# Group 11 Complexes of a Bulky Triazene Ligand

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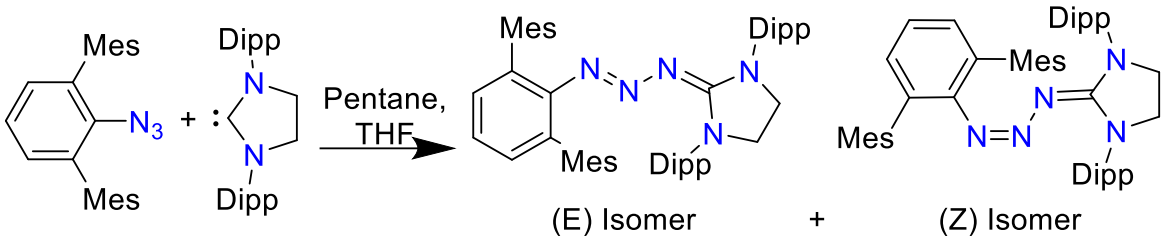
**Supplementary Information**

## Contents

# Synthesis

## Synthesis Compound 1 – π-Conjugated Triazene ligand (L)




**Scheme S1.** Preparation of **1** from $TerMesN_3$ and SIPr carbene.

$TerMesN_3$ (597 mg, 1.68 mmol, 1.00 eq.) was dissolved in a mixture of pentane (3 mL) and THF (3 mL) and added to a solution of SIPr (658 mg, 1.68 mmol) in pentane (7 mL) and THF (2 mL). The solution was stirred for 30 minutes before storage at -35 °C overnight in an attempt to crystallize the product. After no crystals formed, the solution was then dried *in vacuo* to give a glassy yellow colored foam. The solids were broken up, suspended in 5 mL pentane, and the mixture was placed in a -35 °C freezer for 30 minutes. The suspension was then filtered on a coarse glass frit and the solid was washed with 5x1 mL pentane and dried briefly *in vacuo* on the frit. Transferring the solid to a 20 mL scintillation vial was followed with further drying until the solid was a free-flowing powder weighing 730 mg. The filtrate was cooled to -35 °C and additional crystals were isolated by filtration, washed with 2x1 mL cold pentane, and dried to afford another 260 mg as a second crop of pure material. Samples for single crystal X-ray analysis were grown by dissolving the solid in a minimum amount of toluene and storing in a -35°C freezer overnight (*P*-1) and by slow evaporation of a decanted concentrated pentane solution (*C*2/*c*).

Yield: 990 mg (79%)

Analytical Calc. for $C_{51}H_{63}N_5$: C: 82.10%; H: 8.51%; N: 9.39%; Found: C: 79.88%; H: 8.09%; N: 9.08%.

ESI-HRMS (positive ion mode): calculated for $[C_{51}H_{63}N_5Na]^+$ = 768.5091 m/z, observed = 768.4976 m/z.

Melting Point: 170.0-170.8°C.

UV-Vis: 400 nm (ε = 1600 $Lmol^{-1}cm^{-1}$).

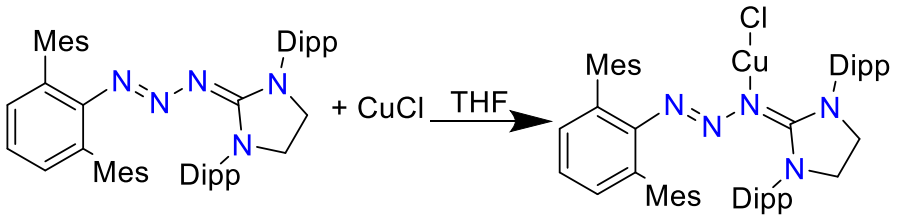
$^1H$ NMR ($C_6D_6$, 300 MHz, 25 °C): δ 7.08 (t, 2H, $^3J_{H-H}$ = 7.6 Hz, *p*-Dipp), 6.95 (d, 2H, $^3J_{H-H}$ = 7.6 Hz, *m*-Dipp), 6.83-6.92 (m, 3H, *p*-TerMes, *m*-TerMes), 6.77 (s, 4H, *m*-Mes), 3.23 (s, 4H, (N-C*H*$_2$)$_2$), 3.06 (q, 4H, $^3J_{H-H}$ = 6.8 Hz, C*H*(CH$_3$)$_2$), 2.32 (s, 6H, *p*-Mes C*H*$_3$), 2.04 (s, 12H, *o*-Mes C*H*$_3$), 1.17 (d, 12H, $^3J_{H-H}$ = 6.8 Hz, CH(C*H*$_3$)$_2$), 1.01 (d, 12H, $^3J_{H-H}$ = 6.8 Hz, CH(C*H*$_3$)$_2$).

$^{13}C\{^1H\}$ NMR ($C_6D_6$, 75 MHz, 25 °C): δ 159.44 (N$_2$-*C*-N), 148.49 (*ipso*-TerMes), 146.93 (*o*-Dipp), 137.85 (*o*-Mes), 136.24 (*ipso*-Dipp), 136.17 (*ipso*-Mes), 135.03 (*p*-Mes), 133.06 (*o*-TerMes), 130.55 (*p*-TerMes), 128.82 (*p*-Dipp), 128.53 (*m*-Mes), 124.87 (*m*-TerMes), 124.46 (*m*-Dipp), 50.18 ((N-*C*H$_2$)$_2$), 29.43 (*C*H(CH$_3$)$_2$), 24.41/24.30 (CH(*C*H$_3$)$_2$), 21.81 (*o*-Mes *C*H$_3$), 21.31 (*p*-Mes *C*H$_3$).

IR (KBr, Transmission, $cm^{-1}$): 2963 (s), 2925 (m), 2868 (m), 1937 (w), 1871 (w), 1721 (w), 1594 (m), 1560 (s, N=N-N=C stretch), 1483 (s), 1441 (s), 1421 (s), 1383 (w), 1326 (m),

1286 (w), 1182 (w), 1158 (w), 1103 (w), 1093 (m), 1046 (s), 1035 (s) 980 (m), 937 (w), 905 (w), 850 (w), 802 (m), 772 (w), 755 (m), 711 (w), 695 (w), 602 (w), 574 (w), 512 (w), 451 (w).

**Synthesis of Compound 2 – L-CuCl**

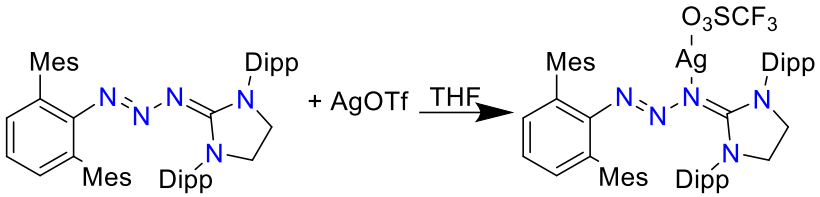



**Scheme S2.** Preparation of **2** from reacting **1** and CuCl in THF.

To **1** (101 mg, 0.135 mmol, 1 eq.) in a 20 mL scintillation vial was added a suspension of CuCl (14 mg, 0.141mmol, 1.04 eq.) in 5 mL THF, and the mixture was stirred for 24 hr. The CuCl appeared to remain undissolved, and 1 mL acetonitrile was added and allowed to stir for an additional hour before drying *in vacuo*. Trituration with 3x2 mL pentane was followed by drying *in vacuo* to give 0.130 g of crude material. Dissolution in 5 mL THF and filtration through a small Kimwipe pipet filter and drying *in vacuo* gave a microcrystalline, yellow solid. Crushing the solid and further drying afforded a solid weighing 0.114 g that was 98% pure by $^{1}$H NMR analysis with a 4:1 ratio of **2**:THF remaining, resulting in a yield of 0.112 g once adjusted for residual solvent. Evaporation of $C_6D_6$ from an NMR sample of **2** gave pale yellow crystals of **2·C$_6$D$_6$**. Analogous attempts to prepare the iodide analogue (**1·CuI**) using Cu(I)I in place of Cu(I)Cl could were unsuccessful in isolating a pure product. The single crystal structure of **1·CuI** was obtained from the
Yield: 112 mg (98%)
Analytical Calc. for $C_{51}H_{63}ClCuN_5$: C: 72.48%; H: 7.51%; N: 8.29%; Found: C: 70.29%; H: 6.97%; N: 8.54%.
ESI-HRMS (positive ion mode): calculated for $[C_{51}H_{63}N_5Cu]^+$ = 808.4374 m/z, observed = 808.4367 m/z.
Melting Point: 311.4 – 316.9 °C.
UV-Vis: 308 nm (ε = 320 Lmol$^{-1}$cm$^{-1}$).
$^{1}$H NMR ($CD_2Cl_2$, 300 MHz, 25 °C): δ 7.40 (t, 2H, $^{3}J_{H\text{-}H}$ = 7.8 Hz, *p*-Dipp), 7.14 (t, 1H, $^{3}J_{H\text{-}H}$ = 7.5 Hz, *p*-TerMes), 7.12 (d, 4H, $^{3}J_{H\text{-}H}$ = 7.8 Hz, *m*-Dipp), 6.81 (d, 2H, $^{3}J_{H\text{-}H}$ = 7.5 Hz, *m*-TerMes), 6.71 (s, 4H, *m*-Mes), 3.83 (s, 4H, (N-C*H*$_2$)$_2$), 2.87 (sept, 4H, $^{3}J_{H\text{-}H}$ = 6.8 Hz, C*H*(CH$_3$)$_2$), 2.26 (s, 6H, *p*-Mes C*H*$_3$), 1.86 (bs, 12H, *o*-Mes C*H*$_3$), 1.18 (d, 12H, $^{3}J_{H\text{-}H}$ = 6.8Hz, CH(C*H*$_3$)$_2$), 0.87 (d, 12H, $^{3}J_{H\text{-}H}$ = 6.8 Hz, CH(C*H*$_3$)$_2$) ppm.
$^{13}$C{$^{1}$H} NMR ($CD_2Cl_2$, 75 MHz, 25 °C): δ 161.80 (N$_2$-*C*-N), 146.20 (*o*-Dipp), 145.86 (*o*-TerMes), 136.40/136.18/136.08/135.90 (m, *ipso*-Mes, *o*-Mes, *ipso*-TerMes, *o*-TerMes), 133.12 (*o*-Dipp), 130.67 (*m*-TerMes), 130.41-130.45 (bs, *p*-Dipp), 128.58-128.68 (bs, *m*-Mes), 128.88 (*m*-Mes), 128.30 (*p*-Mes), 126.32 (*p*-TerMes), 125.86 (*m*-Dipp), 51.47 ((N-*C*H$_2$)$_2$), 29.48 (*C*H(CH$_3$)$_2$), 24.79/24.27 (CH(*C*H$_3$)$_2$), 21.77 (vbr s, width at ½ height = 29 Hz, *o*-Mes *C*H$_3$), 21.13 (*p*-Mes *C*H$_3$) ppm.
IR (KBr, Transmission, cm$^{-1}$): 2963 (s), 2924 (s), 2868 (m), 2732 (m), 1612 (w), 1592 (m), 1558 (s), 1506 (s), 1488 (m), 1457 (s), 1384 (s), 1364 (m), 1344 (m), 1325 (m), 1287 (m),

1260 (m), 1153 (m), 1114 (s), 1043 (m), 1014 (s), 983 (m), 937 (w), 907 (m), 850 (w), 803 (m), 766 (m), 753 (m), 715 (w), 690 (w), 574 (w), 510 (w), 452 (w).

**Synthesis of Compound 3 – L-AgOTf**

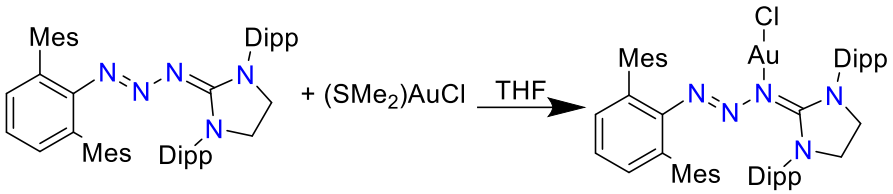



**Scheme S3.** Preparation of **3** from reacting **1** and AgOTf in THF.

**1** (245 mg, 0.33 mmol. 1.0 eq.) was added to a 20 mL scintillation vial with 8 mL of THF and a stir bar. Silver triflate (87 mg, 0.34 mmol, 1.03 eq.) was added to the vial and was stirred for 1 hour. After stirring, the beige reaction mixture was filtered through Celite, and the remaining solution was dried in vacuo. Crystals were grown by dissolving the solids in a minimum amount of THF layered with an equal amount of pentane to produce large beige crystals. The crystals were isolated by decanting the solution, washing with pentane, and drying *in vacuo*.
Yield: 320 mg (97%)
Analytical Calc. for $C_{52}H_{63}AgF_3N_5O_3$: C: 62.27%; H: 6.33%; N: 6.98%. Found: C: 62.30%; H: 5.95%; N: 6.88%.
ESI-HRMS (positive ion mode): calculated for $[C_{51}H_{63}N_5Ag]^+$ = 852.4129 m/z, observed = 852.4150 m/z.
Melting Point: 240.5-257.5°C.
UV-Vis: 360 nm (ε = 590 $Lmol^{-1}cm^{-1}$).
$^1$H NMR ($C_6D_6$, 300 MHz, 25 °C): δ 7.39 (t, 2H, $^3J_{H-H}$ = 7.8 Hz, *p*-Dipp), 7.06 (d, 4H, $^3J_{H-H}$ = 7.8 Hz, *m*-Dipp), 6.86 (t, 1H, $^3J_{H-H}$ = 7.5 Hz, *p*-TerMes), 6.78 (s, 4H, *m*-Mes), 6.70 (d, 2H, $^3J_{H-H}$ = 7.5 Hz, *m*-TerMes), 3.12 (s, 4H, (N-C$H_2$)$_2$), 2.72 (sept, 4H, $^3J_{H-H}$ = 6.9 Hz, C$H$(C$H_3$)$_2$), 2.24 (s, 6H, *p*-Mes C$H_3$), 2.03 (bs, 12H, *o*-Mes C$H_3$), 1.01 (d, 12H, $^3J_{H-H}$ = 6.9 Hz, CH(C$H_3$)$_2$), 0.94 (d, 12H, $^3J_{H-H}$ = 6.9 Hz, CH(C$H_3$)$_2$) ppm.
$^1$H NMR ($CD_2Cl_2$, 300 MHz, 25 °C): δ 7.43 (t, 2H, $^3J_{H-H}$ = 7.8 Hz, *p*-Dipp), 7.19 (t, 1H, $^3J_{H-H}$ = 7.5 Hz, *p*-TerMes), 7.17 (d, 4H, $^3J_{H-H}$ = 7.8 Hz, *m*-Dipp), 6.86 (d, 2H, $^3J_{H-H}$ = 7.5 Hz, *m*-TerMes), 6.72 (s, 4H, *m*-Mes), 3.88 (s, 4H, (N-C$H_2$)$_2$), 2.86 (sept, 4H, $^3J_{H-H}$ = 6.9 Hz, C$H$(C$H_3$)$_2$), 2.26 (s, 6H, *p*-Mes C$H_3$), 1.79 (s, 12H, *o*-Mes C$H_3$), 1.19 (d, 12H, $^3J_{H-H}$ = 6.9 Hz, CH(C$H_3$)$_2$), 0.89 (d, 12H, $^3J_{H-H}$ = 6.9 Hz, CH(C$H_3$)$_2$) ppm.
$^{13}$C{$^1$H} NMR ($CD_2Cl_2$, 75 MHz, 25 °C): δ 158.93 (N$_2$-*C*-N), 146.32 (*o*-Dipp), 143.63 (*ipso*-TerMes), 136.57 (*p*-Mes), 135.71 (*ipso*-Mes), 135.64 (*o*-Mes), 133.98 (*o*-TerMes), 132.63 (*ipso*-Dipp), 130.94 (*p*-Dipp), 130.68 (*m*-TerMes), 128.90 (*m*-Mes), 127.18 (*p*-TerMes), 125.87 (*m*-Dipp), 120.69 (q, $^1J_{F-C}$ = 320 Hz, O$_3$S-*C*F$_3$), 50.88 ((N-*C*H$_2$)$_2$), 29.61 (*C*H(CH$_3$)$_2$), 24.83/24.44 (CH(*C*H$_3$)$_2$), 21.50 (*o*-Mes *C*H$_3$), 21.13 (*p*-Mes *C*H$_3$) ppm.
$^{19}$F NMR ($CD_2Cl_2$, 31 MHz, 25 °C): δ -78.73 ppm (SO$_4$C*F*$_3$).
IR (KBr, Transmission, $cm^{-1}$): 2964 (s), 2925 (m), 2868 (m), 2759 (w), 1613 (m), 1592 (m), 1559 (m), 1505 (s), 1490 (s), 1460 (s), 1384 (m), 1364 (m), 1324 (m), 1287 (m), 1259 (w), 1202 (w), 1181 (w), 1150 (w), 1112 (w), 1095 (w), 1059 (w), 1043 (w), 1001 (s), 984

(m), 937 (w), 905 (w), 850 (w), 803 (w), 766 (w), 754 (w), 712 (w), 574 (w), 557 (w), 453 (w).

**Synthesis of Compound 4 – L-AuCl**




**Scheme S4.** Preparation of **4** from reacting **1** and $(SMe_2)AuCl$ in THF.

**Preparation 1:** This experiment was performed in a light deprived environment to reduce decomposition of the product, and the vial was covered with aluminum foil and placed under a dark container whenever possible. **1** (56 mg, 0.076 mmol, 1 eq.) was added to a 20mL scintillation vial and dissolved in 1 mL THF. In another vial, $(CH_3)_2SAuCl$ (22 mg, 0.076 mmol, 1 eq.) was dissolved in 1 mL THF and the $(CH_3)_2SAuCl$ containing THF solution was quantitatively transferred to the vial containing **1**, and the solution was stirred for 3 hours. The solvent was removed *in vacuo* to give a crude product that was then washed with 2x1 mL pentane, redissolved in a minimum of THF, and filtered through a lint free paper pipet filter and again dried *in vacuo*. The crude product was then recrystallized by layering a dichloromethane solution with pentane. The solvent was removed with a pipet, and two different morphologies were present. The larger blocky-white crystals of the desired compound were manually removed from the dark yellow solids (minor component). The dark yellow material was unidentifiable by SC-XRD owing to its amorphous structure and was discarded.

**Preparation 2**

In minimally visible faint ambient back lighting **1** (106 mg, 0.142 mmol, 1 eq.) was added as a 1.5 mL THF solution dropwise over 5 minutes with stirring to $(CH_3)_2SAuCl$ (41.8 mg, 0.142 mmol, 1 eq.) dissolved in 3 mL THF, rinsing to a total volume of 8 mL. After 1 hour of stirring, the solution was stored at -35 °C for 3 hours. No solid formed, so the solution was concentrated *in vacuo* to 4 mL and carefully layered with 10 mL pentane, storing at -35 °C overnight. Removal of solvent with a pipet and washing with 2x1 mL cold pentane and drying *in vacuo* gave 99 mg glittery golden metallic crystals of **1**.

Yields: **Prep. 1:** 56 mg (71 %) **Prep. 2:** 99 mg (71%)

Analytical Calc. for $C_{51}H_{63}ClAuN_5$: C: 62.60%; H: 6.49%; N: 7.16%; Found: C: 56.74%; H: 6.48%; N: 8.71%.

ESI-HRMS (positive ion mode): calculated for $[C_{51}H_{63}N_5AuClNa]^+$ = 1000.4445 m/z, observed = 1000.4311 m/z.

Melting Point: 235.1-240.5 °C.

UV-Vis: 575 nm (ε = 510 $Lmol^{-1}cm^{-1}$).

$^1H$ NMR ($CD_2Cl_2$, 300 MHz, 25 °C): δ 7.38 (t, 2H, $^3J_{H-H}$ = 7.8 Hz, *p*-Dipp), 7.13 (t, 1H, $^3J_{H-H}$ = 7.5 Hz, *p*-TerMes), 7.09 (d, 4H, $^3J_{H-H}$ = 7.8 Hz, *m*-Dipp), 6.81 (d, 2H, $^3J_{H-H}$ = 7.5 Hz, *m*-TerMes), 6.70 (s, 4H, *m*-Mes), 3.83 (s, 4H, (N-C$H_2$)$_2$), 2.89 (sept, 4H, $^3J_{H-H}$ = 6.8 Hz, C$H$($CH_3$)$_2$), 2.26 (s, 6H, *p*-Mes C$H_3$), 2.03 (bs, 6H, *o*-Mes C$H_3$), 1.76 (bs, 6H, *o*-Mes C$H_3$), 1.18 (d, 12H, $^3J_{H-H}$ = 6.8 Hz, CH(C$H_3$)$_2$), 0.88 (d, 12H, $^3J_{H-H}$ = 6.8 Hz, CH(C$H_3$)$_2$) ppm.

$^{13}C\{^{1}H\}$ NMR ($CD_2Cl_2$, 75 MHz, 25 °C): δ 162.87 ($N_2$-*C*-N), 145.99 (*o*-Dipp), 145.78 (*ipso*-TerMes), 136.61/136.44/136.05/135.79 (*ipso*-Mes, *o*-Mes), 134.74 (*ipso*-Dipp), 133.26 (*o*-TerMes), 130.86 (*m*-TerMes), 130.06 (*p*-Dipp), 128.84 (*m*-Mes), 128.43 (*p*-Mes), 126.30 (*p*-TerMes), 125.30 (*m*-Dipp), 51.96 ((N-$CH_2$)$_2$), 29.30 ($CH(CH_3)_2$), 25.12 ($CH(CH_3)_2$), 23.84 ($CH(CH_3)_2$), 22.38 (*o*-Mes $CH_3$), 21.14 (*p*-Mes $CH_3$), 21.02 (*o*-Mes $CH_3$) ppm.
IR (KBr, Transmission, $cm^{-1}$): 2965 (s), 2926 (m), 2871 (m), 2734 (w), 1611 (w), 1593 (m), 1554 (s), 1506 (s), 1440 (s), 1378 (m), 1366 (m), 1326 (m), 1307 (s), 1288 (s), 1232 (s), 1215 (s), 1169 (s), 1102 (m), 1074 (w), 1045 (m), 1024 (s), 984 (m), 937 (w), 921 (w), 852 (m), 805 (m), 785 (w), 767 (w), 756 (m), 738 (w), 713 (w), 683 (w), 634 (s), 606 (w), 573 (w), 558 (w), 516 (w), 450 (w).

**Isolation of Compound 5 – [(SIPrNH)$_2$Au(I)][Au(I)Cl$_2$]**
The filtrate from **Preparation 2** of **4** was dried to a yellow paste of a considerable proportion. This was suspended in air in isopropanol and left to stir five days, then heated to dissolve the white precipitate. Storage at -20 °C for two days was followed by drying *in vacuo* to a yellow paste that was triturated with 3x1 mL pentane for one extract, and 3x1 mL acetonitrile for the second, filtering through a 2 mL medium glass frit. Both were allowed to dry ambiently, affording 28 mg of an impure mixture with the major component identified as TerMesH (by SC-XRD and matching $^{1}H$ NMR) and minor with unidentified SIPr containing material by $^{1}H$ NMR. The acetonitrile extract dried to 7.3 mg colorless crystalline material identified as [(SIPrNH)$_2$Au(I)][Au(I)Cl$_2$] by SC-XRD.
Yield: 7.3 mg (8%) based on an initial 0.142 mmol of **1**.
Melting Information: beige 120, changing to reddish brown by 140, blackening by 175, progressing between 180-255. Partial melt between 260-265, little change until complete melt at 280 °C.
Melting Information for TerMesH containing first extract: partial melt around colorless crystals at 100, going mostly molten by 175, leaving a very small colorless crystalline component not melting until 205 °C.
IR (diamond, ATR, $cm^{-1}$): 3360 (w), 3311 (w), 3192 (w), 3067 (w), 2962 (s), 2928 (m), 2869 (m), 1755 (w), 1719 (w), 1654 (w), 1610 (s), 1584 (s), 1529 (s), 1494 (w), 1465 (s), 1384 (m), 1362 (m), 1327 (s), 1292 (m), 1269 (m), 1256 (m), 1182 (w), 1155 (w), 1112 (w), 1082 (w), 1058 (m), 1015 (w), 937 (w), 830 (w), 803 (s), 767 (w), 758 (m), 702 (w), 687 (w), 640 (w), 604 (w), 589 (w), 540 (w), 445 (m), 415 (w).

