

## Electronic Supplementary Information

# Geminal Bimetallic Coordination of a Carbene to Main-Group and Transition Metals

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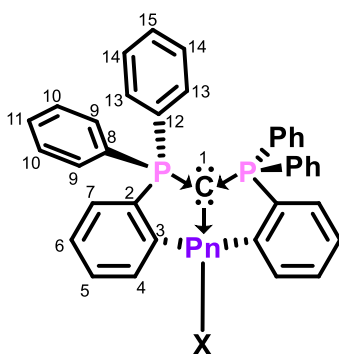
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### Table of Content

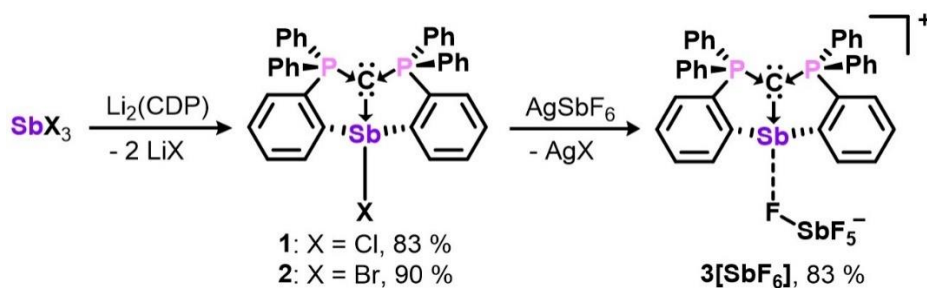
Experimental Procedures .....	2
NMR Spectra .....	7
Crystallographic Refinement Details .....	16
Computational Details .....	19
References.....	28

## Experimental Procedures

*General Considerations* - All manipulations were carried out with the rigorous exclusion of air and moisture under an atmosphere of argon using standard Schlenk techniques or a MBRAUN LABmaster glovebox operating at < 0.1 ppm H<sub>2</sub>O and O<sub>2</sub> and equipped with a -39 °C freezer. All glassware used for experiments or measurements was oven-dried at 190 °C overnight before use. Halogenated solvents were distilled over calcium hydride and others over sodium/benzophenone, then stored over 3 Å molecular sieves. All other solvents were distilled over sodium. NMR spectra were recorded on a Varian Inova 500 MHz (<sup>1</sup>H, 500 MHz, <sup>31</sup>P: 201 MHz), a Varian NMRS 600 MHz (<sup>1</sup>H: 600 MHz, <sup>13</sup>C: 150.9 MHz, <sup>31</sup>P: 243 MHz, <sup>19</sup>F: 564 MHz), and a Bruker Avance III 800 MHz (<sup>1</sup>H, 800 MHz; <sup>13</sup>C, 201 MHz) spectrometers. Proton and carbon chemical shifts are reported in ppm and are referenced using the residual proton and carbon signals of the deuterated solvent (<sup>1</sup>H, CD<sub>2</sub>Cl<sub>2</sub>, δ 5.32; <sup>13</sup>C, CD<sub>2</sub>Cl<sub>2</sub>, δ 53.8). Chemical shifts for other nuclei were referenced to external standards viz 85% H<sub>3</sub>PO<sub>4</sub> for <sup>31</sup>P, and C<sub>6</sub>F<sub>6</sub> for <sup>19</sup>F. Methods and equipment used for the single-crystal X-ray diffraction studies are described under the “[Crystallographic Refinement Details](#)” section. Di(*ortho*)lithiated carbodiphosphorane Li<sub>2</sub>(CDP)<sup>[1]</sup> and (CDP)BiCl<sup>[2]</sup> were synthesized according to the literature. SbCl<sub>3</sub>, SbBr<sub>3</sub>, AgSbF<sub>6</sub>, AgBF<sub>4</sub> and (Me<sub>2</sub>S)AuCl were purchased from commercial sources and used as received. Elemental analysis (EA) was performed using a PerkinElmer Series 2400 II CHNS/O Analyzer, and NMR spectra for all complexes have been provided as further evidence of bulk purity.



**Figure S1.** To simplify assignment of proton and carbon resonances, the numbering scheme above has been adopted.



*Synthesis of (CDP)SbCl (1)* – In a 20 mL scintillation vial equipped with a stir bar, Li<sub>2</sub>(CDP) (190 mg, 0.347 mmol) was dissolved in toluene/Et<sub>2</sub>O (100/1; ~ 5 mL) and cooled to -37 °C in the glovebox freezer. Then a similarly cooled solution of SbCl<sub>3</sub> (80 mg, 0.350 mmol) in THF (~ 2 mL) was rapidly added to the Li<sub>2</sub>(CDP) solution with vigorous stirring for 20 h at room temperature. During this time, a dirty white suspension was observed. Volatiles were removed under vacuum and the desired product was extracted using DCM (~ 12 mL) and completely dried under vacuum to reveal an analytically pure off-white solid. Yield: 200 mg (83 %). Single crystals were obtained from a concentrated DCM solution layered with hexanes at room temperature. <sup>1</sup>H NMR (800 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 9.32 (d, <sup>1</sup>J<sub>HH</sub> 7.7 Hz, 2H, H<sub>4</sub>), 8.05–7.98 (m, 4H, H<sub>6</sub> + H<sub>7</sub>), 7.56 – 7.51 (m, 8H), 7.46 – 7.44 (m, 2H), 7.38 – 7.37 (m, 2H), 7.24 (t, <sup>1</sup>J<sub>HH</sub> 7.4 Hz, 2H, H<sub>15</sub>), 6.94 (t, <sup>1</sup>J<sub>HH</sub> 6.7 Hz, 4H, H<sub>14</sub>), 6.87–6.84 (m, 4H, H<sub>13</sub>). <sup>31</sup>P{<sup>1</sup>H} NMR (201 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 29.5. <sup>13</sup>C{<sup>1</sup>H} NMR (201 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 156.7 – 156.3 (m), 139.9 – 139.0 (m), 138.2 (t, J<sub>PC</sub> = 7.3 Hz), 134.1 – 133.4 (m), 133.3 (t, J<sub>PC</sub> = 5.3 Hz), 132.4 (t, J<sub>PC</sub> = 5.3 Hz), 132.2, 131.3 (t, J<sub>PC</sub> = 7.3 Hz), 131.0, 129.2 (td, J<sub>PC</sub> = 6.1, 2.9 Hz), 128.5 (t, J<sub>PC</sub> = 5.6 Hz), 127.1 – 126.4 (m), 8.3 (t, <sup>1</sup>J<sub>PC</sub> = 100.0 Hz, C<sub>1</sub>). **Anal** (C<sub>37</sub>H<sub>28</sub>ClP<sub>2</sub>Sb; MW 691.79) calc'd for **1**•0.5(CH<sub>2</sub>Cl<sub>2</sub>): C 61.34; H 3.98, found C 61.08; H 3.82.

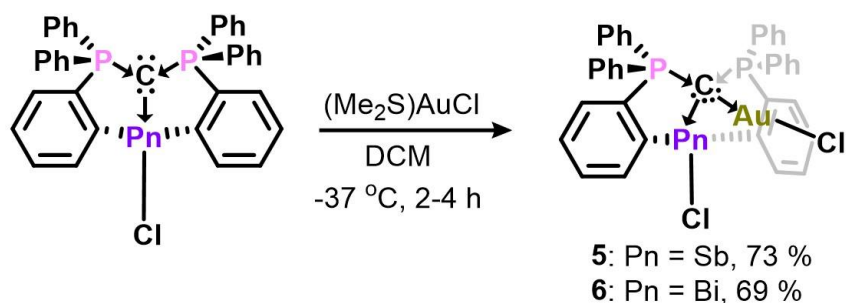
*Synthesis of (CDP)SbBr (2)* – The same procedure for the synthesis of **1** was followed, using SbBr<sub>3</sub> (100 mg, 0.276 mmol) and the corresponding molar equivalent of Li<sub>2</sub>(CDP) (150 mg, 0.273 mmol). Reaction was stirred for 3 days before workup in the same manner as **1**. Yield: 180 mg (90 %). Single crystals were obtained from a concentrated DCM solution layered with hexanes at room temperature. <sup>1</sup>H NMR (800 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 9.31 (d, <sup>1</sup>J<sub>HH</sub> = 7.6 Hz, 2H, H<sub>4</sub>), 8.03 – 8.00 (m, 4H, H<sub>6</sub> + H<sub>7</sub>), 7.59 – 7.50 (m, 8H), 7.47 (t, J = 7.5 Hz, 2H), 7.40 (t, J = 7.4 Hz, 2H), 7.26 (t, <sup>1</sup>J<sub>HH</sub> = 7.4 Hz, 2H, H<sub>15</sub>), 6.96 (t, J = 7.9 Hz, 4H, H<sub>14</sub>), 6.88 – 6.86 (m, 4H, H<sub>13</sub>). <sup>31</sup>P{<sup>1</sup>H} NMR (201 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 31.7. <sup>13</sup>C{<sup>1</sup>H} NMR (201 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 155.6 – 155.2

(m), 140.1 – 139.2 (m), 138.8 (t,  $J_{PC} = 7.5$  Hz), 134.9 – 134.1 (m), 133.9 – 133.0 (m), 132.5 (d,  $J_{PC} = 11.7$  Hz), 132.3 (t,  $J_{PC} = 5.4$  Hz), 131.4 (t,  $J_{PC} = 7.3$  Hz), 131.1, 130.3 (dd,  $J_{PC} = 110.5, 13.4$  Hz), 129.3 (td,  $J_{PC} = 6.3, 3.3$  Hz), 128.7 (t,  $J_{PC} = 5.7$  Hz), 126.4 – 125.7 (m), 6.4 (t,  $^1J_{PC} = 99.1$  Hz,  $C_I$ ). Anal ( $C_{37}H_{28}BrP_2Sb$ ; MW 736.24) calc'd for  $2 \cdot 1.5(CH_2Cl_2)$ : C 53.54; H 3.62, found C 53.89; H 3.53.

*Synthesis of [(CDP)Sb][SbF<sub>6</sub>] (3[SbF<sub>6</sub>])* – In a 20 mL scintillation vial, (CDP)SbBr (25 mg, 0.0339 mmol) and AgSbF<sub>6</sub> (13 mg, 0.0374 mmol) were combined in DCM and stirred in the dark for 30 min at room temperature. AgBr was removed by filtration, and the colorless filtrate was concentrated under vacuum and layered with hexanes to yield colorless single crystals of the title product (25 mg, 83% yield).  $^1H$  NMR (800 MHz,  $CD_2Cl_2$ , 298 K):  $\delta$  8.07 (d,  $^1J_{HH} = 7.5$  Hz, 2H,  $H_4$ ), 8.04 – 7.99 (m, 4H,  $H_6 + H_7$ ), 7.67 (q,  $J = 8.9, 8.2$  Hz, 4H), 7.63 – 7.58 (m, 6H), 7.56 – 7.53 (m, 2H), 7.39 – 7.32 (m, 2H,  $H_{15}$ ), 7.05 – 7.03 (m, 4H,  $H_{14}$ ), 6.96 – 6.87 (m, 4H,  $H_{13}$ ).  $^{31}P\{^1H\}$  NMR (201 MHz,  $C_2D_2Cl_4$ , 323 K):  $\delta$  39.8.  $^{13}C\{^1H\}$  NMR (201 MHz,  $CD_2Cl_2$ , 298 K):  $\delta$  153.9 – 153.5 (m), 139.8 – 138.7 (m), 135.3 (t,  $J = 7.5$  Hz), 133.8 (t,  $J = 5.6$  Hz), 133.7, 133.4, 132.7 – 132.6 (m), 132.4, 132.2 (t,  $J = 5.6$  Hz), 131.7 (d,  $J = 104.3$  Hz), 130.0 – 129.9 (m), 129.8 (q,  $J = 7.0$  Hz), 124.2 (d,  $J = 86.7$  Hz),  $C_I$  was not observed. Anal ( $C_{37}H_{28}F_6P_2Sb_2$ ; MW 892.09) calc'd C 49.82; H 3.16, found C 49.10; H 3.14. Notably, hydrolysis of adventitious moisture during the synthesis of **3[SbF<sub>6</sub>]** results in  $[H(CDP)SbBr][SbF_6]$  (**4[SbF<sub>6</sub>]**), which crystallized in trace amounts and was not intentionally scaled.

