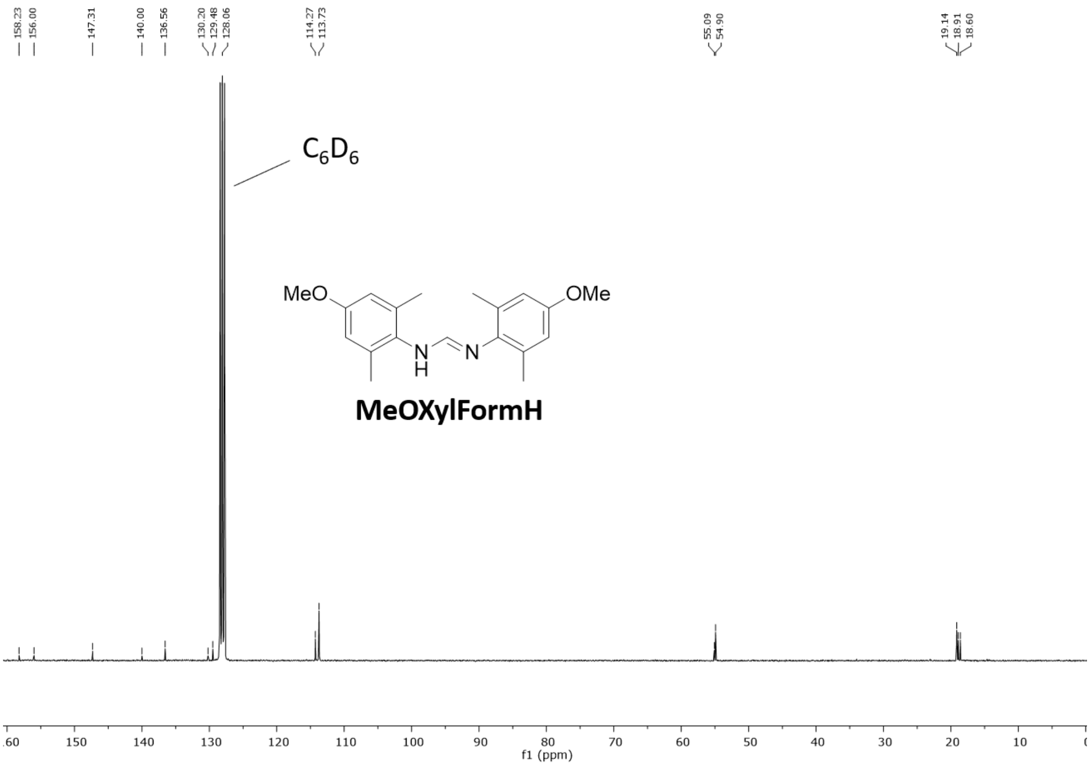


Figure S2: ^{13}C NMR spectrum of **MeOXylFormH** (**L^{1}**) in C_6D_6.

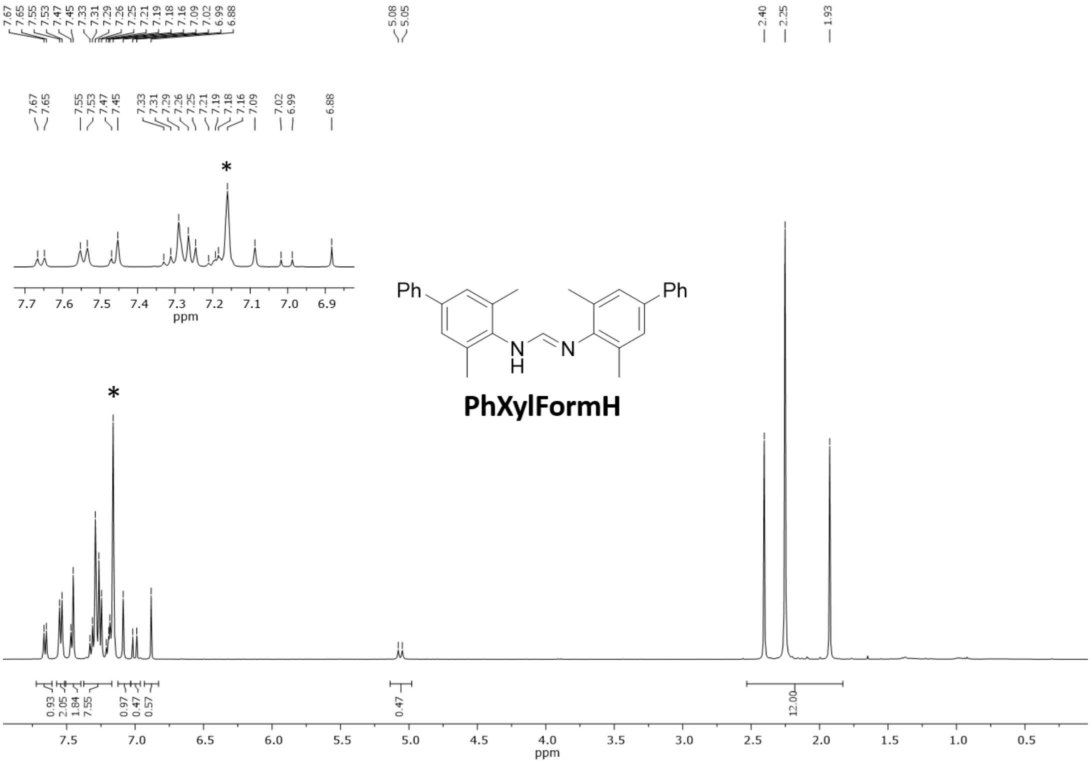


Figure S3: ^{1}H NMR spectrum of **PhXylFormH** (**L^3**) in C_6D_6: *, residual protio solvent signal.

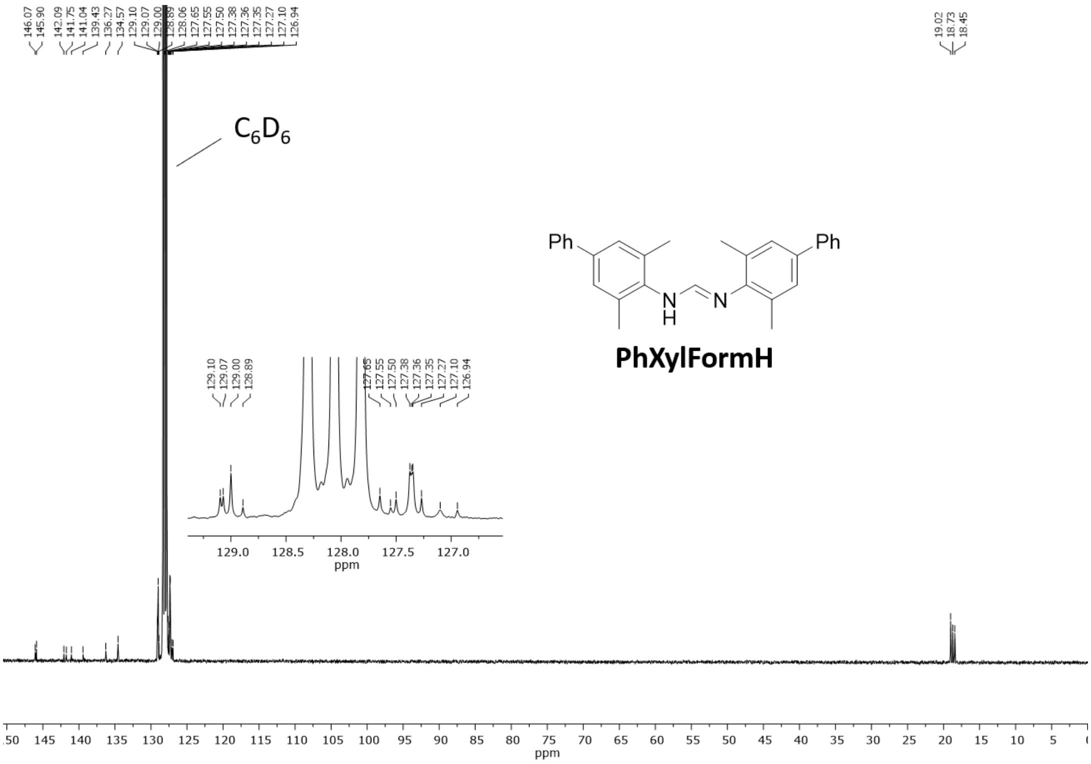


Figure S4: ^{13}C NMR spectrum of **PhXylFormH** (**L^3**) in C_6D_6.

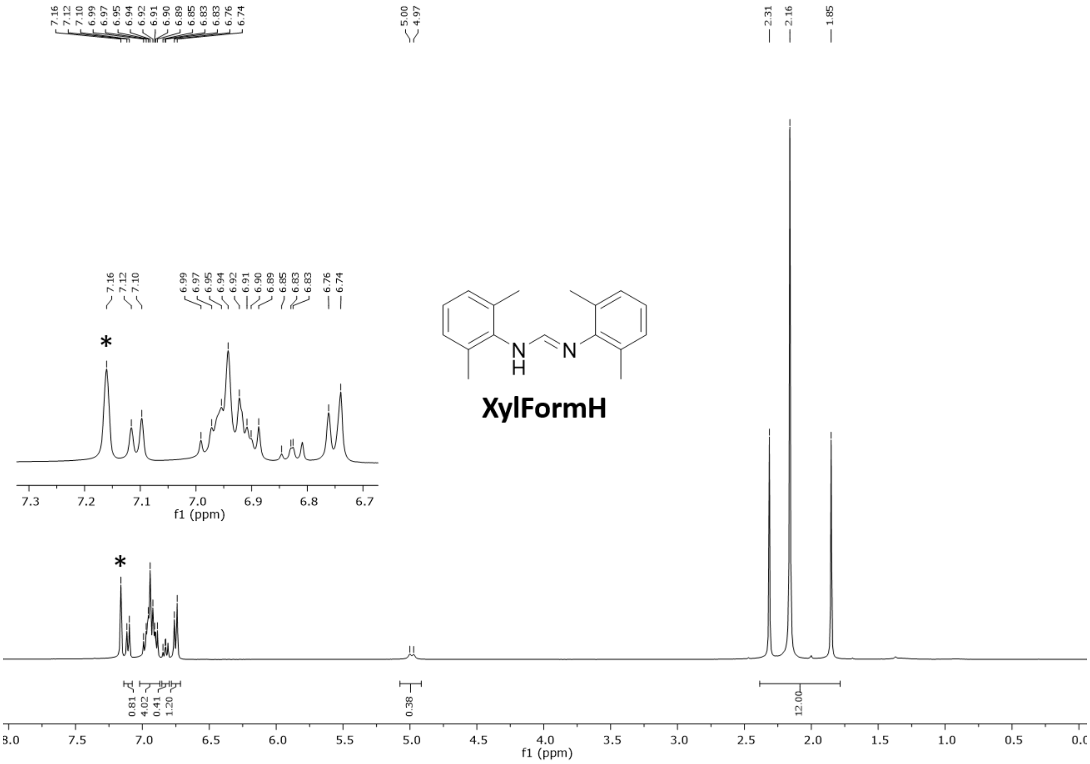


Figure S5: ^{1}H NMR spectrum of **XylFormH** (**L**[4]) in C_6D_6: *, residual protio solvent signal.

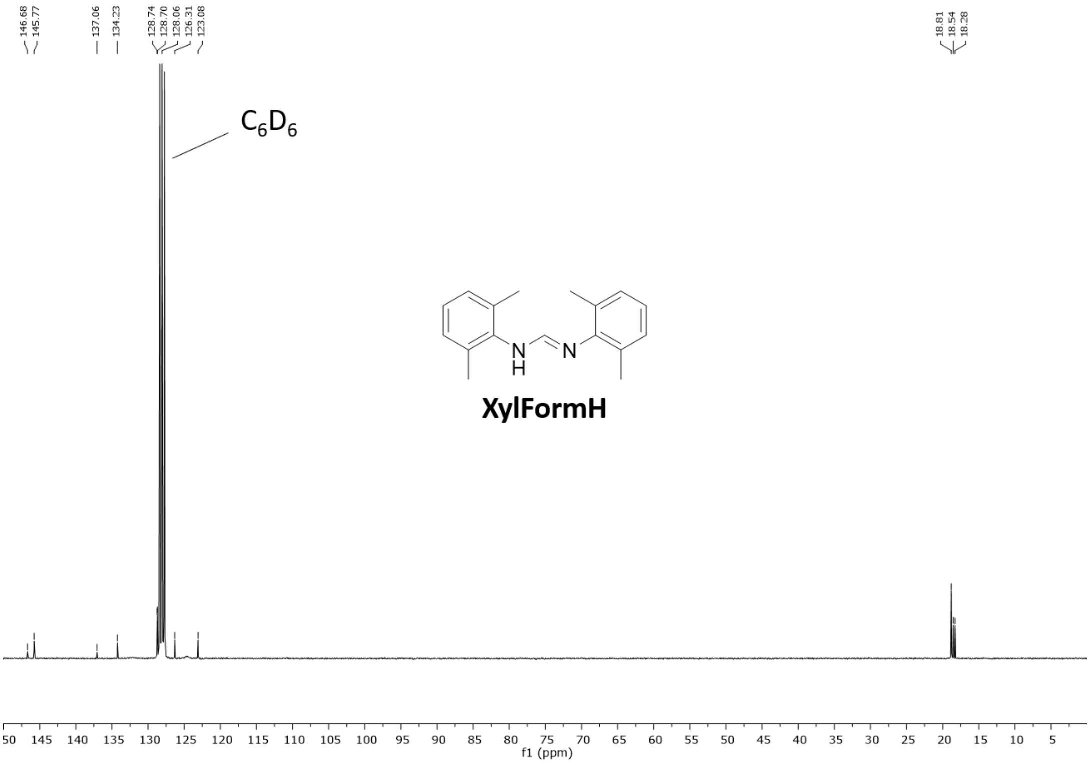


Figure S6: ^{13}C NMR spectrum of **XylFormH** (**L**[4]) in C_6D_6.

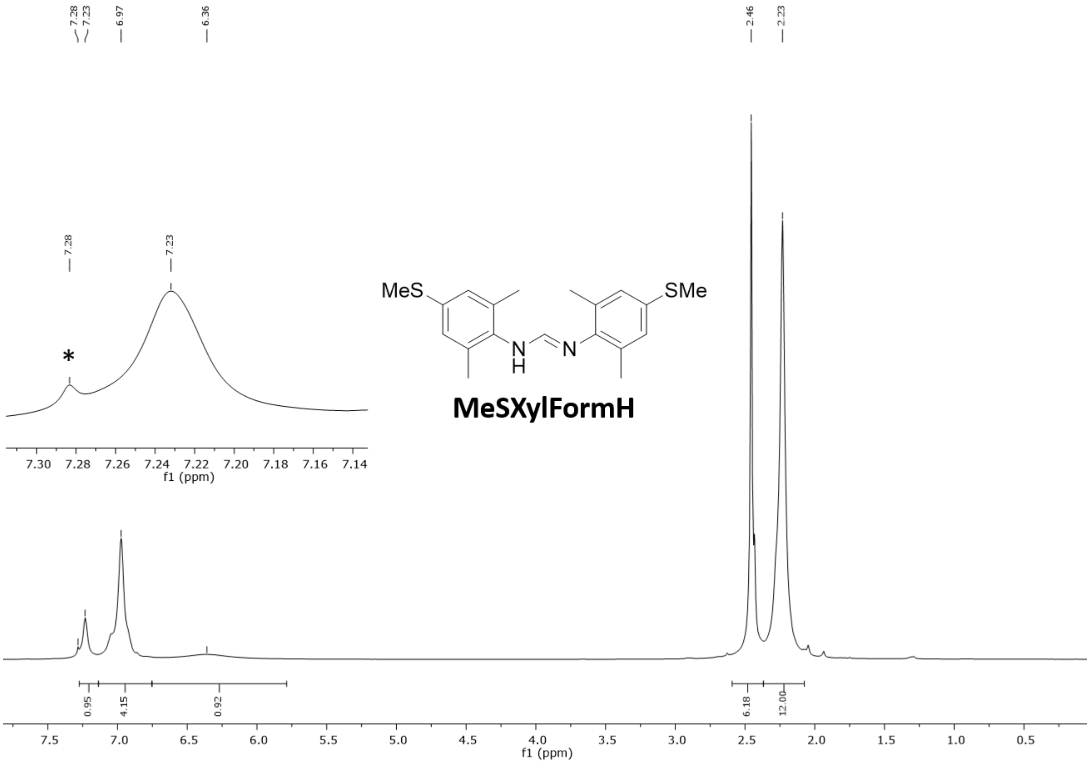


Figure S7: ^{1}H NMR spectrum of **MeSXylFormH** (**L^5**) in $CDCl_3$: *, residual protio solvent signal.

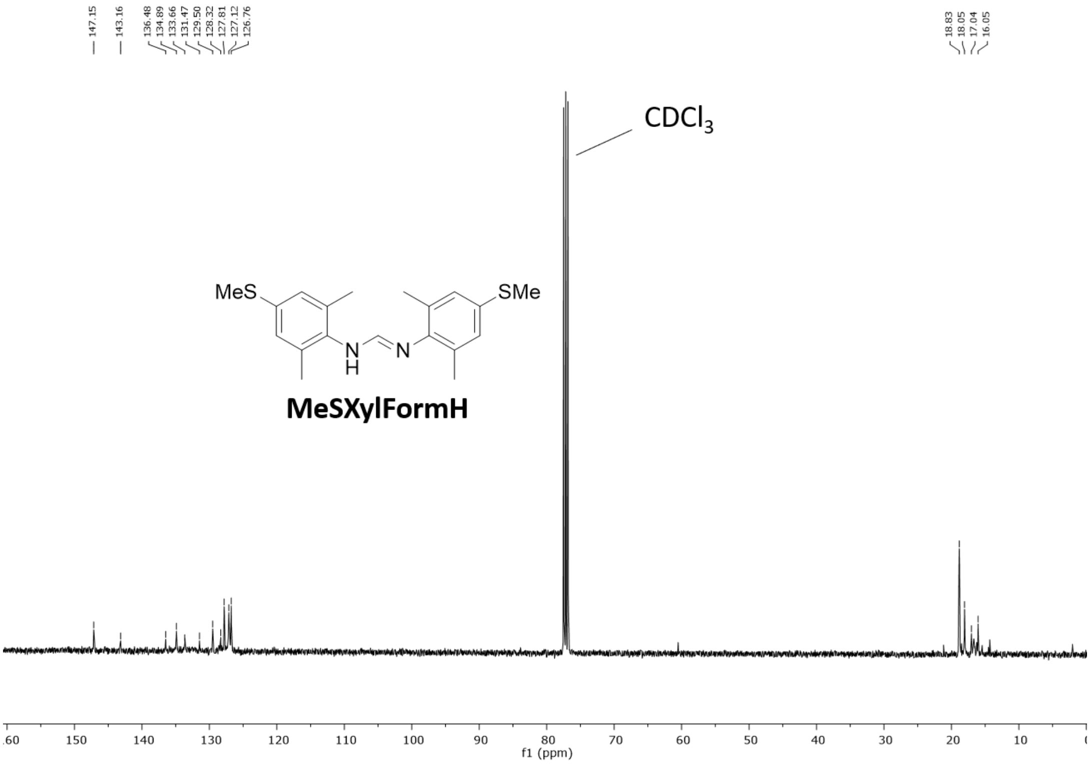


Figure S8: ^{13}C NMR spectrum of **MeSXylFormH** (**L^5**) in $CDCl_3$.

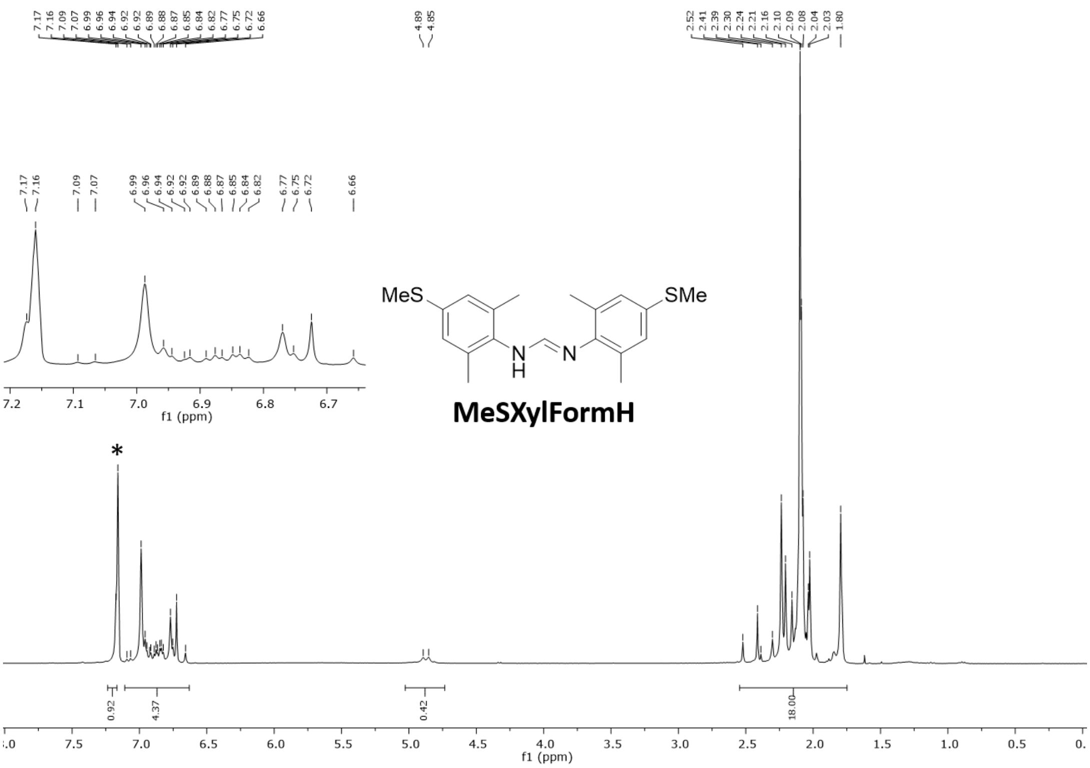


Figure S9: ^{1}H NMR spectrum of **MeSXylFormH** (**L^{5}**) in C_6D_6: *, residual protio solvent signal.

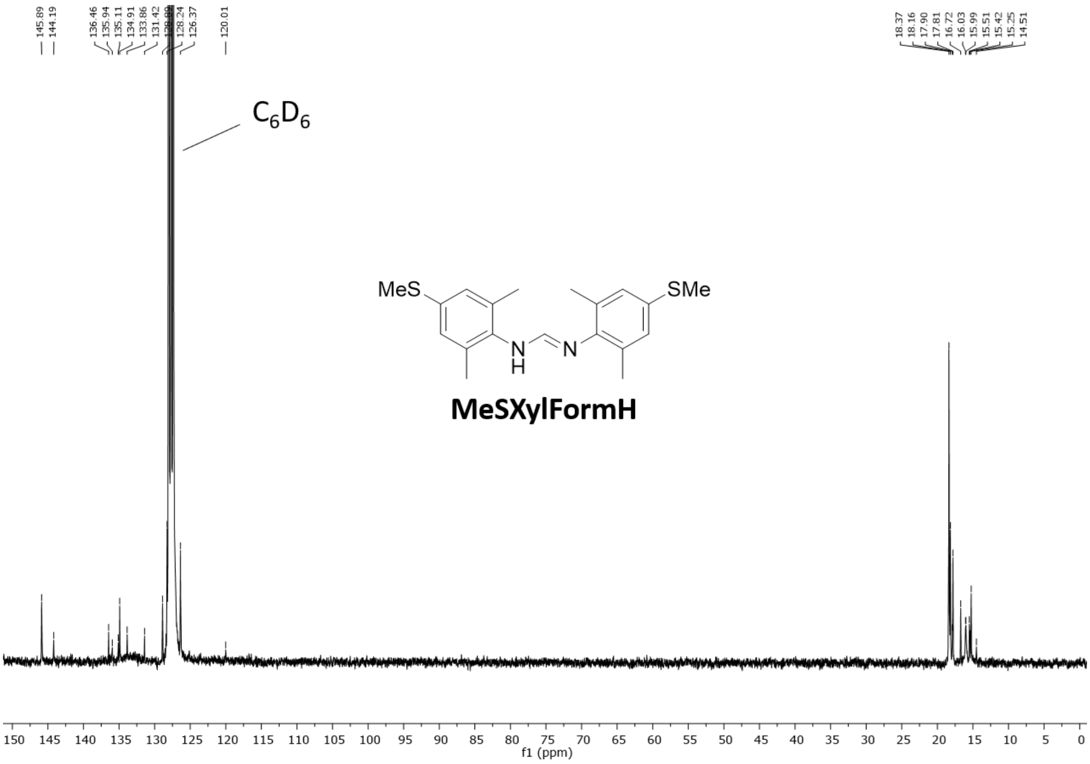


Figure S10: ^{13}C NMR spectrum of **MeSXylFormH** (**L^{5}**) in C_6D_6.

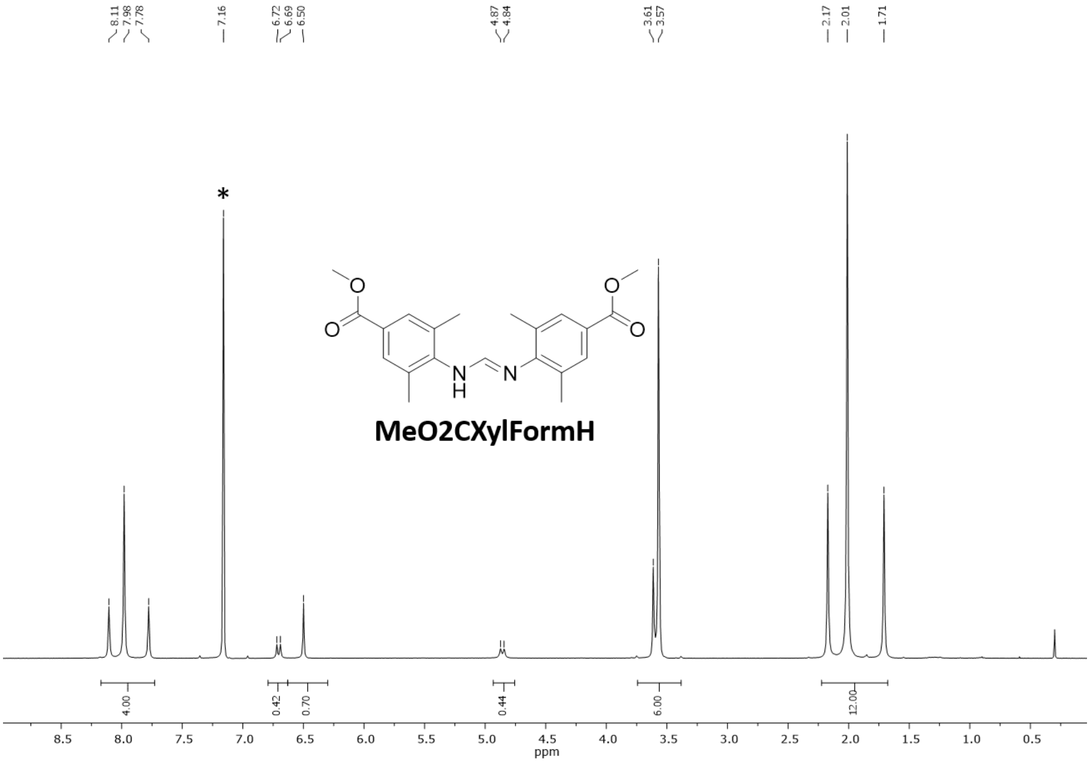


Figure S11: ^{1}H NMR spectrum of **MeO$_2$CXylFormH** (**L^6**) in C_6D_6: *, residual protio solvent signal.

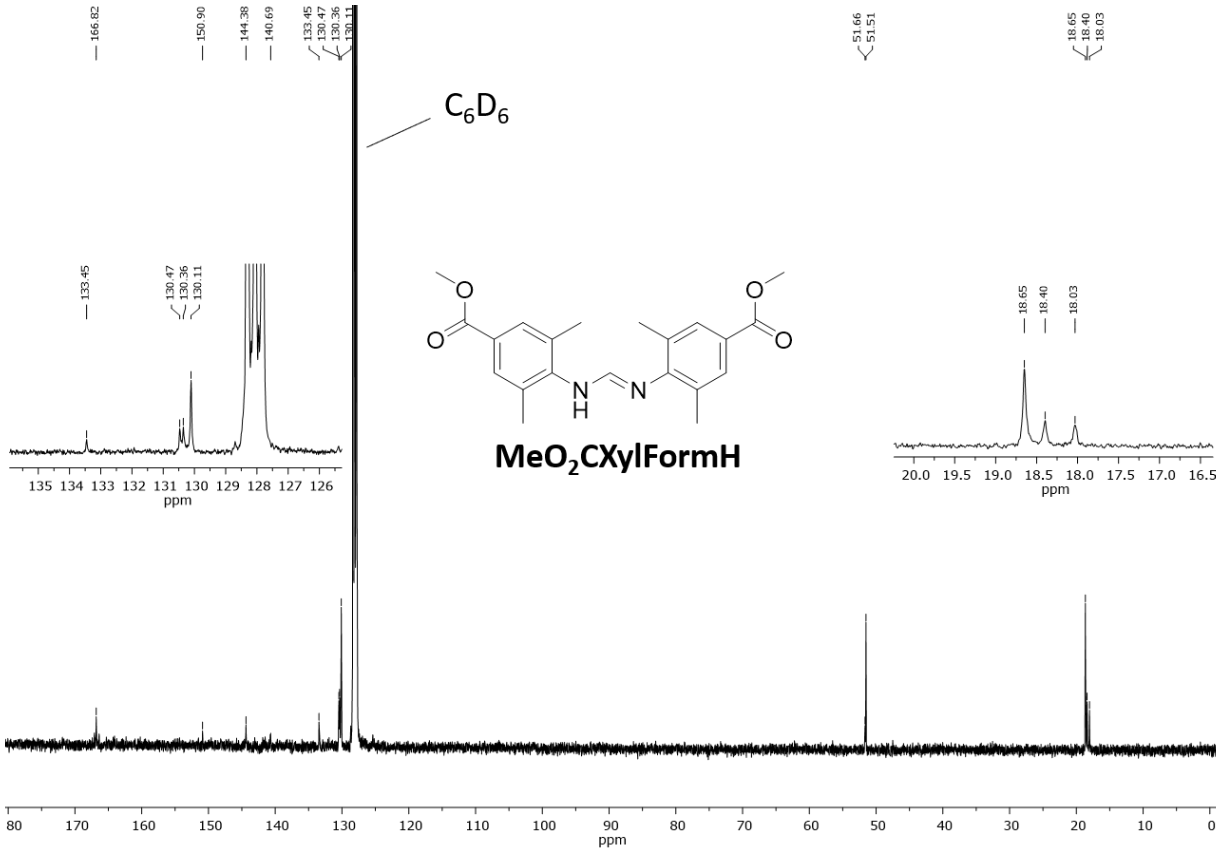


Figure S12: ^{13}C NMR spectrum of **MeO$_2$CXylFormH** (**L^6**) in C_6D_6.

