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Coinage metal amido and thiolate SNS complexes: Consequences of catalyst speciation in Cu(I)-catalysed carbonyl hydroboration†

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I. Experimental

General considerations: All experiments were carried out under dinitrogen, using an MBraun glovebox unless otherwise stated. Diethyl ether, toluene and THF were dried on columns of activated alumina using a J. C. Meyer (formerly Glass Contour) solvent purification system. Anhydrous C_6D_6 was dried with activated alumina (ca. 10 wt %) overnight, followed by filtration. $CDCl_3$ was stored over activated 4 Å molecular sieves (heated at 250 °C for 24 h under vacuum). Anhydrous ethanol was purchased from Aldrich and used as obtained. Other chemicals were used as obtained commercially: CuCl(IPr), AgCl(IPr) and AuCl(IPr) (Sigma Aldrich), triethoxysilane (Sigma Aldrich, 95%), pinacolborane (Sigma Aldrich, 97%), $Li[N(SiMe_3)_2]$ (Sigma Aldrich, 97%), and $Na[N(SiMe_3)_2]$ (Sigma Aldrich, 95%). ^1H, $^{13}C\{^1H\}$ and ^{11}B NMR spectra were recorded on a 300 MHz Bruker Avance or Avance II instrument at room temperature (21−25 °C). ^1H NMR spectra were referenced to solvent residual protons (C_6D_6, δ 7.15; $CDCl_3$, δ 7.26), ^{13}C to solvent resonances and ^{11}B to external $F_3B{\bullet}OEt_2$ at 0 ppm. Proligands **HL¹** and **HL²** were prepared according to literature procedures.[1-2] Mass spectra were recorded on an AB Sciex Q1MS mass spectrometer with electrospray ionization (ESI-MS) in positive mode (ion spray voltage, 5000.0 V; TEM, 400 °C; declustering potential, 11.00 V; focusing potential, 300.0 V) with samples prepared to ca. 0.05 mg/mL in acetonitrile or dichloromethane. For electron impact (EI), solid samples were prepared by drying products under vacuum, and spectra obtained using a Kratos Concept S1 instrument (Hres 7000−10000). X-ray diffraction data were collected on a Bruker Smart or Kappa diffractometer equipped with an ApexII CCD detector and a sealed-tube Mo K source (λ = 0.71073 Å).

Synthesis of Ag-1: A 42 mL glass vial was charged with AgCl(IPr) (200 mg, 0.376 mmol) and 5 mL of THF. To this solution was added dropwise a solution containing **HL¹** (103 mg, 0.376 mmol) and NaHMDS (69 mg, 0.376 mmol) in 5 mL of THF. The final solution turned colorless immediately and was stirred for 6 h. The solvent was then evaporated under vacuum and the product extracted with DCM (2 × 3 mL). The DCM was evaporated under vacuum and the resulting residue was washed with hexane (3 × 3 mL) and filtered, giving 255 mg of **Ag-1** as a white powder (88%). Crystals suitable for X-ray crystallography were grown by hexane layering of a concentrated DCM solution of **Ag-1** after 3 days. ^1H NMR (300 MHz, $CDCl_3$): δ 1.26, 1.32 (d, $^3J_{HH}$ = 7 Hz, 12H, $CH(CH_3)_2$); 2.38, 2.54 (s, 3H, SCH_3); 2.58 (sept, $^3J_{HH}$ = 7 Hz, 4H, $CHMe_2$); 4.48 (s, 2H, N-CH_2); 6.59 (dd, $^3J_{HH}$ = 8, $^4J_{HH}$ = 1 Hz, 1H, Ar–*H*); 6.69 (ddd, $^3J_{HH}$ = 7.5, 7.5, $^4J_{HH}$ = 1 Hz, 1H, Ar–*H*); 7.16 (ov mult, 2H, Ar–*H*); 7.24 (dd, $^3J_{HH}$ = 1.5 Hz, $^4J_{HH}$ = 1 Hz); 7.31 (s, 2H, Ar–*H*); 7.34 (ov mult, 5H, Ar–*H* and dipp Ar-*H*); 7.36 (d mult, $^3J_{HH}$ = 7.5 Hz, 1H, Ar-H), 7.45 (dd, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.5 Hz, 1H, Ar–*H*); 7.52 (d, 8 Hz, 1H, Ar-H), 7.54 (tr, $^3J_{HH}$ = 8 Hz, 2H, dipp Ar–*H*). $^{13}C\{^1H\}$ NMR ($CDCl_3$, 25 °C, 75 MHz): δ 16.0 (s, 1C, SCH_3); 18.4 (s, 1C, SCH_3); 24.0 (s, 4C, $CHCH_3$); 24.8 (s, 4C, $CHCH_3$); 28.8 (s, 4C, $CHCH_3$); 45.9 (s, 1C, NCH_2); 110.5 (s, 1C, Ar–C); 114.4 (s, 1C, Ar–C); 117.2 (s, 1C, Ar–C); 120.0 (s, 2C, H*C*=*C*H); 120.6 (s, 1C, ArC); 123.7 (s, 1C, ArC); 123.8 (s, 1C, ArC); 124.2 (s, 1C, ArC); 125.1 (s, 1C, ArC); 126.0 (s, 1C, ArC); 127.7 (s, 1C, ArC); 127.9 (s, 1C, Ar–C); 129.5 (s, 1C, Ar–C); 130.9 (s, 1C, Ar–C); 134.2 (s, 1C, Ar–C); 134.4 (s, 1C, Ar–C); 145.1 (s, 1C, Ar–C); 157.2 (s, 1C, Cu*C*). EI-MS $[M-H]^+$ 770.3221, Calc'd 770.2760 (Fig. S2).

Attempted Synthesis of Au-1: The reaction was conducted above using AuCl(IPr). After 3 days and reaction work-up as above, the ^1H NMR spectrum showed a significant amount of starting materials and several other products that were not further characterized (Fig. S12).

Synthesis of Ag-2: A 42 mL glass vial was charged with AgCl(IPr) (200 mg, 0.376 mmol) and 5 mL of THF. To this solution was added dropwise a solution containing HL^2 (97 mg, 0.376 mmol) and NaHMDS (69 mg, 0.376 mmol) in 5 mL of THF. The final solution turned orange and was stirred for 6 h. The solvent was then evaporated under vacuum and the residue was extracted with DCM (2 × 3 mL). The DCM was evaporated under vacuum and the resulting solid was washed with hexane (3 × 3 mL) and filtered, giving 266 mg of **Ag-2** as an orange powder (94%). Crystals suitable for X-ray crystallography were grown by hexane layering of a concentrated DCM solution of **Ag-2** after 1 day. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.26, 1.29 (d, $^3J_{HH}$ = 7 Hz, 12H, CH(CH_3)$_2$); 2.43 (s, 3H, SCH_3); 2.62 (sept, $^3J_{HH}$ = 7 Hz, 4H, CHMe$_2$); 6.69 (dd, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1 Hz, 1H, Ar–*H*); 6.85 (ddd, $^3J_{HH}$ = 7.5, 7.5, $^4J_{HH}$ = 1 Hz, 1H, Ar–*H*); 7.15 (ov mult, 2H, Ar–*H*); 7.28 (ov mult, 4H, Ar–*H*); 7.34 (d, $^3J_{HH}$ = 7.5 Hz, 4H, dipp Ar–*H*); 7.50 (dd, $^3J_{HH}$ = 7.5, 7.5 Hz, 1H, Ar–*H*); 7.56 (tr, $^3J_{HH}$ = 7.5 Hz, 2H, dipp Ar–*H*); 8.19 (dd, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.5 Hz, 1H, Ar–*H*); 8.73 (s, 1H, N=C*H*–). ^{13}C{^{1}H} NMR ($CDCl_3$, 25 °C, 75 MHz): δ 17.1 (s, 1C, S*C*H$_3$); 24.1 (s, 4C, CH*C*H$_3$); 24.8 (s, 4C, CH*C*H$_3$); 28.8 (s, 4C, CH–CH$_3$); 118.6 (s, 1C, Ar–C); 122.2 (s, 1C, Ar–C); 122.3 (s, 1C, Ar–C); 124.2 (s, 2C, HC=CH); 125.6 (s, 2C, Ar–C); 126.4 (s, 1C, Ar–C); 127.4 (s, 1C, Ar–C); 129.4 (s, 1C, Ar–C); 129.5 (s, 1C, Ar–C); 130.5 (s, 1C, Ar–C); 130.9 (s, 1C, Ar–C); 131.7 (s, 1C, Ar–C); 134.0 (s, 1C, Ar–C); 134.5 (s, 1C, Ar–C); 134.6 (s, 1C, Ar–C); 145.3 (s, 1C, Ar–C); 145.7 (s, 1C, Ar–C); 152.1 (s, 1C, Ar–C); 158.6 (s, 1C, Cu–C). EI-MS [M]$^+$H 754.2789, Calc'd 754.2427 (Figure S4).

Synthesis of Au-2: A 42 mL glass vial was charged with AuCl(IPr) (233 mg, 0.376 mmol) and 5 mL of THF. To this solution was added dropwise a solution containing HL^2 (97 mg, 0.376 mmol) and NaHMDS (69 mg, 0.376 mmol) in 5 mL of THF. The final solution turned yellow and was stirred for 6 h. The solvent was then evaporated under vacuum and the residue was extracted with DCM (2 × 3 mL). The DCM was evaporated under vacuum and the resulting solid was washed with hexane (3 × 3 mL) and filtered, giving 288 mg of **Au-2** as an orange powder (91%). Crystals suitable for X-ray crystallography were grown by hexane layering of a concentrated DCM solution of **Au-2** after 1 day. ^{1}H NMR (300 MHz, $CDCl_3$): δ 1.27, 1.38 (d, $^3J_{HH}$ = 7 Hz, 12H, CH(CH_3)$_2$); 2.44 (s, 3H, SCH_3); 2.66 (sept, $^3J_{HH}$ = 7 Hz, 4H, CHMe$_2$); 6.53 (ddd, $^3J_{HH}$ = 7.5, 7, $^4J_{HH}$ = 1.5 Hz, 1H, Ar–*H*); 6.70 (dd, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.5 Hz, 1H, Ar–*H*); 6.74 (dd, $^3J_{HH}$ = 8, $^4J_{HH}$ = 1.5 Hz, 1H, Ar–*H);* 6.80 (ddd, $^3J_{HH}$ = 7.5, 7, $^4J_{HH}$ = 1.5 Hz, 1H, Ar–*H*); 7.20 (ov mult, 1H, Ar-*H*); 7.24 (s, 2H, dipp =C–*H*); 7.32 (ov mult, 2H, Ar–*H*); 7.36 (d, $^3J_{HH}$ = 8 Hz, 4H, dipp Ar–*H*); 7.59 (tr, $^3J_{HH}$ = 8 Hz, 2H, dipp Ar–*H*); 8.22 (dd, $^3J_{HH}$ = 7.5, $^4J_{HH}$ = 1.5 Hz, 1H, Ar–*H*); 8.74 (s, 1H, N=C*H*–). ^{13}C{1H} NMR ($CDCl_3$, 25 °C, 300 MHz): δ 17.1 (s, 1C, S–CH$_3$); 24.1 (s, 4C, CH–CH$_3$); 24.8 (s, 4C, CH–CH$_3$); 28.8 (s, 4C, CH–CH$_3$); 118.6 (s, 1C, Ar–C); 122.2 (s, 1C, Ar–C); 122.3 (s, 1C, Ar–C); 124.2 (s, 2C, HC=CH); 125.6 (s, 2C, Ar–C); 126.4 (s, 1C, Ar–C); 127.4 (s, 1C, Ar–C); 129.4 (s, 1C, Ar–C); 129.5 (s, 1C, Ar–C); 130.5 (s, 1C, Ar–C); 130.9 (s, 1C, Ar–C); 131.7 (s, 1C, Ar–C); 134.0 (s, 1C, Ar–C); 134.5 (s, 1C, Ar–C); 134.6 (s, 1C, Ar–C); 145.3 (s, 1C, Ar–C); 145.7 (s, 1C, Ar–C); 152.1 (s, 1C, Ar–C); 158.6 (s, 1C, Cu–C). EI-MS [M]$^+$H 844.3014, Calc'd 844.3033 and [M]$^+$Na 866.2825, Calc'd 866.2853 (Figure S6).