*Isolation of [H(CDP)SbBr][BAr<sup>F</sup><sub>4</sub>] (4[BAr<sup>F</sup><sub>4</sub>])* – In a 20 mL scintillation vial, (CDP)SbBr (35 mg, 0.0476 mmol) and Na[BAr<sup>F</sup><sub>4</sub>] (45 mg, 0.508) were combined in DCM and stirred for 7 h at room temperature. Trace solids presumed to be NaBr were removed by filtration and the filtrate was concentrated under vacuum and layered with hexanes to yield colorless single crystals. In lieu of the expected monocation, the title product was isolated due to protonation of the carbene by trace moisture in the reaction solvent (25 mg, 33% yield).  $^1H$  NMR (500 MHz,  $CD_2Cl_2$ , 298 K):  $\delta$  9.03 (d,  $^1J_{HH} = 5.2$  Hz, 2H,  $H_4$ ), 7.78 (q,  $J = 7.6$  Hz, 4H), 7.74 – 7.69 (m, 7H), 7.70 – 7.56 (m, 8H), 7.54 – 7.51 (m, 6H), 7.49 – 7.46 (m, 2H), 7.22 – 7.17 (m, 6H), 6.90 (dd,  $J = 13.2, 7.7$  Hz, 4H), 3.18 (t,  $^1J_{PH} = 8.1$  Hz, 1H,  $H_I$ ).  $^{31}P\{^1H\}$  NMR (201 MHz,  $C_2D_2Cl_4$ , 323 K):  $\delta$  28.0.  $^{13}C\{^1H\}$  NMR (201 MHz,  $CD_2Cl_2$ , 298 K):  $\delta$  162.2 (q,  $^1J_{BC} = 49.7$  Hz,  $C_{BARF}$ ), 150.1 (d,  $J = 19.9$  Hz), 140.0 (d,  $J =$

15.8 Hz), 135.3, 135.2, 135.0, 134.3 (d,  $J = 15.5$  Hz), 133.8 – 133.1 (m), 132.5 – 132.1 (m), 131.0 (d,  $J = 13.5$  Hz), 131.0 – 130.9 (m), 130.7, 130.5 – 130.27 (m), 130.16, 129.28 (qq,  $^2J_{CF} = 32.4$ , 2.7 Hz,  $C(CF_3)$ ), 125.0 (q,  $^1J_{CF} = 272.4$  Hz,  $CF_3$ ), 124.23 (dd,  $J = 88.6$ , 4.6 Hz), 122.07, 121.67, 117.89 (p,  $J = 3.8$  Hz,  $C_{BARF}$ ), 16.25 (t,  $^1J_{PC} = 62.5$  Hz,  $H_1$ ). Anal ( $C_{69}H_{41}BBRF_{24}P_2Sb$ ; MW 1600.47) calc'd for  $4[BAr^F_4] \cdot (CH_2Cl_2)$ : C 49.89; H 2.57, found C 49.58; H 2.41.



*Synthesis of 5* – In a 20 mL scintillation vial, (CDP)SbCl (20 mg, 0.0289 mmol) was dissolved in minimal DCM (~ 3 mL) and cooled to  $-37\text{ }^\circ\text{C}$  in the glovebox freezer. In the dark,  $(Me_2S)AuCl$  (10 mg, 0.0339 mmol) was added to the colorless solution and shaken together. No color change was observed and reaction was continued at  $-37\text{ }^\circ\text{C}$  for 4 h, during which colorless crystals of the title compound precipitated (19 mg, 73 % yield). Notably, this compound decomposes in DCM at room temperature within 45 minutes, accelerated by ambient light, but is stable enough for rapid spectroscopic analysis. In the solid-state, this compound is stable for several weeks under ambient conditions.  $^1H$  NMR (800 MHz,  $CD_2Cl_2$ , 298 K):  $\delta$  9.00 (d,  $^1J_{HH} = 7.7$  Hz, 2H,  $H_4$ ), 8.13 (dd,  $J = 12.6$ , 7.7 Hz, 4H), 7.67 (t,  $J = 7.4$  Hz, 2H), 7.60 (t,  $J = 7.6$  Hz, 2H), 7.55 – 7.48 (m, 4H), 7.38 – 7.36 (m, 2H), 7.21 (ddt,  $J = 10.0$ , 6.1, 2.0 Hz, 2H), 7.11 – 7.07 (m, 8H), 6.99 (ddd,  $J = 10.9$ , 7.5, 1.2 Hz, 2H).  $^{31}P\{^1H\}$  NMR (201 MHz,  $C_2D_2Cl_4$ , 323 K):  $\delta$  30.1.  $^{13}C\{^1H\}$  NMR (201 MHz,  $CD_2Cl_2$ , 298 K):  $\delta$  180.6, 139.9, 136.8 (m), 134.5, 134.3 – 133.9 (m), 133.7, 133.6, 133.0 (d,  $J = 9.7$  Hz), 132.0 (d,  $J = 96.5$  Hz), 129.9 – 128.8 (m), 128.7 (m),  $C_I$  was not observed. Anal ( $C_{37}H_{28}AuCl_2P_2Sb$ ; MW 924.21) calc'd for  $5 \cdot 0.5(CH_2Cl_2)$ : C 46.59; H 3.02, found C 46.69; H 3.05.

*Synthesis of 6* – In a 20 mL scintillation vial, (CDP)BiCl (25 mg, 0.0321 mmol) was dissolved in minimal DCM (~ 2 mL) and cooled to  $-37\text{ }^\circ\text{C}$  in the glovebox freezer. In the dark,  $(Me_2S)AuCl$  (10 mg, 0.0339 mmol) was added to the colorless solution and shaken together. No color change

was observed and reaction was continued at -37 °C for 2 h, during which colorless crystals of the title compound precipitated (22 mg, 69 % yield). Notably, this compound decomposes in DCM at room temperature within 30 minutes, accelerated by ambient light, but is stable enough for rapid spectroscopic analysis. In the solid-state, this compound is stable for several weeks. **<sup>1</sup>H NMR** (800 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 9.28 (d, *J* = 7.6 Hz, 2H), 8.19 – 8.07 (m, 4H), 7.76 (t, *J* = 7.5 Hz, 2H), 7.67 (t, *J* = 7.4 Hz, 2H), 7.55 – 7.52 (m, 4H), 7.35 (t, *J* = 7.3 Hz, 2H), 7.29 (ddt, *J* = 7.6, 6.2, 2.0 Hz, 2H), 7.14 – 6.99 (m, 10H). **<sup>31</sup>P{<sup>1</sup>H} NMR** (201 MHz, C<sub>2</sub>D<sub>2</sub>Cl<sub>4</sub>, 323 K): δ 32.8. **<sup>13</sup>C{<sup>1</sup>H} NMR** (201 MHz, CD<sub>2</sub>Cl<sub>2</sub>, 298 K): δ 180.7, 141.8 (d, *J* = 106.4 Hz), 139.9, 137.5 – 136.0 (m), 134.53, 134.1 (d, *J* = 5.2 Hz), 133.7, 133.6, 133.0 (d, *J* = 11.2 Hz), 132.0 (dd, *J* = 95.3, 3.7 Hz), 129.6 (q, *J* = 7.0 Hz), 129.4 – 128.9 (m), 128.70 (dt, *J* = 11.4, 6.0 Hz), 15.55 (t, <sup>1</sup>*J*<sub>PC</sub> = 50.9 Hz, *C*<sub>1</sub>). Anal (C<sub>37</sub>H<sub>28</sub>AuCl<sub>2</sub>P<sub>2</sub>Bi; MW 1011.43) calc'd for **6**•(CH<sub>2</sub>Cl<sub>2</sub>): C 41.63; H 2.76, found C 41.81; H 2.62.

## NMR Spectra

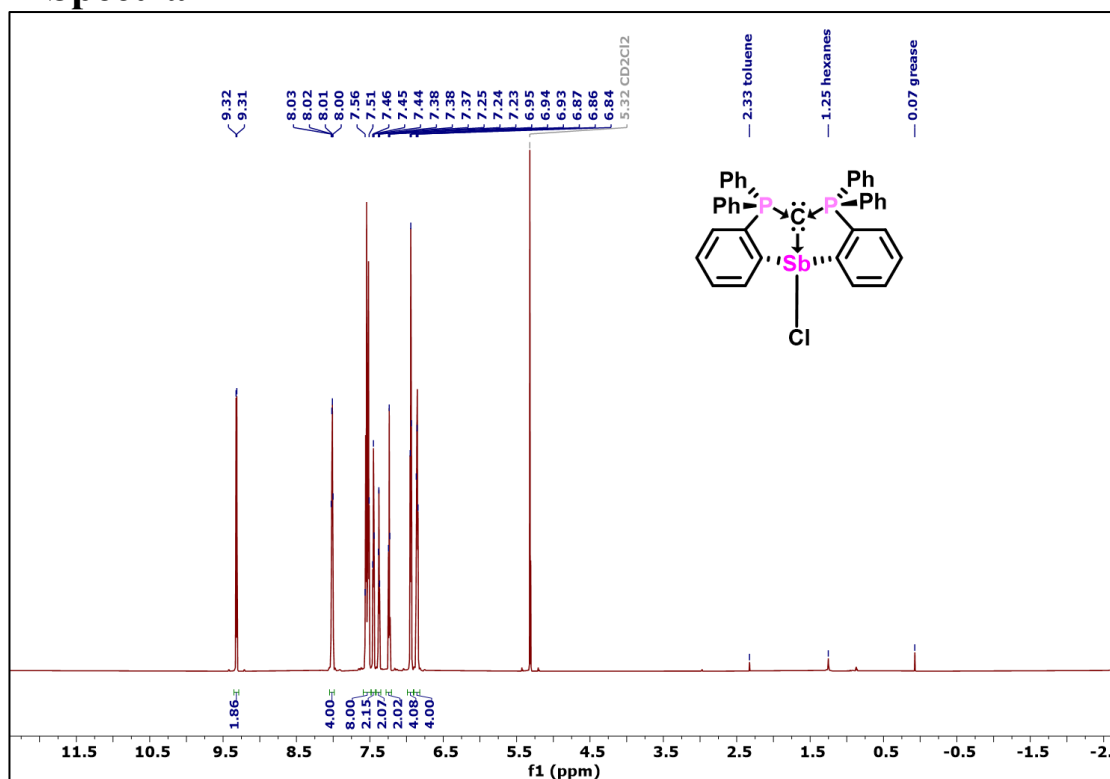


Figure S3.  $^1\text{H}$  NMR spectrum of **1** (800 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

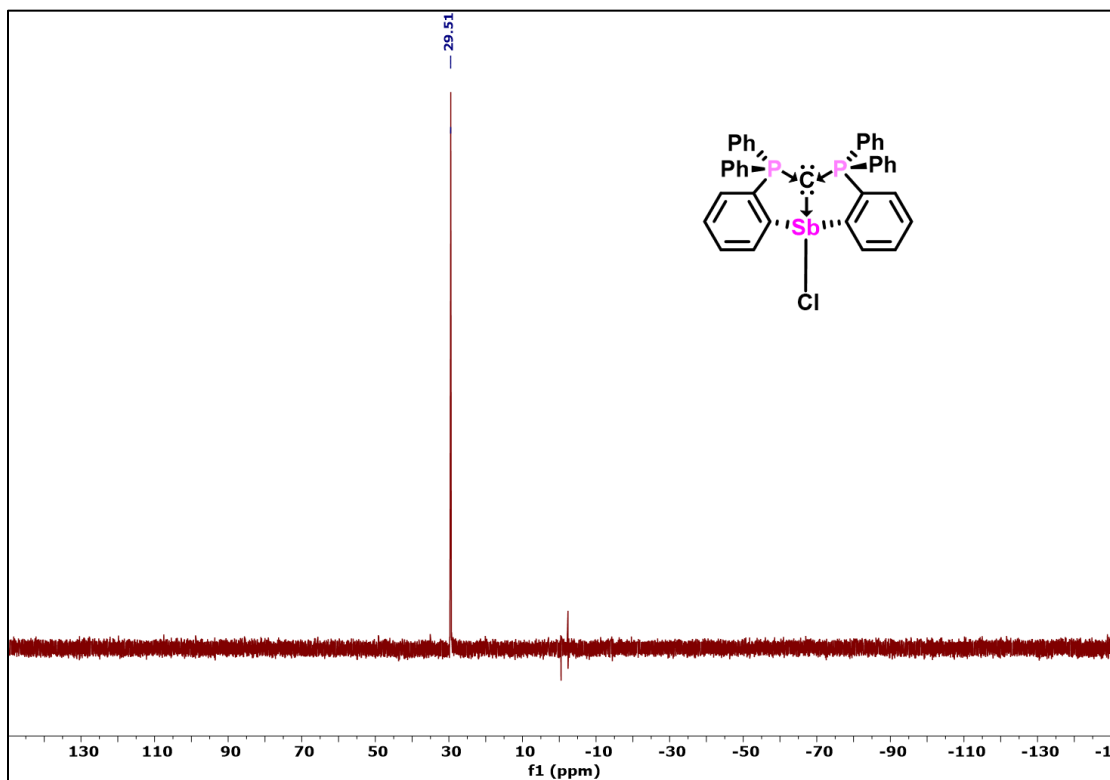


Figure S4.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **1** (201 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