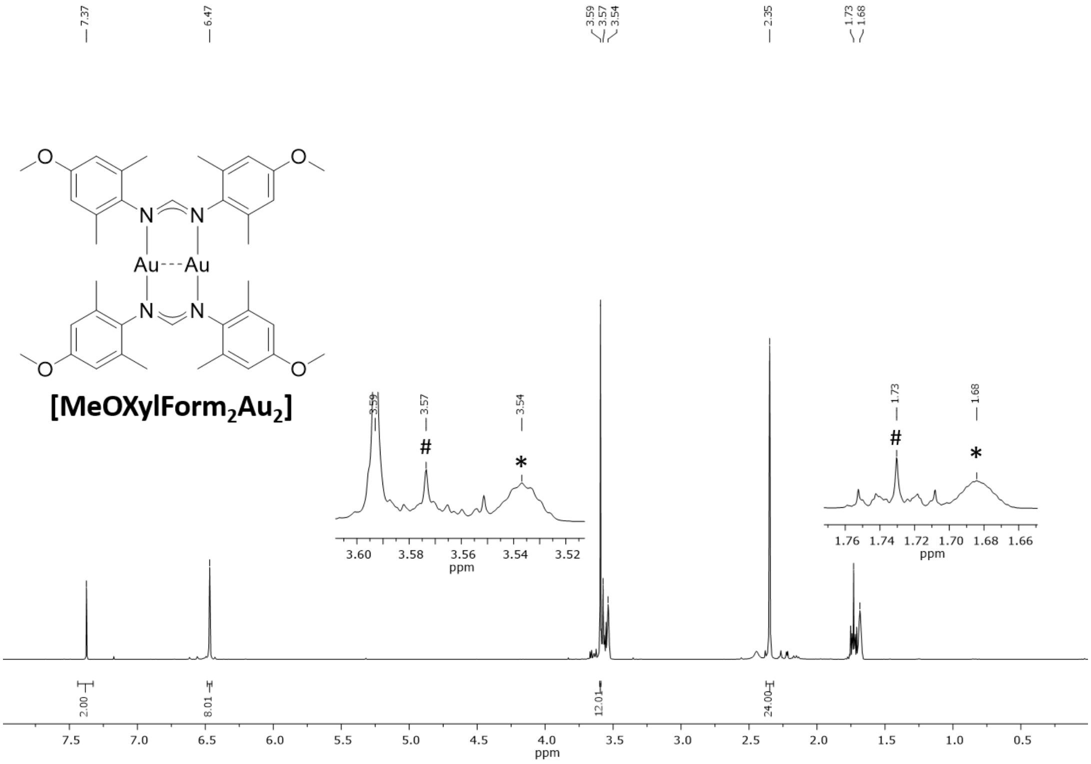


Figure S13: ^{1}H NMR spectrum of **[MeOXylForm$_2$Au$_2$]** (**1**) in THF-d$_8$: *, residual protio solvent signal; #, THF traces that are originating from the crystals.

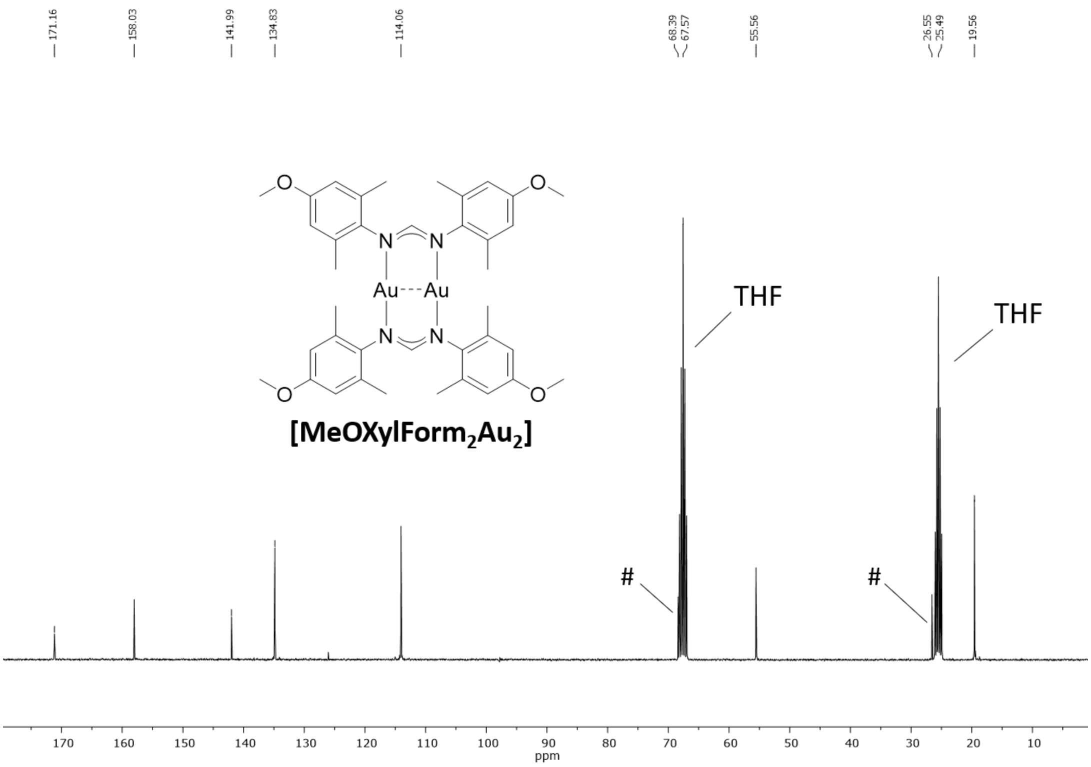


Figure S14: ^{13}C NMR spectrum of **[MeOXylForm$_2$Au$_2$]** (**1**) in THF-d$_8$: #, THF traces that are originating from the crystals.

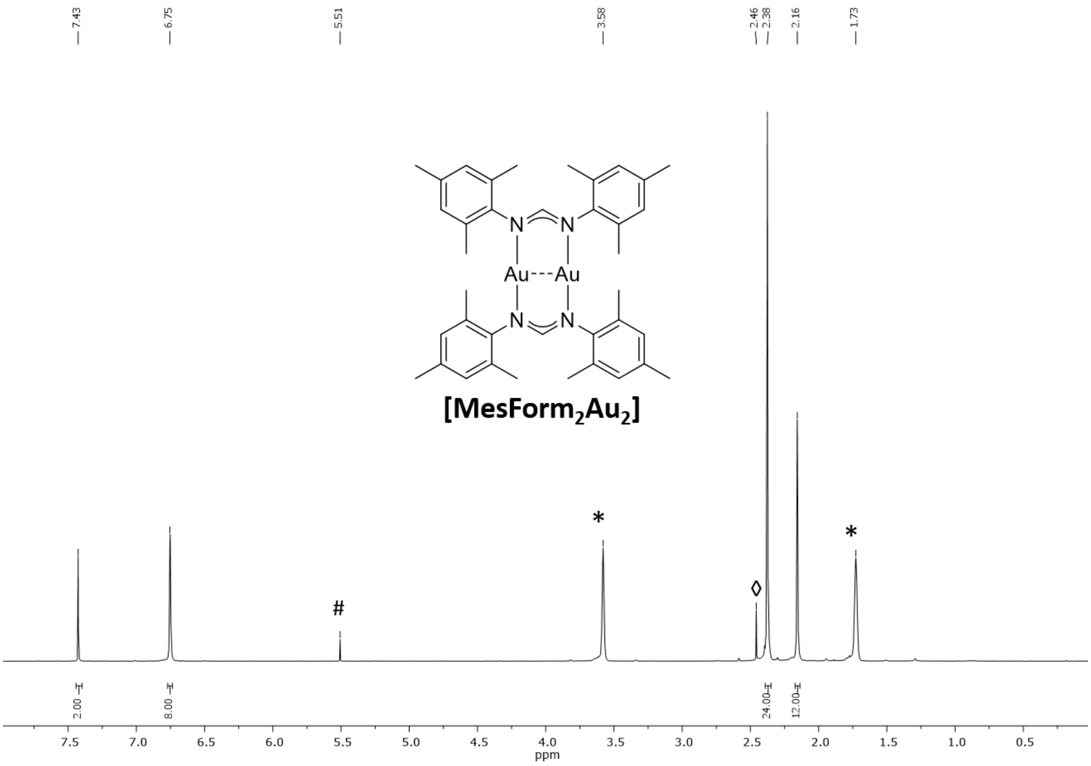


Figure S15: ^{1}H NMR spectrum of **[MesForm$_2$Au$_2$]** (**2**) in THF-d$_8$: *, residual protio solvent signal; #, DCM traces that are originating from the reaction; ◊, water.

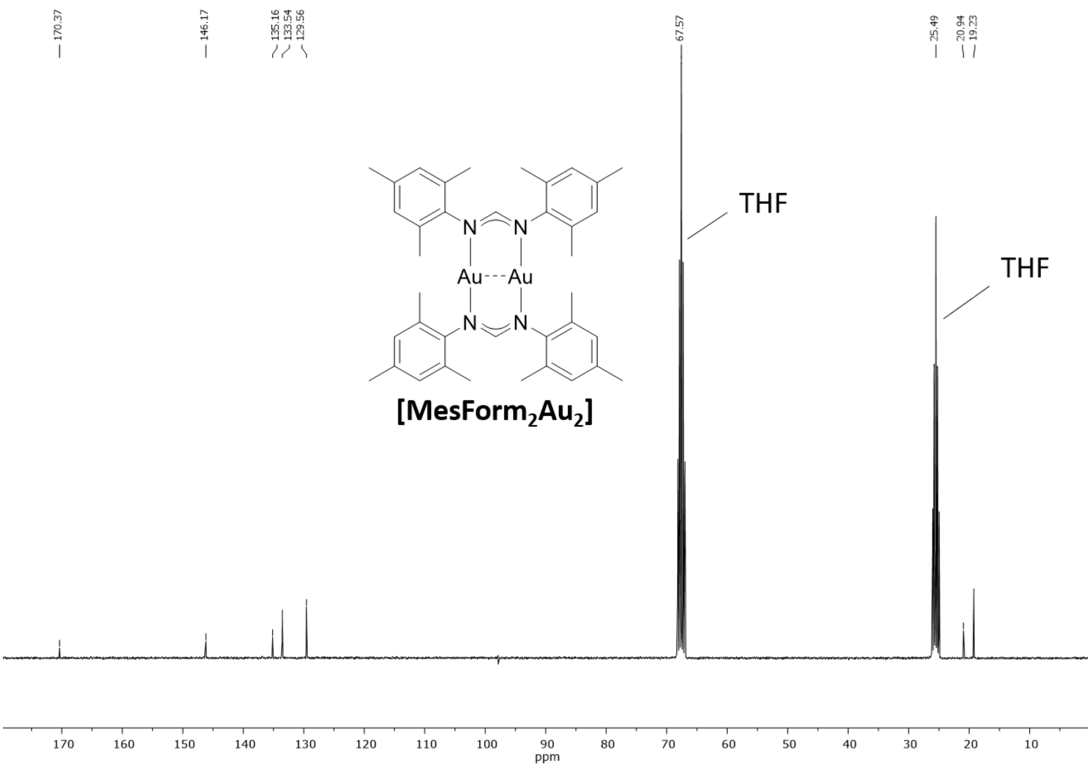


Figure S16: ^{13}C NMR spectrum of **[MesForm$_2$Au$_2$]** (**2**) in THF-d$_8$.

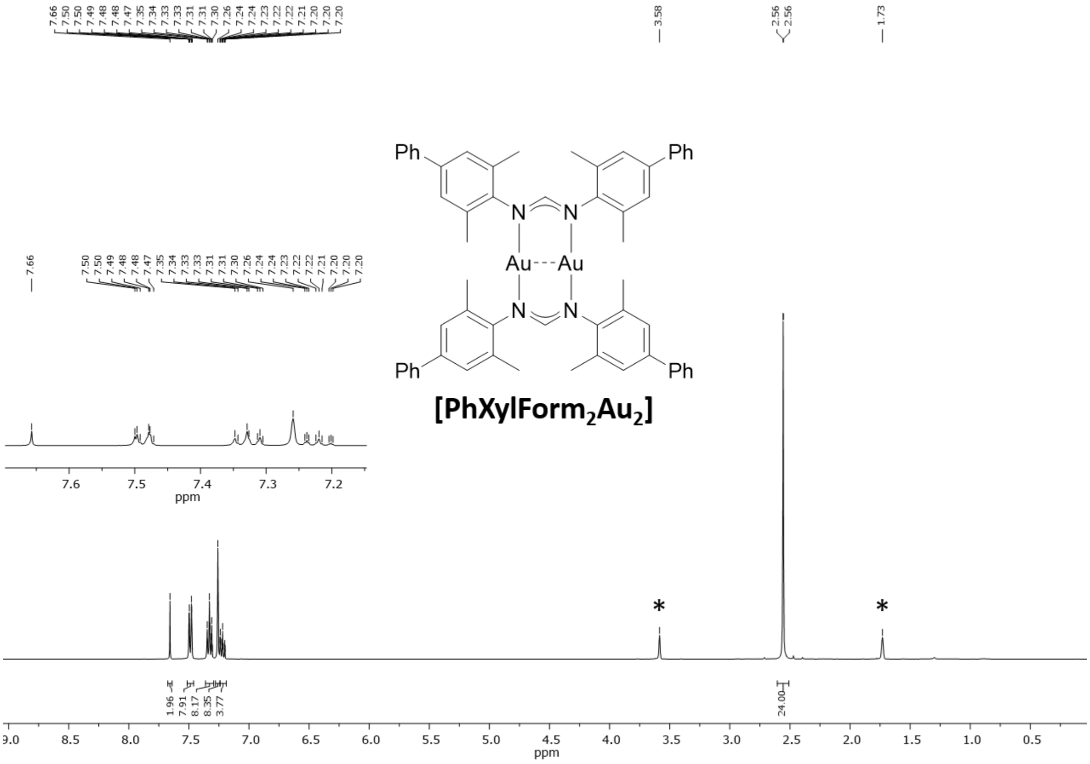


Figure S17: ^{1}H NMR spectrum of **[PhXylForm$_2$Au$_2$]** (**3**) in THF-d_8: *, residual protio solvent signal.

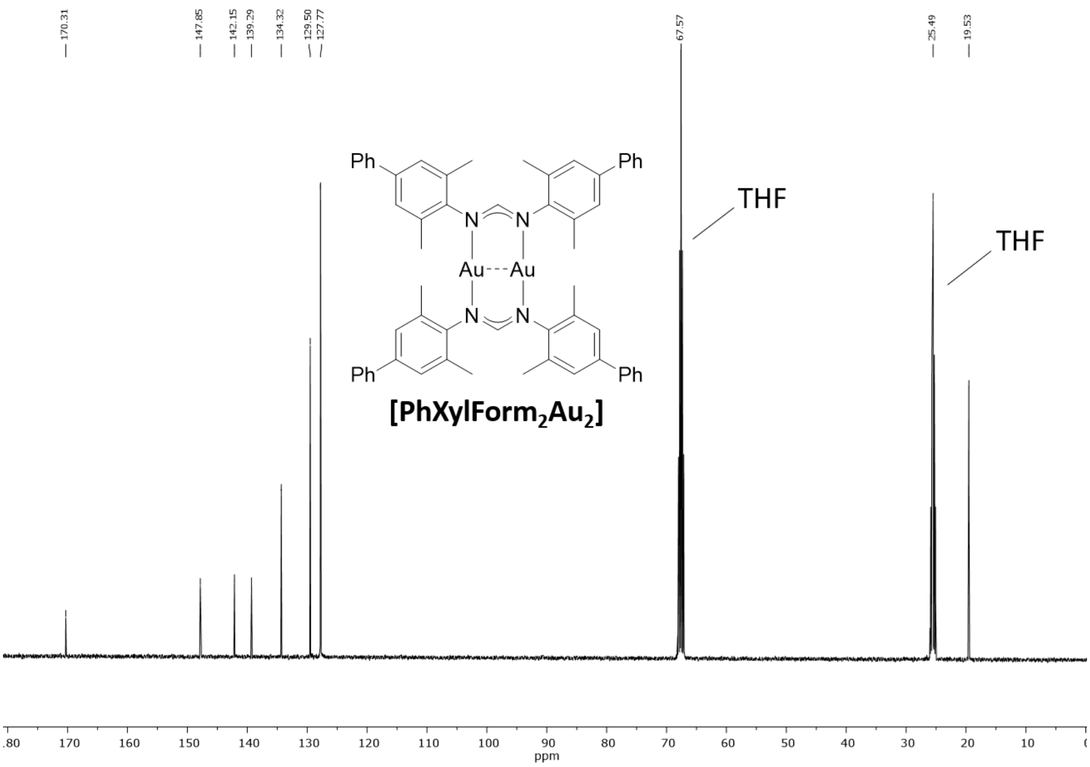


Figure S18: ^{13}C NMR spectrum of **[PhXylForm$_2$Au$_2$]** (**3**) in THF-d_8.

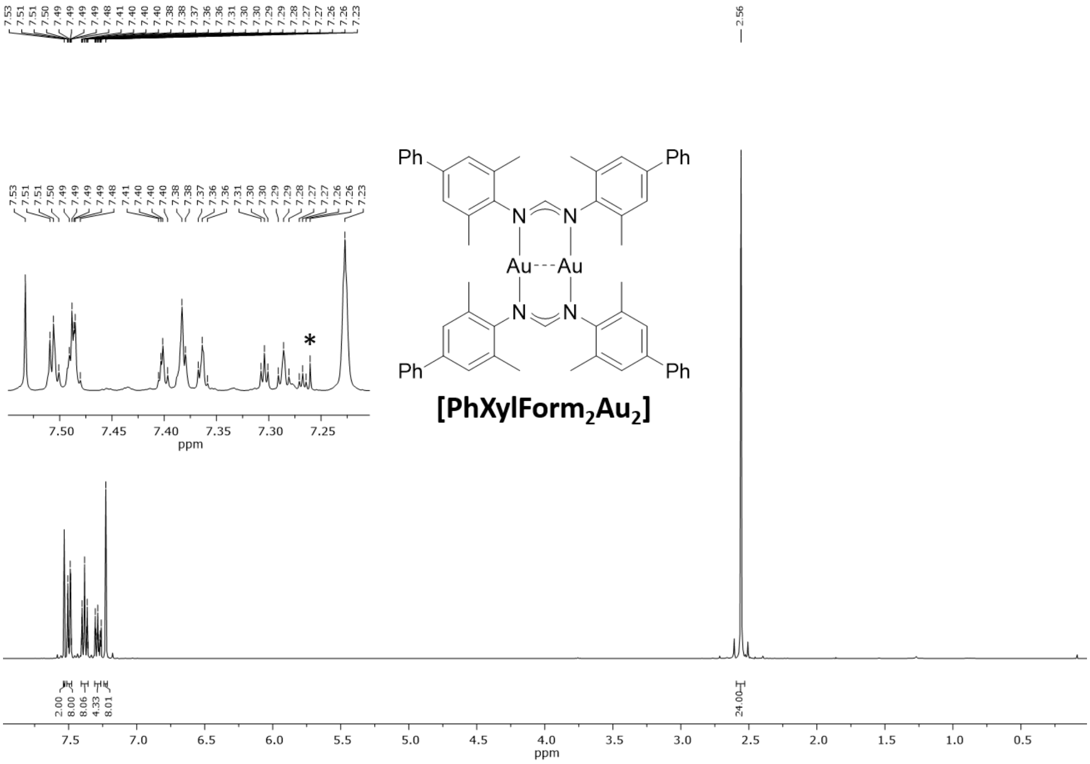


Figure S19: ^{1}H NMR spectrum of **[PhXylForm$_2$Au$_2$]** (**3**) in $CDCl_3$: *, residual protio solvent signal.

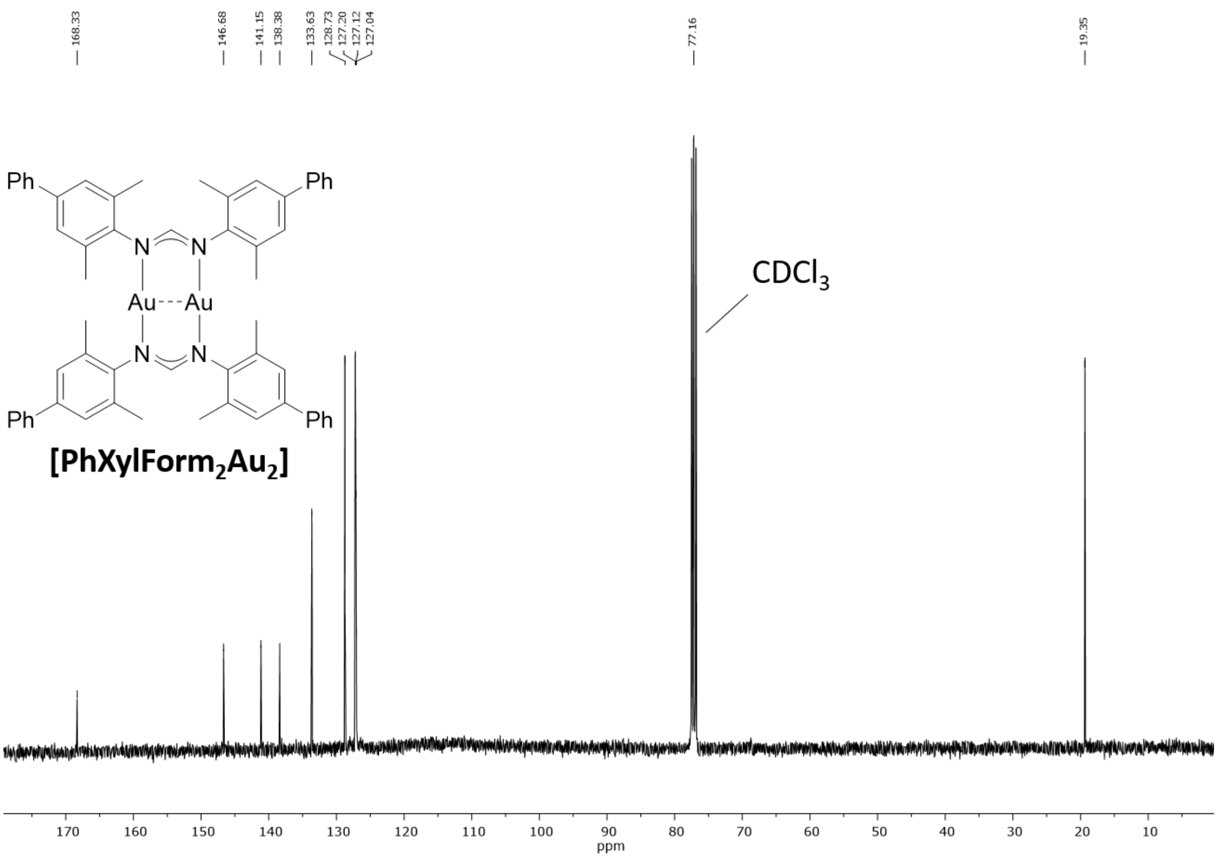


Figure S20: ^{13}C NMR spectrum of **[PhXylForm$_2$Au$_2$]** (**3**) in $CDCl_3$.

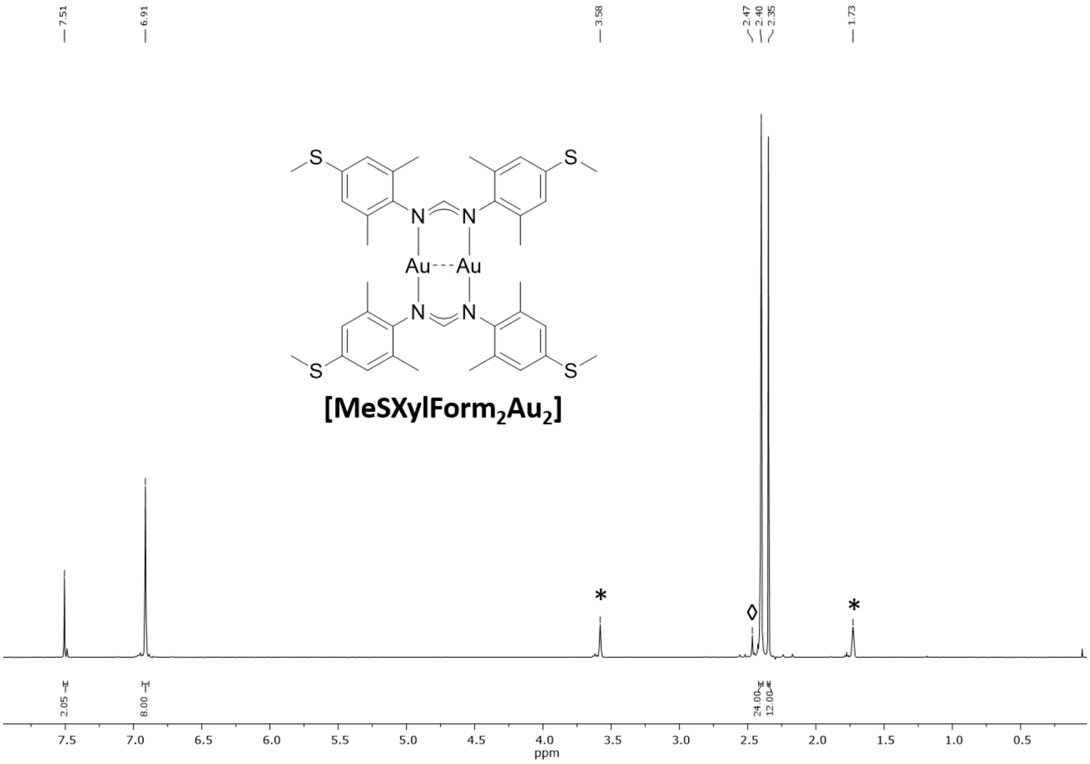


Figure S21: [1]H NMR spectrum of **[MeSXylForm$_2$Au$_2$]** (**5**) in THF-d$_8$: *, residual protio solvent signal; ◊, water.

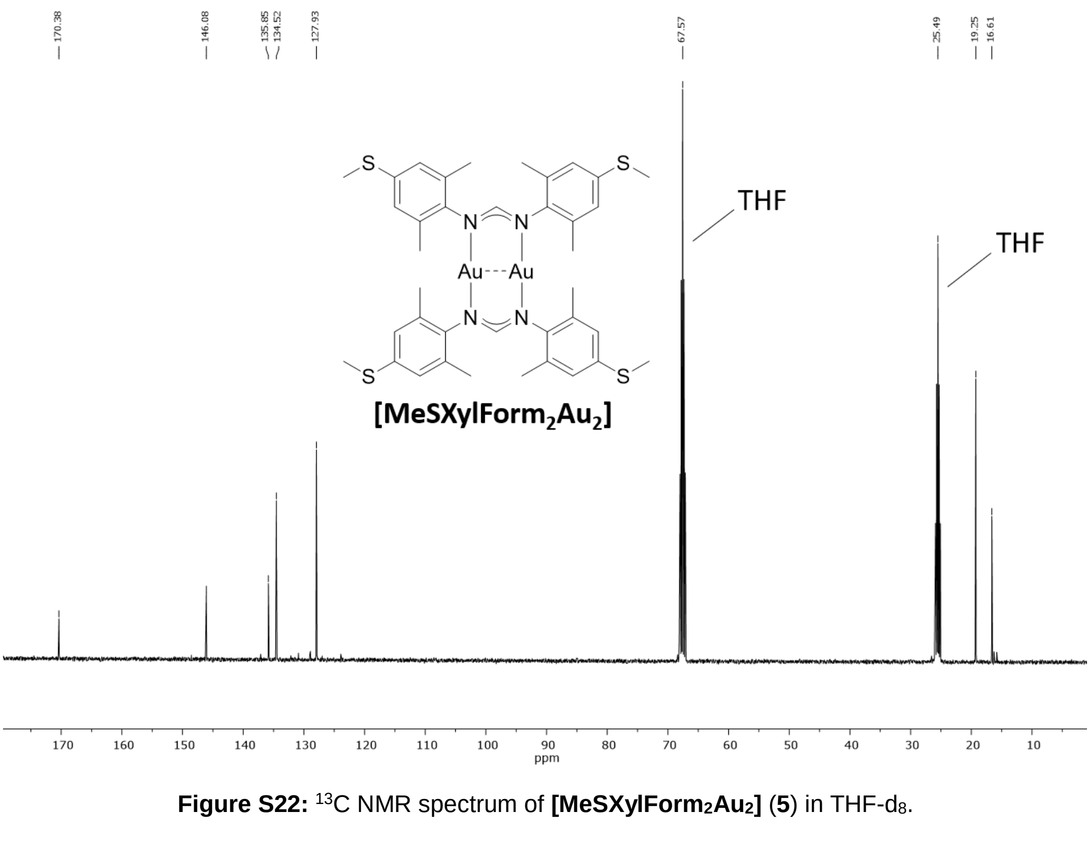


Figure S22: [13]C NMR spectrum of **[MeSXylForm$_2$Au$_2$]** (**5**) in THF-d$_8$.

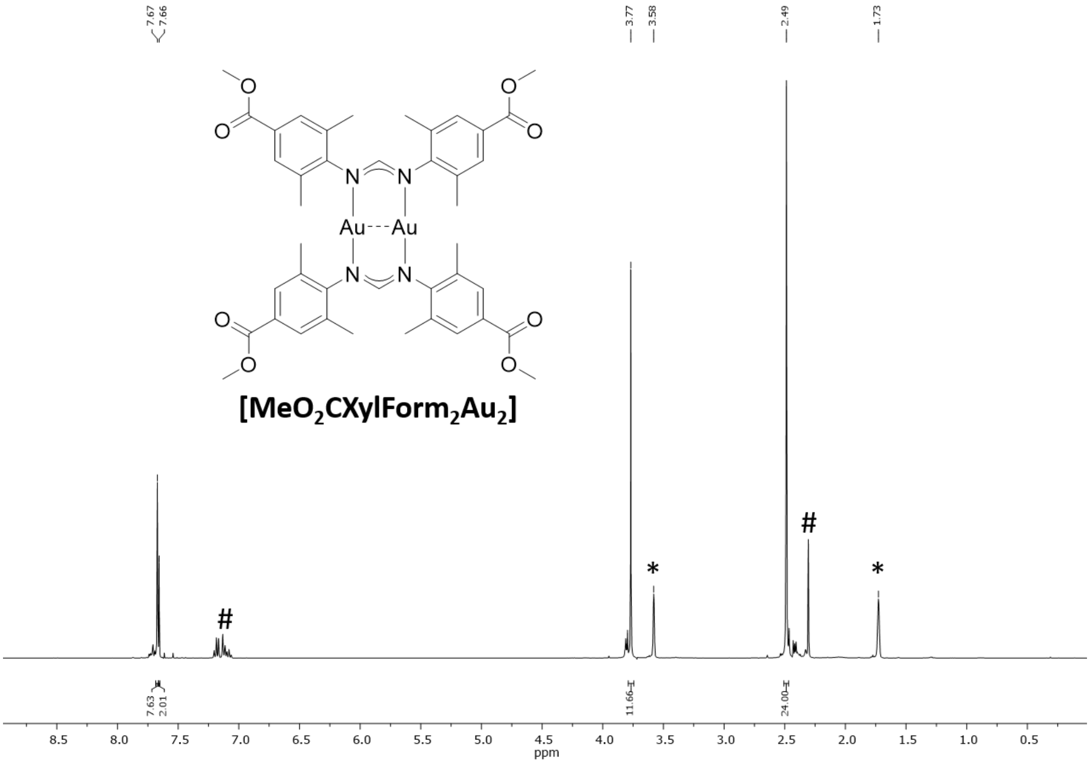


Figure S23: ^{1}H NMR spectrum of **[MeO$_2$CXylForm$_2$Au$_2$]** (**6**) in THF-d$_8$: *, residual protio solvent signal; #, toluene traces that are originating from the crystals.