## Infrared Spectroscopy

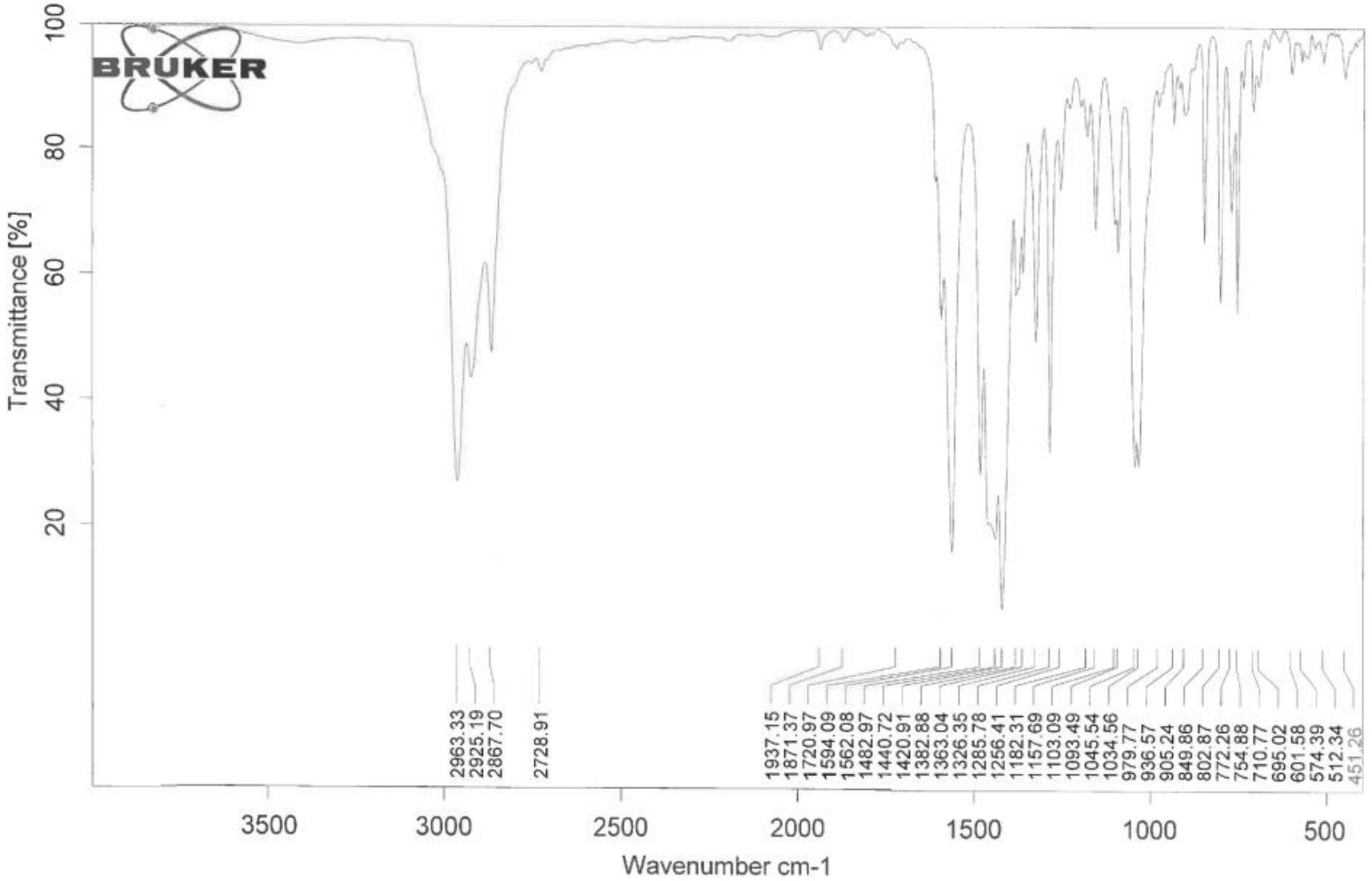



Figure S1 Transmission infrared spectrum of **1** pressed in a KBr pellet.

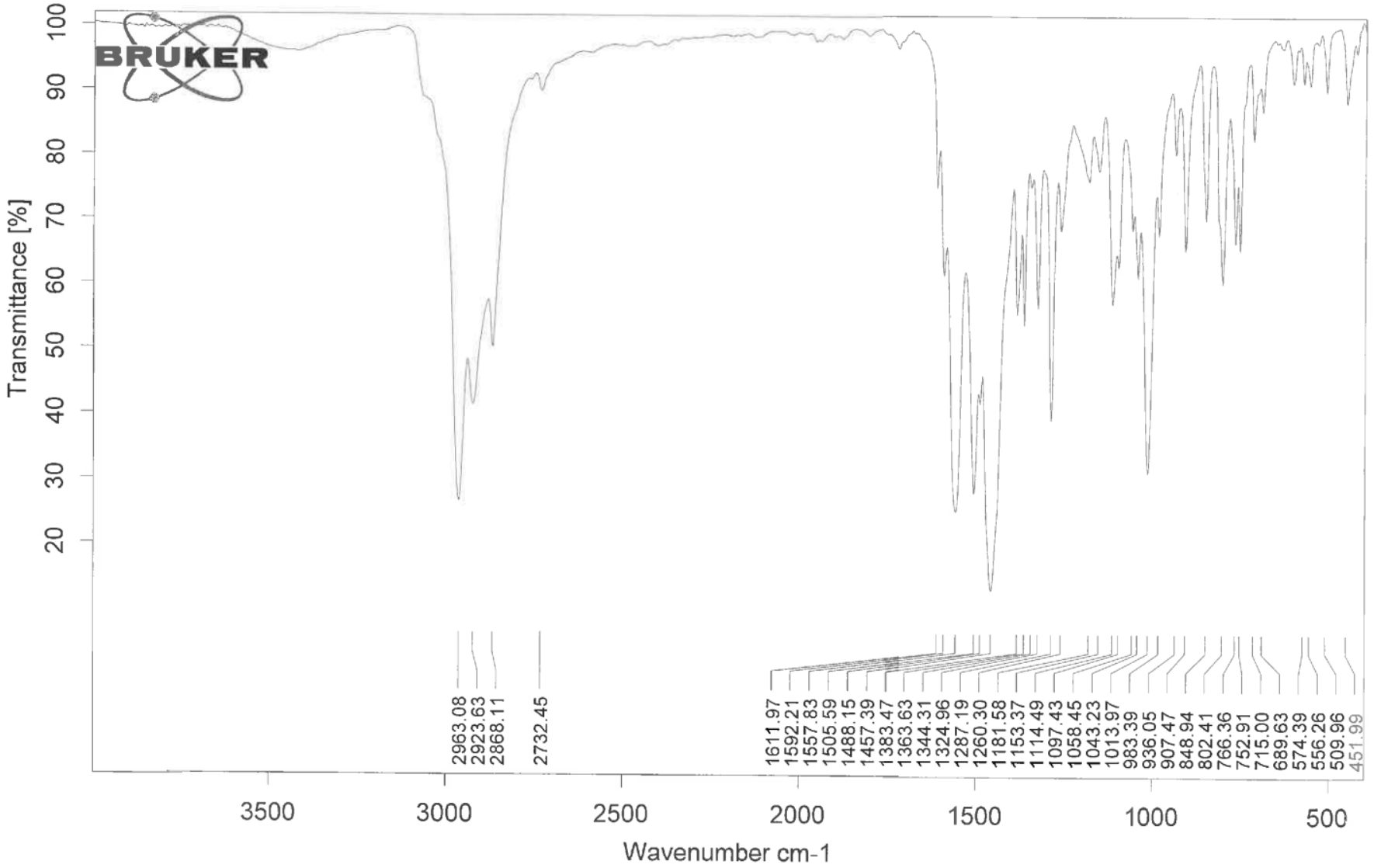



Figure S2 Transmission infrared spectrum of **2** pressed in a KBr pellet.

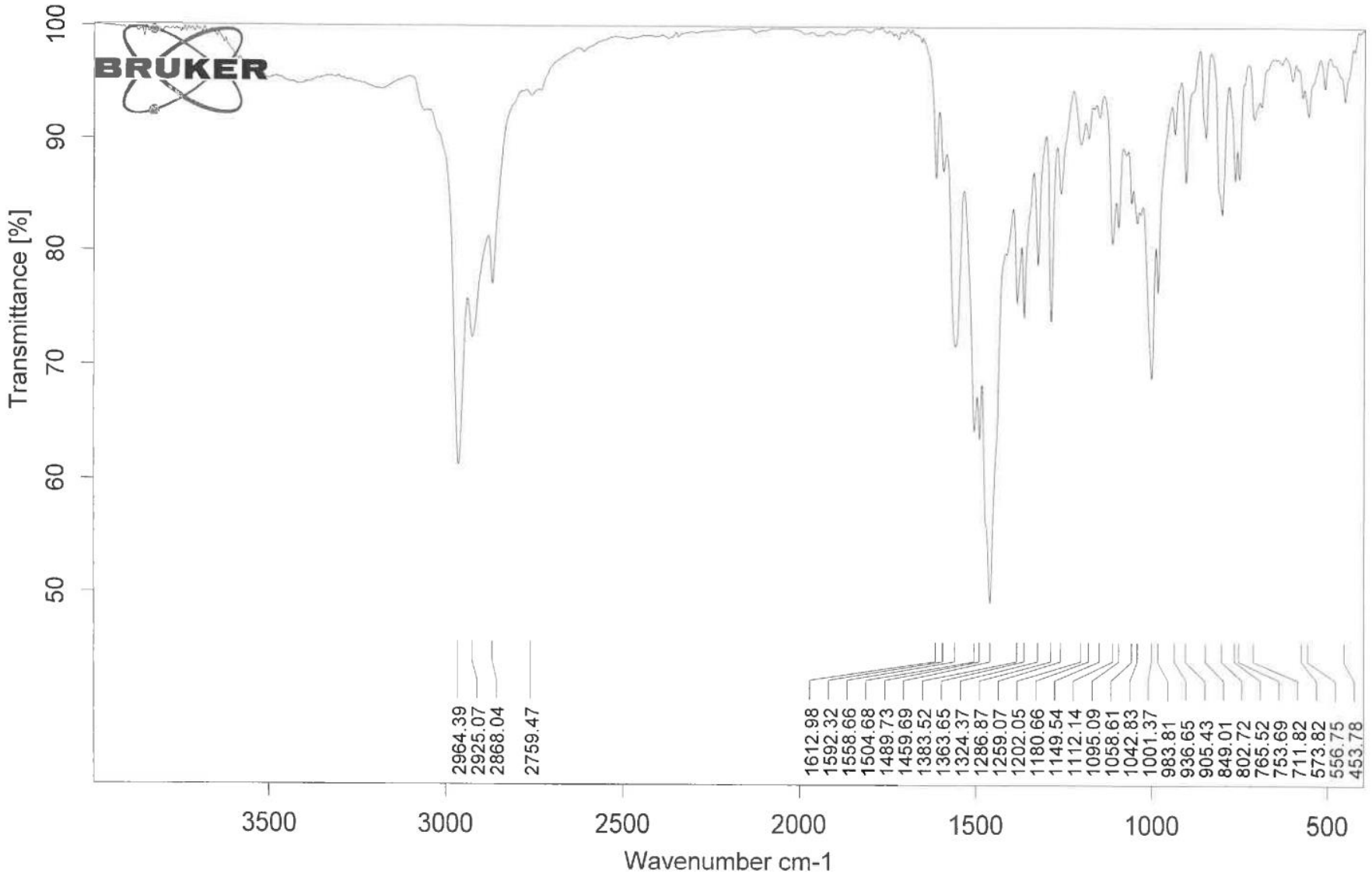



Figure S3 Transmission infrared spectrum of **3** pressed in a KBr pellet.

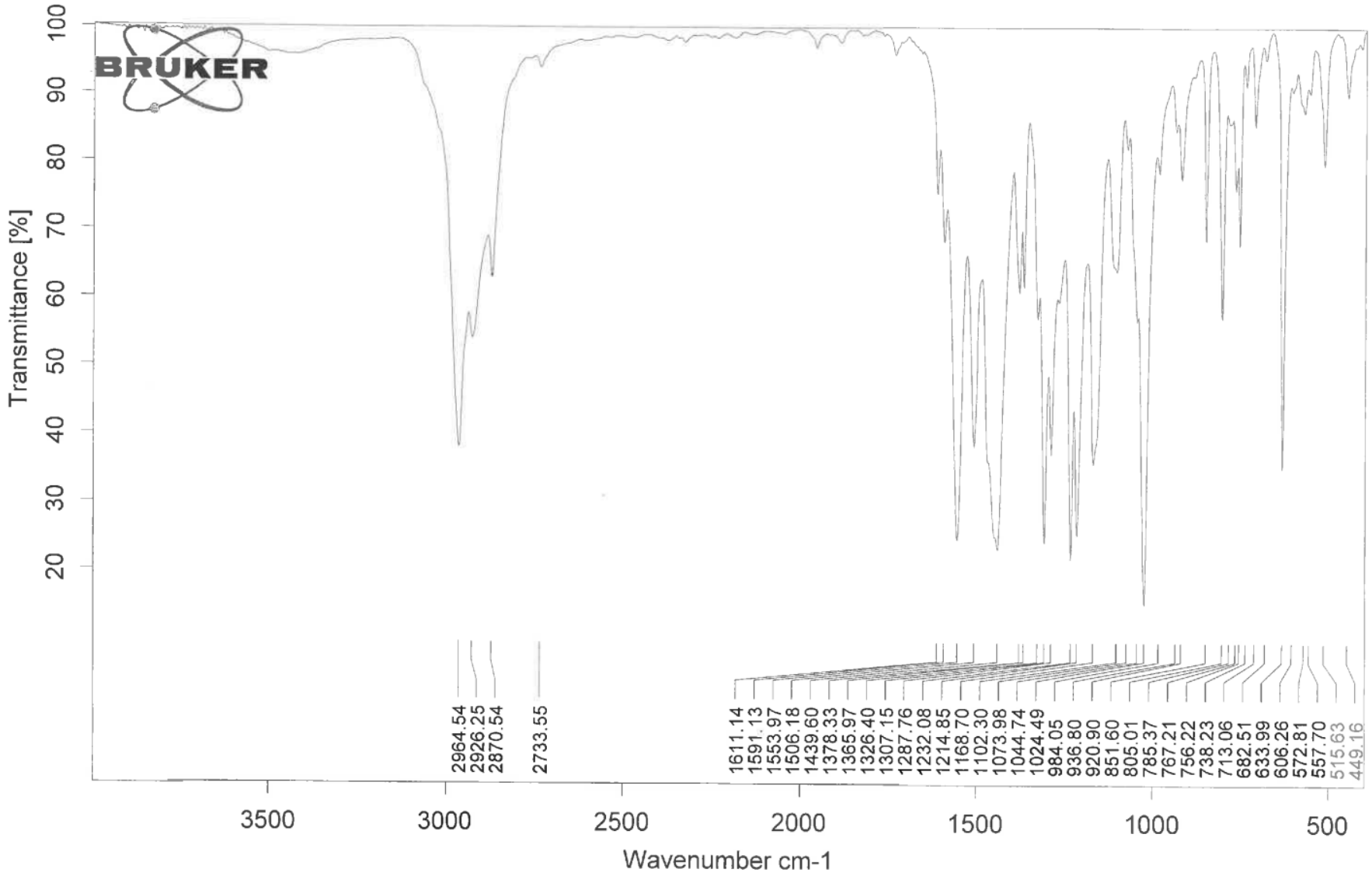



Figure S4 Transmission infrared spectrum of **4** pressed in a KBr pellet.

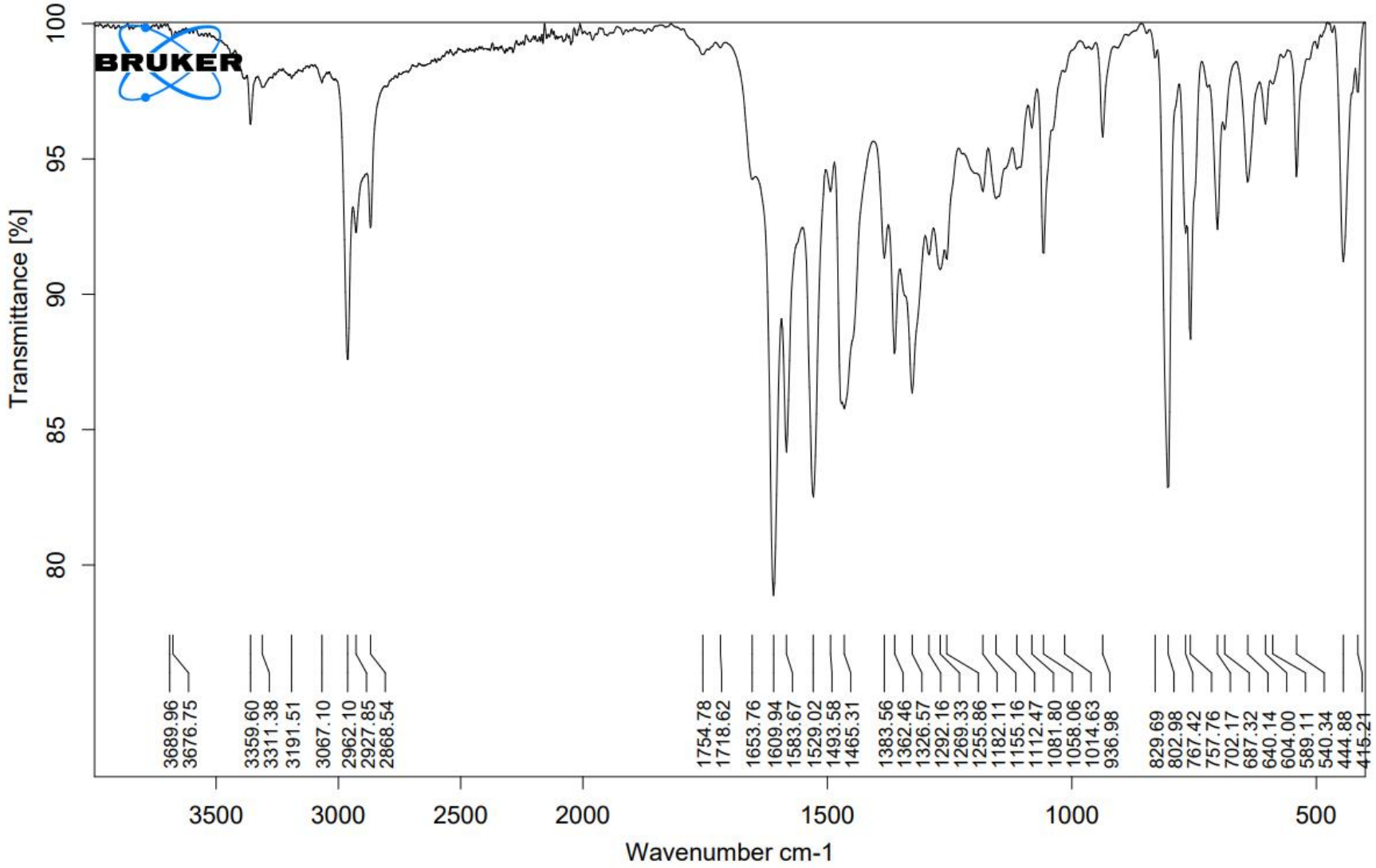



Figure S5 Attenuated total reflectance infrared spectrum of **5**.

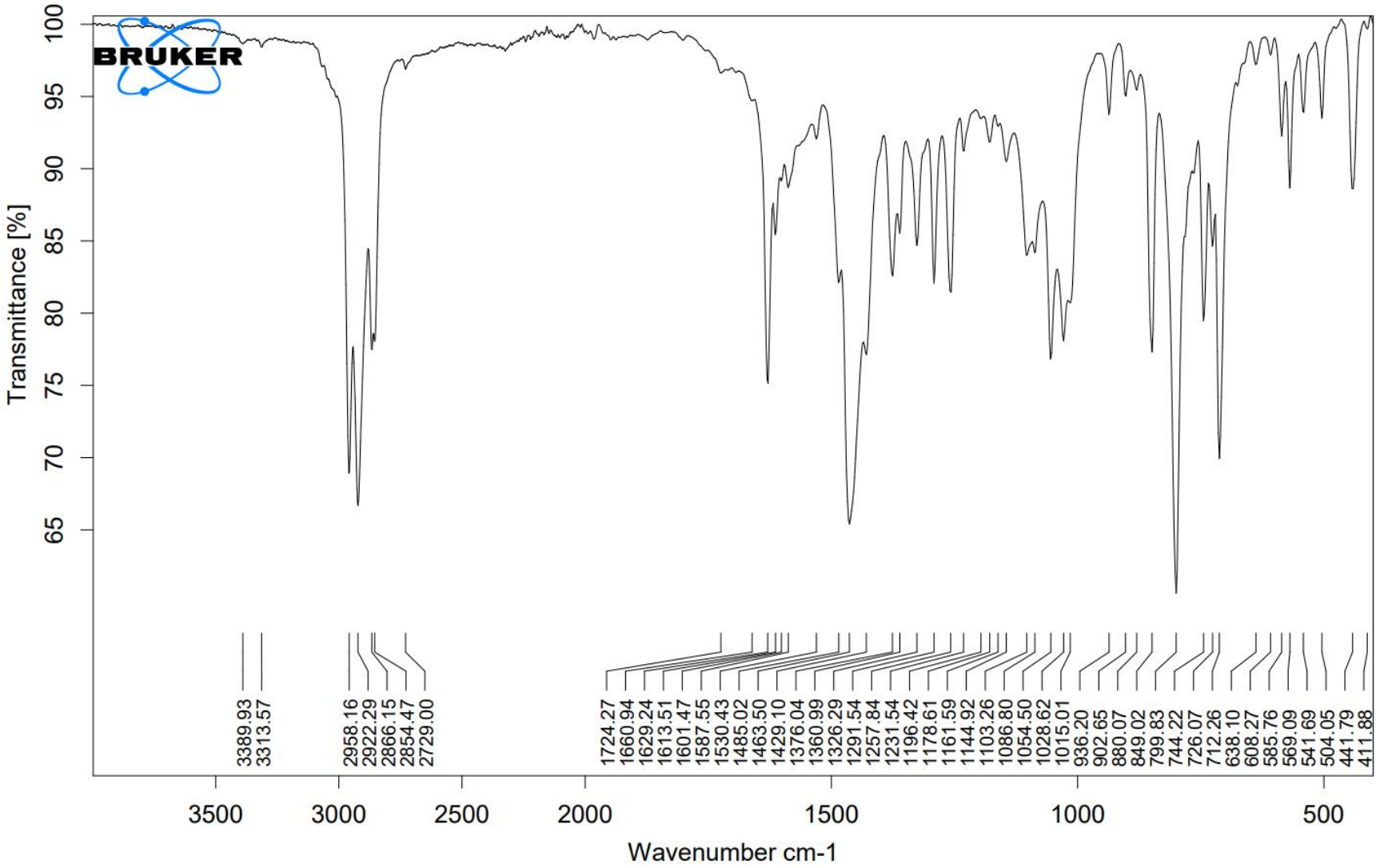



Figure S6 Attenuated total reflectance infrared spectrum of impure TerMesH recovered from the synthesis of compounds **4** and **5.**

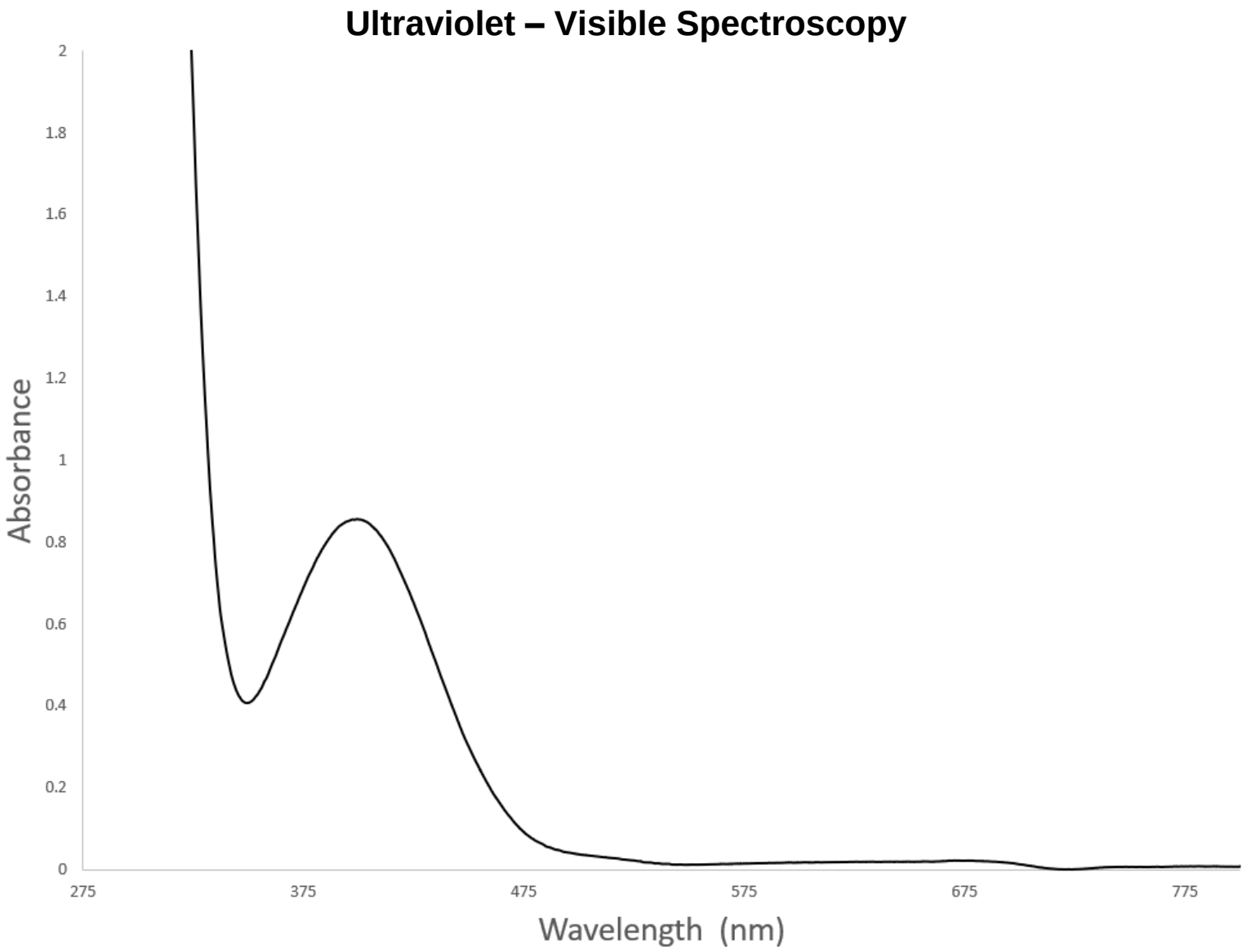



Figure S7 Ultraviolet-visible spectrum of **1** dissolved in THF.