II. Spectroscopic Data

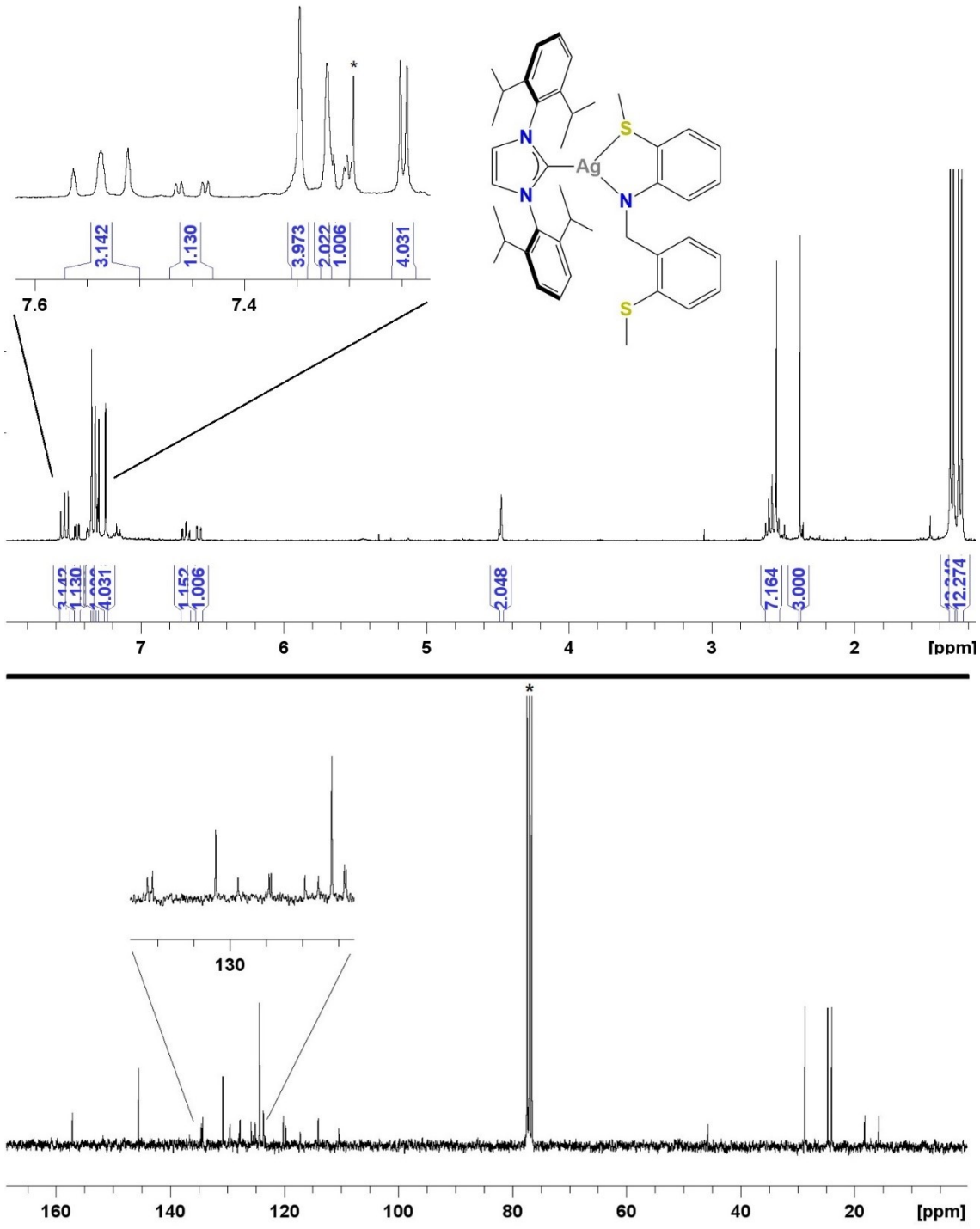

Figure S1. ^{1}H (300 MHz, $CDCl_3$ - top) and $^{13}C\{^{1}H\}$ (75 MHz, $CDCl_3$ - bottom) NMR spectra of **Ag-1**.
* indicates protic impurity in and carbon resonance of $CDCl_3$.

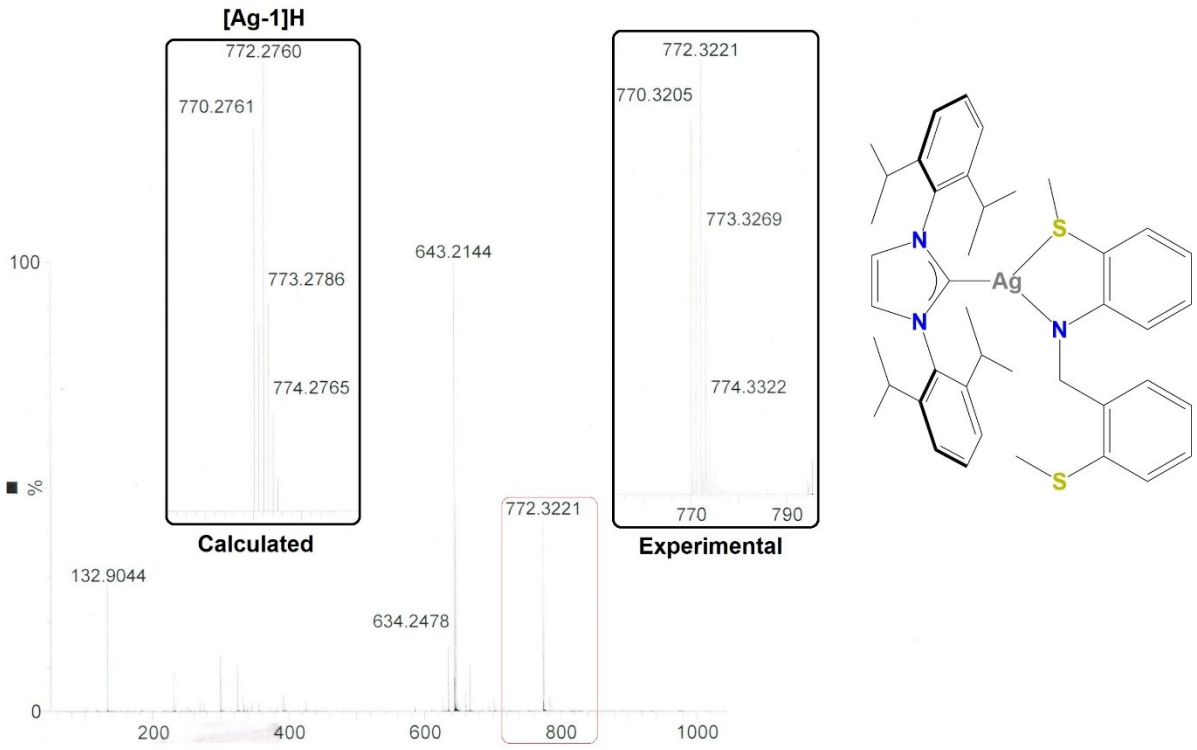

Figure S2. ESI-MS spectrum of [**Ag-1** + H]$^+$.