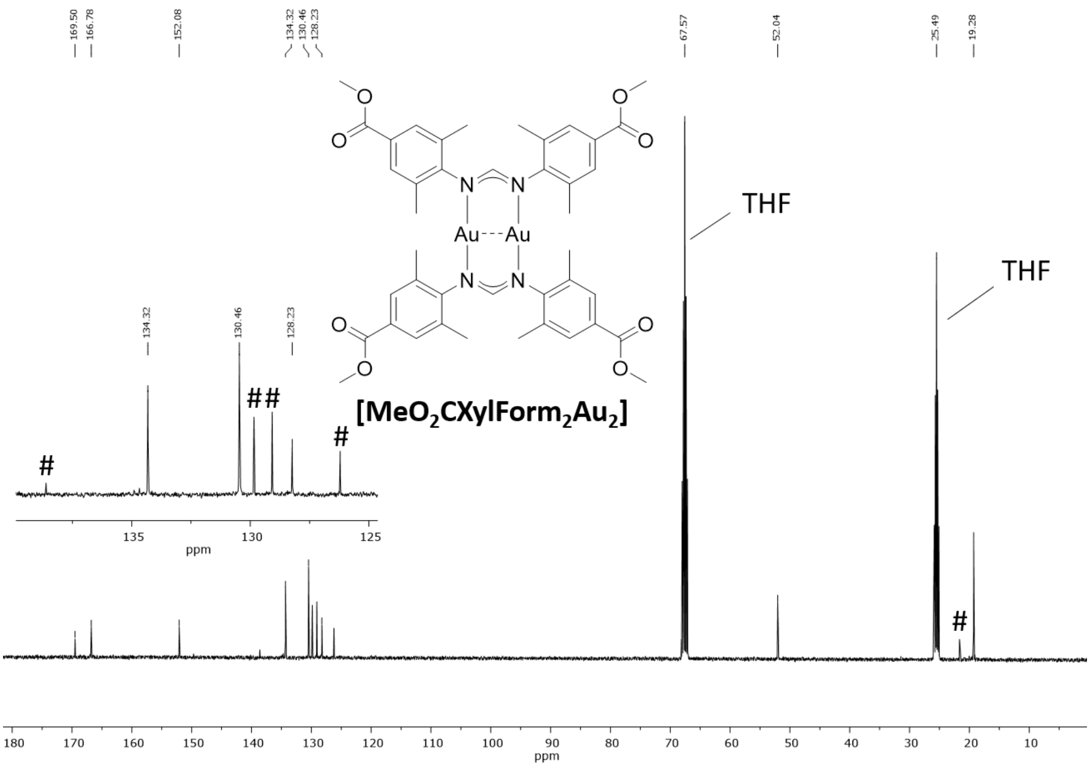


Figure S24: ^{13}C NMR spectrum of **[MeO$_2$CXylForm$_2$Au$_2$]** (**6**) in THF-d$_8$: #, toluene traces that are originating from the crystals.

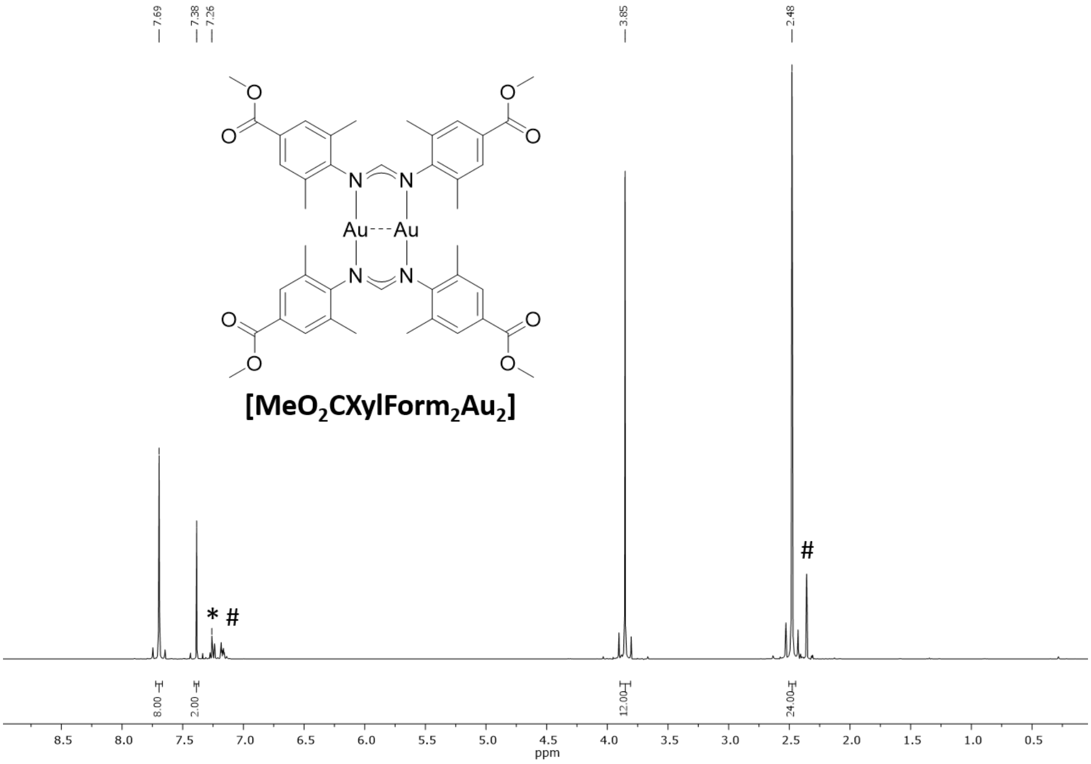


Figure S25: [1]H NMR spectrum of **[MeO$_2$CXylForm$_2$Au$_2$]** (**6**) in $CDCl_3$: *, residual protio solvent signal; #, toluene traces that are originating from the crystals.

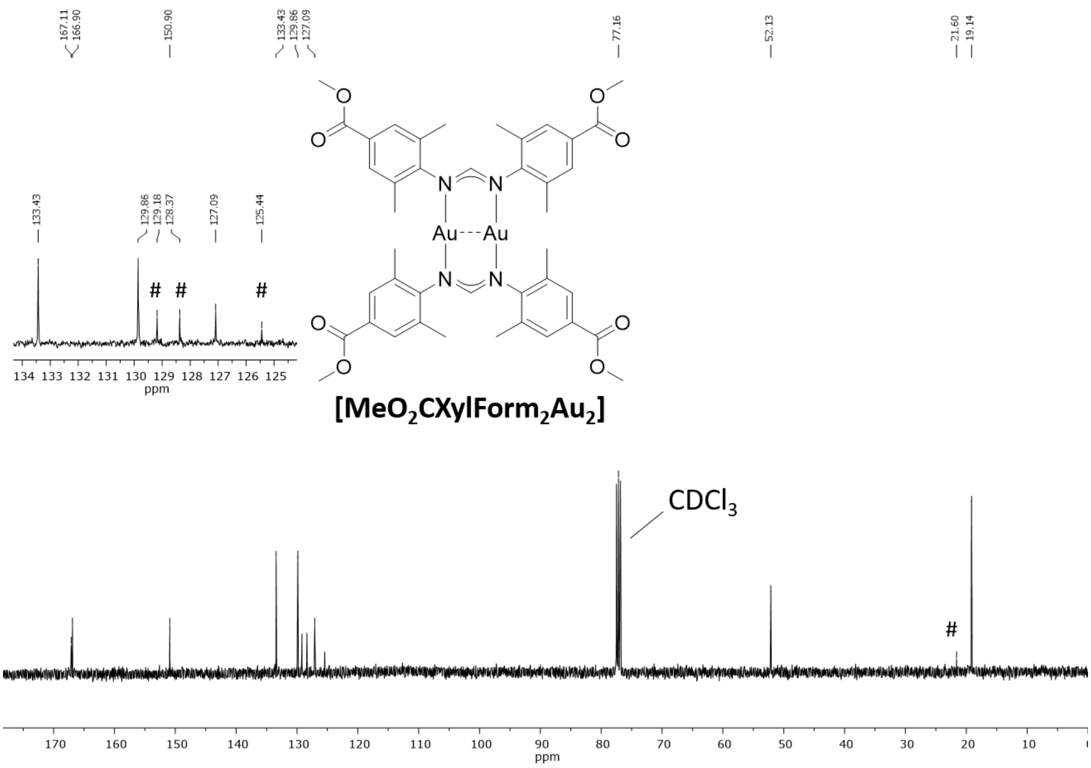


Figure S26: [13]C NMR spectrum of **[MeO$_2$CXylForm$_2$Au$_2$]** (**6**) in $CDCl_3$: #, toluene traces that are originating from the crystals.

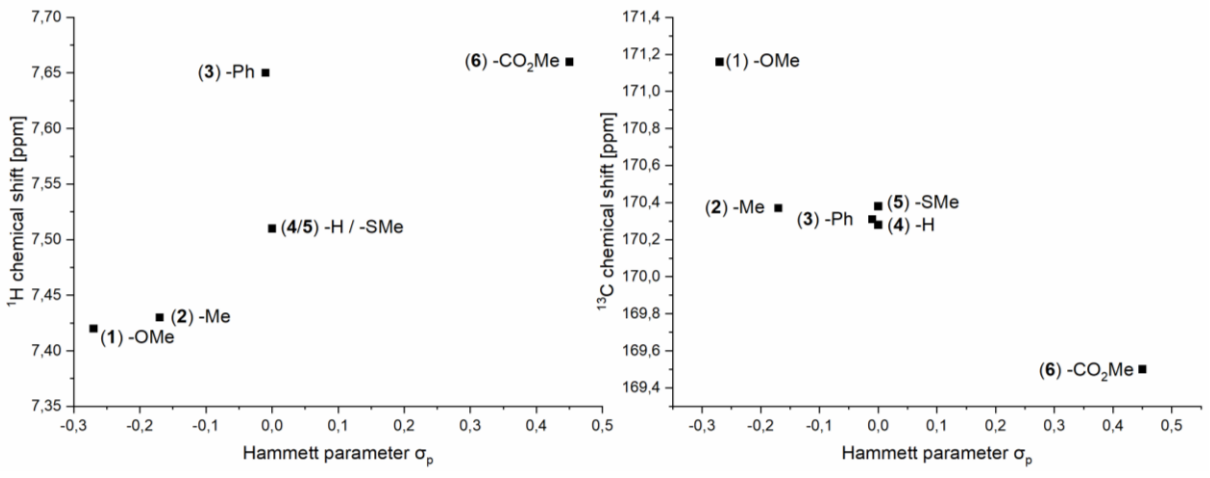


Figure S27: Chemical shift in ^{1}H NMR for NC(*H*)N (left) and ^{13}C NMR for N*C*N (right) compared to σ_p.

Photoluminescence spectra

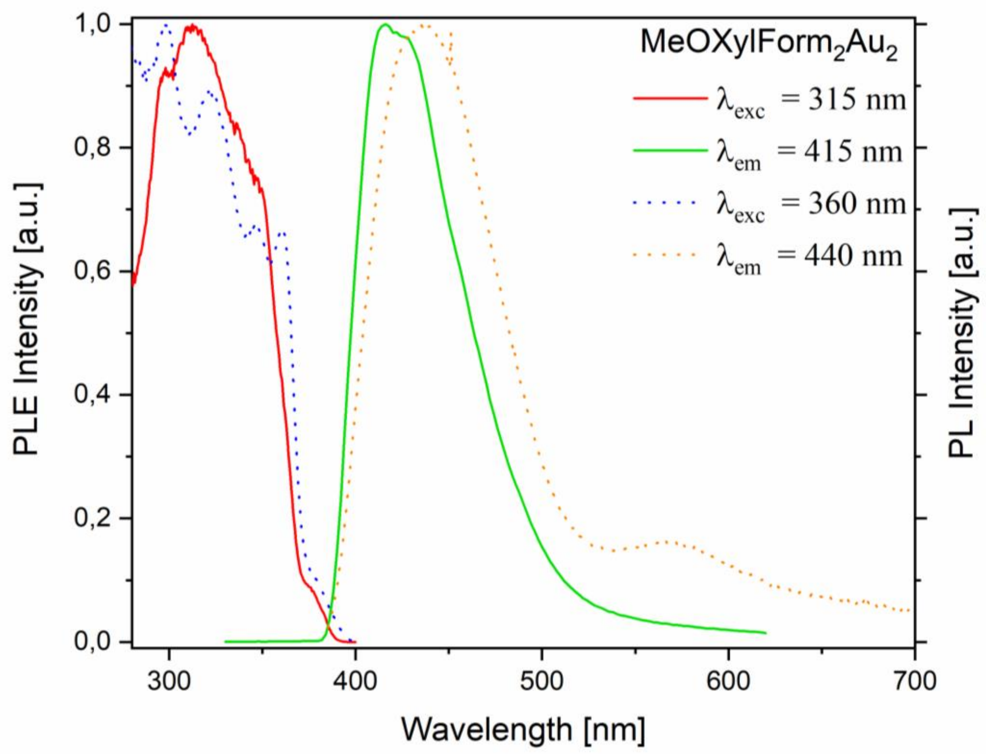


Figure S28: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **1** in solid state and in THF (dotted line) at 77 K.

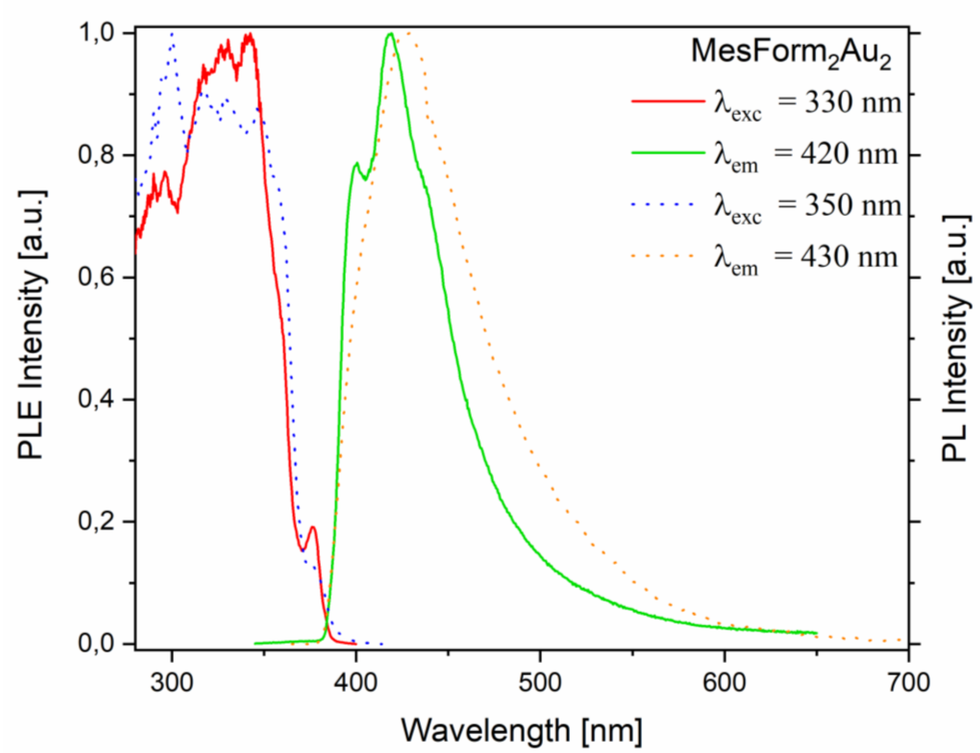


Figure S29: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **2** in solid state and in THF (dotted line) at 77 K.

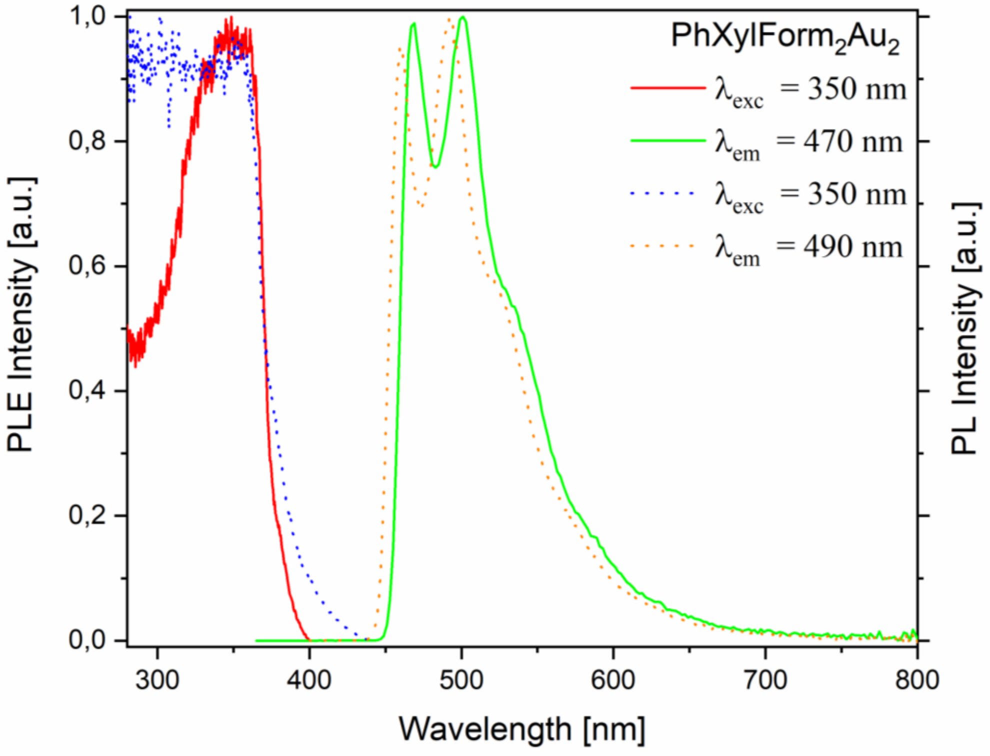


Figure S30: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **3** in solid state and in THF (dotted line) at 77 K.

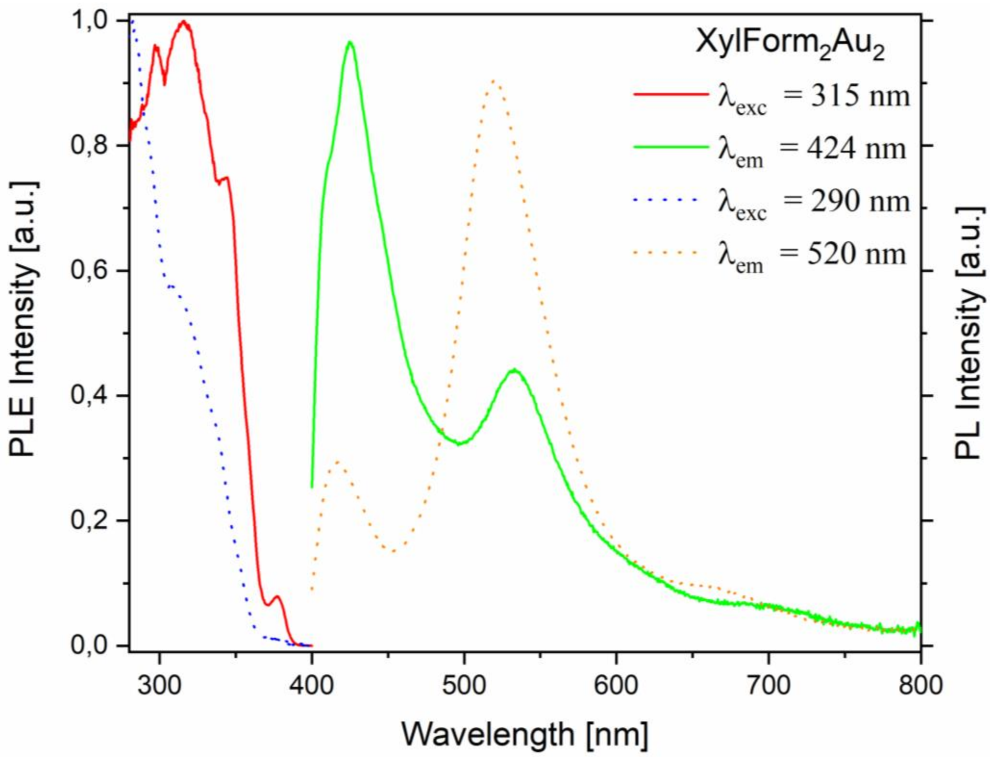


Figure S31: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **4** in solid state and in THF (dotted line) at 77 K.

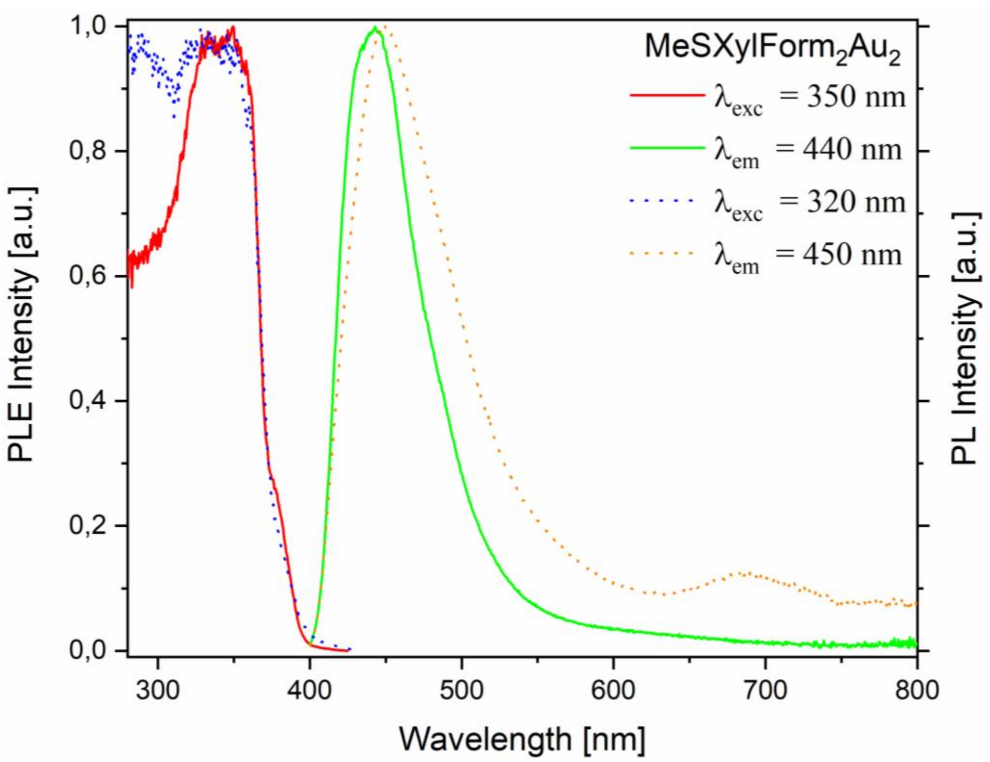


Figure S32: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **5** in solid state and in THF (dotted line) at 77 K.

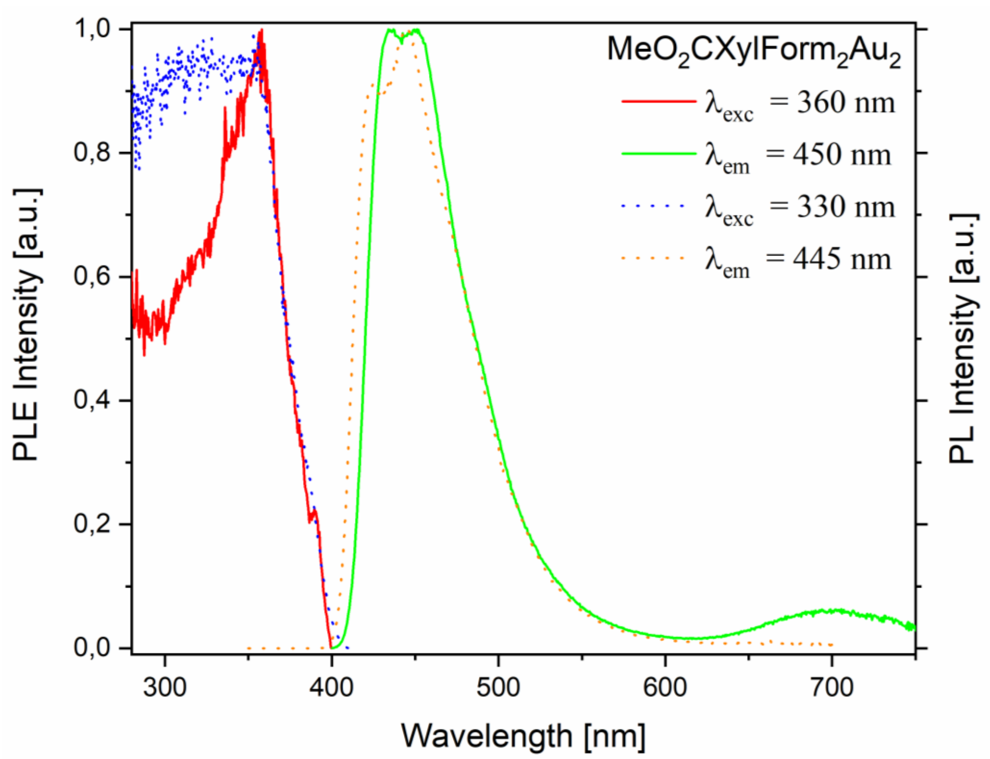


Figure S33: Photoluminescence emission (PL) and excitation (PLE) spectra of compound **6** in solid state and in THF (dotted line) at 77 K.

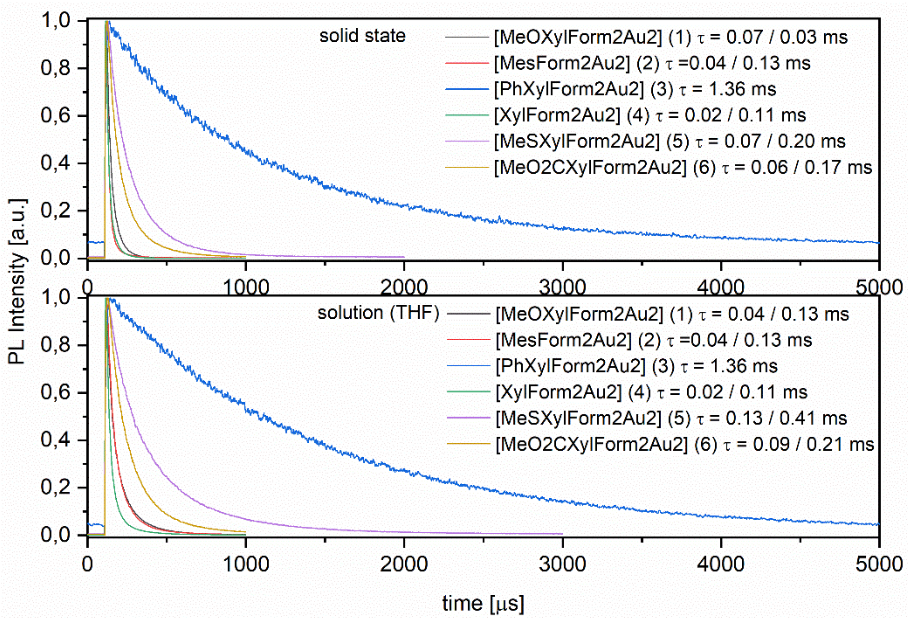
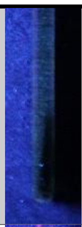
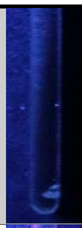
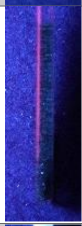
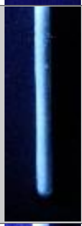
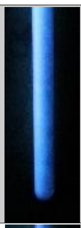
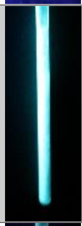
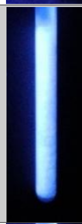
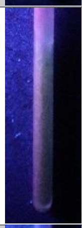
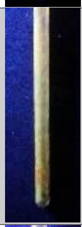
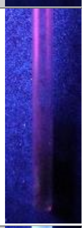
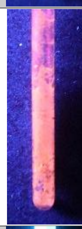
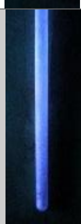
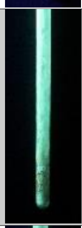
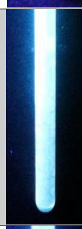
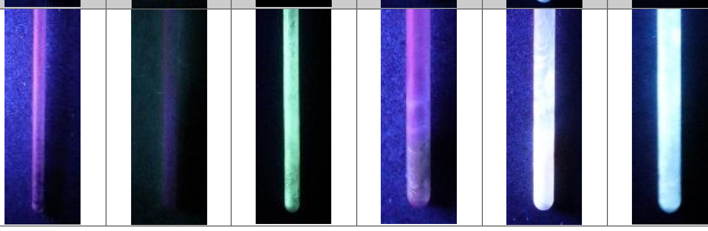


Figure S34: Phosphorescence decay times in solution and in solid state for compounds **1**-**6**.

Table S1: Experimental data of the LU spectra and the decay times for compounds **1**-**6**.

		1	2	3	4	5	6
λ (Exc, solution)	**[nm]**	360	350	350	290	320	330
λ (Em, solution)	**[nm]**	440	430	490	520	450	445
λ (Max_{exc}, solution, 77 K)	**[nm]**	298	300	282	284	334	353
λ (Max_{em}, solution, 77 K)	**[nm]**	437	429	492	519	449	446
λ (Exc, solid)	**[nm]**	315	330	350	315	350	360
λ (Em, solid)	**[nm]**	415	420	470	424	440	450
λ (Max_{exc}, solid, 77 K)	**[nm]**	313	343	349	316	350	358
λ (Max_{em}, solid, 77 K)	**[nm]**	416	419	501	425	443	451
τ_1, Phos (solution, 77 K)	**[ms]**	0.04	0.04	1.36	0.02	0.13	0.09
τ_2, Phos (solution, 77 K)	**[ms]**	0.13	0.13	--	0.11	0.41	0.21
τ_1, Phos (solid, 77 K)	**[ms]**	0.07	0.14	0.44	0.06	0.07	0.06
τ_2/τ_3, Phos (solid, >77 K)	**[ms]**	0.03	0.02/ 0.02	1.23	0.02	0.20	0.17

Table S2: Visual luminescence under UV light with short (254 nm) and long (360 nm) Wavelength, in solution and in solid state at low temperatures (77 K) and room temperature.

