In Silico Screening of *P,N*-Ligands Facilitates Optimization of Au(III)-Mediated *S*-Arylation

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General Experimental Information

Materials

All chemicals were used as purchased unless otherwise noted from Acros, Alfa Aesar, Chem-Impex, Combi-Blocks, Fisher Scientific, Millipore Sigma, Oakwood Chemical, Strem Chemicals, or TCI Chemicals. Hydrogen tetrachloroaurate(III) trihydrate was stored in a desiccator under an argon atmosphere in a sealed scintillation vial. Anhydrous toluene was distilled over CaH_2 and stored under argon. Anhydrous THF was obtained by passing through an activated alumina column prior to use. Chlorodicyclopentylphosphine was purchased from Millipore Sigma and used as received and stored under an argon atmosphere. Silver hexafluoroantimonate ($AgSbF_6$), dicyclohexylphosphine, and di-1-adamantylphosphine were stored in a Vacuum Atmospheres Genesis stainless steel glove box under nitrogen atmosphere. Representative procedures are provided for each reaction.

Instrumentation

NMR spectra were recorded on the following: AV400 Bruker spectrometer at 400 (^{1}H) and 101 MHz (^{13}C{^{1}H}); AV300 Bruker spectrometer at 300 (^{1}H) and 121 MHz (^{31}P{^{1}H}); NEO600 Bruker spectrometer at 600 (^{1}H), 151 (^{13}C{^{1}H}), and 243 MHz (^{31}P{^{1}H}). Spectra are reported in δ (parts per million) relative to residual proteo-solvent signals for ^{1}H and H_3PO_4 (δ 0.00 ppm) for ^{31}P{^{1}H}. The following abbreviations were used to explain multiplicities: s = singlet, d = doublet, t = triplet, q = quartet, m = multiplet. Deuterated solvents were purchased from Cambridge Isotope Laboratories and used as received for all NMR experiments. Column chromatography was performed on a Biotage Isolera One 3.0 autocolumn instrument. All silica chromatography was carried out on the Biotage using KP-Sil high-performance columns repacked using the Silicycle silica (P60, particle size 40–63 μm, column sizes described in experimental). Reverse phase purification was carried out on an Agilent 1290 Infinity II liquid chromatography system equipped with a UV detector using a Luna 5 μm C18 100 Å column (Preparatory: 5 μm, 250 × 21.2 mm) with monitoring at λ = 215 and 254 nm and with a flow rate of 20 mL/min.

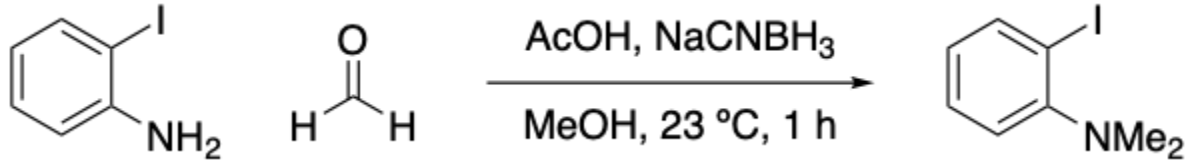
High-resolution mass spectrometry data was collected using either an Agilent 1260 Infinity 6530 Q-TOF ESI instrument (ESI/QTOF), a Waters LCT premier mass spectrometer with a direct inject port (ESI), or a Thermo Exactive Plus Orbitrap instrument with IonSense ID-CUBE DART source (DART).

UV-Vis and Stopped-Flow Kinetics experiments were carried out using an Applied Photophysics SX20, using the Absorbance Photomultiplier or Photodiode Array detectors for single-wavelength and multiwavelength data collection, respectively. For single-wavelength data collection, the monochromator was set to a pre-defined wavelength, and the slit width to 1.0 mm. The instrument was configured setting the cell path-length to 10 mm. When taking full spectra with the Photodiode Array, 1:1 MeCN-buffered reaction solvent was used as the reference sample. For single wavelength measurements, 1000 data points were collected for durations ranging from 50 ms to 120 s. For full spectra, a minimum of 10 spectra were taken to determine the best wavelengths for single wavelength monitoring. Trigger mode was set to external, and a pressure hold was used for

reactions below 5 s to remove artifacts observed due to cavitation. Instrument syringes and lines were rinsed firstly with Milli-Q® water, and then reaction buffer system prior to use. For any given bioconjugation reaction, the concentration of **GSH** was at least 100 times larger than the concentration of bioconjugation reagent to ensure pseudo first-order conditions. Raw data was exported as ProData CSV files and processed in OriginPro 9.1. Data was plotted for presentation using Prism 10.

Synthesis of *Ortho*-Halo-*N*,*N*-Dimethylanilines with Varying Aryl Substituents

Synthesis of 2-iodo-*N*,*N*-dimethylaniline (34)



A one neck 1 L round bottom flask was charged with a stir bar, then 2-iodoaniline (10.000 g, 1 Eq, 45.656 mmol) was dissolved in 400 mL of methanol. Formaldehyde (34.09 mL, 10 Eq, 456.56 mmol, 37% weight in water) and acetic acid (13.1 mL, 5 Eq, 228.28 mmol) were added to the flask and left to stir for ten minutes at 23 ºC. Sodium cyanoborohydride (11.48 g, 4 Eq, 182.62 mmol) was added in portions over a 15 minute period, then this was left to stir for one hour at 23 ºC. The reaction was concentrated under vacuum and carefully pH adjusted to ca. pH 8 using 1 M $NaHCO_3$. The product was transferred to a separatory with ethyl acetate (300 mL), then the organic layer was washed with $NaHCO_3$ (2 x 75 mL) and brine (100 mL). The organic layer was collected, dried with anhydrous magnesium sulfate, filtered, and concentrated under vacuum. The resulting product was further purified *via* vacuum distillation at 85 ºC to afford a clear, colorless liquid (9.445 g, 84% yield).

Physical state: Clear, colorless liquid
TLC (UV): R_f 0.67 (5:1 hexanes-ethyl acetate)
^{1}H NMR (400 MHz, $CDCl_3$): δ 7.84 (dd, *J* = 7.8, 1.5 Hz, 1H), 7.31 (m, 1H), 7.10 (dd, *J* = 8.0, 1.5 Hz, 1H), 6.77 (m, 1H), 2.77 (s, 6H).
^{13}C{^{1}H} NMR (101 MHz, $CDCl_3$): δ 155.10, 140.33, 129.19, 125.12, 120.61, 97.27, 45.12.
HRMS (ESI/QTOF): $[M+H]^+$ calculated for $C_8H_{11}IN^+$ 247.9936, observed 247.9963.

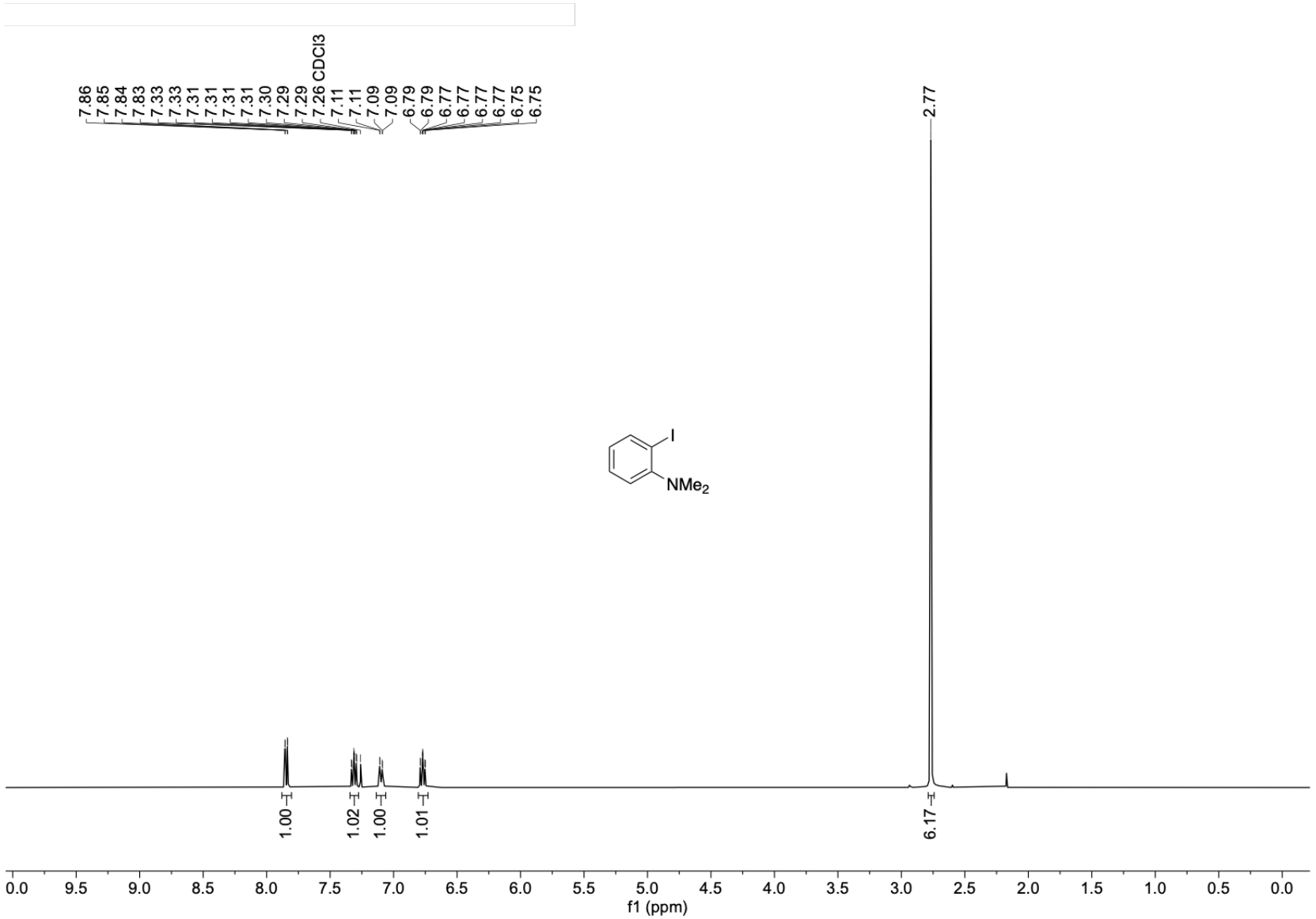


Figure S1. ^{1}H NMR of **34** in $CDCl_3$ at 298 K.

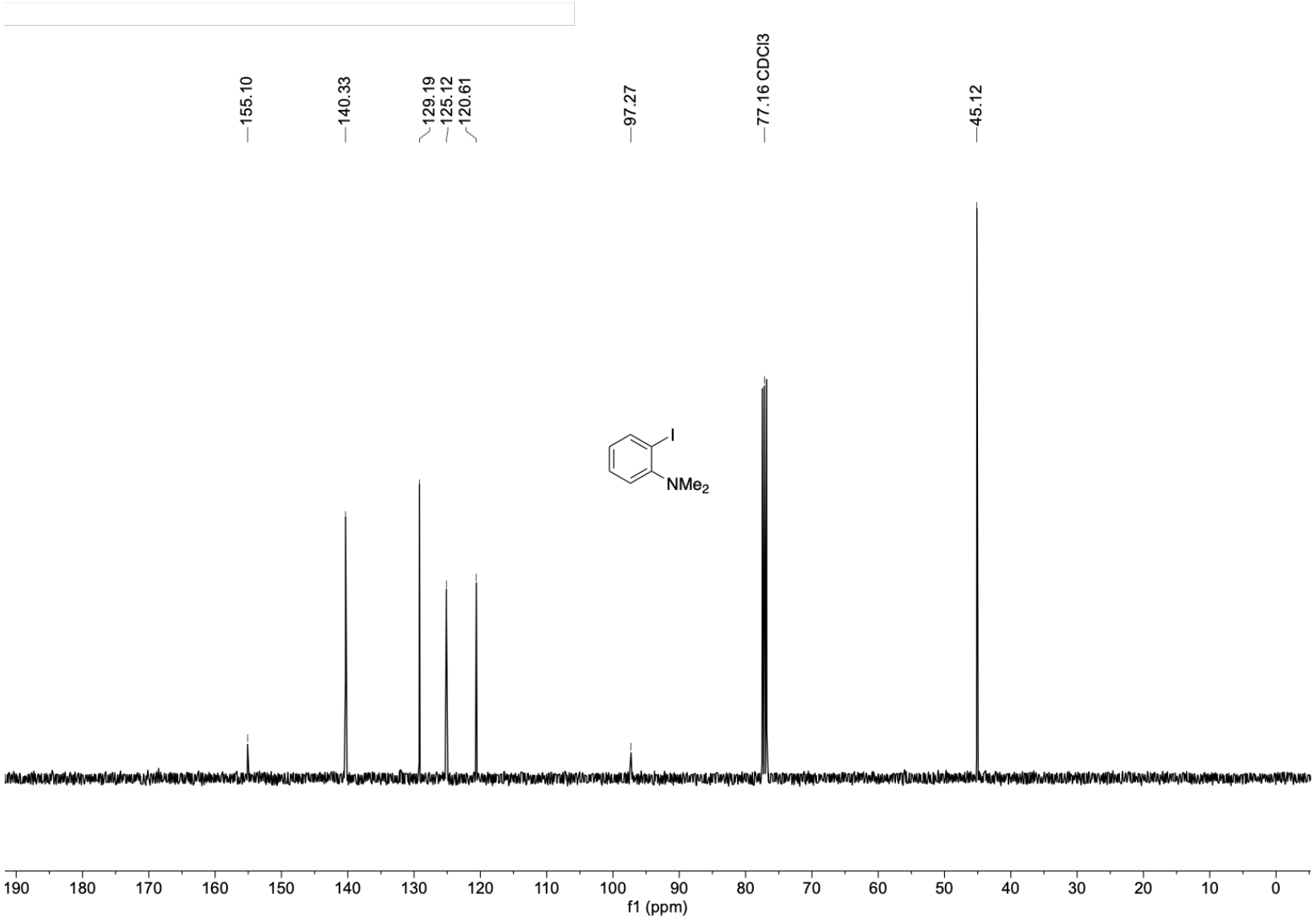
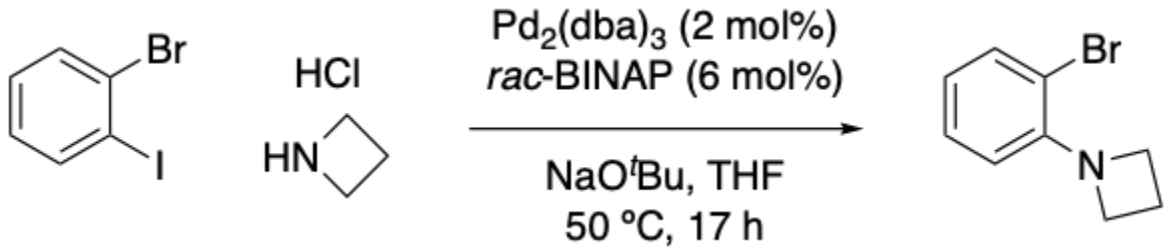


Figure S2. $^{13}C\{^{1}H\}$ NMR of **34** in $CDCl_3$ at 298 K.

Synthesis of 1-(2-bromophenyl)azetidine (35)



A flame dried scintillation vial was charged with a stir bar and placed under an inert atmosphere, then *rac*-BINAP (187 mg, 0.06 Eq, 300 µmol) and $Pd_2(dba)_3$ (91.6 mg, 0.02 Eq, 100 µmol) were suspended in 5 mL of anhydrous THF, creating a dark orange suspension. After stirring at 23 ºC for five minutes, sodium *tert*-butoxide (1.44 g, 3 Eq, 15.0 mmol) was added under positive pressure of argon, then 2-bromo-iodobenzene (1.41 g, 637 µL, 1 Eq, 5.00 mmol) was added to the flask followed by azetidine hydrochloride (555 mg, 1.2 Eq, 6.00 mmol). The flask was then heated at 50 ºC under a static argon atmosphere. After 17 hours, the reaction was cooled to ambient temperature and filtered through a pad of Celite, then the flow through was dried with anhydrous magnesium sulfate, filtered, and concentrated under vacuum. The product was further purified using flash column chromatography (50 g silica gel, 0-50% gradient of ethyl acetate against hexanes) to afford the product as a yellow liquid (550 mg, 2.59 mmol, 52% yield).

Physical state: Yellow liquid
TLC (UV): R_f 0.63 (6:1 hexanes-ethyl acetate)
^{1}H NMR (600 MHz, $CDCl_3$): δ 7.41 (dd, *J* = 7.9, 1.5 Hz, 1H), 7.21 – 7.15 (m, 1H), 6.67 (td, *J* = 7.6, 1.5 Hz, 1H), 6.55 (dd, *J* = 8.1, 1.5 Hz, 1H), 4.07 (t, *J* = 7.3 Hz, 4H), 2.27 (p, *J* = 7.3 Hz, 2H).
^{13}C{^{1}H} NMR (151 MHz, $CDCl_3$): δ 149.53, 134.18, 127.86, 120.27, 114.90, 108.82, 54.34, 16.96.
HRMS (DART): $[M+H]^+$ calculated for $C_9H_{11}BrN^+$ 212.0075, observed 212.0083.

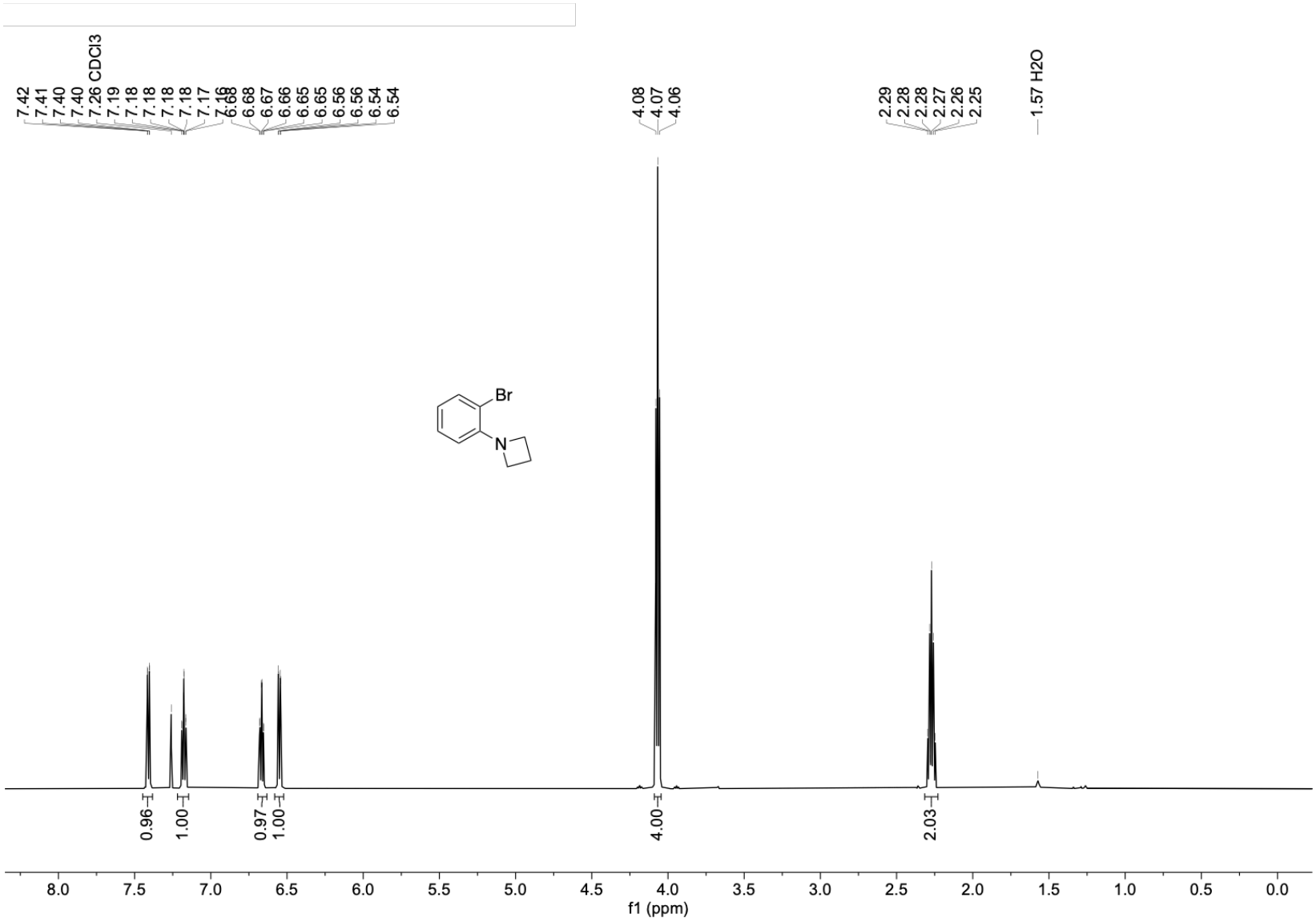


Figure S3. ^{1}H NMR of **35** in $CDCl_3$ at 298 K.

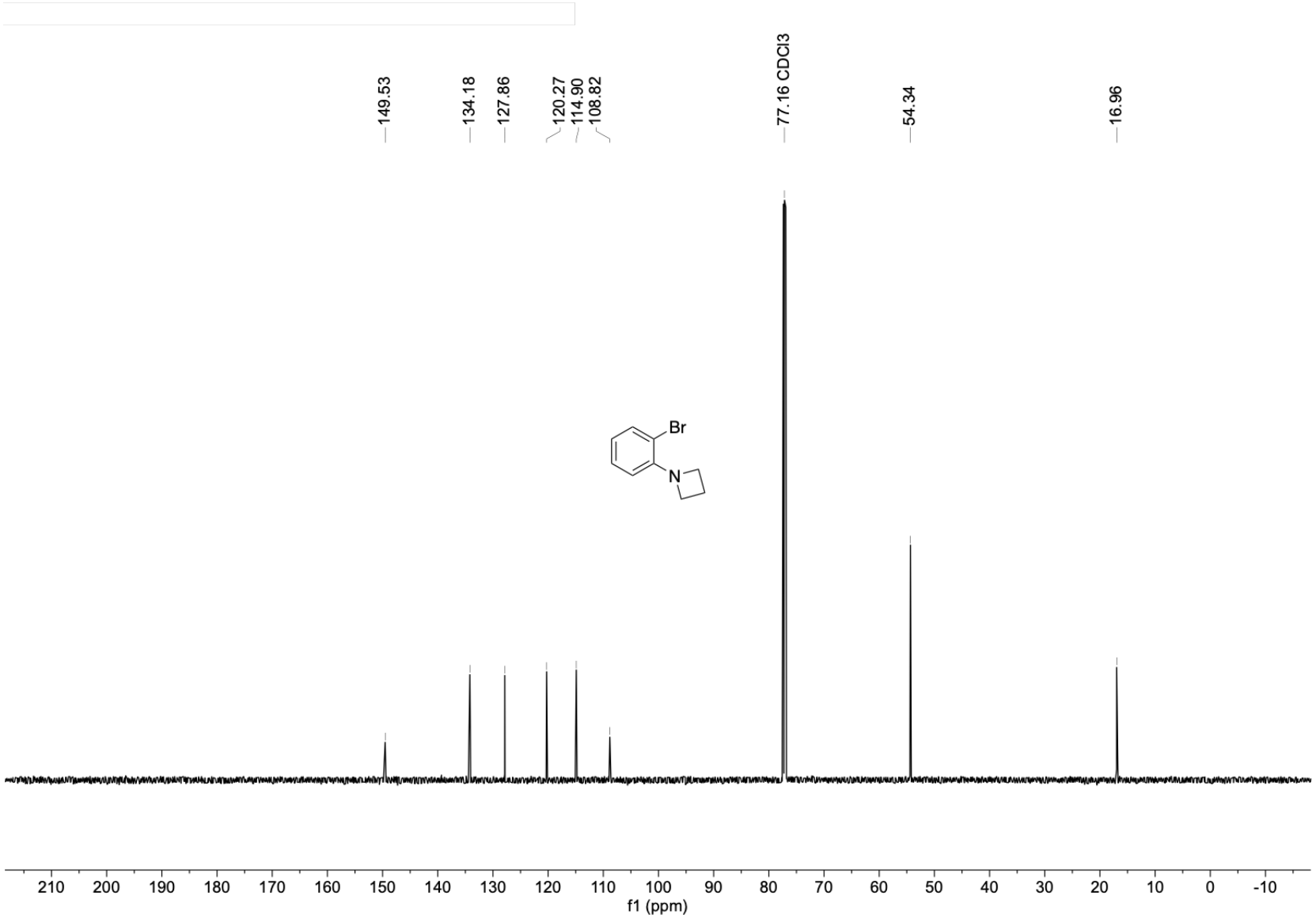
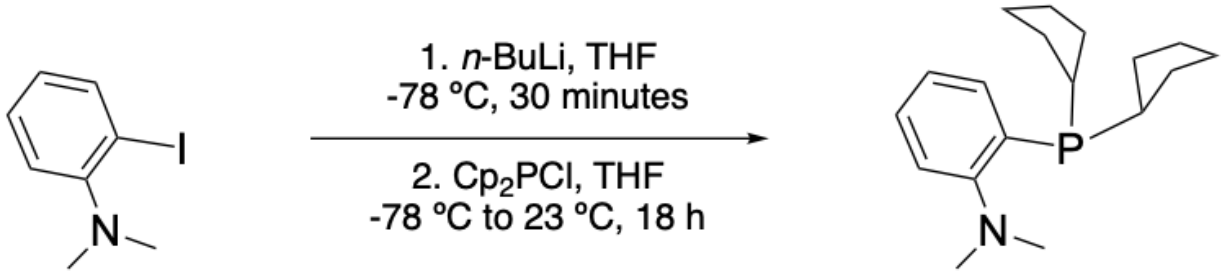


Figure S4. $^{13}C\{^{1}H\}$ NMR of **34** in $CDCl_3$ at 298 K.