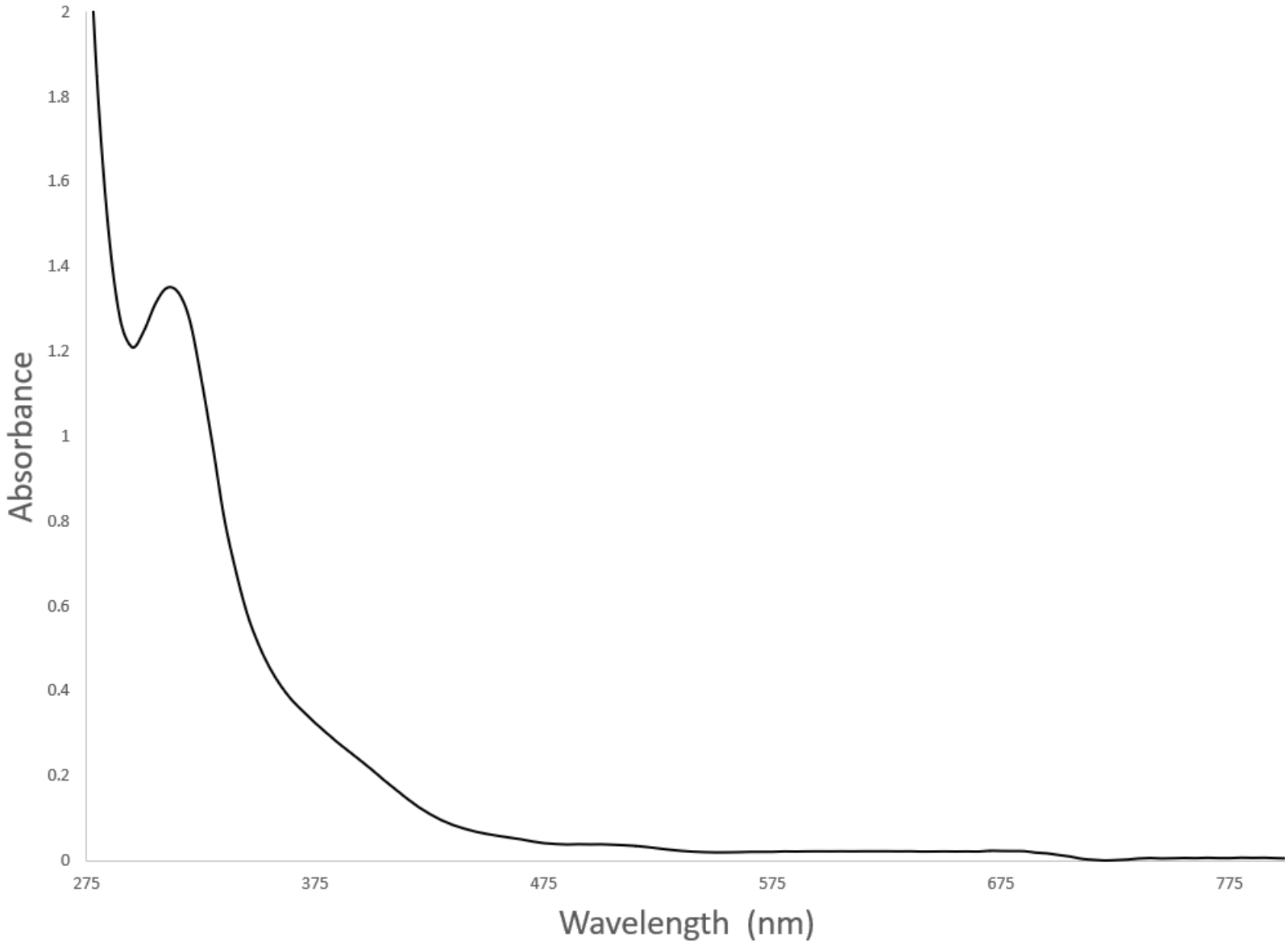



Figure S8 Ultraviolet-visible spectrum of **2** dissolved in THF.

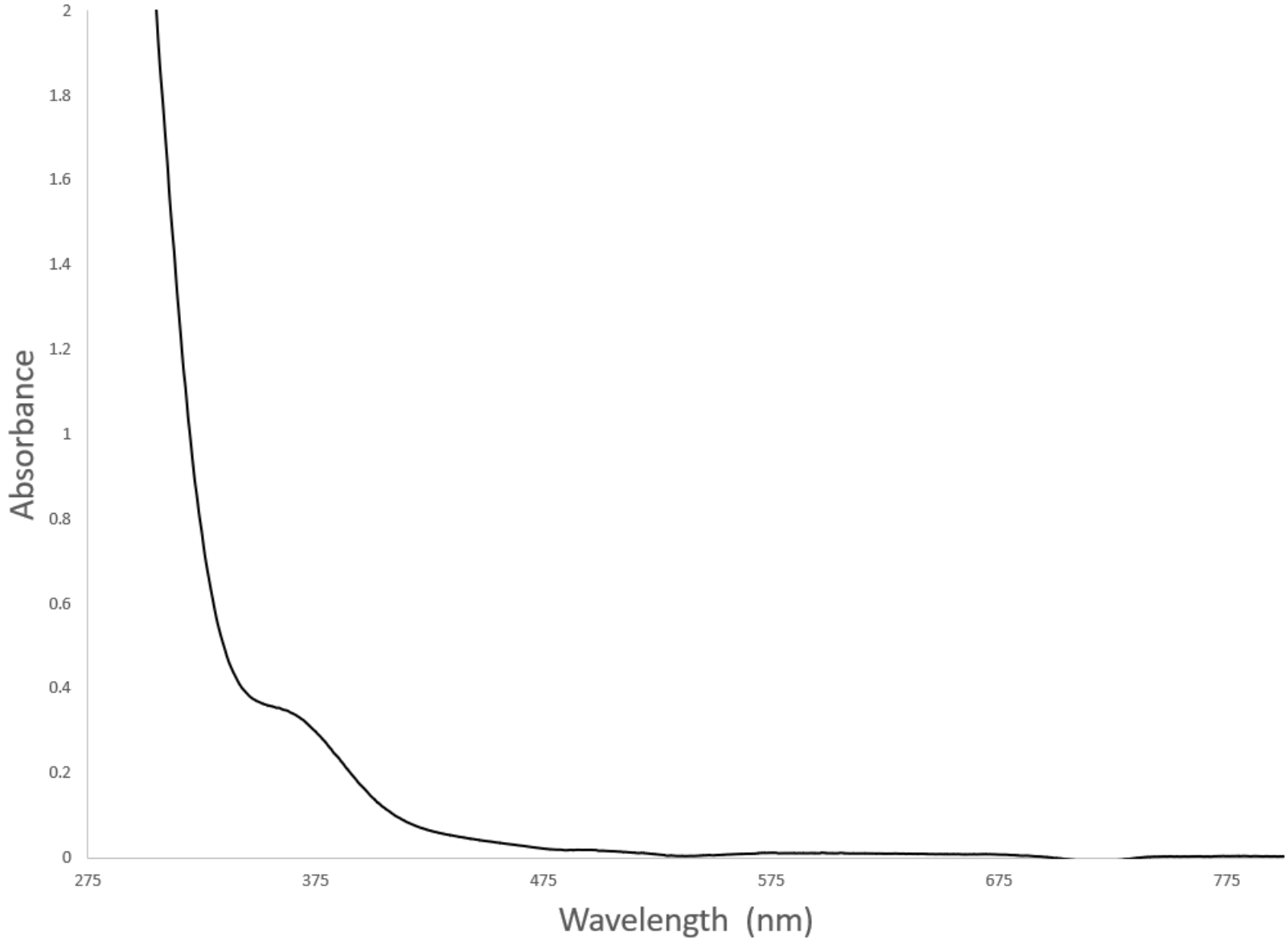



Figure S9 Ultraviolet-visible spectrum of **3** dissolved in THF.

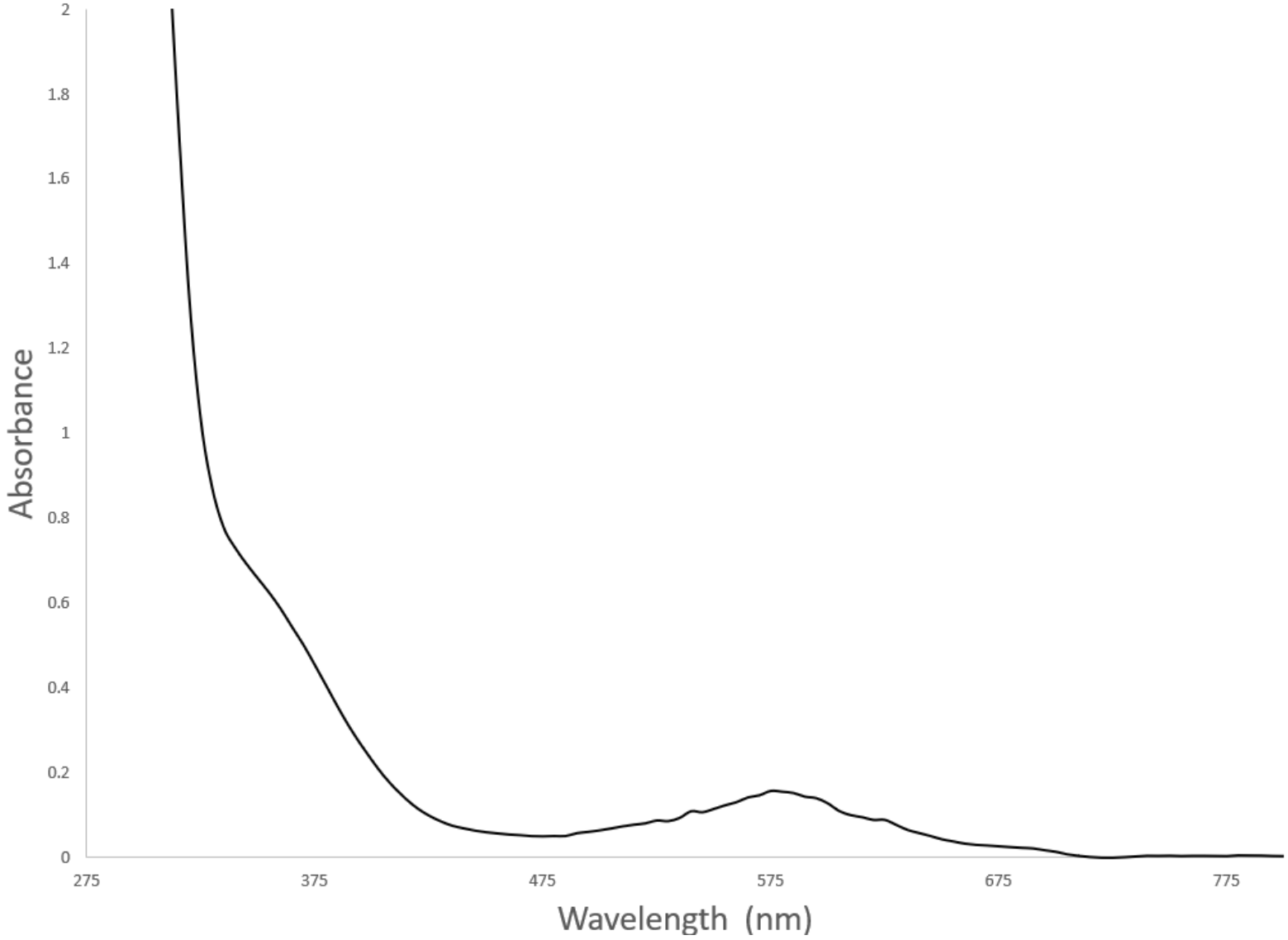



Figure S10 Ultraviolet-visible spectrum of **4** dissolved in THF.

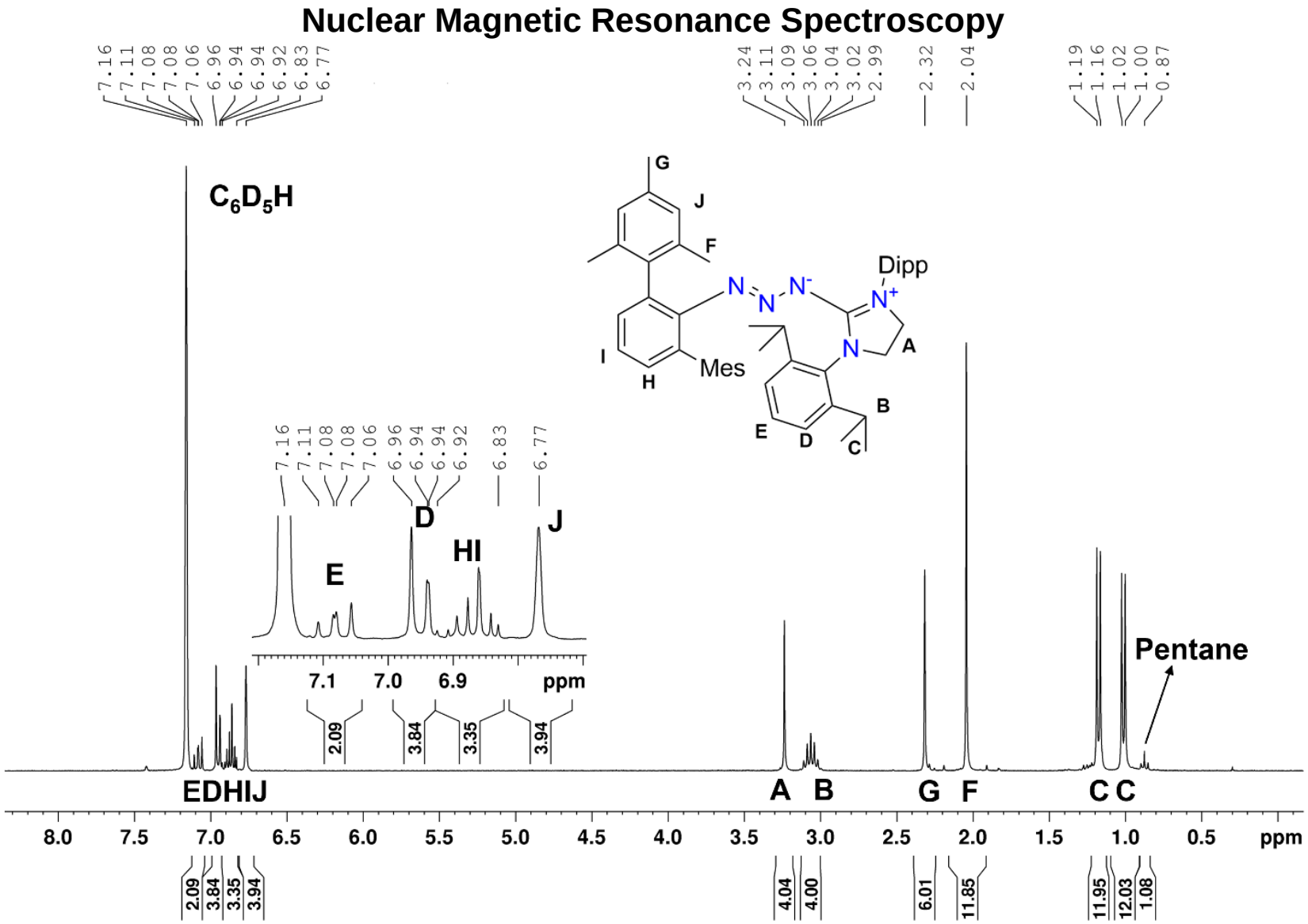



Figure S11 Assigned $^{1}$H NMR spectrum of **1** dissolved in $C_6D_6$.

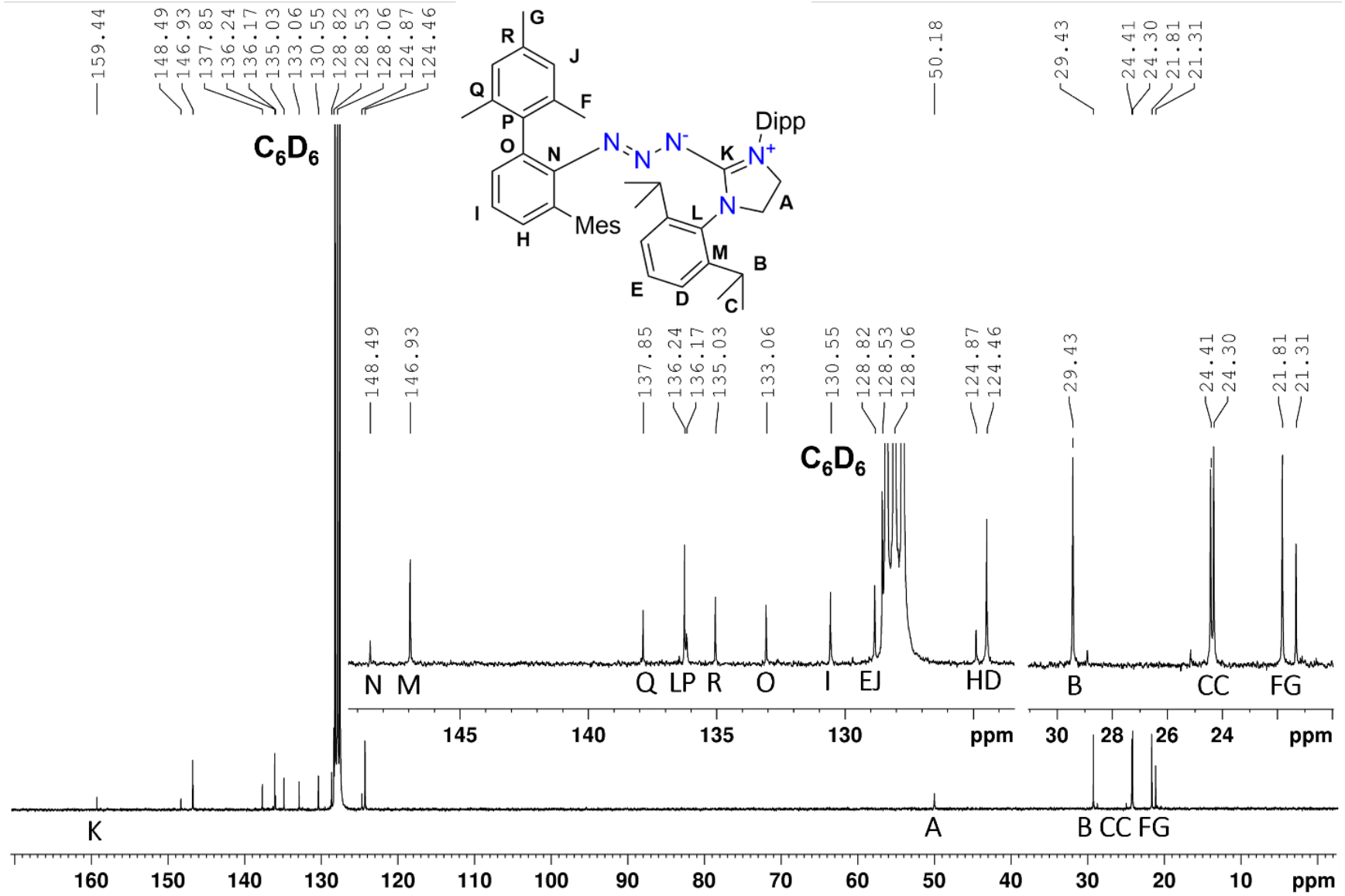



Figure S12 Assigned $^{13}C$ NMR spectrum of **1** dissolved in $C_6D_6$.

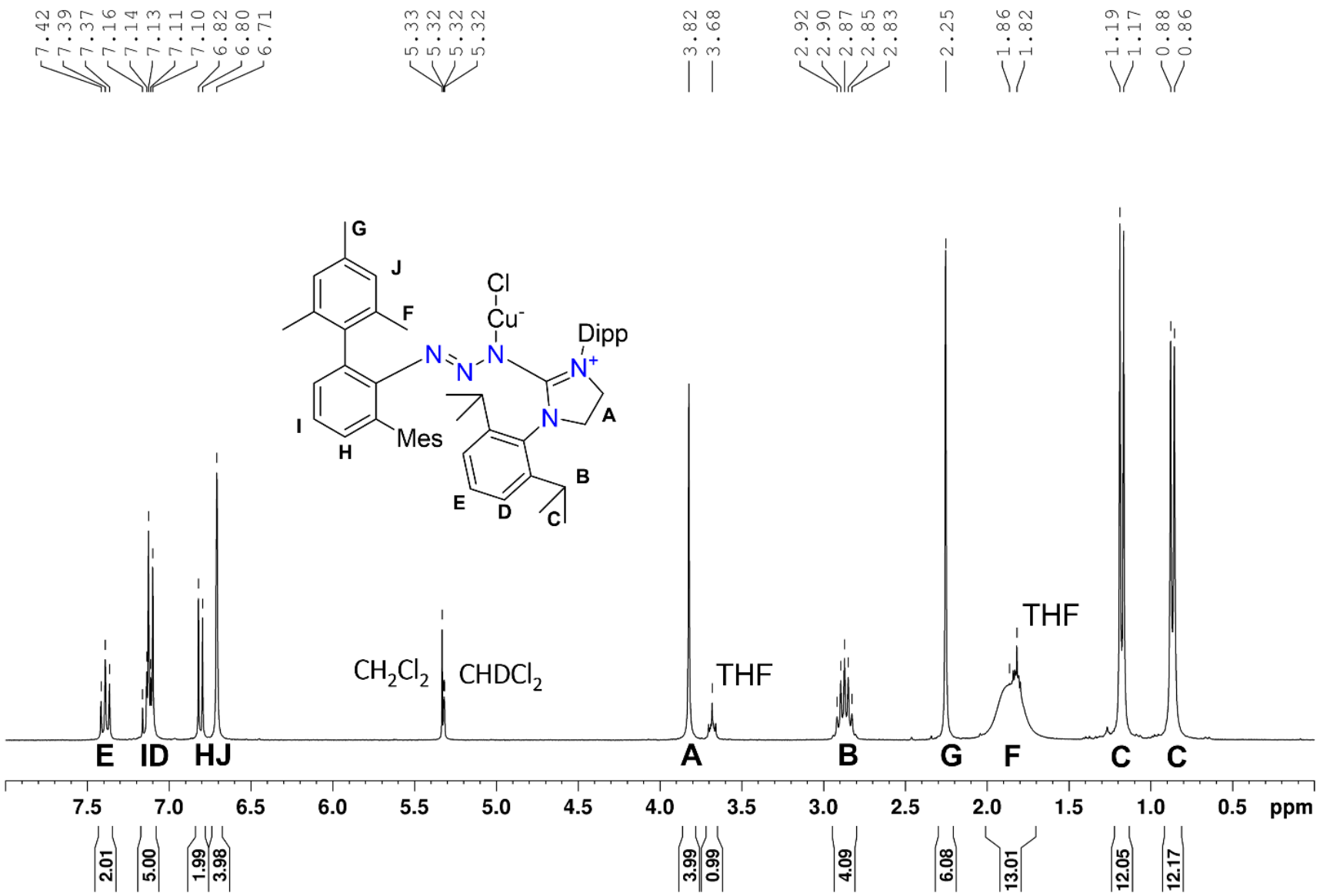



Figure S13 Assigned $^{1}H$ NMR spectrum of **2** dissolved in $CD_2Cl_2$.