	1	2	3	4	5	6
Solution, rt, 254 nm						
Solution, rt, 360 nm						
Solution, 77 K, 254 nm						
Solution, 77 K, 360 nm						
Solid, rt, 254 nm						
Solid, rt, 360 nm						
Solid, 77 K, 254 nm						
Solid, 77 K, 360 nm						

IR spectra

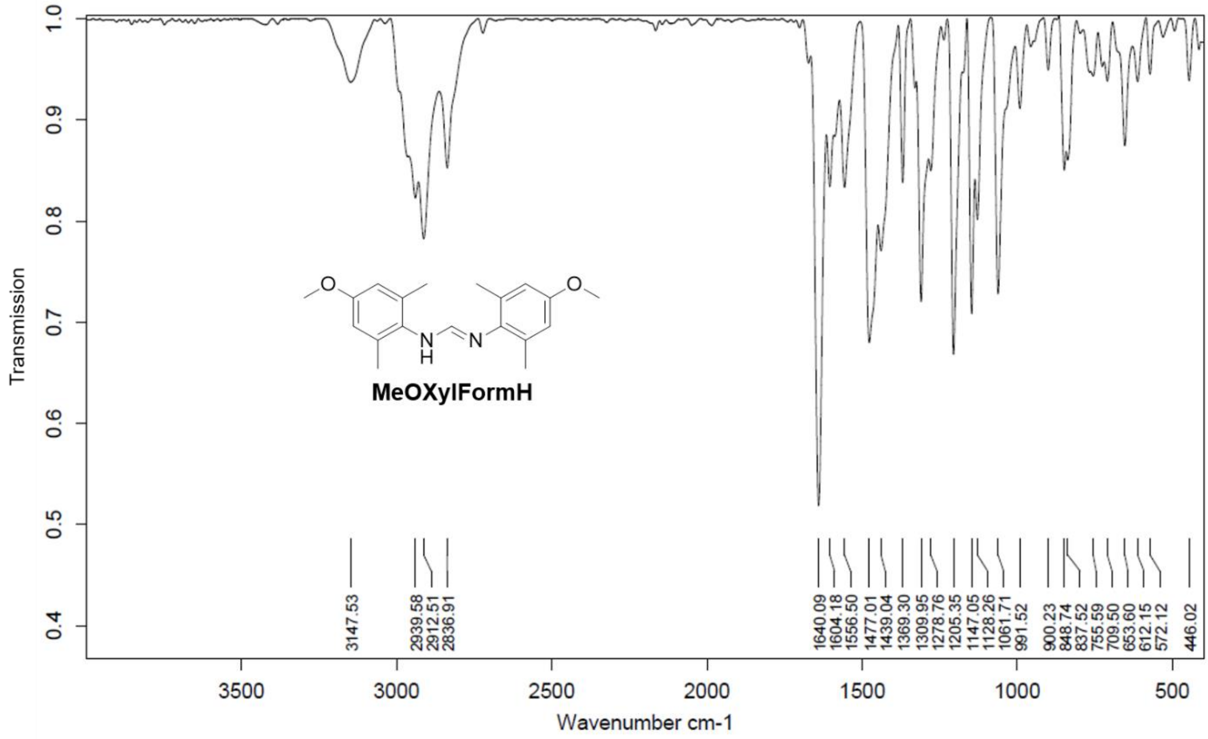


Figure S35: IR spectrum of **MeOXylFormH** (**L[1]**).

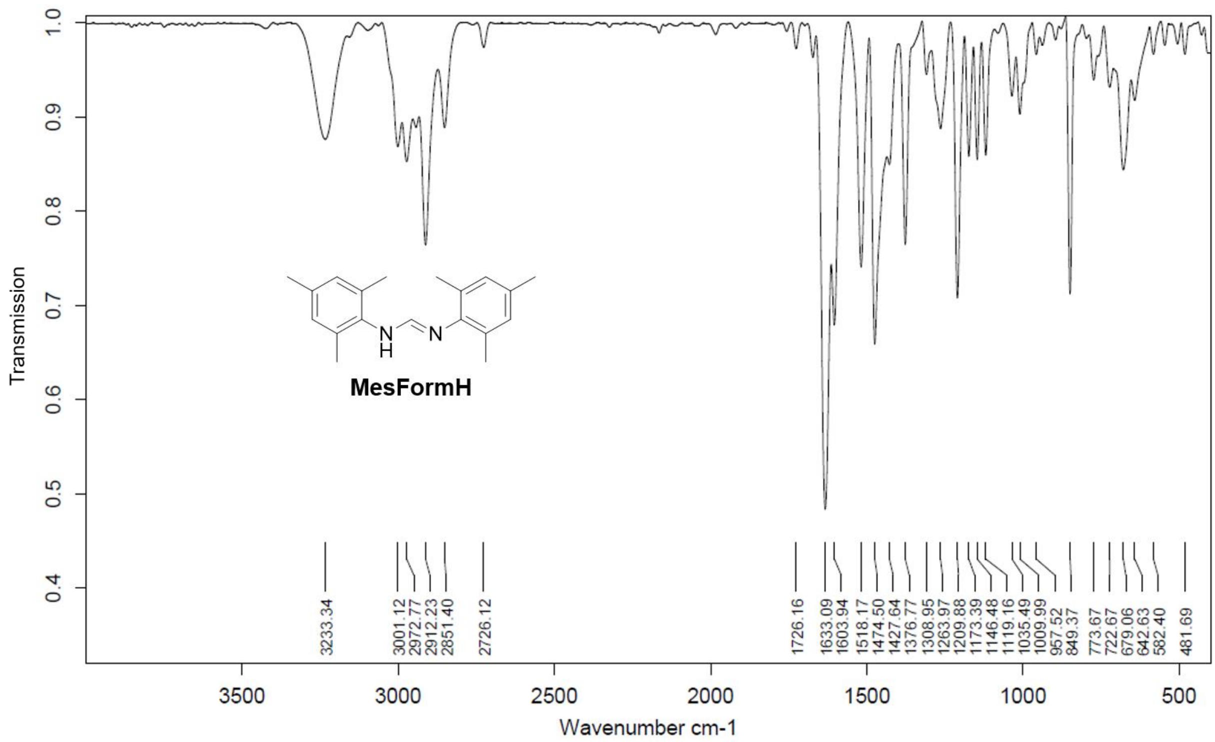


Figure S36: IR spectrum of **MesFormH** (**L[2]**).

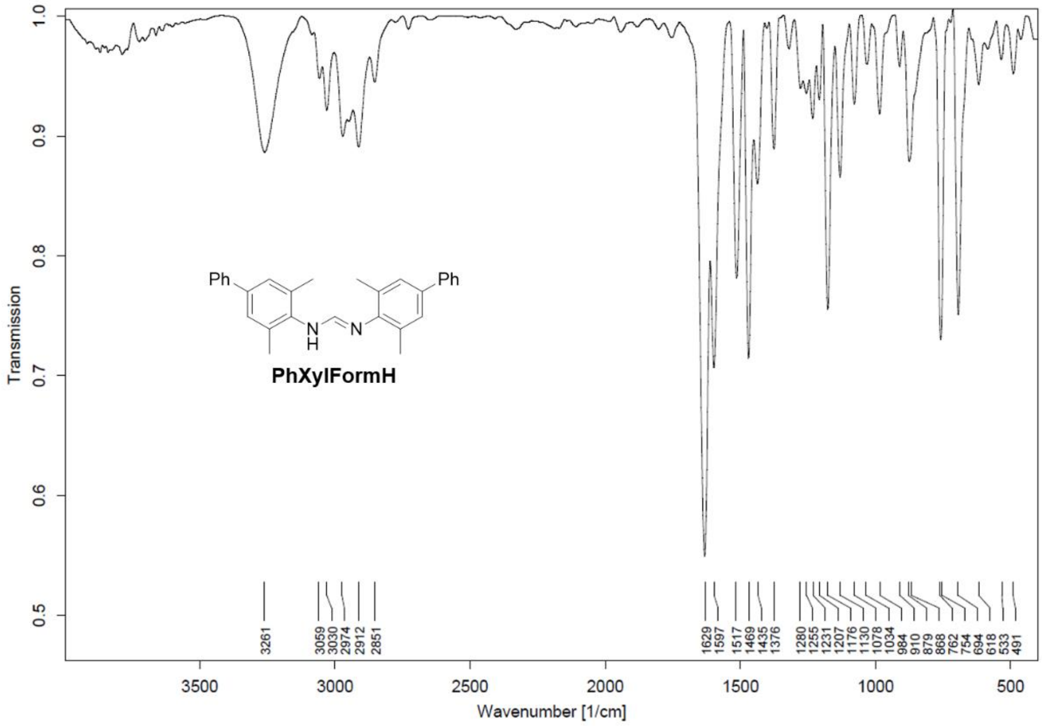


Figure S37: IR spectrum of **PhXylFormH** (**L**[3]).

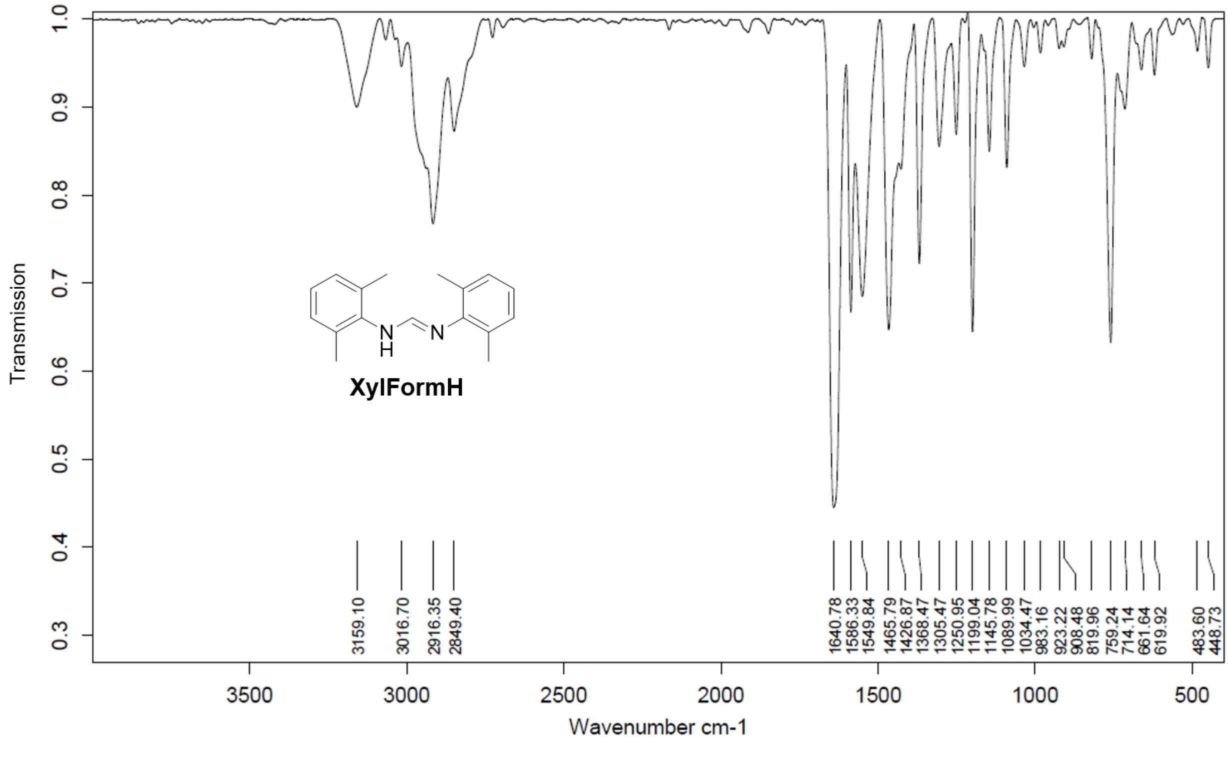


Figure S38: IR spectrum of **XylFormH** (**L**[4]).

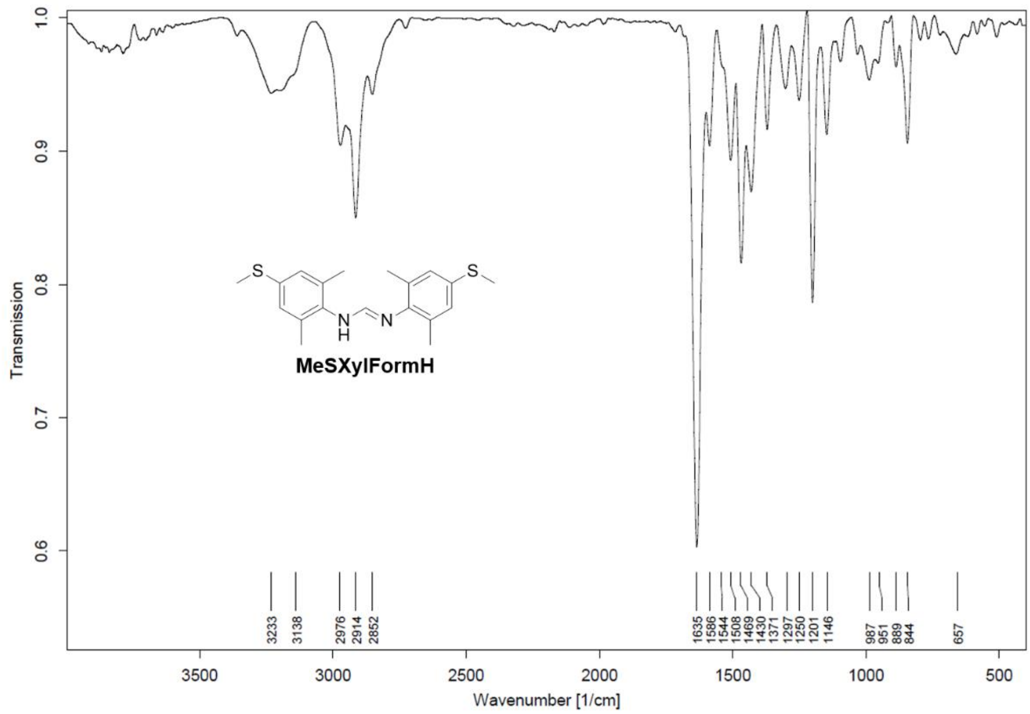


Figure S39: IR spectrum of **MeSXylFormH** (**L⁵**).

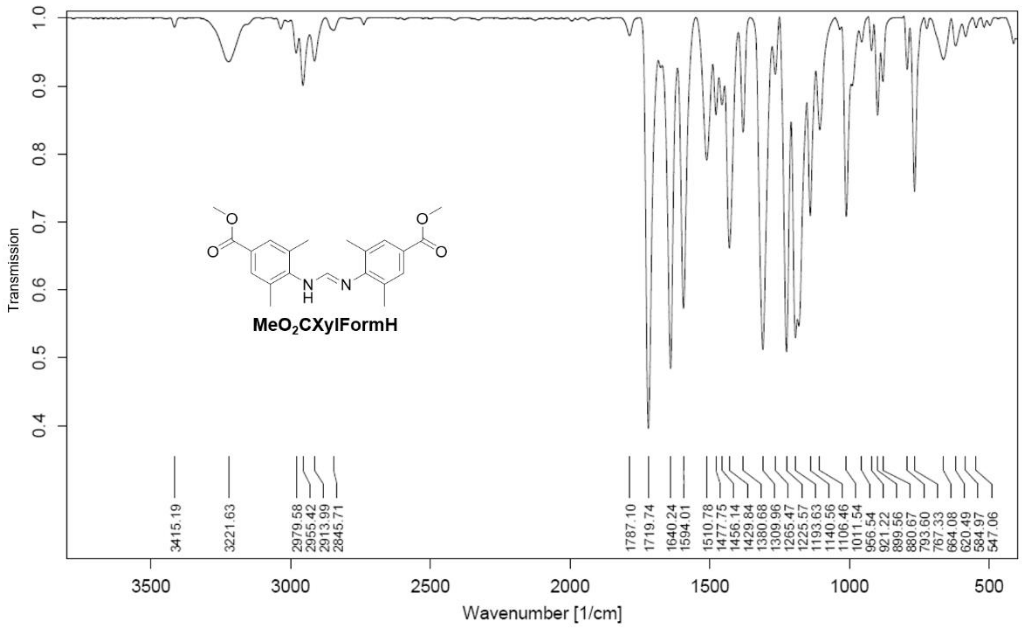


Figure S40: IR spectrum of **MeO$_2$CXylFormH** (**L⁶**).

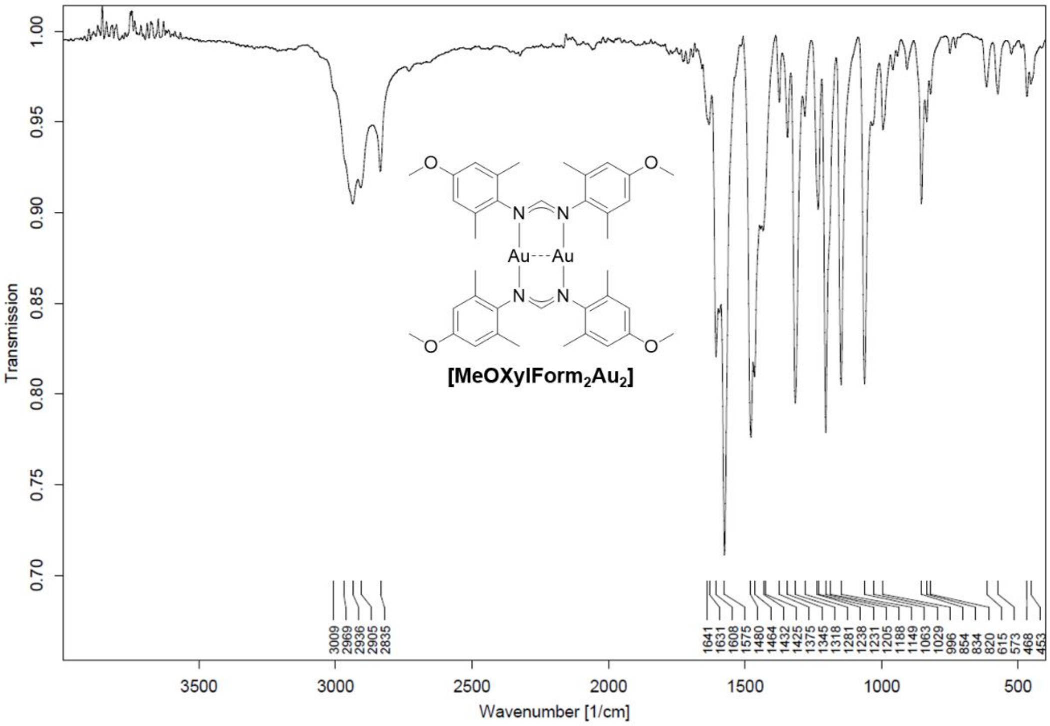


Figure S41: IR spectrum of **[MeOXylForm$_2$Au$_2$]** (**1**).

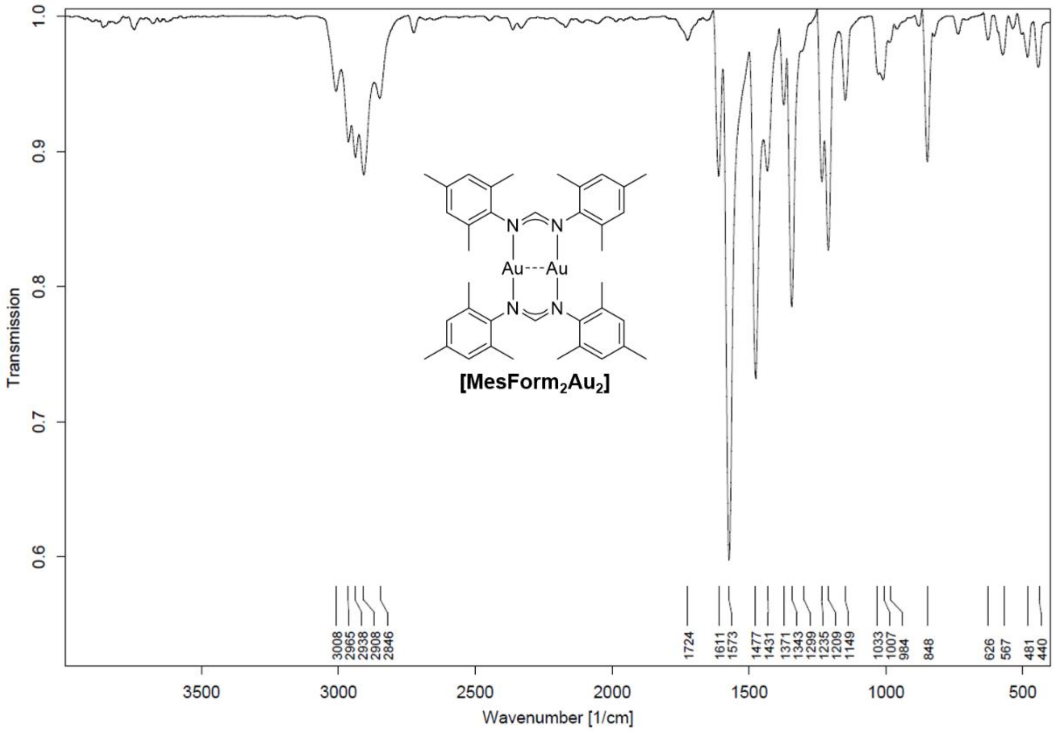


Figure S42: IR spectrum of **[MesForm$_2$Au$_2$]** (**2**).

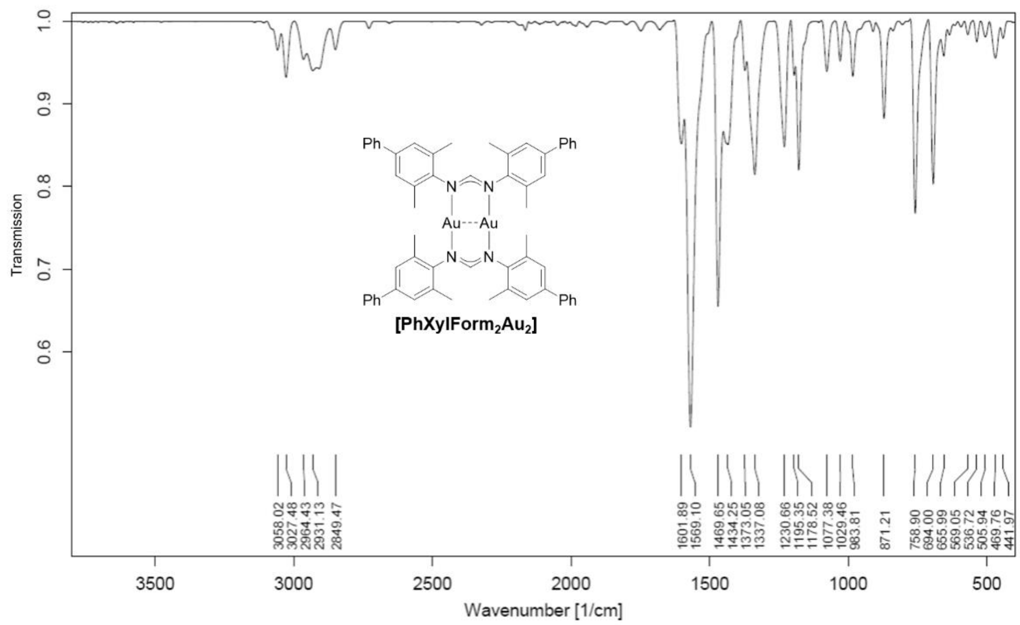


Figure S43: IR spectrum of **[PhXylForm$_2$Au$_2$]** (**3**).

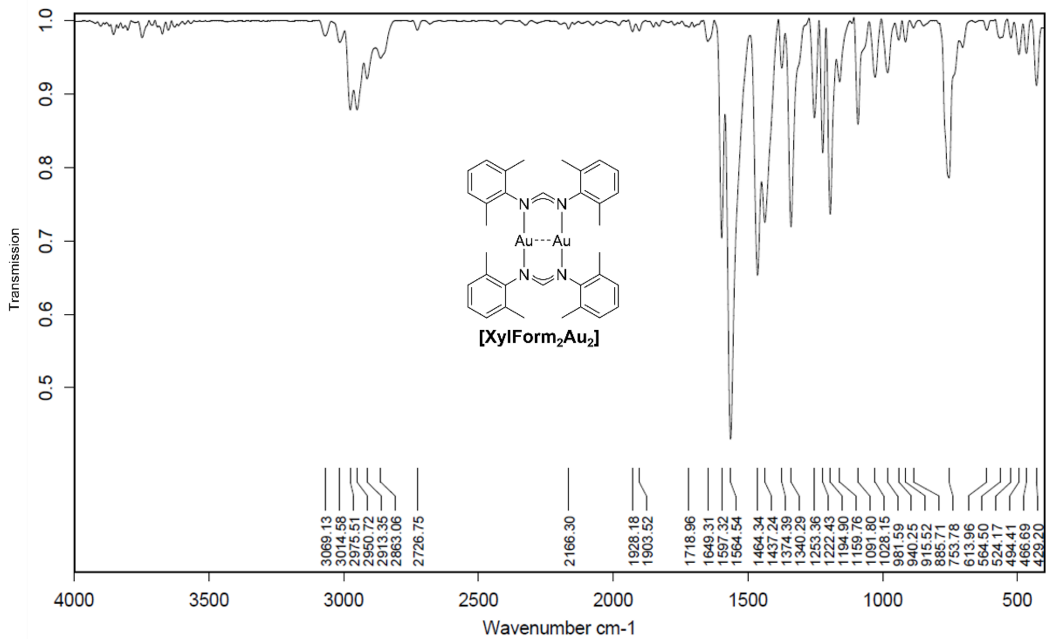


Figure S44: IR spectrum of **[XylForm$_2$Au$_2$]** (**4**).

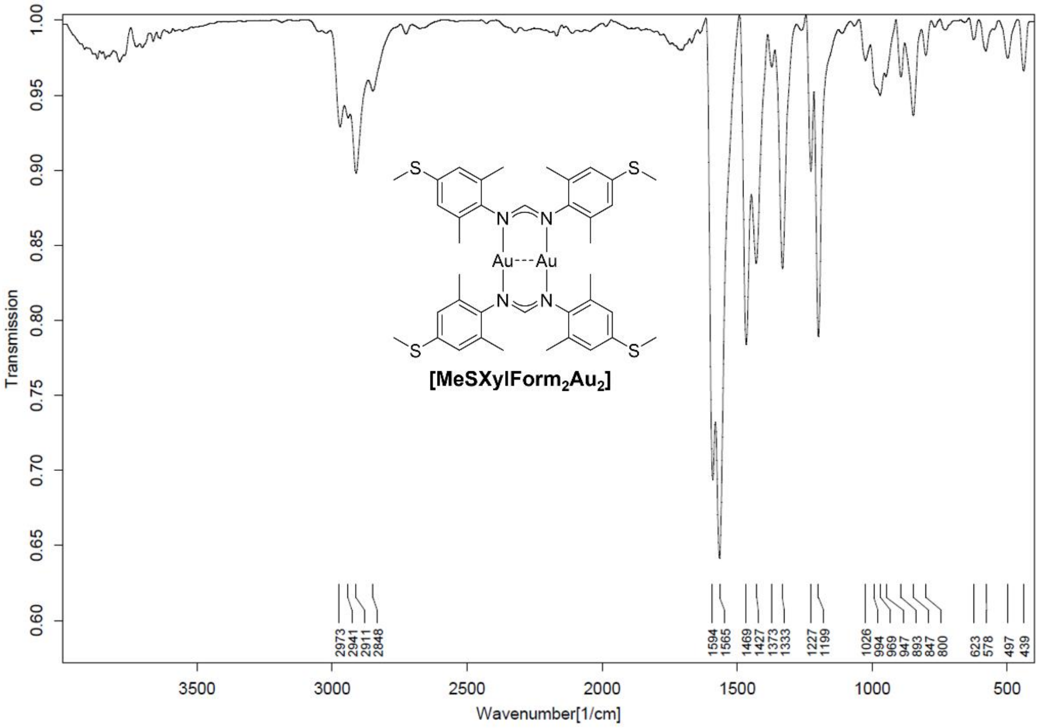


Figure S45: IR spectrum of **[MeSXylForm$_2$Au$_2$]** (**5**).

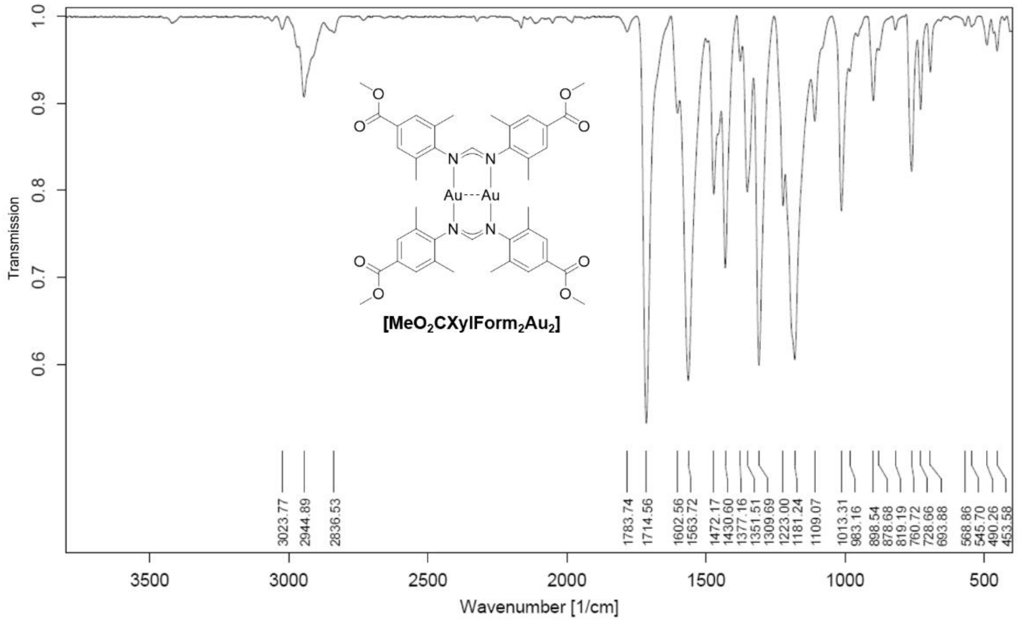


Figure S46: IR spectrum of **[MeO$_2$CXylForm$_2$Au$_2$]** (**6**).

UV-Vis spectra

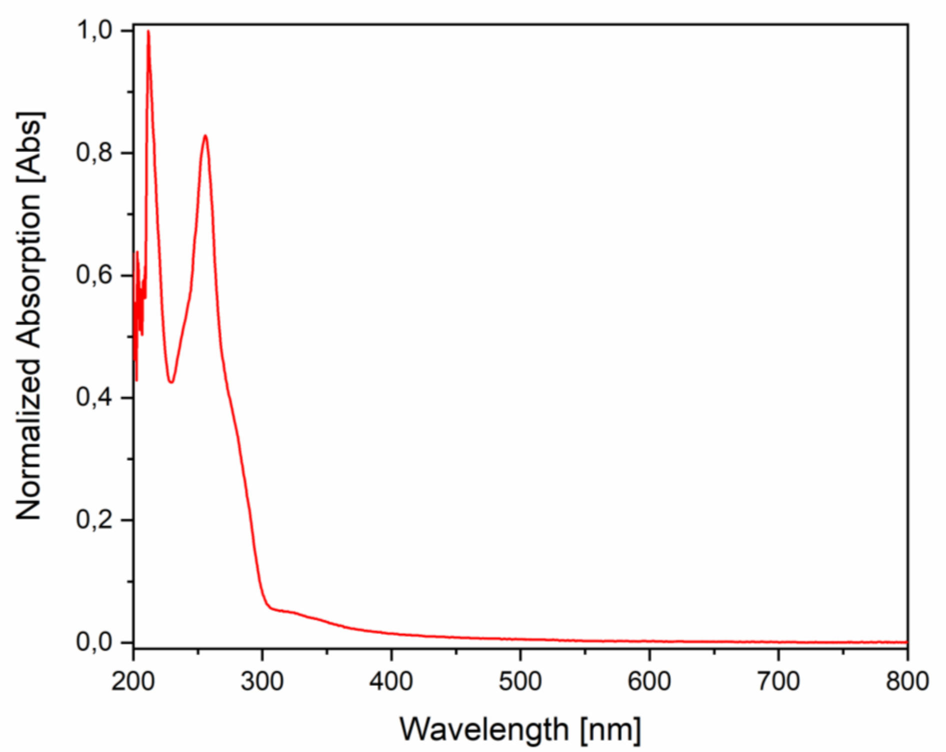


Figure S47: UV-Vis spectrum of **[MeOXylForm$_2$Au$_2$]** (**1**) in THF.