Synthesis of Substituted *P,N*-Ligands

Synthesis of (PCp_2)Me-DalPhos (21)



A 15 mL, two neck round bottom flask was charged with a stir bar then flame dried three times under vacuum. **34** (370.6 mg, 231.6 µL, 1 Eq, 1.500 mmol) was added to the flask dissolved in 3 mL of anhydrous THF. This clear, colorless solution was cooled to -78 ºC, then *n*-BuLi (115.3 mg, 720.0 µL, 2.5 molar in hexanes, 1.2 Eq, 1.800 mmol) was added to the flask, immediately forming a yellow, clear solution. This was left to stir at -78 ºC for 30 minutes under argon. After 30 minutes, chlorodicyclopentylphosphine (368.4 mg, 344.6 µL, 1.2 Eq, 1.800 mmol) was added to the flask at -78 ºC with no observable exotherm and formation of a darker, yellow solution. After 30 minutes of stirring at -78 ºC, the flask was removed from the cooling bath and left to stir at 23 ºC under a static argon atmosphere overnight. After 18 hours, the clear, yellow reaction was removed from argon and quenched with 3 mL of methanol with no observable exotherm or color change. This was diluted with diethyl ether (150 mL) and transferred to a separatory funnel where the organic layer was washed once with saturated sodium bicarbonate (30 mL), then the organic layer was collected and the aqueous layer was extracted once with DCM (50 mL). The organic layers were combined, dried with anhydrous magnesium sulfate, filtered, and concentrated under vacuum. The resulting product was further purified using flash column chromatography (25 g silica gel, 0-80% ethyl acetate against hexanes). UV active products that eluted between 20-60% ethyl acetate were collected and concentrated under vacuum. The resulting orange oil was purified *via* preparative HPLC using a 10-100% gradient of acetonitrile against water, both with 0.1% TFA additive. Pure fractions as determined by mass spectrometry were collected and concentrated under vacuum to remove the acetonitrile. The resulting mixture was transferred to a separatory funnel with DCM (50 mL), then the organic layer was washed with saturated sodium carbonate (25 mL). The organic layer was collected, dried with anhydrous magnesium sulfate, filtered, and concentrated under vacuum to afford the product as a clear, colorless oil (87 mg, 0.30 mmol, 20% yield).

Physical state: Colorless oil
^{1}H NMR (600 MHz, CD_2Cl_2): δ 7.46 – 7.38 (m, 1H), 7.29 – 7.21 (m, 1H), 7.12 – 7.05 (m, 1H), 7.05 – 6.99 (m, 1H), 2.73 (s, 6H), 2.15 – 2.03 (m, 2H), 1.98 – 1.87 (m, 2H), 1.69 – 1.63 (m, 2H), 1.61 – 1.55 (m, 4H), 1.53 – 1.49 (m, 4H), 1.47 – 1.39 (m, 2H), 1.23 – 1.14 (m, 2H).
^{31}P{^{1}H} NMR (243 MHz, CD_2Cl_2): δ -12.27.
HRMS (DART): $[M+H]^+$ calculated for $C_{18}H_{29}NP^+$ 290.2038, observed 290.2035.

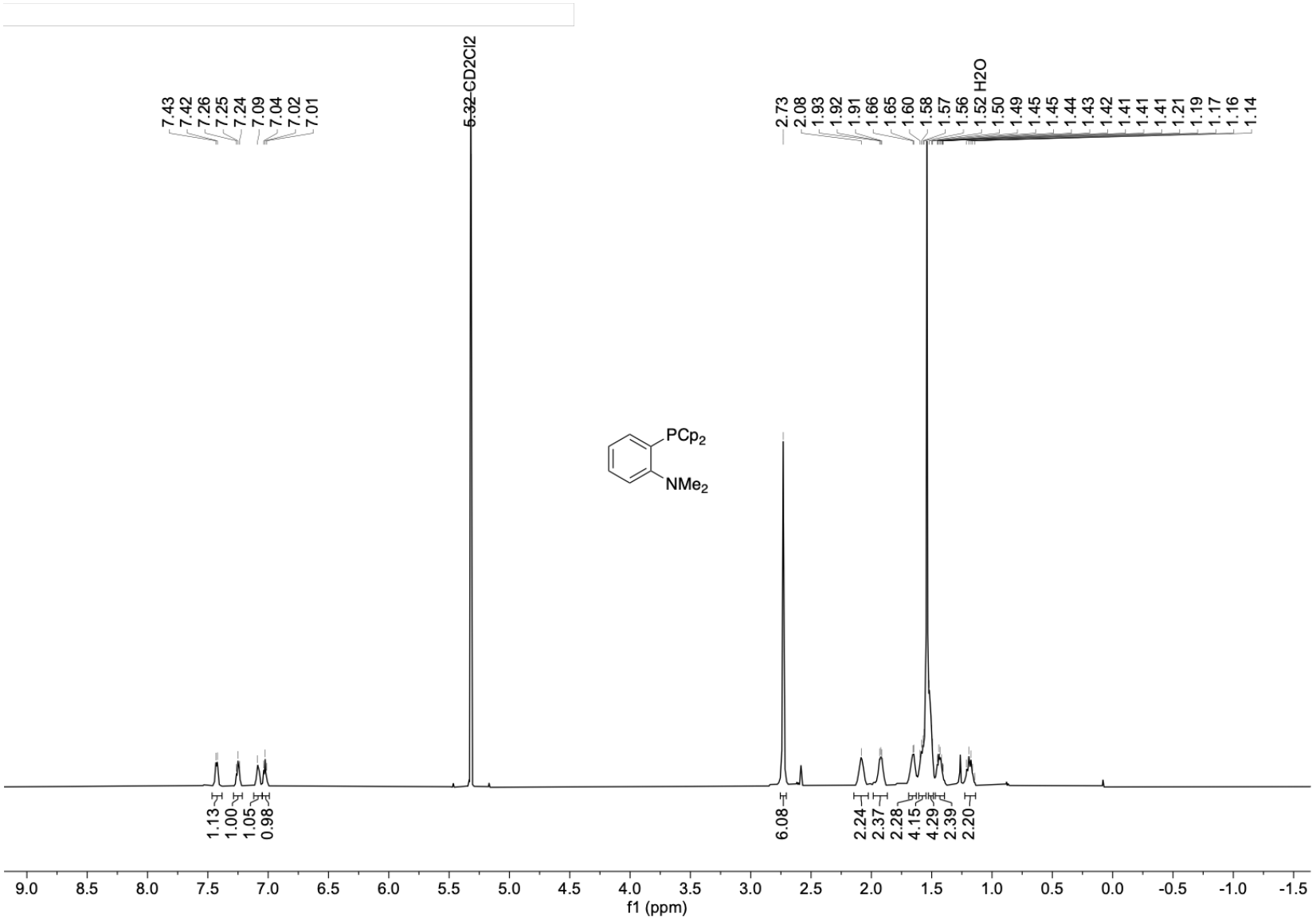


Figure S5. ^{1}H NMR of **21** in CD_2Cl_2 at 298 K.

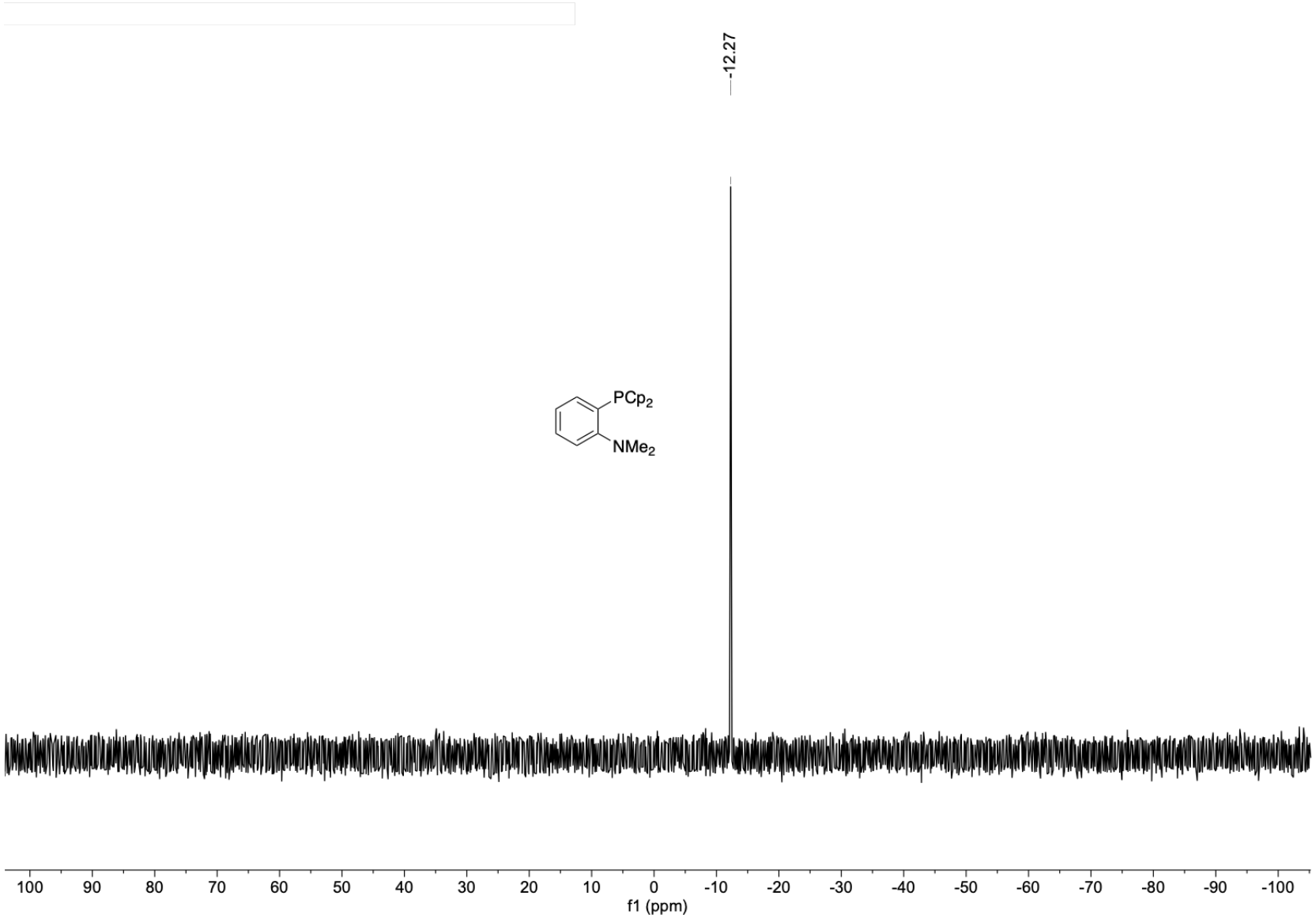
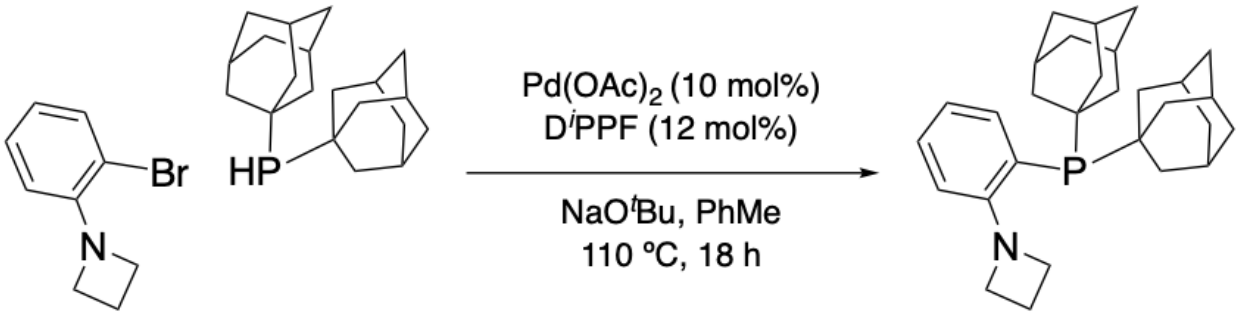


Figure S6. $^{31}P\{^{1}H\}$ NMR of **21** in CD_2Cl_2 at 298 K.

Synthesis of Azet-DalPhos (22)



Inside of a nitrogen-filled glovebox, $Pd(OAc)_2$ (5.6 mg, 0.10 Eq, 24.8 µmol) and D^{i}PPF (12.4 mg, 0.12 Eq, 29.8 µmol) were added as solids to a one dram vial charged with a stir bar, then the solids were dissolved in 450 µL of anhydrous toluene and left to stir at 23 ºC for ca. 15 minutes. Separately, di-1-adamantylphosphine (75 mg, 1 Eq, 248 µmol) and NaO^{t}Bu (36 mg, 1.5 Eq, 372 µmol) were added as solids to a one dram vial charged with a stir bar and suspended in 750 µL of anhydrous toluene and left to stir for ca. 15 minutes. **35** (55 mg, 1.05 Eq, 260 µmol) was weighed out into a two dram vial charged with a stir bar and diluted with 300 µL of anhydrous toluene. The $Pd(OAc)_2$/D^{i}PPF solution was transferred to the dram vial containing **35**, then the $HPAd_2$/NaO^{t}Bu solution was transferred to the vial containing **35** and the Pd/L complex, then the $HPAd_2$/NaO^{t}Bu vial was washed twice with 750 µL of anhydrous toluene (1.5 mL total) to give a total reaction volume of 3 mL of anhydrous toluene. The two dram vial was sealed with electrical tape and removed from the glovebox where it was refluxed in a sealed vial at 110 ºC for 18 hours. After 18 hours, the reaction was cooled to 23 ºC, and the reaction was filtered through a plug of Celite and the eluent was concentrated under vacuum. The resulting product was further purified using flash column chromatography (25 g silica gel, 0-80% ethyl acetate against hexanes). UV active products that eluted between 20-60% ethyl acetate were collected and concentrated under vacuum. The resulting yellow solid was then suspended in 5 mL of methanol to remove any residual aniline and Pd/L. The vial was sonicated for ca. 10 seconds, then the vial was centrifuged (60 seconds, 4400 rpm, 23 ºC) and the supernatant was decanted off. This was repeated two additional times to afford the product as an off-white solid (86 mg, 0.20 mmol, 80% yield).

Physical state: Off-white solid

^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.59 – 7.51 (m, 1H), 7.22 – 7.13 (m, 1H), 6.74 – 6.64 (m, 1H), 6.43 (dd, *J* = 8.4, 4.3 Hz, 1H), 4.06 (t, *J* = 7.2 Hz, 4H), 2.18 (p, *J* = 7.3 Hz, 2H), 2.02 – 1.92 (m, 6H), 1.93 – 1.82 (m, 12H), 1.72 – 1.63 (m, 12H).

^{31}P{^{1}H} NMR (121 MHz, CD_2Cl_2): δ 18.23.

HRMS (DART): $[M+H]^+$ calculated for $C_{29}H_{41}NP^+$ 434.2977, observed 4234.2969.

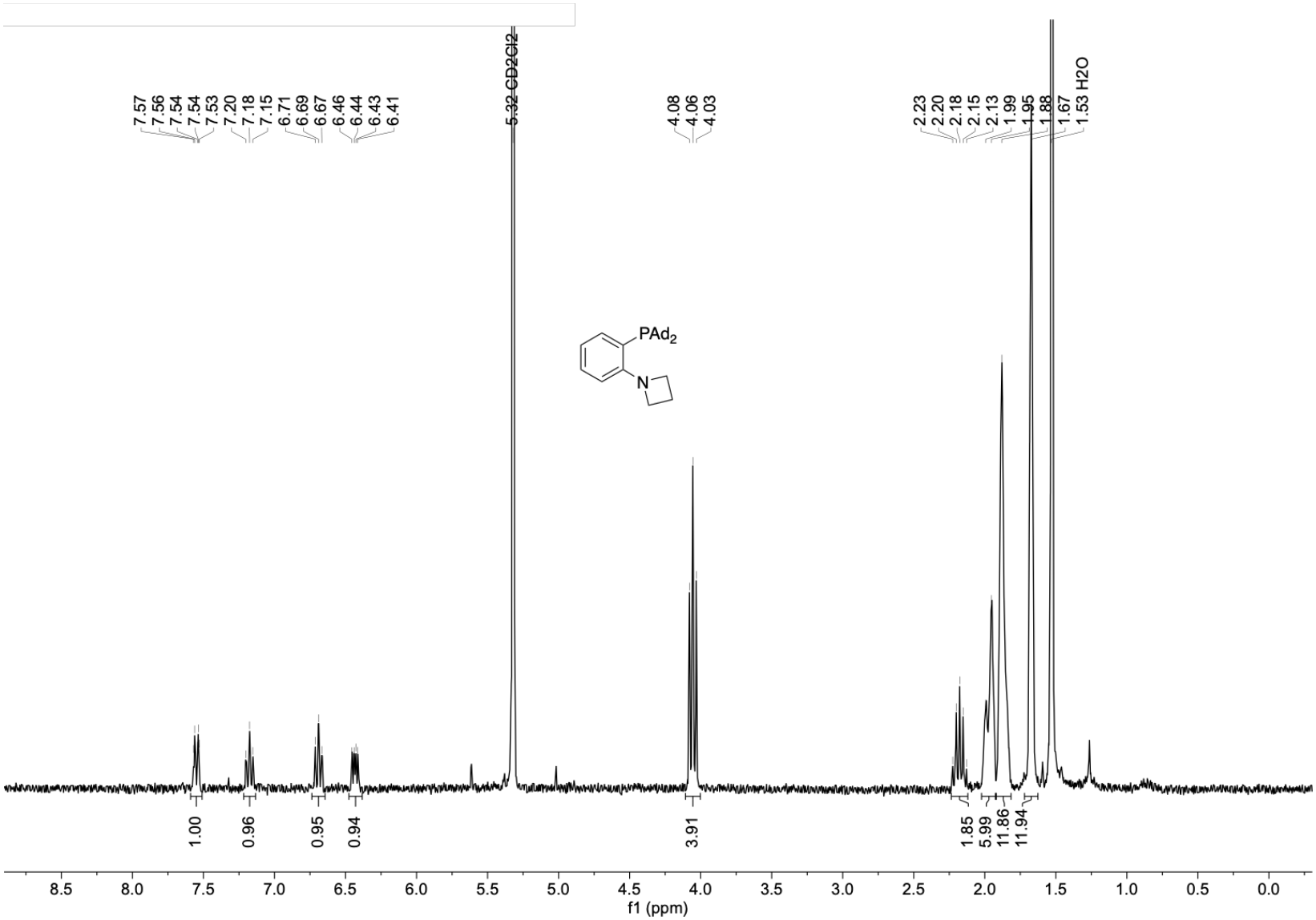


Figure S7. ^{1}H NMR of **22** in CD_2Cl_2 at 298 K.

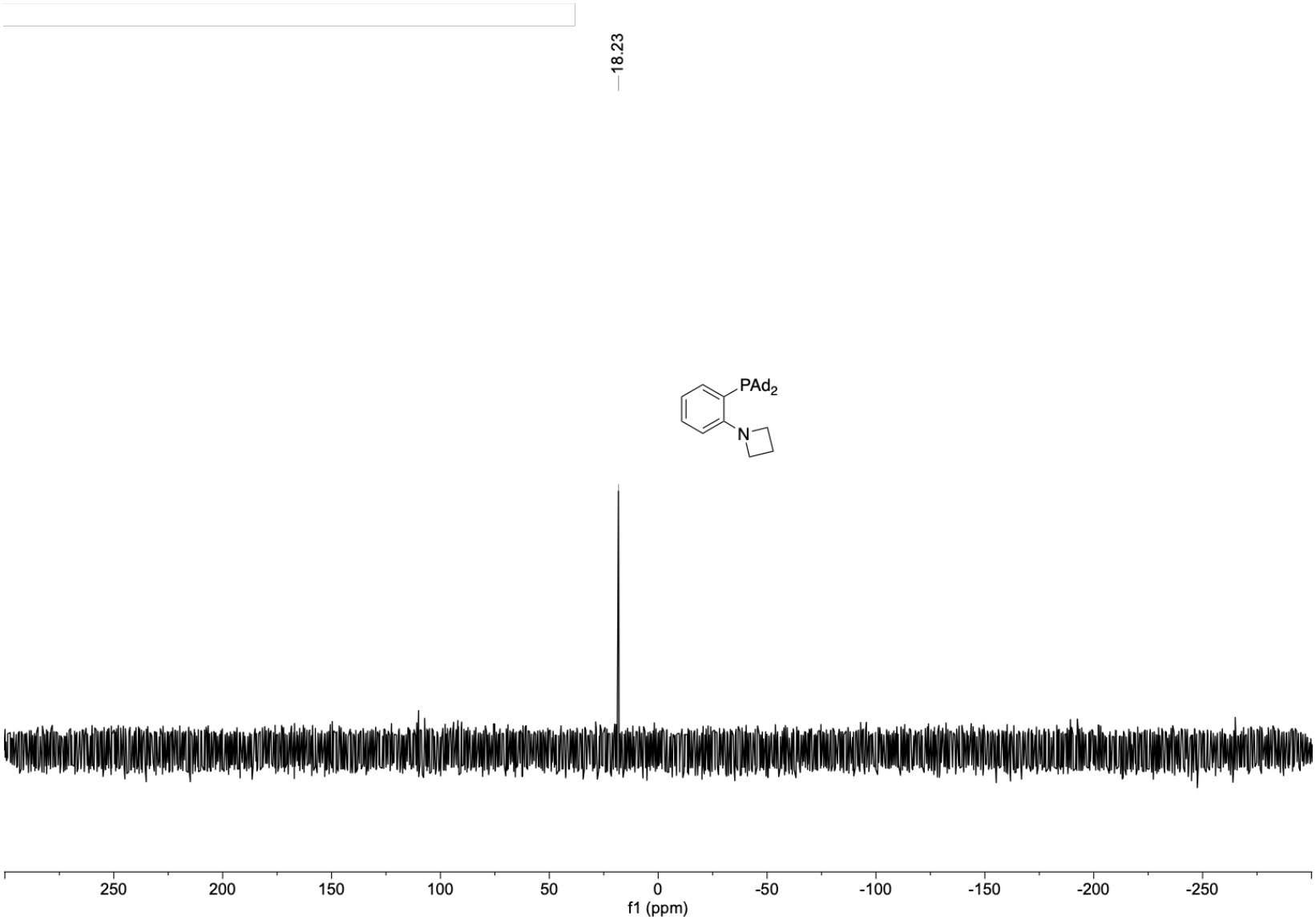
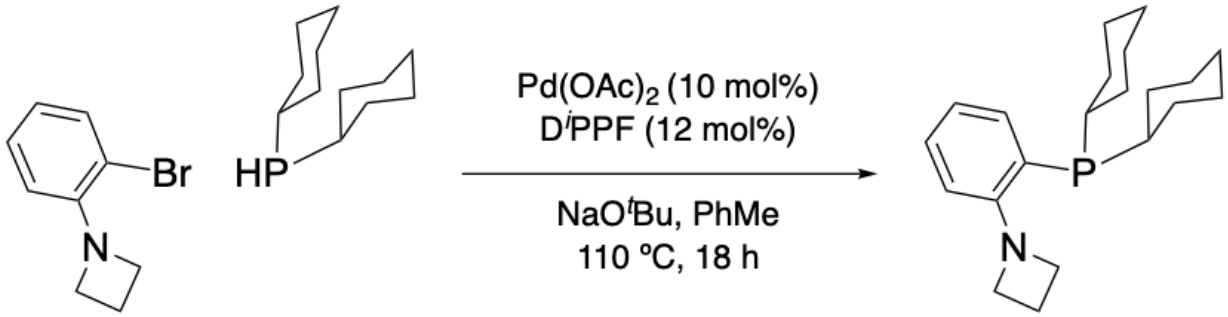


Figure S8. $^{31}P\{^{1}H\}$ NMR of **22** in CD_2Cl_2 at 298 K.

Synthesis of (PCy_2)Azet-DalPhos (23)



Inside of a nitrogen-filled glovebox, $Pd(OAc)_2$ (8.5 mg, 0.10 Eq, 37.8 µmol) and D^{i}PPF (19.0 mg, 0.12 Eq, 15.9 µmol) were added as solids to a one dram vial charged with a stir bar, then the solids were dissolved in 450 µL of anhydrous toluene and left to stir at 23 ºC for ca. 15 minutes. Separately, dicyclohexylphosphine (75 mg, 49.5 µL, 1 Eq, 378 µmol) and NaO^{t}Bu (36 mg, 1.5 Eq, 372 µmol) were added as solids to a one dram vial charged with a stir bar and suspended in 750 µL of anhydrous toluene and left to stir for ca. 15 minutes. **35** (84 mg, 1.05 Eq, 397 µmol) was weighed out into a two dram vial charged with a stir bar and diluted with 300 µL of anhydrous toluene. The $Pd(OAc)_2$/D^{i}PPF solution was transferred to the dram vial containing **35**, then the $HPCy_2$/NaO^{t}Bu solution was transferred to the vial containing **35** and the Pd/L complex, then the $HPCy_2$/NaO^{t}Bu vial was washed twice with 750 µL of anhydrous toluene (1.5 mL total) to give a total reaction volume of 3 mL of anhydrous toluene. The two dram vial was sealed with electrical tape and removed from the glovebox where it was refluxed in a sealed vial at 110 ºC for 18 hours. After 18 hours, the reaction was cooled to 23 ºC, and the reaction was filtered through a plug of Celite and the eluent was concentrated under vacuum. The resulting product was further purified using flash column chromatography (25 g silica gel, 0-80% ethyl acetate against hexanes). UV active products that eluted between 20-60% ethyl acetate were collected and concentrated under vacuum. The resulting orange oil was purified *via* preparative HPLC using a 10-100% gradient of acetonitrile against water, both with 0.1% TFA additive. Pure fractions as determined by mass spectrometry were collected and concentrated under vacuum to remove the acetonitrile. The resulting mixture was transferred to a separatory funnel with DCM (50 mL), then the organic layer was washed with saturated sodium carbonate (25 mL). The organic layer was collected, dried with anhydrous magnesium sulfate, filtered, and concentrated under vacuum to afford the product as an orange oil (78 mg, 0.24 mmol, 63% yield).