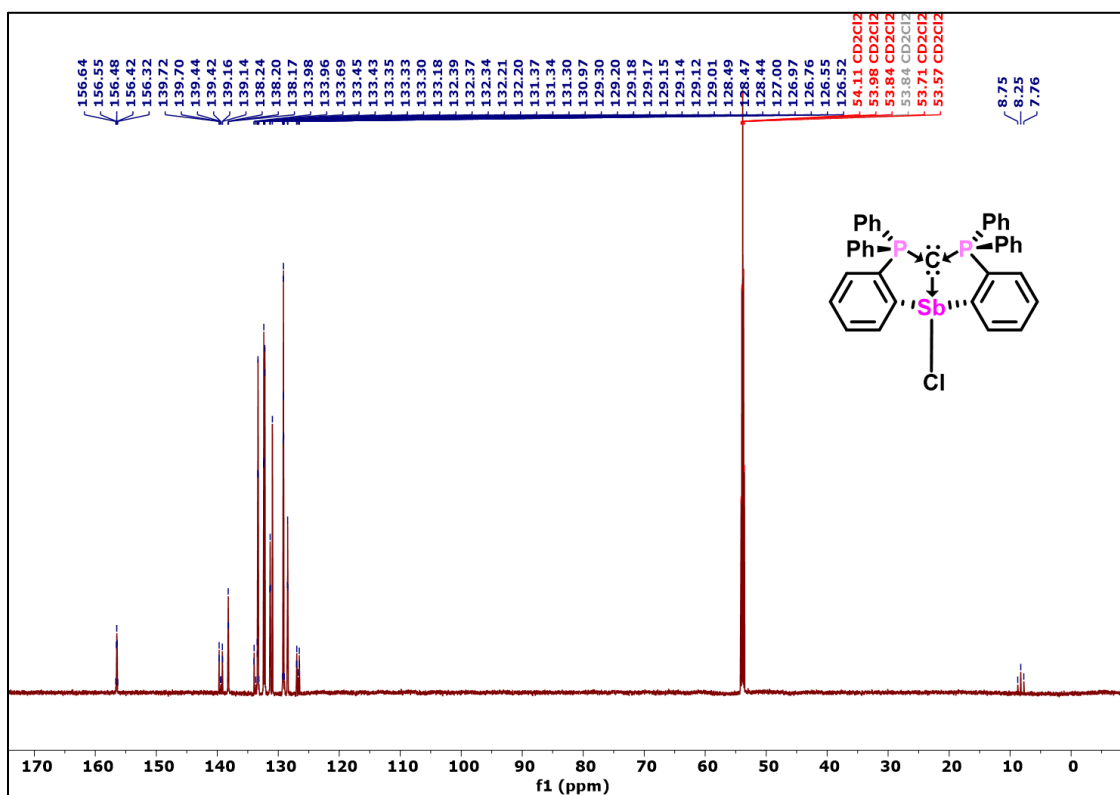


Figure S5.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **1** (200 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

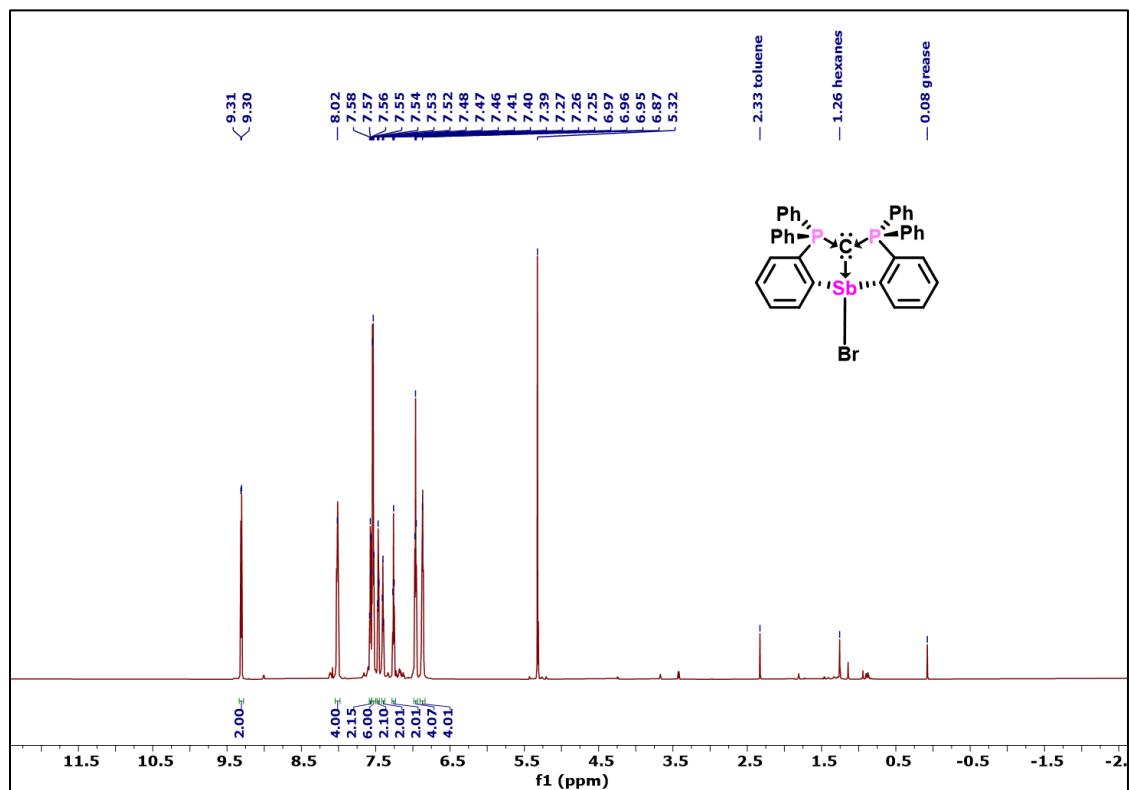


Figure S6.  $^1\text{H}$  NMR spectrum of **2** (800 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).



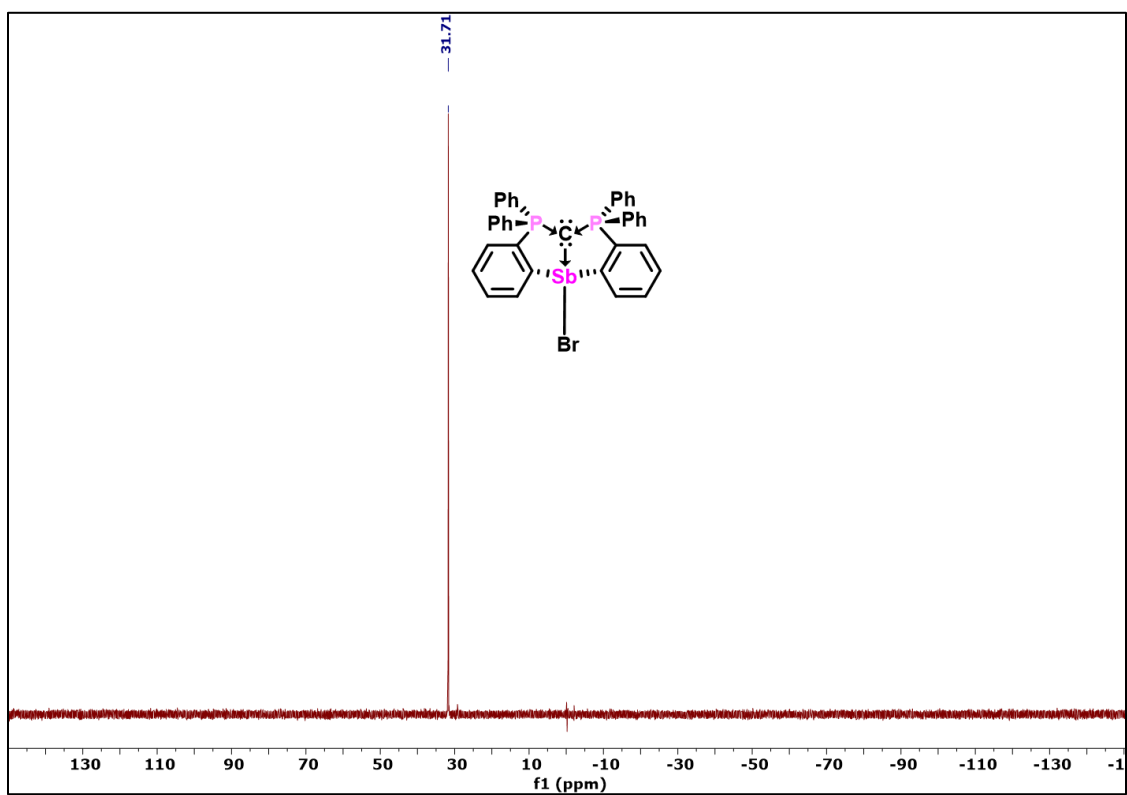


Figure S7.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **2** (201 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

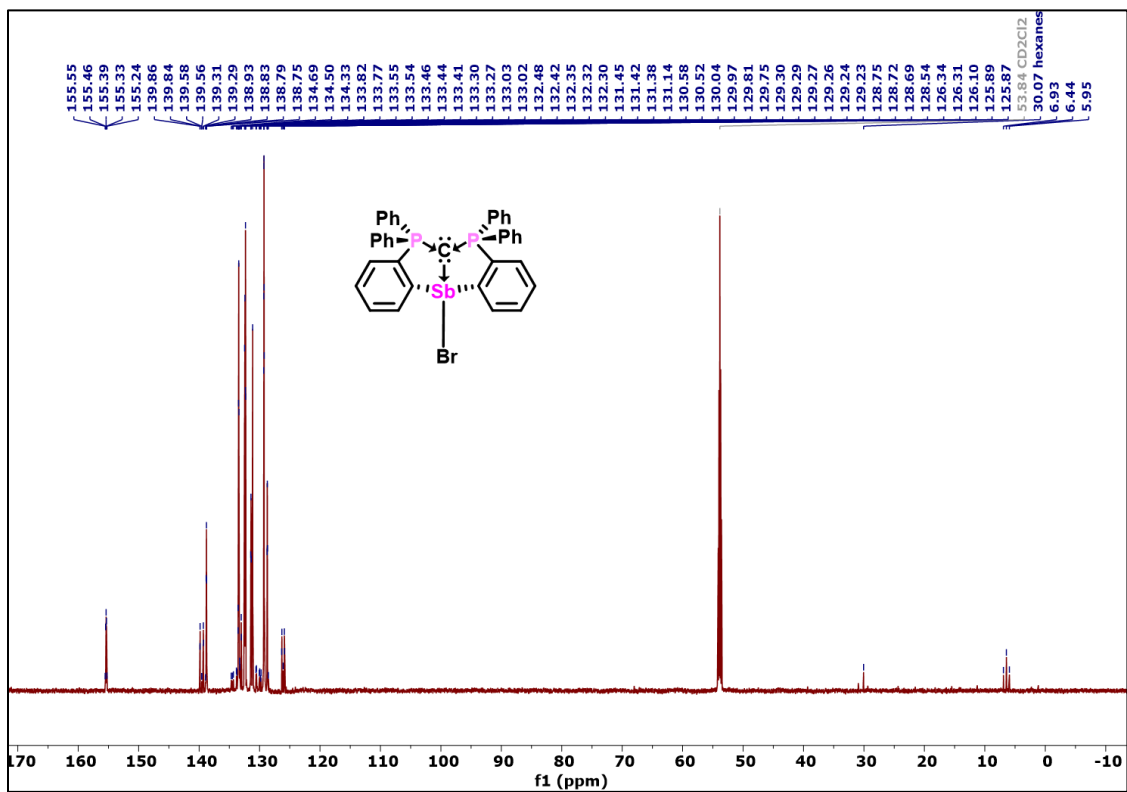


Figure S8.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **2** (200 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