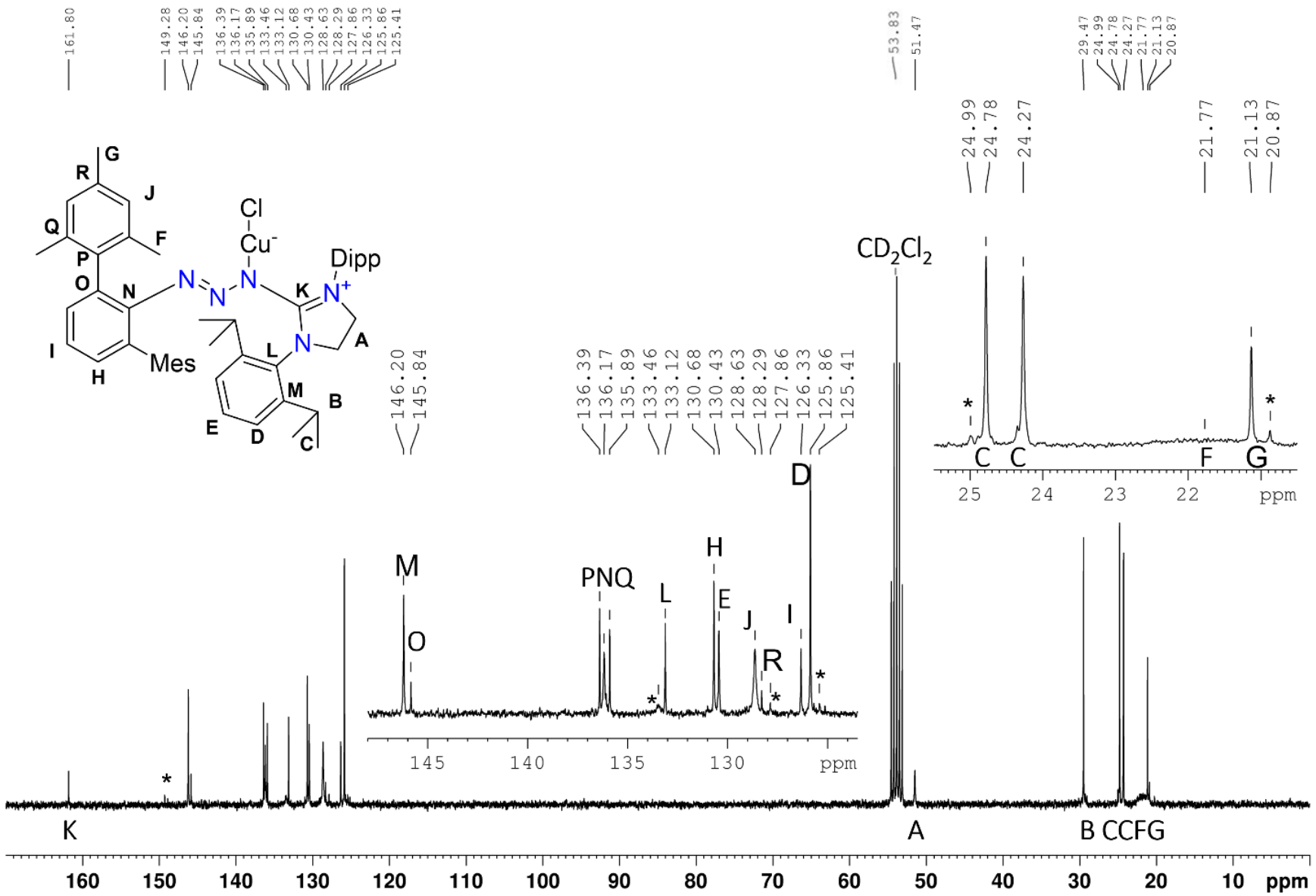



Figure S14 Assigned $^{13}C$ NMR spectrum of **2** dissolved in $CD_2Cl_2$.

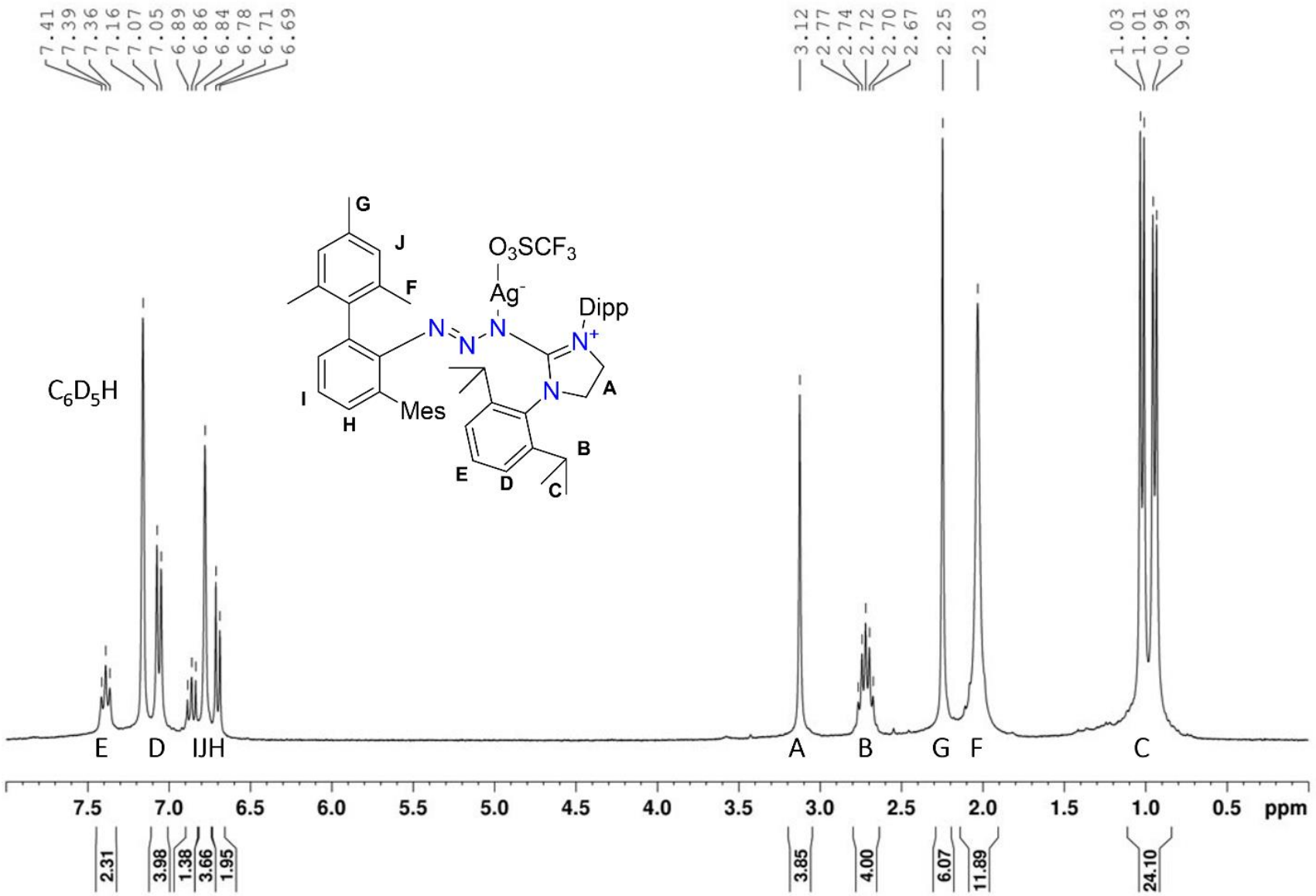



Figure S15 Assigned $^{1}H$ NMR spectrum of **3** dissolved in $C_6D_6$.

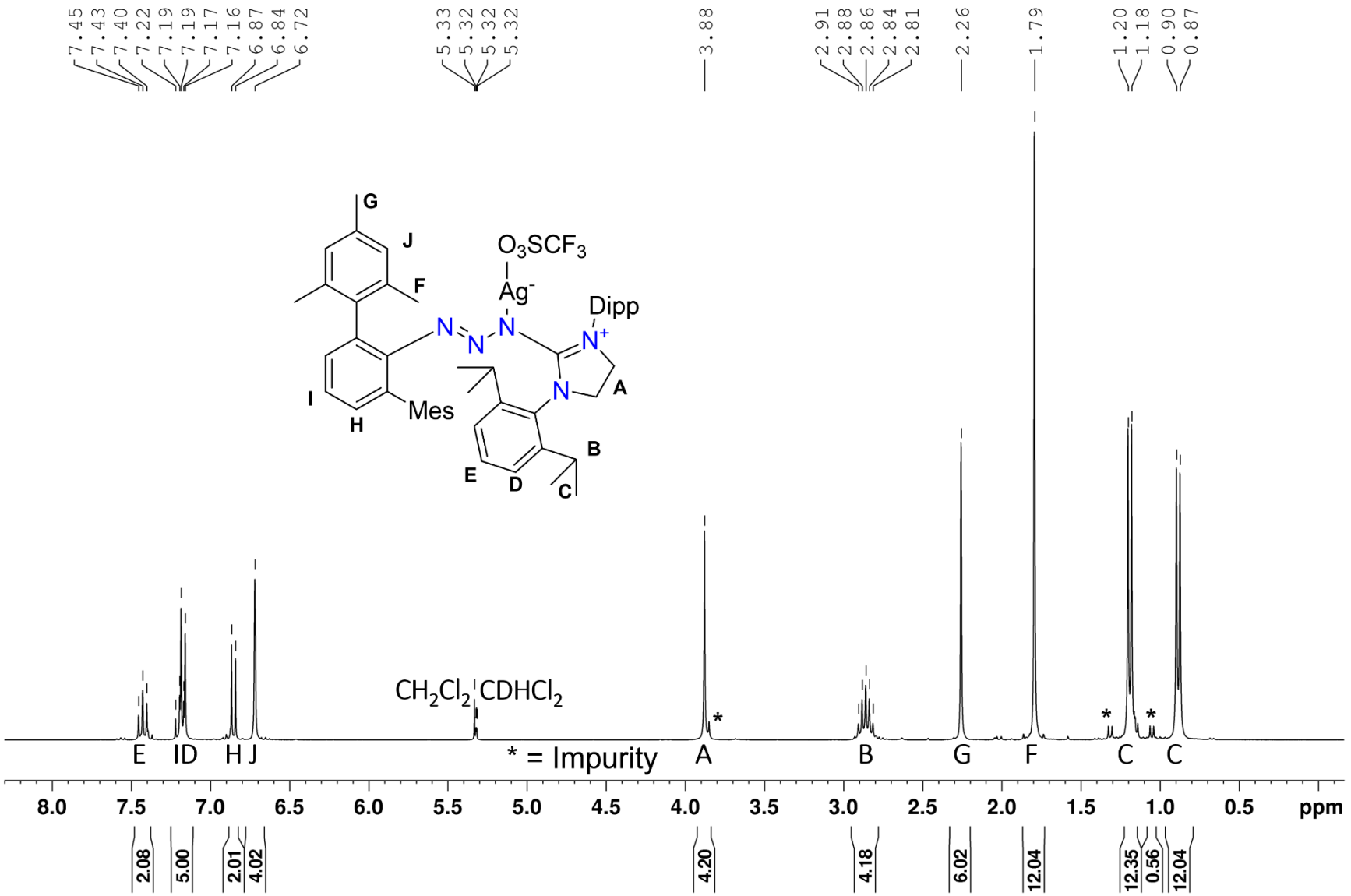



Figure S16 Assigned $^{1}H$ NMR spectrum of **3** dissolved in $CD_2Cl_2$.

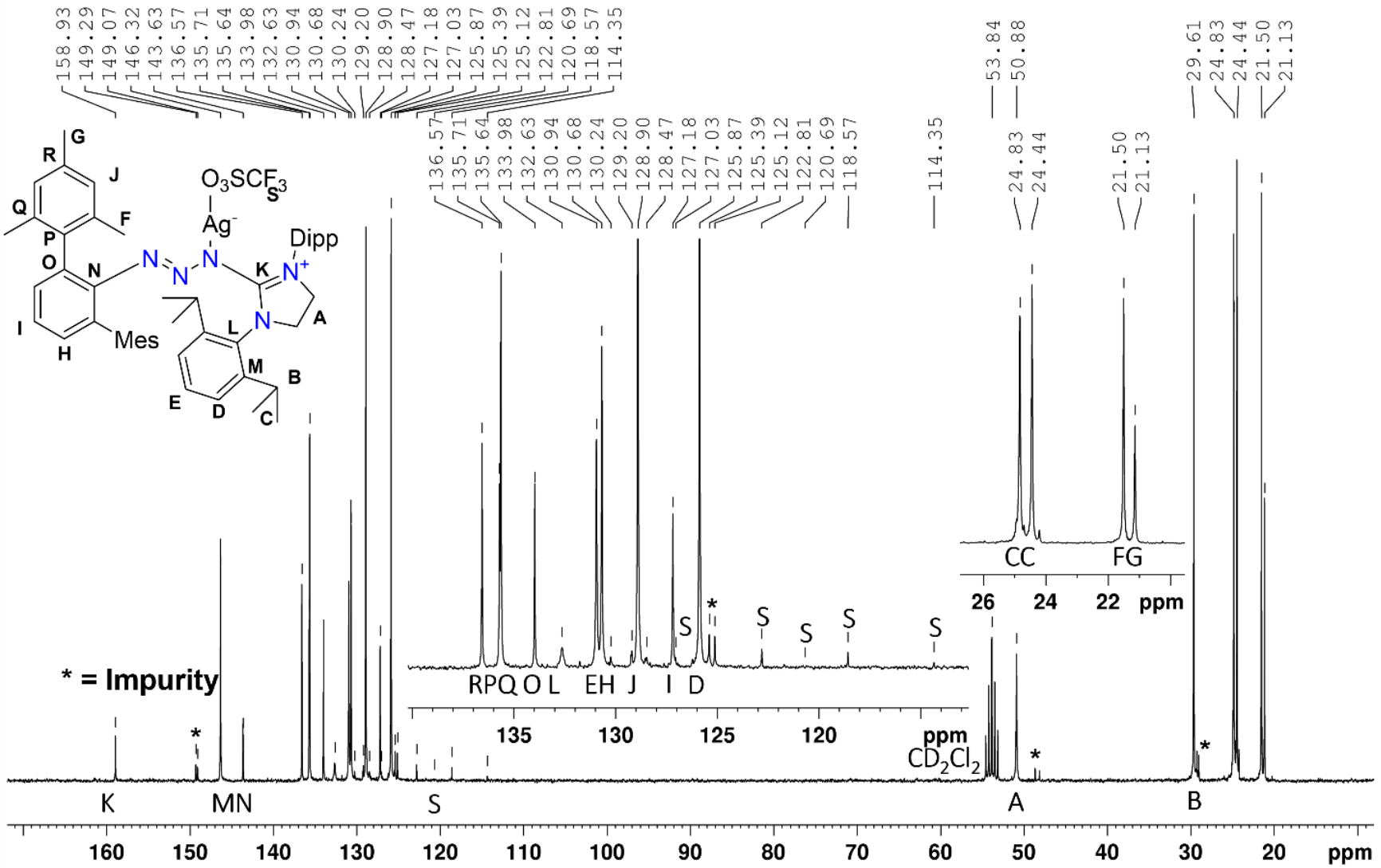



Figure S17 Assigned $^{13}C$ NMR spectrum of **3** dissolved in $CD_2Cl_2$.

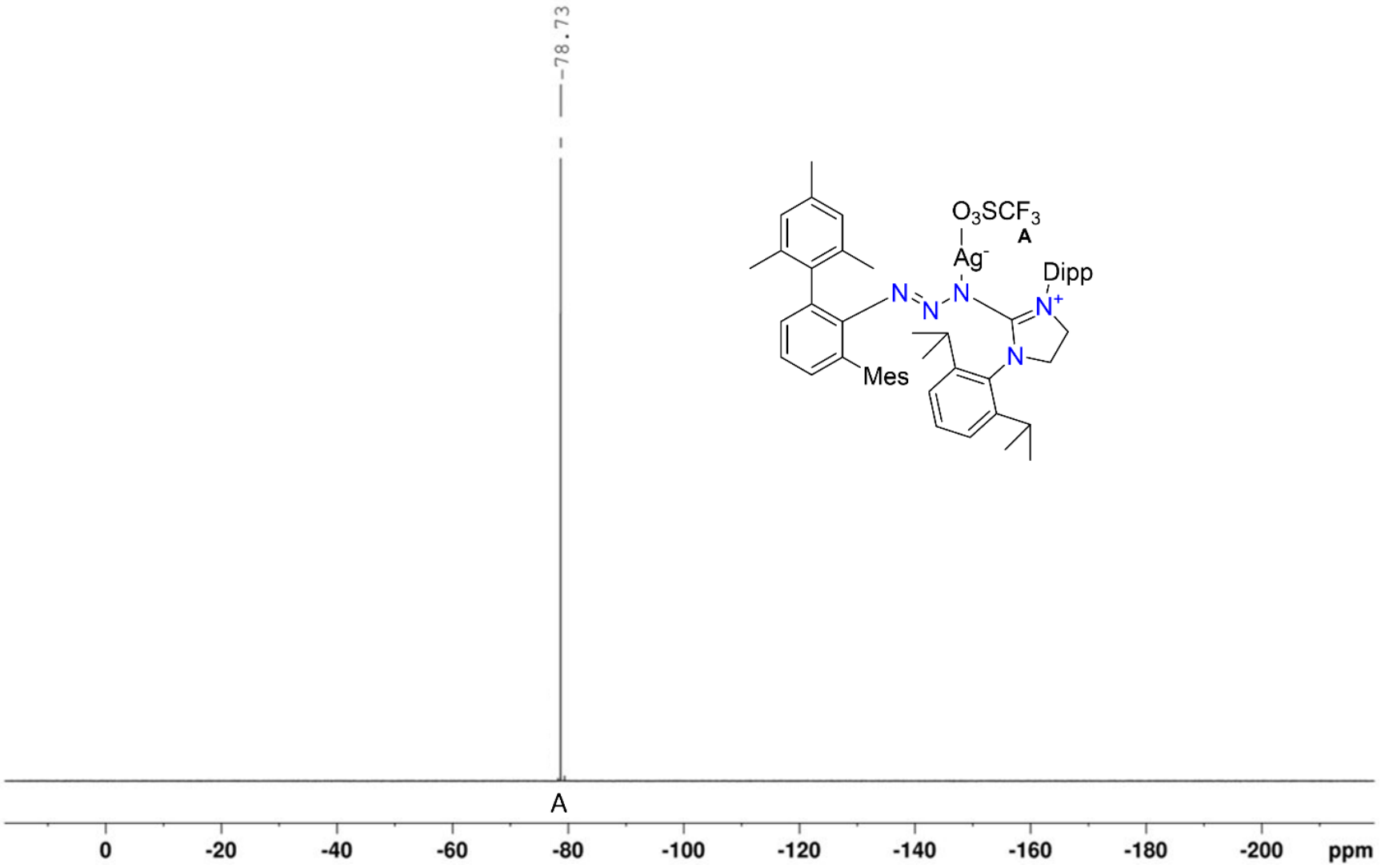



Figure S18 Assigned $^{19}F$ NMR spectrum of **3** dissolved in $CD_2Cl_2$.

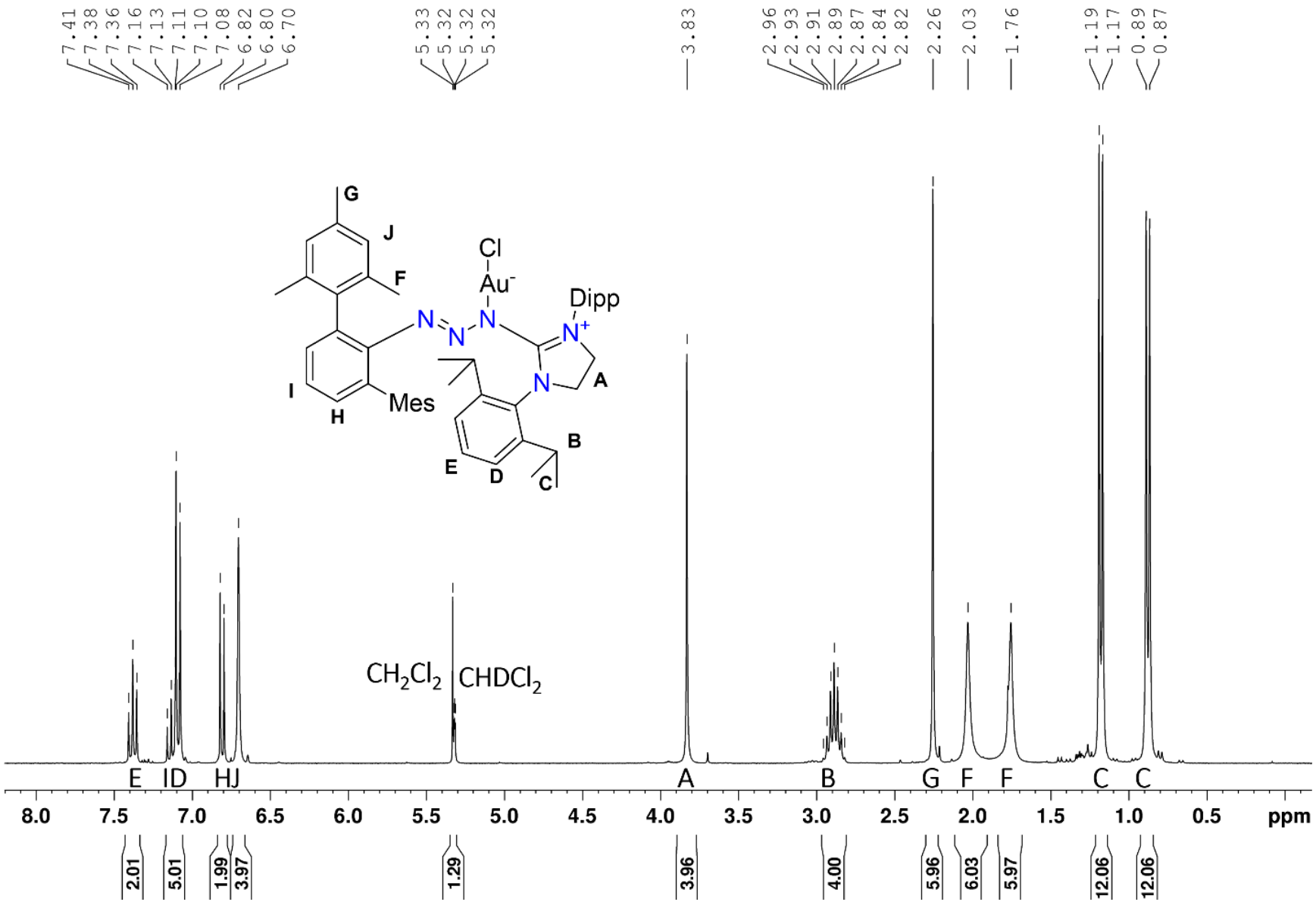



Figure S19 Assigned $^{1}H$ NMR spectrum of **4** dissolved in $CD_2Cl_2$.