Physical state: Orange oil

^{1}H NMR (300 MHz, CD_2Cl_2): δ 7.28 (ddd, *J* = 7.6, 3.1, 1.6 Hz, 1H), 7.19 – 7.12 (m, 1H), 6.71 (td, *J* = 7.4, 1.2 Hz, 1H), 6.42 (ddd, *J* = 8.2, 4.6, 1.2 Hz, 1H), 4.03 (t, *J* = 7.2 Hz, 4H), 2.21 (p, *J* = 7.2 Hz, 2H), 1.93 – 1.70 (m, 6H), 1.70 – 1.58 (m, 4H), 1.38 – 0.91 (m, 12H).

^{31}P{^{1}H} NMR (121 MHz, CD_2Cl_2): δ -14.72.

HRMS (ESI): $[M+H]^+$ calculated for $C_{21}H_{33}NP^+$ 330.2351, observed 330.2407.

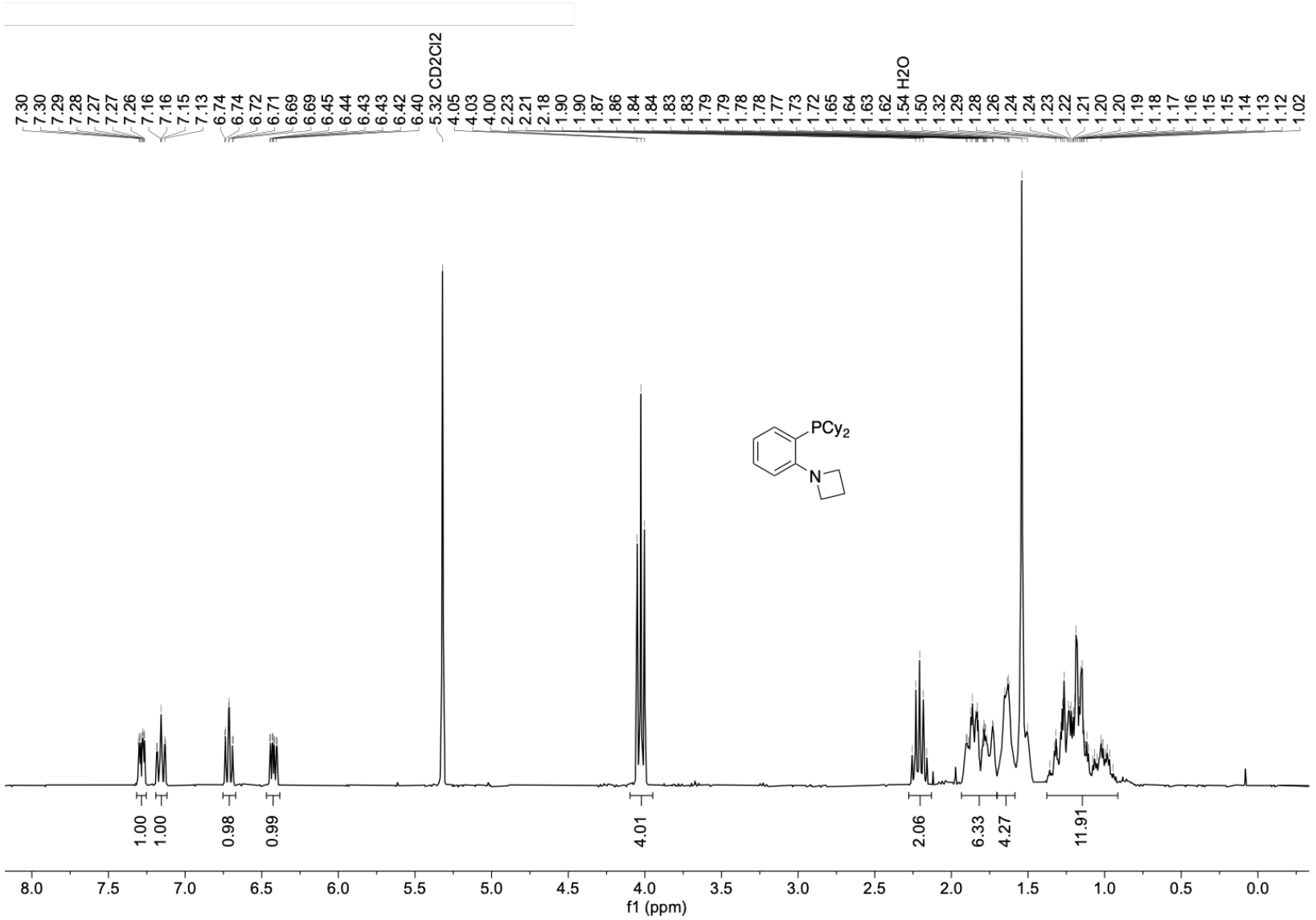


Figure S9. ^{1}H NMR of **23** in CD_2Cl_2 at 298 K.

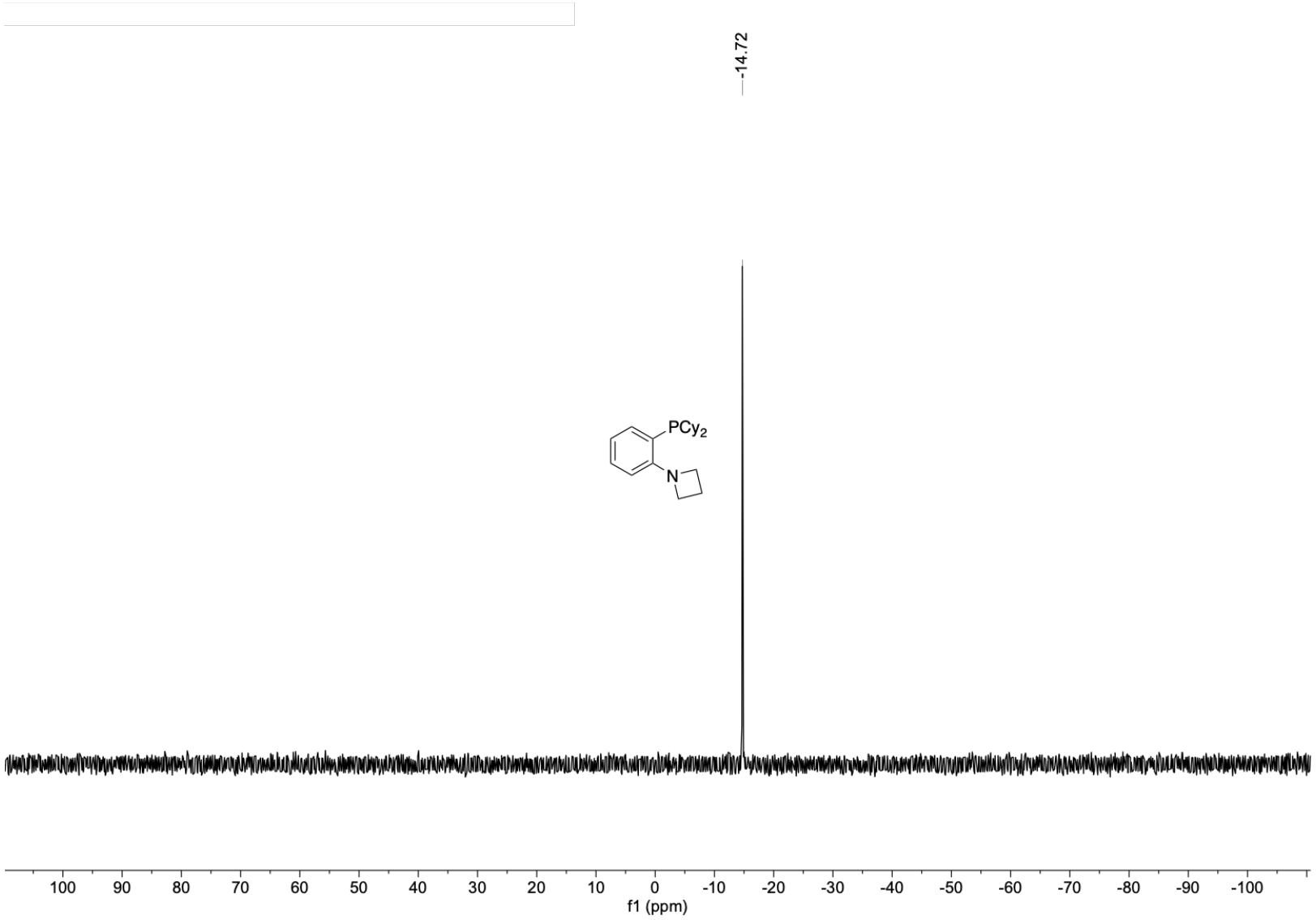
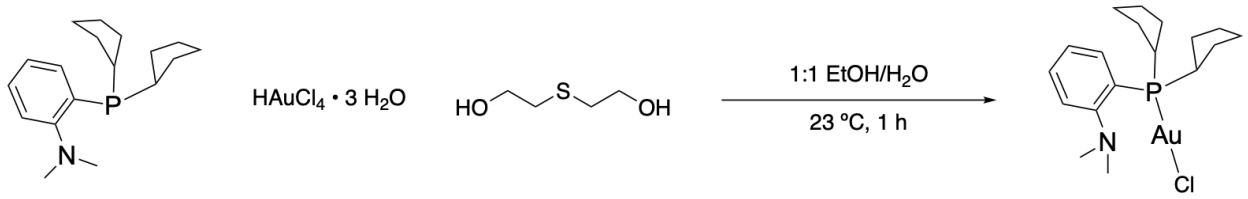


Figure S10. $^{31}P\{^{1}H\}$ NMR of **23** in CD_2Cl_2 at 298 K.

Synthesis of *P*,*N*-Ligated Au^{I}Cl Reagents

Synthesis of [(PCp$_2$)Me-DalPhos]Au^{I}Cl (24)



21 (35 mg, 1 Eq, 0.12 mmol) was added to a one dram vial charged with a stir bar. The ligand was suspended in 500 µL of ethanol. Hydrogen tetrachloroaurate(III) trihydrate (48 mg, 1 Eq, 0.12 mmol) was added to a separate one dram vial charged with a stir bar, then this was dissolved in 250 µL of DI water, forming a yellow solution. To this, 2,2'-thiodiethanol (44 mg, 37 µL, 3 Eq, 0.36 mmol) was added in five portions of 7.4 µL over two minutes. With each added portion, the reaction solution turned yellow and opaque and then eventually became clear and colorless. The Au solution was then added into the ligand, forming a white suspension. The Au vial was washed twice with 125 µL of DI water (250 µL total), then these washes were transferred to the vial containing the ligand. This was left to stir for one hour at 23 ºC under ambient conditions. After one hour, the white suspension was transferred onto a medium-grain fritted filter funnel, and the solid was washed five times with 2 mL of methanol. The white solid was then dissolved in DCM and filtered through the fritted funnel. The eluent was subsequently filtered through a pad of Celite to remove any gold nanoparticles that may have formed. The product was then concentrated under vacuum to afford a white solid (40 mg, 76 µmol, 64% yield).

Physical state: White solid
^{1}H NMR (600 MHz, CD_2Cl_2): δ 8.05 – 7.97 (m, 1H), 7.57 – 7.51 (m, 1H), 7.47 – 7.41 (m, 1H), 7.32 – 7.27 (m, 1H), 2.94 – 2.80 (m, 2H), 2.62 (s, 6H), 2.15 – 2.04 (m, 2H), 1.93 – 1.79 (m, 4H), 1.74 – 1.63 (m, 4H), 1.59 – 1.48 (m, 4H), 1.49 – 1.38 (m, 2H).
^{31}P{^{1}H} NMR (243 MHz, CD_2Cl_2): δ 59.36.
HRMS (DART): $[M+H]^+$ calculated for $C_{18}H_{29}AuClNP^+$ 522.1392, observed 522.1389.

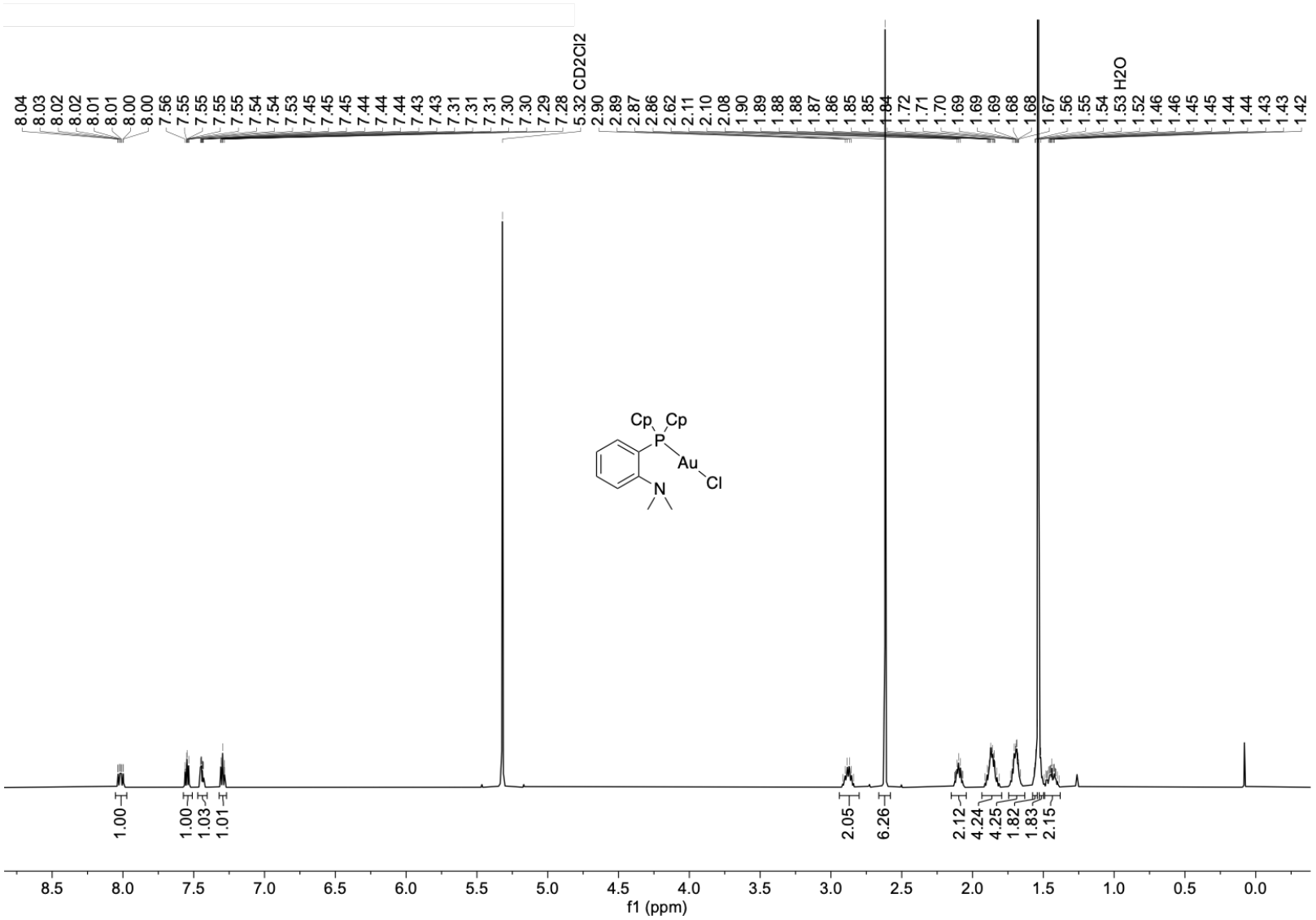


Figure S11. ^{1}H NMR of **24** in CD_2Cl_2 at 298 K.

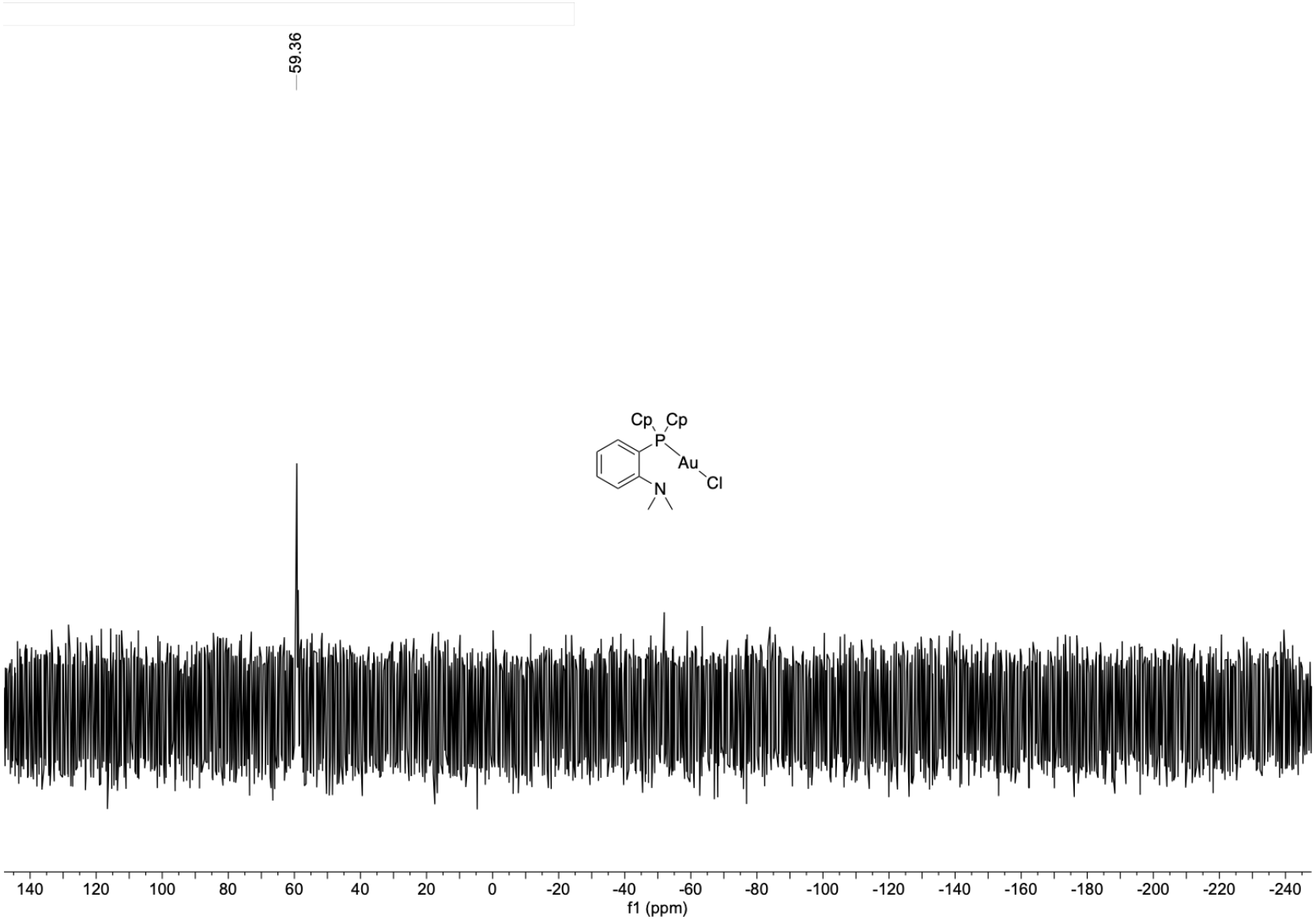
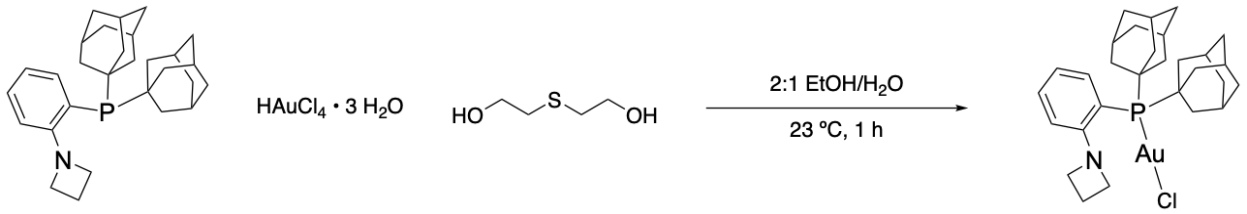


Figure S12. $^{31}P\{^{1}H\}$ NMR of **24** in CD_2Cl_2 at 298 K.

Synthesis of [Azet-DalPhos]Au^{I}Cl (25)



Hydrogen tetrachloroaurate(III) trihydrate (36 mg, 1 Eq, 92 μmol) was added to a two dram vial charged with a stir bar, then this was dissolved in 1 mL of DI water, forming a yellow solution. To this, 2,2'-thiodiethanol (34 mg, 28 μL, 3 Eq, 0.28 mmol) was added in five portions of 5.6 μL over two minutes. With each added portion, the reaction solution turned yellow and opaque and then eventually became clear and colorless. Next, **22** (40 mg, 1 Eq, 92 μmol) was added as a solid to the vial, then 2 mL of ethanol was added to the reaction, forming a white, opaque suspension. This was left to stir for one hour at 23 ºC under ambient conditions. After one hour, the white suspension was transferred onto a medium-grain fritted filter funnel, and the solid was washed five times with 2 mL of methanol. The white solid was then dissolved in DCM and filtered through the fritted funnel. The eluent was subsequently filtered through a pad of Celite to remove any gold nanoparticles that may have formed. The product was then concentrated under vacuum to afford a white solid (60 mg, 90 μmol, 98% yield).

Physical state: White solid

^{1}H NMR (600 MHz, CD_2Cl_2): δ 7.73 – 7.68 (m, 1H), 7.67 – 7.63 (m, 1H), 7.60 – 7.55 (m, 1H), 7.25 – 7.20 (m, 1H), 3.82 (t, *J* = 7.0 Hz, 4H), 2.34 (p, *J* = 7.0 Hz, 2H), 2.24 – 2.17 (m, 6H), 2.12 – 2.04 (m, 6H), 2.00 – 1.95 (m, 6H), 1.73 – 1.64 (m, 12H).

^{31}P{^{1}H} NMR (243 MHz, CD_2Cl_2): δ 57.44.

HRMS (DART): $[M+H]^+$ calculated for $C_{29}H_{41}AuClNP^+$ 666.2331, observed 666.2342.

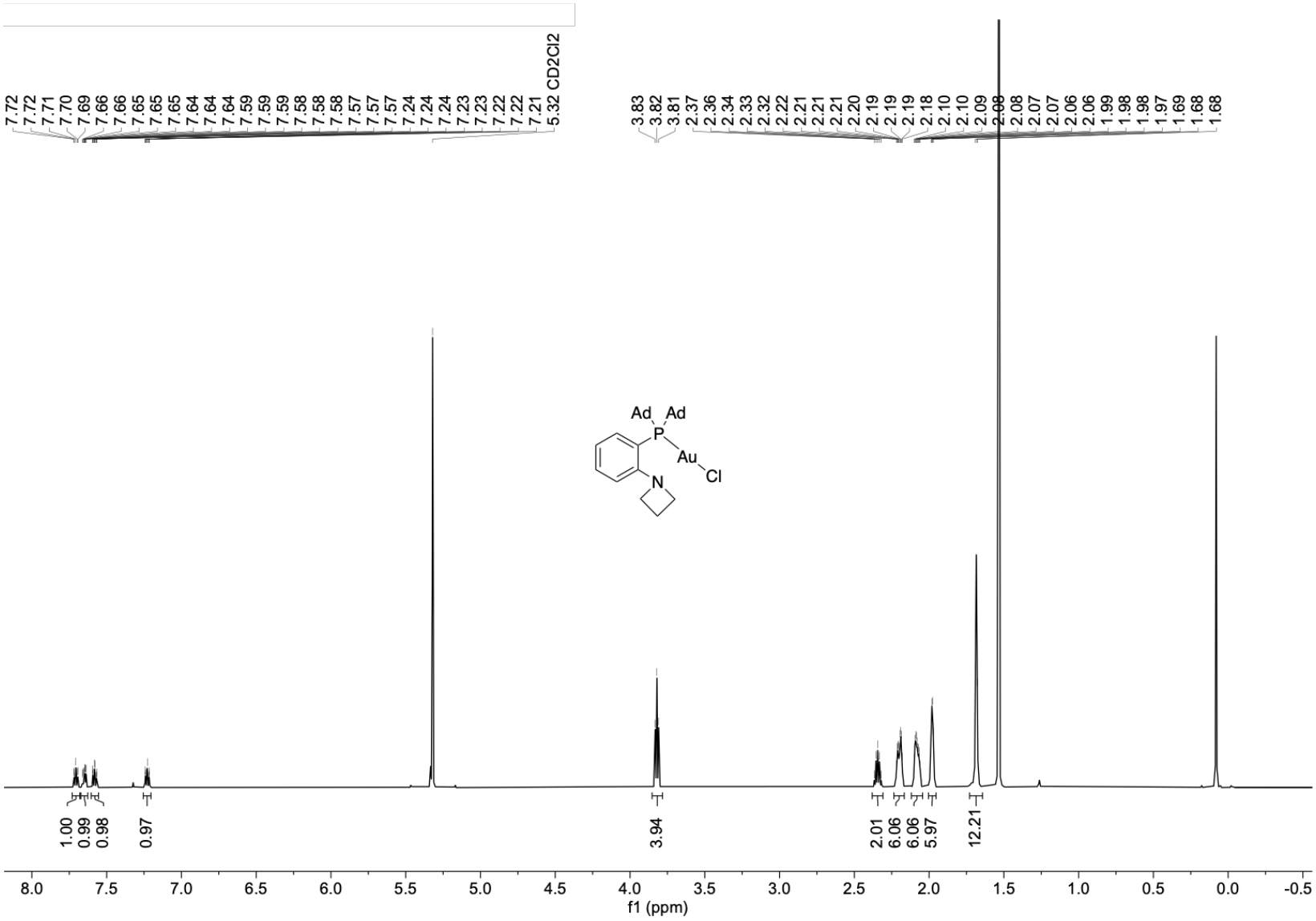


Figure S13. ^{1}H NMR of **25** in CD_2Cl_2 at 298 K.