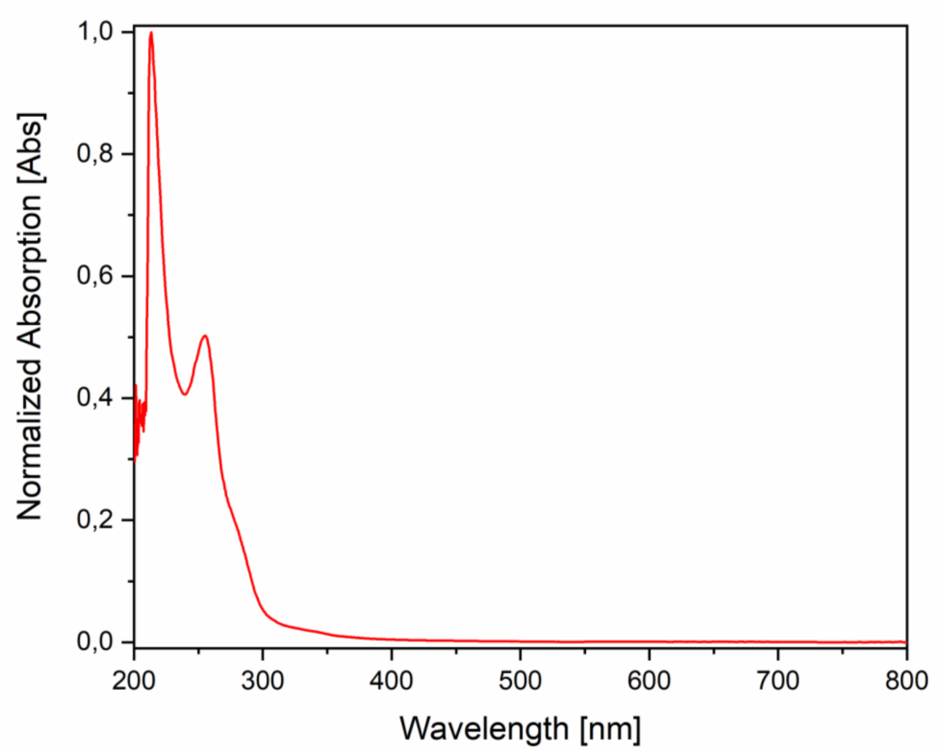


Figure S48: UV-Vis spectrum of **[MesForm$_2$Au$_2$]** (**2**) in THF.

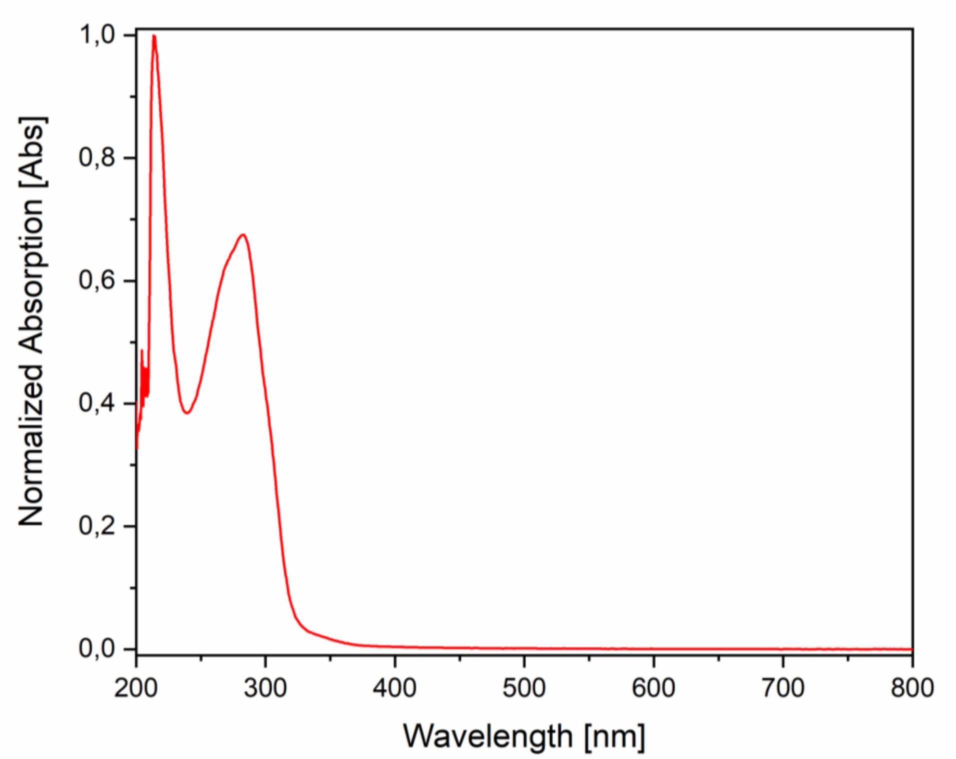


Figure S49: UV-Vis spectrum of **[PhXylForm$_2$Au$_2$]** (**3**) in THF.

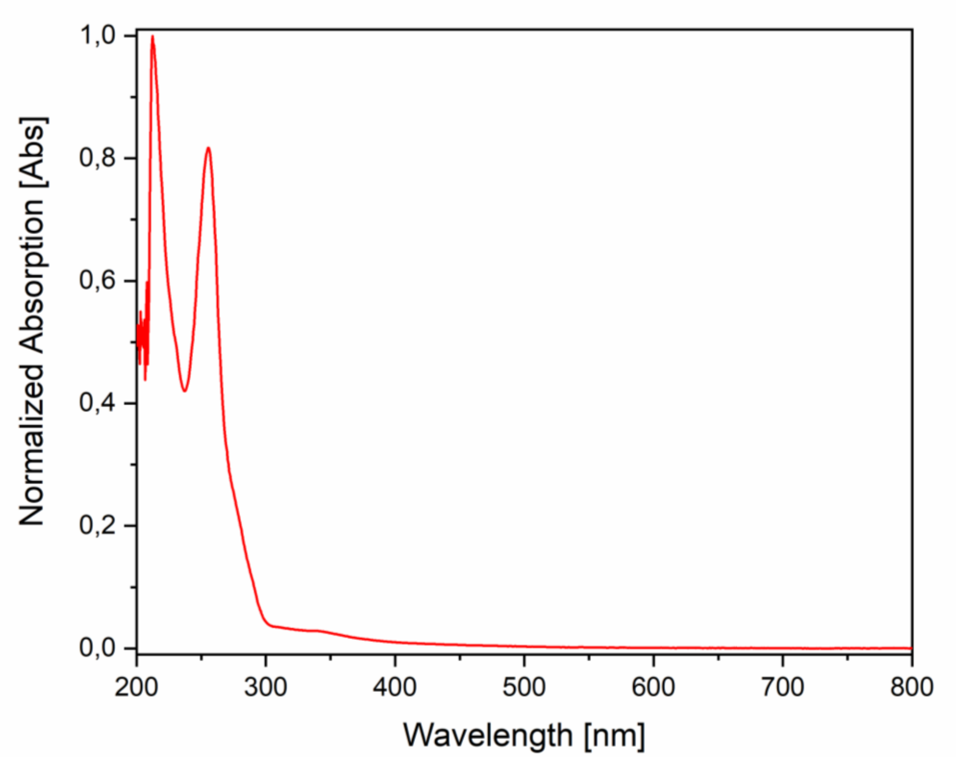


Figure S50: UV-Vis spectrum of **[XylForm$_2$Au$_2$]** (**4**) in THF.

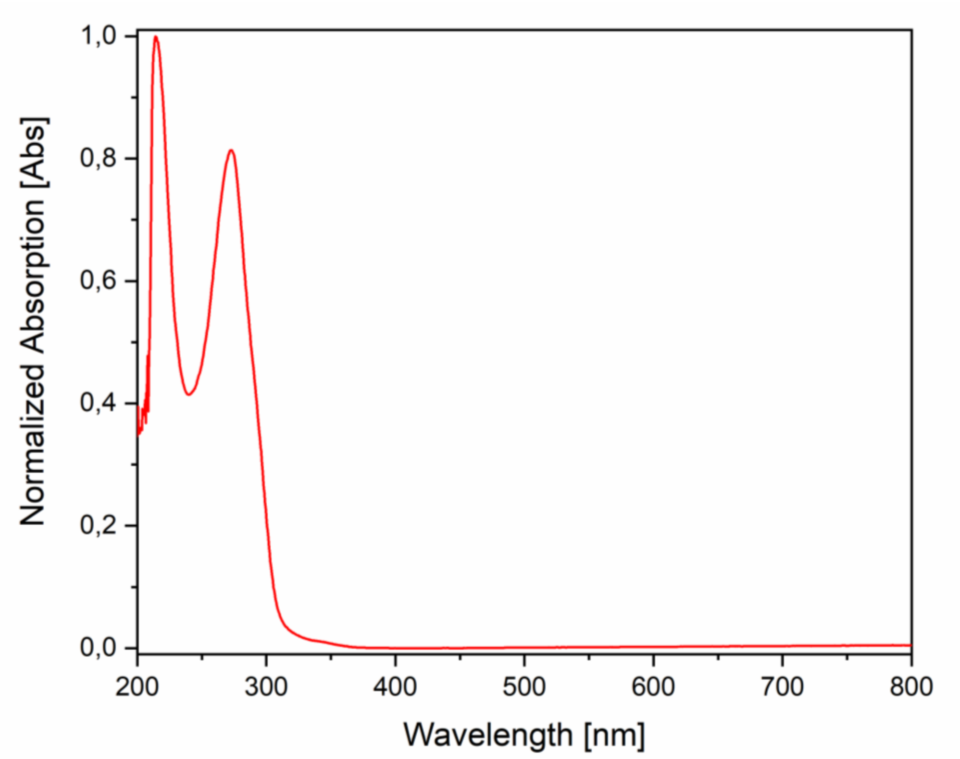


Figure S51: UV-Vis spectrum of **[MeSXylForm$_2$Au$_2$]** (**5**) in THF.

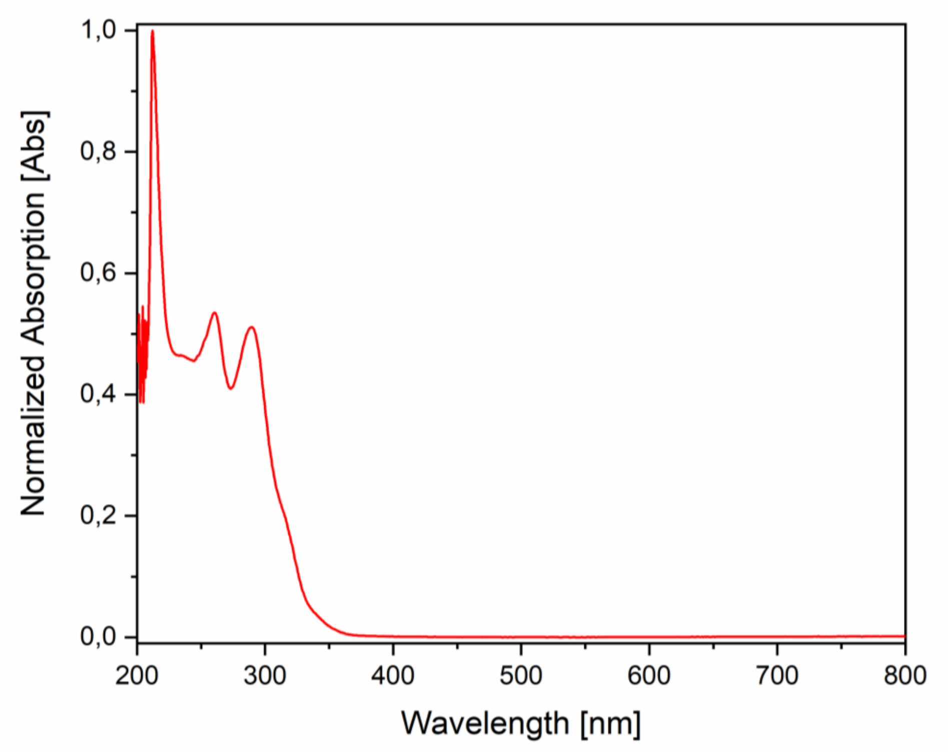


Figure S52: UV-Vis spectrum of **[MeO$_2$CXylForm$_2$Au$_2$]** (**6**) in THF.

Mass spectra

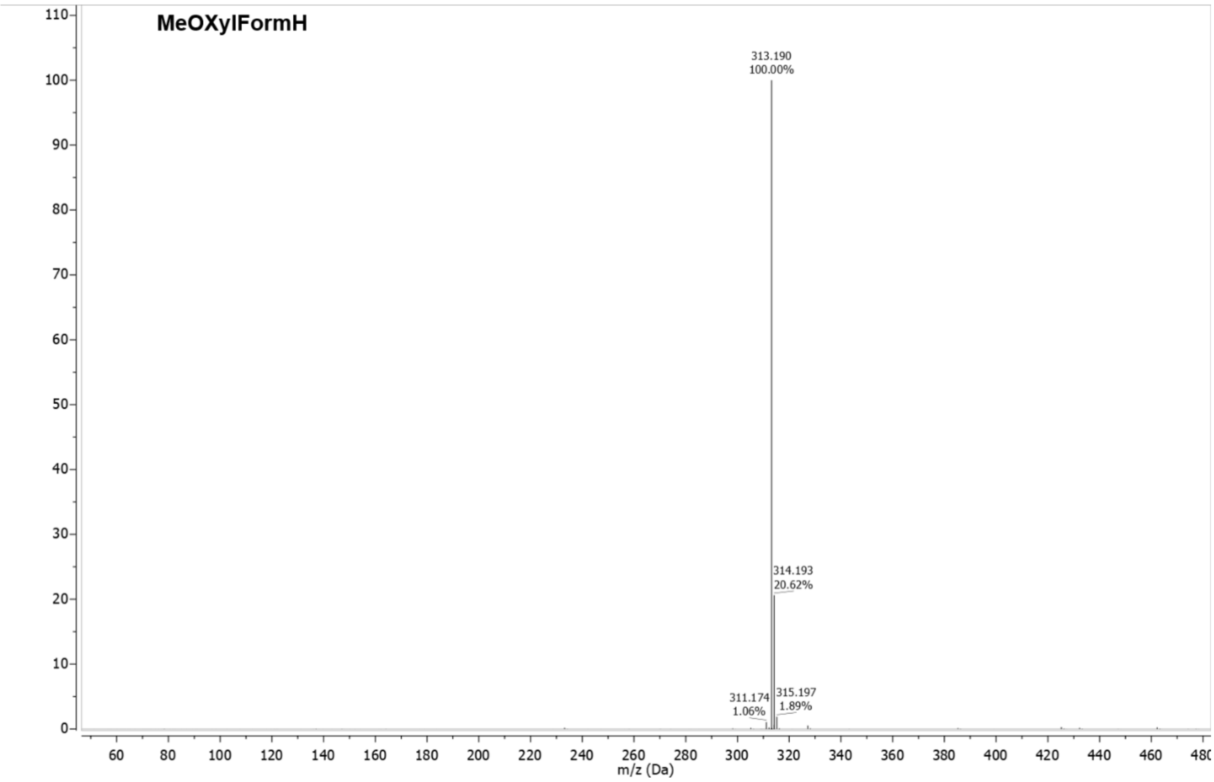


Figure S53: ESI mass spectrum of **MeOXylFormH** (**L^1**).

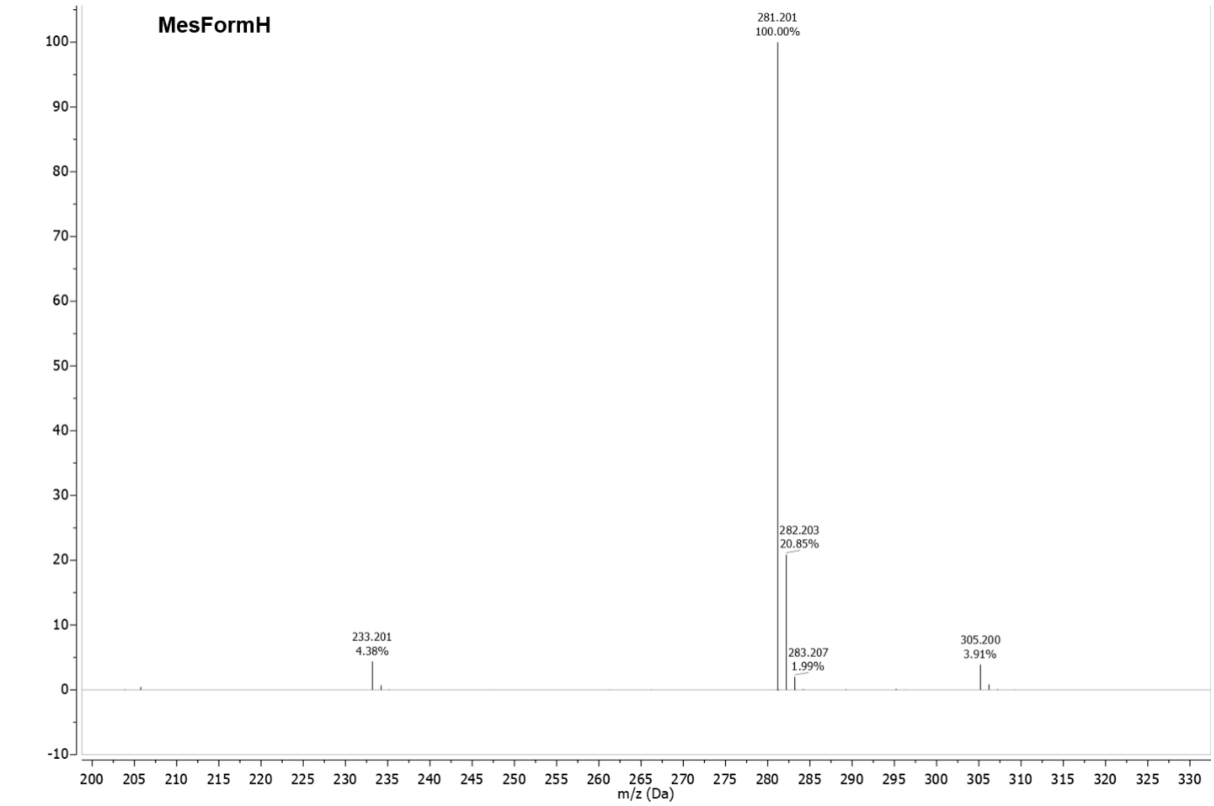


Figure S54: ESI mass spectrum of **MesFormH** (**L^2**).

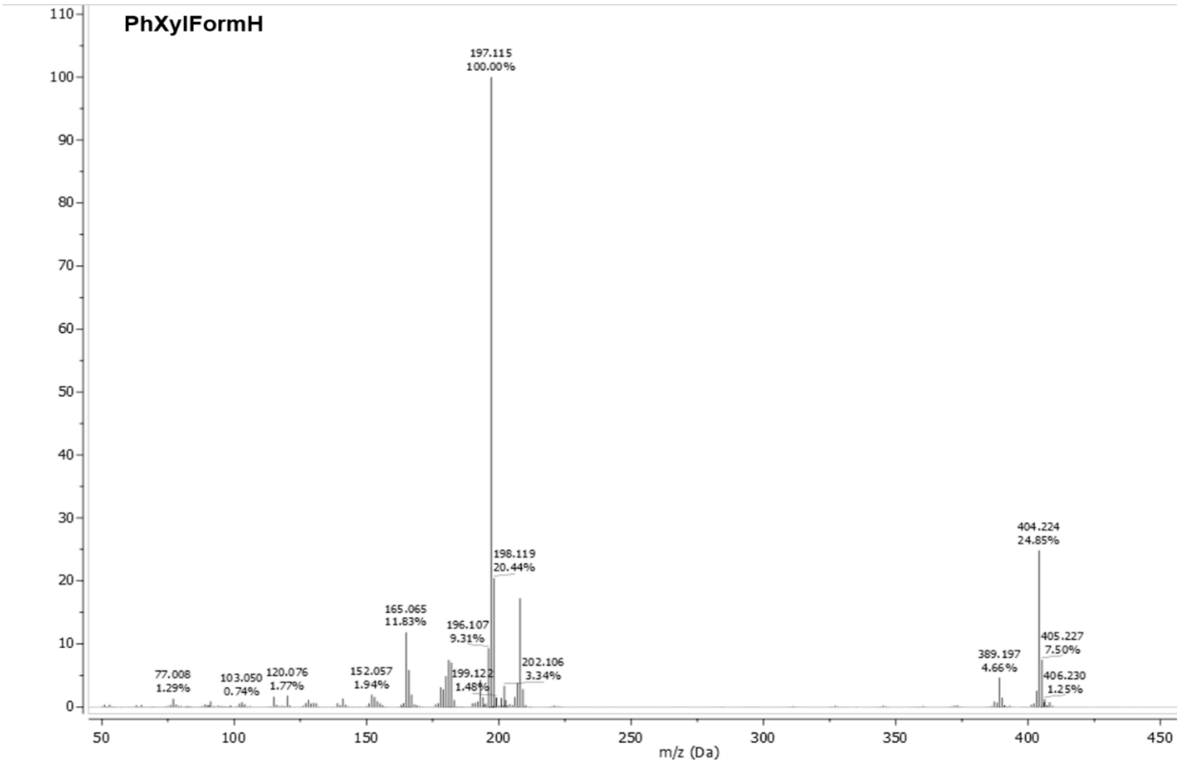


Figure S55: EI mass spectrum of **PhXylFormH** (**L**[3]).

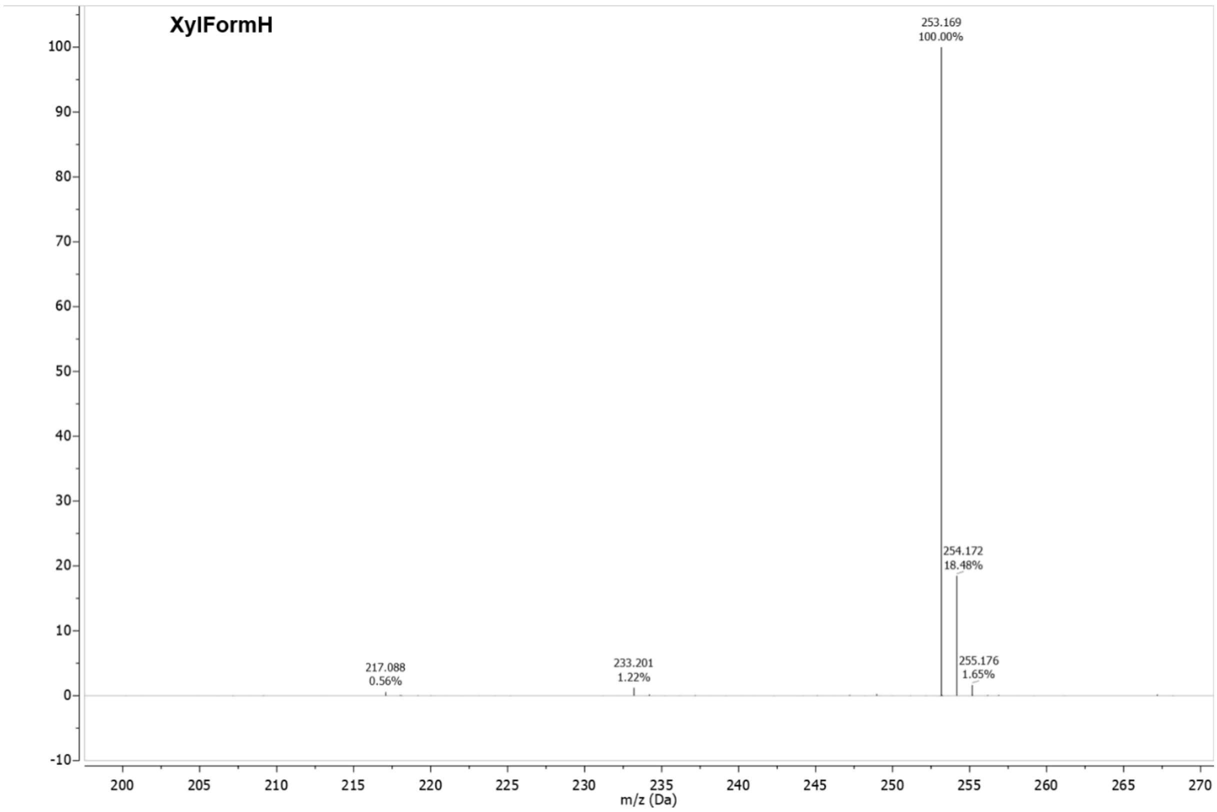


Figure S56: ESI mass spectrum of **XylFormH** (**L**[4]).

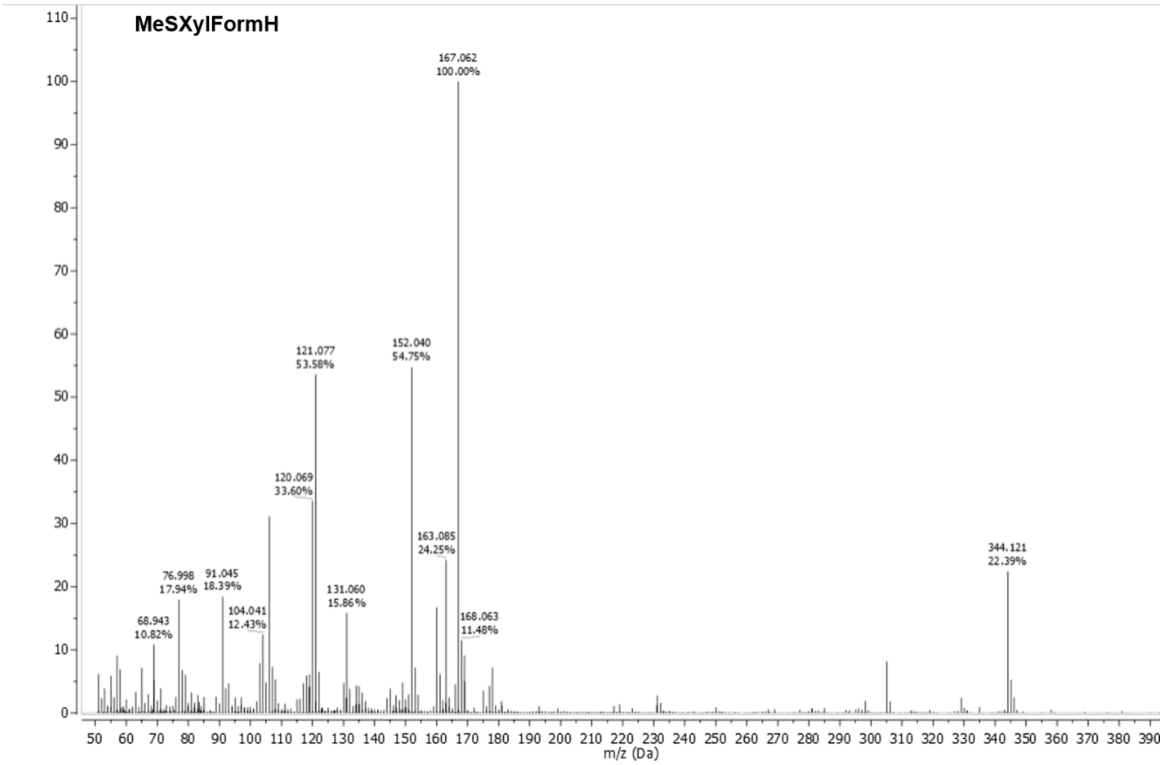


Figure S57: EI mass spectrum of **MeSXylFormH** (**L⁵**).

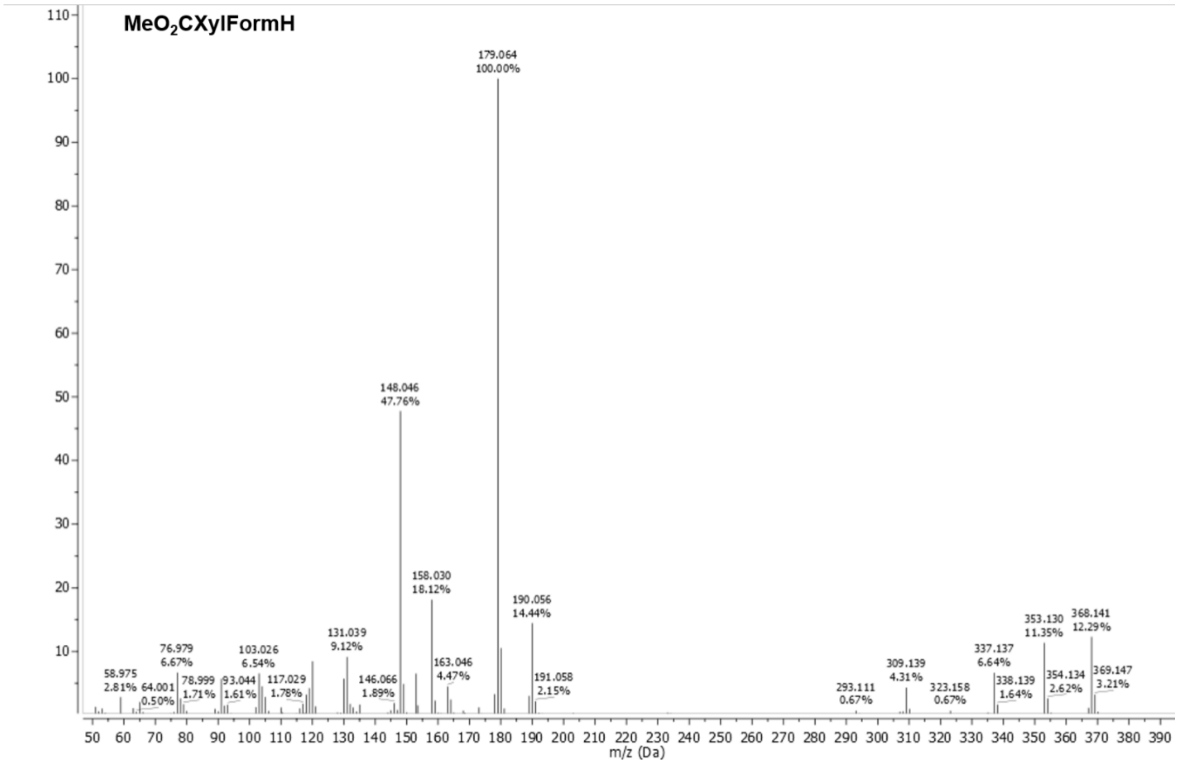


Figure S58: EI mass spectrum of **$MeO_2CXylFormH$** (**L⁶**).