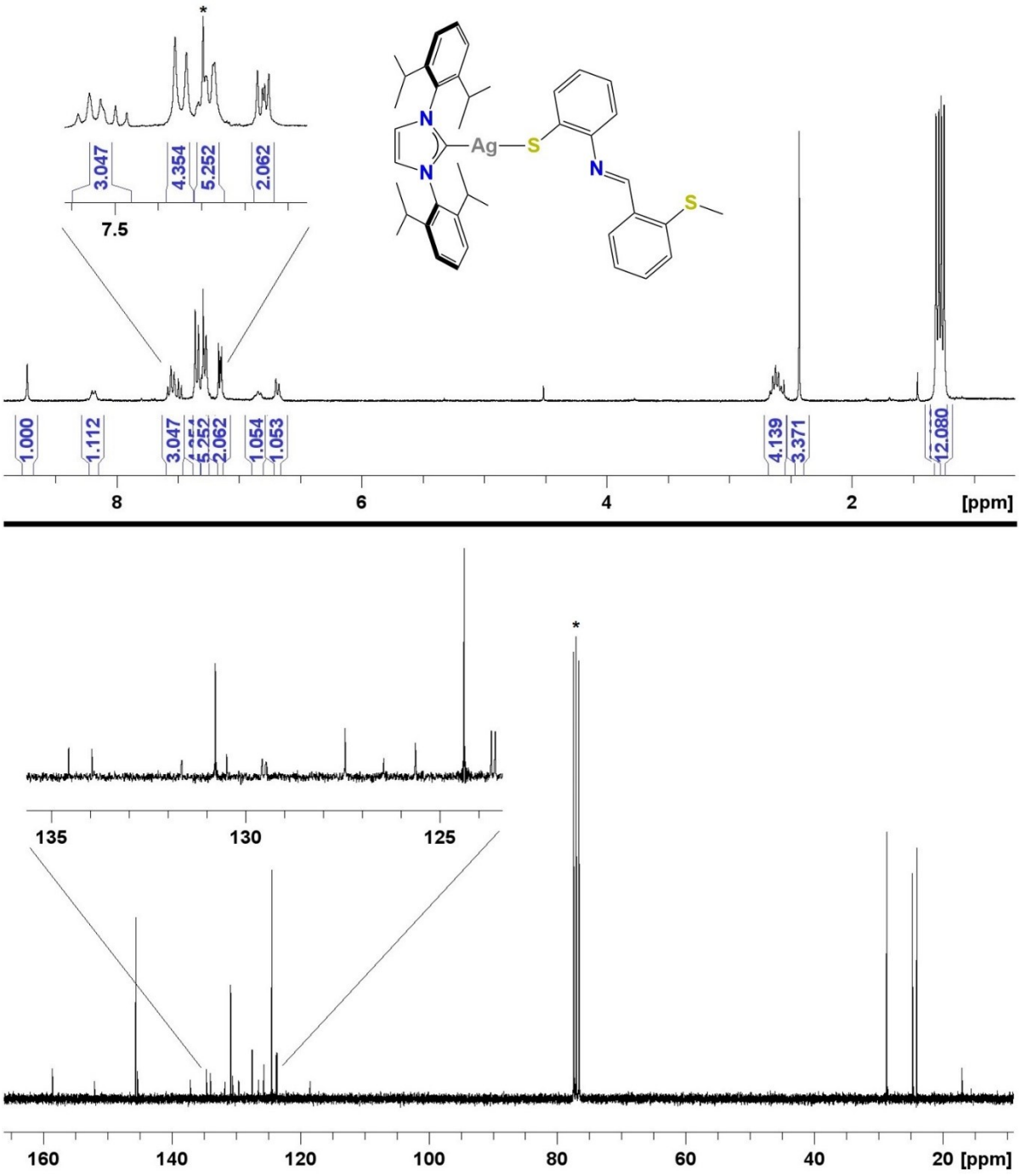

Figure S3. ^{1}H (300 MHz, $CDCl_3$ - top) and $^{13}C\{^{1}H\}$ (75 MHz, $CDCl_3$ - bottom) NMR spectra of **Ag-2**.
* indicates protic impurity in and carbon resonance of $CDCl_3$.

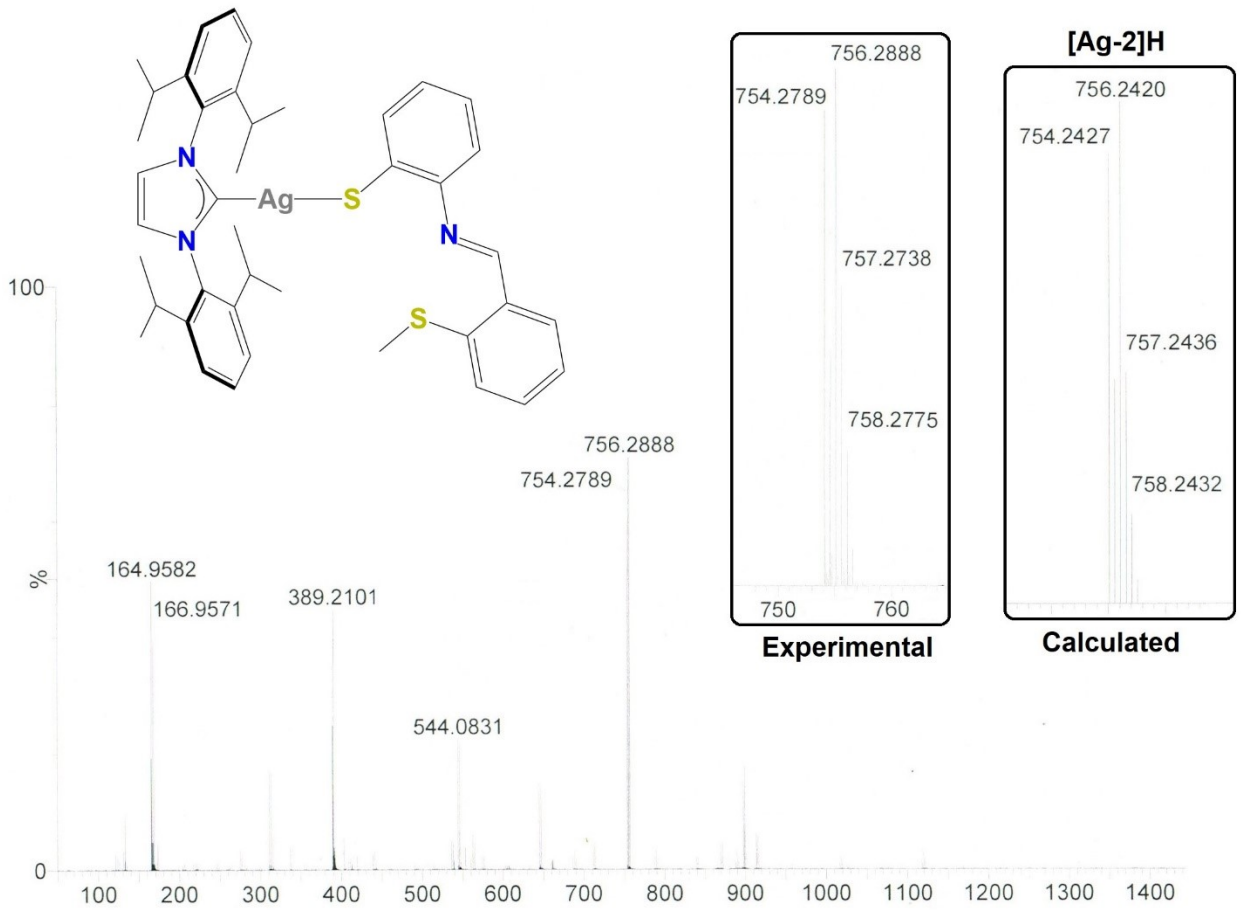

Figure S4. ESI-MS spectrum of [**Ag-2** + H]$^+$.

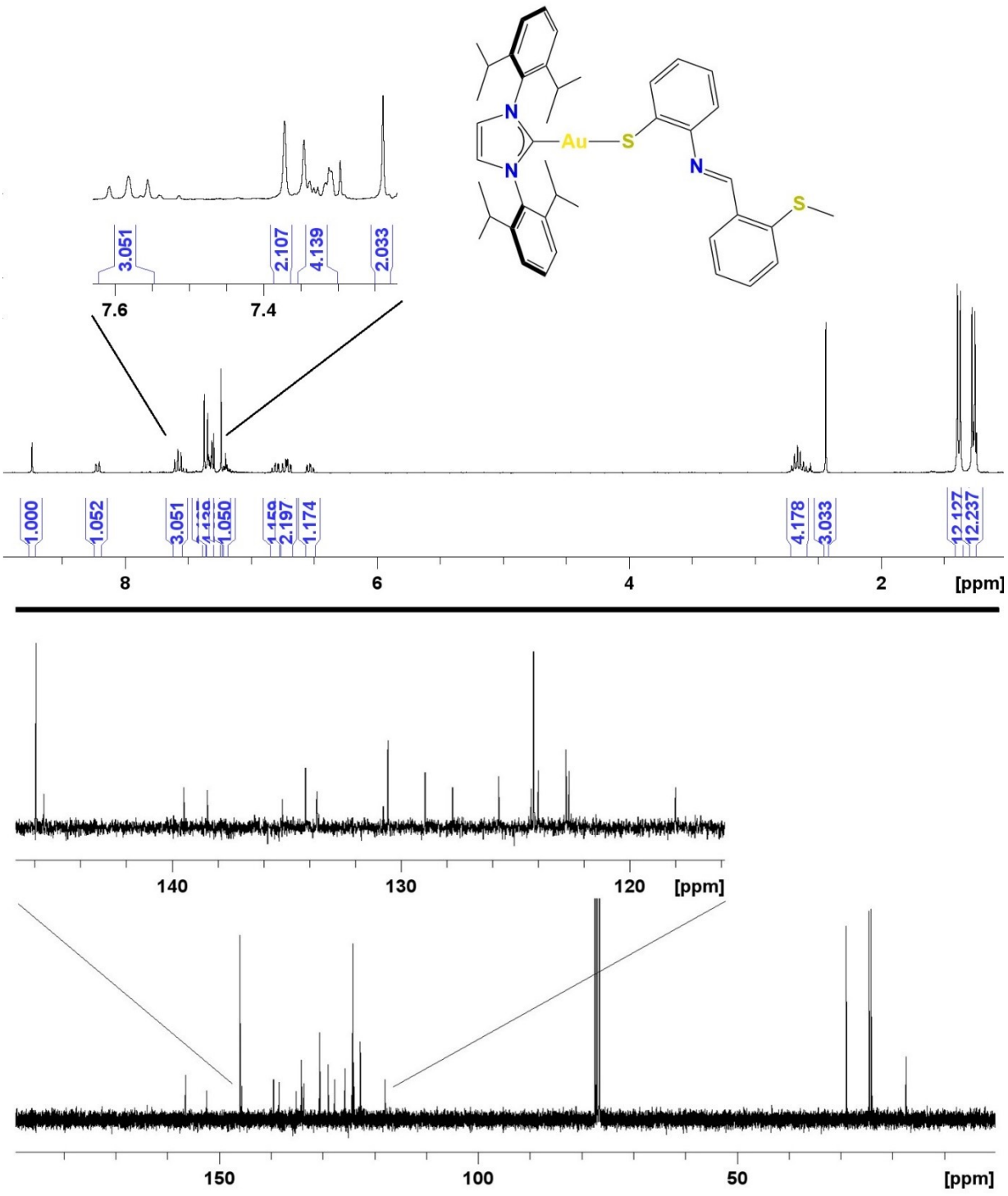

Figure S5. ^{1}H (300 MHz, $CDCl_3$ - top) and $^{13}C\{^{1}H\}$ (75 MHz, $CDCl_3$ - bottom) NMR spectra of **Au-2**.
* indicates protic impurity in and carbon resonance of $CDCl_3$.