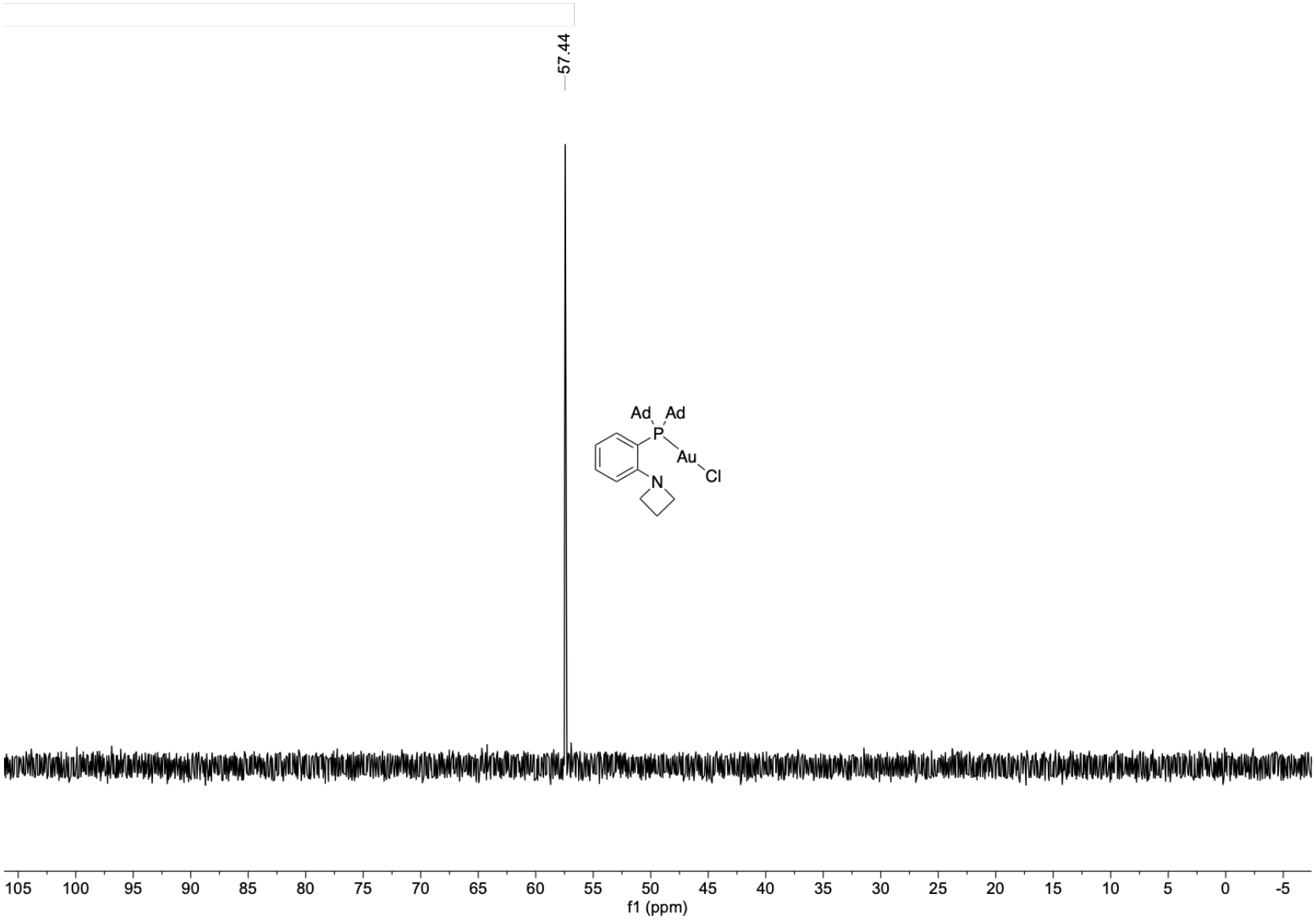
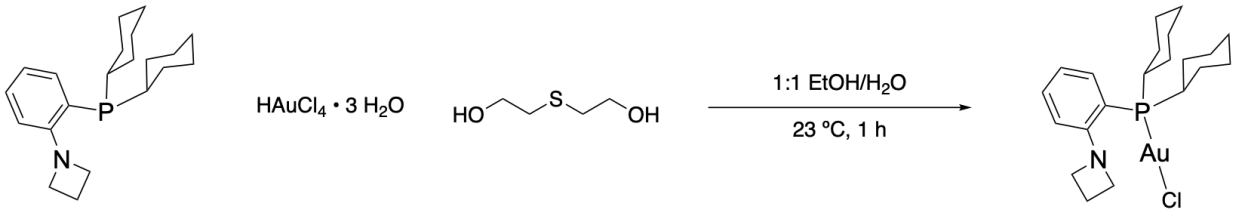


Figure S14. $^{31}P\{^{1}H\}$ NMR of **25** in CD_2Cl_2 at 298 K.

Synthesis of [(PCy$_2$)Azet-DalPhos]Au^{I}Cl (26)



23 (18 mg, 1 Eq, 55 µmol) was added to a one dram vial charged with a stir bar. The ligand was suspended in 500 µL of ethanol. Hydrogen tetrachloroaurate(III) trihydrate (22 mg, 1 Eq, 55 µmol) was added to a separate one dram vial charged with a stir bar, then this was dissolved in 250 µL of DI water, forming a yellow solution. To this, 2,2'-thiodiethanol (20 mg, 17 µL, 3 Eq, 0.36 mmol) was added in five portions of 3.4 µL over two minutes. With each added portion, the reaction solution turned yellow and opaque and then eventually became clear and colorless. The Au solution was then added into the ligand, forming a white suspension. The Au vial was washed twice with 125 µL of DI water (250 µL total), then these washes were transferred to the vial containing the ligand. This was left to stir for one hour at 23 ºC under ambient conditions. After one hour, the white suspension was transferred onto a medium-grain fritted filter funnel, and the solid was washed five times with 2 mL of methanol. The white solid was then dissolved in DCM and filtered through the fritted funnel. The eluent was subsequently filtered through a pad of Celite to remove any gold nanoparticles that may have formed. The product was then concentrated under vacuum to afford a white solid (18 mg, 32 µmol, 58% yield).

Physical state: White solid
^{1}H NMR (600 MHz, CD_2Cl_2): δ 7.66 (dd, *J* = 12.4, 7.7 Hz, 1H), 7.55 – 7.49 (m, 1H), 7.40 (dd, *J* = 8.4, 4.3 Hz, 1H), 7.18 – 7.14 (m, 1H), 3.85 (t, *J* = 7.1 Hz, 4H), 2.48 – 2.40 (m, 2H), 2.30 (p, *J* = 7.1 Hz, 2H), 2.16 – 2.10 (m, 2H), 1.90 – 1.84 (m, 2H), 1.73 – 1.70 (m, 2H), 1.69 – 1.64 (m, 2H), 1.62 – 1.53 (m, 2H), 1.49 – 1.46 (m, 2H), 1.43 – 1.33 (m, 2H), 1.31 – 1.20 (m, 6H).
^{31}P{^{1}H} NMR (243 MHz, CD_2Cl_2): δ 47.52.
HRMS (DART): $[M+H]^+$ calculated for $C_{21}H_{33}AuClNP^+$ 562.1705, observed 562.1719.

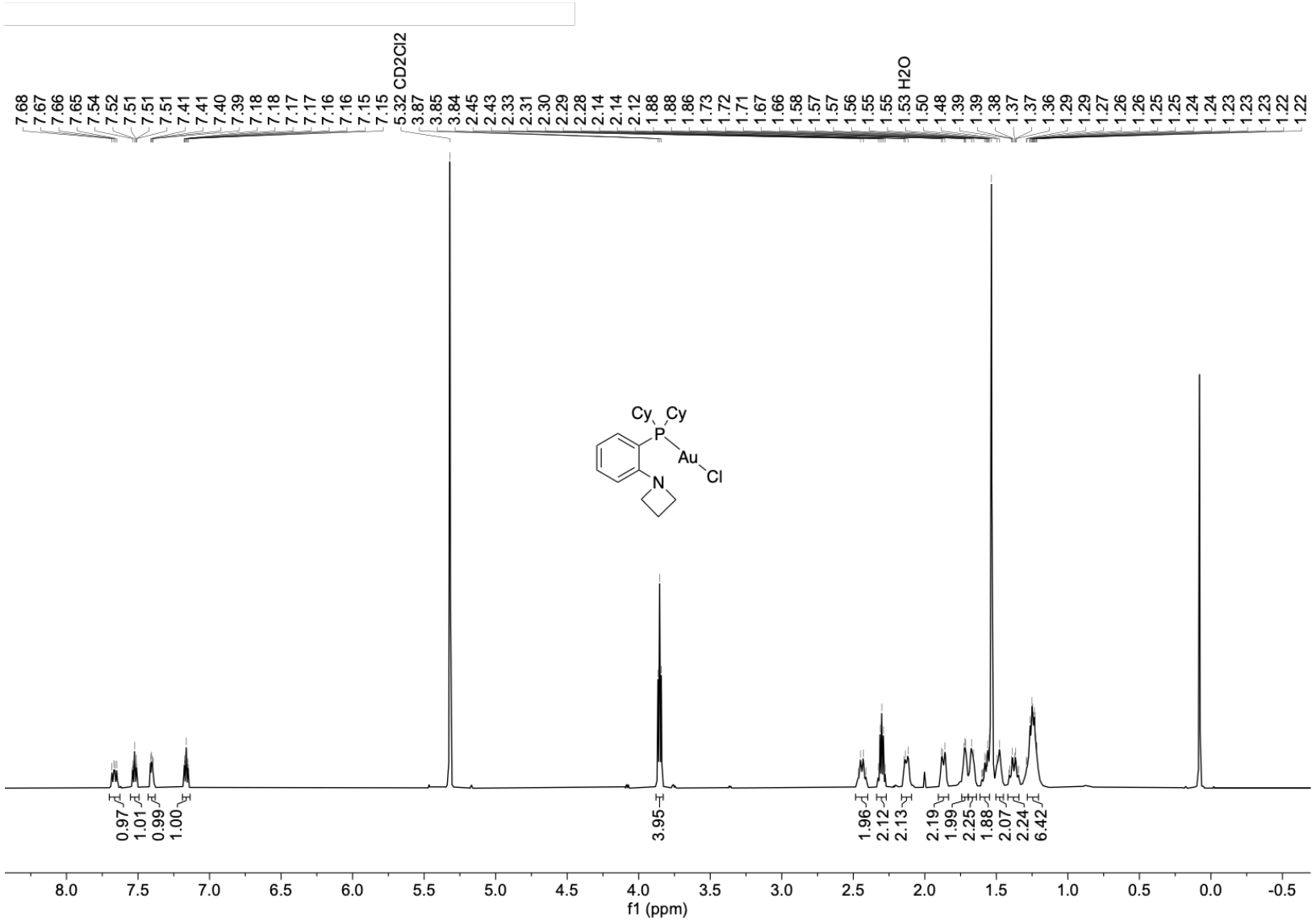


Figure S15. ^{1}H NMR of **26** in CD_2Cl_2 at 298 K.

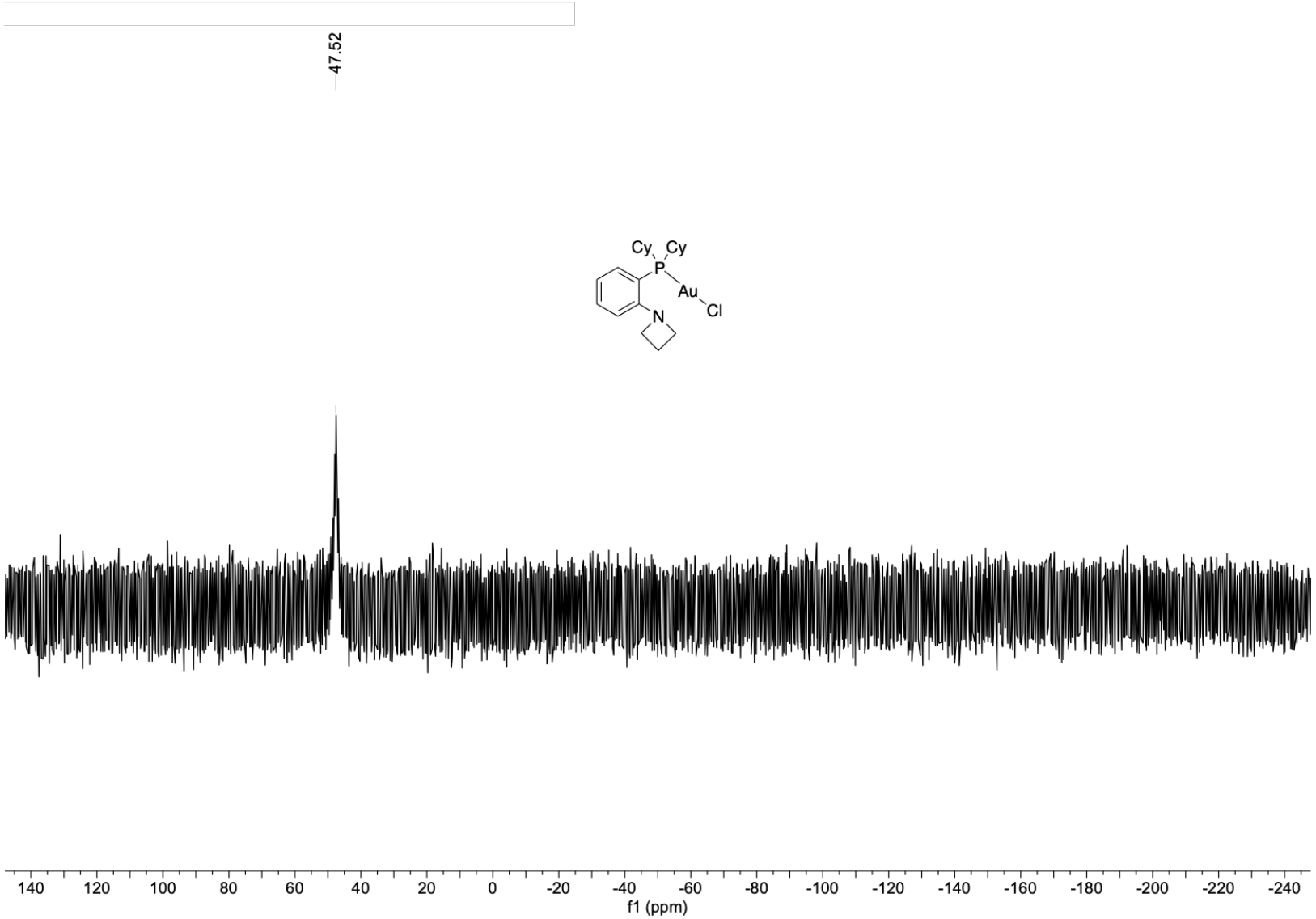
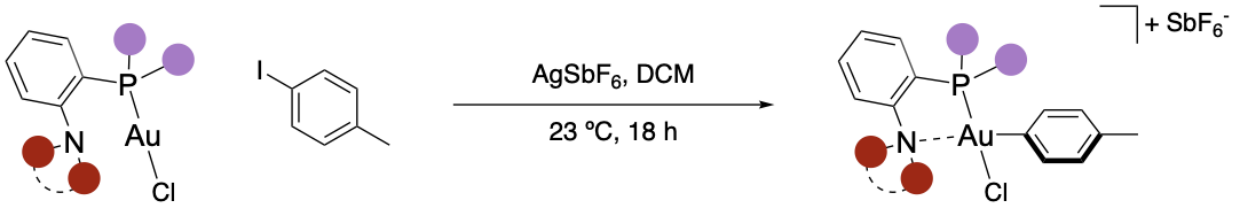


Figure S16. $^{31}P\{^{1}H\}$ NMR of **26** in CD_2Cl_2 at 298 K.

Synthesis of Au(III) Oxidative Complexes

General Procedure A



$AgSbF_6$ (1 Eq) was weighed out in a one dram vial inside of a nitrogen-filled glovebox in the absence of light, then the vial was sealed, covered with electrical tape, and removed from the glovebox. This vial was charged with a stir bar, and the $AgSbF_6$ was dissolved in 500 µL of DCM. [(*P*,*N*-Ligand)$Au^{I}Cl$] (10.0 mg, 1 Eq) was weighed out in a separate one dram vial, then *p*-iodotoluene (5 Eq) was added to the Au-containing vial and these compounds were dissolved in 500 µL of DCM. Both vials were stored at -20 ºC for ca. two minutes, then the vials were removed from the freezer and the Au^{I}/ArI solution was transferred to the $AgSbF_6$ vial, immediately forming a yellow color and white precipitates. The Au^{I}/ArI vial was washed twice with 250 µL of DCM (500 µL of DCM), then both washes were transferred to the $AgSbF_6$ vial to give a total reaction volume of 1.5 mL of anhydrous DCM. The vial was left to stir for 18 hours in the absence of light at 23 ºC. After 18 hours, the opaque, yellow suspension was filtered through a pad of Celite to remove any liberated AgCl and gold nanoparticles that may have formed, then the flow through was collected in a scintillation vial and concentrated under vacuum. 5 mL of pentane was added to the vial and it was sonicated for ca. 10 seconds, then the vial was centrifuged (60 seconds, 4400 rpm, 23 ºC) and the supernatant was decanted off. This was repeated three additional times with 5 mL of 3:2 (v/v) pentane-diethyl ether, then this was performed two more times with 5 mL of pentyl. The resulting material was further dried under vacuum to yield the title compound as a solid. Individual yield and characterization data are provided for each compound.

Synthesis of [((PCp$_2$)Me-DalPhos)Au^{III}(*p*-Toluene)Cl]$^+$ SbF$_6^-$ (27)

27 was synthesized according to General Procedure A and isolated as a white solid (14.3 mg, 16.8 µmol, 83% yield, 92% purity). *8 mol% 4-iodotoluene was unable to be removed despite multiple rounds of washing.

Physical State: White solid
^{1}H NMR (600 MHz, CD$_3$CN): δ 8.04 – 7.99 (m, 1H), 7.99 – 7.91 (m, 1H), 7.85 – 7.78 (m, 1H), 7.72 – 7.66 (m, 1H), 7.24 (d, *J* = 8.1 Hz, 2H), 7.16 (d, *J* = 8.1 Hz, 2H), 3.43 (s, 6H), 3.05 – 2.92 (m, 2H), 2.34 (s, 3H), 2.12 – 2.11 (m, 2H), 2.09 – 2.00 (m, 2H), 1.91 – 1.82 (m, 2H), 1.72 – 1.58 (m, 6H), 1.53 – 1.44 (m, 2H), 0.95 – 0.79 (m, 2H).
^{31}P{^{1}H} NMR (243 MHz, CD$_3$CN): δ 55.83.
HRMS (ESI): [M-SbF$_6$]$^+$ calculated for $C_{25}H_{35}AuClNP^+$ 612.1861, observed 612.1906.

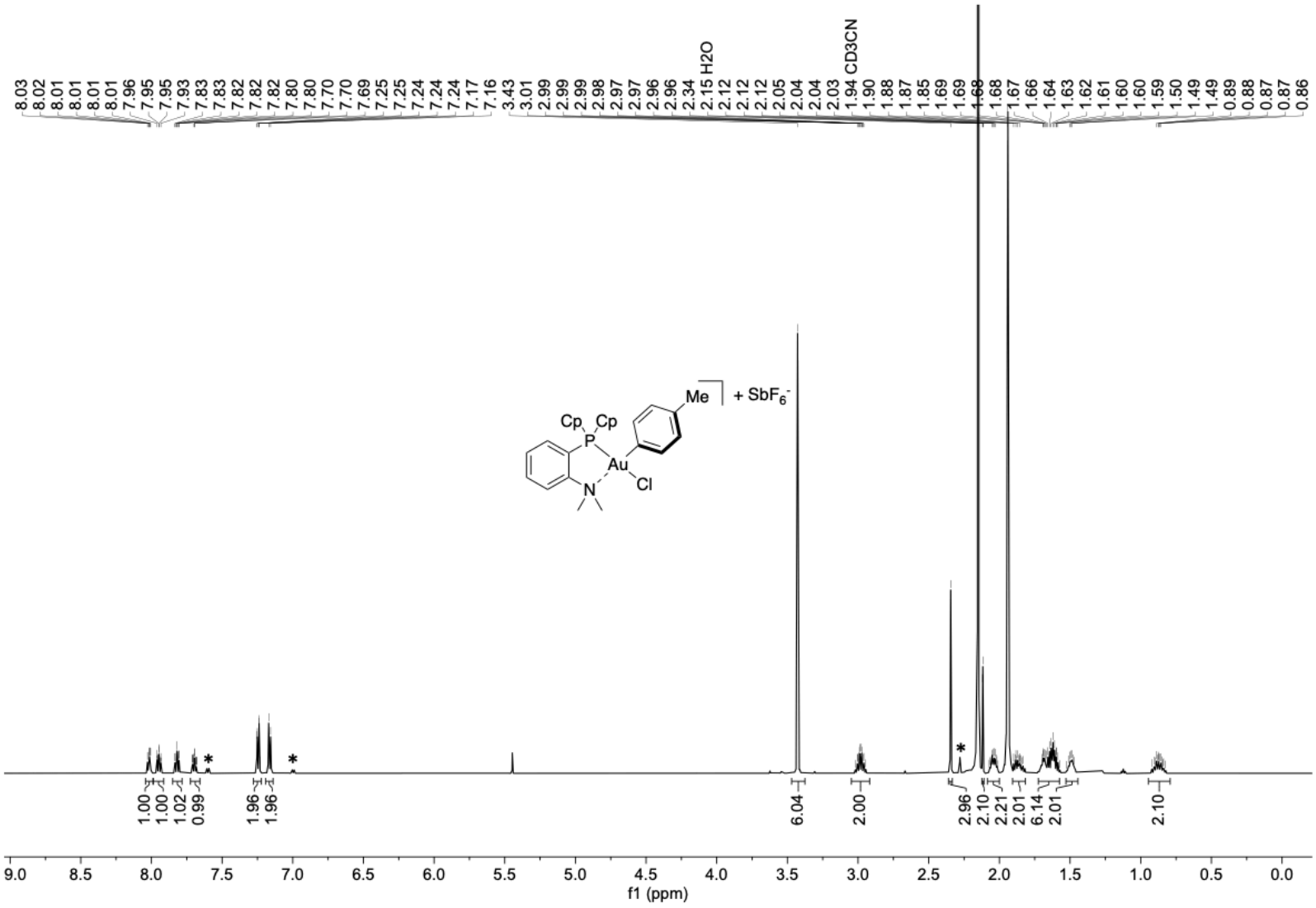


Figure S17. ^{1}H NMR of **27** in CD_3CN at 298 K.