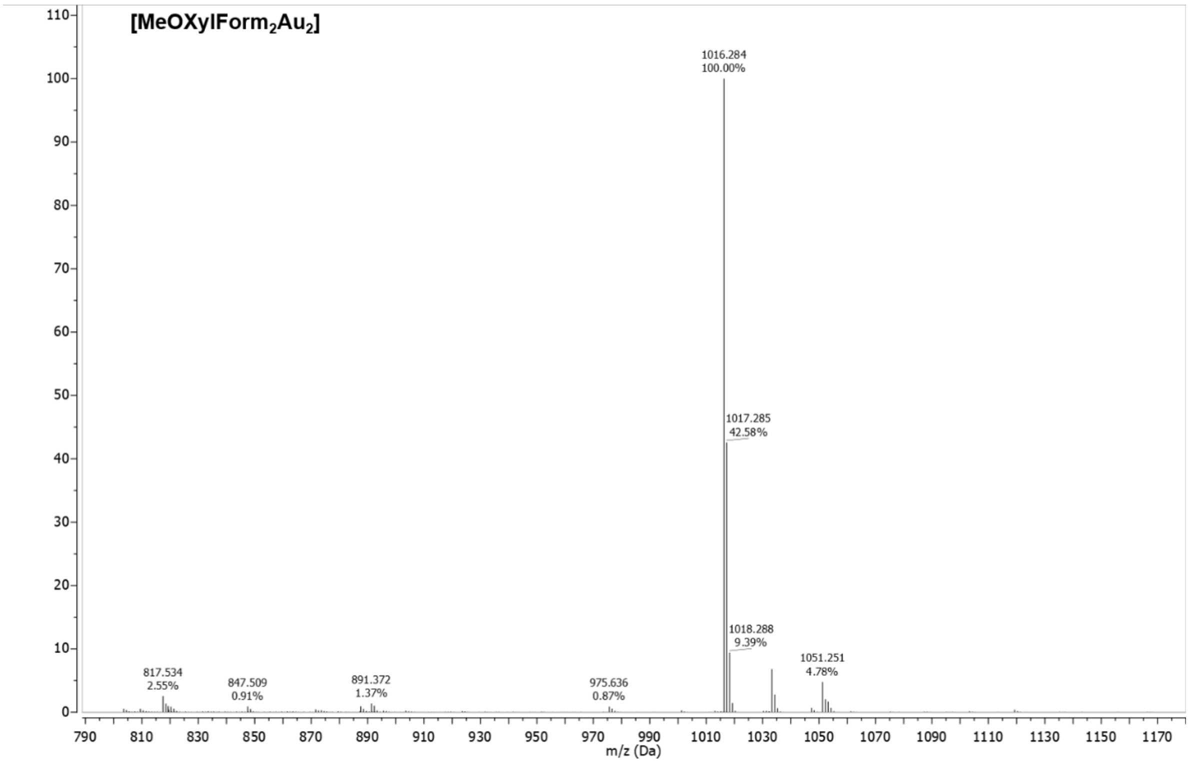


Figure S59: ESI mass spectrum of **[MeOXylForm$_2$Au$_2$]** (**1**).

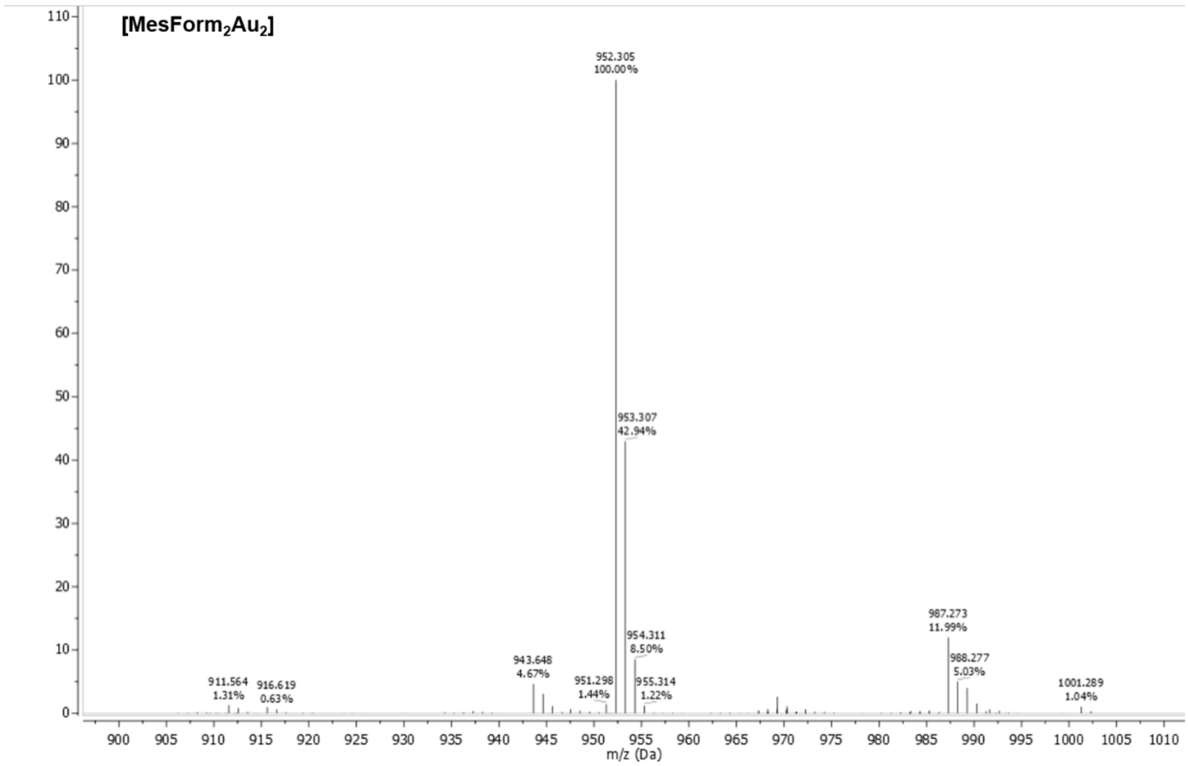


Figure S60: ESI mass spectrum of **[MesForm$_2$Au$_2$]** (**2**).

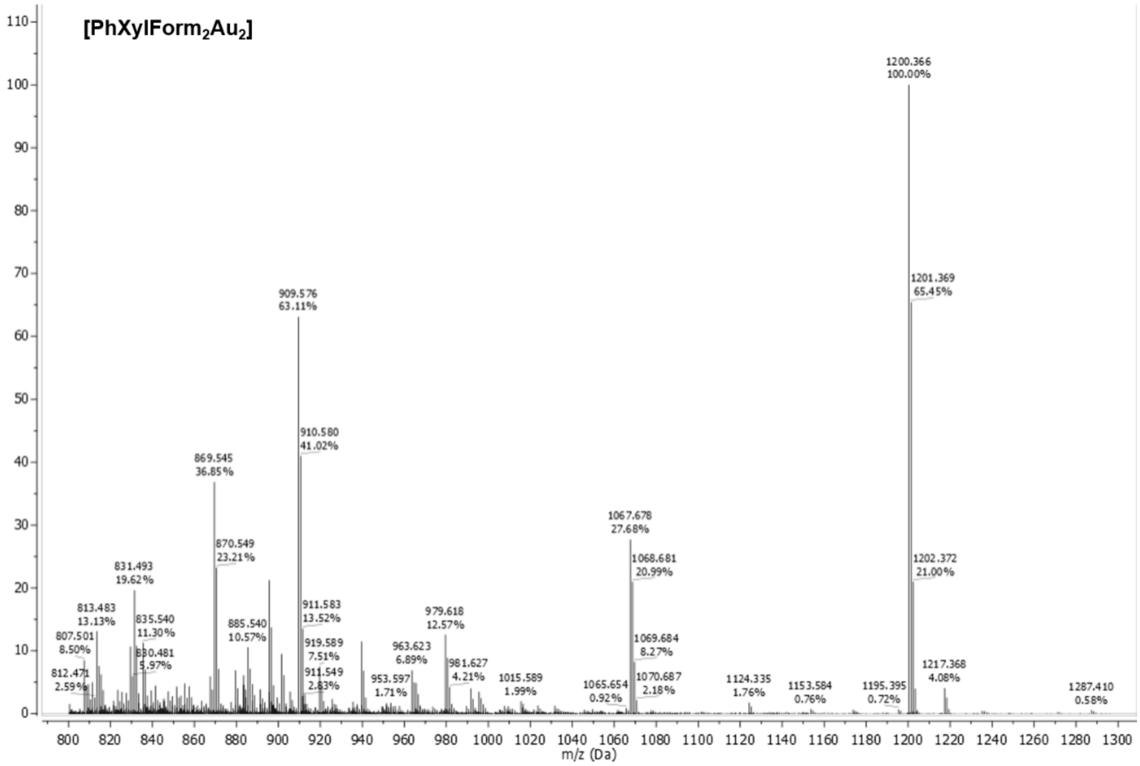


Figure S61: ESI mass spectrum of **[PhXylForm$_2$Au$_2$]** (**3**).

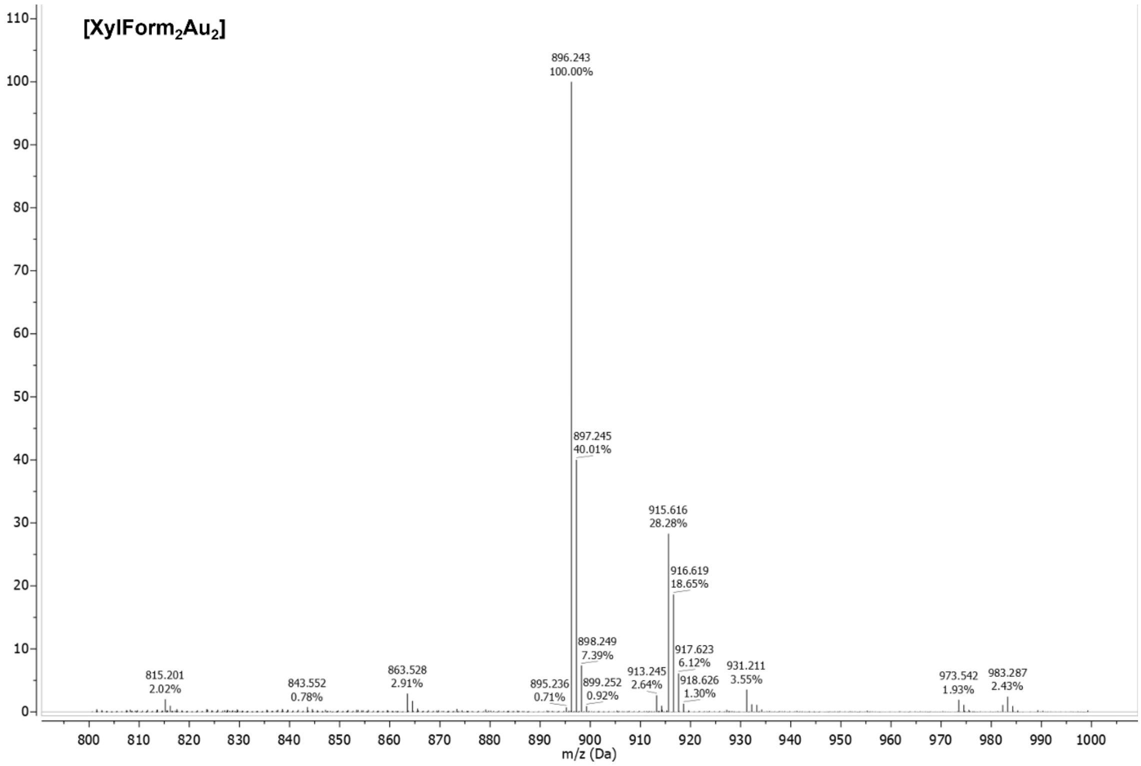


Figure S62: ESI mass spectrum of **[XylForm$_2$Au$_2$]** (**4**).

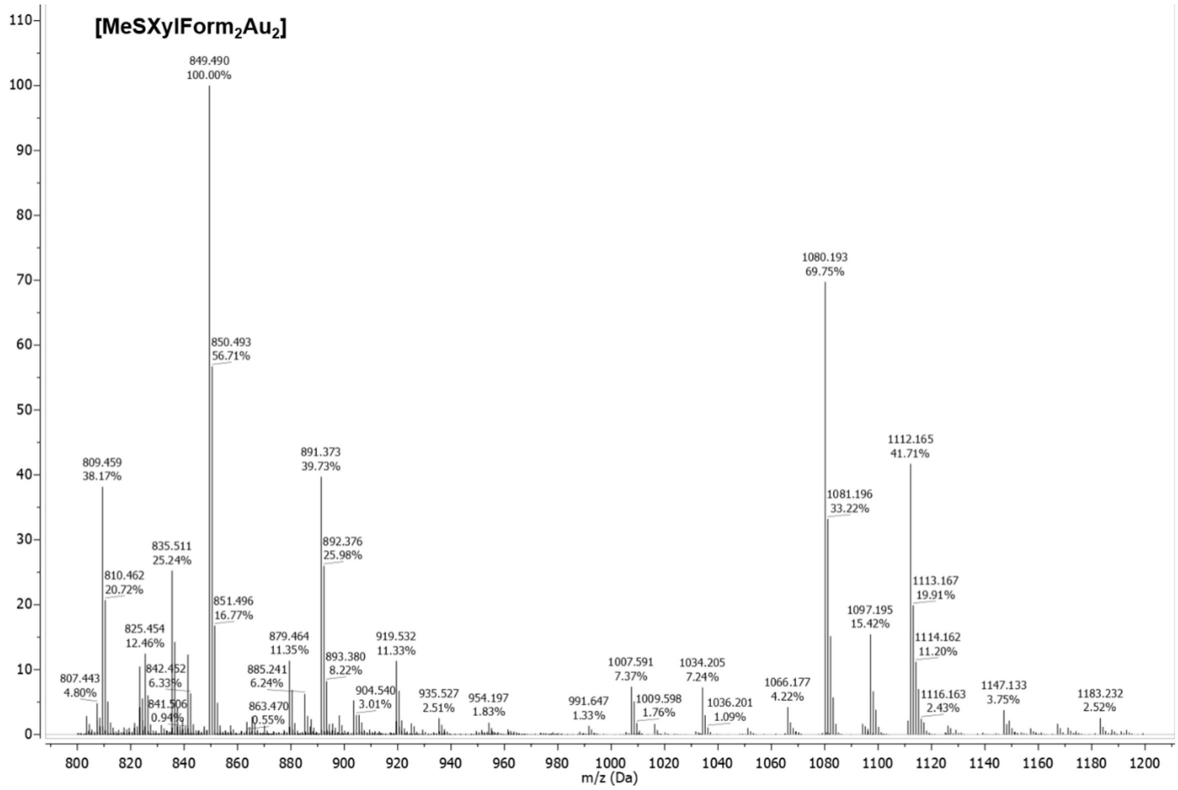


Figure S63: ESI mass spectrum of **[MeSXylForm$_2$Au$_2$]** (**5**).

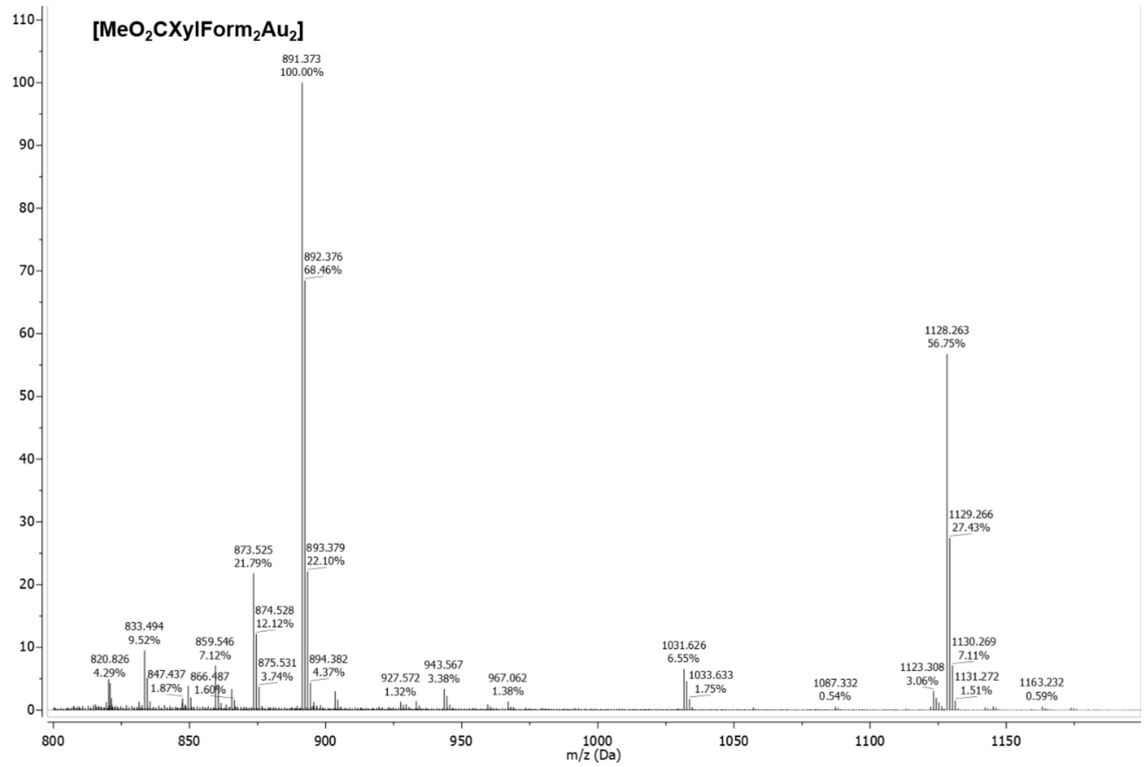


Figure S64: ESI mass spectrum of **[MeO$_2$CXylForm$_2$Au$_2$]** (**6**).

X-ray crystallography

General methods

Suitable crystals for the X-ray analysis of all compounds were obtained as described above. A suitable crystal was covered in mineral oil (Aldrich) and mounted on a glass fibre. The crystal was transferred directly to the cold stream of a STOE StadiVari (100, 130 or 150 K) diffractometer. All structures were solved by using the program SHELXS/T[13] and Olex[2].[14] The remaining non-hydrogen atoms were located from successive difference Fourier map calculations. The refinements were carried out by using full-matrix least-squares techniques on F^2 by using the program SHELXL.[3-4] The H-atoms were introduced into the geometrically calculated positions (SHELXL procedures) unless otherwise stated and refined riding on the corresponding parent atoms. In each case, the locations of the largest peaks in the final difference Fourier map calculations, as well as the magnitude of the residual electron densities, were of no chemical significance. Specific comments for each data set are given below. Summary of the crystal data, data collection and refinement for compounds are given in **Table S3** and **Table S4**. Crystallographic data for the structures reported in this paper have been deposited with the Cambridge Crystallographic Data Centre as a supplementary publication no. CCDC 2120940-2120944. Copies of the data can be obtained free of charge on application to CCDC, 12 Union Road, Cambridge CB21EZ, UK (fax: (+(44)1223-336-033; email: deposit@ccdc.cam.ac.uk).

Summary of crystal data

Table S3: Crystal data, data collection and refinement for compounds **1**-**3.**

Compounds	**1**	**2**	**3**
Chemical formular	$C_{46}H_{62}Au_2N_4O_6$	$C_{38}H_{46}Au_2N_4$	$C_{66}H_{70}Au_2N_4O_2$
CCDC Number	2120940	2120941	2120942
Formular Mass	1160.93	952.72	1345.19
Radiation type	MoKα	MoKα	MoKα
Wavelength/nm	0.71073	0.71073	0.71073
Crystal system	triclinic	monoclinic	monoclinic
a/Å	12.724(3)	21.050(3)	15.3524(3)
b/Å	13.217(3)	11.1793(13)	18.6578(6)
c/Å	14.196(3)	17.033(3)	9.9186(2)
α/Å	79.36(3)	90	90
β/Å	88.97(3)	120.17(2)	104.188(2)
γ/Å	74.33(3)	90	90
Unit cell volume/$Å^3$	2257.9(9)	3465.2(10)	2754.44(12)
Temperatur/K	150	150	100
Space Group	P-1	C2/c	$P2_1/c$
Z	2	4	2
Absorption coefficient, *μ*/mm	6.541	8.489	5.369
No. of reflections measured	25906	12658	34907
No. of independent reflections	12466	4809	7686
R_{int}	0.0335	0.0310	0.0258
Final R_1 values ($I > 2\sigma(I)$)	0.0304	0.0287	0.0229
Final $wR(F^2)$ values ($I > 2\sigma(I)$)	0.0685	0.0705	0.0572
Final R_1 values (all data)	0.0474	0.0361	0.0315
Final $wR(F^2)$ values (all data)	0.0728	0.0731	0.0600
Goodness of fit on F^2	0.975	1.042	1.021

Table S4: Crystal data, data collection and refinement for compounds **5** and **6.**

Compounds	**5**	**6**
Chemical formular	$C_{38}H_{46}Au_2N_4S_4$	$C_{42}H_{46}Au_2N_4O_8$
CCDC Number	2120943	2120944
Formular Mass	1080.96	1128.76
Radiation type	MoKα	MoKα
Wavelength/nm	0.71073	0.71073
Crystal system	trigonal	triclinic
a/Å	32.805(2)	7.1610(3)
b/Å	32.805(2)	12.6256(6)
c/Å	20.4318(12)	12.9627(7)
α/Å	90	83.032(4)
β/Å	90	78.583(4)
γ/Å	120	83.304(4)
Unit cell volume/$Å^3$	19042(2)	1135.13(10)
Temperatur/K	150	160
Space Group	R-3c	P-1
Z	18	1
Absorption coefficient, *µ*/mm	7.153	6.506
No. of reflections measured	19962	15857
No. of independent reflections	6132	6716
R_{int}	0.0904	0.0191
Final R_1 values ($I > 2\ \sigma(I)$)	0.0772	0.0210
Final $wR(F^2)$ values ($I > 2\ \sigma(I)$)	0.2172	0.0426
Final R_1 values (all data)	0.1384	0.0275
Final $wR(F^2)$ values (all data)	0.2675	0.0434
Goodness of fit on F^2	1.030	0.957

Crystal structures

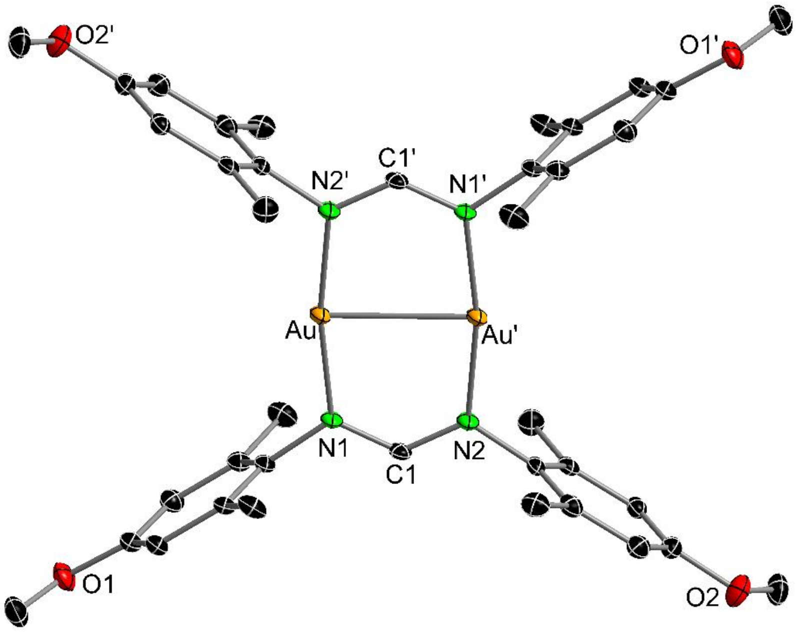


Figure S65: Molecular structure of **1** in the solid state with ellipsoids drawn at 30 % probability. Hydrogen atoms and non-coordinating solvent molecules are omitted for clarity. Selected bond lengths [Å] and angles [°]: Au-Au 2.7079(7), Au-N1 2.034(3), Au'-N2 2.035(3), N1-C1 1.321(4), N2-C1 1.317(4), N1-C1-N2 126.7(3), N1-Au-N2' 170.11(11), N1-Au-Au' 84.42(8), N2-Au'-Au 85.70(8), C1-N1-C2-C7 85.85, C1-N2-C10-C11 101.03.

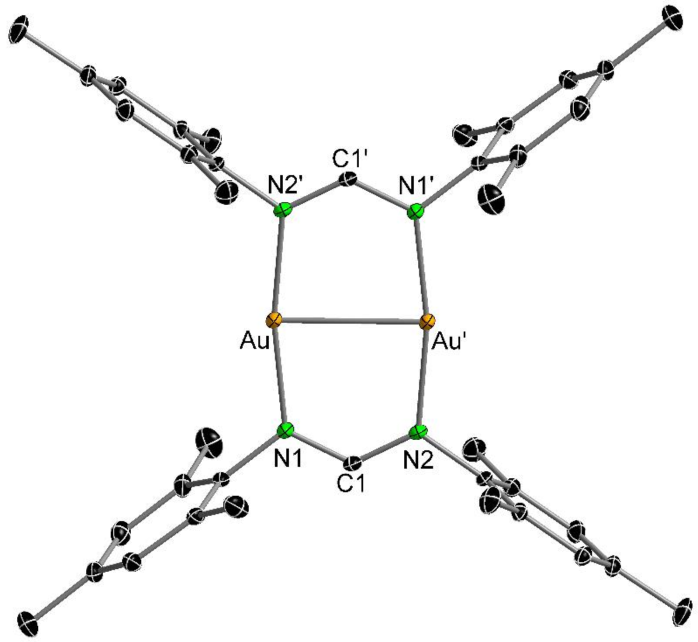


Figure S66: Molecular structure of **2** in the solid state with ellipsoids drawn at 30 % probability. Hydrogen atoms are omitted for clarity. Selected bond lengths [Å] and angles [°]: AU-Au' 2.7277(4), Au-N1 2.024(3), Au'-N2 2.028(3), N1-C1 1.331(4), N2-C1 1.306(5), N1-C1-N2 127.2(3), N1-Au-N2' 169.66(12), N2-Au'-Au 85.08(8), C1-N1-C2-C7 100.91, C1-N2-C10-C11 99.57.

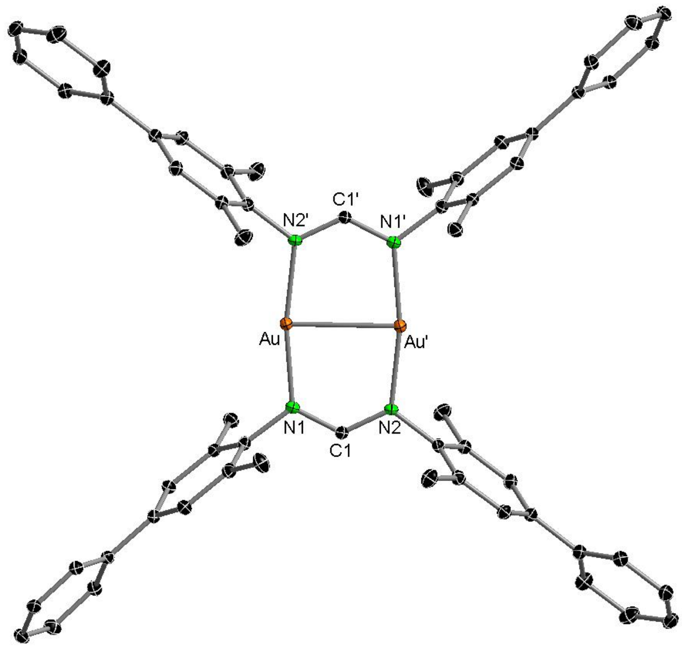


Figure S67: Molecular structure of **3** in the solid state with ellipsoids drawn at 30 % probability. Hydrogen atoms and non-coordinating solvent molecules are omitted for clarity. Selected bond lengths [Å] and angles [°]: Au-Au’ 2.7366(2), Au-N1 2.028(2), Au’-N2 2.031(2), N1-C1 1.326(3), N2-C1 1.318(3), N1-C1-N2 127.4(2), N1-Au-N2 169.64(8), N1-Au-Au‘ 84.71(6), N2-Au‘-Au 84.93(6), C1-N1-C2-C7 102.52, C1-N2-C10-C11 81.53.

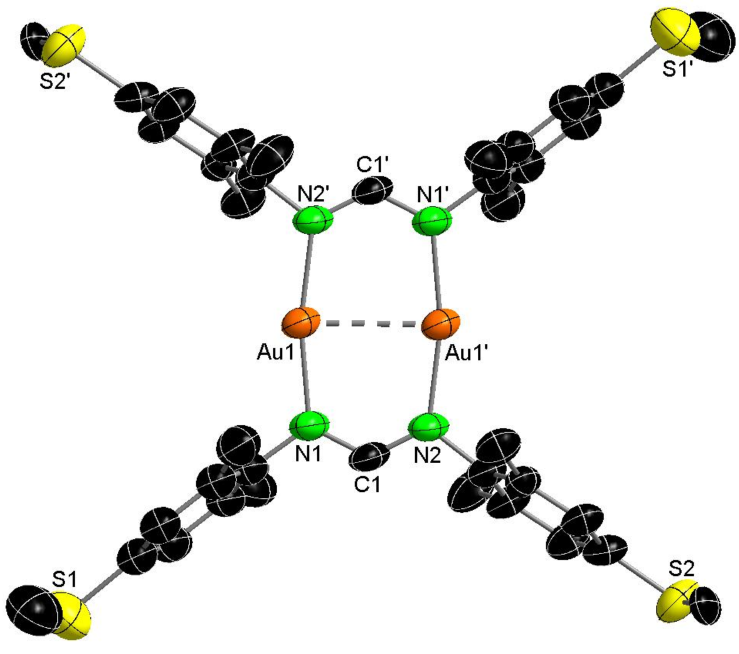


Figure S68: Molecular structure of **5** in the solid state with ellipsoids drawn at 30 % probability. Hydrogen atoms and non-coordinating solvent molecules are omitted for clarity. Selected bond lengths [Å] and angles [°]: Au-Au’ 2.7359(12), Au-N1 2.024(11), Au’-N2 2.023(10), N1-C1 1.32(2), N2-C1 1.447(15), N1-C1-N2 125.8(13), N1-Au-N2’ 168.4(5), N1-Au-Au‘ 84.6(4), N2-Au‘-Au 83.8(4), C1-N1-C2-C7 96.3(15), C1-N2-C11-C12 84.1(13).