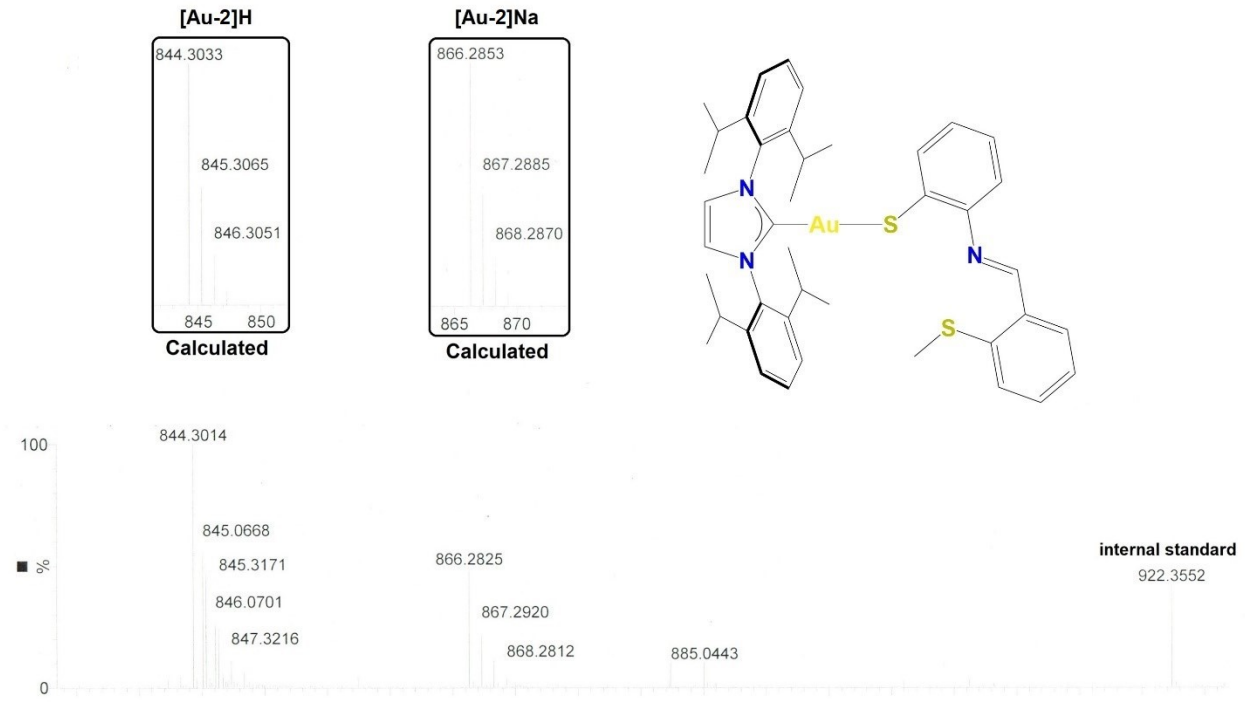

Figure S6. ESI-MS spectrum of [**Au-2** + H]$^+$ and [**Au-2** + Na]$^+$

III. Mechanistic Studies

Stoichiometric Reaction of Cu-1 with HBpin: A pale-yellow solution of **Cu-1** (0.01 g, 0.014 mmol) in C_6D_6 was charged with pinacolborane (0.002 g, 2 µl, 0.014 mmol), resulting in an immediate color change to deep yellow. The crude ^{1}H NMR spectrum showed complete conversion of **Cu-1** to $[CuH(IPr)]_2$ and N-borylated **L^1** (Fig. S7).

Stoichiometric Reaction of Ag-1 with HBpin: A colorless solution of **Ag-1** (0.01 g, 0.014 mmol) in C_6D_6 was charged with pinacolborane (0.002 g, 2 µl, 0.014 mmol), resulting in an immediate colour change to black which then became a colourless solution with insoluble black precipitate. The crude ^{1}H NMR spectrum showed complete conversion of **Ag-1** into N-borylated **L^1** and presumably silver metal (Fig. S8).

Stoichiometric Reaction of Ag-2 with HBpin: An orange solution of **Ag-2** (0.01 g, 0.014 mmol) in C_6D_6 was charged with pinacolborane (0.002 g, 2 µl, 0.014 mmol), resulting in an a slow colour change to deep brown. The crude ^{1}H and ^{11}B NMR spectra showed complete conversion of **Ag-2** into a mixture of products that were not characterized further (Figs. S9,S10).

Stoichiometric Reaction of Au-2 with HBpin: An orange solution of **Au-2** (0.011 g, 0.014 mmol) in C_6D_6 was charged with pinacolborane (0.002 g, 2 µl, 0.014 mmol), resulting in no colour change. The crude ^{1}H NMR spectrum showed no reaction (Fig. S11).

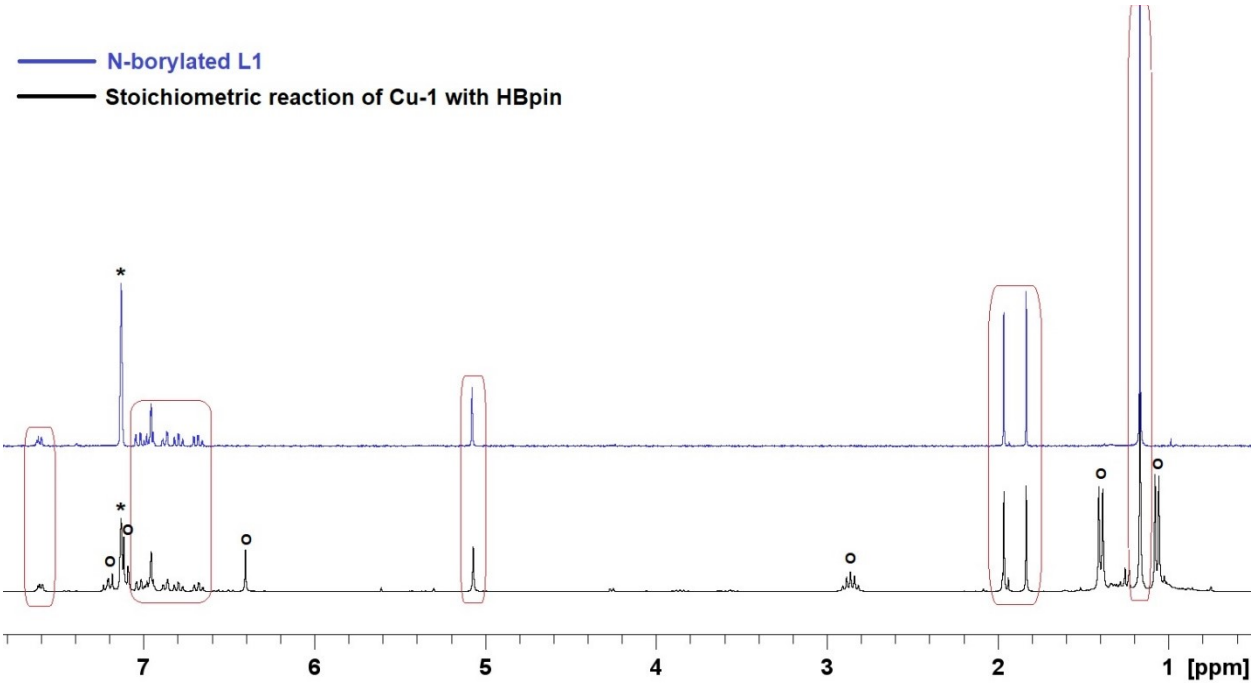

Figure S7. Stacked plot of ^{1}H NMR spectra of N-borylated **L^{1}** and reaction mixture of stoichiometric reaction of **Cu-1** with HBpin in C_6D_6. **o** indicates $[CuH(IPr)]_2$, and * indicates protic impurity in C_6D_6.

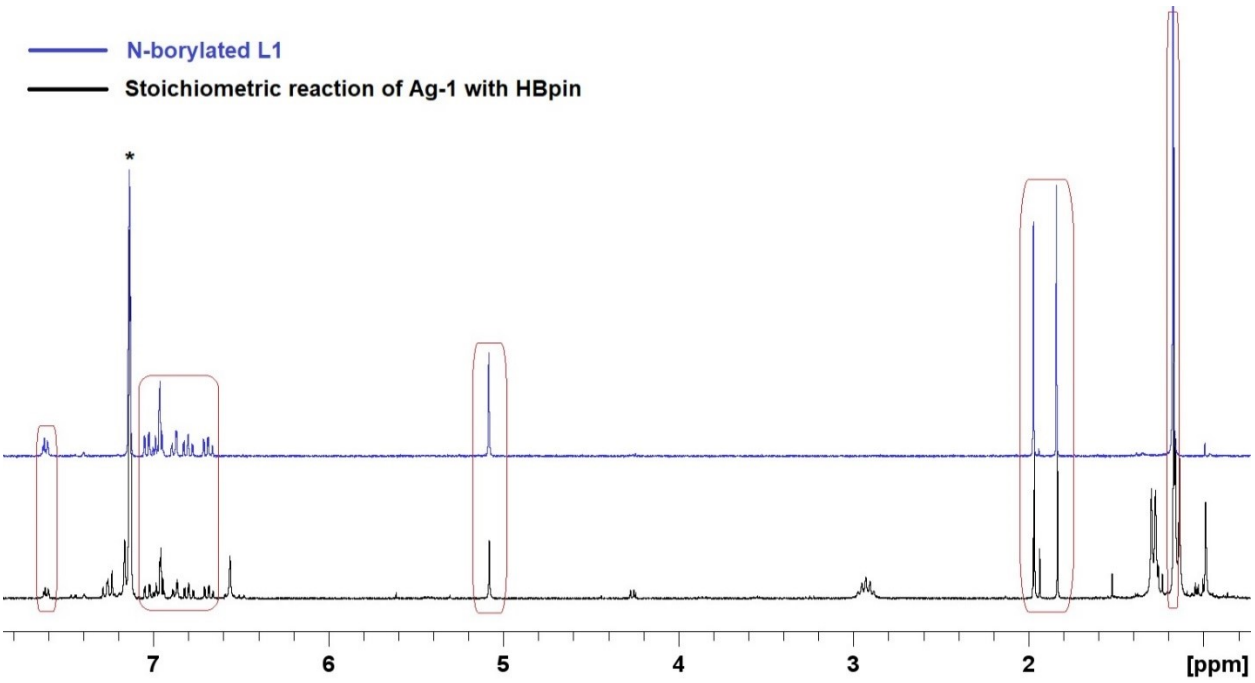

Figure S8. Stacked plot of ^{1}H NMR spectra of N-borylated **L^{1}** and reaction mixture of stoichiometric reaction of **Ag-1** with HBpin in C_6D_6. * indicates protic impurity in C_6D_6.

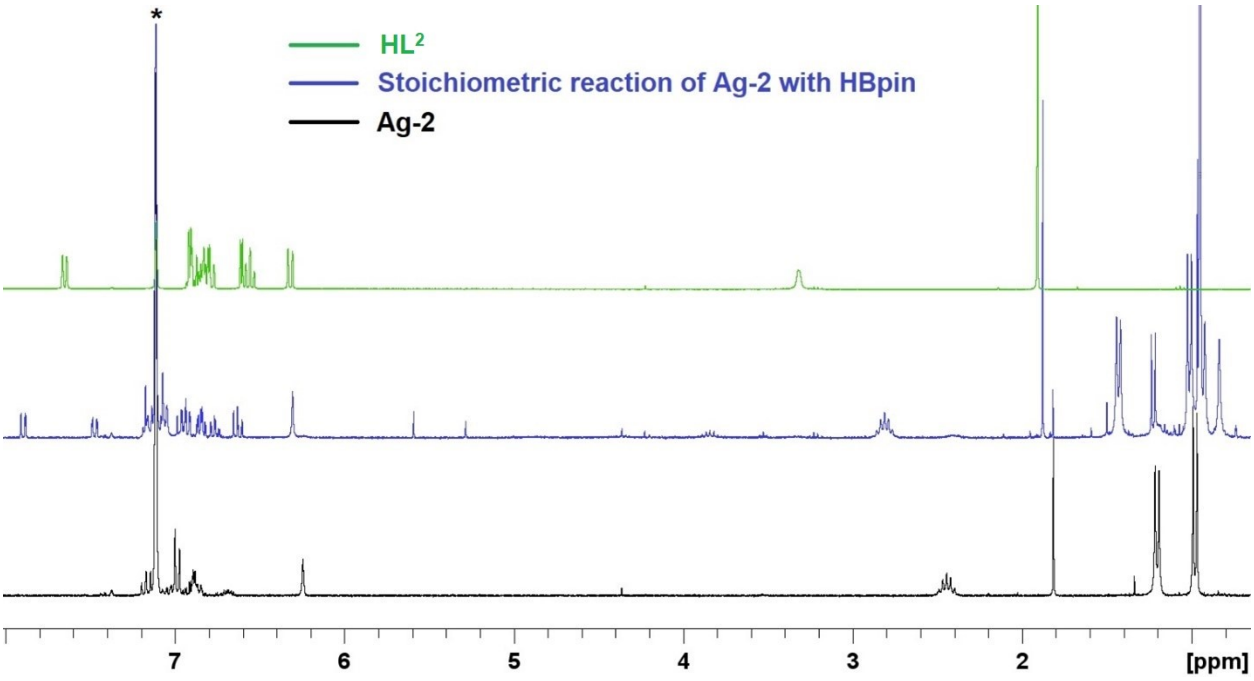

Figure S9. Stacked plot of ^{1}H NMR spectra of H**L²**, **Ag-2** and reaction mixture of stoichiometric reaction of **Ag-2** with HBpin in C_6D_6. * indicates protic impurity in C_6D_6.