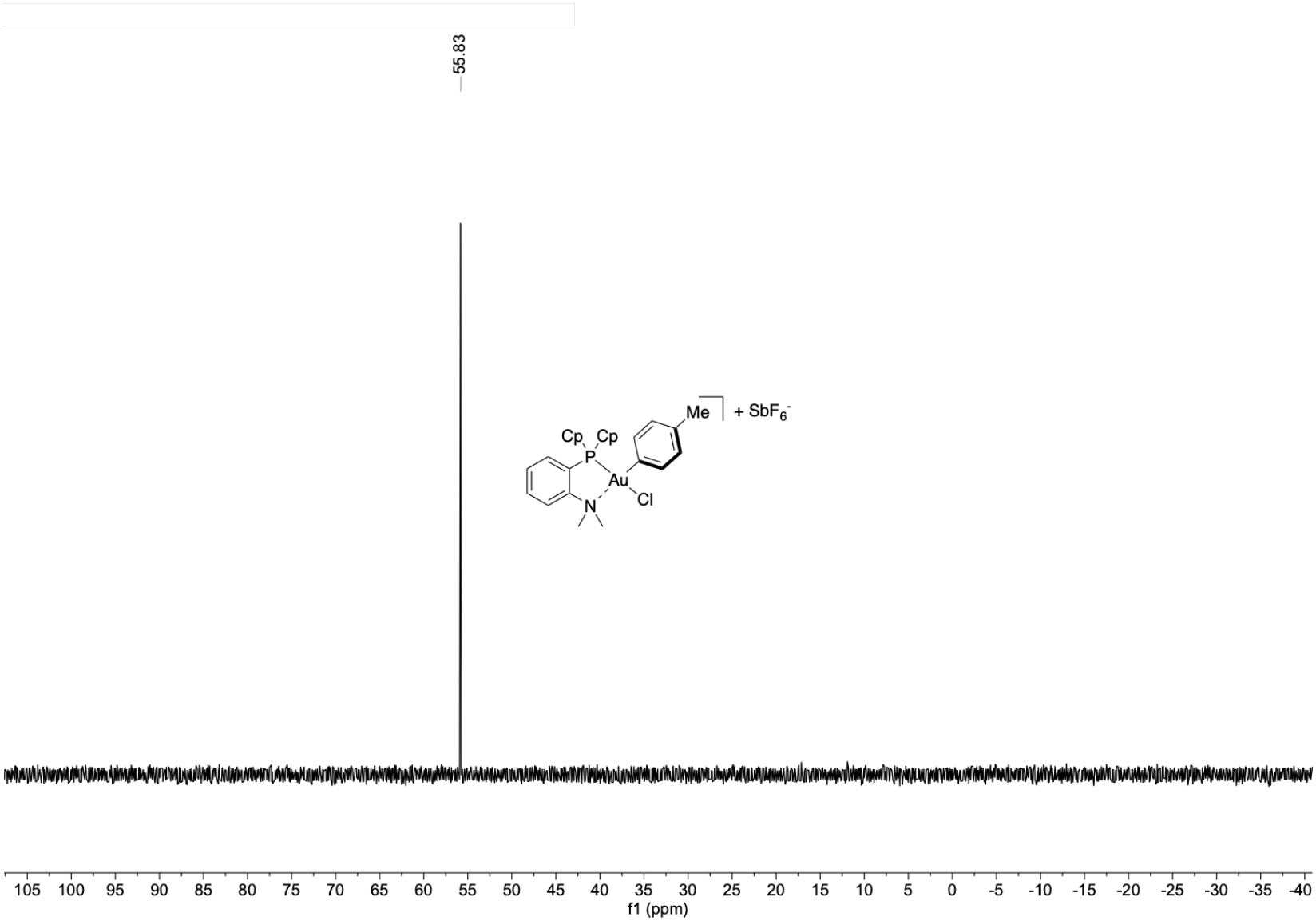
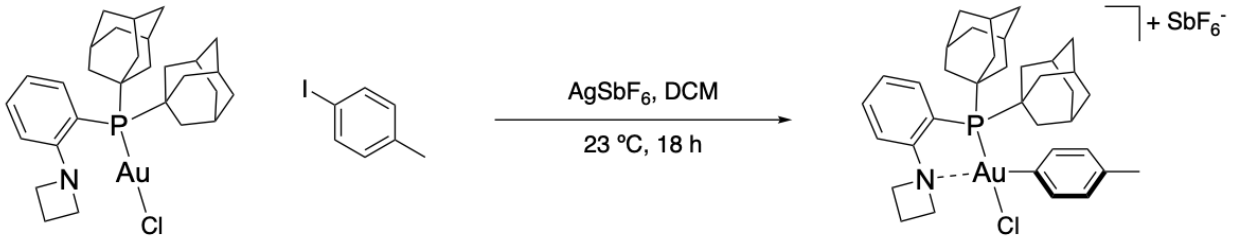


Figure S18. $^{31}P\{^{1}H\}$ NMR of **27** in CD_3CN at 298 K.

Synthesis of [(Azet-DalPhos)Au^{III}(*p*-Toluene)Cl]$^{+}$ SbF_6^{-} (28)



28 was synthesized according to General Procedure A and isolated as a yellow solid (13.0 mg, 13.1 µmol, 87% yield).

Physical State: Yellow solid
^{1}H NMR (600 MHz, CD_3CN): δ 8.56 – 8.35 (m, 1H), 8.11 – 7.93 (m, 1H), 7.94 – 7.84 (m, 1H), 7.73 – 7.59 (m, 1H), 7.44 (d, *J* = 8.3 Hz, 2H), 7.15 (d, *J* = 8.1 Hz, 2H), 5.51 (td, *J* = 10.8, 7.6 Hz, 2H), 4.51 (td, *J* = 10.9, 6.8 Hz, 2H), 3.10 – 2.99 (m, 1H), 2.89 – 2.79 (m, 1H), 2.35 (s, 3H), 2.25 – 2.21 (m, 6H), 2.03 – 1.96 (m, 12H), 1.75 – 1.68 (m, 12H).
^{31}P{^{1}H} NMR (243 MHz, CD_3CN): δ 75.18.
HRMS (ESI): $[M\text{-}SbF_6^{-}]^{+}$ calculated for $C_{36}H_{47}AuClNP^{+}$ 756.2800, observed 756.2811.

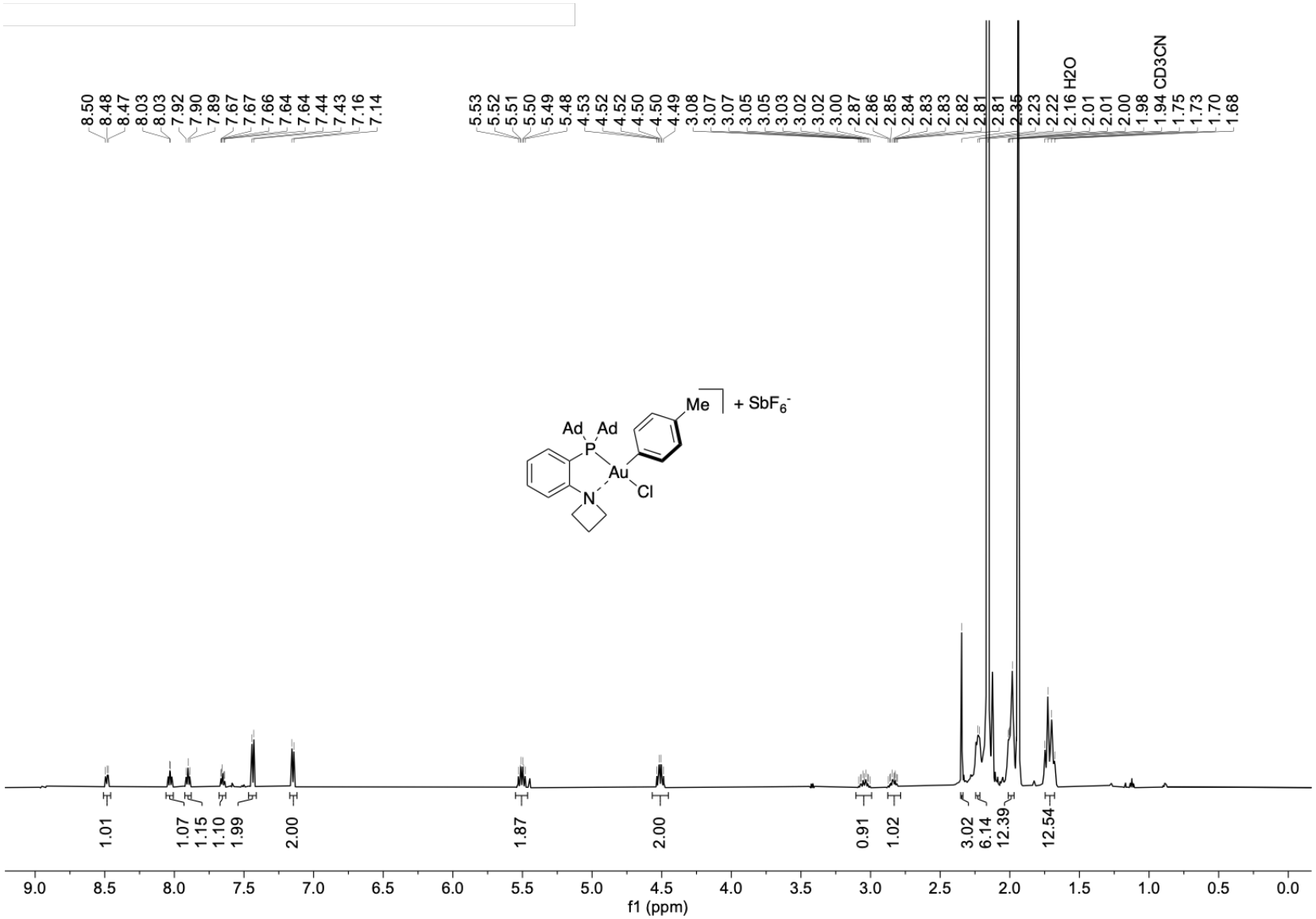


Figure S19. ^{1}H NMR of **28** in CD_3CN at 298 K.

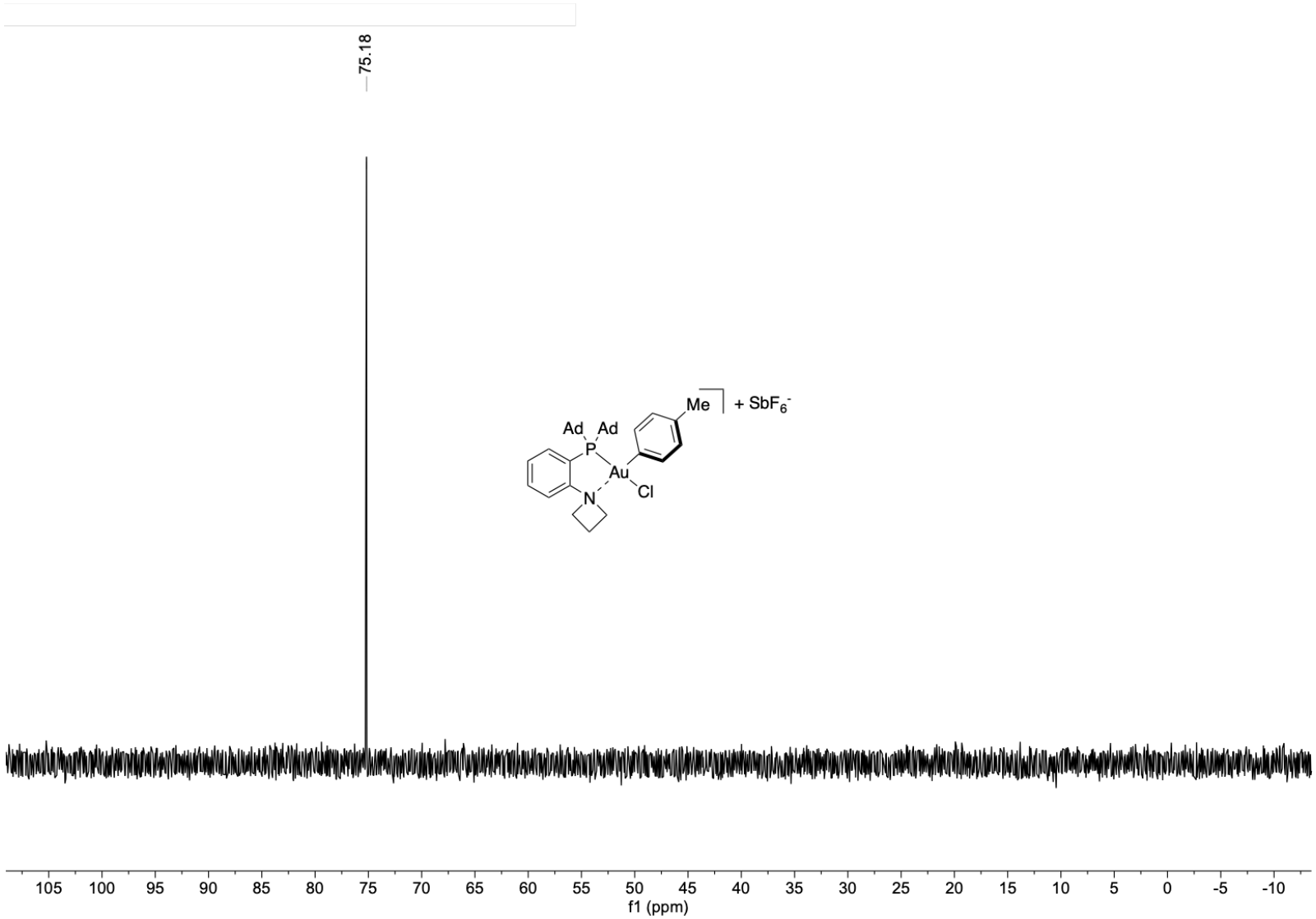
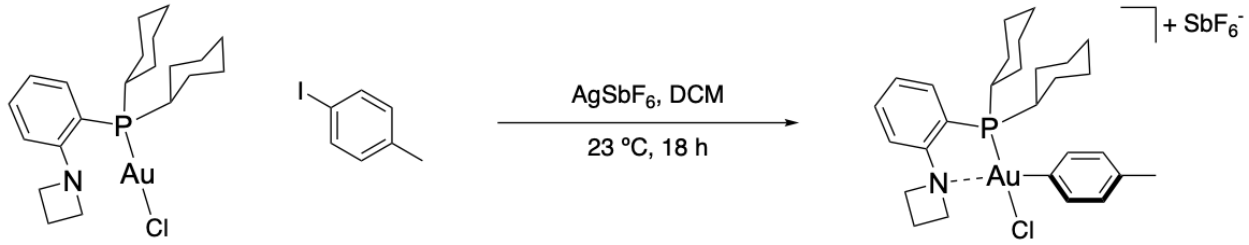


Figure S20. $^{31}P\{^{1}H\}$ NMR of **28** in CD_3CN at 298 K.

Synthesis of [((PCy$_2$)Azet-DalPhos)Au^{III}(*p*-Toluene)Cl]$^+$ SbF$_6^-$ (29)



29 was synthesized according to General Procedure A and isolated as a white solid (10.0 mg, 11.2 µmol, 63% yield).

Physical State: White solid
^{1}H NMR (600 MHz, CD$_3$CN): δ 8.48 – 8.41 (m, 1H), 8.08 – 8.00 (m, 1H), 7.74 – 7.64 (m, 2H), 7.26 – 7.17 (m, 4H), 5.37 (td, *J* = 10.6, 7.2 Hz, 2H), 4.55 (td, *J* = 10.8, 7.1 Hz, 2H), 2.99 – 2.91 (m, 1H), 2.91 – 2.81 (m, 1H), 2.76 – 2.67 (m, 2H), 2.36 (s, 3H), 1.84 – 1.77 (m, 2H), 1.75 – 1.71 (m, 2H), 1.70 – 1.59 (m, 6H), 1.51 – 1.41 (m, 2H), 1.32 – 1.24 (m, 4H), 1.09 – 0.97 (m, 2H), 0.58 – 0.45 (m, 2H).
^{31}P{^{1}H} NMR (243 MHz, CD$_3$CN): δ 58.64.
HRMS (ESI): [M-SbF$_6^-$]$^+$ calculated for $C_{28}H_{39}AuClNP^+$ 652.2174, observed 652.2193.

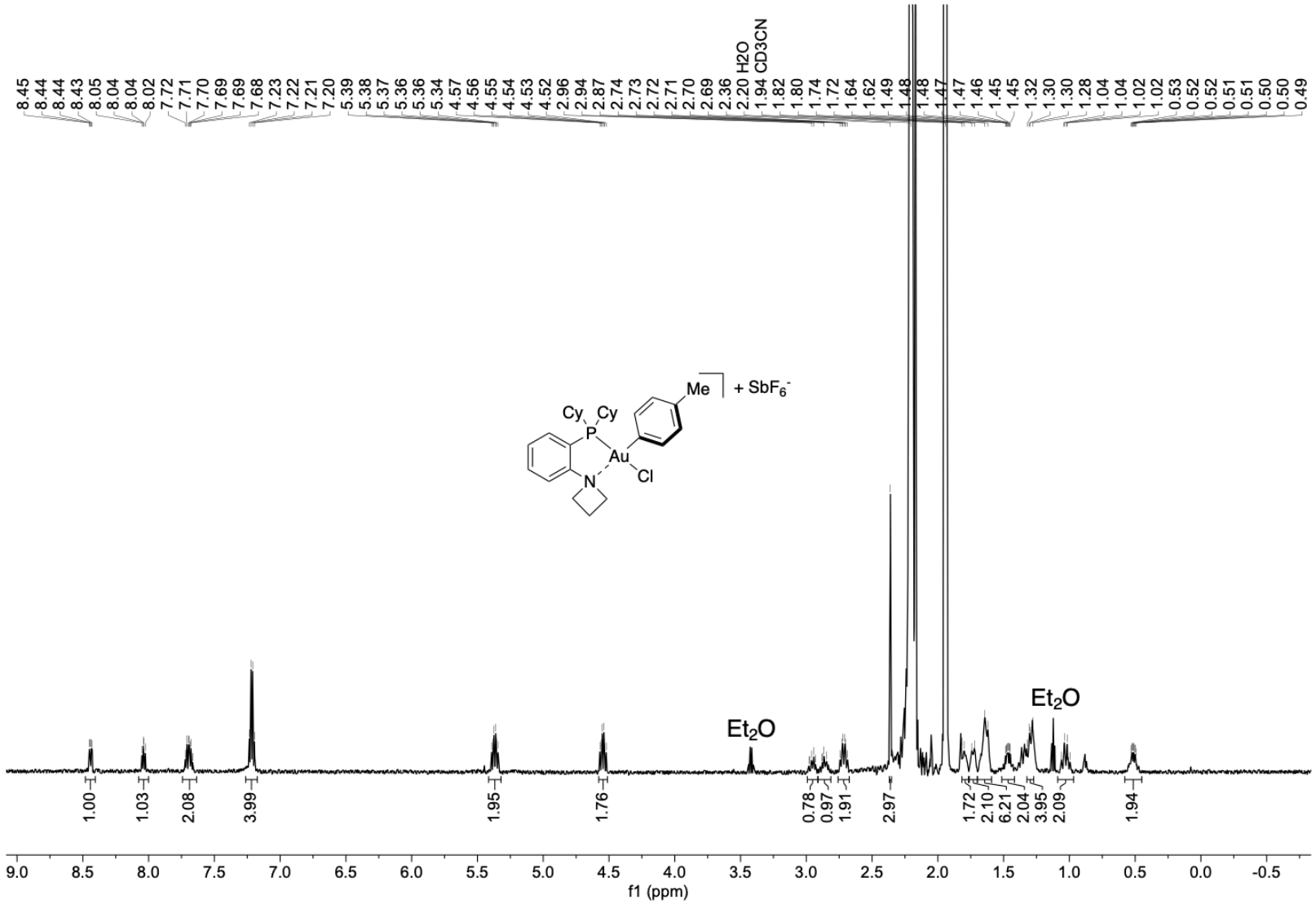


Figure S21. ^{1}H NMR of **29** in CD_3CN at 298 K.

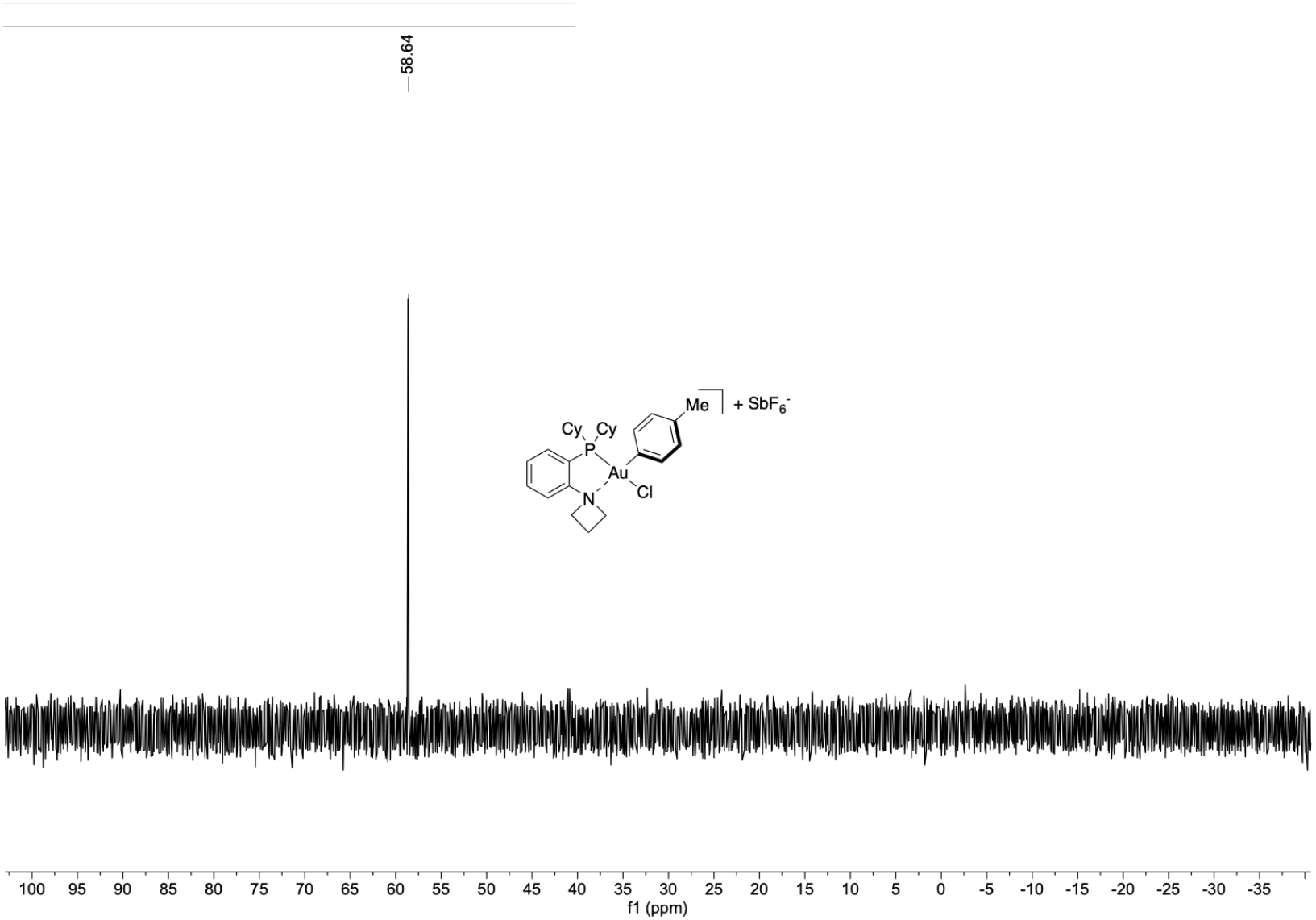


Figure S22. $^{31}P\{^{1}H\}$ NMR of **29** in CD_3CN at 298 K.

Stopped-Flow Kinetics

General Procedure

Solution Preparation: Stock solutions of Au(III) OACs were made at ca. 1 mg/mL in MeCN, then this was diluted to a final concentration of 10 μM in 1:1 MeCN/100 mM Tris buffer at pH 7.4 (10 mL of 10 μM Au(III) OAC solution is generally sufficient for five replicates across five different concentrations of **GSH**). Separately, a 5 mL of a 40 mM **GSH** stock solution was prepared in 1:1 MeCN/100 mM Tris buffer at pH 7.4, then this was used to make 5 mL of 1 mM, 2 mM, 4 mM, 5 mM, 6 mM, and 8 mM **GSH**. Each stock solution was freshly prepared before performing the stopped-flow experiments.

Data Collection – Wavelength Selection: Temperature was set to 20 ºC. Trigger mode was set to external and for runs less than 5 s, a pressure hold was enabled to prevent effects from cavitation. The stopped flow was equipped with a photodiode array detector, then the reference solution (1:1 MeCN/100 mM Tris buffer at pH 7.4) was driven into the chamber five times and the baseline was set. 10 μM Au(III) OAC was loaded into one syringe while 1 mM **GSH** was loaded into the other syringe, then the solutions were driven into the chamber five times to prime the chamber. The wavelength data (175 nm – 720 nm) was then acquired using a time scan of 50 ms to 10 s depending on the desired time frame. The optimal wavelength for single wavelength measurements was determined by examining the absorbance traces across the different spectra.

Data Collection – Single Wavelength: Temperature was set to 20 ºC. The stopped flow was equipped with a monochromator, then the reference solution (1:1 MeCN/100 mM Tris buffer at pH 7.4) was driven into the chamber five times and the baseline was set at the desired wavelength previously determined. 10 μM Au(III) OAC was loaded into one syringe while 1 mM **GSH** was loaded into the other syringe, then the solutions were driven into the chamber five times to prime the chamber. The single wavelength data was then acquired using a time scan of 50 ms to 120 s depending on the desired time frame. Replicates were performed at n = 3 or n = 5 depending on the time frame of the run (i.e. shorter runs allowed for more replicates). This process was repeated for each concentration of **GSH** – beginning with lower concentrations of **GSH** prevents dilution and cross-contamination between runs.

Data Processing: Raw data was exported as ProData CSV files and processed in OriginPro 9.1. k_{RE} was calculated using previously published methods.[1] k_{Co}, k_{Dis}, and K_{Eq} were calculated using previously published methods.[2]

S-Arylation of GSH with [((PCp$_2$)Me-DalPhos)Au^{III}(*p*-Toluene)Cl]$^+$ SbF_6^- (27)

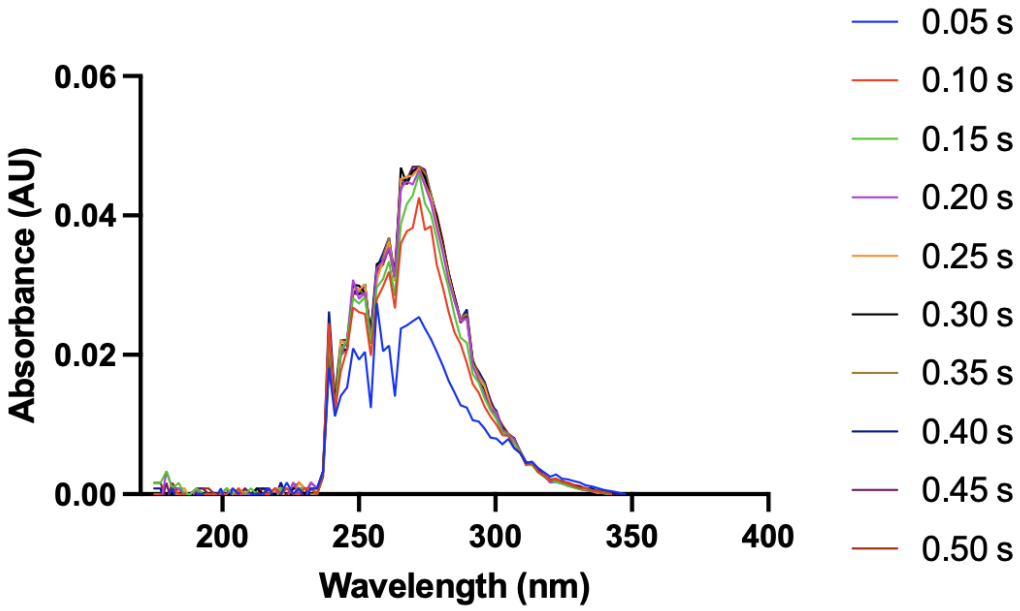


Figure S23. UV-Vis spectrum for 10 µM **27** with 1 mM **GSH** in 1:1 MeCN/100 mM Tris buffer at pH 7.4 over 500 ms. Spectra: 10. Sample period: 500 ms.