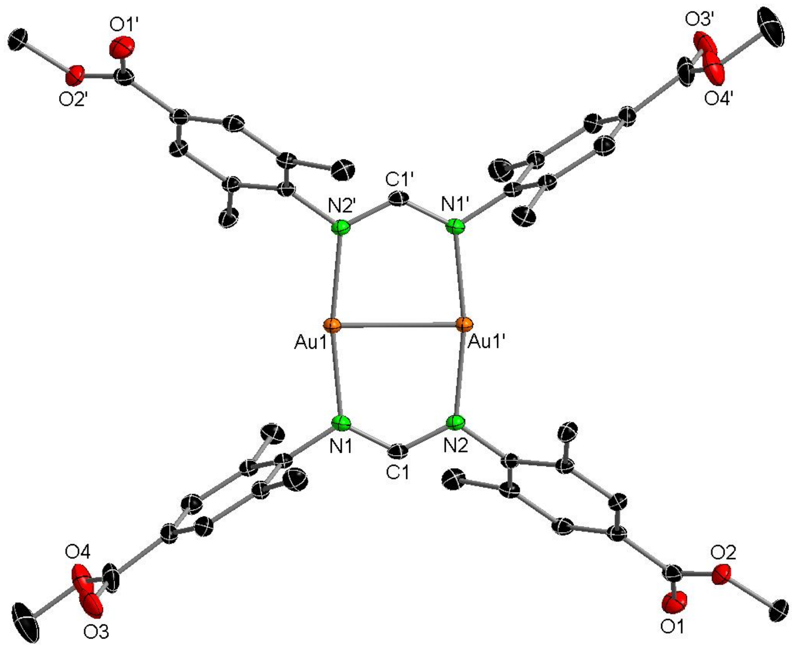


Figure S69: Molecular structure of **6** in the solid state with ellipsoids drawn at 30 % probability. Hydrogen atoms and non-coordinating solvent molecules are omitted for clarity. Selected bond lengths [Å] and angles [°]: Au-Au‘ 2.7195(2), Au-N1 2.035(2), Au’-N2 2.036(2), N1-C1 1.315(3), N2-C1 1.326(3), N1-C1-N2 126.7(2), N1-Au-N2’ 169.87(8), N1-Au-Au‘ 84.50(6), N2-Au‘-Au 85.38(6), C1-N2-C2-C7 58.5(3), C1-N1-C12A-C13A 91.4(5), C1-N1-C12B-C13B 104.1(4).

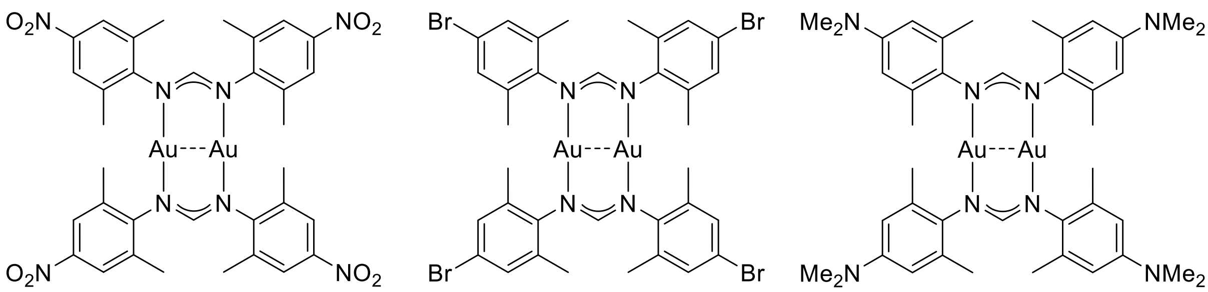
Quantum chemical calculations

General procedures

All quantum-chemical calculations were performed with the TURBOMOLE program package.[15, 16] The resolution-of-the-identity (RI) approximation was used for all two-electron integrals. The equilibrium geometries were optimized at the PBE0-D3(BJ) level of theory,[17-19] and the electronic excitations were calculated at the CD-ev*GW*(10)/BSE level of theory (eigenvalue-only self-consistent *GW* (ev*GW*) [20] employing contour deformation (CD) [21] for highest 10 occupied and lowest 10 unoccupied orbitals followed by the Bethe–Salpeter equation (BSE) [21-23] approach). For non- and scalar-relativistic one-component (1c) calculations, the def2-TZVP basis set [24] was used with effective core potentials (ECPs) [25] for gold. For quasirelativistic two-component (2c) calculations, the dhf-TZVP-2c basis set [26] together with the underlying dhf-ecp-2c ECPs [27] was used.

All orbital and auxiliary basis sets were taken from the TURBOMOLE basis-set library. [12] The "Coulomb-fitting" auxiliary basis sets (denoted jbas) were used in the ground-state DFT computations, and the "MP2-fitting" auxiliary basis sets (denoted cbas) were used in the excited-state TDDFT and *GW*/BSE computations. The ground-state density functional theory (DFT) computations were carried out with the modules DSCF and RIDFT, and the self-consistent field convergence criterion scfconv = 8 and DFT grid 4 were used. The geometry optimization was considered converged when the change in energy and cartesian gradients reached thresholds of 10^{-7} and 10^{-4} Hartree, respectively. The excited-state TDDFT and *GW*/BSE computations were carried out with the ESCF module, and the convergence criterion rpaconv = 6 was used. Furthermore, in ev*GW*, the damping parameter was set to $\eta = 0.001$ in order to achieve rapid convergence. In CD-*GW*, 128 grid points were used, also 128 parameters were taken in the Padé approximant.

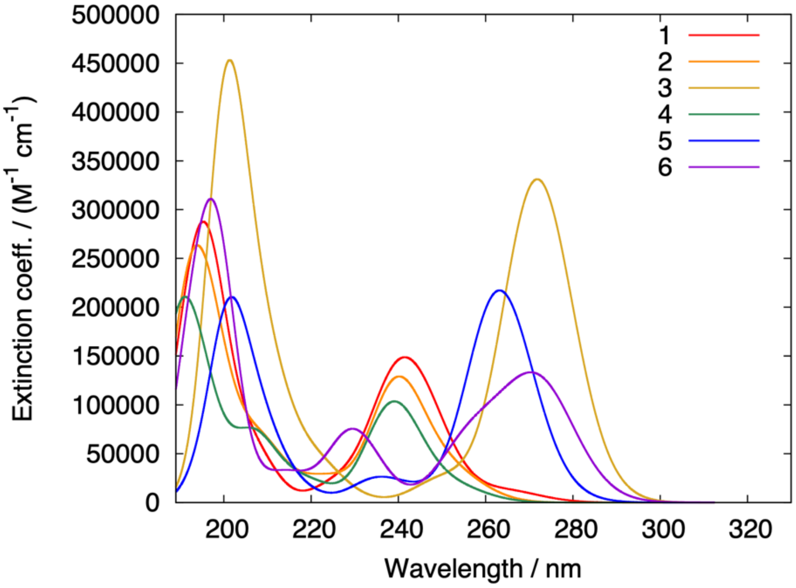
Excited state calculations at the S_0 geometry



7 **8** **9**

Figure S70: Calculated complexes with nitroso- (7), bromo- (8) and dimethylamino-(9) groups in para position.

At the ground-state geometries, the absorption spectra were calculated with CD-ev*GW*/BSE employing the PBE0 functional and def2-TZVP basis set.



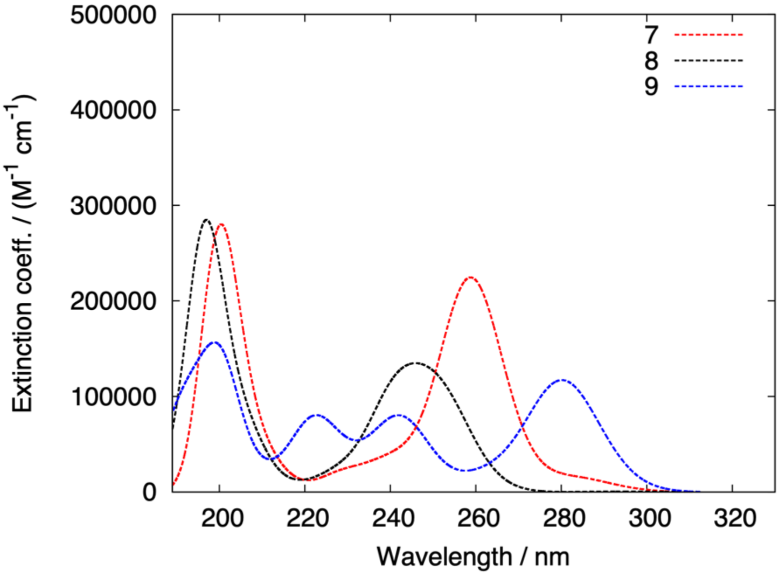
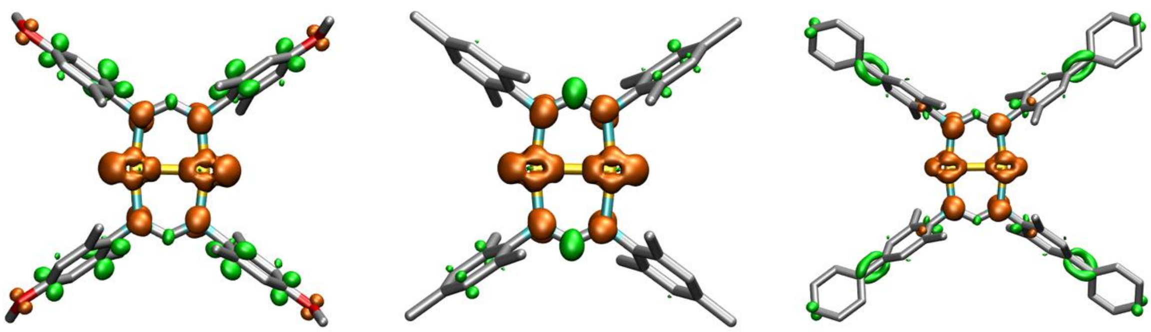
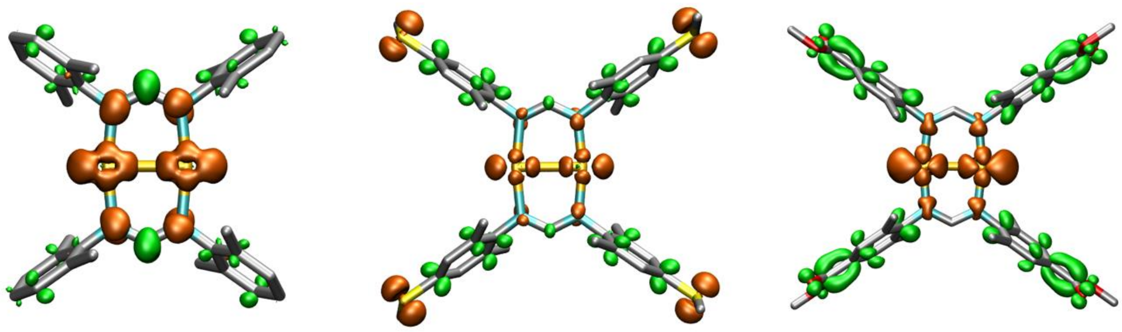


Figure S71: Absorption spectra (FWHM = 0.3 eV) calculated using PBE0 ev*GW*-BSE/def2-TZVP at the optimized S_0 geometries.



1 **2** **3**



4 5 6

Figure S72: Unrelaxed difference density plots (iso-value: 0.0015 a_0^{-3}) for the MLCT absorption bands. Green represents a loss of electron density while orange represents a gain of electron density. All hydrogen atoms are omitted for clarity.

The electron donating and withdrawing properties of the substituents are reflected in the change of electron density. However, the charge-transfer from the gold center to the aromatic groups of the amidinate ligands does not obviously differ, and is actually quite similar among all the complexes. Therefore, the electronic effects of the ligands on the absorption properties are very limited.

Two-component excited state calculations at the T_1 geometry

The optimized structure of the first triplet excited state (T_1) removes the coplanarity of the ground-state geometry. The central carbon atom of one amidinate ligand is located out of the Au_2N_4 plane. At the optimized T_1 geometries, two-component (2c) CD-ev*GW*/BSE calculations using the dhf-TZVP-2c basis set were performed to investigate luminescence properties. Note that for complex **3**, the dhf-SV(P)-2c basis set was used for all atoms in the *para*-substituted phenyl rings in order to facilitate the computation.

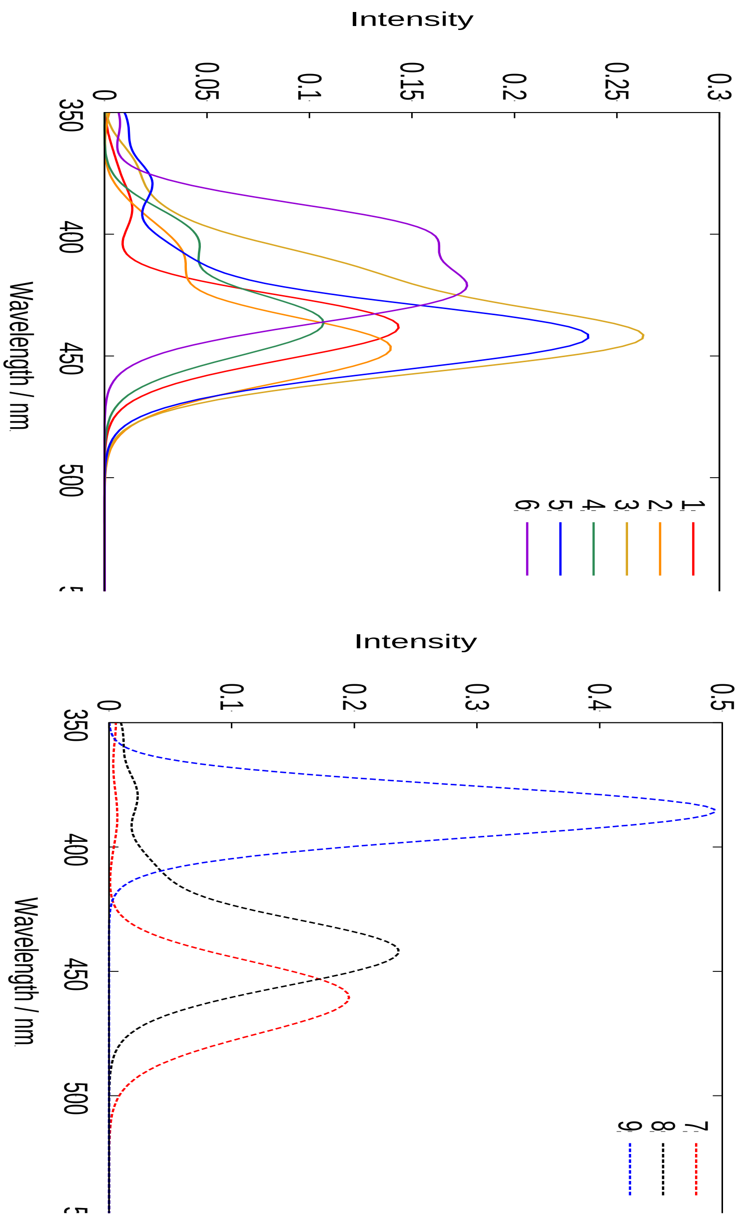
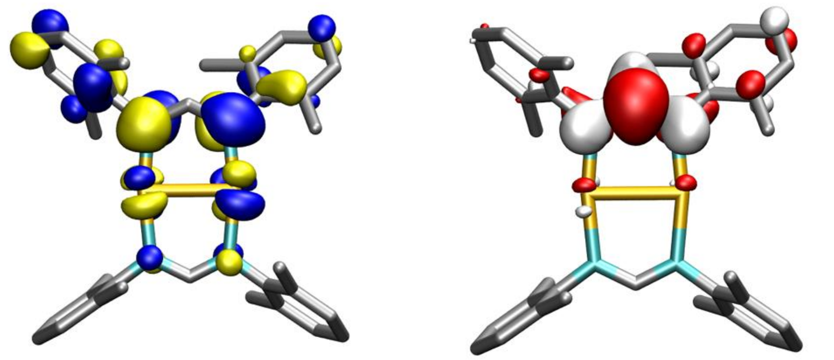


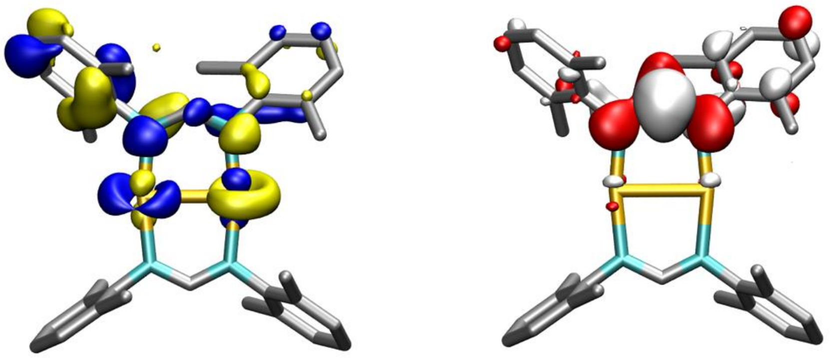
Figure S73: Emission spectra (FWHM = 0.2 eV) calculated using PBE0 ev*GW*-BSE/dhf-TZVP-2c at the optimized T_1 geometries.

As can be seen, the typical MLCT peak in the visible range is now split into two distinct (shoulder) peaks (except complex **9**), and the high-energy peak consists of one component of the second triplet excited state (T_2), which starts to gain intensity from strong mixing with the singlet states. This is also the most intense triplet excitation in the energetic range between S_1 and T_1.

An NTO analysis further confirms the MLCT character of the triplet excited states. The NTOs are quite similar among all the complexes, and those of complex **4** are presented as an example. Due to the distorted symmetry, the electron density is not evenly distributed on two amidinate ligands anymore, but exclusively centered on one side where the central carbon atom is located out of the Au_2N_4 plane.



T_1



T_2

Figure S74: Dominating occupied (blue/yellow) and virtual (red/white) natural transition orbitals (NTOs, iso-value: 0.04 $a_0^{-3/2}$) of the first and second triplet excitations of complex **4**. All hydrogen atoms are omitted for clarity.

The calculated triplet excitation energies as well as oscillator strengths and lifetimes (in the mixed velocity/length representation) are listed in Table S5.

Table S5: First and second triplet excitations T_1 and T_2 at the optimized T_1 geometries. Excitation energies of triplets are given at their center of mass. Oscillator strengths f and electric dipole radiative lifetime τ are taken from the most intense component.

	1	**2**	**3**	**4**
T_1 / eV (nm)	2.05 (606)	1.98 (626)	2.07 (599)	2.04 (608)
f_1 / a.u.	3.335×10^{-5}	4.146×10^{-5}	9.473×10^{-5}	4.451×10^{-5}
τ_1 / µs	165	142	56.8	124
T_2 / eV (nm)	3.16 (392)	2.99 (414)	2.95 (420)	3.04 (408)
f_2 / a.u.	1.249×10^{-2}	3.189×10^{-2}	1.052×10^{-1}	3.551×10^{-2}
τ_2 / µs	0.183	0.079	0.025	0.069
	5	**6**	**7**	**8**
T_1 / eV (nm)	2.07 (599)	2.25 (550)	2.01 (616)	2.04 (608)
f_1 / a.u.	6.219×10^{-5}	1.431×10^{-4}	2.100×10^{-5}	5.060×10^{-5}
τ_1 / µs	86.4	31.7	271	110
T_2 / eV (nm)	3.00 (413)	3.06 (405)	3.17 (391)	2.98 (416)
f_2 / a.u.	3.592×10^{-2}	1.349×10^{-1}	3.973×10^{-3}	6.403×10^{-2}
τ_2 / µs	0.070	0.018	0.577	0.040
	9			
T_1 / eV (nm)	3.09 (402)			
f_1 / a.u.	7.458×10^{-6}			
τ_1 / µs	325			
T_2 / eV (nm)	3.10 (400)			
f_2 / a.u.	7.901×10^{-6}			
τ_2 / µs	303			

Table S6: Frontier orbital energies and MLCT absorption/emission maxima with respect to the Hammett parameter of the substituents.

	1	2	3	4	5	6	7	8	9
HOMO / eV	-5.46	-5.64	-5.78	-5.80	-5.50	-6.20	-4.92	-6.15	-6.88
LUMO / eV	-0.53	-0.59	-1.01	-0.71	-0.71	-1.52	-0.24	-1.14	-2.72
$\lambda_{abs,}$/ nm	241	240	272	239	263	270	259	246	280
λ_{em}/ nm	438	446	442	437	442	421	460	441	386

Geometry optimizations

All ground-state (S_0) geometries were optimized in C_i symmetry except for complex **8** (in C_2 symmetry).

Table S7: Intermetallic Au···Au distances based on quantum chemical calculations (DFT).

	1	2	3	4	5	6	7	8	9
r/Å	2.752	2.753	2.752	2.753	2.751	2.751	2.751	2.751	2.751

Table S8: Calculated partial charges of Au atoms based on a natural population analysis (NPA).

	1	2	3	4	5	6	7	8	9
e	0.494	0.498	0.502	0.502	0.498	0.510	0.491	0.502	0.515

Cartesian coordinates

Cartesian coordinates in Å. All structure parameters are optimized at the PBE0-D3(BJ)/def2-TZVP level of theory

MeOXylForm$_2$Au$_2$ (1)

Au	-1.3742798	0.0480549	0.0437818
O	5.8127331	4.8159593	-1.7575896
O	-5.5835303	5.0280341	-1.9029259
N	-1.1382841	1.9403484	-0.6759063
C	0.0562172	2.4412091	-0.9101163
H	0.0797547	3.4655567	-1.2921719
C	3.9390880	4.3464539	-0.2918358
H	4.2442881	5.0808594	0.4420619
N	1.2259005	1.8615166	-0.7413676
C	-4.4872652	4.2635374	-1.6804504
C	-3.7622277	3.6272049	-2.6775478
H	-4.0543813	3.7081997	-3.7163877
C	4.6819150	4.1383028	-1.4448957
C	4.2747879	3.1753004	-2.3633053

H	4.8724693	3.0255290	-3.2550610
C	2.3829255	2.6478103	-0.9849481
C	3.1335032	2.4249774	-2.1475974
C	-2.2587230	2.7412811	-1.0217765
C	-2.6453885	2.8583367	-2.3550878
C	-4.0981214	4.1282527	-0.3512267
H	-4.6816834	4.6297012	0.4122482
C	-2.9919247	3.3728832	-0.0078638
C	-1.8850852	2.1485998	-3.4329997
H	-1.6809898	1.1136166	-3.1478119
H	-0.9155336	2.6183664	-3.6237730
H	-2.4446702	2.1523716	-4.3688972
C	2.7868715	3.5999718	-0.0515085
C	-2.5845198	3.2214712	1.4229458
H	-2.6119355	2.1695753	1.7249644
H	-3.2447535	3.7890861	2.0787689
H	-1.5576562	3.5583298	1.5844281
C	2.0072315	3.8078720	1.2105680
H	2.5789219	4.3996455	1.9261352
H	1.7490406	2.8507873	1.6703223
H	1.0646355	4.3315691	1.0250860
C	-6.0152880	5.1804691	-3.2308790
H	-6.2886106	4.2183076	-3.6781990
H	-5.2485697	5.6577659	-3.8513664
H	-6.8952157	5.8205082	-3.1944127
C	6.2620952	5.7905462	-0.8513112
H	6.4972621	5.3537956	0.1256780
H	5.5220926	6.5874900	-0.7173456
H	7.1685960	6.2129304	-1.2815415
C	2.7063004	1.3841614	-3.1326013
H	1.6935692	1.5709735	-3.4980034
H	2.6848858	0.3939612	-2.6661507
H	3.3843797	1.3524095	-3.9854693

Au	1.3742798	-0.0480549	-0.0437818
O	-5.8127331	-4.8159593	1.7575896
O	5.5835303	-5.0280341	1.9029259
N	1.1382841	-1.9403484	0.6759063
C	-0.0562172	-2.4412091	0.9101163
H	-0.0797547	-3.4655567	1.2921719
C	-3.9390880	-4.3464539	0.2918358
H	-4.2442881	-5.0808594	-0.4420619
N	-1.2259005	-1.8615166	0.7413676
C	4.4872652	-4.2635374	1.6804504
C	3.7622277	-3.6272049	2.6775478
H	4.0543813	-3.7081997	3.7163877
C	-4.6819150	-4.1383028	1.4448957
C	-4.2747879	-3.1753004	2.3633053
H	-4.8724693	-3.0255290	3.2550610
C	-2.3829255	-2.6478103	0.9849481
C	-3.1335032	-2.4249774	2.1475974
C	2.2587230	-2.7412811	1.0217765
C	2.6453885	-2.8583367	2.3550878
C	4.0981214	-4.1282527	0.3512267
H	4.6816834	-4.6297012	-0.4122482
C	2.9919247	-3.3728832	0.0078638
C	1.8850852	-2.1485998	3.4329997
H	1.6809898	-1.1136166	3.1478119
H	0.9155336	-2.6183664	3.6237730
H	2.4446702	-2.1523716	4.3688972
C	-2.7868715	-3.5999718	0.0515085
C	2.5845198	-3.2214712	-1.4229458
H	2.6119355	-2.1695753	-1.7249644
H	3.2447535	-3.7890861	-2.0787689
H	1.5576562	-3.5583298	-1.5844281
C	-2.0072315	-3.8078720	-1.2105680
H	-2.5789219	-4.3996455	-1.9261352

H	-1.7490406	-2.8507873	-1.6703223
H	-1.0646355	-4.3315691	-1.0250860
C	6.0152880	-5.1804691	3.2308790
H	6.2886106	-4.2183076	3.6781990
H	5.2485697	-5.6577659	3.8513664
H	6.8952157	-5.8205082	3.1944127
C	-6.2620952	-5.7905462	0.8513112
H	-6.4972621	-5.3537956	-0.1256780
H	-5.5220926	-6.5874900	0.7173456
H	-7.1685960	-6.2129304	1.2815415
C	-2.7063004	-1.3841614	3.1326013
H	-1.6935692	-1.5709735	3.4980034
H	-2.6848858	-0.3939612	2.6661507
H	-3.3843797	-1.3524095	3.9854693

$MesForm_2Au_2$ (2)

Au	0.3750013	-1.3122474	0.1780512
N	-1.6282965	-1.6875221	0.1389527
N	-2.2728844	0.5691907	-0.1551789
C	-2.5055805	-0.7179354	-0.0109649
H	-3.5568248	-1.0187835	-0.0160384
C	-2.1265985	-3.0158598	0.1807184
C	-2.5457545	-3.6371207	-0.9984306
C	-3.0036845	-4.9479294	-0.9331298
H	-3.3236047	-5.4359315	-1.8491613
C	-3.0489023	-5.6509208	0.2631052
C	-2.6100045	-5.0105220	1.4161822
H	-2.6270888	-5.5456913	2.3611454
C	-2.1473354	-3.7019827	1.3986595
C	-2.4740017	-2.9154443	-2.3087560
H	-2.6303310	-3.6064253	-3.1376035
H	-1.5035712	-2.4283478	-2.4338926
H	-3.2311702	-2.1293725	-2.3850590

C	-1.6691970	-3.0375074	2.6500359
H	-1.7809484	-3.6996450	3.5090359
H	-2.2172212	-2.1133474	2.8491857
H	-0.6148251	-2.7547525	2.5638367
C	-3.3985815	1.4319170	-0.2144585
C	-3.7763887	1.9818843	-1.4421687
C	-4.8627087	2.8463524	-1.4765954
H	-5.1588139	3.2752474	-2.4294194
C	-5.5762305	3.1762935	-0.3309367
C	-5.1674503	2.6247194	0.8764950
H	-5.6990234	2.8847716	1.7872747
C	-4.0855970	1.7568812	0.9584562
C	-3.0150710	1.6520991	-2.6863451
H	-1.9708812	1.9705635	-2.6012210
H	-3.4570286	2.1423874	-3.5541422
H	-2.9909296	0.5752075	-2.8701159
C	-3.6446348	1.2026235	2.2778511
H	-4.1491844	1.7136949	3.0983004
H	-2.5645257	1.3111285	2.4055277
H	-3.8643858	0.1344793	2.3662551
Au	-0.3750013	1.3122474	-0.1780512
N	1.6282965	1.6875221	-0.1389527
N	2.2728844	-0.5691907	0.1551789
C	2.5055805	0.7179354	0.0109649
H	3.5568248	1.0187835	0.0160384
C	2.1265985	3.0158598	-0.1807184
C	2.5457545	3.6371207	0.9984306
C	3.0036845	4.9479294	0.9331298
H	3.3236047	5.4359315	1.8491613
C	3.0489023	5.6509208	-0.2631052
C	2.6100045	5.0105220	-1.4161822
H	2.6270888	5.5456913	-2.3611454
C	2.1473354	3.7019827	-1.3986595

C	2.4740017	2.9154443	2.3087560
H	2.6303310	3.6064253	3.1376035
H	1.5035712	2.4283478	2.4338926
H	3.2311702	2.1293725	2.3850590
C	1.6691970	3.0375074	-2.6500359
H	1.7809484	3.6996450	-3.5090359
H	2.2172212	2.1133474	-2.8491857
H	0.6148251	2.7547525	-2.5638367
C	3.3985815	-1.4319170	0.2144585
C	3.7763887	-1.9818843	1.4421687
C	4.8627087	-2.8463524	1.4765954
H	5.1588139	-3.2752474	2.4294194
C	5.5762305	-3.1762935	0.3309367
C	5.1674503	-2.6247194	-0.8764950
H	5.6990234	-2.8847716	-1.7872747
C	4.0855970	-1.7568812	-0.9584562
C	3.0150710	-1.6520991	2.6863451
H	1.9708812	-1.9705635	2.6012210
H	3.4570286	-2.1423874	3.5541422
H	2.9909296	-0.5752075	2.8701159
C	3.6446348	-1.2026235	-2.2778511
H	4.1491844	-1.7136949	-3.0983004
H	2.5645257	-1.3111285	-2.4055277
H	3.8643858	-0.1344793	-2.3662551
C	-3.5737512	-7.0534990	0.3152313
H	-3.0464358	-7.6480281	1.0638352
H	-4.6359685	-7.0651499	0.5790920
H	-3.4710159	-7.5520289	-0.6501296
C	3.5737512	7.0534990	-0.3152313
H	3.0464358	7.6480281	-1.0638352
H	4.6359685	7.0651499	-0.5790920
H	3.4710159	7.5520289	0.6501296
C	-6.7655201	4.0854209	-0.3982687

H	-7.6912004	3.5122899	-0.5110395
H	-6.8614721	4.6825033	0.5106455
H	-6.6973003	4.7667191	-1.2481264
C	6.7655201	-4.0854209	0.3982687
H	7.6912004	-3.5122899	0.5110395
H	6.8614721	-4.6825033	-0.5106455
H	6.6973003	-4.7667191	1.2481264

PhXylForm$_2$Au$_2$ (3)

Au	-1.3747367	-0.0618057	0.0002441
N	-1.1814168	-0.0455635	2.0300278
C	0.0003158	-0.0002263	2.6074775
H	0.0006247	-0.0006365	3.7006934
C	3.8029434	-1.2644725	4.2818101
H	4.0947758	-2.2085245	4.7293921
N	1.1818243	0.0454996	2.0295645
C	-4.5939748	0.1383857	4.4886625
C	-3.8029443	1.2644990	4.2818356
H	-4.0949100	2.2086392	4.7291364
C	4.5939318	-0.1383460	4.4887400
C	4.2253332	1.0486722	3.8601755
H	4.8138787	1.9442703	4.0280089
C	2.3209476	-0.0163396	2.8718254
C	3.1002767	1.1306094	3.0537809
C	-2.3204282	0.0162631	2.8724479
C	-2.6719919	1.2267611	3.4779295
C	-4.2253119	-1.0485616	3.8600818
H	-4.8141829	-1.9440176	4.0274441
C	-3.0999773	-1.1305866	3.0541221
C	-1.8675167	2.4663881	3.2335099
H	-1.6493350	2.5871125	2.1694718
H	-0.9040218	2.4384235	3.7510436
H	-2.4048484	3.3477861	3.5842628