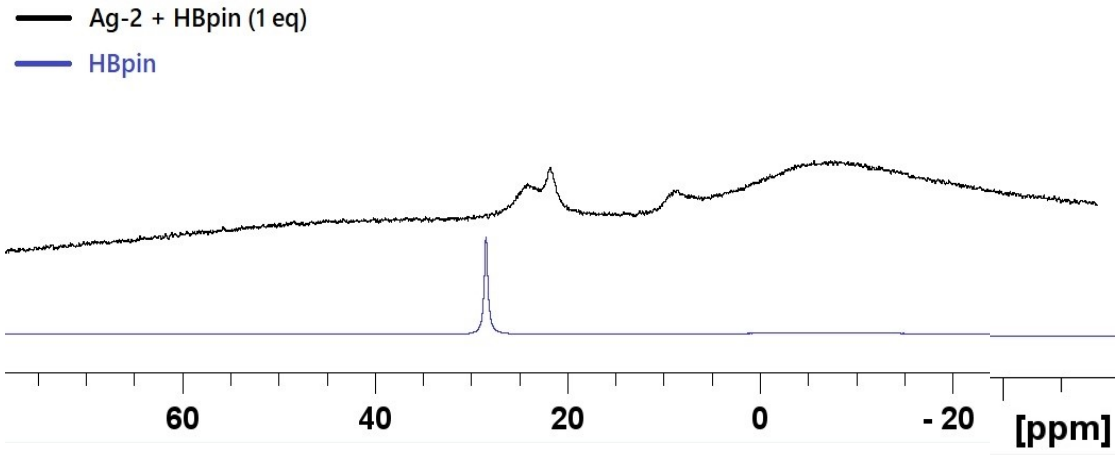

Figure S10. Stacked plot of ^{1}B NMR spectra of HBpin and reaction mixture of stoichiometric reaction of **Ag-2** with HBpin in C_6D_6.

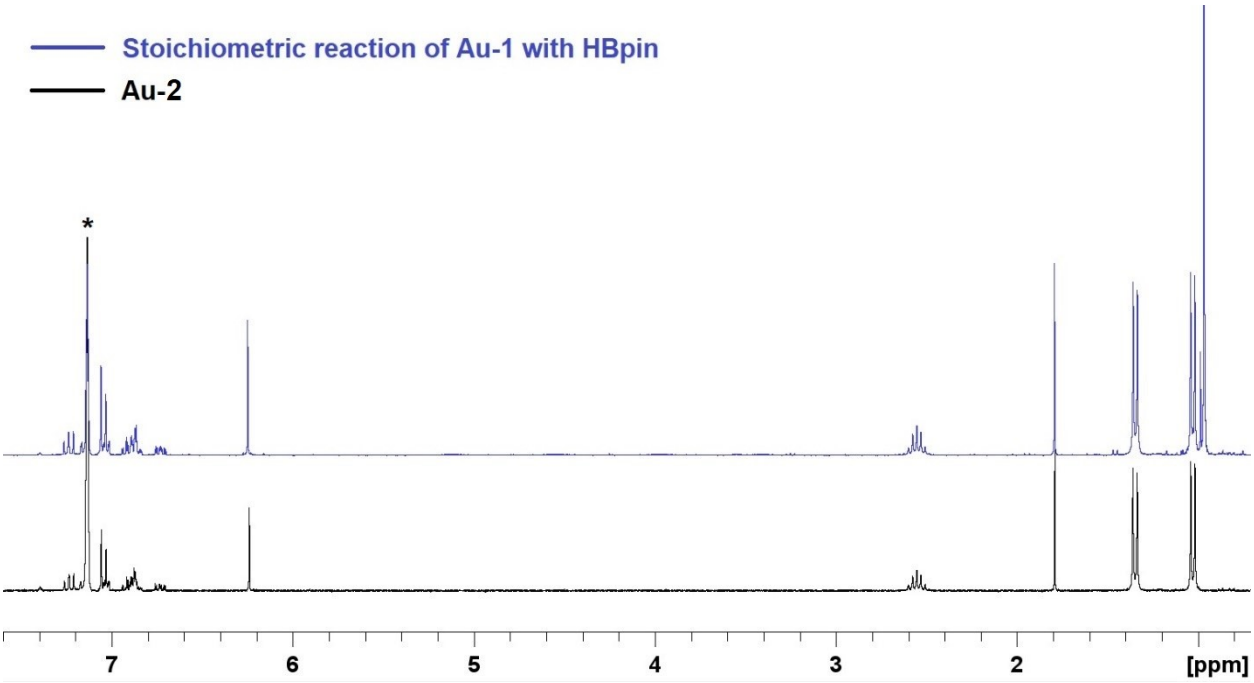

Figure S11. Stacked plot of ^{1}H NMR spectra of **Au-2** and reaction mixture of stoichiometric reaction of **Au-2** with HBpin in C_6D_6. * indicates protic impurity in C_6D_6.

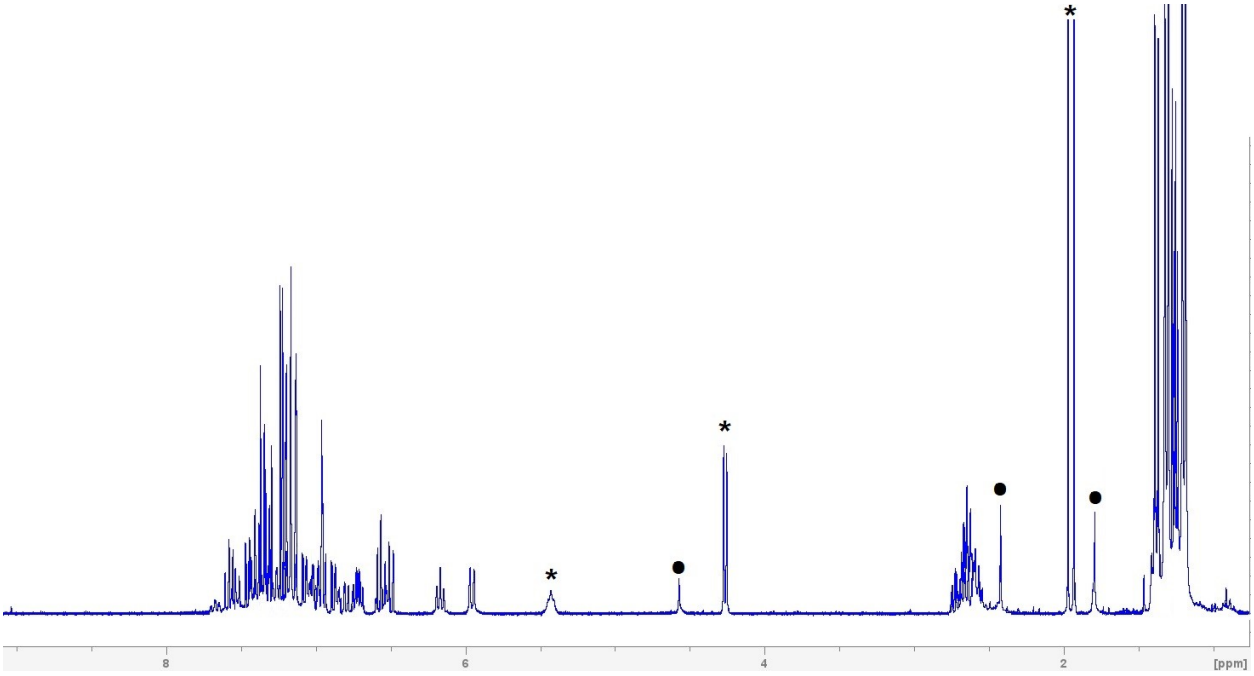

Figure S12. ^{1}H NMR spectrum (300 MHz) of reaction mixture of AuCl(IPr), H**L**^{1} and Na[N(SiMe$_3$)$_2$] in C_6D_6. * indicates free H**L**^{1} and • indicates possible **Au-1**.

V. Crystallographic Details

Crystallographic data for all compounds were collected from a single crystal mounted on a MiTeGen dual thickness MicroMount using Parabar oil. Data were collected on Bruker Smart (**Au-2**) or Kappa (**Ag-1** and **Ag-2**) ApexII single crystal diffractometers equipped with a graphite monochromator. The instrument was equipped with a sealed tube Mo Kα source ($\lambda =$ 0.71073 Å), an ApexII CCD detector and a dry compressed air-cooling system operating at 200 (**Ag-1** and **Ag-2**) and 208 K (**Au-2**). Raw data collection and processing were performed with the Apex3 software package from Bruker.[3] Initial unit cell parameters were determined from 36 data frames from select ω scans. Semi-empirical absorption corrections based on equivalent reflections were applied.[4] Systematic absences in the diffraction data-set and unit-cell parameters were consistent with the assigned space group. The initial structural solutions were determined using ShelxT direct methods,[5] and refined with full-matrix least-squares procedures based on F^2 using ShelXL or ShelXle.[6] Hydrogen atoms were placed geometrically and refined using a riding model. Additional crystallographic information is given in Table S1. For **Ag-1**, one co-crystallized molecule of dichloromethane was found disordered and close to a crystallographic inversion center (ratio 0.57:0.43 for part -1/part -2), accounting for 0.5 DCM per asymmetric unit (i.e., per Ag complex). Deposition Numbers: 2201238-2201240.

Table S1: X-ray crystallographic data collection and refinement details.