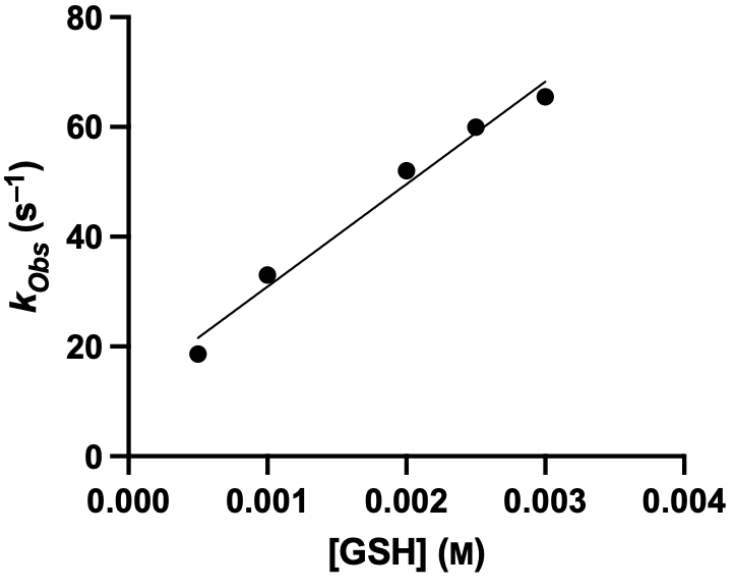


Figure S24. Plot of k_{Obs} against [**GSH**] for **27**. k_{Obs} measured from 100 ms to 500 ms. k_{Co} = 18,700 ± 539 $M^{-1}s^{-1}$, k_{Dis} = 12.2 ± 1.09 s^{-1}, K_{Eq} = 1,530 ± 181 M^{-1}. Single wavelength spectra were collected at 255 nm from 100 ms to 500 ms with 1000 samples per spectrum, n = 5 – some error bars are smaller than the markers.

S-Arylation of GSH with [(Azet-DalPhos)Au^{III}(*p*-Toluene)Cl]$^{+}$ SbF_6^{-} (28)

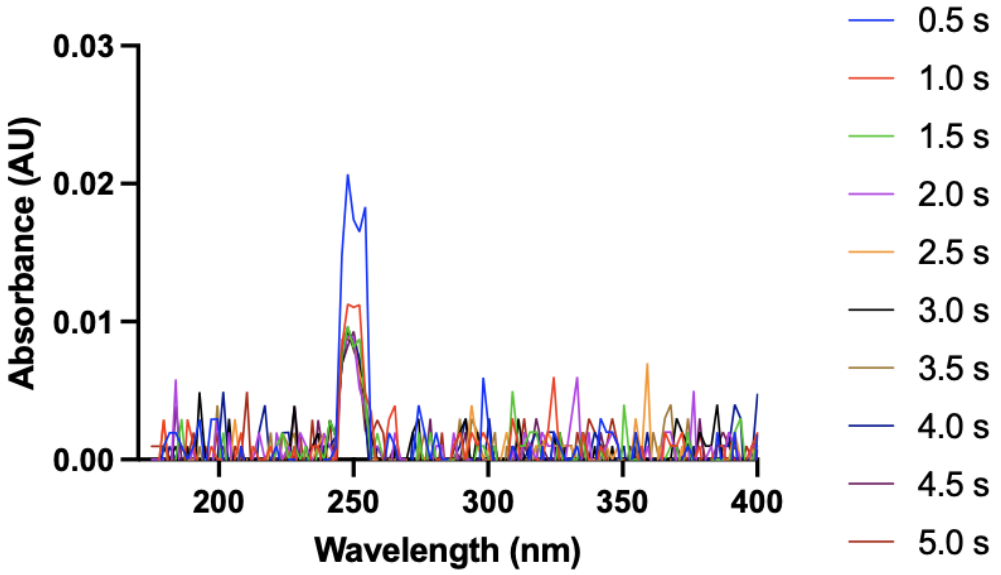


Figure S25. UV-Vis spectrum for 10 µM **28** with 1 mM **GSH** in 1:1 MeCN/100 mM Tris buffer at pH 7.4 over 5 s. Spectra: 10. Sample period: 5 s.

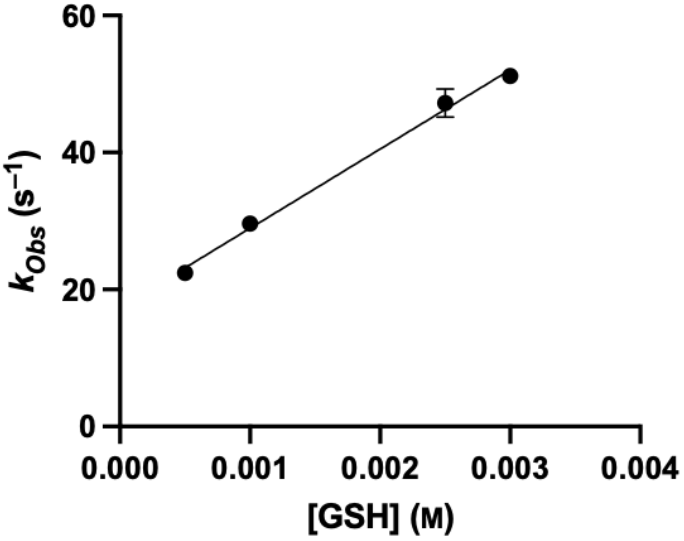


Figure S26. Plot of k_{Obs} against [**GSH**] for **28**. k_{Obs} measured over 1 s. k_{Co} = 11,600 ± 307 $M^{-1}s^{-1}$, k_{Dis} = 17.4 ± 0.624 s^{-1}, K_{Eq} = 670 ± 41.6 M^{-1}. Single wavelength spectra were collected at 250 nm over 1 s with 1000 samples per spectrum, n = 5 – some error bars are smaller than the markers.

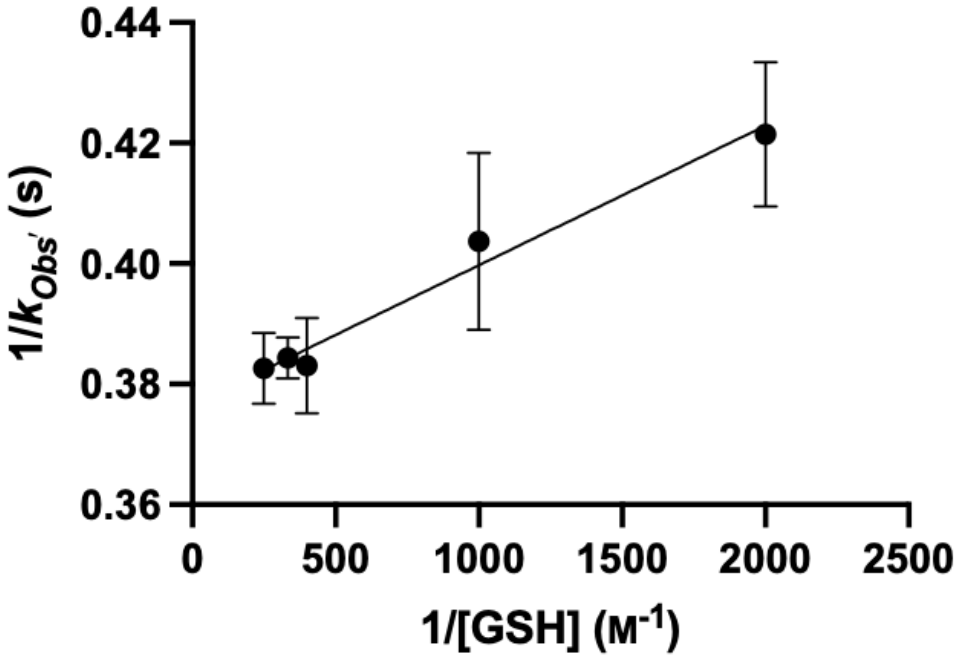


Figure S27. Plot of $1/k_{Obs'}$ against 1/[**GSH**] for **28**. $k_{Obs'}$ measured over 3 s. k_{RE} = 2.66 ± 0.0207 s^{-1}. Single wavelength spectra were collected at 250 nm over 3 s with 1000 samples per spectrum, n = 5.

S-Arylation of GSH with [((PCy$_2$)Azet-DalPhos)Au^{III}(*p*-Toluene)Cl]$^+$ SbF_6^- (29)

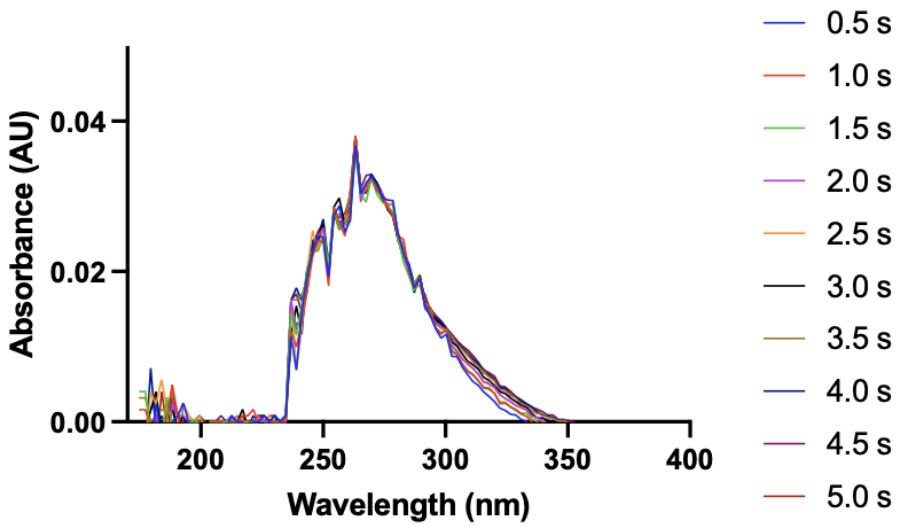


Figure S28. UV-Vis spectrum for 10 µM **29** with 1 mM **GSH** in 1:1 MeCN/100 mM Tris buffer at pH 7.4 over 5.0 s. Spectra: 10. Sample period: 500 ms.

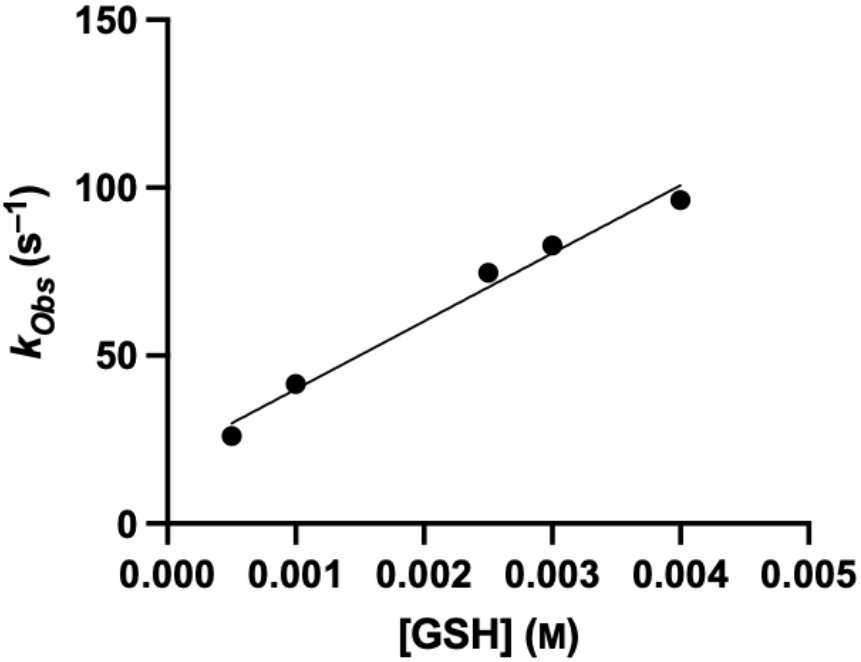


Figure S29. Plot of k_{Obs} against [**GSH**] for **29**. k_{Obs} measured from 50 ms to 200 ms. k_{Co} = 20,200 ± 595 $M^{-1}s^{-1}$, k_{Dis} = 19.8 ± 1.52 s^{-1}, K_{Eq} = 1,020 ± 108 M^{-1}. Single wavelength spectra were collected at 263 nm from 50 ms to 200 ms with 1000 samples per spectrum, n = 5 – some error bars are smaller than the markers.

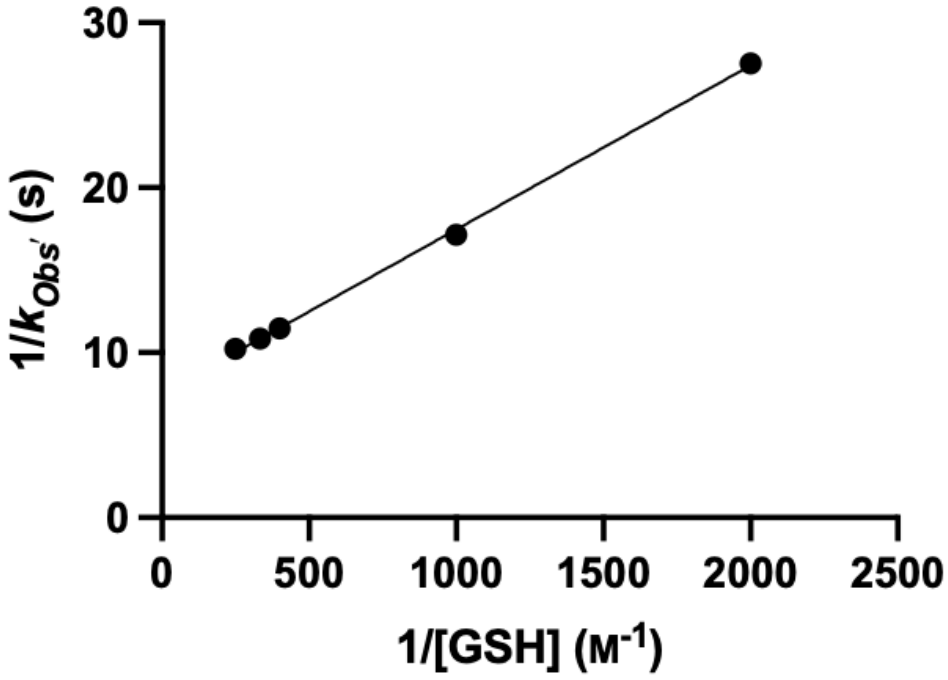


Figure S30. Plot of 1/k_{Obs} against 1/[**GSH**] for **29**. k_{Obs} measured from 60 s to 120 s. k_{RE} = 0.133 ± 0.00269 s^{-1}. Single wavelength spectra were collected at 305 nm from 60 s to 120 s with 1000 samples per spectrum, n = 3 – some error bars are smaller than the markers.

Competition Experiments

General Procedure

All competition experiments were performed in a similar manner to those reported by our groups previously.[1,3,4] [(Ligand)Au^{III}(Ar)Cl]$^+$ SbF_6^- complexes were prepared as 3.0 mM solutions in 500 µL of MeCN in two separate microcentrifuge tubes. 100 µL of each of the Au(III) complexes was added to a separate 500 µL microcentrifuge tube, then this mixture was vortexed for 15 seconds and centrifuged to ensure thorough mixing. Separately, a 1.0 mM **GSH** solution was prepared in 100 mM Tris buffer at pH 7.4 (Milli-Q water). To perform the competition experiment, a 25 µL of 1.0 mM **GSH** was added to a 500 µL microcentrifuge tube along with 25 µL of 100 mM Tris buffer at pH 7.4. 50 µL of the mixture of Au(III) complexes was added to the microcentrifuge tube containing **GSH** and vortexed for 15 seconds to ensure complete mixing. This was left to stand at 23 ºC for 15 minutes (250 µM **GSH**, 750 µM of each Au(III) reagent).

After 15 minutes, the solution was vortexed again for 15 seconds and then centrifuged down. A 10 µL aliquot of the reaction mixture was removed and diluted with 90 µL of 1:1 water-MeCN, both containing 0.1% TFA. The 100 µL of solution was analyzed using LC-MS with a 10 µL injection and a 1-99% gradient of MeCN against water, both containing 0.1% formic acid (0-1 minutes: 1% MeCN; 1-12 minutes: 1-99% MeCN; 12-15 minutes: 99% MeCN).

The percent product distributions were determined by integrating the total ion chromatogram for each *S*-arylation product and determining the ratio between the ion counts. Each reaction was repeated in triplicate, and the percentage of product is reported as an average of three independent runs.

Individual control experiments for each Au(III) complex were performed similarly to the above procedure, but 25 µL of the 3.0 mM Au(III) stock solution was added to the final microcentrifuge tube along with 25 µL of MeCN. These experiments were used to determine whether each Au(III) reagent was independently capable of performing the *S*-arylation.

Compounds **30** and **31** were synthesized according to previously described procedures.[3–5]

S-Arylation of GSH with [((PCp$_2$)Me-DalPhos)Au^{III}(*p*-Toluene)Cl]$^+$ SbF$_6^-$ (27) and [((PCy$_2$)Me-DalPhos)Au^{III}(*p*-Ethylbenzene)Cl]$^+$ SbF$_6^-$ (30)

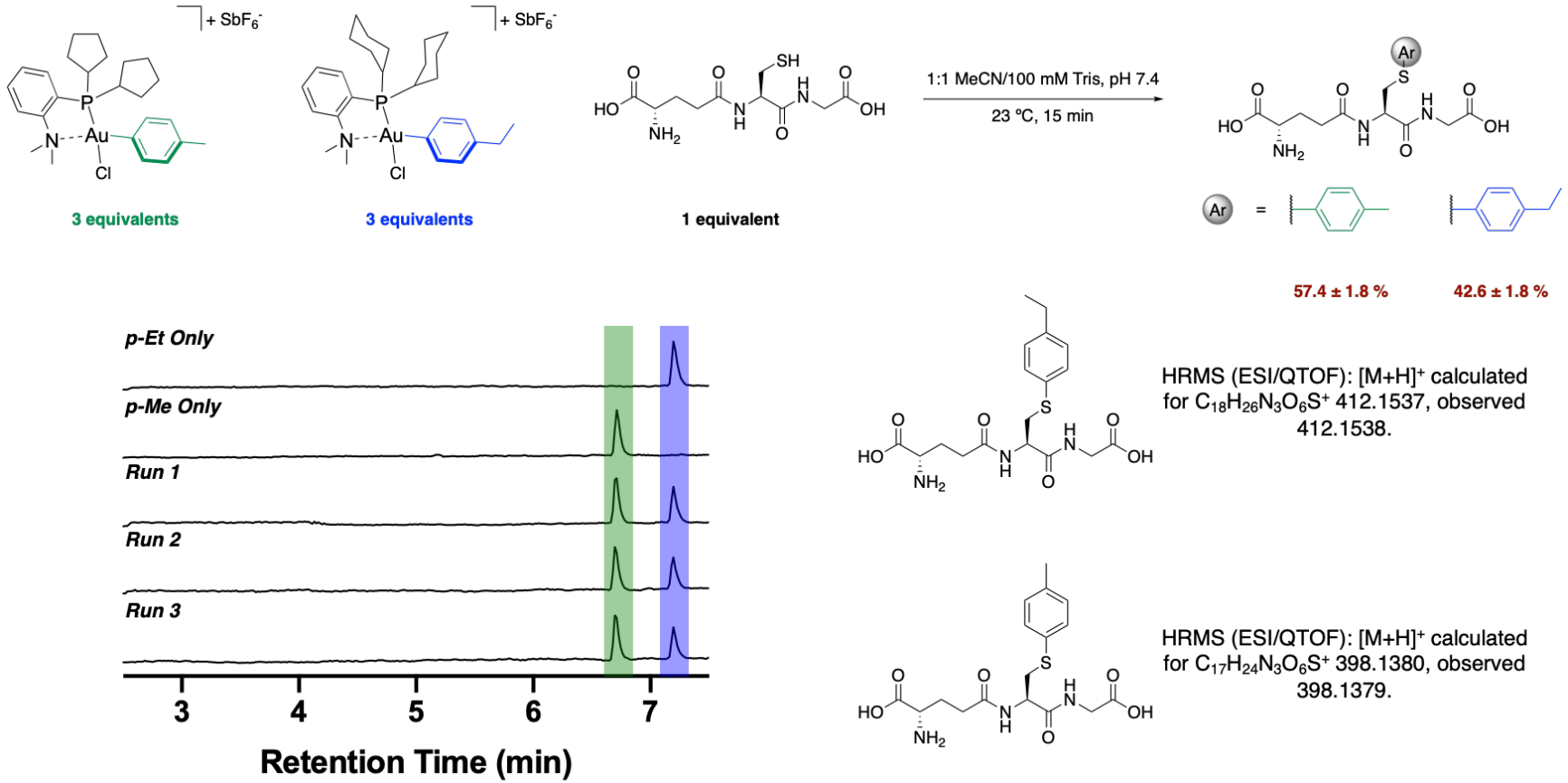


Figure S31. Scheme of the *S*-arylation of **GSH** in the presence of both **27** and **30** and the corresponding LC-MS as well as the LC-MS traces of the *S*-arylation products of **GSH** in the presence of each independent Au(III) oxidative addition complex.

S-Arylation of GSH with [(Azet-DalPhos)Au^{III}(*p*-Toluene)Cl]$^{+}$ SbF_6^{-} (28) and [(Me-DalPhos)Au^{III}(*p*-Ethylbenzene)Cl]$^{+}$ SbF_6^{-} (31)

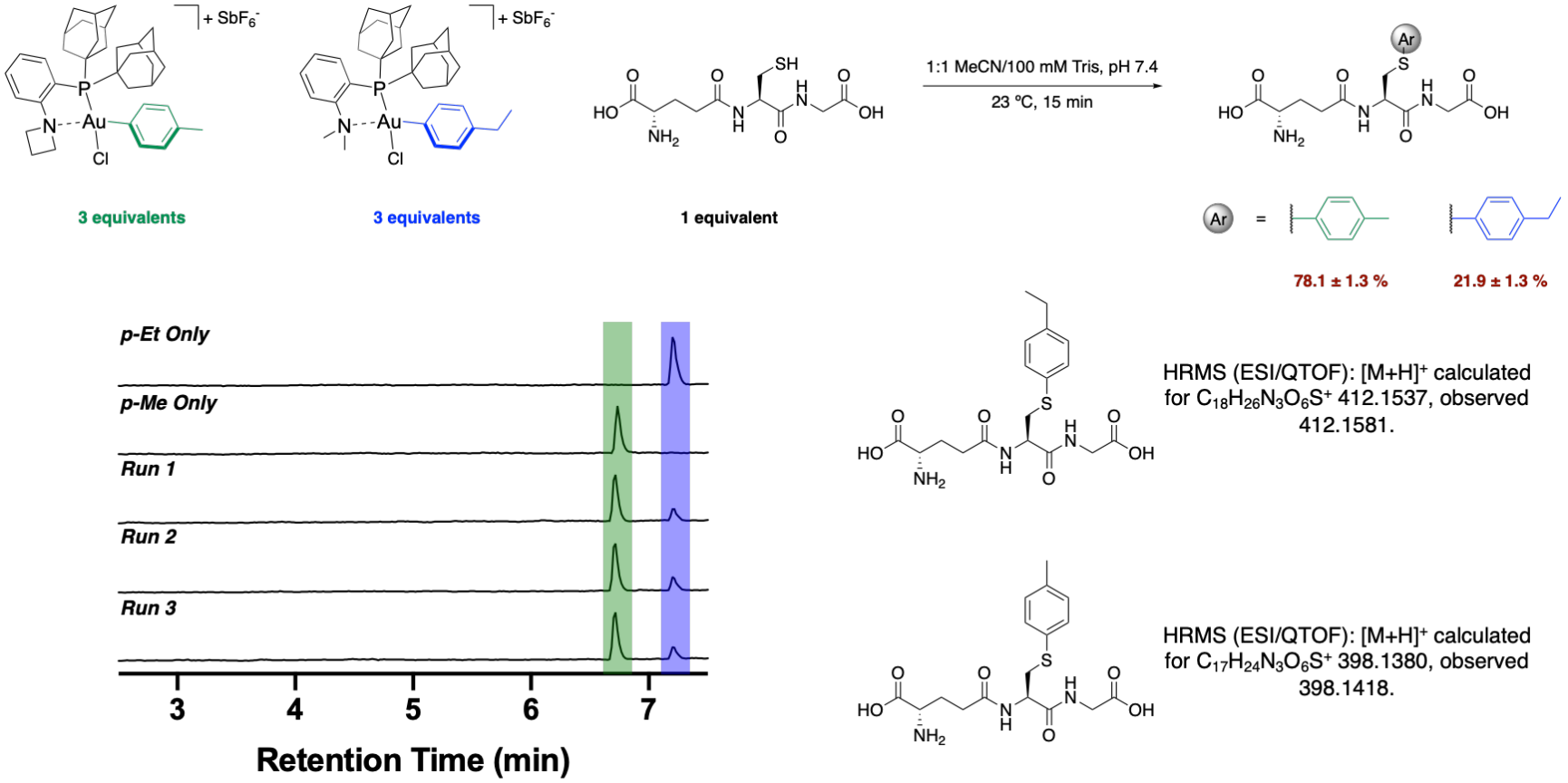


Figure S32. Scheme of the *S*-arylation of **GSH** in the presence of both **28** and **31** and the corresponding LC-MS as well as the LC-MS traces of the *S*-arylation products of **GSH** in the presence of each independent Au(III) oxidative addition complex.