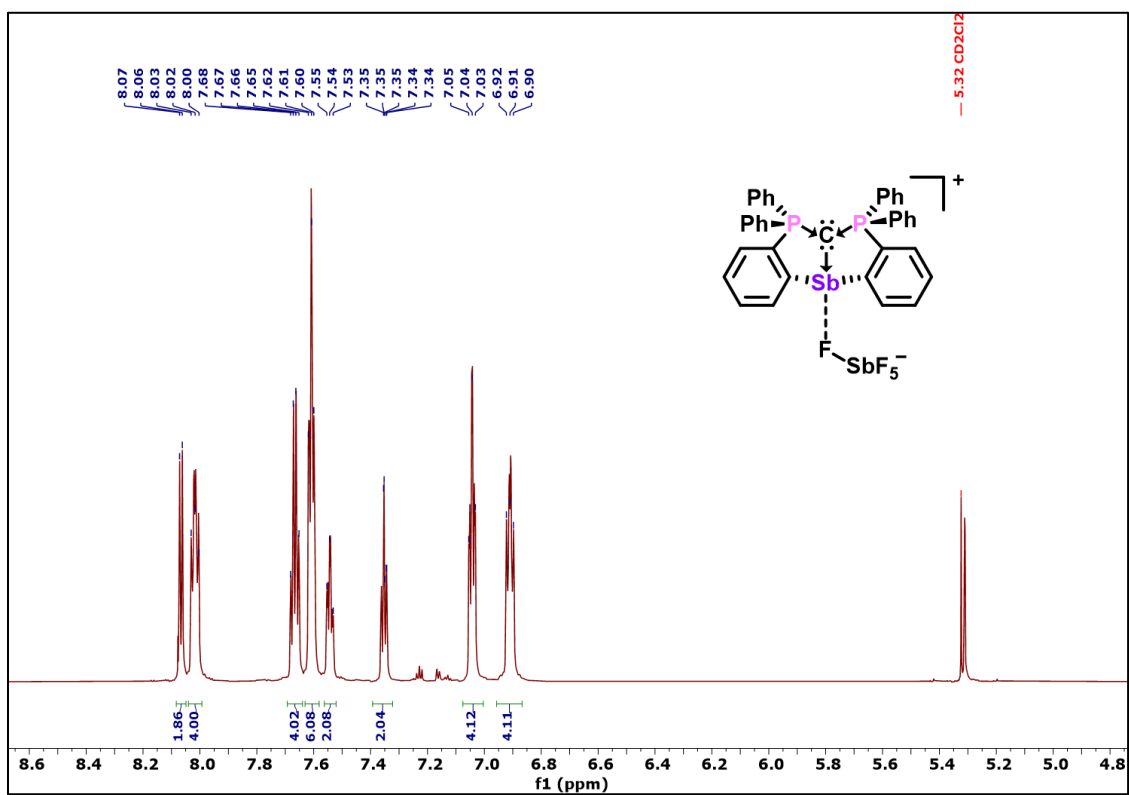


Figure S9.  $^1\text{H}$  NMR spectrum of  $3[\text{SbF}_6]$  (800 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

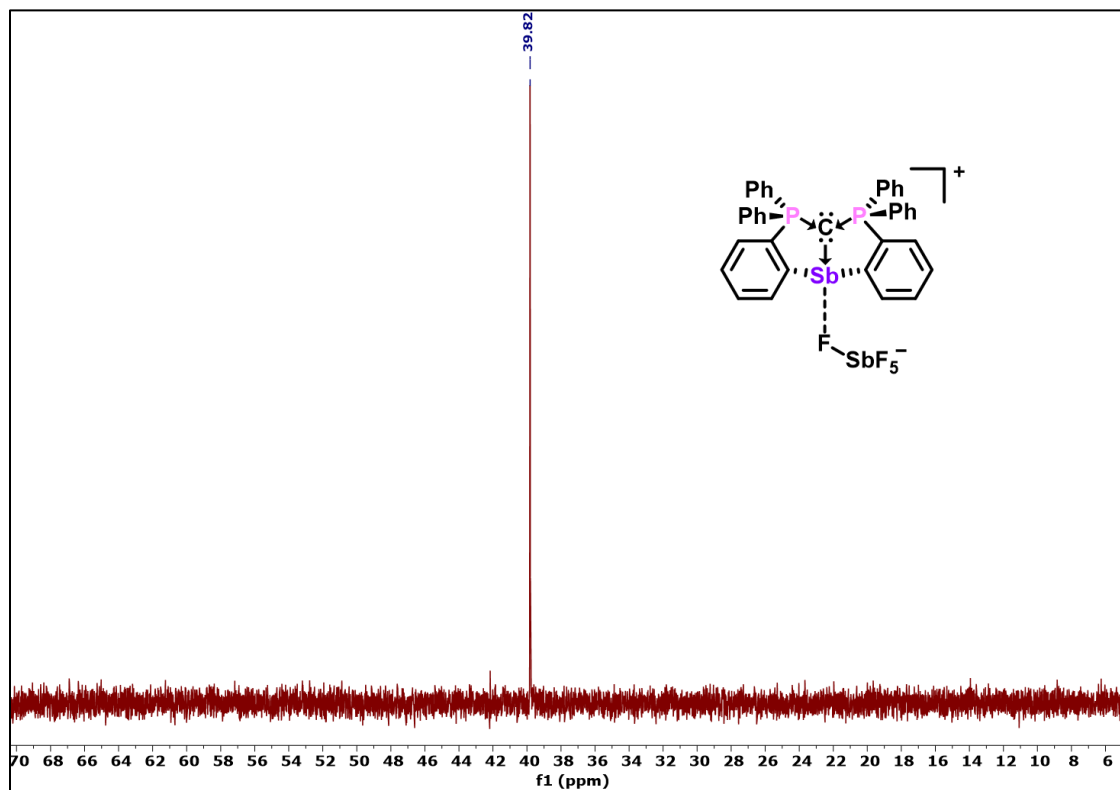


Figure S10.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of  $3[\text{SbF}_6]$  (201 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

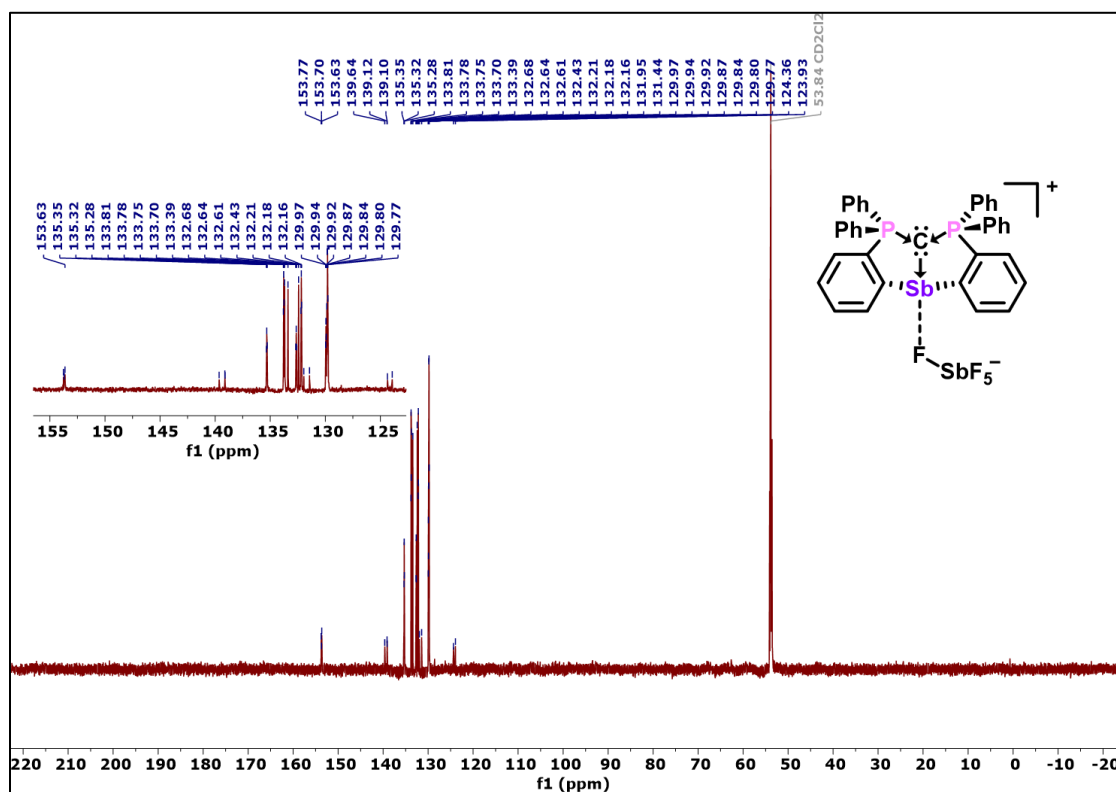


Figure S11.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $3[\text{SbF}_6]$  (200 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

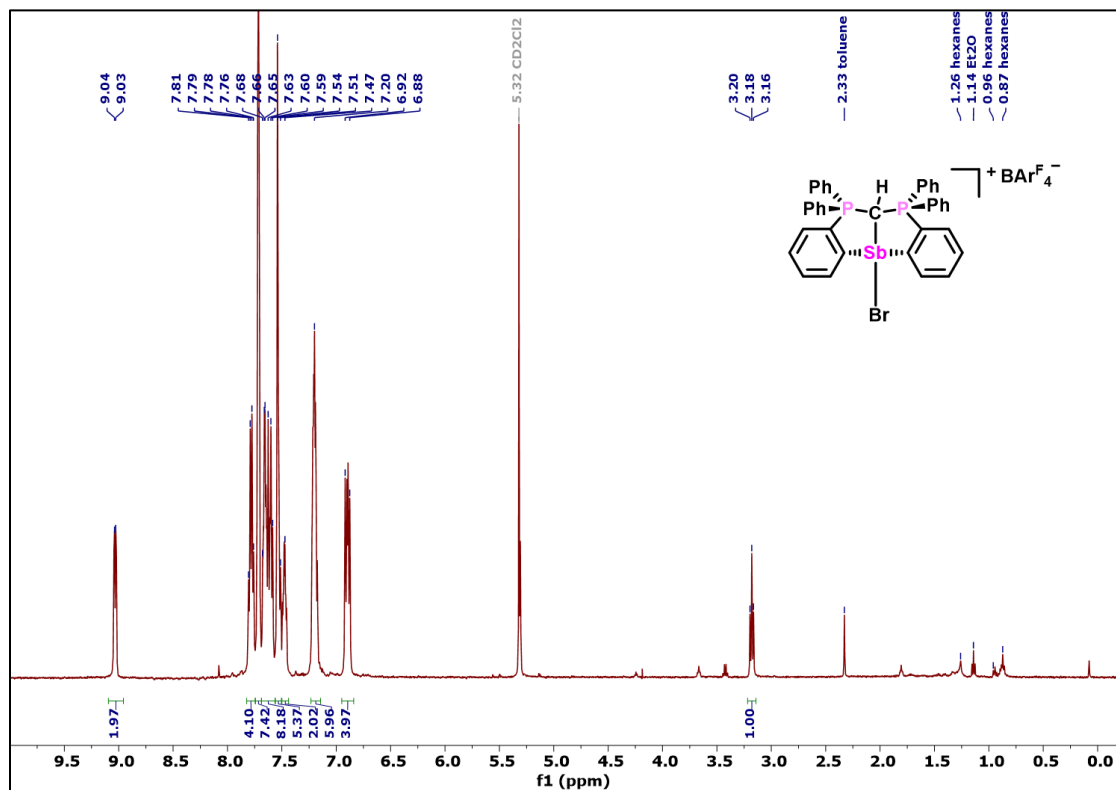


Figure S12.  $^1\text{H}$  NMR spectrum of  $4[\text{BArF}_4]$  (500 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

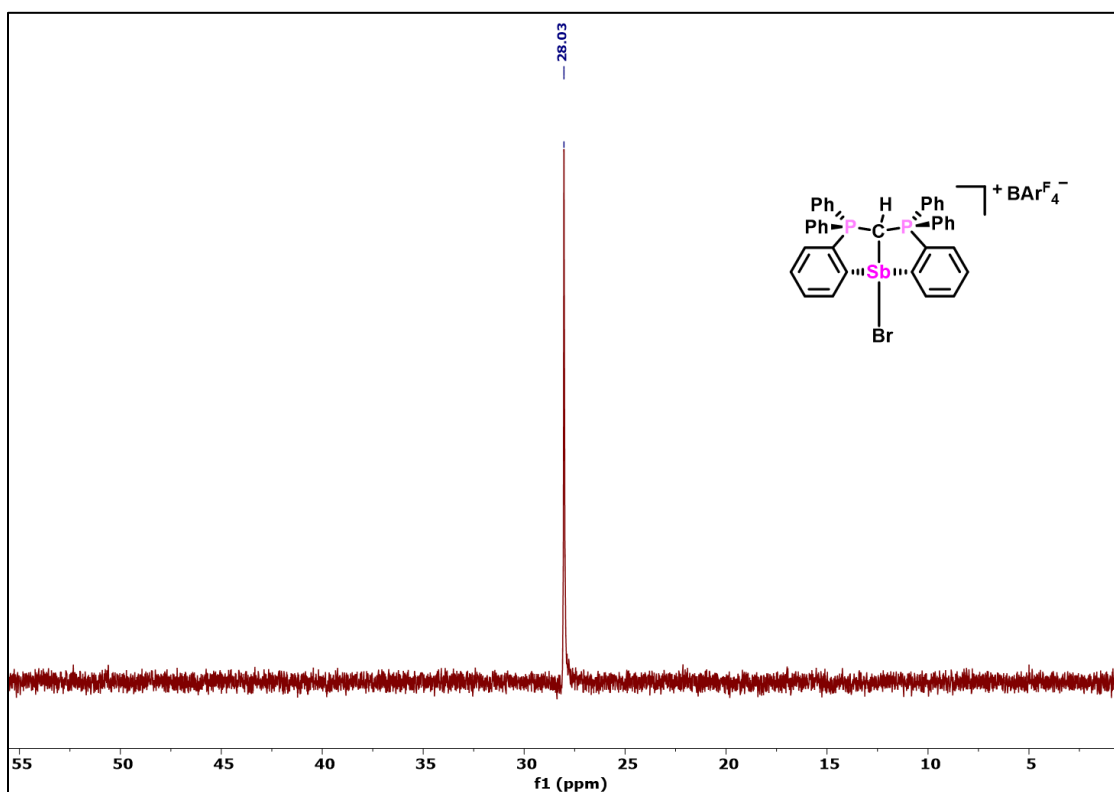


Figure S13.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of  $4[\text{BArF}_4]$  (201 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