	Ag-1	**Ag-2**	**Au-2**
empirical formula	$C_{42.50}H_{53}AgClN_3S_2$	$C_{41}H_{48}AgN_3S_2$	$C_{41}H_{48}AuN_3S_2$
formula weight ($g \cdot mol^{-1}$)	813.32	754.81	843.91
crystal system	monoclininc	monoclininc	monoclininc
space group	$P\ 2_1/c$	$P\ 2_1/c$	$P\ 2_1/c$
a (A)	16.9305(4)	11.7400(3)	11.7500(2)
b (A)	12.5740(3)	9.7942(5)	19.7459(3)
c (A)	19.3854(5)	16.5946(4)	16.6374(3)
α (deg)	90	90	90
β (deg)	98.8880(10)	100.436(1)	100.484(1)
γ (deg)	90	90	90
V (A^3)	4077.29(17)	3792.53(16)	3795.67(11)
Z	4	4	4
T (K)	200.05	200	208
p_{calcd}($g \cdot cm^{-3}$)	1.325	1.322	1.477
μ(mm^{-1})	0.695	0.673	4.018
$2\theta_{max}$ (deg)	62.096	50.054	50.048
total/unique reflections	31548/11390	23875/6682	23366/6690
Reflections [$I_o \geq 2\sigma(I_o)$]	8604	5634	5675
R_1, wR_2 [$I_o \geq 2\sigma(I_o)$]	0.0328, 0.0813	0.0264, 0.0585	0.0213, 0.0400
goodness of fit	1.013	1.026	1.021
CCDC number	2201240	2201238	2201239

Table S2. Bond lengths for **Ag-1**.

Atom 1	Atom 2	**Length (Å)**
Ag1	S1	2.8031(7)
Ag1	N1	2.104(2)
Ag1	C1	2.069(2)
S1	C2	1.788(4)
S1	C3	1.770(2)
S2	C15	1.767(2)
S2	C16	1.784(3)
N1	C4	1.347(2)
N1	C9	1.450(2)
N2	C1	1.353(2)
N2	C18	1.384(2)
N2	C31	1.445(2)
N3	C1	1.352(2)
N3	C17	1.392(3)
N3	C19	1.443(2)
C2	H2A	0.979
C2	H2B	0.98
C2	H2C	0.981
C3	C4	1.427(3)
C3	C8	1.389(3)
C4	C5	1.425(3)
C5	H5	0.95
C5	C6	1.379(3)
C6	H6	0.95
C6	C7	1.378(4)
C7	H7	0.95
C7	C8	1.380(4)
C8	H8	0.95
C9	H9A	0.99
C9	H9B	0.99
C9	C10	1.520(3)
C10	C11	1.374(3)
C10	C15	1.404(3)
C11	H11	0.95
C11	C12	1.386(3)
C12	H12	0.95
C12	C13	1.372(4)
C13	H13	0.95
C13	C14	1.381(3)
C14	H14	0.95
C14	C15	1.392(3)
C16	H16A	0.98

C16	H16B	0.98
C16	H16C	0.98
C17	H17	0.95
C17	C18	1.343(3)
C18	H18	0.95
C19	C20	1.391(3)
C19	C24	1.399(3)
C20	C21	1.397(3)
C20	C28	1.513(3)
C21	H21	0.95
C21	C22	1.377(4)
C22	H22	0.95
C22	C23	1.366(4)
C23	H23	0.95
C23	C24	1.395(3)
C24	C26	1.511(3)
C25	H25A	0.98
C25	H25B	0.98
C25	H25C	0.98
C25	C26	1.525(3)
C26	H26	1
C26	C27	1.526(4)
C27	H27A	0.98
C27	H27B	0.98
C27	H27C	0.98
C28	H28	1
C28	C29	1.524(4)
C28	C30	1.527(3)
C29	H29A	0.98
C29	H29B	0.98
C29	H29C	0.98
C30	H30A	0.98
C30	H30B	0.98
C30	H30C	0.98
C31	C32	1.393(3)
C31	C36	1.398(3)
C32	C33	1.390(3)
C32	C37	1.514(3)
C33	H33	0.95
C33	C34	1.376(3)
C34	H34	0.95
C34	C35	1.368(4)
C35	H35	0.95
C35	C36	1.392(3)
C36	C40	1.514(3)

C37	H37	1
C37	C38	1.531(3)
C37	C39	1.524(3)
C38	H38A	0.98
C38	H38B	0.98
C38	H38C	0.98
C39	H39A	0.98
C39	H39B	0.98
C39	H39C	0.98
C40	H40	1
C40	C41	1.529(5)
C40	C42	1.525(4)
C41	H41A	0.98
C41	H41B	0.98
C41	H41C	0.98
C42	H42A	0.98
C42	H42B	0.98
C42	H42C	0.98
Cl1B	C43B	1.78(2)
Cl1B	C43B	1.58(2)
Cl2B	C43B	1.77(2)
Cl2B	C43B	1.49(3)
C43B	H43A	0.99
C43B	H43B	0.99
C43B	Cl1B	1.58(2)
C43B	Cl2B	1.49(3)
C43B	C43B	1.61(2)
Cl1B	C43B	1.78(2)
Cl2B	C43B	1.77(2)
C43B	H43A	0.99
C43B	H43B	0.99

Table S3. Bond angles for **Ag-1.**

Atom1	**Atom2**	**Atom3**	**Angle**
S1	Ag1	N1	75.86(5)
S1	Ag1	C1	126.08(5)
N1	Ag1	C1	158.05(7)
Ag1	S1	C2	94.3(1)
Ag1	S1	C3	93.80(7)
C2	S1	C3	102.0(1)
C15	S2	C16	104.1(1)
Ag1	N1	C4	127.6(1)
Ag1	N1	C9	115.0(1)

C4	N1	C9	117.4(2)
C1	N2	C18	111.6(1)
C1	N2	C31	122.0(1)
C18	N2	C31	126.4(1)
C1	N3	C17	111.1(2)
C1	N3	C19	123.8(2)
C17	N3	C19	125.1(2)
Ag1	C1	N2	124.5(1)
Ag1	C1	N3	131.3(1)
N2	C1	N3	104.2(1)
S1	C2	H2A	109.5
S1	C2	H2B	109.5
S1	C2	H2C	109.4
H2A	C2	H2B	109.5
H2A	C2	H2C	109.5
H2B	C2	H2C	109.4
S1	C3	C4	120.7(2)
S1	C3	C8	117.9(2)
C4	C3	C8	121.4(2)
N1	C4	C3	121.8(2)
N1	C4	C5	123.5(2)
C3	C4	C5	114.7(2)
C4	C5	H5	118.8
C4	C5	C6	122.4(2)
H5	C5	C6	118.8
C5	C6	H6	119.4
C5	C6	C7	121.2(2)
H6	C6	C7	119.4
C6	C7	H7	120.8
C6	C7	C8	118.5(2)
H7	C7	C8	120.8
C3	C8	C7	121.6(2)
C3	C8	H8	119.2
C7	C8	H8	119.2
N1	C9	H9A	108.3
N1	C9	H9B	108.4
N1	C9	C10	115.7(2)
H9A	C9	H9B	107.4
H9A	C9	C10	108.3
H9B	C9	C10	108.4
C9	C10	C11	121.7(2)
C9	C10	C15	119.4(2)
C11	C10	C15	118.9(2)
C10	C11	H11	119.4
C10	C11	C12	121.2(2)

H11	C11	C12	119.4
C11	C12	H12	120.2
C11	C12	C13	119.6(2)
H12	C12	C13	120.2
C12	C13	H13	119.7
C12	C13	C14	120.6(2)
H13	C13	C14	119.7
C13	C14	H14	120.1
C13	C14	C15	119.9(2)
H14	C14	C15	120.1
S2	C15	C10	116.8(1)
S2	C15	C14	123.5(2)
C10	C15	C14	119.8(2)
S2	C16	H16A	109.5
S2	C16	H16B	109.5
S2	C16	H16C	109.5
H16A	C16	H16B	109.5
H16A	C16	H16C	109.5
H16B	C16	H16C	109.5
N3	C17	H17	126.7
N3	C17	C18	106.7(2)
H17	C17	C18	126.7
N2	C18	C17	106.5(2)
N2	C18	H18	126.8
C17	C18	H18	126.8
N3	C19	C20	118.7(2)
N3	C19	C24	118.3(2)
C20	C19	C24	123.0(2)
C19	C20	C21	117.2(2)
C19	C20	C28	123.0(2)
C21	C20	C28	119.7(2)
C20	C21	H21	119.5
C20	C21	C22	120.9(2)
H21	C21	C22	119.6
C21	C22	H22	119.8
C21	C22	C23	120.5(2)
H22	C22	C23	119.8
C22	C23	H23	119.3
C22	C23	C24	121.5(2)
H23	C23	C24	119.2
C19	C24	C23	116.8(2)
C19	C24	C26	121.8(2)
C23	C24	C26	121.3(2)
H25A	C25	H25B	109.5
H25A	C25	H25C	109.4

H25A	C25	C26	109.5
H25B	C25	H25C	109.5
H25B	C25	C26	109.5
H25C	C25	C26	109.5
C24	C26	C25	113.6(2)
C24	C26	H26	107.6
C24	C26	C27	110.3(2)
C25	C26	H26	107.6
C25	C26	C27	110.0(2)
H26	C26	C27	107.6
C26	C27	H27A	109.4
C26	C27	H27B	109.5
C26	C27	H27C	109.5
H27A	C27	H27B	109.5
H27A	C27	H27C	109.4
H27B	C27	H27C	109.5
C20	C28	H28	107.6
C20	C28	C29	111.6(2)
C20	C28	C30	111.1(2)
H28	C28	C29	107.6
H28	C28	C30	107.6
C29	C28	C30	111.2(2)
C28	C29	H29A	109.5
C28	C29	H29B	109.5
C28	C29	H29C	109.5
H29A	C29	H29B	109.5
H29A	C29	H29C	109.5
H29B	C29	H29C	109.5
C28	C30	H30A	109.5
C28	C30	H30B	109.5
C28	C30	H30C	109.5
H30A	C30	H30B	109.5
H30A	C30	H30C	109.5
H30B	C30	H30C	109.5
N2	C31	C32	118.7(2)
N2	C31	C36	118.3(2)
C32	C31	C36	122.9(2)
C31	C32	C33	117.2(2)
C31	C32	C37	122.3(2)
C33	C32	C37	120.5(2)
C32	C33	H33	119.5
C32	C33	C34	121.0(2)
H33	C33	C34	119.5
C33	C34	H34	119.8
C33	C34	C35	120.5(2)