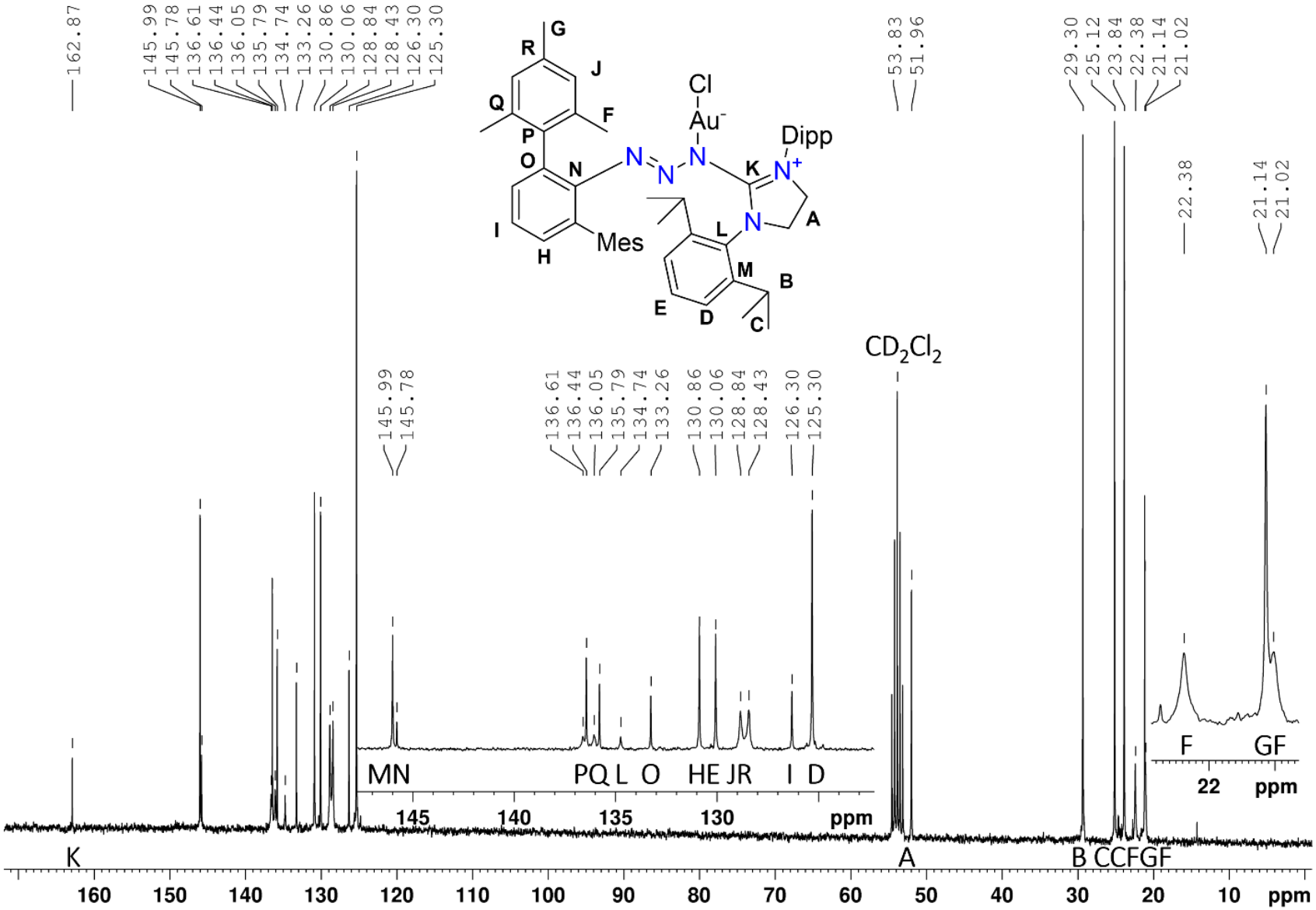



Figure S20 Assigned $^{13}C$ NMR spectrum of **4** dissolved in $CD_2Cl_2$.

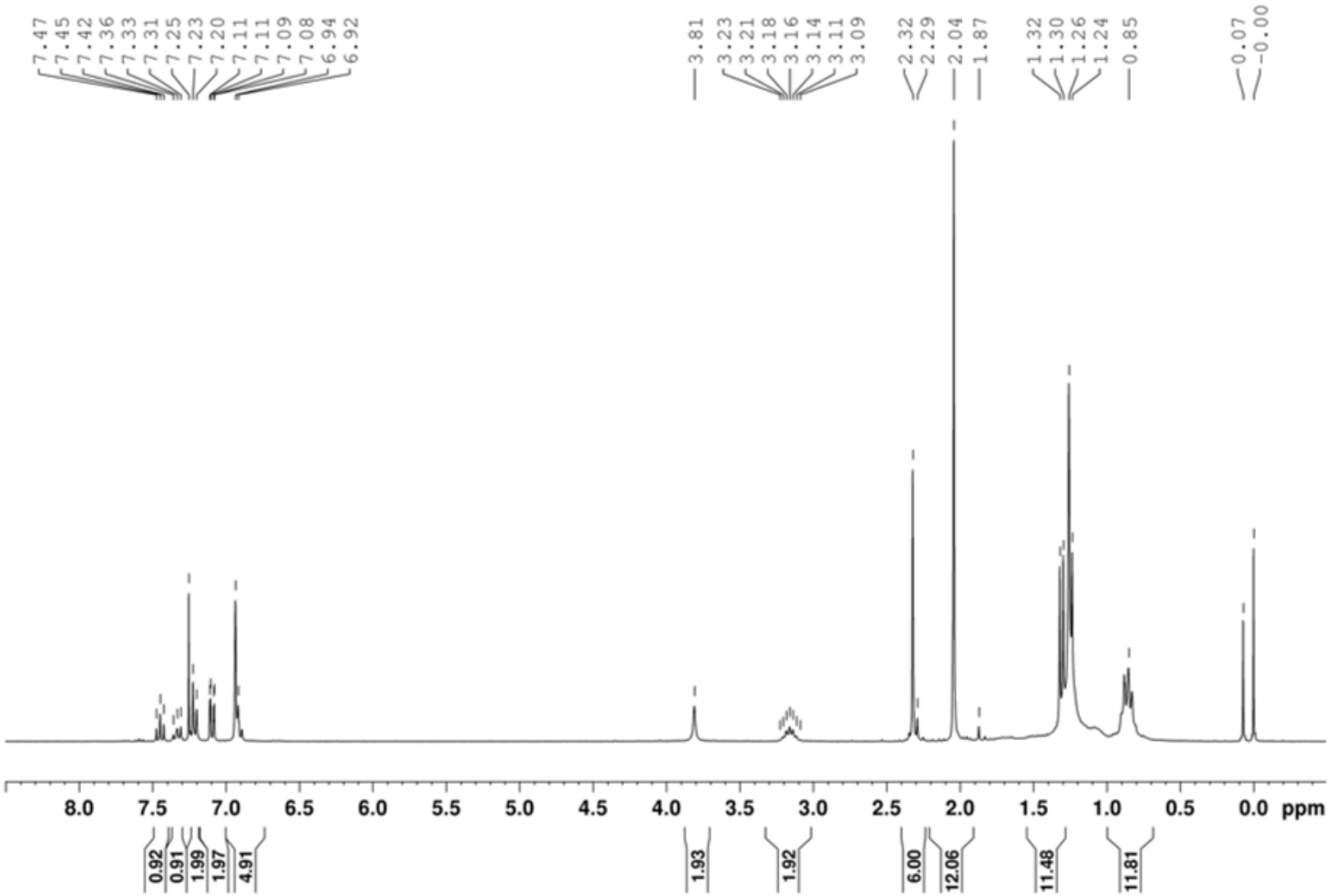



Figure S21 $^{1}H$ NMR spectrum in $CDCl_3$ of crude TerMesH dominant residue with unidentified SIPr containing material, along with pentane and silicone grease. Residue is derived from the preparation of **4** via crystallization and rinsing the crystals.

## Additional NMR Analysis

Analysis of **1** was done in $C_6D_6$, resulting in a $^{1}H$ NMR spectrum featuring nearly complete symmetry of the peaks observed. The only outlier is each of the isopropyl methyl peaks appears as two doublets centered at 1.17 and 1.01 ppm respectively. For each of the compounds **1**-**4**, a minimal shift in the N-C-N (previous carbene) $^{13}C$ NMR signal is observed. Chemical shifts barely differ, spanning a ~4 ppm range for the ligand **1** and the three metal complexes **2**-**4**. Of the three metal complexes, the silver complex **3** has the closest signal to the free ligand **1**, while the copper and gold complexes are slightly more deshielded.

The $^{1}H$ NMR spectrum of **3** was taken in both $C_6D_6$ and $CD_2Cl_2$ to explore potential solvent dependent differences. In $C_6D_6$, the compound exhibits symmetric equivalence of the TerMes fragment with a broad singlet centered at 2.03 ppm for the *ortho*-mesityl methyl protons. The SIPr fragment likewise features primarily symmetric signals, however, minor inequivalence of the Dipp methyl groups is observed with doublets centered at 0.94 and 1.02 ppm. *Meta*-mesityl protons, *meta*-Dipp protons, and the *para*-TerMes proton nearly overlap, but are resolved enough to observe the distinct singlet (6.78 ppm), doublet (6.70 ppm), and triplet (6.86 ppm) respectively. In $CD_2Cl_2$, **3** exhibits similar symmetry, however, peaks such as the *ortho*-mesityl methyl peak is far sharper and is observed upfield shifted compared to $C_6D_6$ solution (1.79 vs 2.03 ppm respectively). Greater separation of the inequivalent Dipp methyl signals is also observed in $CD_2Cl_2$ with the doublets appearing at 1.19 and 0.88 ppm. Chemical shifts of the aryl protons also differ, with the *meta*-TerMes aryl protons occurring more upfield vs. $C_6D_6$ solution (6.85 vs 6.70 ppm respectively). The other significant shift occurs for the *para*-TerMes triplet which is downfield shifted to 7.19 ppm in $CD_2Cl_2$ solution vs. 6.86 ppm in $C_6D_6$. The $^{19}F$ NMR signal for the trifluoromethyl group of the anion is observed at -78.73 ppm.

The $^{1}H$ NMR spectrum of **2** is very similar to that of **4**. The only notable difference is that the *ortho*-mesityl methyl protons are observed as a single broad singlet at 1.86 ppm rather than two distinct separate broad signals for the gold analogue. For **4**, asymmetry is observed for the protons of the *ortho*-mesityl methyl protons which appear as broad singlets at 1.76 and 2.03 ppm, along with the Dipp methyl groups with doublets centered at 0.88 and 1.18 ppm. All other protons are well enough resolved for complete identification, despite minor overlap of the *para*-TerMes triplet and the *meta*-Dipp doublet.

# High Resolution Mass Spectrometry

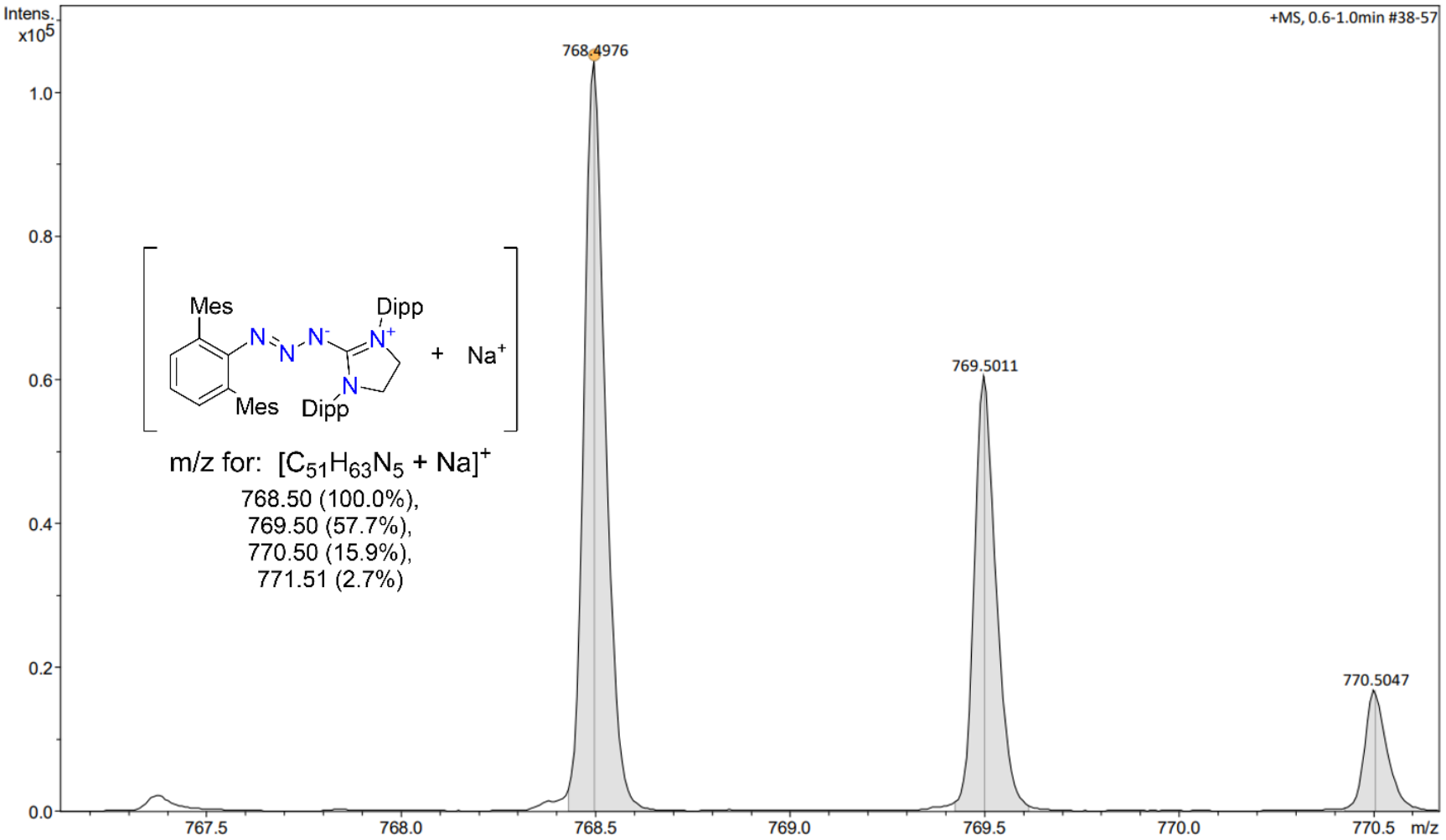



Figure S22 High resolution mass spectrum of **1**.

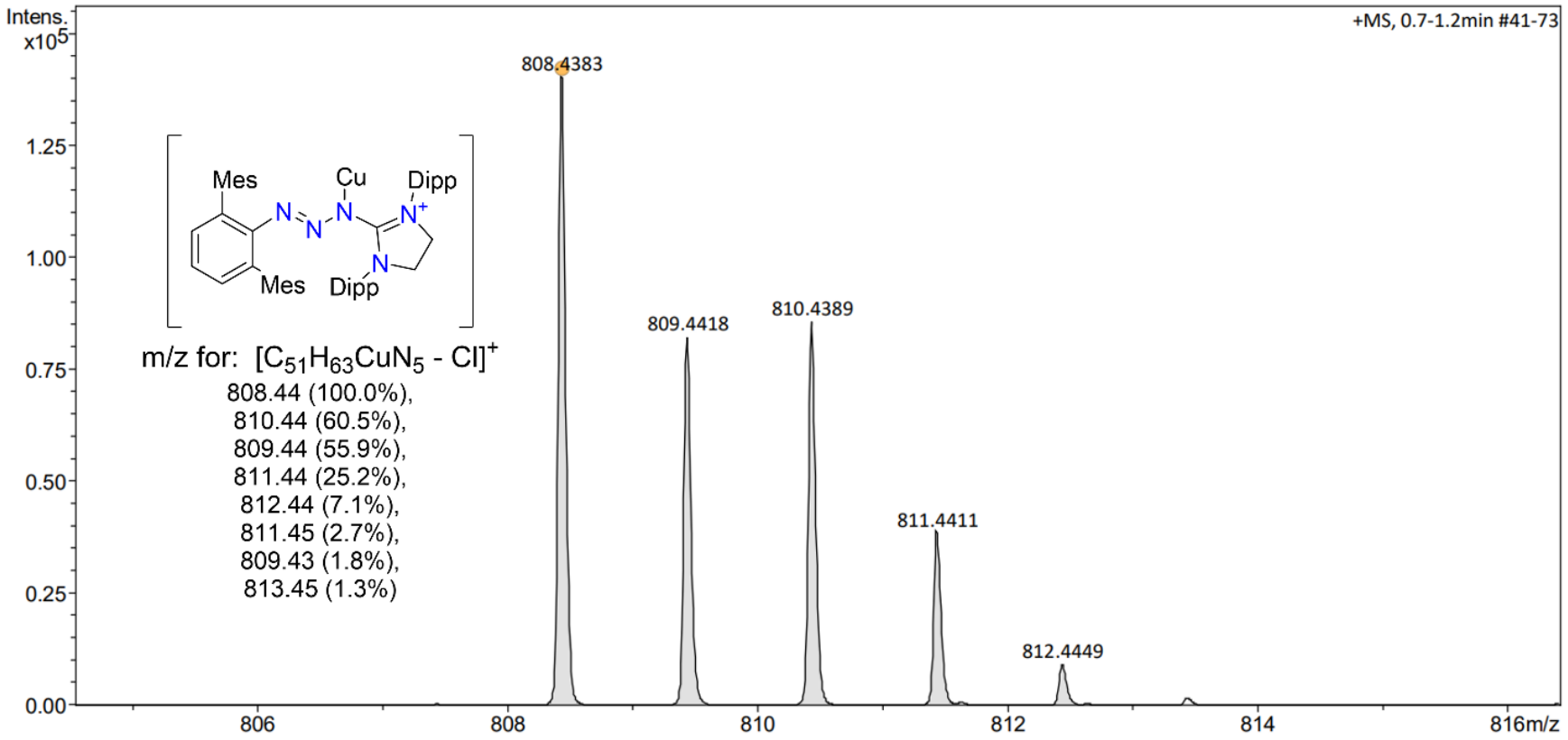



Figure S23 High resolution mass spectrum of **2**.

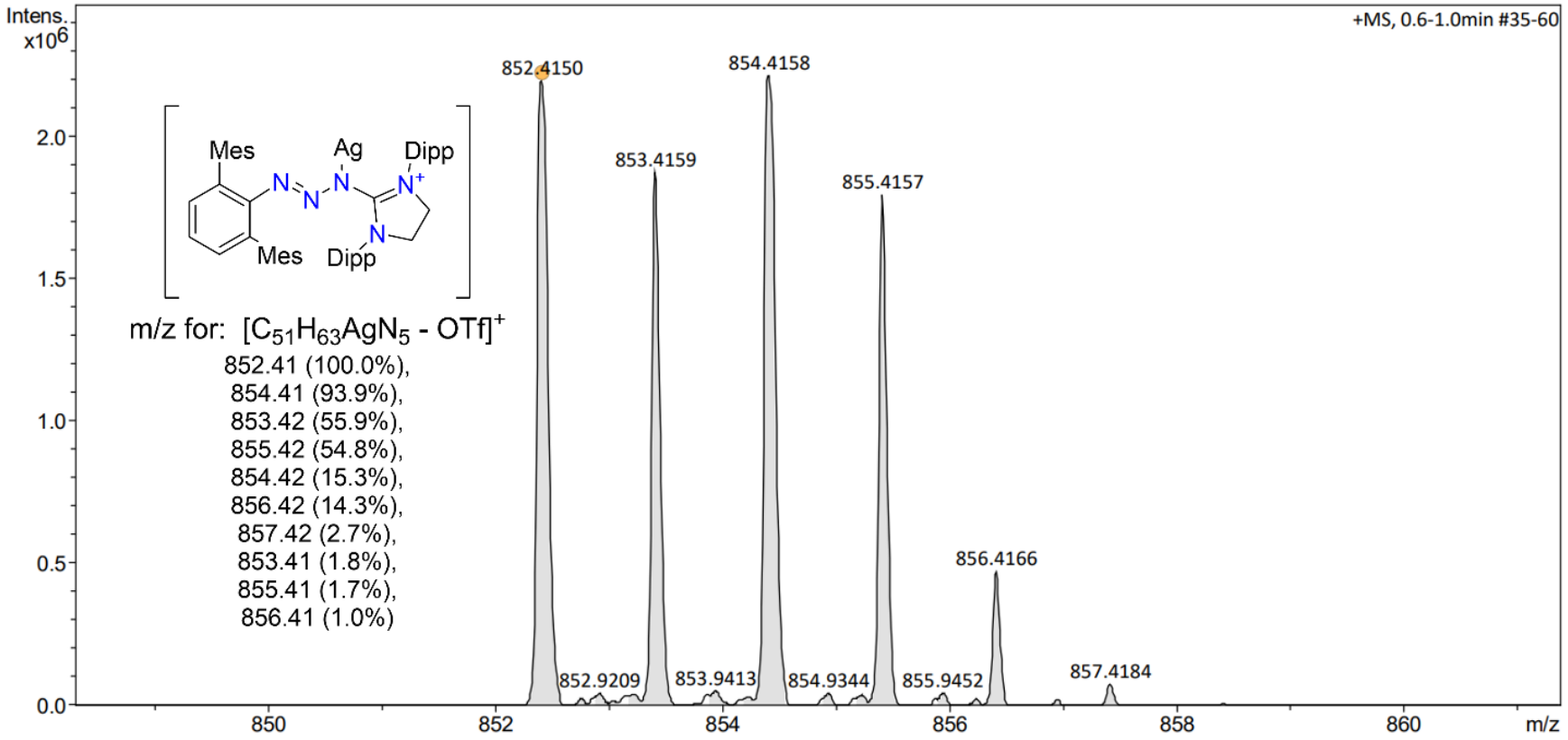



Figure S24 High resolution mass spectrum of **3**.

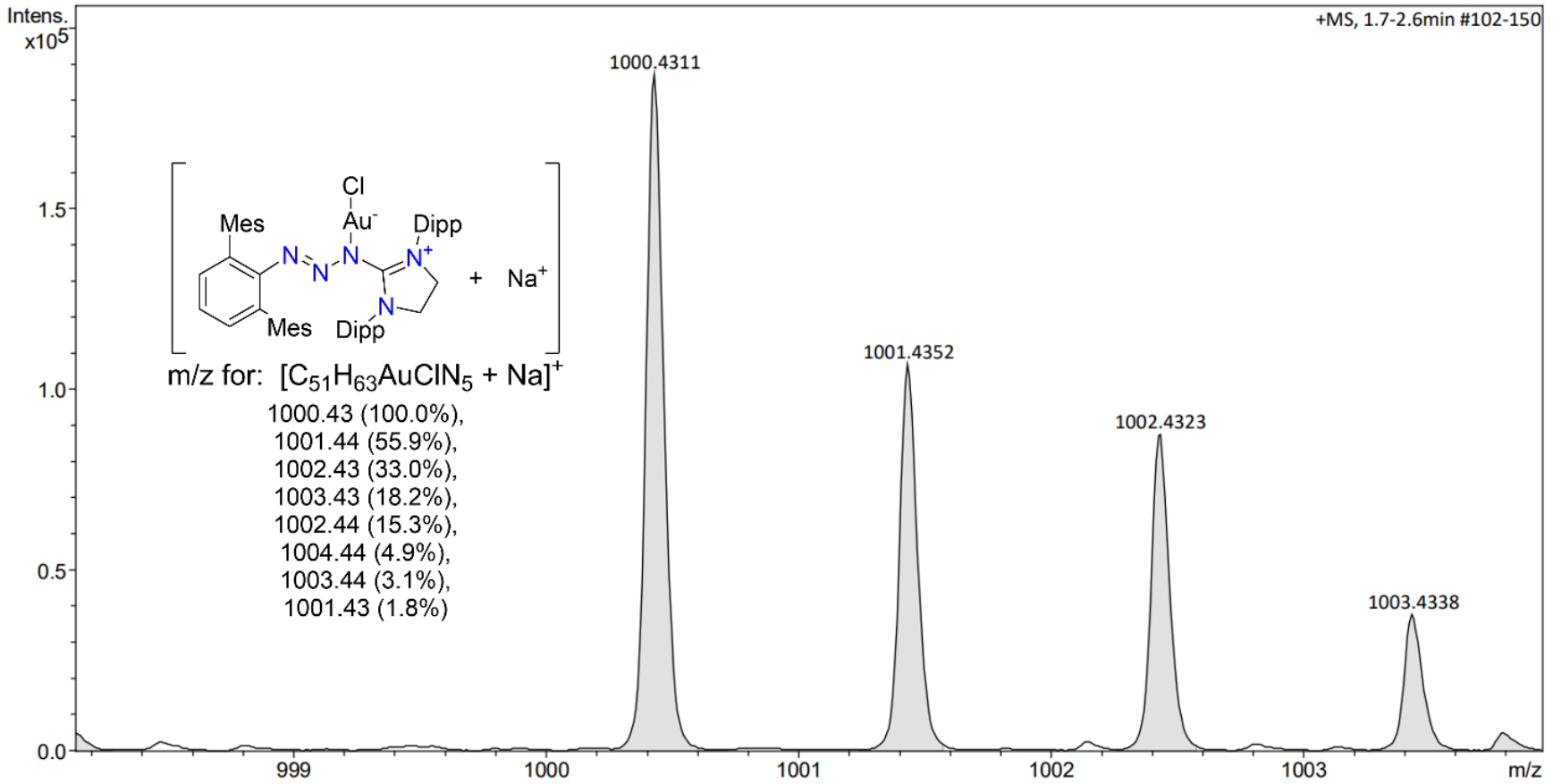



Figure S25 High resolution mass spectrum of **4**.