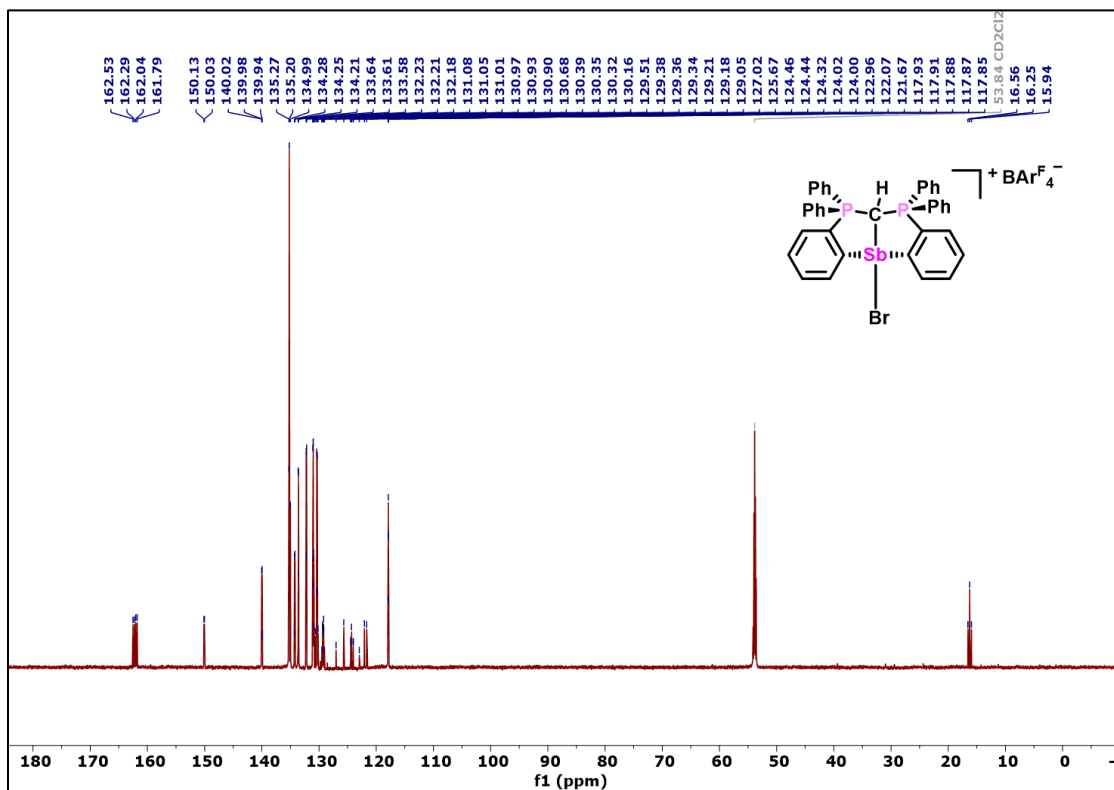
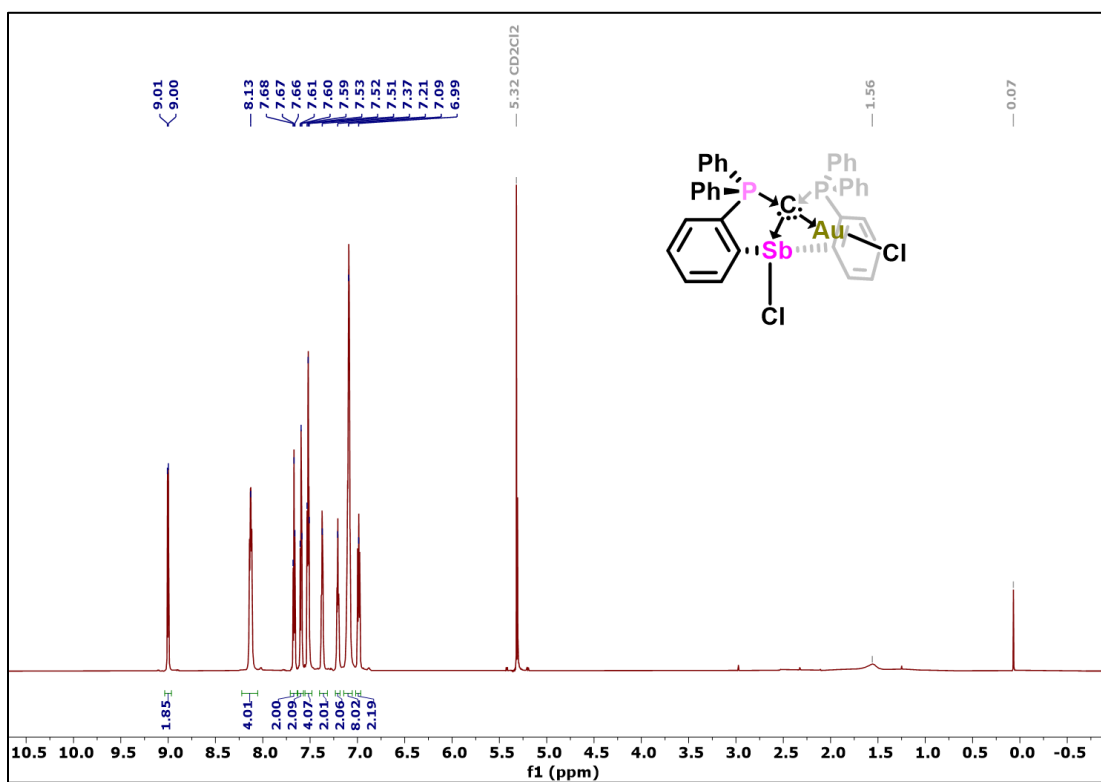
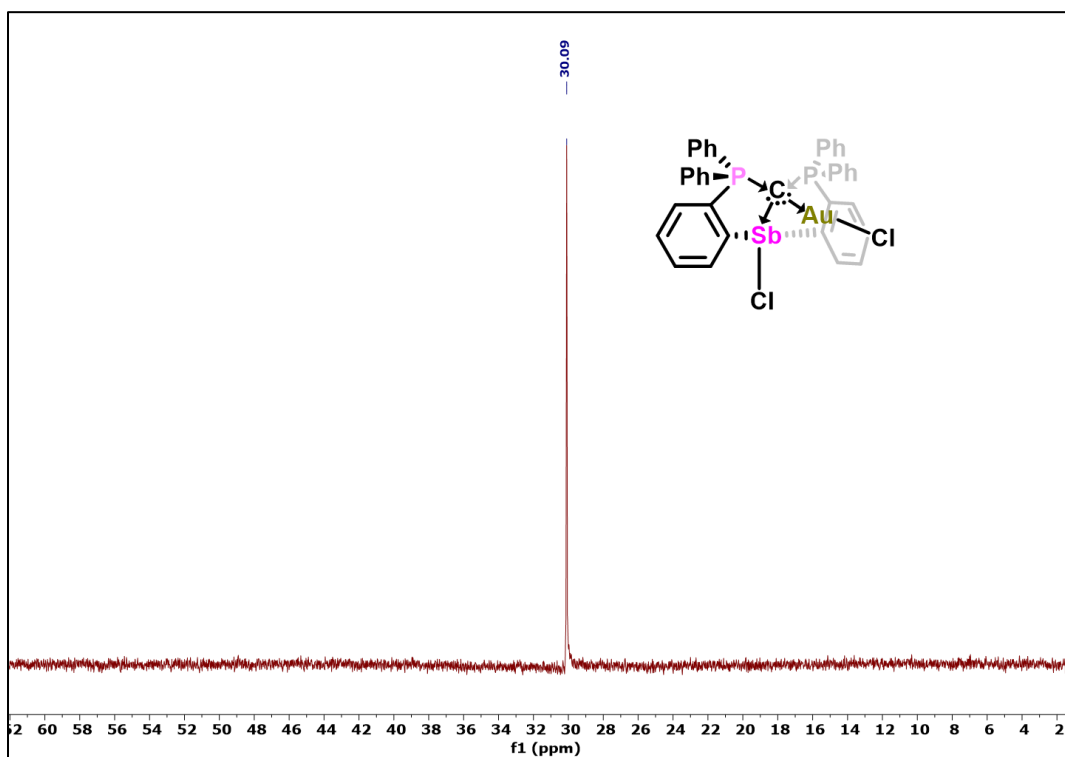


Figure S14.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of  $4[\text{BArF}_4]$  (200 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).



**Figure S15.**  $^1\text{H}$  NMR spectrum of **5** (800 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K) showing residual  $(\text{Me}_2\text{S})$  ( $\delta$  1.56 ppm) and grease ( $\delta$  0.07 ppm).



**Figure S16.**  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **5** (201 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

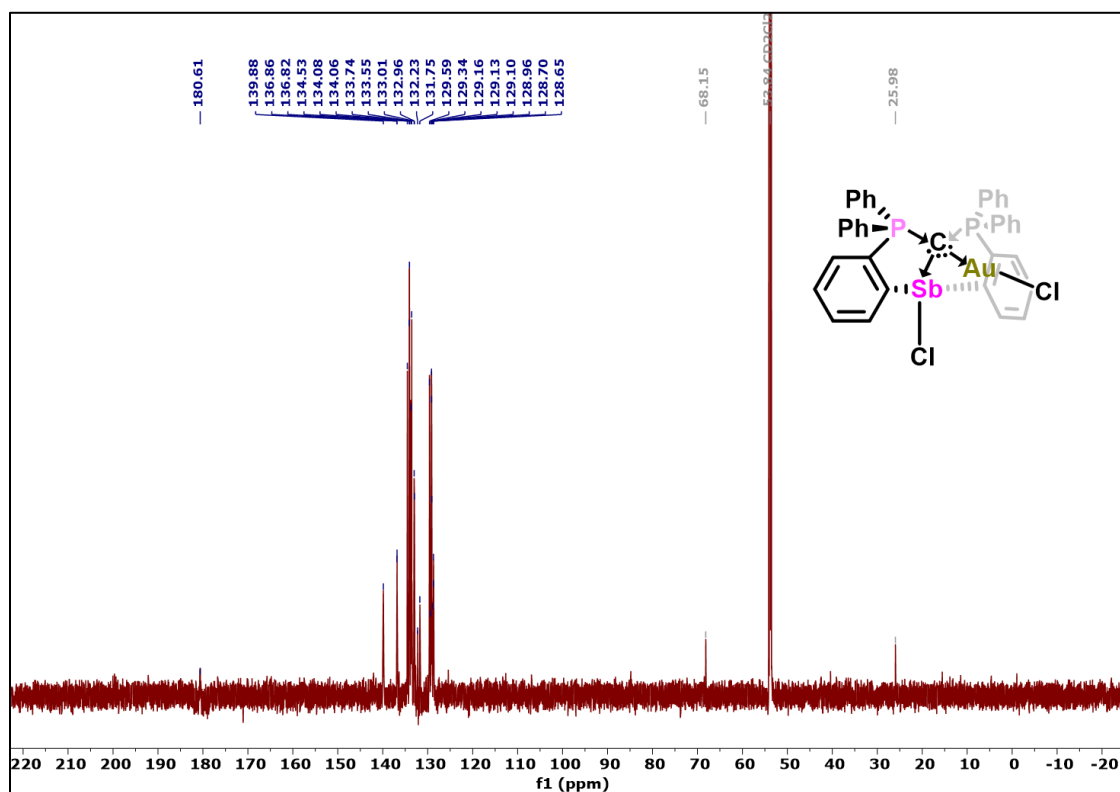


Figure S17.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of 5 (200 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