C	2.6722440	-1.2267670	3.4775581
C	-2.7192493	-2.4181876	2.3961732
H	-2.7293845	-2.3173179	1.3058961
H	-3.4077433	-3.2158180	2.6759485
H	-1.7050170	-2.7229394	2.6651138
C	1.8672949	-2.4661257	3.2334021
H	2.4042386	-3.3477352	3.5842079
H	1.6488127	-2.5868716	2.1694395
H	0.9039011	-2.4376069	3.7510998
C	2.7191603	2.4182045	2.3959955
H	1.7048675	2.7225677	2.6652009
H	2.7290135	2.3175026	1.3056902
H	3.4073928	3.2160684	2.6757007
Au	1.3747367	0.0618057	-0.0002441
N	1.1814168	0.0455635	-2.0300278
C	-0.0003158	0.0002263	-2.6074775
H	-0.0006247	0.0006365	-3.7006934
C	-3.8029434	1.2644725	-4.2818101
H	-4.0947758	2.2085245	-4.7293921
N	-1.1818243	-0.0454996	-2.0295645
C	4.5939748	-0.1383857	-4.4886625
C	3.8029443	-1.2644990	-4.2818356
H	4.0949100	-2.2086392	-4.7291364
C	-4.5939318	0.1383460	-4.4887400
C	-4.2253332	-1.0486722	-3.8601755
H	-4.8138787	-1.9442703	-4.0280089
C	-2.3209476	0.0163396	-2.8718254
C	-3.1002767	-1.1306094	-3.0537809
C	2.3204282	-0.0162631	-2.8724479
C	2.6719919	-1.2267611	-3.4779295
C	4.2253119	1.0485616	-3.8600818
H	4.8141829	1.9440176	-4.0274441
C	3.0999773	1.1305866	-3.0541221

C	1.8675167	-2.4663881	-3.2335099
H	1.6493350	-2.5871125	-2.1694718
H	0.9040218	-2.4384235	-3.7510436
H	2.4048484	-3.3477861	-3.5842628
C	-2.6722440	1.2267670	-3.4775581
C	2.7192493	2.4181876	-2.3961732
H	2.7293845	2.3173179	-1.3058961
H	3.4077433	3.2158180	-2.6759485
H	1.7050170	2.7229394	-2.6651138
C	-1.8672949	2.4661257	-3.2334021
H	-2.4042386	3.3477352	-3.5842079
H	-1.6488127	2.5868716	-2.1694395
H	-0.9039011	2.4376069	-3.7510998
C	-2.7191603	-2.4182045	-2.3959955
H	-1.7048675	-2.7225677	-2.6652009
H	-2.7290135	-2.3175026	-1.3056902
H	-3.4073928	-3.2160684	-2.6757007
C	-5.7918452	0.2015356	5.3447784
C	-6.9475957	-0.5066855	5.0140606
C	-8.0733897	-0.4472741	5.8187877
C	-8.0677128	0.3224028	6.9728901
C	-6.9255284	1.0319471	7.3138081
C	-5.8003606	0.9716002	6.5082474
H	-6.9697699	-1.0896408	4.1004039
H	-8.9636991	-0.9983005	5.5379930
H	-8.9484853	0.3695548	7.6024751
H	-6.9072763	1.6298201	8.2178920
H	-4.9037188	1.5089775	6.7953748
C	5.7917807	-0.2016588	5.3448898
C	6.9475558	0.5064388	5.0140226
C	8.0733607	0.4471600	5.8187322
C	8.0678233	-0.3226002	6.9727739
C	6.9256740	-1.0321711	7.3137581

C	5.8003203	-0.9716020	6.5084522
H	6.9696345	1.0892540	4.1002730
H	8.9635335	0.9984615	5.5380341
H	8.9485198	-0.3694151	7.6024943
H	6.9075506	-1.6301603	8.2177687
H	4.9035789	-1.5085952	6.7959950
C	-5.7917807	0.2016588	-5.3448898
C	-5.8003203	0.9716020	-6.5084522
C	-6.9256740	1.0321711	-7.3137581
C	-8.0678233	0.3226002	-6.9727739
C	-8.0733607	-0.4471600	-5.8187322
C	-6.9475558	-0.5064388	-5.0140226
H	-4.9035789	1.5085952	-6.7959950
H	-6.9075506	1.6301603	-8.2177687
H	-8.9485198	0.3694151	-7.6024943
H	-8.9635335	-0.9984615	-5.5380341
H	-6.9696345	-1.0892540	-4.1002730
C	5.7918452	-0.2015356	-5.3447784
C	5.8003606	-0.9716002	-6.5082474
C	6.9255284	-1.0319471	-7.3138081
C	8.0677128	-0.3224028	-6.9728901
C	8.0733897	0.4472741	-5.8187877
C	6.9475957	0.5066855	-5.0140606
H	4.9037188	-1.5089775	-6.7953748
H	6.9072763	-1.6298201	-8.2178920
H	8.9484853	-0.3695548	-7.6024751
H	8.9636991	0.9983005	-5.5379930
H	6.9697699	1.0896408	-4.1004039

XylForm$_2$Au$_2$ (4)

Au	0.3754909	-1.3116426	0.1810811
N	-1.6278550	-1.6892471	0.1327399
N	-2.2726961	0.5660136	-0.1663061

C	-2.5056893	-0.7206981	-0.0208939
H	-3.5566844	-1.0218978	-0.0276796
C	-2.1241514	-3.0179862	0.1761898
C	-2.5754727	-3.6260728	-0.9999583
C	-3.0351092	-4.9368891	-0.9335354
H	-3.3834081	-5.4192685	-1.8406069
C	-3.0395222	-5.6299419	0.2645734
H	-3.3977187	-6.6522302	0.2991940
C	-2.5784901	-5.0160664	1.4177072
H	-2.5780194	-5.5572597	2.3578255
C	-2.1144599	-3.7069024	1.3938496
C	-2.5384339	-2.8918668	-2.3049507
H	-2.7028457	-3.5785142	-3.1358392
H	-1.5766967	-2.3923287	-2.4458752
H	-3.3073979	-2.1155895	-2.3613352
C	-1.6095162	-3.0448141	2.6357407
H	-1.7179994	-3.7031275	3.4980450
H	-2.1410897	-2.1122773	2.8397361
H	-0.5521681	-2.7779873	2.5345303
C	-3.3972404	1.4300329	-0.2273076
C	-3.7655193	1.9811233	-1.4590056
C	-4.8520213	2.8461516	-1.4982985
H	-5.1481061	3.2766373	-2.4489256
C	-5.5550778	3.1596763	-0.3466251
H	-6.3998694	3.8369082	-0.3938063
C	-5.1724431	2.6114467	0.8654983
H	-5.7140046	2.8643384	1.7707622
C	-4.0890574	1.7435641	0.9469175
C	-2.9989327	1.6471190	-2.6986836
H	-1.9548693	1.9651552	-2.6109526
H	-3.4371450	2.1357426	-3.5692644
H	-2.9750838	0.5698612	-2.8800341
C	-3.6545936	1.1761948	2.2628271

H	-4.1633607	1.6799977	3.0850748
H	-2.5752415	1.2835524	2.3976217
H	-3.8754362	0.1075208	2.3409856
Au	-0.3754909	1.3116426	-0.1810811
N	1.6278550	1.6892471	-0.1327399
N	2.2726961	-0.5660136	0.1663061
C	2.5056893	0.7206981	0.0208939
H	3.5566844	1.0218978	0.0276796
C	2.1241514	3.0179862	-0.1761898
C	2.5754727	3.6260728	0.9999583
C	3.0351092	4.9368891	0.9335354
H	3.3834081	5.4192685	1.8406069
C	3.0395222	5.6299419	-0.2645734
H	3.3977187	6.6522302	-0.2991940
C	2.5784901	5.0160664	-1.4177072
H	2.5780194	5.5572597	-2.3578255
C	2.1144599	3.7069024	-1.3938496
C	2.5384339	2.8918668	2.3049507
H	2.7028457	3.5785142	3.1358392
H	1.5766967	2.3923287	2.4458752
H	3.3073979	2.1155895	2.3613352
C	1.6095162	3.0448141	-2.6357407
H	1.7179994	3.7031275	-3.4980450
H	2.1410897	2.1122773	-2.8397361
H	0.5521681	2.7779873	-2.5345303
C	3.3972404	-1.4300329	0.2273076
C	3.7655193	-1.9811233	1.4590056
C	4.8520213	-2.8461516	1.4982985
H	5.1481061	-3.2766373	2.4489256
C	5.5550778	-3.1596763	0.3466251
H	6.3998694	-3.8369082	0.3938063
C	5.1724431	-2.6114467	-0.8654983
H	5.7140046	-2.8643384	-1.7707622

C	4.0890574	-1.7435641	-0.9469175
C	2.9989327	-1.6471190	2.6986836
H	1.9548693	-1.9651552	2.6109526
H	3.4371450	-2.1357426	3.5692644
H	2.9750838	-0.5698612	2.8800341
C	3.6545936	-1.1761948	-2.2628271
H	4.1633607	-1.6799977	-3.0850748
H	2.5752415	-1.2835524	-2.3976217
H	3.8754362	-0.1075208	-2.3409856

MeSXylForm$_2$Au$_2$ (5)

Au	-1.3706108	0.0669362	0.0937925
S	6.1648801	4.9354027	-2.0088306
S	-5.9261083	5.2961286	-1.7960822
N	-1.1345179	1.9567932	-0.6338128
C	0.0570062	2.4426214	-0.9104566
H	0.0807900	3.4668332	-1.2924088
C	3.9710840	4.3007182	-0.4134719
H	4.2957610	5.0389754	0.3085790
N	1.2234479	1.8461009	-0.7836181
C	-4.5026280	4.3024245	-1.5424084
C	-3.7923916	3.6743590	-2.5563211
H	-4.1033504	3.7671335	-3.5890320
C	4.6977938	4.0767459	-1.5747415
C	4.2563448	3.1055401	-2.4726725
H	4.8208329	2.9213394	-3.3811255
C	2.3832634	2.6158908	-1.0574384
C	3.1091858	2.3704567	-2.2300739
C	-2.2576903	2.7653776	-0.9462233
C	-2.6712226	2.9004068	-2.2715919

C	-4.0801000	4.1459689	-0.2227924
H	-4.6320581	4.6303878	0.5763009
C	-2.9674404	3.3849190	0.0903374
C	-1.9368014	2.2026323	-3.3749027
H	-1.7421874	1.1594308	-3.1137604
H	-0.9647300	2.6635528	-3.5734877
H	-2.5119605	2.2320791	-4.3007769
C	2.8150954	3.5749881	-0.1410824
C	-2.5306027	3.2186741	1.5106408
H	-2.5602860	2.1648633	1.8058355
H	-3.1725084	3.7859359	2.1847505
H	-1.4982099	3.5470513	1.6529726
C	2.0629155	3.8067226	1.1334033
H	2.6511289	4.4112477	1.8244132
H	1.8155108	2.8585800	1.6171958
H	1.1167253	4.3278385	0.9601961
C	-6.1552594	5.2415506	-3.5705727
H	-6.3418214	4.2251981	-3.9203835
H	-5.3034600	5.6712779	-4.0996890
H	-7.0371830	5.8496855	-3.7723592
C	6.4077201	6.0561335	-0.6343143
H	6.5542633	5.5168511	0.3026200
H	5.5797234	6.7599277	-0.5379140
H	7.3164004	6.6123958	-0.8649848
C	2.6524037	1.3261510	-3.1977592
H	1.6320833	1.5159824	-3.5394962
H	2.6386665	0.3382871	-2.7259616
H	3.3092195	1.2861733	-4.0668152

Au	1.3706108	-0.0669362	-0.0937925
S	-6.1648801	-4.9354027	2.0088306
S	5.9261083	-5.2961286	1.7960822
N	1.1345179	-1.9567932	0.6338128
C	-0.0570062	-2.4426214	0.9104566
H	-0.0807900	-3.4668332	1.2924088
C	-3.9710840	-4.3007182	0.4134719
H	-4.2957610	-5.0389754	-0.3085790
N	-1.2234479	-1.8461009	0.7836181
C	4.5026280	-4.3024245	1.5424084
C	3.7923916	-3.6743590	2.5563211
H	4.1033504	-3.7671335	3.5890320
C	-4.6977938	-4.0767459	1.5747415
C	-4.2563448	-3.1055401	2.4726725
H	-4.8208329	-2.9213394	3.3811255
C	-2.3832634	-2.6158908	1.0574384
C	-3.1091858	-2.3704567	2.2300739
C	2.2576903	-2.7653776	0.9462233
C	2.6712226	-2.9004068	2.2715919
C	4.0801000	-4.1459689	0.2227924
H	4.6320581	-4.6303878	-0.5763009
C	2.9674404	-3.3849190	-0.0903374
C	1.9368014	-2.2026323	3.3749027
H	1.7421874	-1.1594308	3.1137604
H	0.9647300	-2.6635528	3.5734877
H	2.5119605	-2.2320791	4.3007769
C	-2.8150954	-3.5749881	0.1410824
C	2.5306027	-3.2186741	-1.5106408

H	2.5602860	-2.1648633	-1.8058355
H	3.1725084	-3.7859359	-2.1847505
H	1.4982099	-3.5470513	-1.6529726
C	-2.0629155	-3.8067226	-1.1334033
H	-2.6511289	-4.4112477	-1.8244132
H	-1.8155108	-2.8585800	-1.6171958
H	-1.1167253	-4.3278385	-0.9601961
C	6.1552594	-5.2415506	3.5705727
H	6.3418214	-4.2251981	3.9203835
H	5.3034600	-5.6712779	4.0996890
H	7.0371830	-5.8496855	3.7723592
C	-6.4077201	-6.0561335	0.6343143
H	-6.5542633	-5.5168511	-0.3026200
H	-5.5797234	-6.7599277	0.5379140
H	-7.3164004	-6.6123958	0.8649848
C	-2.6524037	-1.3261510	3.1977592
H	-1.6320833	-1.5159824	3.5394962
H	-2.6386665	-0.3382871	2.7259616
H	-3.3092195	-1.2861733	4.0668152

$MeO_2CXylForm_2Au_2$ (6)

Au	0.3915883	-1.2995974	0.2238678
N	-1.6099255	-1.6848923	0.2949927
N	-2.2821455	0.5503031	-0.0703274
C	-2.5016638	-0.7288891	0.1451421
C	-2.0864531	-3.0139240	0.4061846
C	-2.5908656	-3.6625336	-0.7274570
C	-3.0307744	-4.9721690	-0.5997508
C	-2.9674929	-5.6286466	0.6225554

C	-2.4524282	-4.9707410	1.7327338
C	-2.0047140	-3.6634608	1.6445937
C	-2.6263042	-2.9699764	-2.0551183
C	-1.4461143	-2.9580764	2.8384672
C	-3.4042326	1.4145695	-0.0890026
C	-3.8229074	1.9568542	-1.3099950
C	-4.9045787	2.8236978	-1.3126822
C	-5.5587753	3.1508508	-0.1306959
C	-5.1229693	2.6088175	1.0709339
C	-4.0439773	1.7400490	1.1137282
C	-3.1149585	1.6064182	-2.5794344
C	-3.5546771	1.1880286	2.4170052
Au	-0.3915883	1.2995974	-0.2238678
N	1.6099255	1.6848923	-0.2949927
N	2.2821455	-0.5503031	0.0703274
C	2.5016638	0.7288891	-0.1451421
C	2.0864531	3.0139240	-0.4061846
C	2.5908656	3.6625336	0.7274570
C	3.0307744	4.9721690	0.5997508
C	2.9674929	5.6286466	-0.6225554
C	2.4524282	4.9707410	-1.7327338
C	2.0047140	3.6634608	-1.6445937
C	2.6263042	2.9699764	2.0551183
C	1.4461143	2.9580764	-2.8384672
C	3.4042326	-1.4145695	0.0890026
C	3.8229074	-1.9568542	1.3099950
C	4.9045787	-2.8236978	1.3126822
C	5.5587753	-3.1508508	0.1306959

C	5.1229693	-2.6088175	-1.0709339
C	4.0439773	-1.7400490	-1.1137282
C	3.1149585	-1.6064182	2.5794344
C	3.5546771	-1.1880286	-2.4170052
O	3.8975543	7.5579841	0.3395412
C	3.4275293	7.0256150	-0.7973335
O	3.3910453	7.6308595	-1.8385404
C	4.3529620	8.9006831	0.2332168
O	7.0415293	-4.5388191	1.3085356
C	6.7153358	-4.0755180	0.0938026
O	7.3079841	-4.3876759	-0.9077522
C	8.1437928	-5.4365582	1.3352453
O	-3.8975543	-7.5579841	-0.3395412
C	-3.4275293	-7.0256150	0.7973335
O	-3.3910453	-7.6308595	1.8385404
C	-4.3529620	-8.9006831	-0.2332168
O	-7.0415293	4.5388191	-1.3085356
C	-6.7153358	4.0755180	-0.0938026
O	-7.3079841	4.3876759	0.9077522
C	-8.1437928	5.4365582	-1.3352453

$Me_2NXylForm_2Au_2$ (7)

Au	-1.3738674	0.0530097	0.0464239
N	-1.1361185	1.9276522	-0.7173793
C	0.0598025	2.4187192	-0.9651995
H	0.0854246	3.4350410	-1.3680768
C	3.9384441	4.3374771	-0.3945710
H	4.2260300	5.0923067	0.3249061
N	1.2289797	1.8397259	-0.7888166

C	-4.5124103	4.2622694	-1.7480138
C	-3.7633989	3.5992210	-2.7281057
H	-4.0468235	3.6655726	-3.7699840
C	4.7179864	4.1155999	-1.5364339
C	4.2849481	3.1291551	-2.4327474
H	4.8438217	2.9297785	-3.3372141
C	2.3864115	2.6206017	-1.0480968
C	3.1408718	2.3822592	-2.1987668
C	-2.2544258	2.7290201	-1.0700431
C	-2.6535022	2.8323126	-2.4036389
C	-4.0855937	4.1440840	-0.4183970
H	-4.6205697	4.6501809	0.3739678
C	-2.9779129	3.3859329	-0.0725653
C	-1.9001576	2.1076792	-3.4767502
H	-1.7200322	1.0685001	-3.1901945
H	-0.9188753	2.5558528	-3.6590357
H	-2.4529976	2.1231532	-4.4165553
C	2.7918829	3.5992663	-0.1389384
C	-2.5608446	3.2668109	1.3591449
H	-2.5818979	2.2213849	1.6835984
H	-3.2186269	3.8457093	2.0081774
H	-1.5341717	3.6105098	1.5077245
C	2.0065268	3.8415049	1.1136705
H	2.5650327	4.4735904	1.8048465
H	1.7687173	2.8978931	1.6111541
H	1.0523283	4.3354275	0.9072463
C	2.7171165	1.3254204	-3.1690273
H	1.7058634	1.5058869	-3.5418873

H	2.6932249	0.3428677	-2.6866966
H	3.3982821	1.2784651	-4.0192546
Au	1.3738674	-0.0530097	-0.0464239
N	1.1361185	-1.9276522	0.7173793
C	-0.0598025	-2.4187192	0.9651995
H	-0.0854246	-3.4350410	1.3680768
C	-3.9384441	-4.3374771	0.3945710
H	-4.2260300	-5.0923067	-0.3249061
N	-1.2289797	-1.8397259	0.7888166
C	4.5124103	-4.2622694	1.7480138
C	3.7633989	-3.5992210	2.7281057
H	4.0468235	-3.6655726	3.7699840
C	-4.7179864	-4.1155999	1.5364339
C	-4.2849481	-3.1291551	2.4327474
H	-4.8438217	-2.9297785	3.3372141
C	-2.3864115	-2.6206017	1.0480968
C	-3.1408718	-2.3822592	2.1987668
C	2.2544258	-2.7290201	1.0700431
C	2.6535022	-2.8323126	2.4036389
C	4.0855937	-4.1440840	0.4183970
H	4.6205697	-4.6501809	-0.3739678
C	2.9779129	-3.3859329	0.0725653
C	1.9001576	-2.1076792	3.4767502
H	1.7200322	-1.0685001	3.1901945
H	0.9188753	-2.5558528	3.6590357
H	2.4529976	-2.1231532	4.4165553
C	-2.7918829	-3.5992663	0.1389384
C	2.5608446	-3.2668109	-1.3591449

H	2.5818979	-2.2213849	-1.6835984
H	3.2186269	-3.8457093	-2.0081774
H	1.5341717	-3.6105098	-1.5077245
C	-2.0065268	-3.8415049	-1.1136705
H	-2.5650327	-4.4735904	-1.8048465
H	-1.7687173	-2.8978931	-1.6111541
H	-1.0523283	-4.3354275	-0.9072463
C	-2.7171165	-1.3254204	3.1690273
H	-1.7058634	-1.5058869	3.5418873
H	-2.6932249	-0.3428677	2.6866966
H	-3.3982821	-1.2784651	4.0192546
N	-5.6370454	4.9934684	-2.0769156
C	-5.8877085	5.2981500	-3.4595521
H	-6.0120958	4.3845400	-4.0471721
H	-6.8153489	5.8635716	-3.5367997
H	-5.0833293	5.8897871	-3.9218082
C	-6.2192213	5.8571309	-1.0855647
H	-7.0994671	6.3403233	-1.5073357
H	-6.5465056	5.2876918	-0.2114627
H	-5.5286184	6.6404520	-0.7388528
N	-5.8770203	-4.8319597	1.7636504
C	-6.4986368	-4.7551836	3.0579993
H	-7.4017902	-5.3638715	3.0554515
H	-5.8461647	-5.1093365	3.8701817
H	-6.7968611	-3.7293799	3.2904154
C	-6.1381166	-5.9996685	0.9661373
H	-7.0910484	-6.4315396	1.2688040
H	-6.2180641	-5.7423169	-0.0934431

H	-5.3608896	-6.7718909	1.0680885
N	5.6370454	-4.9934684	2.0769156
C	5.8877085	-5.2981500	3.4595521
H	6.0120958	-4.3845400	4.0471721
H	6.8153489	-5.8635716	3.5367997
H	5.0833293	-5.8897871	3.9218082
C	6.2192213	-5.8571309	1.0855647
H	7.0994671	-6.3403233	1.5073357
H	6.5465056	-5.2876918	0.2114627
H	5.5286184	-6.6404520	0.7388528
N	5.8770203	4.8319597	-1.7636504
C	6.4986368	4.7551836	-3.0579993
H	7.4017902	5.3638715	-3.0554515
H	5.8461647	5.1093365	-3.8701817
H	6.7968611	3.7293799	-3.2904154
C	6.1381166	5.9996685	-0.9661373
H	7.0910484	6.4315396	-1.2688040
H	6.2180641	5.7423169	0.0934431
H	5.3608896	6.7718909	-1.0680885

BrXylForm$_2$Au$_2$ (8)

Au	1.3732557	-0.0761093	-0.0050521
Br	6.1204260	0.1129511	-5.5433813
Br	-6.1204260	-0.1129511	-5.5433813
N	-1.1802351	0.0609529	-2.0347525
C	4.5768039	0.0604556	-4.4544921
N	1.1802351	-0.0609529	-2.0347525
C	-4.2140188	1.1293477	-3.8491703
H	-4.8108204	2.0202488	-4.0003674

C	4.2140188	-1.1293477	-3.8491703
H	4.8108204	-2.0202488	-4.0003674
C	2.3228217	-0.0196407	-2.8733898
C	2.6978096	1.1864225	-3.4737771
C	3.8351476	1.2125321	-4.2730602
H	4.1435879	2.1375416	-4.7442997
C	0.0000000	0.0000000	-2.6138329
H	0.0000000	0.0000000	-3.7070053
C	3.0805124	-1.1824363	-3.0484556
C	1.9080681	2.4376538	-3.2420393
H	0.9564577	2.4251642	-3.7814005
H	2.4653622	3.3124413	-3.5770267
H	1.6689456	2.5558659	-2.1823948
C	-2.3228217	0.0196407	-2.8733898
C	-3.0805124	1.1824363	-3.0484556
C	-2.6978096	-1.1864225	-3.4737771
C	-2.6813093	2.4581312	-2.3789622
H	-1.6595861	2.7437475	-2.6396715
H	-2.7025027	2.3481780	-1.2896273
H	-3.3522665	3.2705570	-2.6574938
C	2.6813093	-2.4581312	-2.3789622
H	1.6595861	-2.7437475	-2.6396715
H	2.7025027	-2.3481780	-1.2896273
H	3.3522665	-3.2705570	-2.6574938
C	-4.5768039	-0.0604556	-4.4544921
C	-3.8351476	-1.2125321	-4.2730602
H	-4.1435879	-2.1375416	-4.7442997
C	-1.9080681	-2.4376538	-3.2420393

H	-0.9564577	-2.4251642	-3.7814005
H	-2.4653622	-3.3124413	-3.5770267
H	-1.6689456	-2.5558659	-2.1823948
Au	-1.3732557	0.0761093	-0.0050521
Br	-6.0623244	0.7910834	5.5442400
Br	6.0623244	-0.7910834	5.5442400
N	1.1798446	-0.0699084	2.0246152
C	-4.5368252	0.5675165	4.4514283
N	-1.1798446	0.0699084	2.0246152
C	3.6718972	-1.6299434	4.2685063
H	3.8739525	-2.5831755	4.7410987
C	-3.6718972	1.6299434	4.2685063
H	-3.8739525	2.5831755	4.7410987
C	-2.3096773	0.2378281	2.8647129
C	-3.1914968	-0.8335416	3.0414023
C	-4.3101316	-0.6549794	3.8449285
H	-5.0017616	-1.4741304	3.9977111
C	0.0000000	0.0000000	2.6034406
H	0.0000000	0.0000000	3.6966227
C	-2.5465507	1.4777787	3.4663569
C	-2.9378053	-2.1454487	2.3709110
H	-1.9530903	-2.5422452	2.6284976
H	-3.6934829	-2.8789124	2.6515984
H	-2.9500129	-2.0336251	1.2816272
C	2.3096773	-0.2378281	2.8647129
C	2.5465507	-1.4777787	3.4663569
C	3.1914968	0.8335416	3.0414023
C	1.6225898	-2.6331559	3.2332095

H	0.6752311	-2.5120245	3.7665324
H	1.3777725	-2.7274634	2.1724301
H	2.0761706	-3.5637870	3.5740493
C	-1.6225898	2.6331559	3.2332095
H	-0.6752311	2.5120245	3.7665324
H	-1.3777725	2.7274634	2.1724301
H	-2.0761706	3.5637870	3.5740493
C	4.5368252	-0.5675165	4.4514283
C	4.3101316	0.6549794	3.8449285
H	5.0017616	1.4741304	3.9977111
C	2.9378053	2.1454487	2.3709110
H	1.9530903	2.5422452	2.6284976
H	3.6934829	2.8789124	2.6515984
H	2.9500129	2.0336251	1.2816272

$O_2NXylForm_2Au_2$ (9)

Au	-1.3712826	0.0630338	0.0841562
N	-1.1340068	1.9526147	-0.6472124
C	0.0564105	2.4467097	-0.9115503
H	0.0799484	3.4704892	-1.2932830
C	3.9203240	4.3262172	-0.3067420
H	4.2543456	5.0857600	0.3873387
N	1.2219298	1.8524686	-0.7704082
C	-4.4772555	4.2043393	-1.6389980
C	-3.7444160	3.6194420	-2.6526996
H	-4.0633345	3.7465167	-3.6785471
C	4.6679344	4.0684072	-1.4386746
C	4.3052526	3.1003334	-2.3558135
H	4.9249891	2.9368091	-3.2271810
C	2.3849795	2.6238033	-1.0047816
C	3.1524987	2.3605247	-2.1475538
C	-2.2614506	2.7361745	-0.9905210

C	-2.6206826	2.8699602	-2.3384082
C	-4.1326846	4.0671260	-0.3077231
H	-4.7396979	4.5455798	0.4490632
C	-3.0137705	3.3252231	0.0347075
C	-1.8294050	2.1961705	-3.4161517
H	-1.6147594	1.1580720	-3.1513036
H	-0.8663391	2.6871347	-3.5829572
H	-2.3745978	2.2128630	-4.3593316
C	2.7624915	3.5996902	-0.0724792
C	-2.6159723	3.1565316	1.4653890
H	-2.6517963	2.1021752	1.7580995
H	-3.2791500	3.7192173	2.1214801
H	-1.5898838	3.4891597	1.6375395
C	1.9541817	3.8356775	1.1656056
H	2.5117662	4.4441865	1.8768854
H	1.6875437	2.8900562	1.6436197
H	1.0176979	4.3574695	0.9485024
C	2.7349181	1.3050978	-3.1197623
H	1.7204492	1.4771587	-3.4862733
H	2.7283717	0.3186056	-2.6448079
H	3.4126434	1.2725984	-3.9721211
Au	1.3712826	-0.0630338	-0.0841562
N	1.1340068	-1.9526147	0.6472124
C	-0.0564105	-2.4467097	0.9115503
H	-0.0799484	-3.4704892	1.2932830
C	-3.9203240	-4.3262172	0.3067420
H	-4.2543456	-5.0857600	-0.3873387
N	-1.2219298	-1.8524686	0.7704082
C	4.4772555	-4.2043393	1.6389980
C	3.7444160	-3.6194420	2.6526996
H	4.0633345	-3.7465167	3.6785471
C	-4.6679344	-4.0684072	1.4386746
C	-4.3052526	-3.1003334	2.3558135

H	-4.9249891	-2.9368091	3.2271810
C	-2.3849795	-2.6238033	1.0047816
C	-3.1524987	-2.3605247	2.1475538
C	2.2614506	-2.7361745	0.9905210
C	2.6206826	-2.8699602	2.3384082
C	4.1326846	-4.0671260	0.3077231
H	4.7396979	-4.5455798	-0.4490632
C	3.0137705	-3.3252231	-0.0347075
C	1.8294050	-2.1961705	3.4161517
H	1.6147594	-1.1580720	3.1513036
H	0.8663391	-2.6871347	3.5829572
H	2.3745978	-2.2128630	4.3593316
C	-2.7624915	-3.5996902	0.0724792
C	2.6159723	-3.1565316	-1.4653890
H	2.6517963	-2.1021752	-1.7580995
H	3.2791500	-3.7192173	-2.1214801
H	1.5898838	-3.4891597	-1.6375395
C	-1.9541817	-3.8356775	-1.1656056
H	-2.5117662	-4.4441865	-1.8768854
H	-1.6875437	-2.8900562	-1.6436197
H	-1.0176979	-4.3574695	-0.9485024
C	-2.7349181	-1.3050978	3.1197623
H	-1.7204492	-1.4771587	3.4862733
H	-2.7283717	-0.3186056	2.6448079
H	-3.4126434	-1.2725984	3.9721211
N	-5.6624149	4.9917378	-1.9861790
O	-5.9425968	5.0949276	-3.1612154
O	-6.2893938	5.4917333	-1.0769487
N	5.8890387	4.8426905	-1.6717544
O	6.1858547	5.6827377	-0.8495048
O	6.5269777	4.5956948	-2.6726722
N	5.6624149	-4.9917378	1.9861790
O	5.9425968	-5.0949276	3.1612154

O	6.2893938	-5.4917333	1.0769487
N	-5.8890387	-4.8426905	1.6717544
O	-6.1858547	-5.6827377	0.8495048
O	-6.5269777	-4.5956948	2.6726722

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