# Single Crystal X-ray Diffraction

**Table S1.** Crystallographic data related to the single crystal X-ray diffraction of (E)- and (Z)- isomers of **1** and the $C_6D_6$ solvate of **2**. A crystal of the iodide analogue of solvent free **2** was also isolated but could not be prepared clean.

| Identification code | **1-(*E*)** | **1-(*Z*)** | **2·$C_6D_6$** | **1·CuI** |
|---|---|---|---|---|
| Empirical formula | $C_{51}H_{63}N_5$ | $C_{51}H_{63}N_5$ | $C_{57}H_{63}N_5CuClD_6$ | $C_{51}H_{63}N_5CuI$ |
| Formula weight | 746.06 | 746.06 | 929.19 | 936.5 |
| Temperature/K | 125 | 150 | 125 | 300 |
| Crystal system | triclinic | monoclinic | Monoclinic | monoclinic |
| Space group | P-1 | C2/c | P21/n | P21 |
| a/Å | 11.2025(4) | 39.281(2) | 10.6515(3) | 11.7942(3) |
| b/Å | 11.2154(4) | 11.3290(7) | 19.6951(5) | 18.1027(6) |
| c/Å | 19.5845(8) | 20.6762(12) | 24.8627(7) | 12.4614(5) |
| α/° | 88.4840(10) | 90 | 90 | 90 |
| β/° | 81.3940(10) | 105.449(2) | 99.2710(10) | 112.8800(10) |
| γ/° | 65.5370(10) | 90 | 90 | 90 |
| Volume/Å3 | 2212.77(14) | 8868.8(9) | 5147.6(2) | 2451.26(14) |
| Z | 2 | 8 | 4 | 2 |
| ρcalcg/cm3 | 1.12 | 1.118 | 1.199 | 1.269 |
| μ/mm-1 | 0.065 | 0.065 | 0.517 | 1.112 |
| F(000) | 808 | 3232 | 1968 | 972 |
| Crystal size/mm3 | 0.1 × 0.1 × 0.1 | 0.1 × 0.09 × 0.06 | 0.35 × 0.24 × 0.18 | 0.32 × 0.17 × 0.04 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.992 to 55.006 | 4.08 to 52.744 | 4.454 to 69.94 | 4.036 to 72.526 |
| Index ranges | -14 ≤ h ≤ 14, -14 ≤ k ≤ 14, -25 ≤ l ≤ 25 | -48 ≤ h ≤ 48, -14 ≤ k ≤ 14, -25 ≤ l ≤ 25 | -17 ≤ h ≤ 15, -31 ≤ k ≤ 31, -40 ≤ l ≤ 40 | -19 ≤ h ≤ 19, -29 ≤ k ≤ 29, -20 ≤ l ≤ 20 |
| Reflections collected | 121195 | 224787 | 239862 | 178176 |
| Independent reflections | 10166 [Rint = 0.0388, Rsigma = 0.0273] | 9075 [Rint = 0.1124, Rsigma = 0.0325] | 22589 [Rint = 0.0386, Rsigma = 0.0211] | 23181 [Rint = 0.0503, Rsigma = 0.0268] |
| Data/restraints/parameters | 10166/0/519 | 9075/0/520 | 22589/5/591 | 23181/1/537 |
| Goodness-of-fit on F2 | 1.035 | 1.049 | 1.082 | 1.085 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0772, wR2 = 0.1982 | R1 = 0.0693, wR2 = 0.1659 | R1 = 0.0437, wR2 = 0.1223 | R1 = 0.0250, wR2 = 0.0572 |
| Final R indexes [all data] | R1 = 0.0897, wR2 = 0.2113 | R1 = 0.0999, wR2 = 0.1865 | R1 = 0.0620, wR2 = 0.1413 | R1 = 0.0336, wR2 = 0.0633 |
| Largest diff. peak/hole / e Å-3 | 0.99/-0.36 | 0.70/-0.28 | 0.75/-0.80 | 0.91/-0.66 |
| Flack parameter | | | | 0.009(2) |

**Table S2.** Crystallographic data related to the single crystal X-ray diffraction of silver(I) triflate complex **3**, solvent free and $C_6D_6$ co-crystallized gold complex **4**, and unexpected gold salt **5** and **TerMesH** that were isolated from the hydrolyzed residue left from the synthesis of **4**.

| Identification code | **3** | **4** | **4-$C_6D_6$** | **5** | **TerMesH** |
|---|---|---|---|---|---|
| Empirical formula | $C_{52}H_{63}N_5AgF_3O_3S$ | $C_{51}H_{63}N_5AuCl$ | $C_{57}H_{63}N_5AuClD_6$ | $C_{54}H_{78}N_6Au_2Cl_2$ | $C_{24}H_{26}$ |
| Formula weight | 1003 | 978.48 | 1062.62 | 1276.05 | 314.45 |
| Temperature/K | 125 | 150 | 100 | 150 | 150 |
| Crystal system | Orthorhombic | monoclinic | Monoclinic | monoclinic | triclinic |
| Space group | Pca21 | P21/n | P21/n | P21/n | P-1 |
| a/Å | 22.0453(16) | 10.7224(7) | 10.6309(2) | 15.0715(14) | 9.0095(10) |
| b/Å | 11.9742(8) | 19.5925(13) | 19.3993(5) | 12.0259(11) | 11.7459(14) |
| c/Å | 18.6052(15) | 25.0634(17) | 25.4245(7) | 16.7031(13) | 18.4967(18) |
| α/° | 90 | 90 | 90 | 90 | 98.261(5) |
| β/° | 90 | 99.514(3) | 99.2860(10) | 115.525(3) | 95.617(5) |
| γ/° | 90 | 90 | 90 | 90 | 106.614(5) |
| Volume/Å$^3$ | 4911.3(6) | 5192.9(6) | 5174.6(2) | 2731.9(4) | 1836.2(4) |
| Z | 4 | 4 | 4 | 2 | 4 |
| ρcalcg/cm$^3$ | 1.356 | 1.252 | 1.364 | 1.551 | 1.137 |
| μ/mm$^{-1}$ | 0.511 | 2.92 | 2.935 | 5.501 | 0.064 |
| F(000) | 2096 | 2000 | 2168 | 1272 | 680 |
| Crystal size/mm$^3$ | 0.29 × 0.2 × 0.15 | 0.07 × 0.04 × 0.03 | 0.22 × 0.07 × 0.07 | 0.33 × 0.07 × 0.02 | 0.2 × 0.08 × 0.06 |
| Radiation | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) | MoKα (λ = 0.71073) |
| 2Θ range for data collection/° | 3.87 to 72.694 | 3.896 to 54.206 | 3.866 to 57 | 4.522 to 54.324 | 4.644 to 50.05 |
| Index ranges | -36 ≤ h ≤ 36, -19 ≤ k ≤ 19, -31 ≤ l ≤ 31 | -13 ≤ h ≤ 13, -25 ≤ k ≤ 25, -32 ≤ l ≤ 32 | -14 ≤ h ≤ 14, -26 ≤ k ≤ 26, -34 ≤ l ≤ 34 | -19 ≤ h ≤ 19, -15 ≤ k ≤ 15, -21 ≤ l ≤ 21 | -10 ≤ h ≤ 10, -13 ≤ k ≤ 13, -22 ≤ l ≤ 22 |
| Reflections collected | 262752 | 134659 | 163551 | 66080 | 64785 |
| Independent reflections | 23773 [Rint = 0.0533, Rsigma = 0.0248] | 11462 [Rint = 0.0902, Rsigma = 0.0378] | 13114 [Rint = 0.0309, Rsigma = 0.0132] | 6062 [Rint = 0.0523, Rsigma = 0.0271] | 6451 [Rint = 0.1108, Rsigma = 0.0530] |
| Data / restraints / parameters | 23773/7/621 | 11462/0/537 | 13114/0/618 | 6062/0/316 | 6451/0/445 |
| Goodness-of-fit on F2 | 1.159 | 1.173 | 1.106 | 1.058 | 1.2 |
| Final R indexes [I>=2σ (I)] | R1 = 0.0298, wR2 = 0.0745 | R1 = 0.0532, wR2 = 0.1414 | R1 = 0.0357, wR2 = 0.0819 | R1 = 0.0261, wR2 = 0.0577 | R1 = 0.0945, wR2 = 0.1754 |
| Final R indexes [all data] | R1 = 0.0411, wR2 = 0.0860 | R1 = 0.0852, wR2 = 0.1770 | R1 = 0.0413, wR2 = 0.0888 | R1 = 0.0349, wR2 = 0.0638 | R1 = 0.1446, wR2 = 0.2025 |
| Largest diff. peak/hole / e Å$^{-3}$ | 0.90/-0.80 | 3.38/-2.02 | 1.74/-0.93 | 2.04/-1.57 | 0.27/-0.25 |
| Flack Parameter | -0.020(4) | - | - | - | - |

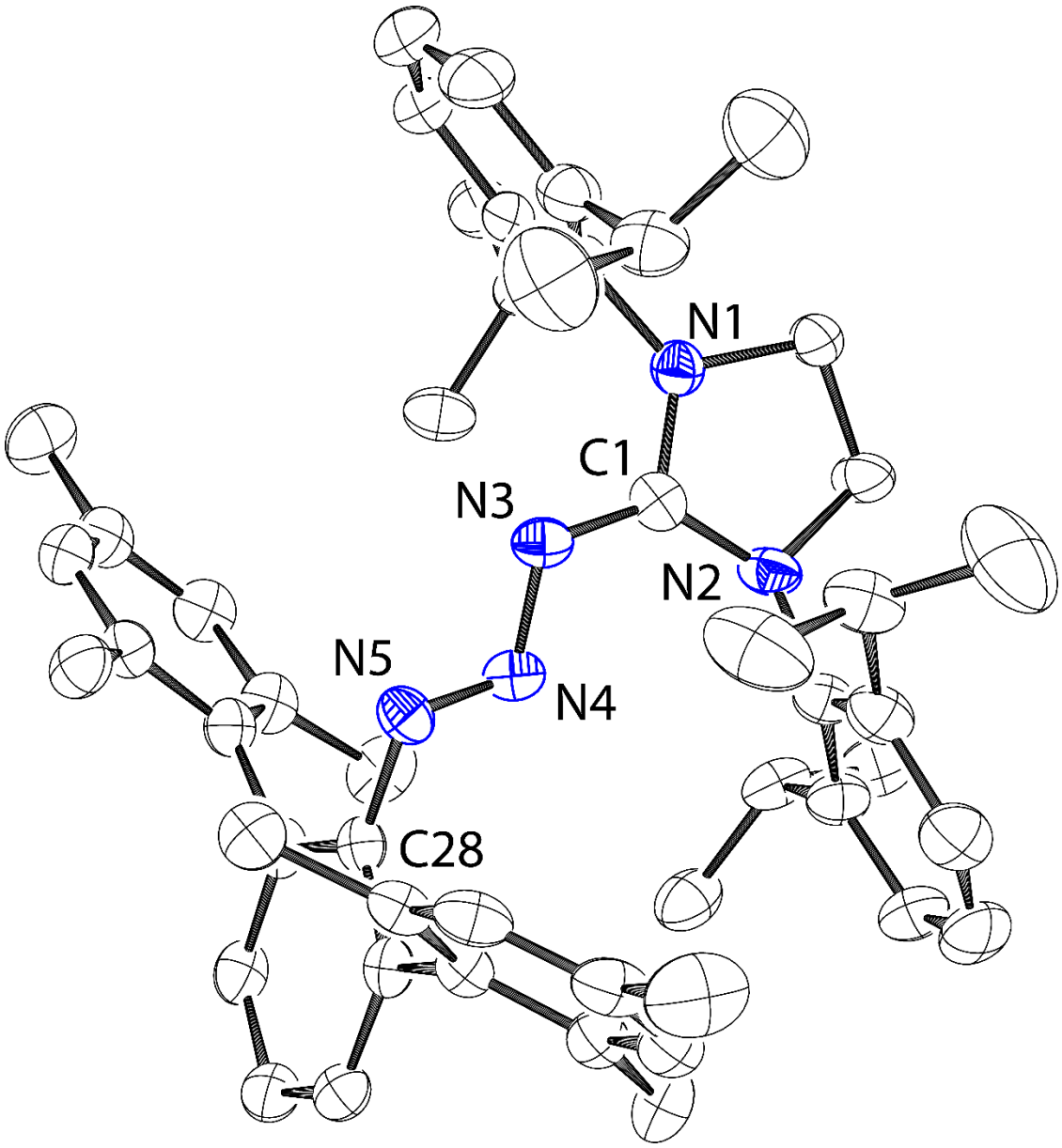



Figure S26 Molecular structure of **1** as the (*E*)-isomer with anisotropic displacement ellipsoids projected at the 50% probability level. Hydrogen atoms have been omitted for clarity.

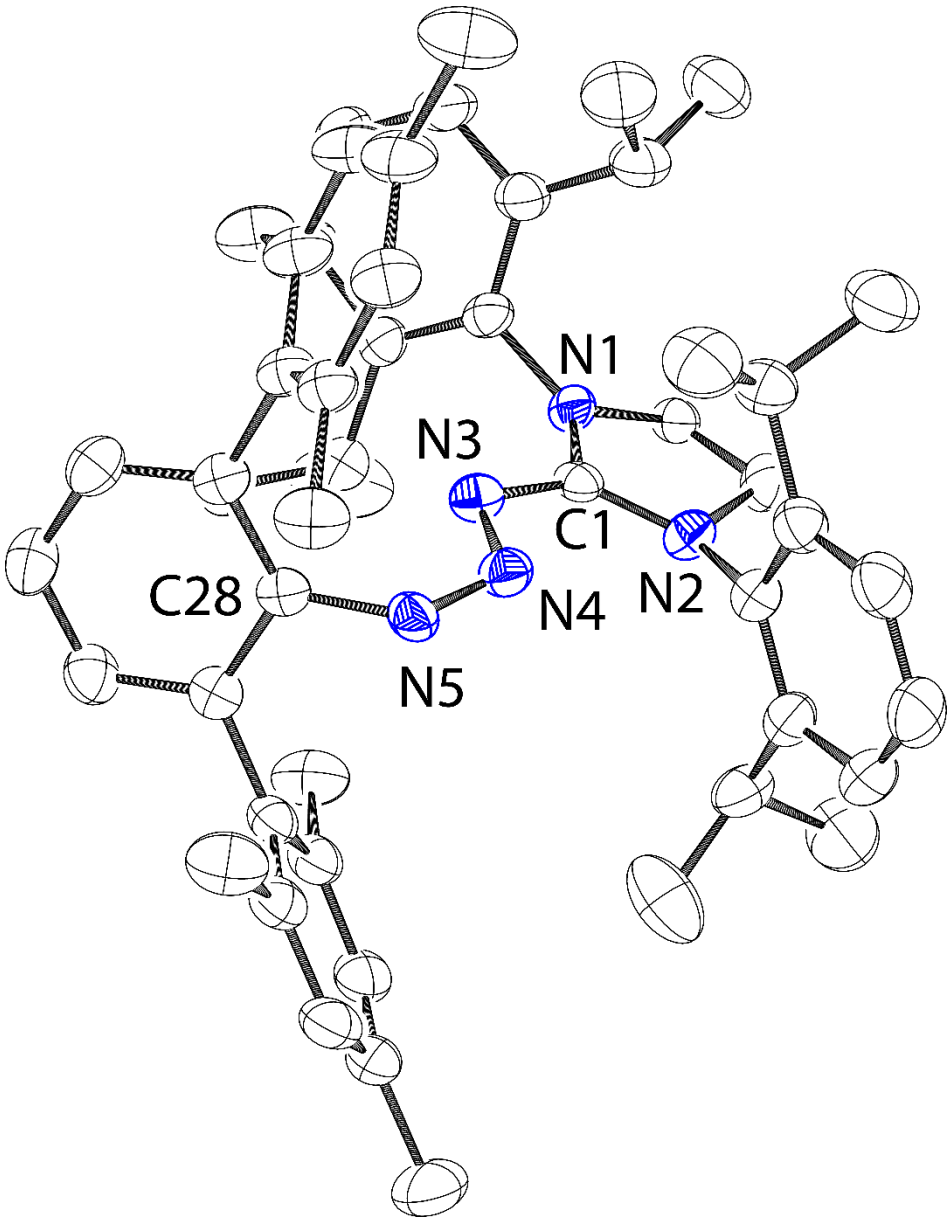



Figure S27 Molecular structure of **1** as the (*Z*)-isomer with anisotropic displacement ellipsoids projected at the 50% probably level. Hydrogen atoms have been omitted for clarity.

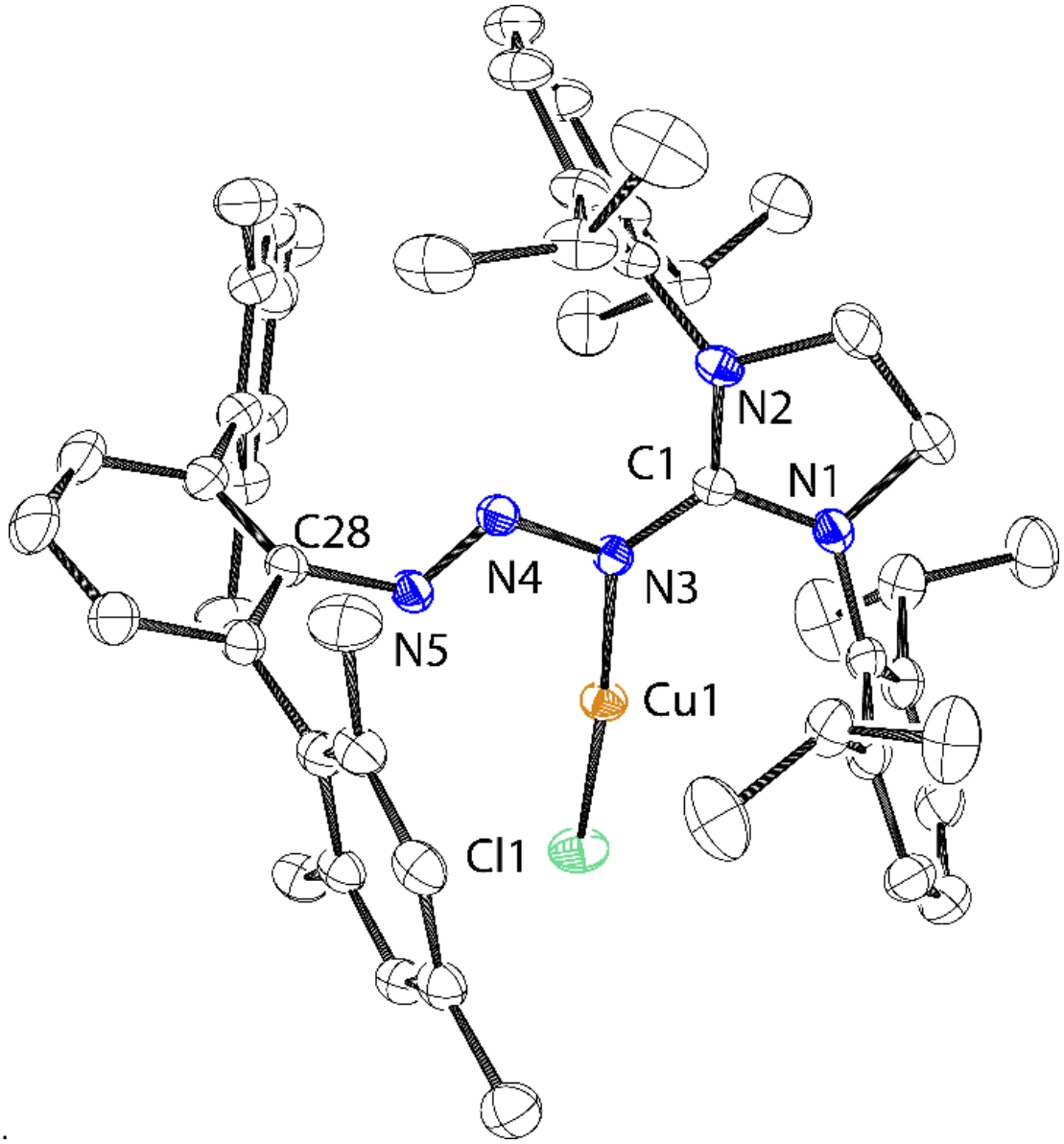



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Figure S28 Molecular structure of **2** with anisotropic displacement ellipsoids projected at the 50% probability level. Hydrogen atoms and $C_6D_6$ have been omitted for clarity.

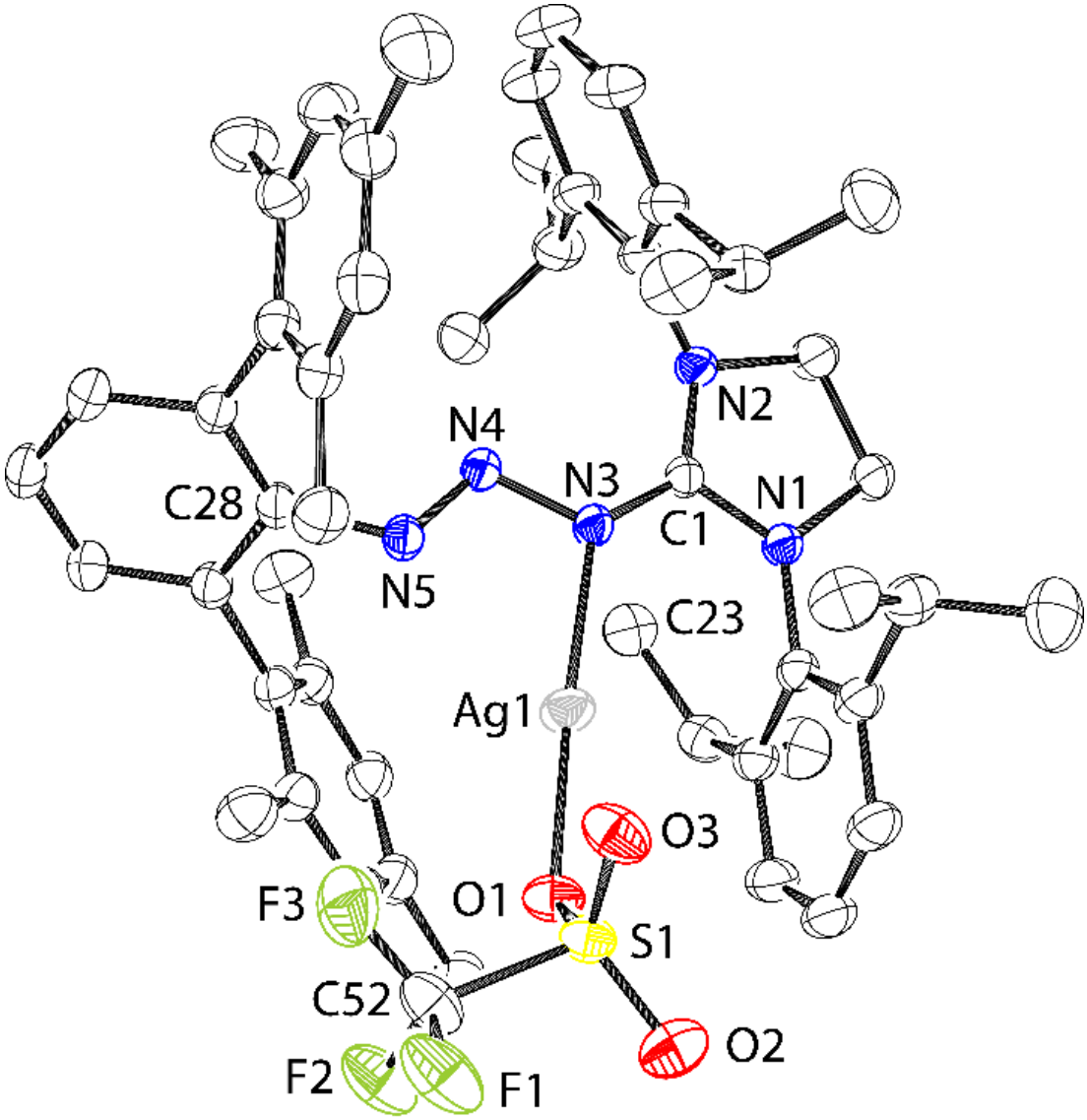



Figure S29 Molecular structure of **3** with anisotropic displacement ellipsoids projected at the 50% probability level. Hydrogen have been omitted for clarity.