S-Arylation of GSH with [((PCy$_2$)Azet-DalPhos)Au^{III}(*p*-Toluene)Cl]$^+$ SbF$_6^-$ (29) and [((PCy$_2$)Me-DalPhos)Au^{III}(*p*-Ethylbenzene)Cl]$^+$ SbF$_6^-$ (30)

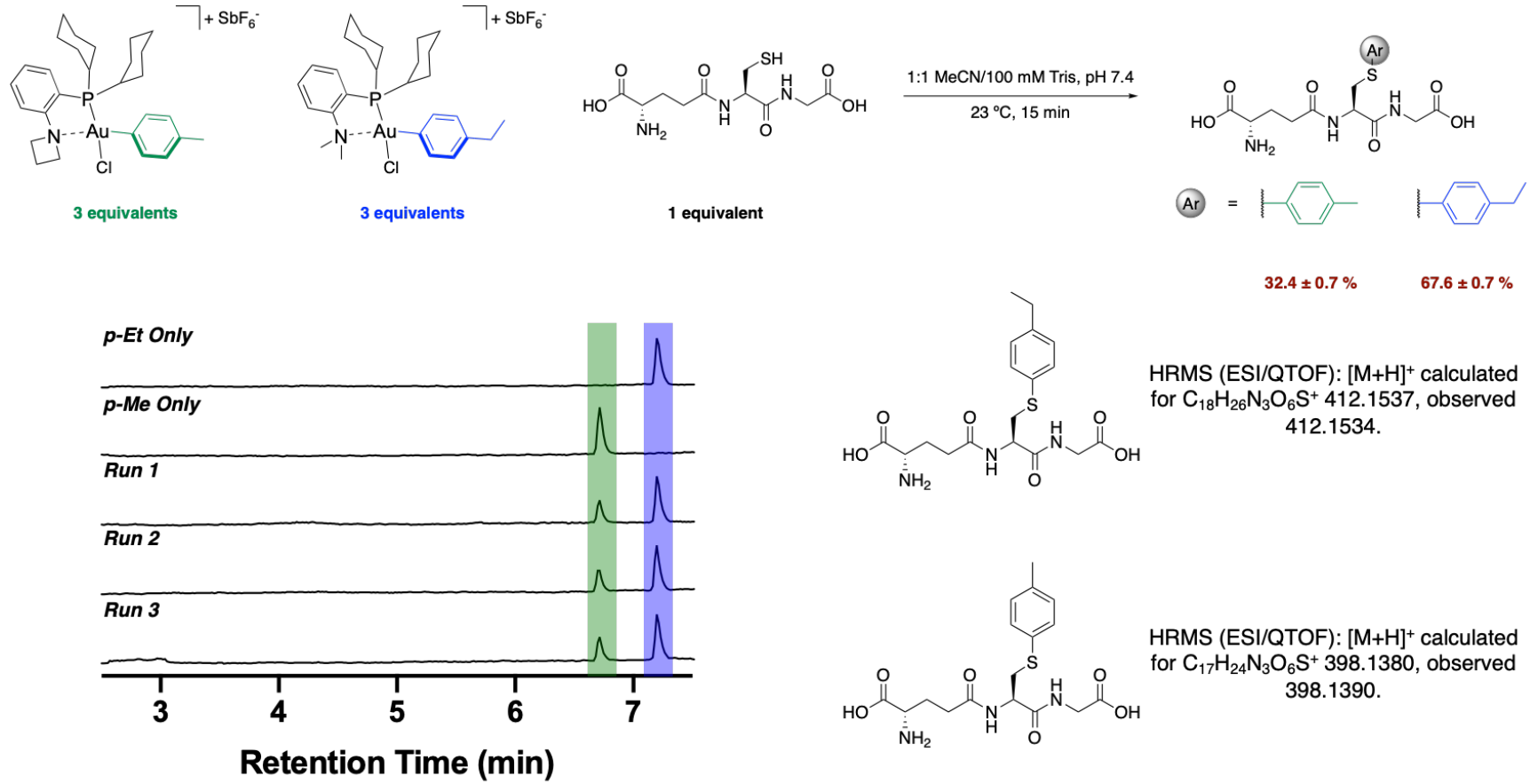


Figure S33. Scheme of the *S*-arylation of **GSH** in the presence of both **29** and **30** and the corresponding LC-MS as well as the LC-MS traces of the *S*-arylation products of **GSH** in the presence of each independent Au(III) oxidative addition complex.

Computations

General Computational Details

All calculations were carried out with the Gaussian 09 software package.[5] An ultrafine grid was applied for all calculations to ensure accuracy. Ground state geometries were optimized in water with the CPCM solvation model[6] using the B3LYP functional[7,8] with the D3 correction for dispersion.[9] The LANL2DZ basis set was used for the Au atom, and the 6-31G(d) basis set was used for all other atoms in the system. Frequency calculations were carried out at the same level of theory to ensure that stationary points were truly minima or saddle points on the potential energy surface. Thermal corrections to free energies were calculated using Grimme's quasi-rigid rotor-harmonic oscillator approximation at 298 K[10] using the Goodvibes program.[11] Single point energy calculations were performed using the ωB97X-D functional[12] with the CPCM solvation model in water. The single point calculations used an SDD basis set for the Au atom, and the 6-311+G(d,p) basis set was used for all other atoms. Conformational searches were carried out using the conformer-rotamer ensemble sampling tool (CREST)[13,14] version 2.7.1 with XTB version 6.2 RC2 (SAW190805).[15–17] All transition states were verified using intrinsic reaction coordinate (IRC) calculations. Images of molecular structures were rendered in CYLview with C-H hydrogens omitted on the Au-containing complexes for clarity.[18]

Computed energies and calculated coordinates for [(Me-DalPhos)Au(Phenyl)Cl]$^+$ (**5**), [((P^{t}Bu$_2$)Me-DalPhos)Au(Phenyl)Cl]$^+$ (**6**), and [((PCy$_2$)Me-DalPhos)Au(Phenyl)Cl]$^+$ (**7**) were previously published.[1]

Buried Volume Calculations

Computational Details

Conformational searches were carried out using the conformer-rotamer ensemble sampling tool (CREST)[13,14] version 2.7.1 with XTB version 6.2 RC2 (SAW190805).[15–17] The best conformers were then optimized in water with the CPCM solvation model[6] using the B3LYP functional[7,8] with the D3 correction for dispersion.[9] The LANL2DZ basis set was used for the Au atom, and the 6-31G(d) basis set was used for all other atoms in the system. Frequency calculations were carried out at the same level of theory to ensure that stationary points were truly minima or saddle points on the potential energy surface. Thermal corrections to free energies were calculated using Grimme's quasi-rigid rotor-harmonic oscillator approximation at 298 K[10] using the Goodvibes program.[11] Single point energy calculations were performed using the ωB97X-D functional[12] with the CPCM solvation model in water. The single point calculations used an SDD basis set for the Au atom, and the 6-311+G(d,p) basis set was used for all other atoms. The $\%V_{Bur}$ calculations were performed using Cavallo's SambVca 2.0 web tool[19] using each DFT calculated structure. The following parameters were used to calculate the percent buried volume.

- Atom coordinated to center of sphere: Au
- Atom for z-axis definition: N
- Atom for xz plane definition: P
- Atoms to be deleted: Au and Cl
- Bond radii scaled by 1.17
- Sphere radius set to 3.5 Å
- Distance of the coordination point from the center of the sphere: 0.0 Å
- Mesh spacing for numerical integration: 0.10
- No H atoms included in calculation

Computed Energies – *S*-Arylation

Diphosphine Variation

S-Arylation of Methanethiol with [((P^{i}Pr$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (8)

Table S1. Computed energies for the *S*-arylation of methanethiol with [((P^{i}Pr$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**8**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-1771.323794	0.45306	-1770.84268	0.084561	0.080855	-1770.927241	-1770.923535	-1771.578513
Int1	-1749.208128	0.490689	-1748.686917	0.090704	0.085897	-1748.777621	-1748.772814	-1749.4536
TS_{RE}	-1749.190828	0.488194	-1748.67228	0.091304	0.086052	-1748.763584	-1748.758333	-1749.434298
Int2	-1749.246301	0.489613	-1748.725746	0.094166	0.08769	-1748.819911	-1748.813435	-1749.492706
P_{Au}	-1539.860104	0.358087	-1539.477959	0.079331	0.074283	-1539.557289	-1539.552241	-1540.149991
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

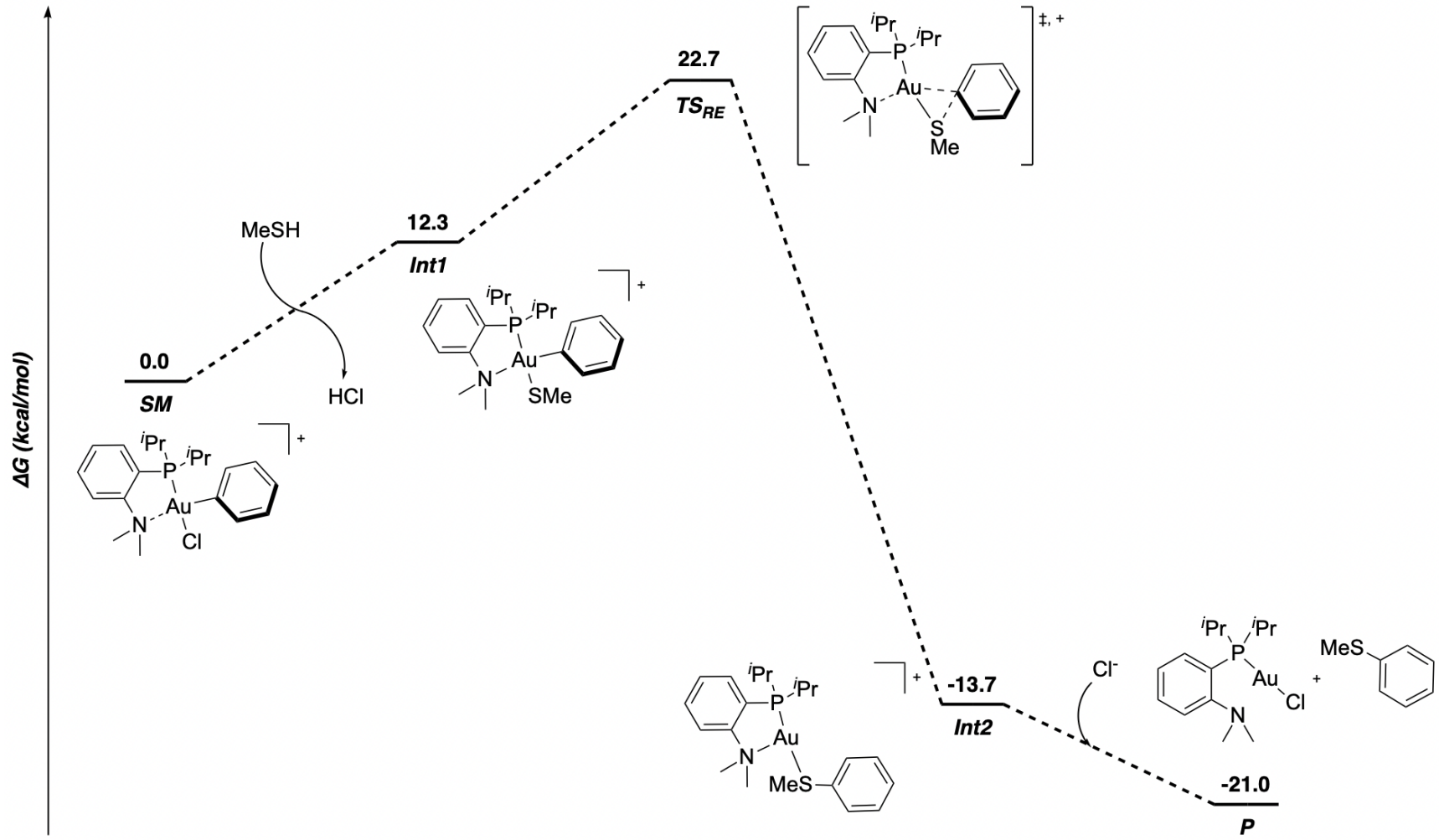


Figure S34. Free energy diagram for the *S*-arylation of methanethiol with [((P^{i}Pr$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**8**) with methanethiol calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. ^{i}Pr = isopropyl.

S-Arylation of Methanethiol with [((PCp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (9)

Table S2. Computed energies for the *S*-arylation of methanethiol with [((PCp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**9**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-1926.164127	0.527978	-1925.606648	0.088676	0.084084	-1925.695324	-1925.690732	-1926.408369
Int1	-1904.054993	0.56545	-1903.457452	0.095747	0.089487	-1903.553199	-1903.54694	-1904.290209
TS_{RE}	-1904.03061	0.562251	-1903.435987	0.098115	0.090829	-1903.534102	-1903.526817	-1904.263182
Int2	-1904.085289	0.563079	-1903.489356	0.100966	0.092298	-1903.590322	-1903.581654	-1904.321258
P_{Au}	-1694.702193	0.432406	-1694.244085	0.084818	0.078301	-1694.328902	-1694.322386	-1694.981653
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

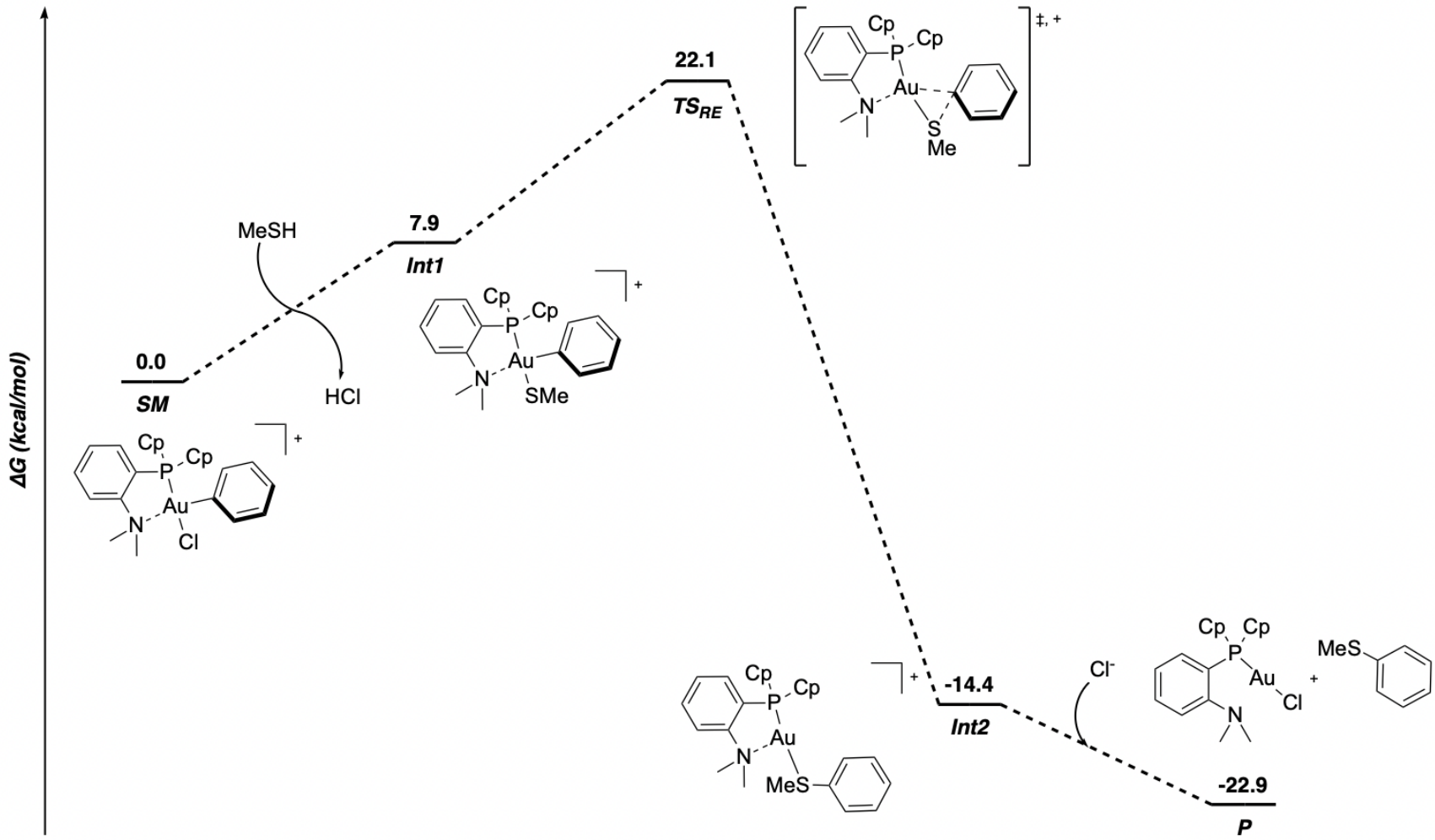


Figure S35. Free energy diagram for the *S*-arylation of methanethiol with [((PCp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**9**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Cp = cyclopentyl.

S-Arylation of Methanethiol with [((PCubane$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (15)

Table S3. Computed energies for the *S*-arylation of methanethiol with [((PCubane$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**15**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-2151.986825	0.511631	-2151.445389	0.09097	0.085059	-2151.536359	-2151.530448	-2152.220292
Int1	-2129.877109	0.549459	-2129.295533	0.09629	0.089516	-2129.391823	-2129.385048	-2130.102472
TS_{RE}	-2129.851613	0.546462	-2129.272882	0.098472	0.090627	-2129.371354	-2129.363509	-2130.074906
Int2	-2129.907936	0.548583	-2129.326863	0.098796	0.090929	-2129.425659	-2129.417792	-2130.134659
P_{Au}	-1920.522946	0.4176	-1920.080023	0.082782	0.077121	-1920.162805	-1920.157144	-1920.794082
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

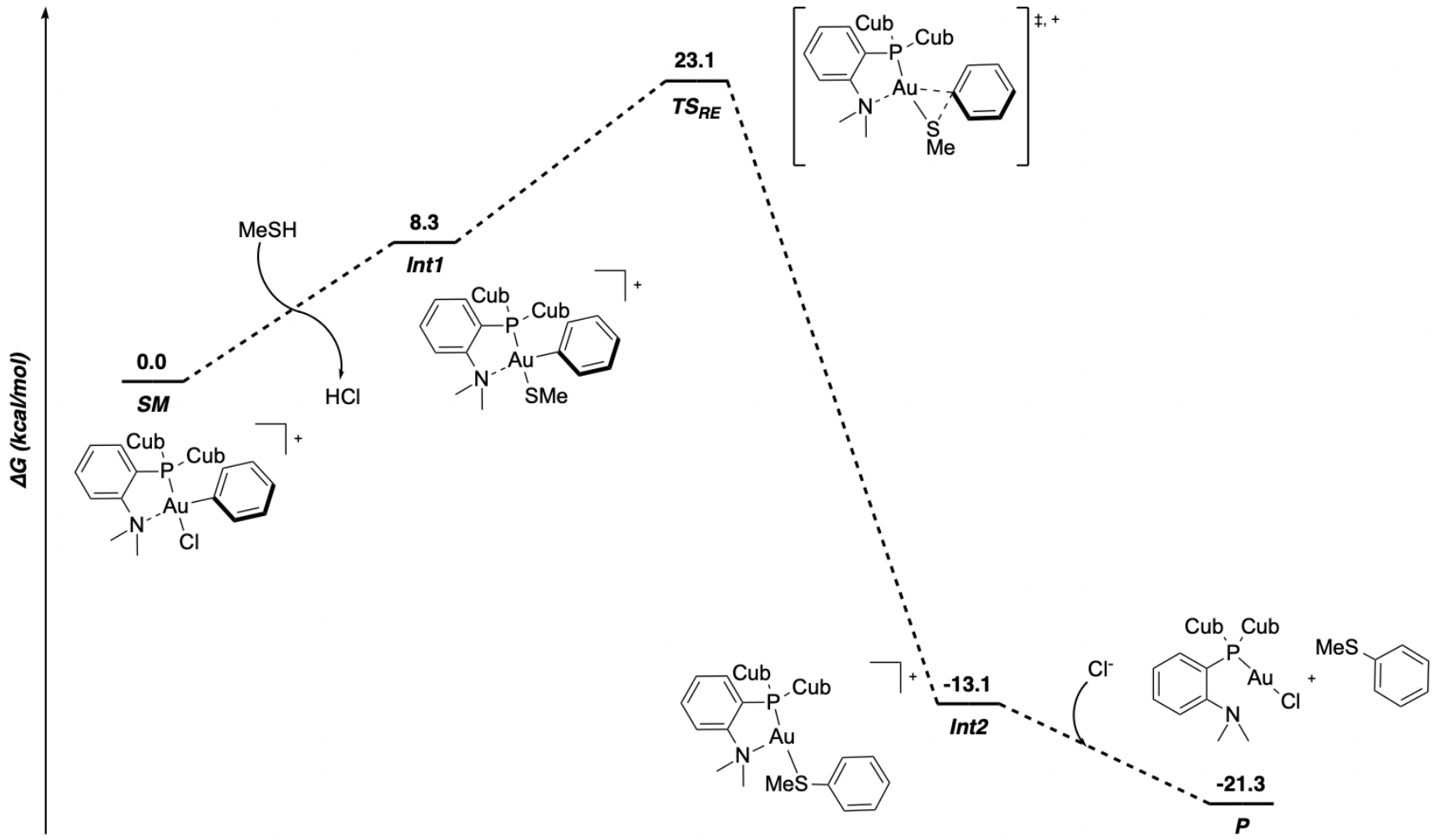


Figure S36. Free energy diagram for the *S*-arylation of methanethiol with [((PCubane$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**15**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Cub = cubyl.

S-Arylation of Methanethiol with [((PCyb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (10)

Table S4. Computed energies for the *S*-arylation of methanethiol with [((PCyb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**10**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-1847.46885	0.466365	-1846.974287	0.087426	0.082048	-1847.061713	-1847.056335	-1847.718089
Int1	-1825.36063	0.504727	-1824.825614	0.091791	0.086038	-1824.917406	-1824.911652	-1825.601607
TS_{RE}	-1825.339988	0.501792	-1824.807764	0.094152	0.087302	-1824.901916	-1824.895066	-1825.577599
Int2	-1825.395005	0.503909	-1824.860454	0.095046	0.087827	-1824.9555	-1824.948281	-1825.635117
P_{Au}	-1616.009244	0.373031	-1615.612748	0.077565	0.073449	-1615.690313	-1615.686197	-1616.2948
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

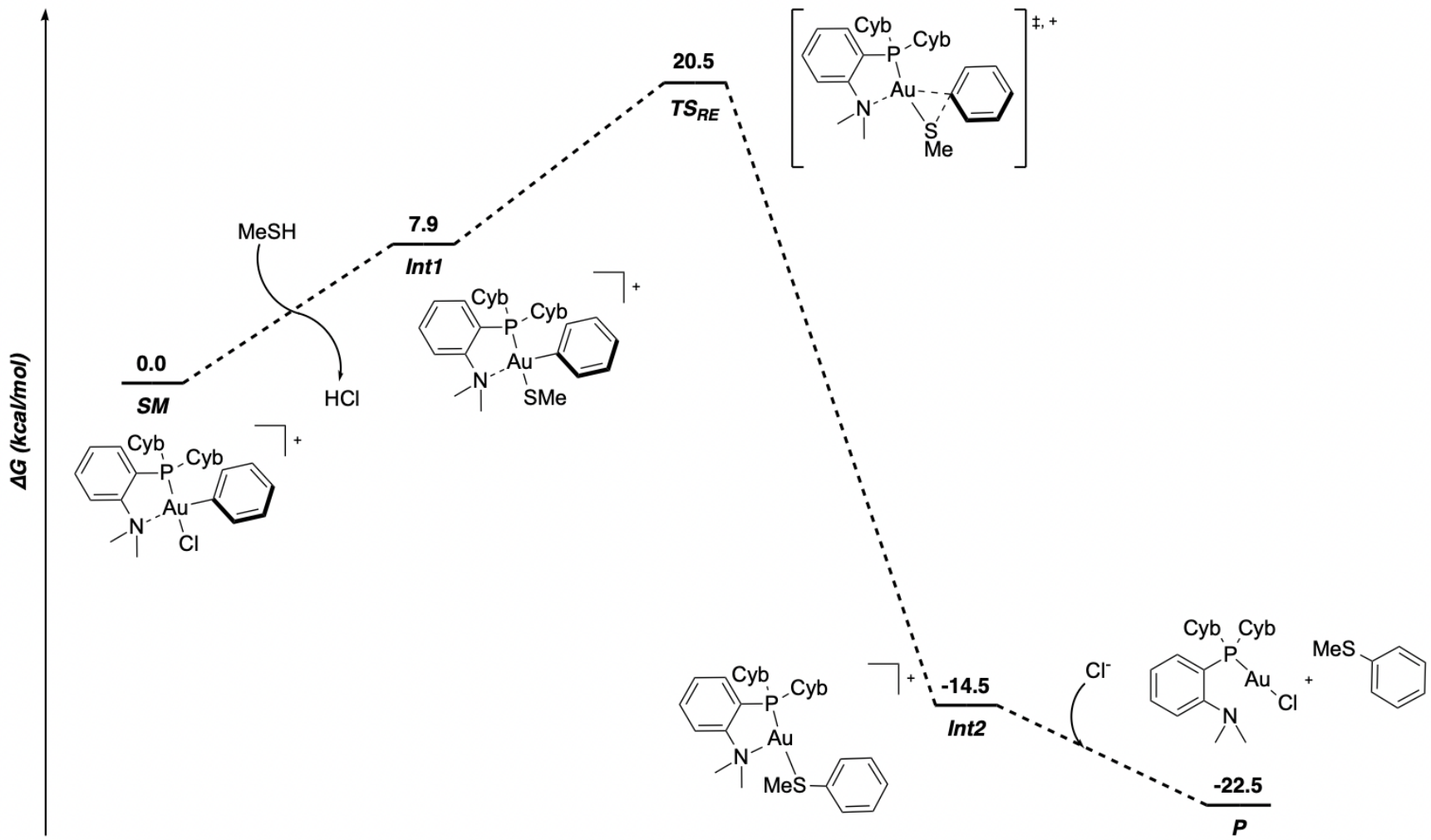


Figure S37. Free energy diagram for the *S*-arylation of methanethiol with [((PCyb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**10**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Cyb = cyclobutyl.