H34	C34	C35	119.8
C34	C35	H35	119.3
C34	C35	C36	121.3(2)
H35	C35	C36	119.3
C31	C36	C35	117.0(2)
C31	C36	C40	122.9(2)
C35	C36	C40	120.1(2)
C32	C37	H37	107.7
C32	C37	C38	110.8(2)
C32	C37	C39	113.2(2)
H37	C37	C38	107.7
H37	C37	C39	107.7
C38	C37	C39	109.5(2)
C37	C38	H38A	109.5
C37	C38	H38B	109.5
C37	C38	H38C	109.5
H38A	C38	H38B	109.5
H38A	C38	H38C	109.5
H38B	C38	H38C	109.5
C37	C39	H39A	109.5
C37	C39	H39B	109.5
C37	C39	H39C	109.5
H39A	C39	H39B	109.5
H39A	C39	H39C	109.5
H39B	C39	H39C	109.5
C36	C40	H40	107.9
C36	C40	C41	111.4(2)
C36	C40	C42	111.0(2)
H40	C40	C41	107.9
H40	C40	C42	107.9
C41	C40	C42	110.5(2)
C40	C41	H41A	109.4
C40	C41	H41B	109.5
C40	C41	H41C	109.5
H41A	C41	H41B	109.5
H41A	C41	H41C	109.5
H41B	C41	H41C	109.5
C40	C42	H42A	109.5
C40	C42	H42B	109.5
C40	C42	H42C	109.5
H42A	C42	H42B	109.5
H42A	C42	H42C	109.5
H42B	C42	H42C	109.5
C43B	Cl1B	C43B	57.1(9)
C43B	Cl2B	C43B	59(1)

Cl1B	C43B	Cl2B	107(1)
Cl1B	C43B	H43A	110
Cl1B	C43B	H43B	110
Cl1B	C43B	Cl1B	123(1)
Cl1B	C43B	Cl2B	14.6(9)
Cl1B	C43B	C43B	55.1(9)
Cl2B	C43B	H43A	110
Cl2B	C43B	H43B	110
Cl2B	C43B	Cl1B	16.1(8)
Cl2B	C43B	Cl2B	121(1)
Cl2B	C43B	C43B	52(1)
H43A	C43B	H43B	109
H43A	C43B	Cl1B	103
H43A	C43B	Cl2B	104
H43A	C43B	C43B	127
H43B	C43B	Cl1B	100
H43B	C43B	Cl2B	101
H43B	C43B	C43B	124
Cl1B	C43B	Cl2B	137(1)
Cl1B	C43B	C43B	68(1)
Cl2B	C43B	C43B	70(1)
C43B	Cl1B	C43B	57.1(9)
C43B	Cl2B	C43B	59(1)
Cl1B	C43B	Cl2B	137(1)
Cl1B	C43B	C43B	68(1)
Cl1B	C43B	Cl1B	123(1)
Cl1B	C43B	Cl2B	16.1(8)
Cl1B	C43B	H43A	103
Cl1B	C43B	H43B	100
Cl2B	C43B	C43B	70(1)
Cl2B	C43B	Cl1B	14.6(9)
Cl2B	C43B	Cl2B	121(1)
Cl2B	C43B	H43A	104
Cl2B	C43B	H43B	101
C43B	C43B	Cl1B	55.1(9)
C43B	C43B	Cl2B	52(1)
C43B	C43B	H43A	127
C43B	C43B	H43B	124
Cl1B	C43B	Cl2B	107(1)
Cl1B	C43B	H43A	110
Cl1B	C43B	H43B	110
Cl2B	C43B	H43A	110
Cl2B	C43B	H43B	110
H43A	C43B	H43B	109

Table S4. Bond lengths for **Ag-2**.

Atom1	Atom2	Length (Å)
Ag1	S1	2.3477(7)
Ag1	C1	2.090(2)
S1	C28	1.768(2)
S2	C40	1.771(2)
S2	C41	1.764(5)
N1	C33	1.419(3)
N1	C34	1.267(3)
N2	C1	1.359(3)
N2	C2	1.382(3)
N2	C4	1.444(2)
N3	C1	1.348(2)
N3	C3	1.382(3)
N3	C16	1.443(2)
C2	H2	0.95
C2	C3	1.342(3)
C3	H3	0.95
C4	C5	1.399(3)
C4	C9	1.394(3)
C5	C6	1.399(3)
C5	C13	1.514(3)
C6	H6	0.95
C6	C7	1.375(4)
C7	H7	0.95
C7	C8	1.367(4)
C8	H8	0.95
C8	C9	1.393(3)
C9	C10	1.521(4)
C10	H10	1
C10	C11	1.513(5)
C10	C12	1.525(5)
C11	H11A	0.98
C11	H11B	0.98
C11	H11C	0.98
C12	H12A	0.98
C12	H12B	0.98
C12	H12C	0.98
C13	H13	1
C13	C14	1.538(3)
C13	C15	1.534(3)
C14	H14A	0.98
C14	H14B	0.98
C14	H14C	0.98

C15	H15A	0.98
C15	H15B	0.98
C15	H15C	0.98
C16	C17	1.393(3)
C16	C21	1.397(3)
C17	C18	1.397(3)
C17	C25	1.515(3)
C18	H18	0.95
C18	C19	1.374(4)
C19	H19	0.95
C19	C20	1.370(3)
C20	H20	0.95
C20	C21	1.395(3)
C21	C22	1.516(3)
C22	H22	1
C22	C23	1.514(3)
C22	C24	1.519(4)
C23	H23A	0.98
C23	H23B	0.98
C23	H23C	0.98
C24	H24A	0.981
C24	H24B	0.98
C24	H24C	0.98
C25	H25	1
C25	C26	1.521(4)
C25	C27	1.527(3)
C26	H26A	0.98
C26	H26B	0.98
C26	H26C	0.981
C27	H27A	0.98
C27	H27B	0.98
C27	H27C	0.98
C28	C29	1.402(3)
C28	C33	1.408(3)
C29	H29	0.95
C29	C30	1.375(3)
C30	H30	0.95
C30	C31	1.377(3)
C31	H31	0.95
C31	C32	1.381(3)
C32	H32	0.95
C32	C33	1.386(3)
C34	H34	0.95
C34	C35	1.466(3)
C35	C36	1.389(3)

C35	C40	1.403(3)
C36	H36	0.95
C36	C37	1.376(4)
C37	H37	0.95
C37	C38	1.381(4)
C38	H38	0.95
C38	C39	1.366(4)
C39	H39	0.95
C39	C40	1.388(4)
C41	H41A	0.98
C41	H41B	0.98
C41	H41C	0.98

Table S5. Bond angles for **Ag-2**.

Atom1	**Atom2**	**Atom3**	**Angle**
S1	Ag1	C1	178.33(6)
Ag1	S1	C28	103.17(7)
C40	S2	C41	102.0(2)
C33	N1	C34	117.0(2)
C1	N2	C2	111.1(2)
C1	N2	C4	122.5(2)
C2	N2	C4	125.9(2)
C1	N3	C3	111.5(2)
C1	N3	C16	124.5(2)
C3	N3	C16	124.0(2)
Ag1	C1	N2	125.7(1)
Ag1	C1	N3	130.1(1)
N2	C1	N3	104.1(2)
N2	C2	H2	126.7
N2	C2	C3	106.7(2)
H2	C2	C3	126.7
N3	C3	C2	106.6(2)
N3	C3	H3	126.7
C2	C3	H3	126.7
N2	C4	C5	119.2(2)
N2	C4	C9	117.5(2)
C5	C4	C9	123.2(2)
C4	C5	C6	116.4(2)
C4	C5	C13	121.8(2)
C6	C5	C13	121.8(2)
C5	C6	H6	119.4
C5	C6	C7	121.2(2)
H6	C6	C7	119.4

C6	C7	H7	119.5
C6	C7	C8	121.0(2)
H7	C7	C8	119.5
C7	C8	H8	119.6
C7	C8	C9	120.7(2)
H8	C8	C9	119.7
C4	C9	C8	117.5(2)
C4	C9	C10	122.7(2)
C8	C9	C10	119.8(2)
C9	C10	H10	107.6
C9	C10	C11	111.3(2)
C9	C10	C12	110.9(2)
H10	C10	C11	107.6
H10	C10	C12	107.7
C11	C10	C12	111.5(3)
C10	C11	H11A	109.5
C10	C11	H11B	109.5
C10	C11	H11C	109.5
H11A	C11	H11B	109.5
H11A	C11	H11C	109.5
H11B	C11	H11C	109.4
C10	C12	H12A	109.4
C10	C12	H12B	109.4
C10	C12	H12C	109.5
H12A	C12	H12B	109.5
H12A	C12	H12C	109.5
H12B	C12	H12C	109.5
C5	C13	H13	107.4
C5	C13	C14	113.1(2)
C5	C13	C15	112.0(2)
H13	C13	C14	107.3
H13	C13	C15	107.3
C14	C13	C15	109.5(2)
C13	C14	H14A	109.5
C13	C14	H14B	109.5
C13	C14	H14C	109.5
H14A	C14	H14B	109.5
H14A	C14	H14C	109.5
H14B	C14	H14C	109.5
C13	C15	H15A	109.5
C13	C15	H15B	109.5
C13	C15	H15C	109.4
H15A	C15	H15B	109.5
H15A	C15	H15C	109.4
H15B	C15	H15C	109.5

N3	C16	C17	119.1(2)
N3	C16	C21	117.8(2)
C17	C16	C21	123.1(2)
C16	C17	C18	117.1(2)
C16	C17	C25	122.9(2)
C18	C17	C25	120.0(2)
C17	C18	H18	119.6
C17	C18	C19	120.8(2)
H18	C18	C19	119.6
C18	C19	H19	119.5
C18	C19	C20	120.9(2)
H19	C19	C20	119.6
C19	C20	H20	119.5
C19	C20	C21	121.0(2)
H20	C20	C21	119.5
C16	C21	C20	117.0(2)
C16	C21	C22	122.7(2)
C20	C21	C22	120.3(2)
C21	C22	H22	108.1
C21	C22	C23	111.5(2)
C21	C22	C24	110.0(2)
H22	C22	C23	108.1
H22	C22	C24	108.1
C23	C22	C24	111.0(2)
C22	C23	H23A	109.5
C22	C23	H23B	109.4
C22	C23	H23C	109.5
H23A	C23	H23B	109.5
H23A	C23	H23C	109.5
H23B	C23	H23C	109.4
C22	C24	H24A	109.5
C22	C24	H24B	109.5
C22	C24	H24C	109.5
H24A	C24	H24B	109.5
H24A	C24	H24C	109.4
H24B	C24	H24C	109.5
C17	C25	H25	107.8
C17	C25	C26	111.4(2)
C17	C25	C27	111.5(2)
H25	C25	C26	107.8
H25	C25	C27	107.8
C26	C25	C27	110.3(2)
C25	C26	H26A	109.5
C25	C26	H26B	109.5
C25	C26	H26C	109.4