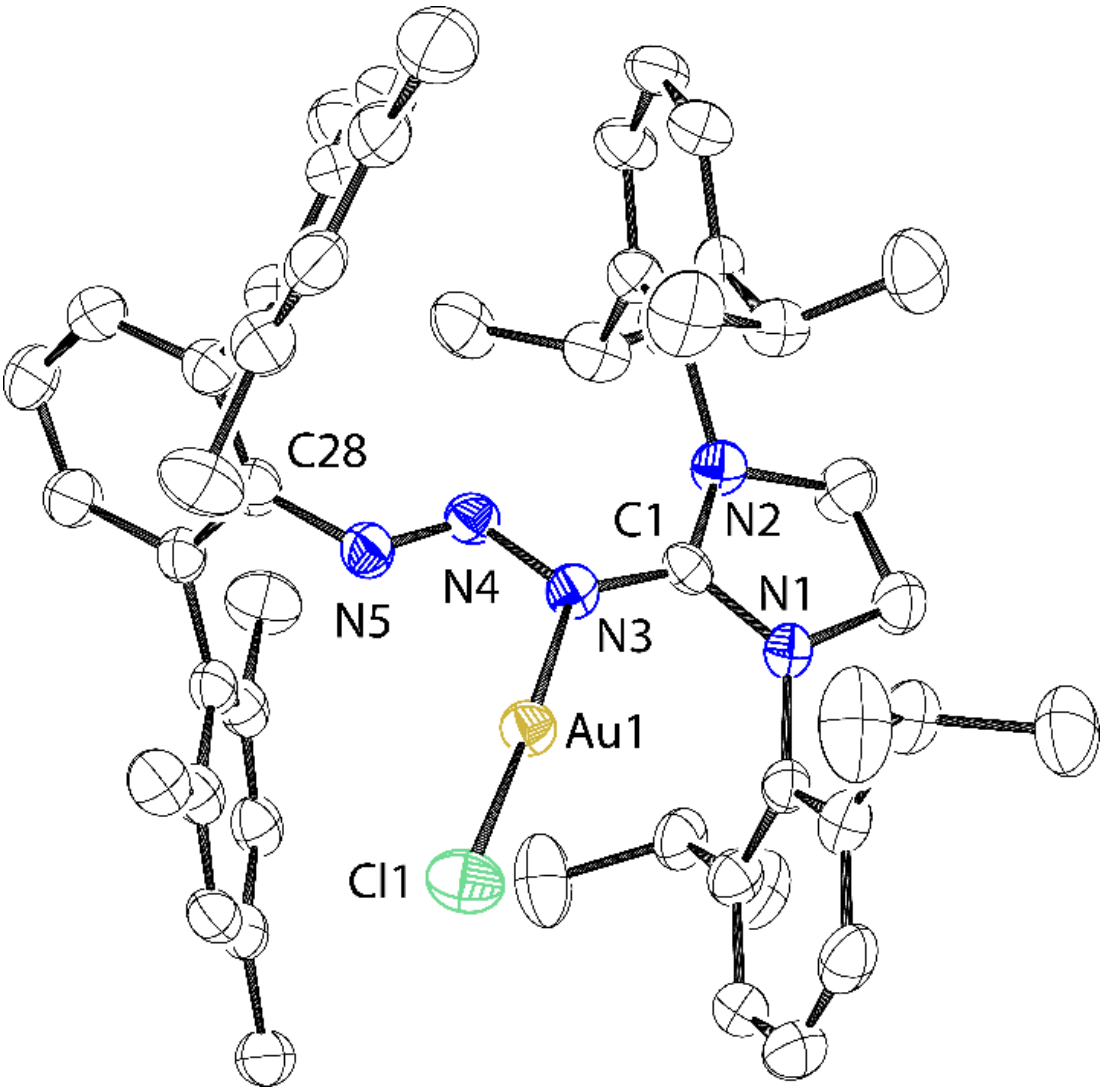



Figure S30 Molecular structure of **4** with anisotropic displacement ellipsoids projected at the 50% probability level. Hydrogen atoms have been omitted for clarity.

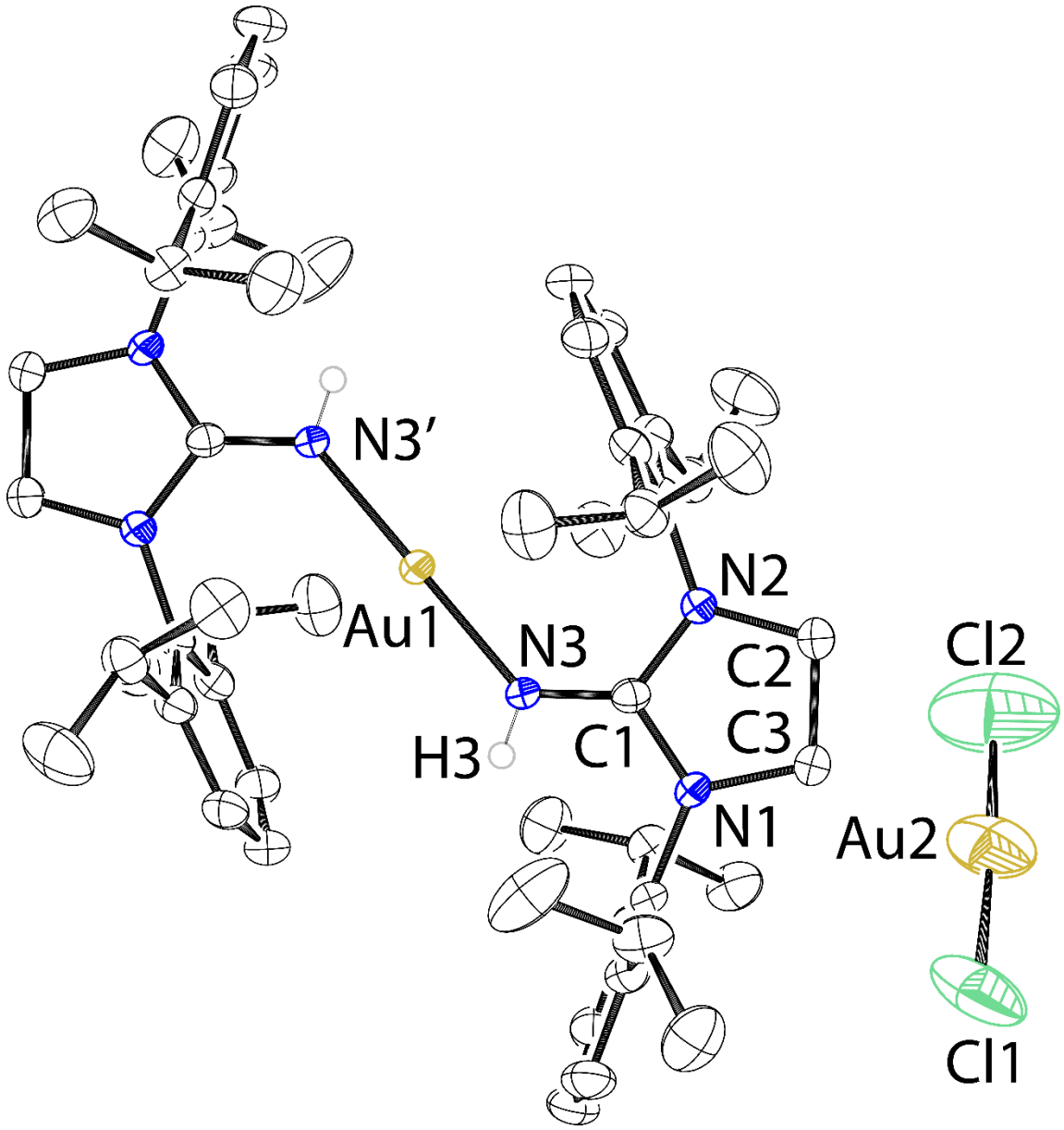



Figure S31 Molecular structure of **5** with anisotropic displacement ellipsoids projected at the 50% probability level with the inversion symmetry centered on Au1 grown. Hydrogen atoms have been omitted for clarity except for the protons (H3) on nitrogen (N3) bound directly to the Au(I) center of the cation. The gold(I) dichloride anion has been modelled with two component disorder in equal ratios, displacing Au2 from the inversion center due to the initial large anisotropic displacement ellipsoids when the inversion was centered on Au2.

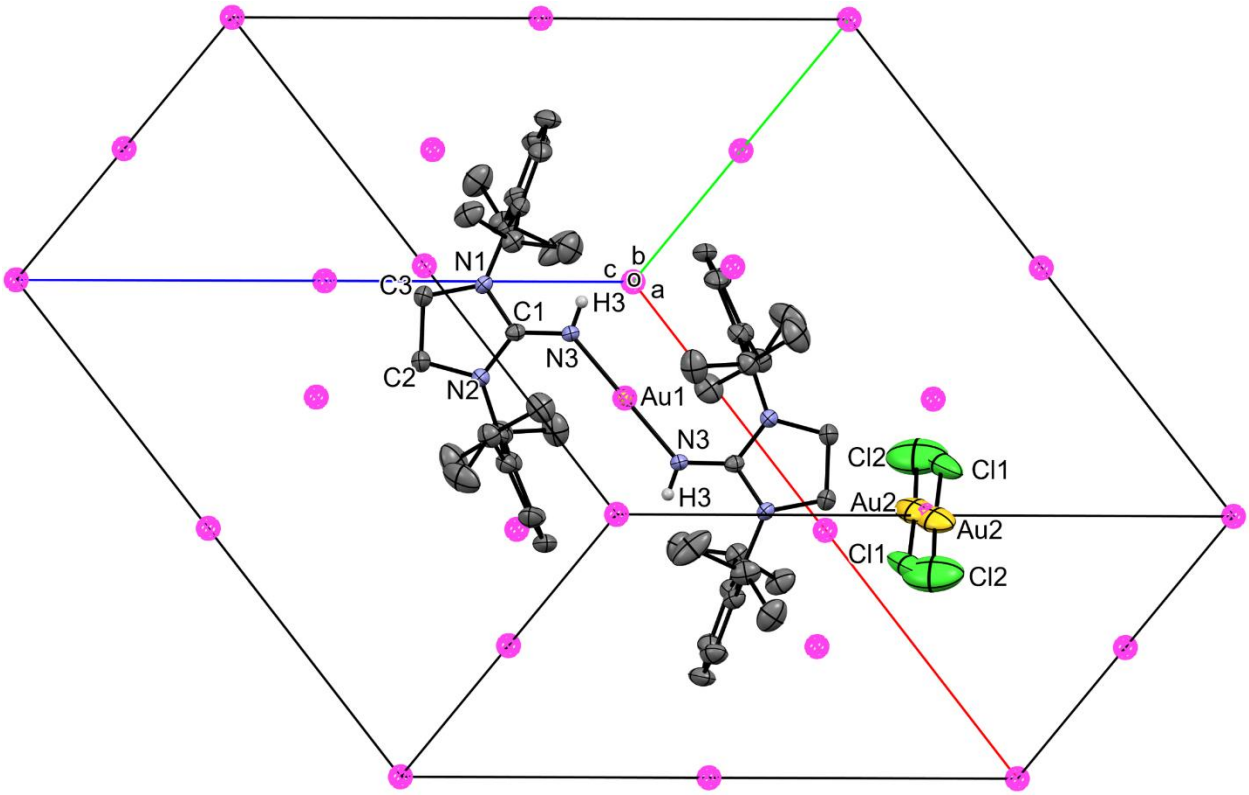



Figure S32 Diagram of one molecule of **5** with inversion centers surrounding the unit cell outlined, detailing the exact centering of Au1 and the slightly offset two. The unit cell reference has the optic axis in the back of the molecule.

# Scanning Electron Microscopy

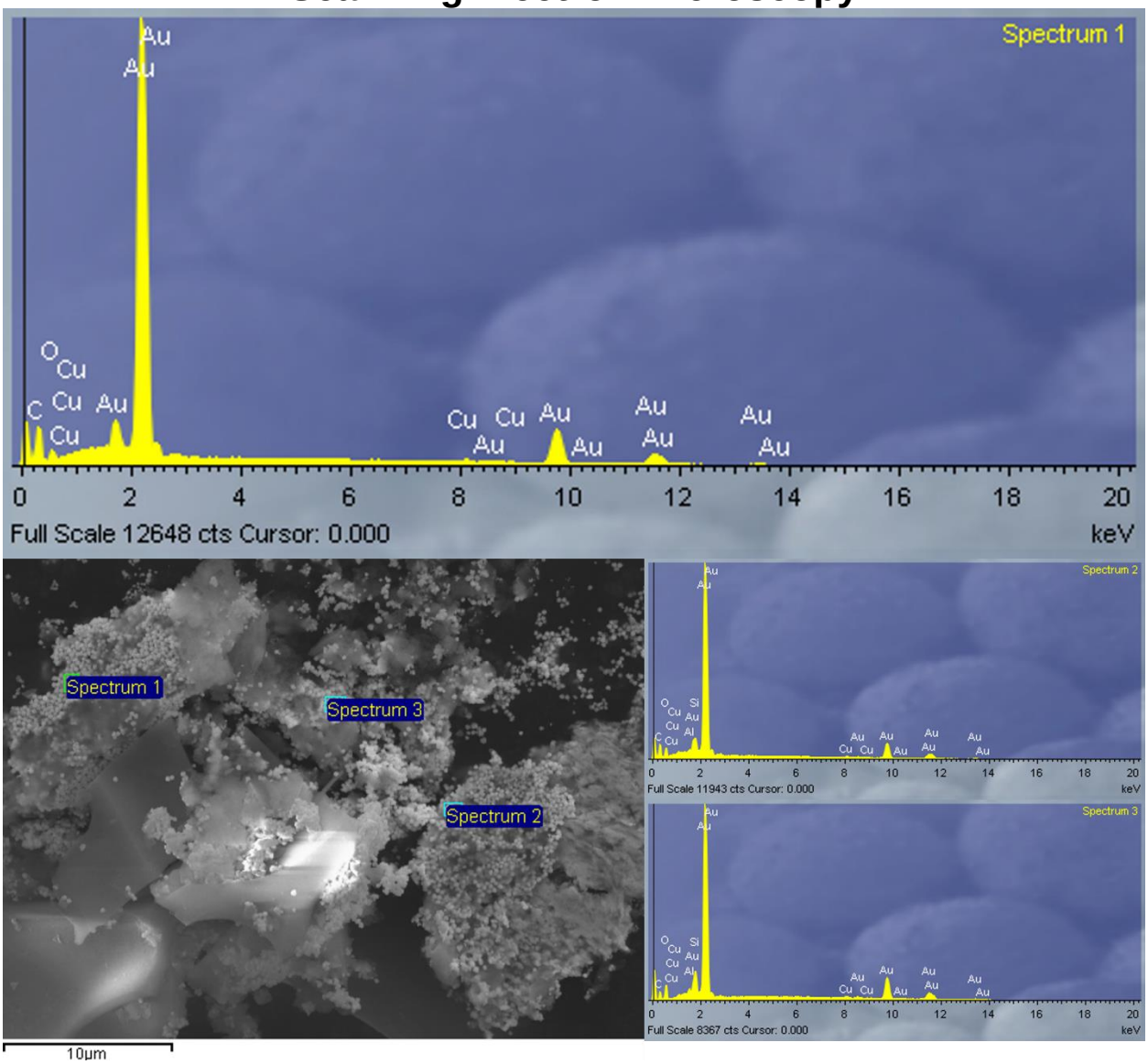



Figure S33 SEM-EDS analysis of gold nanoparticles formed on decomposition of **4** in THF under ambient lighting on glass.

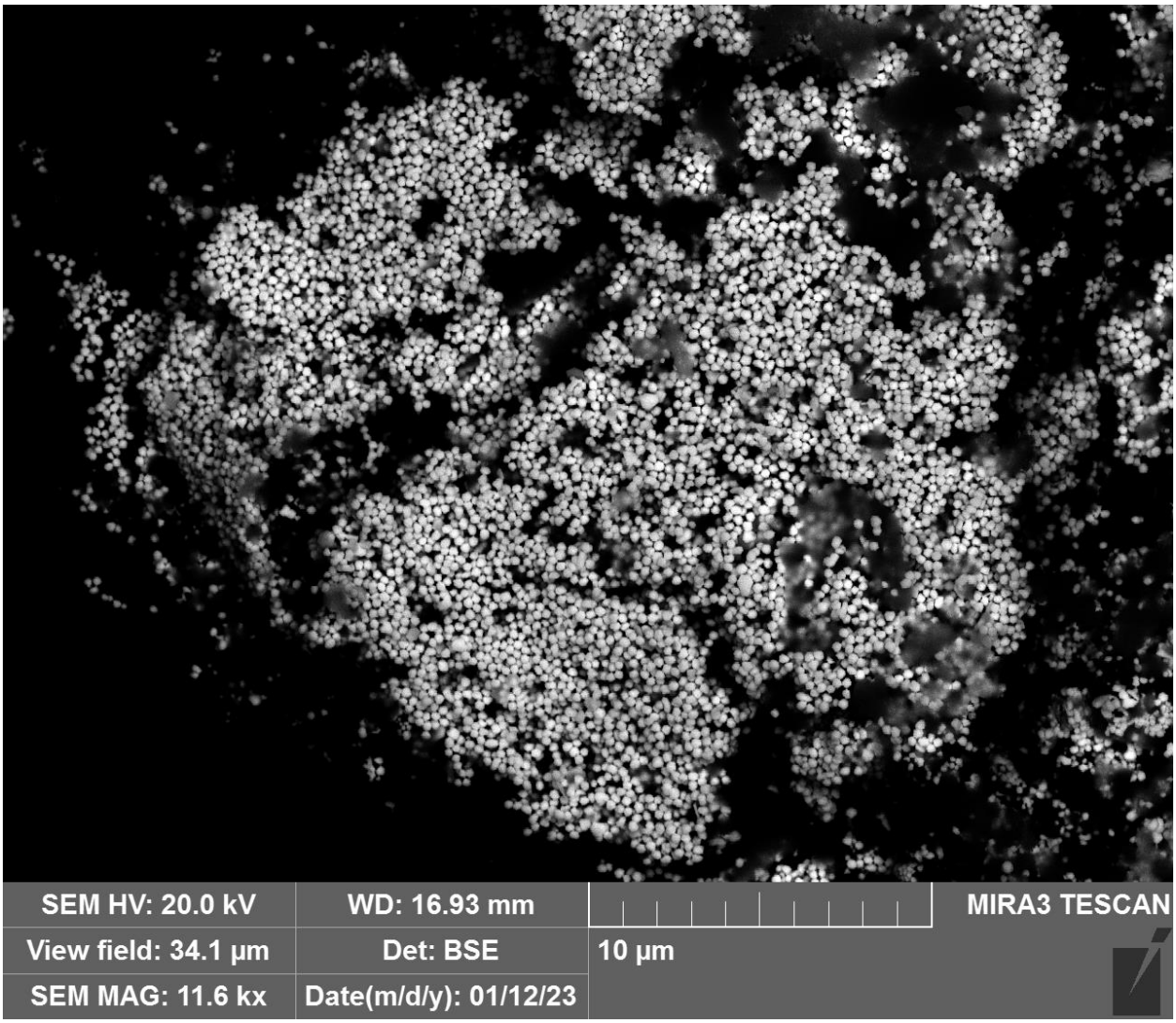



Figure S34 SEM back scattered electron (BSE) image of gold nanoparticles derived from **4**.

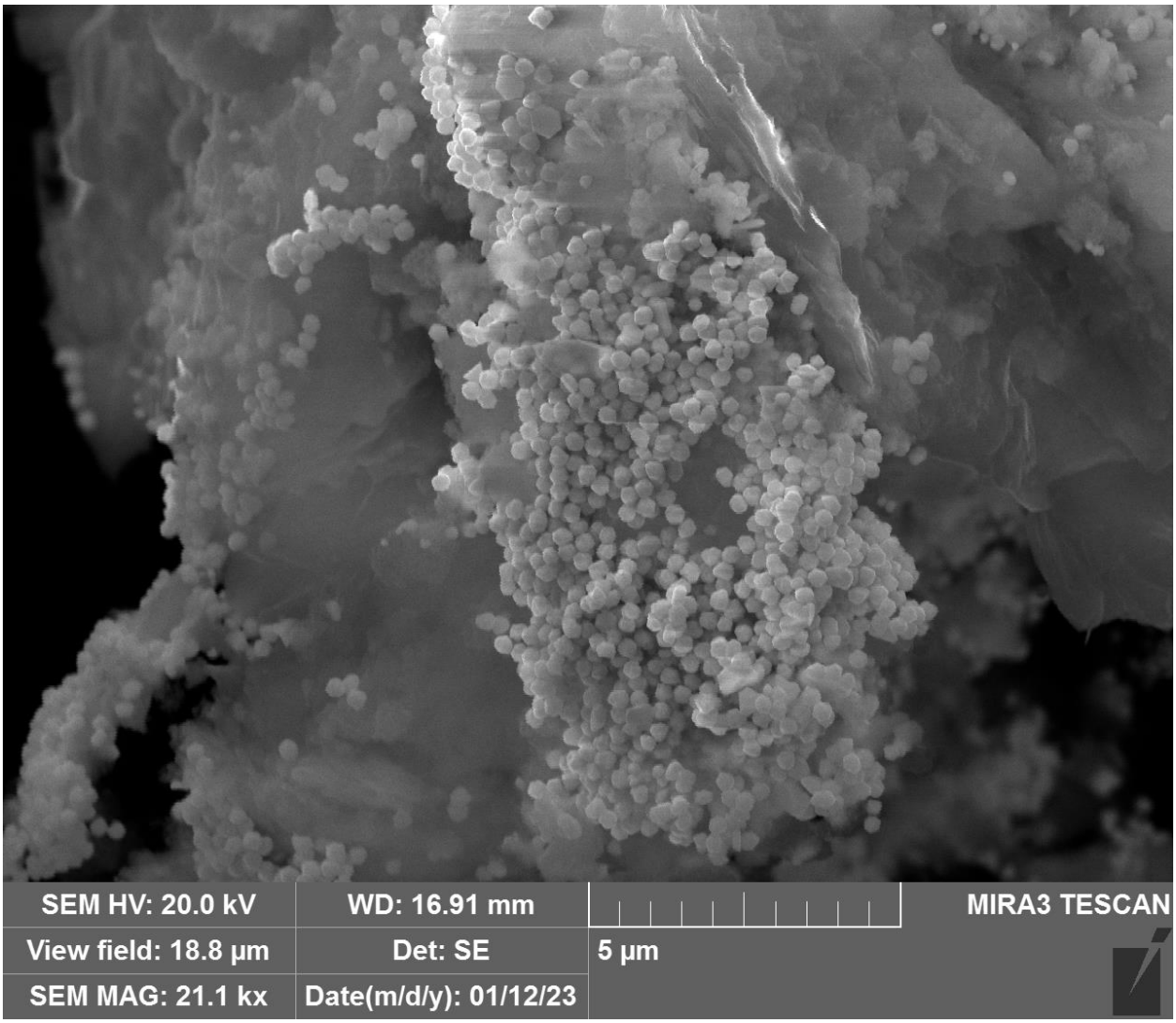



Figure S35 SEM secondary electron (SE) image of gold nanoparticles derived from **4**.

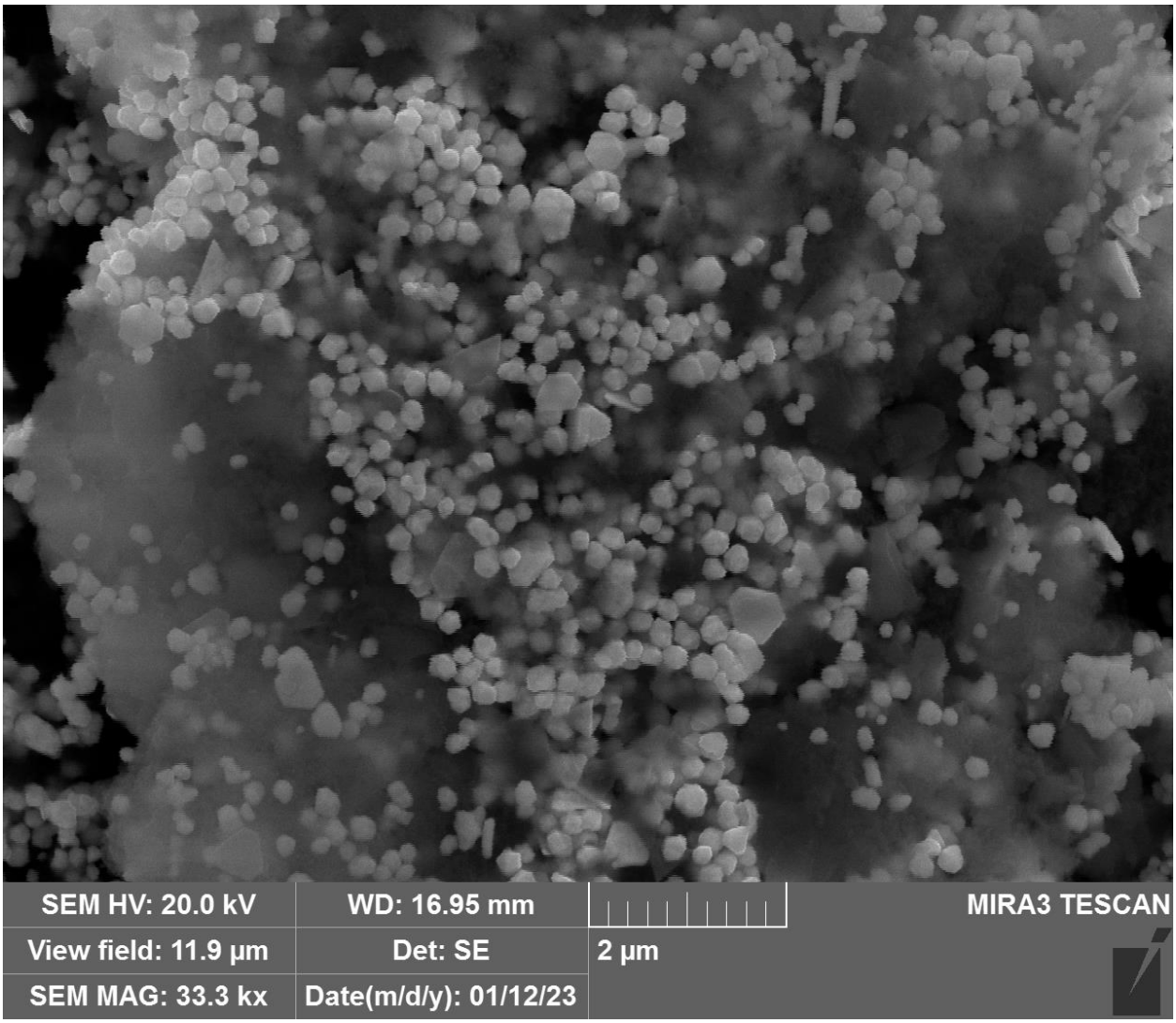
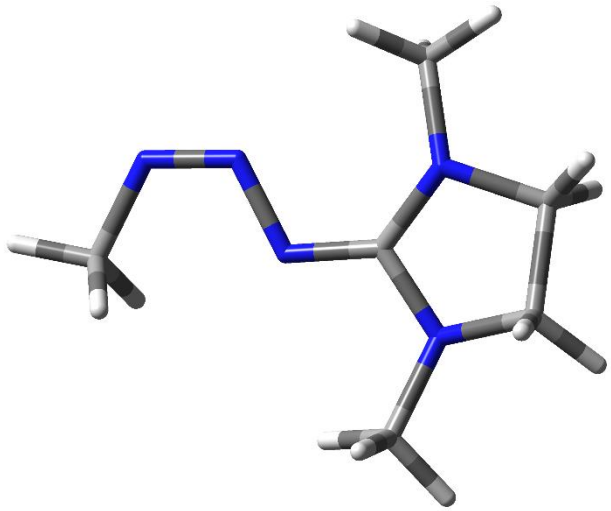



Figure S36 SEM SE image of gold nanoparticles derived from **4**. The larger prismatic particles are ~300-600 nm in diameter, and a random selection of 20 smaller round particles gave a distribution in size of 180 +/- 40 nm.