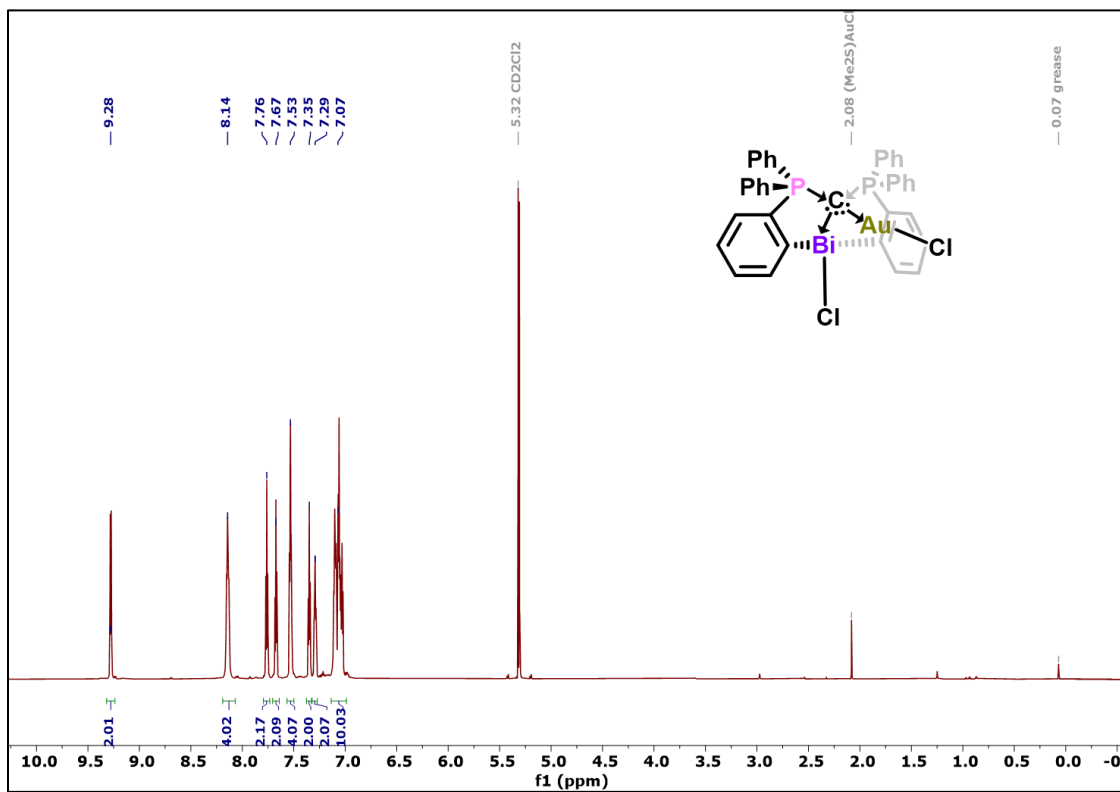


Figure S18.  $^1\text{H}$  NMR spectrum of 6 (800 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

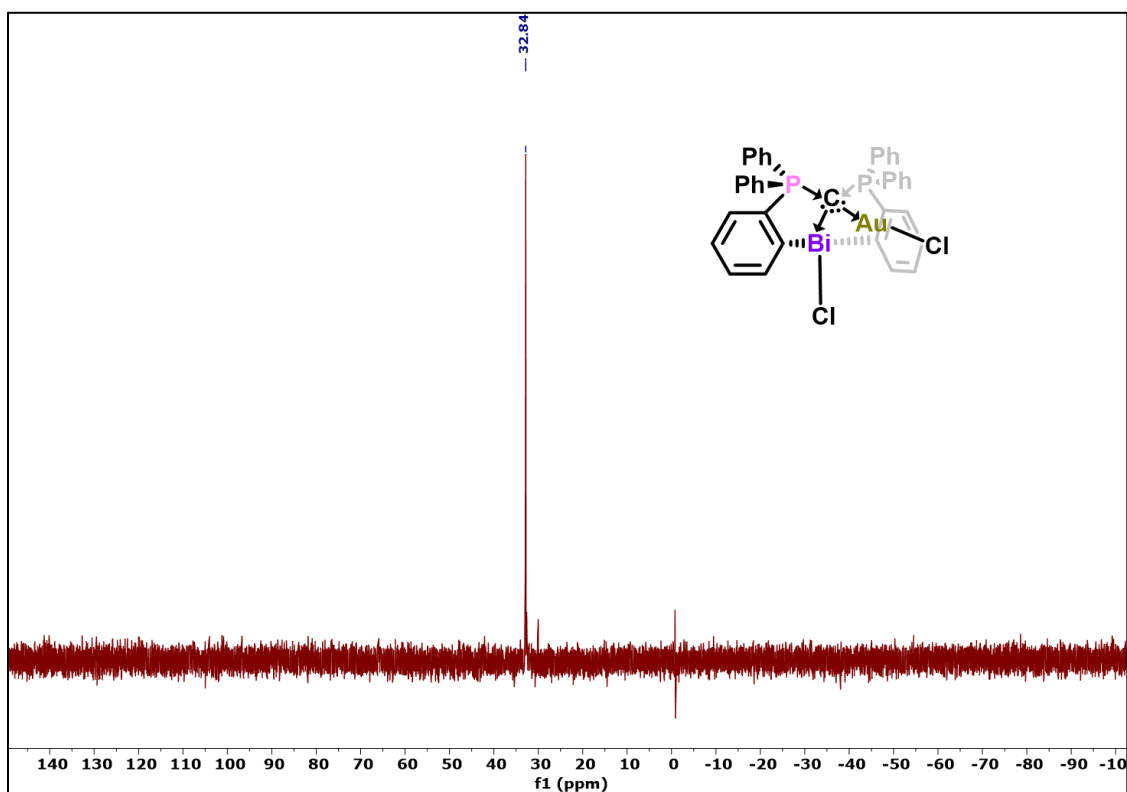


Figure S19.  $^{31}\text{P}\{^1\text{H}\}$  NMR spectrum of **6** (201 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

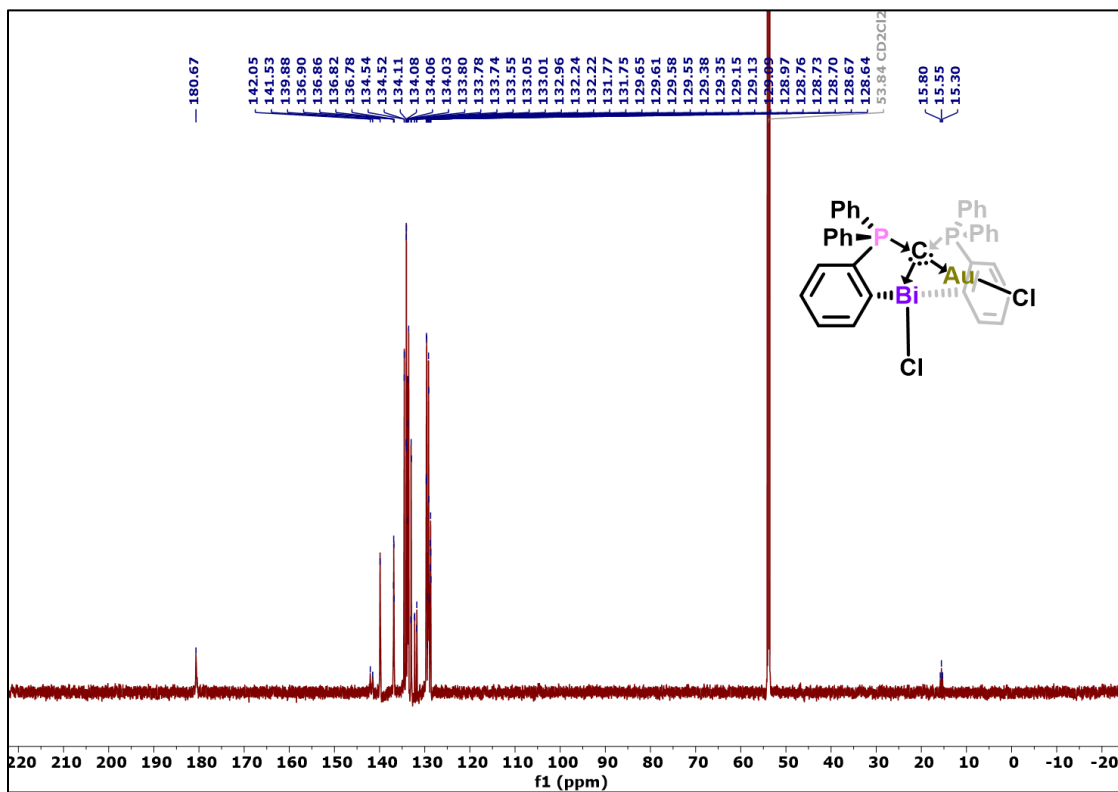


Figure S20.  $^{13}\text{C}\{^1\text{H}\}$  NMR spectrum of **6** (200 MHz,  $\text{CD}_2\text{Cl}_2$ , 298 K).

## Crystallographic Refinement Details

Single crystals of **1**, **2**, **3**[SbF<sub>6</sub>], **4**[SbF<sub>6</sub>], **4**[BArF], **5** or **6** were coated with Paratone oil and mounted on a MiTeGen MicroLoop. The X-ray intensity data were measured for **1**, **2**, **4**[BArF], and **5** were measured on a Bruker Kappa APEXII Duo system equipped with a fine-focus sealed tube (Mo K<sub>α</sub>, λ = 0.71073 Å) and a graphite monochromator. Data for **3**[SbF<sub>6</sub>], **4**[SbF<sub>6</sub>] and **6** were measured on a Bruker D8 Venture PhotonIII Kappa four-circle diffractometer system equipped with an Incoatec IμS 3.0 micro-focus sealed X-ray tube (Mo K<sub>α</sub>, λ = 0.71073 Å) and a HELIOS double bounce multilayer mirror monochromator. The frames were integrated with the Bruker SAINT software package<sup>[3]</sup> using a narrow-frame algorithm. Data were corrected for absorption effects using the Multi-Scan method (SADABS).<sup>[4]</sup> Each structure was solved and refined using the Bruker SHELXTL Software Package<sup>[5]</sup> within APEX4<sup>[3]</sup> and OLEX2.<sup>[6]</sup> Non-hydrogen atoms were refined anisotropically. Hydrogen atoms were placed in geometrically calculated positions with  $U_{iso} = 1.2U_{equiv}$  of the parent atom ( $1.5U_{equiv}$  for methyl).

For **1**, **3**[SbF<sub>6</sub>], **4**[BArF], the relative occupancy of the disordered atoms was freely refined with the sum of all parts in each group set to equal one. Constraints and restraints were used as needed on the anisotropic displacement parameters and bond lengths of the disordered atoms. For **2** and **6**, the relative occupancy of the disordered dichloromethane molecules were freely refined. No constraints or restraints were needed.