H26A	C26	H26B	109.5
H26A	C26	H26C	109.4
H26B	C26	H26C	109.5
C25	C27	H27A	109.5
C25	C27	H27B	109.5
C25	C27	H27C	109.5
H27A	C27	H27B	109.5
H27A	C27	H27C	109.5
H27B	C27	H27C	109.5
S1	C28	C29	122.9(2)
S1	C28	C33	120.4(2)
C29	C28	C33	116.7(2)
C28	C29	H29	118.9
C28	C29	C30	122.2(2)
H29	C29	C30	118.9
C29	C30	H30	119.8
C29	C30	C31	120.5(2)
H30	C30	C31	119.7
C30	C31	H31	120.6
C30	C31	C32	118.7(2)
H31	C31	C32	120.6
C31	C32	H32	119.2
C31	C32	C33	121.5(2)
H32	C32	C33	119.3
N1	C33	C28	120.2(2)
N1	C33	C32	119.4(2)
C28	C33	C32	120.4(2)
N1	C34	H34	118.8
N1	C34	C35	122.4(2)
H34	C34	C35	118.8
C34	C35	C36	119.4(2)
C34	C35	C40	121.9(2)
C36	C35	C40	118.7(2)
C35	C36	H36	119.4
C35	C36	C37	121.3(2)
H36	C36	C37	119.4
C36	C37	H37	120.3
C36	C37	C38	119.5(2)
H37	C37	C38	120.3
C37	C38	H38	119.9
C37	C38	C39	120.3(2)
H38	C38	C39	119.9
C38	C39	H39	119.5
C38	C39	C40	121.1(2)
H39	C39	C40	119.4

S2	C40	C35	120.1(2)
S2	C40	C39	120.8(2)
C35	C40	C39	119.1(2)
S2	C41	H41A	109.5
S2	C41	H41B	109.5
S2	C41	H41C	109.5
H41A	C41	H41B	109.5
H41A	C41	H41C	109.4
H41B	C41	H41C	109.5

Table S6. Bond lengths for **Au-2**.

Atom1	**Atom2**	**Length (Å)**
Au1	S1	2.2981(7)
Au1	C1	2.008(3)
S1	C28	1.765(2)
S2	C40	1.772(3)
S2	C41	1.773(5)
N1	C1	1.349(3)
N1	C2	1.384(3)
N1	C10	1.451(3)
N2	C1	1.361(3)
N2	C3	1.382(3)
N2	C4	1.448(4)
N3	C33	1.425(3)
N3	C34	1.277(4)
C2	H2	0.94
C2	C3	1.341(4)
C3	H3	0.94
C4	C5	1.400(4)
C4	C9	1.394(5)
C5	C6	1.396(4)
C5	C22	1.521(5)
C6	H6	0.941
C6	C7	1.376(5)
C7	H7	0.94
C7	C8	1.379(5)
C8	H8	0.94
C8	C9	1.394(4)
C9	C26	1.512(5)
C10	C11	1.397(4)
C10	C15	1.391(4)
C11	C12	1.399(4)
C11	C16	1.514(4)

C12	H12	0.94
C12	C13	1.368(5)
C13	H13	0.94
C13	C14	1.377(5)
C14	H14	0.94
C14	C15	1.390(4)
C15	C19	1.522(4)
C16	H16	0.99
C16	C17	1.528(4)
C16	C18	1.530(5)
C17	H17A	0.97
C17	H17B	0.97
C17	H17C	0.971
C18	H18A	0.97
C18	H18B	0.97
C18	H18C	0.97
C19	H19	0.99
C19	C20	1.526(5)
C19	C21	1.513(4)
C20	H20A	0.97
C20	H20B	0.97
C20	H20C	0.97
C21	H21A	0.97
C21	H21B	0.97
C21	H21C	0.97
C22	H22	0.99
C22	C23	1.531(4)
C22	C24	1.535(5)
C23	H23A	0.97
C23	H23B	0.97
C23	H23C	0.97
C24	H24A	0.971
C24	H24B	0.97
C24	H24C	0.97
C25	H25A	0.97
C25	H25B	0.969
C25	H25C	0.97
C25	C26	1.526(6)
C26	H26	0.99
C26	C27	1.526(5)
C27	H27A	0.97
C27	H27B	0.97
C27	H27C	0.97
C28	C29	1.402(4)
C28	C33	1.404(4)

C29	H29	0.94
C29	C30	1.378(5)
C30	H30	0.94
C30	C31	1.378(5)
C31	H31	0.94
C31	C32	1.387(4)
C32	H32	0.94
C32	C33	1.393(5)
C34	H34	0.94
C34	C35	1.464(4)
C35	C36	1.396(4)
C35	C40	1.399(4)
C36	H36	0.94
C36	C37	1.378(4)
C37	H37	0.94
C37	C38	1.376(5)
C38	H38	0.94
C38	C39	1.378(5)
C39	H39	0.94
C39	C40	1.399(4)
C41	H41A	0.97
C41	H41B	0.97
C41	H41C	0.97

Table S7. Bond Angles for **Au-2**.

Atom1	**Atom2**	**Atom3**	**Angle**
S1	Au1	C1	179.21(8)
Au1	S1	C28	104.37(9)
C40	S2	C41	102.0(2)
C1	N1	C2	111.4(2)
C1	N1	C10	124.7(2)
C2	N1	C10	123.8(2)
C1	N2	C3	110.7(2)
C1	N2	C4	122.6(2)
C3	N2	C4	126.2(2)
C33	N3	C34	117.3(2)
Au1	C1	N1	129.6(2)
Au1	C1	N2	126.0(2)
N1	C1	N2	104.3(2)
N1	C2	H2	126.8
N1	C2	C3	106.5(2)
H2	C2	C3	126.8
N2	C3	C2	107.2(2)

N2	C3	H3	126.4
C2	C3	H3	126.4
N2	C4	C5	118.8(3)
N2	C4	C9	117.2(3)
C5	C4	C9	124.0(3)
C4	C5	C6	116.2(3)
C4	C5	C22	122.1(3)
C6	C5	C22	121.7(3)
C5	C6	H6	119.3
C5	C6	C7	121.3(3)
H6	C6	C7	119.3
C6	C7	H7	119.7
C6	C7	C8	120.8(3)
H7	C7	C8	119.5
C7	C8	H8	119.6
C7	C8	C9	120.8(3)
H8	C8	C9	119.6
C4	C9	C8	116.8(3)
C4	C9	C26	123.4(3)
C8	C9	C26	119.8(3)
N1	C10	C11	118.4(2)
N1	C10	C15	118.2(2)
C11	C10	C15	123.3(2)
C10	C11	C12	116.5(2)
C10	C11	C16	123.2(2)
C12	C11	C16	120.3(3)
C11	C12	H12	119.4
C11	C12	C13	121.3(3)
H12	C12	C13	119.4
C12	C13	H13	119.6
C12	C13	C14	120.8(3)
H13	C13	C14	119.6
C13	C14	H14	119.7
C13	C14	C15	120.6(3)
H14	C14	C15	119.7
C10	C15	C14	117.4(2)
C10	C15	C19	122.6(2)
C14	C15	C19	119.9(2)
C11	C16	H16	107.8
C11	C16	C17	111.6(3)
C11	C16	C18	111.3(3)
H16	C16	C17	107.8
H16	C16	C18	107.8
C17	C16	C18	110.5(3)
C16	C17	H17A	109.5

C16	C17	H17B	109.5
C16	C17	H17C	109.4
H17A	C17	H17B	109.5
H17A	C17	H17C	109.5
H17B	C17	H17C	109.4
C16	C18	H18A	109.5
C16	C18	H18B	109.5
C16	C18	H18C	109.5
H18A	C18	H18B	109.5
H18A	C18	H18C	109.5
H18B	C18	H18C	109.4
C15	C19	H19	107.9
C15	C19	C20	109.9(3)
C15	C19	C21	112.3(3)
H19	C19	C20	107.8
H19	C19	C21	107.9
C20	C19	C21	110.9(3)
C19	C20	H20A	109.5
C19	C20	H20B	109.5
C19	C20	H20C	109.5
H20A	C20	H20B	109.5
H20A	C20	H20C	109.4
H20B	C20	H20C	109.4
C19	C21	H21A	109.5
C19	C21	H21B	109.5
C19	C21	H21C	109.5
H21A	C21	H21B	109.4
H21A	C21	H21C	109.5
H21B	C21	H21C	109.4
C5	C22	H22	107.3
C5	C22	C23	112.1(3)
C5	C22	C24	112.5(3)
H22	C22	C23	107.3
H22	C22	C24	107.3
C23	C22	C24	110.0(3)
C22	C23	H23A	109.5
C22	C23	H23B	109.5
C22	C23	H23C	109.5
H23A	C23	H23B	109.5
H23A	C23	H23C	109.5
H23B	C23	H23C	109.5
C22	C24	H24A	109.5
C22	C24	H24B	109.5
C22	C24	H24C	109.5
H24A	C24	H24B	109.4

H24A	C24	H24C	109.4
H24B	C24	H24C	109.5
H25A	C25	H25B	109.5
H25A	C25	H25C	109.4
H25A	C25	C26	109.4
H25B	C25	H25C	109.5
H25B	C25	C26	109.5
H25C	C25	C26	109.4
C9	C26	C25	111.8(3)
C9	C26	H26	107.5
C9	C26	C27	111.2(3)
C25	C26	H26	107.5
C25	C26	C27	111.2(3)
H26	C26	C27	107.5
C26	C27	H27A	109.4
C26	C27	H27B	109.5
C26	C27	H27C	109.5
H27A	C27	H27B	109.5
H27A	C27	H27C	109.4
H27B	C27	H27C	109.5
S1	C28	C29	123.1(2)
S1	C28	C33	120.0(2)
C29	C28	C33	116.9(2)
C28	C29	H29	119
C28	C29	C30	122.0(3)
H29	C29	C30	119
C29	C30	H30	119.7
C29	C30	C31	120.6(3)
H30	C30	C31	119.7
C30	C31	H31	120.6
C30	C31	C32	118.9(3)
H31	C31	C32	120.5
C31	C32	H32	119.6
C31	C32	C33	120.9(3)
H32	C32	C33	119.5
N3	C33	C28	120.5(2)
N3	C33	C32	118.8(3)
C28	C33	C32	120.7(3)
N3	C34	H34	118.8
N3	C34	C35	122.4(2)
H34	C34	C35	118.8
C34	C35	C36	119.1(2)
C34	C35	C40	121.8(2)
C36	C35	C40	119.1(3)
C35	C36	H36	119.6

C35	C36	C37	120.8(3)
H36	C36	C37	119.6
C36	C37	H37	120
C36	C37	C38	119.9(3)
H37	C37	C38	120.1
C37	C38	H38	119.8
C37	C38	C39	120.5(3)
H38	C38	C39	119.7
C38	C39	H39	119.8
C38	C39	C40	120.4(3)
H39	C39	C40	119.8
S2	C40	C35	120.5(2)
S2	C40	C39	120.2(2)
C35	C40	C39	119.3(3)
S2	C41	H41A	109.5
S2	C41	H41B	109.5
S2	C41	H41C	109.5
H41A	C41	H41B	109.5
H41A	C41	H41C	109.4
H41B	C41	H41C	109.5

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