# Computational Analysis of Parent Compounds and Compound 1

Calculations were performed using Gaussian 16 (Revision B.01)[1] using the M06-2X[2] functional and def2-TZVP[3] basis set. Initial structures were optimized at the B3LYP/6-31G(d)[4,5] level with the GD3BJ dispersion correction[6] as a starting point for the higher-level calculations. All are local minima from frequency calculations (no imaginary frequencies).

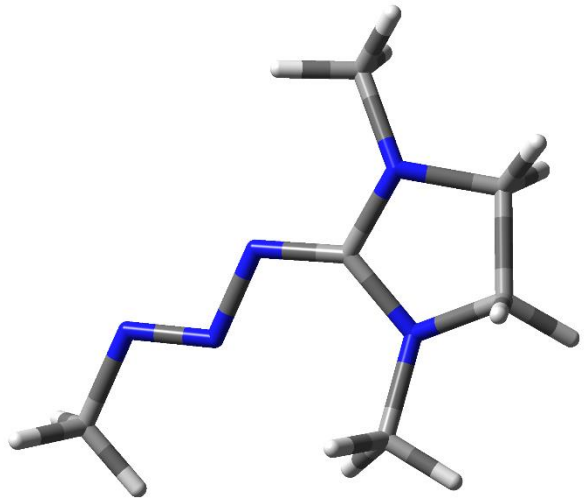
Parent Z-isomer, Energy: -509.948805 Hartrees



| | | | |
|---|---|---|---|
| N | 1.209400 | 1.113300 | 0.213700 |
| N | 1.035400 | -1.073600 | -0.163700 |
| N | -0.953700 | 0.324600 | 0.065300 |
| N | -1.729500 | -0.803000 | -0.090600 |
| N | -2.951600 | -0.631300 | -0.105200 |
| C | 0.324700 | 0.078500 | 0.038300 |
| C | 2.448300 | -0.809400 | 0.080400 |
| H | 3.072400 | -1.398000 | -0.590600 |
| H | 2.713000 | -1.052400 | 1.116800 |
| C | 2.539800 | 0.686900 | -0.171700 |
| H | 3.303700 | 1.179200 | 0.428900 |
| H | 2.728100 | 0.900700 | -1.232200 |
| C | 0.556400 | -2.426300 | 0.073700 |
| H | 0.188300 | -2.550600 | 1.095000 |
| H | -0.245400 | -2.679400 | -0.609300 |
| H | 1.400200 | -3.097900 | -0.084500 |
| C | 0.803400 | 2.481500 | -0.003200 |
| H | 0.740600 | 2.719100 | -1.071400 |
| H | -0.173200 | 2.636600 | 0.446300 |
| H | 1.531100 | 3.143000 | 0.466000 |

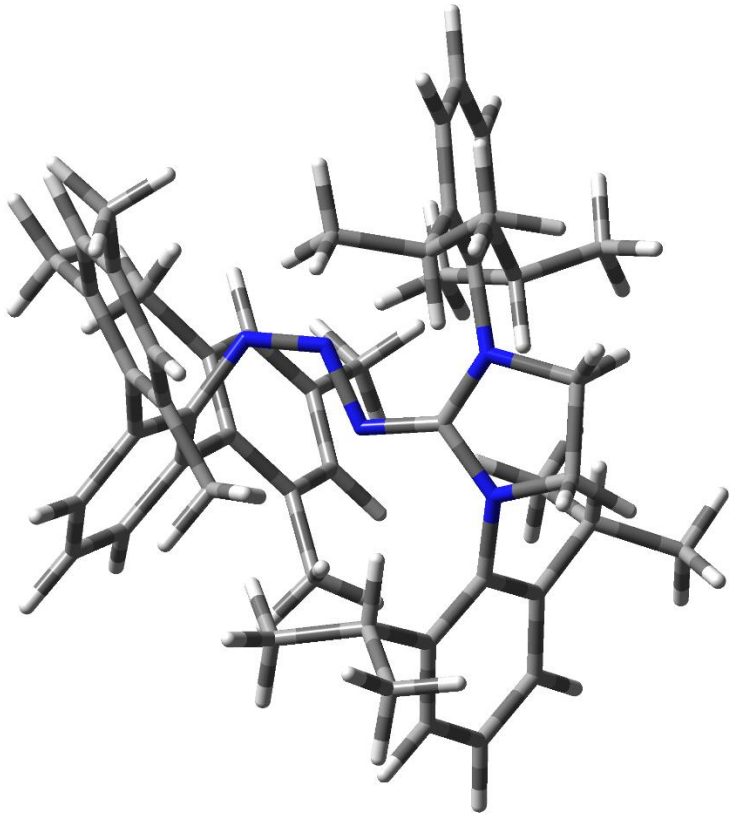
| | | | |
|---|---|---|---|
| C | -3.464300 | 0.733000 | 0.042600 |
| H | -4.548700 | 0.676900 | 0.006200 |
| H | -3.139500 | 1.170400 | 0.988700 |
| H | -3.091500 | 1.376300 | -0.756900 |

Parent E-isomer, Energy: -509.950604 Hartrees



| | | | |
|---|---|---|---|
| N | -2.791300 | -0.824900 | -0.045800 |
| N | -1.772300 | -0.136100 | 0.021500 |
| N | 1.666300 | -0.834800 | -0.209800 |
| N | 0.703100 | 1.139900 | 0.175300 |
| N | -0.636200 | -0.883900 | -0.136500 |
| C | 0.460100 | -0.193000 | -0.059800 |
| C | 2.737100 | 0.035700 | 0.229500 |
| H | 3.649800 | -0.140000 | -0.338900 |
| H | 2.949800 | -0.109900 | 1.297200 |
| C | 2.123400 | 1.401700 | -0.027400 |
| H | 2.476900 | 2.169200 | 0.659900 |
| H | 2.313600 | 1.730500 | -1.056700 |
| C | 1.776900 | -2.260400 | -0.007300 |
| H | 1.801900 | -2.514000 | 1.058800 |
| H | 0.919600 | -2.748500 | -0.461300 |
| H | 2.694200 | -2.613000 | -0.478300 |
| C | -0.217700 | 2.222500 | -0.128900 |
| H | -0.579400 | 2.169500 | -1.159200 |
| H | -1.074000 | 2.203300 | 0.535500 |
| H | 0.325300 | 3.157600 | 0.007500 |
| C | -3.997900 | -0.033100 | 0.127300 |
| H | -4.618500 | -0.152100 | -0.762600 |
| H | -4.558300 | -0.438900 | 0.971200 |
| H | -3.780900 | 1.024400 | 0.294100 |

**Compound 1** Z-isomer, Energy: -2254.019281 Hartrees



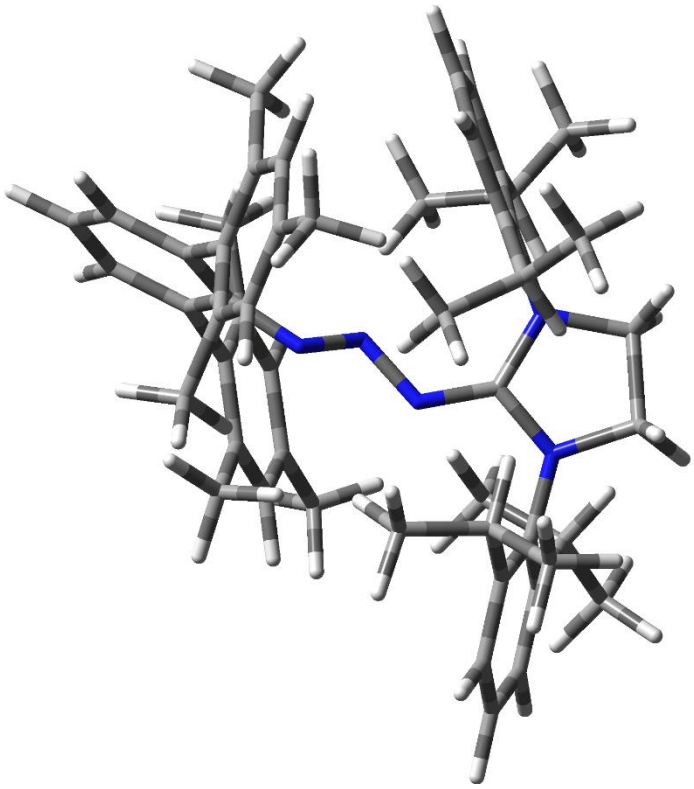
| | | | |
|---|---|---|---|
| N | -1.467100 | 0.880800 | -2.084900 |
| N | -0.180500 | 2.300100 | -0.968300 |
| N | -0.252900 | -0.041000 | -0.317100 |
| N | 0.567500 | 0.352800 | 0.711800 |
| N | 1.220800 | -0.506300 | 1.309200 |
| C | -0.609800 | 1.000100 | -1.030400 |
| C | -0.889800 | 3.122100 | -1.944600 |
| H | -0.200000 | 3.815700 | -2.425500 |
| H | -1.674400 | 3.703500 | -1.445400 |
| C | -1.463300 | 2.085400 | -2.903400 |
| H | -2.471400 | 2.326800 | -3.239000 |
| H | -0.828200 | 1.944100 | -3.783700 |
| C | -2.387400 | -0.174400 | -2.368700 |
| C | -3.740600 | 0.047000 | -2.057800 |
| C | -4.672700 | -0.910900 | -2.435700 |
| H | -5.718400 | -0.761800 | -2.199000 |
| C | -4.279500 | -2.065400 | -3.093500 |
| H | -5.017100 | -2.803200 | -3.382300 |
| C | -2.942500 | -2.276900 | -3.368300 |
| H | -2.638900 | -3.187100 | -3.870400 |
| C | -1.972200 | -1.339700 | -3.016700 |
| C | -4.191000 | 1.239100 | -1.237500 |

| | | | |
|---|---|---|---|
| H | -3.404600 | 1.994700 | -1.254000 |
| C | -5.465100 | 1.896400 | -1.765200 |
| H | -5.370800 | 2.163000 | -2.819200 |
| H | -5.675600 | 2.804400 | -1.197800 |
| H | -6.330200 | 1.240300 | -1.660000 |
| C | -4.359500 | 0.788600 | 0.215400 |
| H | -5.144500 | 0.031200 | 0.283900 |
| H | -4.638000 | 1.628000 | 0.855900 |
| H | -3.436500 | 0.348600 | 0.599300 |
| C | -0.522400 | -1.635700 | -3.329000 |
| H | 0.077200 | -0.802700 | -2.959400 |
| C | -0.293000 | -1.758500 | -4.837000 |
| H | -0.827200 | -2.617800 | -5.247200 |
| H | 0.770000 | -1.897100 | -5.043000 |
| H | -0.634400 | -0.867300 | -5.366400 |
| C | -0.076600 | -2.906000 | -2.597500 |
| H | -0.017500 | -2.733400 | -1.521800 |
| H | 0.905200 | -3.226100 | -2.944100 |
| H | -0.773500 | -3.726700 | -2.776400 |
| C | 0.406500 | 3.007000 | 0.134700 |
| C | 1.721600 | 3.459300 | 0.011600 |
| C | 2.249800 | 4.233700 | 1.040900 |
| H | 3.272100 | 4.584500 | 0.969200 |
| C | 1.495300 | 4.547500 | 2.156300 |
| H | 1.922800 | 5.145100 | 2.951200 |
| C | 0.191400 | 4.090100 | 2.256400 |
| H | -0.392500 | 4.329600 | 3.136900 |
| C | -0.380000 | 3.320900 | 1.250400 |
| C | 2.593000 | 3.095700 | -1.170700 |
| H | 1.995600 | 2.489200 | -1.853700 |
| C | 3.066100 | 4.339900 | -1.925100 |
| H | 2.225300 | 4.952900 | -2.254700 |
| H | 3.649500 | 4.054300 | -2.802100 |
| H | 3.701200 | 4.962100 | -1.291300 |
| C | 3.782000 | 2.246700 | -0.717500 |
| H | 4.428300 | 2.812300 | -0.042300 |
| H | 4.379900 | 1.940800 | -1.577400 |
| H | 3.453300 | 1.346500 | -0.193600 |
| C | -1.804300 | 2.828400 | 1.411600 |
| H | -2.095300 | 2.304800 | 0.499700 |
| C | -2.776200 | 3.995500 | 1.602500 |
| H | -2.572400 | 4.527200 | 2.533500 |
| H | -3.804300 | 3.632200 | 1.649700 |
| H | -2.701100 | 4.715800 | 0.785500 |
| C | -1.915200 | 1.827000 | 2.564700 |
| H | -1.297000 | 0.945400 | 2.387600 |

| | | | |
|---|---|---|---|
| H | -2.948500 | 1.495000 | 2.683300 |
| H | -1.596200 | 2.283100 | 3.504600 |
| C | 1.153400 | -1.885900 | 0.947800 |
| C | 2.282000 | -2.450900 | 0.341000 |
| C | 2.258900 | -3.809500 | 0.036300 |
| H | 3.126300 | -4.249900 | -0.441400 |
| C | 1.168900 | -4.597400 | 0.371000 |
| H | 1.170400 | -5.654600 | 0.140100 |
| C | 0.096100 | -4.033400 | 1.044500 |
| H | -0.735000 | -4.652600 | 1.360100 |
| C | 0.070800 | -2.676100 | 1.353000 |
| C | -1.053900 | -2.130900 | 2.170300 |
| C | -2.357700 | -2.114800 | 1.654900 |
| C | -3.402000 | -1.677500 | 2.463100 |
| H | -4.407700 | -1.667400 | 2.055600 |
| C | -3.193600 | -1.254300 | 3.768700 |
| C | -1.898400 | -1.288300 | 4.264700 |
| H | -1.712900 | -0.975700 | 5.287200 |
| C | -0.824500 | -1.719900 | 3.492100 |
| C | -2.642800 | -2.560400 | 0.247400 |
| H | -1.886300 | -2.171300 | -0.431600 |
| H | -3.619500 | -2.204200 | -0.081900 |
| H | -2.637300 | -3.649500 | 0.160900 |
| C | -4.331200 | -0.740900 | 4.607500 |
| H | -4.170900 | -0.954400 | 5.664300 |
| H | -5.278200 | -1.187800 | 4.305300 |
| H | -4.428000 | 0.343000 | 4.502700 |
| C | 0.549400 | -1.730100 | 4.103500 |
| H | 1.145300 | -2.571100 | 3.748100 |
| H | 0.482700 | -1.783900 | 5.189500 |
| H | 1.086300 | -0.817200 | 3.837000 |
| C | 3.538500 | -1.675300 | 0.098800 |
| C | 3.951700 | -1.353500 | -1.199200 |
| C | 5.179200 | -0.731600 | -1.392600 |
| H | 5.489200 | -0.485600 | -2.403400 |
| C | 6.001100 | -0.390300 | -0.327900 |
| C | 5.573200 | -0.709400 | 0.953700 |
| H | 6.203800 | -0.461000 | 1.800800 |
| C | 4.362700 | -1.354000 | 1.186700 |
| C | 3.074500 | -1.653600 | -2.381100 |
| H | 3.058400 | -2.722400 | -2.604400 |
| H | 3.426700 | -1.127700 | -3.268300 |
| H | 2.046400 | -1.353700 | -2.175400 |
| C | 7.291700 | 0.346100 | -0.556900 |
| H | 7.986300 | 0.194200 | 0.268700 |
| H | 7.108100 | 1.420300 | -0.643000 |

| | | | |
|---|---|---|---|
| H | 7.774900 | 0.020300 | -1.478300 |
| C | 3.960200 | -1.699700 | 2.592200 |
| H | 3.121200 | -1.076600 | 2.904800 |
| H | 4.788800 | -1.541700 | 3.281000 |
| H | 3.638500 | -2.740300 | 2.666800 |

**Compound 1** E-isomer, Energy: -2254.021432 Hartrees



| | | | |
|---|---|---|---|
| N | -0.850300 | 0.635500 | -1.012900 |
| N | -0.053300 | 0.556800 | -0.067500 |
| N | 2.197100 | -2.024200 | 0.785200 |
| N | 0.762900 | -1.069600 | 2.171900 |
| N | 0.718900 | -0.555600 | -0.197300 |
| C | -3.635100 | -0.396100 | -2.300600 |
| C | 1.173700 | -1.126800 | 0.873800 |
| C | -1.515900 | 1.869400 | -1.197500 |
| C | 0.688400 | 3.168700 | -1.257100 |
| C | -0.796000 | 3.063700 | -1.377100 |
| C | -3.699800 | 0.574400 | -1.290900 |
| C | -2.902700 | 1.831200 | -1.406600 |
| C | 1.240200 | 4.081700 | -0.340700 |
| C | -1.502100 | 4.208000 | -1.747000 |
| H | -0.947200 | 5.122000 | -1.917400 |
| C | -0.479700 | -0.544800 | 2.634000 |

| | | | |
|---|---|---|---|
| C | 2.269900 | -2.857500 | 1.973100 |
| H | 3.305100 | -3.051800 | 2.252100 |
| H | 1.773100 | -3.820200 | 1.802200 |
| C | -3.567000 | 3.002700 | -1.748400 |
| H | -4.638900 | 2.966000 | -1.902100 |
| C | 4.809600 | -0.972500 | 0.557100 |
| H | 4.421800 | -1.303000 | 1.523300 |
| C | -4.597500 | 0.421200 | -0.228400 |
| C | -2.873600 | 4.189700 | -1.924800 |
| H | -3.396700 | 5.089400 | -2.221200 |
| C | 1.537300 | 2.442000 | -2.104300 |
| C | -4.465100 | -1.508600 | -2.219900 |
| H | -4.415200 | -2.256700 | -3.004400 |
| C | -5.360500 | -1.683100 | -1.171200 |
| C | -2.705600 | -0.231300 | -3.470100 |
| H | -2.841100 | 0.744500 | -3.941300 |
| H | -2.882000 | -1.004400 | -4.216700 |
| H | -1.666900 | -0.290700 | -3.139200 |
| C | 2.619400 | 4.226600 | -0.270200 |
| H | 3.036100 | 4.923600 | 0.450500 |
| C | 1.526700 | -2.000100 | 3.003300 |
| H | 0.847900 | -2.585500 | 3.624000 |
| H | 2.214200 | -1.455600 | 3.657500 |
| C | 1.025000 | 1.460600 | -3.122300 |
| H | 1.696000 | 1.425500 | -3.980300 |
| H | 0.025300 | 1.716600 | -3.472800 |
| H | 0.977800 | 0.456900 | -2.688100 |
| C | -5.414400 | -0.706100 | -0.186500 |
| H | -6.109500 | -0.820700 | 0.639400 |
| C | 2.907100 | -2.334200 | -0.411000 |
| C | 3.476600 | 3.513500 | -1.099600 |
| C | 4.229900 | -1.876400 | -0.514300 |
| C | 4.327100 | 0.464600 | 0.330300 |
| H | 4.730500 | 0.843600 | -0.611100 |
| H | 4.670600 | 1.119100 | 1.134700 |
| H | 3.239600 | 0.530700 | 0.266500 |
| C | -0.472500 | 0.635700 | 3.380600 |
| C | 0.811900 | 1.386400 | 3.662100 |
| H | 1.643900 | 0.759000 | 3.339900 |
| C | 2.913600 | 2.633100 | -2.009400 |
| H | 3.560700 | 2.070800 | -2.675000 |
| C | -1.655600 | -1.261800 | 2.378200 |
| C | 6.333100 | -1.013100 | 0.635100 |
| H | 6.707800 | -2.034300 | 0.718900 |
| H | 6.672800 | -0.450000 | 1.505300 |
| H | 6.788800 | -0.553400 | -0.243800 |

| | | | |
|---|---|---|---|
| C | -4.707400 | 1.465900 | 0.849900 |
| H | -5.239400 | 2.349600 | 0.491100 |
| H | -3.722000 | 1.793700 | 1.183300 |
| H | -5.250600 | 1.072000 | 1.708700 |
| C | 0.859300 | 2.665800 | 2.829200 |
| H | 0.743600 | 2.435200 | 1.769100 |
| H | 1.809900 | 3.185600 | 2.969900 |
| H | 0.054000 | 3.342500 | 3.124400 |
| C | -1.692000 | 1.128200 | 3.833000 |
| H | -1.718500 | 2.047700 | 4.404600 |
| C | 0.990600 | 1.681600 | 5.151200 |
| H | 0.216600 | 2.358600 | 5.516800 |
| H | 1.955400 | 2.160800 | 5.325700 |
| H | 0.946100 | 0.768400 | 5.747000 |
| C | -2.855700 | -0.716900 | 2.824000 |
| H | -3.786700 | -1.226600 | 2.605700 |
| C | 2.302200 | -3.089900 | -1.418200 |
| C | 0.382700 | 4.922500 | 0.571800 |
| H | 0.072000 | 5.847500 | 0.081100 |
| H | 0.943600 | 5.196900 | 1.465000 |
| H | -0.521700 | 4.398200 | 0.877300 |
| C | -1.644700 | -2.592900 | 1.652400 |
| H | -0.610000 | -2.940900 | 1.597300 |
| C | 4.953200 | -2.214800 | -1.650500 |
| H | 5.977200 | -1.883400 | -1.757000 |
| C | 3.063400 | -3.396100 | -2.545300 |
| H | 2.618000 | -3.978000 | -3.343000 |
| C | 0.868600 | -3.572700 | -1.333900 |
| H | 0.441900 | -3.220300 | -0.394500 |
| C | -2.873800 | 0.465600 | 3.545900 |
| H | -3.816400 | 0.872700 | 3.889200 |
| C | 4.965700 | 3.703600 | -1.008300 |
| H | 5.236900 | 4.750100 | -1.158300 |
| H | 5.485400 | 3.108300 | -1.758700 |
| H | 5.338300 | 3.406500 | -0.025700 |
| C | 4.373600 | -2.971300 | -2.659400 |
| H | 4.949100 | -3.224900 | -3.540600 |
| C | -6.206600 | -2.922700 | -1.079400 |
| H | -6.485000 | -3.285700 | -2.068700 |
| H | -7.117800 | -2.739500 | -0.510300 |
| H | -5.657200 | -3.723900 | -0.577700 |
| C | 0.795900 | -5.101300 | -1.339700 |
| H | 1.164300 | -5.509200 | -2.283100 |
| H | -0.238300 | -5.428800 | -1.216200 |
| H | 1.393000 | -5.532400 | -0.534000 |
| C | -2.177500 | -2.450200 | 0.226700 |

| | | | |
|---|---|---|---|
| H | -2.174700 | -3.421100 | -0.276000 |
| H | -1.585000 | -1.751600 | -0.366600 |
| H | -3.203700 | -2.081500 | 0.248700 |
| C | 0.028700 | -2.976100 | -2.465400 |
| H | 0.036500 | -1.887500 | -2.403400 |
| H | -1.006200 | -3.316000 | -2.392100 |
| H | 0.414800 | -3.280700 | -3.440500 |
| C | -2.436400 | -3.657000 | 2.415800 |
| H | -3.503300 | -3.427100 | 2.418700 |
| H | -2.105600 | -3.738000 | 3.452600 |
| H | -2.312100 | -4.628900 | 1.935300 |

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