**Table S1.** Crystallographic data for 1-6

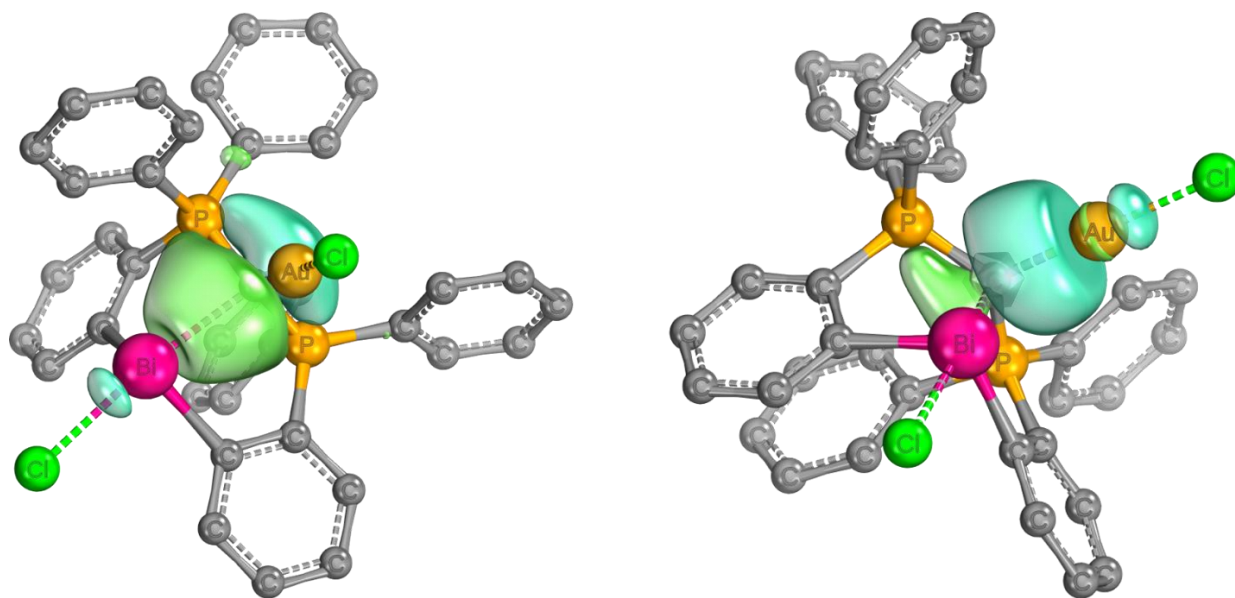
	1	2	3[SbF6]	4[SbF6]	4[BArF]	5	6
CCDC number	2312268	2312269	2312270	2312271	2312272	2312273	2312274
Formula	C <sub>77</sub> H <sub>62</sub> Cl <sub>8</sub> P <sub>4</sub> Sb <sub>2</sub>	C <sub>77</sub> H <sub>62</sub> Br <sub>2</sub> Cl <sub>6</sub> P <sub>4</sub> Sb <sub>2</sub>	C <sub>39</sub> H <sub>32</sub> Cl <sub>4</sub> F <sub>6</sub> P <sub>2</sub> Sb <sub>2</sub>	C <sub>41</sub> H <sub>37</sub> BrF <sub>6</sub> O P <sub>2</sub> Sb <sub>2</sub>	C <sub>141</sub> H <sub>88</sub> B <sub>2</sub> Br <sub>2</sub> Cl <sub>6</sub> F 48P <sub>4</sub> Sb <sub>2</sub>	C <sub>40</sub> H <sub>34</sub> AuCl 8P <sub>2</sub> Sb	C <sub>40</sub> H <sub>34</sub> AuBi Cl <sub>8</sub> P <sub>2</sub>
FW (g/mol)	1634.21	1727.16	1061.88	1045.05	3452.93	1178.93	1266.16
Temp (K)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)	100(2)
λ (Å)	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073	0.71073
Size (mm)	0.202 x 0.223 x 0.277	0.132 x 0.237 x 0.292	0.063 x 0.187 x 0.396	0.056 x 0.085 x 0.089	0.172 x 0.227 x 0.444	0.090 x 0.166 x 0.191 m	0.107 x 0.158 x 0.235
Crystal habit	colourless block	colourless block	colourless plate	yellow plate	colourless plate	colourless rod	colourless block
Crystal system	orthorhombic	orthorhombic	monoclinic	monoclinic	triclinic	monoclinic	monoclinic
Space group	F d d 2	F d d 2	P 2 <sub>1</sub> /n	P2 <sub>1</sub> /c	P -1	P2 <sub>1</sub> /c	P2 <sub>1</sub> /c
a (Å)	28.250(2)	27.674(4)	14.6987(6)	10.3202(8)	12.1350(9)	11.6084(8)	11.6409(4)
b (Å)	31.290(3)	31.304(4)	15.5168(7)	20.6841(13)	16.6073(12)	23.1906(16)	23.1633(9)
c (Å)	15.7735(12)	16.183(2)	17.5220(7)	18.5080(13)	18.5495(13)	15.8524(11)	15.8194(7)
α (°)	90	90	90	90	107.079(2)	90	90
β (°)	90	90	93.9750(10)	92.122(2)	95.331(2)	97.164(2)	97.161(2)
γ (°)	90	90	90	90	99.299(2)	90	90
Volume (Å <sup>3</sup> )	13943.(2)	14019.(3)	3986.7(3)	3948.1(5)	3487.2(4)	4234.2(5)	4232.3(3)
Z	8	8	4	4	1	4	4
Density (g/cm <sup>3</sup> )	1.557	1.637	1.769	1.758	1.644	1.849	1.987
μ (mm <sup>-1</sup> )	1.214	2.275	1.761	2.522	1.234	4.709	8.225
F(000)	6560	6864	2080	2048.0	1709	2280	2408
θ range (°)	1.61 to 30.56	1.60 to 28.28	2.19 to 28.34	1.48 to 27.94	1.16 to 28.36	1.56 to 26.41	1.76 to 28.32
Index ranges	-40 ≤ h ≤ 40 -44 ≤ k ≤ 44 -22 ≤ l ≤ 22	-36 ≤ h ≤ 36 -33 ≤ k ≤ 41 -21 ≤ l ≤ 21	-19 ≤ h ≤ 19 -20 ≤ k ≤ 20 -23 ≤ l ≤ 20	-13 ≤ h ≤ 13 -27 ≤ k ≤ 27 -24 ≤ l ≤ 24	-15 ≤ h ≤ 16 -21 ≤ k ≤ 22 -24 ≤ l ≤ 24	-14 ≤ h ≤ 14 -29 ≤ k ≤ 25 -19 ≤ l ≤ 19	-14 ≤ h ≤ 15 -30 ≤ k ≤ 30 -21 ≤ l ≤ 21
Reflns collected	57234	52053	64871	109972	88634	50354	69871
Independent reflns	10638 [R <sub>int</sub> = 0.0498]	8532 [R <sub>int</sub> = 0.0655]	9927 [R <sub>int</sub> = 0.0591]	9453 [R <sub>int</sub> = 0.0599]	17385 [R <sub>int</sub> = 0.0698]	8666 [R <sub>int</sub> = 0.0689]	10507 [R <sub>int</sub> = 0.0734]
Data / restraints / parameters	10638 / 31 / 473	8532 / 1 / 430	9927 / 0 / 476	9453/0/478	17385 / 284 / 1041	8666 / 0 / 469	10507 / 0 / 479
GOF on F <sup>2</sup>	1.045	1.023	1.191	1.023	1.007	1.065	1.033
R <sub>1</sub> (I > 2σ(I))	0.0308	0.0338	0.0642	0.0253	0.0391	0.0409	0.0315

wR <sub>2</sub> (all data)	0.0646	0.0627	0.1687	0.0580	0.0875	0.0974	0.0681
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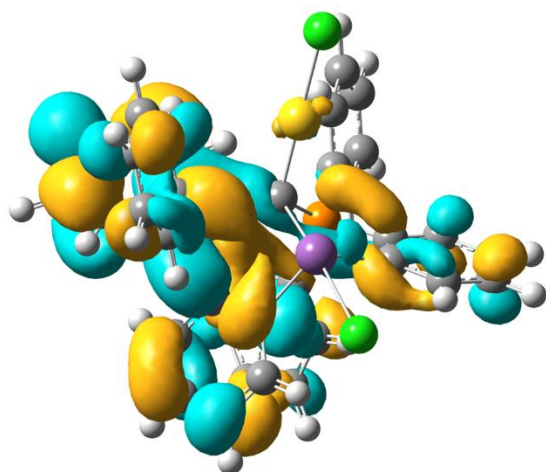
## Computational Details

### General

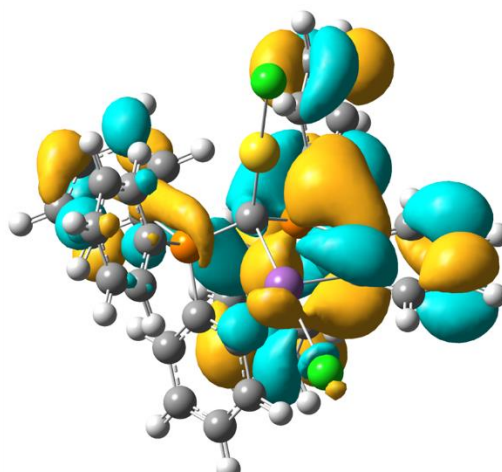
All geometries were optimized with Orca 5.0.4,<sup>[7]</sup> using the BP86 functional in conjunction with a valence triple-zeta polarization (def2-TZVP). The dispersion corrections were introduced using the Grimme D3-parametrized correction<sup>[8]</sup> and the Becke Johnson damping to the DFT energy.<sup>[9]</sup> The RIJCOSX approximation<sup>[10]</sup> was used to reduce the computational cost of calculations. The initial structures were generated from the above X-ray crystallography data while the counter ions were not included. The solvation effect was included by polarizable continuum model (PCM) using CH<sub>2</sub>Cl<sub>2</sub> as solvent. The bond lengths errors for all optimized structures are within 0.02 Å when compared to the crystal structure. In addition, characterization of stationary points as minima were verified by analytical vibrational mode analysis. Quantum theory of atoms-in-molecules (QTAIM) analysis<sup>[11]</sup> were conducted using Multiwfn program<sup>[12]</sup> For the intrinsic bond orbitals (IBOs) calculations,<sup>[13]</sup> wave functions were obtained in the ORCA 5.0.4 and structural depictions were made using the IboView.<sup>[14]</sup> All the wave functions analysis were carried out at the BP86-D3(BJ)/def2-TZVPP level of theory. The fluoride ion affinity (FIA) for **3**<sup>+</sup> was calculated (atPW6B95-(D3BJ)/def2-TZVPP//BP86-D3(BJ)/def2-TZVP level of theory) towards the isodesmic reaction with the TMS<sup>+</sup>/TMSF system<sup>[15]</sup> (where FIA of TMS<sup>+</sup> 952.5 kJ/mol) and the CPCM (CH<sub>2</sub>Cl<sub>2</sub>) method implemented in ORCA were used.



**Figure S20.** Selected IBOs of **6** with enclosing 80% of the density of the orbital electron.

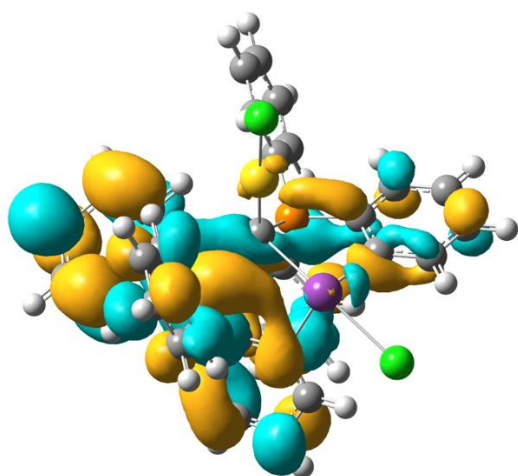


**LUMO (-2.58 eV)**

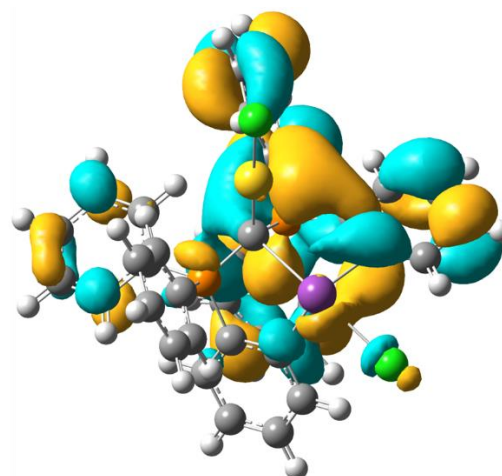


**LUMO+1 (-2.45 eV)**

**Figure S21.** The lowest unoccupied molecular orbitals (LUMO) of compound 5.



**LUMO (-2.55 eV)**



**LUMO+1 (-2.42 eV)**

**Figure S22.** The LUMOs of compound 6.

## QTAIM

QTAIM<sup>[11]</sup> analyses were conducted based on the optimized geometries of **5** and **6**. A bonding critical point (BCP) in accordance with the AIM theory locates between two atoms containing the considered bond. The most important parameters for description of the interaction are the electron density  $\rho(r)$  and the Laplacian of the electron density [ $\nabla^2\rho(r)$ ]. In general, large values of the electron density  $\rho(r)$  indicate a strong bonding interaction (for the same type of chemical bond). A negative  $\nabla^2\rho(r)$  shows the excess potential energy at the BCP which means that the electronic charge is contracted between two nuclei (covalent interaction), while a positive  $\nabla^2\rho(r)$  reveals that the kinetic energy contribution is greater than the potential energy (closed-shell interaction). QTAIM topological parameter  $G(r)$  is the Lagrangian kinetic energy and  $V(r)$  is the local potential electron energy density. The sign of electronic energy  $H(r)$  on the Hamiltonian at BCP determines whether the accumulation of charge at a given point is stabilizing [ $H(r) < 0$ ] or destabilizing [ $H(r) > 0$ ]. The nature of bond can be evaluated by means of the  $|V(r)|/G(r)$ .<sup>[16]</sup> If  $|V(r)|/G(r) > 2$ , then the bond has covalent character,  $1 < |V(r)|/G(r) < 2$  suggests that bond has partially covalent character, and  $|V(r)|/G(r) < 1$  suggests that the bonding is a closed-shell interaction (Tables S2 & S3).

**Table S2.** Values of the density of all electrons  $\rho(r)$ , Laplacian of electron density  $\nabla^2\rho(r)$ , local potential electron energy density  $V(r)$ , energy density  $H(r)$ , Lagrangian kinetic energy  $G(r)$  (in a.u.) at the bond critical points (BCPs) for respective bonds of **5**, calculated at PCM(DCM)-BP86-D3(BJ)/def2-TZVPP level of theory

<b>5</b>						
	$\rho(r)$	$\nabla^2\rho(r)$	$V(r)$	$H(r)$	$G(r)$	$ V(r) /G(r)$
C <sub>carbone</sub> -Au	0.1299	0.1711	-0.1635	-0.6079	0.1027	1.592016
C <sub>carbone</sub> -Sb	0.0561	0.0554	-0.0397	-0.0129	0.0267	1.486891
C <sub>Ph</sub> -Sb	0.0992	0.0559	-0.0927	-0.0394	0.0533	1.739212
C <sub>Ph</sub> -Sb	0.1024	0.0581	-0.0981	-0.0418	0.0563	1.742451
Au-Cl	0.0956	0.2206	-0.1176	-0.0315	0.0861	1.365854
Sb-Cl	0.0511	0.0725	-0.0390	-0.0104	0.0285	1.368421

**Table S3** Values of the density of all electrons  $\rho(r)$ , Laplacian of electron density  $\nabla^2\rho(r)$ , local potential electron energy density  $V(r)$ , energy density  $H(r)$ , Lagrangian kinetic energy  $G(r)$  (in a.u.) at the bond critical points (BCPs) for respective bonds of **6**, calculated at PCM(DCM)-BP86-D3(BJ)/def2-TZVPP level of theory

	<b>6</b>					
	$\rho(r)$	$\nabla^2\rho(r)$	$V(r)$	$H(r)$	$G(r)$	$ V(r) /G(r)$
C <sub>carbone</sub> -Au	0.1305	0.1688	-0.1642	-0.0615	0.1028	1.597276
C <sub>carbone</sub> -Bi	0.0479	0.0709	-0.0334	-0.0078	0.0256	1.304688
C <sub>Ph</sub> -Bi	0.0895	0.0794	-0.0778	-0.0290	0.0488	1.594262
C <sub>Ph</sub> -Bi	0.0930	0.0824	-0.0831	-0.0312	0.0518	1.604247
Au-Cl	0.0954	0.2207	-0.1174	-0.0314	0.0860	1.365116
Bi-Cl	0.0486	0.0933	-0.0387	-0.0077	0.0310	1.248387

## Cartesian Coordinates

**Table S4.** Cartesian coordinates for compound **5**

Atom	X	Y	Z
Au	0.77809021	-1.78716849	-1.35586135
Sb	-2.16866833	-0.17872155	-0.85516764
Cl	-4.65470781	0.54725749	-1.44021439
Cl	1.30986295	-3.56054715	-2.76078807
P	0.86551914	1.32746293	-0.55861576
P	-0.09756951	-0.58913401	1.54970775
C	0.21925379	-0.24239503	-0.12904651
C	-0.06003030	1.86698243	-2.01019662
C	-1.39833315	1.44163231	-2.12126135
C	-2.16786730	1.94492732	-3.17762162
H	-3.20894189	1.63130860	-3.27429546
C	-1.61714852	2.84391270	-4.09735295
H	-2.23290833	3.22230605	-4.91566896
C	-0.28353313	3.24866828	-3.98268204
H	0.14829290	3.93986169	-4.70791772
C	0.49799950	2.76335565	-2.93382964
H	1.53848705	3.07654710	-2.83494210
C	2.64148457	1.44081073	-0.95068047
C	3.37169182	0.33544370	-1.40921405
H	2.87722886	-0.63805186	-1.50383759
C	4.72045497	0.47179574	-1.73997443
H	5.27858138	-0.39828050	-2.08866942
C	5.34941323	1.71533402	-1.62618279
H	6.40460610	1.82037125	-1.88365948
C	4.62388399	2.82486230	-1.18120735
H	5.10759534	3.79869011	-1.09225317
C	3.27645207	2.69212723	-0.84162753
H	2.72320262	3.56104553	-0.48465396
C	0.60891585	2.59308179	0.71888531
C	1.48843570	2.67272214	1.81204918
H	2.35949353	2.02104617	1.86719584
C	1.25108498	3.59297990	2.83230004
H	1.93612799	3.64757356	3.67953491
C	0.14015955	4.43941753	2.76662948
H	-0.04833670	5.15530754	3.56817959
C	-0.73028045	4.36884223	1.67504728
H	-1.59900850	5.02598569	1.62222773
C	-0.49802420	3.45178921	0.64942348
H	-1.18123678	3.39444022	-0.19765480
C	-1.36178071	0.59933775	2.06850674
C	-2.35051398	0.85953071	1.09432953
C	-3.40165144	1.71848932	1.42340016
H	-4.18231040	1.91046998	0.68452089

C	-3.44536818	2.33653362	2.67823730
H	-4.25993922	3.02457962	2.91323846
C	-2.44420710	2.09514348	3.62309293
H	-2.46841857	2.59616805	4.59176981
C	-1.40171393	1.21550624	3.32464019
H	-0.61417701	1.03564958	4.05646748
C	-0.84821399	-2.23560756	1.68738483
C	-0.03429105	-3.35886406	1.46085449
H	1.02828148	-3.23217983	1.24732734
C	-0.58958167	-4.63643111	1.50442447
H	0.04163843	-5.50623189	1.31822052
C	-1.95262115	-4.79971585	1.78130094
H	-2.38554455	-5.80095737	1.80885007
C	-2.75730823	-3.68481763	2.02804350
H	-3.81791553	-3.80966543	2.25024528
C	-2.20811852	-2.39990684	1.98473283
H	-2.83784243	-1.53114467	2.17778435
C	1.32617638	-0.64969395	2.66014854
C	1.15228567	-0.90819068	4.03062787
H	0.15533773	-1.07928923	4.43969426
C	2.26614752	-0.97165543	4.86835354
H	2.13096000	-1.16258386	5.93385447
C	3.55260436	-0.80483676	4.34151403
H	4.42071635	-0.86026031	5.00011764
C	3.72792010	-0.58798384	2.97162991
H	4.72985992	-0.48127992	2.55381303
C	2.61647712	-0.51161154	2.13011502
H	2.75072141	-0.35842211	1.05900411

**Table S5.** Cartesian coordinates for compound **6**

Atom	X	Y	Z
Bi	2.21146884	-0.00908680	-0.36921699
Au	-0.41064749	1.89413438	-1.38264115
Cl	4.68238551	-1.14208752	-0.46551980
Cl	-0.34182253	3.72806624	-2.80986309
P	-1.05399866	-1.19080190	-0.77170971
P	-0.36135959	0.52414112	1.59837380
C	-0.38032730	0.28119436	-0.12177575
C	0.07719294	-1.80751474	-2.04092883
C	1.45389821	-1.57178954	-1.86876035
C	2.35142825	-2.16226214	-2.76575842
H	3.42358981	-1.99724776	-2.63644561
C	1.88708145	-2.96385777	-3.81503819
H	2.60056834	-3.41486873	-4.50774058
C	0.51587362	-3.17787126	-3.98745885



H	0.15264495	-3.79041971	-4.81403246
C	-0.39264560	-2.60506371	-3.09652526
H	-1.46292118	-2.77441096	-3.22399645
C	-2.71459156	-1.08291618	-1.51596069
C	-3.21855831	0.12560072	-2.01625881
H	-2.61728592	1.03764448	-1.93305091
C	-4.47876519	0.16810312	-2.61437751
H	-4.86179658	1.11619452	-2.99466235
C	-5.24305484	-0.99746572	-2.72511233
H	-6.22911087	-0.96279455	-3.19124579
C	-4.74255810	-2.20838359	-2.23605091
H	-5.33344626	-3.12165751	-2.32026331
C	-3.48529419	-2.25458470	-1.63142397
H	-3.10844812	-3.20114657	-1.24281517
C	-1.20242022	-2.51502385	0.46332369
C	-2.30328679	-2.53866174	1.33607334
H	-3.10312502	-1.80629370	1.23406045
C	-2.37902483	-3.50637931	2.33739871
H	-3.23491659	-3.51702081	3.01375909
C	-1.36145132	-4.45568274	2.47109750
H	-1.41824650	-5.20911064	3.25830886
C	-0.26983913	-4.43983830	1.59774218
H	0.52718300	-5.17687378	1.70180748
C	-0.18821293	-3.47560760	0.59284910
H	0.66697430	-3.46097403	-0.08250059
C	0.62678196	-0.81058998	2.32776781
C	1.79383111	-1.14340382	1.60961590
C	2.65216485	-2.11254766	2.13121731
H	3.56745881	-2.36392453	1.58973928
C	2.33446890	-2.76699839	3.32809085
H	3.00179974	-3.53906925	3.71682145
C	1.15942527	-2.45223761	4.01627729
H	0.90169880	-2.98018540	4.93551994
C	0.30384937	-1.46426956	3.52341491
H	-0.61783883	-1.22718234	4.05512774
C	0.52365517	2.06906936	1.96068879
C	-0.08539967	3.28403190	1.60140643
H	-1.08375039	3.28753027	1.16124740
C	0.59185991	4.48541936	1.80230723
H	0.12113725	5.42552585	1.51188413
C	1.87244086	4.48285076	2.36920534
H	2.40287400	5.42460524	2.51879859
C	2.46832970	3.27821359	2.74966017
H	3.46195580	3.27341242	3.19976450
C	1.79526356	2.06868036	2.55085209
H	2.26221295	1.12990015	2.84982504
C	-1.96079909	0.72753283	2.41855390
C	-2.03137350	0.95014005	3.80450773
H	-1.12045625	1.00185477	4.40307340
C	-3.27368150	1.12983957	4.41351191
H	-3.32931976	1.29407028	5.49058682

C	-4.44317415	1.11223335	3.64362023
H	-5.41203527	1.25758825	4.12396807
C	-4.37012934	0.92861131	2.25974113
H	-5.27716172	0.93704682	1.65378642
C	-3.13017626	0.73833195	1.64632366
H	-3.06688566	0.61225293	0.56497914

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**Table S6.** Cartesian coordinates for compound **3<sup>+</sup>**

Atom	X	Y	Z
Sb	-0.30522786	-2.47481553	0.53238668
P	-1.51231530	0.36010298	0.07610234
P	1.55270971	0.11945009	0.16853587
C	-0.03883305	-0.32741720	0.60078565
C	-1.70875035	-2.08268563	-1.10410938
C	-2.18713075	-0.76055342	-1.18773651
C	-3.14347223	-0.40538335	-2.14959857
H	-3.51972270	0.61743761	-2.20966874
C	-3.60313014	-1.37189717	-3.04847927
H	-4.33237893	-1.09746405	-3.81197105
C	-3.13358991	-2.68732160	-2.96741669
H	-3.49482739	-3.43766505	-3.67302687
C	-2.20381792	-3.04847623	-1.98405870
H	-1.86034429	-4.08323193	-1.92061252
C	-2.71151361	0.33598212	1.43911430
C	-4.08887971	0.42947197	1.18275547
H	-4.45748985	0.48754949	0.15749586
C	-4.99137809	0.43544181	2.24611326
H	-6.06200363	0.50335115	2.04766192
C	-4.52509669	0.34757734	3.56392082
H	-5.23513738	0.34885239	4.39249931
C	-3.15414490	0.25233820	3.81929490
H	-2.79012715	0.18061785	4.84532443
C	-2.24577840	0.24569451	2.75761381
H	-1.17192264	0.16737327	2.93459548
C	-1.47772402	2.05379609	-0.53504313
C	-1.63779747	3.10727503	0.37965796
H	-1.79517913	2.89310257	1.43781064
C	-1.60404036	4.42661037	-0.07232142
H	-1.72690204	5.24558342	0.63763053
C	-1.42173173	4.69486914	-1.43241372
H	-1.40099187	5.72699871	-1.78545952
C	-1.25968276	3.64514550	-2.34203710
H	-1.10605587	3.85559049	-3.40080655
C	-1.28218557	2.32331363	-1.89836403

H	-1.14325966	1.50671107	-2.60657344
C	1.54636332	-2.52479763	-0.60591244
C	2.28979182	-1.33223953	-0.63894060
C	3.54847113	-1.29320038	-1.25803839
H	4.12820442	-0.36890855	-1.28091970
C	4.05147285	-2.44314124	-1.86828570
H	5.02234457	-2.41230132	-2.36455681
C	3.31352309	-3.63245597	-1.84094147
H	3.71004500	-4.52978626	-2.31925472
C	2.07296971	-3.67931239	-1.19597143
H	1.51905335	-4.61983418	-1.16298939
C	2.57726911	0.47482936	1.62480757
C	2.08597890	0.13612408	2.89236005
H	1.08070667	-0.28094054	2.97640721
C	2.87720398	0.33979236	4.02541661
H	2.49075431	0.07792721	5.01158530
C	4.15871515	0.88289755	3.89333656
H	4.77567225	1.04613386	4.77841902
C	4.65121102	1.22321108	2.62749062
H	5.64901349	1.65243148	2.52538000
C	3.86557096	1.01967526	1.49268188
H	4.25121487	1.29871392	0.51084239
C	1.75927154	1.53192162	-0.93641821
C	1.81810845	2.83164440	-0.40857240
H	1.74857407	2.99006102	0.66830146
C	1.97141801	3.91911122	-1.26816838
H	2.00761533	4.92959796	-0.85974306
C	2.08060856	3.71349870	-2.64729104
H	2.21122221	4.56663729	-3.31468329
C	2.01098772	2.42027647	-3.17405873
H	2.08654164	2.26078640	-4.25048758
C	1.83964418	1.32801307	-2.32314683
H	1.77667390	0.31919595	-2.73264628

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