S-Arylation of Methanethiol with [((PBcp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (13)

Table S5. Computed energies for the *S*-arylation of methanethiol with [((PBcp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**13**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-1923.570568	0.478385	-1923.063858	0.088389	0.082446	-1923.152247	-1923.146304	-1923.815087
Int1	-1901.461957	0.516453	-1900.914981	0.093092	0.086564	-1901.008072	-1901.001544	-1901.69811
TS_{RE}	-1901.437915	0.513364	-1900.893861	0.094828	0.087531	-1900.988689	-1900.981393	-1901.671958
Int2	-1901.492973	0.51472	-1900.946879	0.09898	0.08982	-1901.045859	-1901.036699	-1901.730823
P_{Au}	-1692.109008	0.38432	-1691.700818	0.079485	0.074138	-1691.780304	-1691.774956	-1692.39031
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

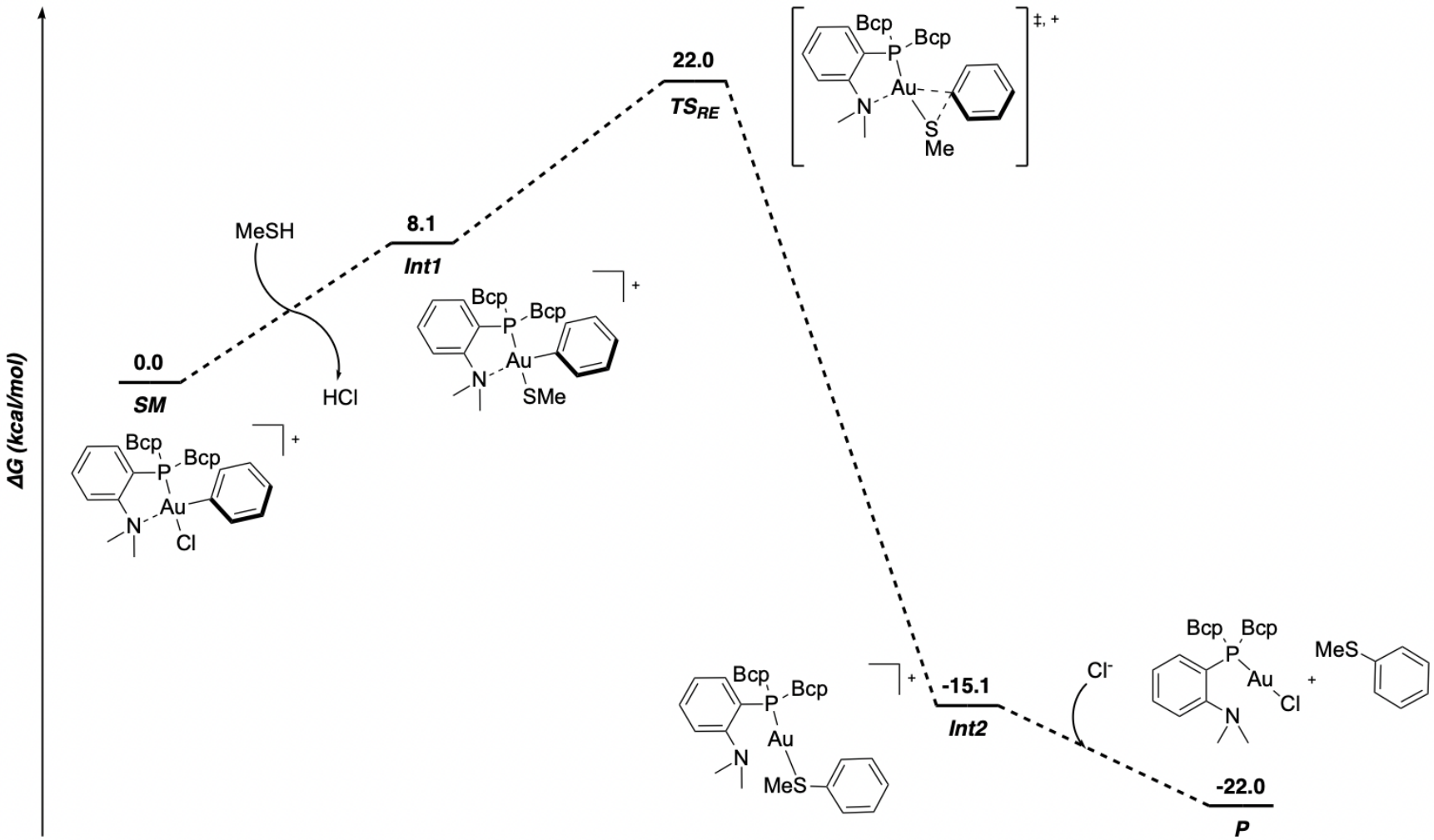


Figure S38. Free energy diagram for the *S*-arylation of methanethiol with [((PBcp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**13**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Bcp = bicyclo[1.1.1]pentyl.

S-Arylation of Methanethiol with [((PBcb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (14)

Table S6. Computed energies for the *S*-arylation of methanethiol with [((PBcb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**14**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-1844.943566	0.417676	-1844.498412	0.086076	0.080643	-1844.584488	-1844.579055	-1845.18624
Int1	-1822.833264	0.455802	-1822.347697	0.091565	0.08517	-1822.439262	-1822.432867	-1823.067563
TS_{RE}	-1822.812335	0.453364	-1822.329318	0.091895	0.085387	-1822.421213	-1822.414705	-1823.043927
Int2	-1822.870005	0.455145	-1822.38492	0.092855	0.086034	-1822.477775	-1822.470954	-1823.105268
P_{Au}	-1613.485407	0.324403	-1613.138334	0.075916	0.071666	-1613.21425	-1613.21	-1613.765165
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

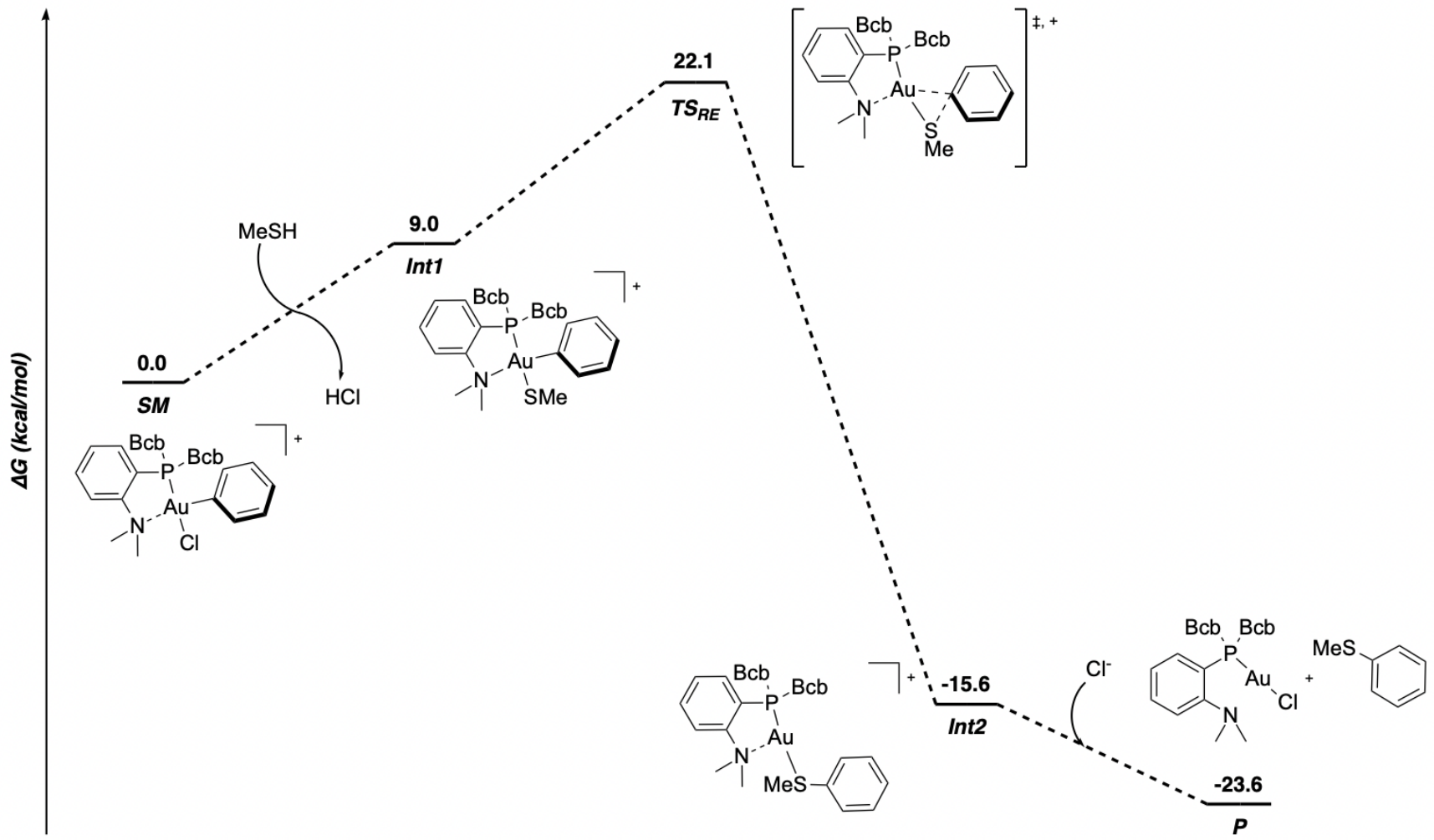


Figure S39. Free energy diagram for the *S*-arylation of methanethiol with [((PBcb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**14**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Bcb = bicyclo[1.1.0]butyl.

S-Arylation of Methanethiol with [((PCyp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (11)

Table S7. Computed energies for the *S*-arylation of methanethiol with [((PCyp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**11**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-1768.826821	0.407514	-1768.393198	0.081987	0.077749	-1768.475186	-1768.470947	-1769.081672
Int1	-1746.716879	0.445486	-1746.242984	0.087525	0.082286	-1746.330509	-1746.32527	-1746.963158
TS_{RE}	-1746.696941	0.44318	-1746.225574	0.087408	0.082265	-1746.312982	-1746.30784	-1746.939235
Int2	-1746.754958	0.444977	-1746.281452	0.08877	0.083103	-1746.370222	-1746.364555	-1747.000908
P_{Au}	-1537.370784	0.313871	-1537.035474	0.072777	0.069225	-1537.10825	-1537.104699	-1537.660927
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

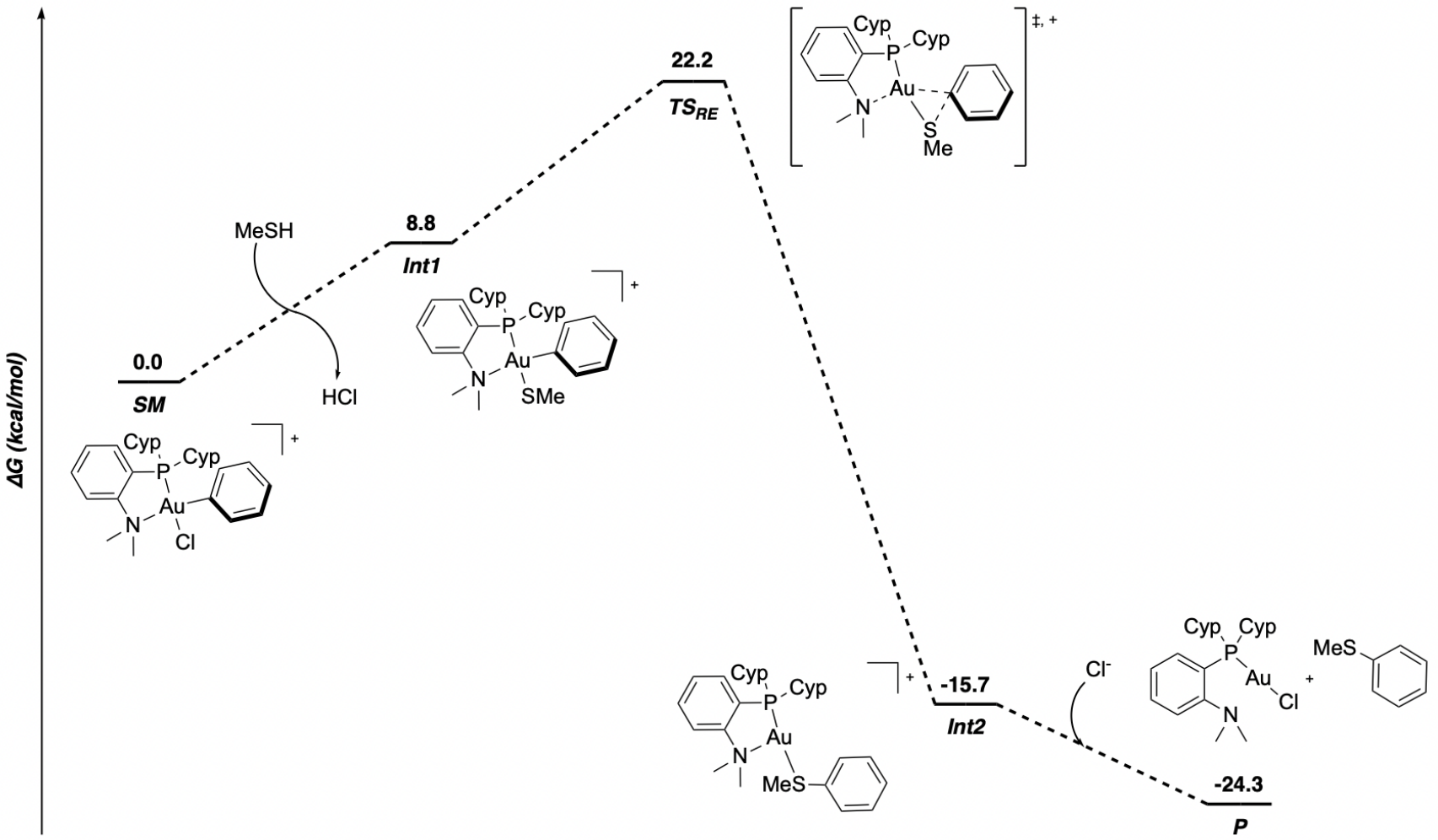


Figure S40. Free energy diagram for the *S*-arylation of methanethiol with [((PCyp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**11**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Cyp = cyclopropyl.

S-Arylation of Methanethiol with [((PMe$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (12)

Table S8. Computed energies for the *S*-arylation of methanethiol with [((PMe$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**12**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-1614.052993	0.336946	-1613.692866	0.075512	0.072014	-1613.768378	-1613.764881	-1614.321425
Int1	-1591.9441	0.374896	-1591.5436	0.081456	0.076822	-1591.6251	-1591.6205	-1592.2036
TS_{RE}	-1591.917881	0.372685	-1591.519864	0.081302	0.07687	-1591.601166	-1591.596733	-1592.174652
Int2	-1591.975972	0.374675	-1591.575715	0.083332	0.077813	-1591.659047	-1591.653528	-1592.235988
P_{Au}	-1382.592548	0.243553	-1382.330385	0.066903	0.063743	-1382.397288	-1382.394127	-1382.895644
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

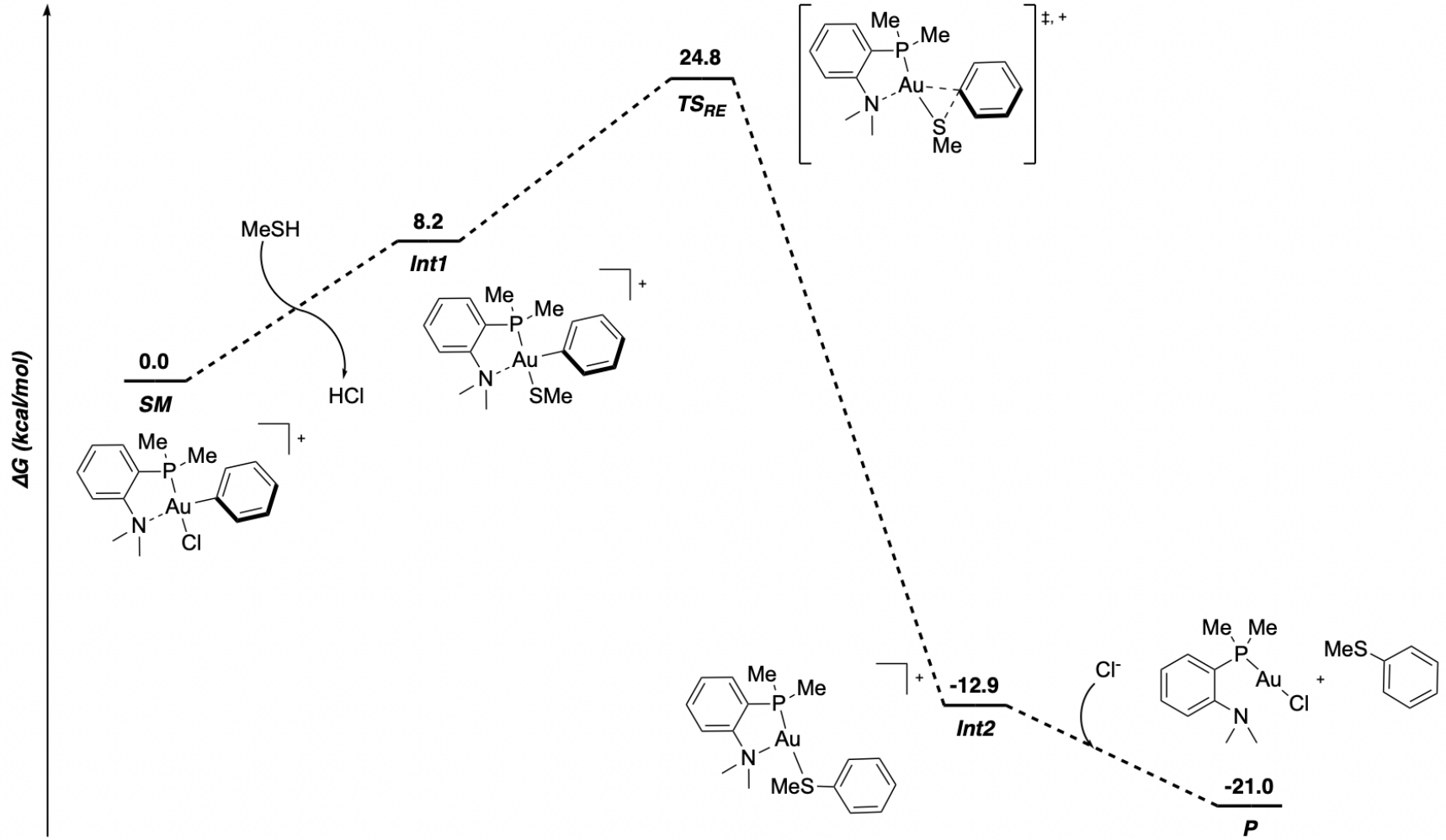


Figure S41. Free energy diagram for the *S*-arylation of methanethiol with [((PMe$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**12**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Me = methyl.

Amine Variation

S-Arylation of Methanethiol with [(Mor-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (16)

Table S9. Computed energies for the *S*-arylation of methanethiol with [(Mor-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**16**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-2467.145076	0.776337	-2466.33254	0.101898	0.095952	-2466.434438	-2466.428492	-2467.351315
Int1	-2445.037104	0.814518	-2444.184236	0.106877	0.100135	-2444.291113	-2444.284371	-2445.234987
TS_{RE}	-2445.021143	0.811672	-2444.171153	0.106934	0.100107	-2444.278087	-2444.27126	-2445.217085
Int2	-2445.088789	0.812665	-2444.237346	0.109253	0.101382	-2444.346598	-2444.338728	-2445.289119
P_{Au}	-2235.700414	0.68201	-2234.986877	0.093118	0.087564	-2235.079995	-2235.074441	-2235.945015
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

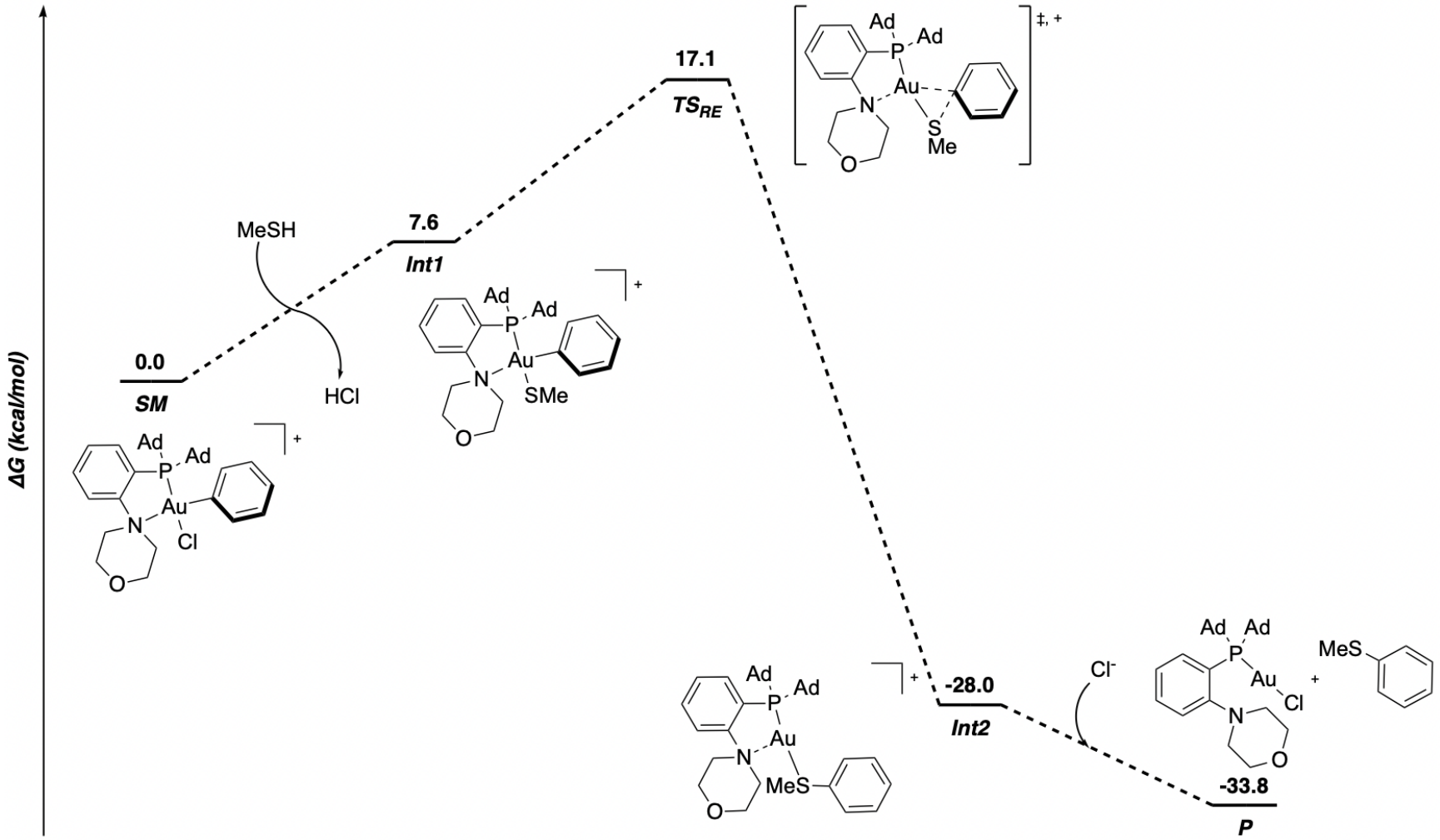


Figure S42. Free energy diagram for the *S*-arylation of methanethiol with [(Mor-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**16**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Ad = 1-adamantyl.

S-Arylation of Methanethiol with [(Pip-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (17)

Table S10. Computed energies for the *S*-arylation of methanethiol with [(Pip-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**17**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-2431.25601	0.800551	-2430.418936	0.103923	0.097162	-2430.522858	-2430.516098	-2431.45953
Int1	-2409.147904	0.838582	-2408.270712	0.107151	0.100452	-2408.377863	-2408.371164	-2409.344055
TS_{RE}	-2409.142034	0.83639	-2408.267292	0.106412	0.099988	-2408.373704	-2408.36728	-2409.334655
Int2	-2409.201308	0.836731	-2408.325576	0.109898	0.101875	-2408.435474	-2408.427451	-2409.398051
P_{Au}	-2199.812185	0.706041	-2199.07439	0.093305	0.087829	-2199.167696	-2199.16222	-2200.052995
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

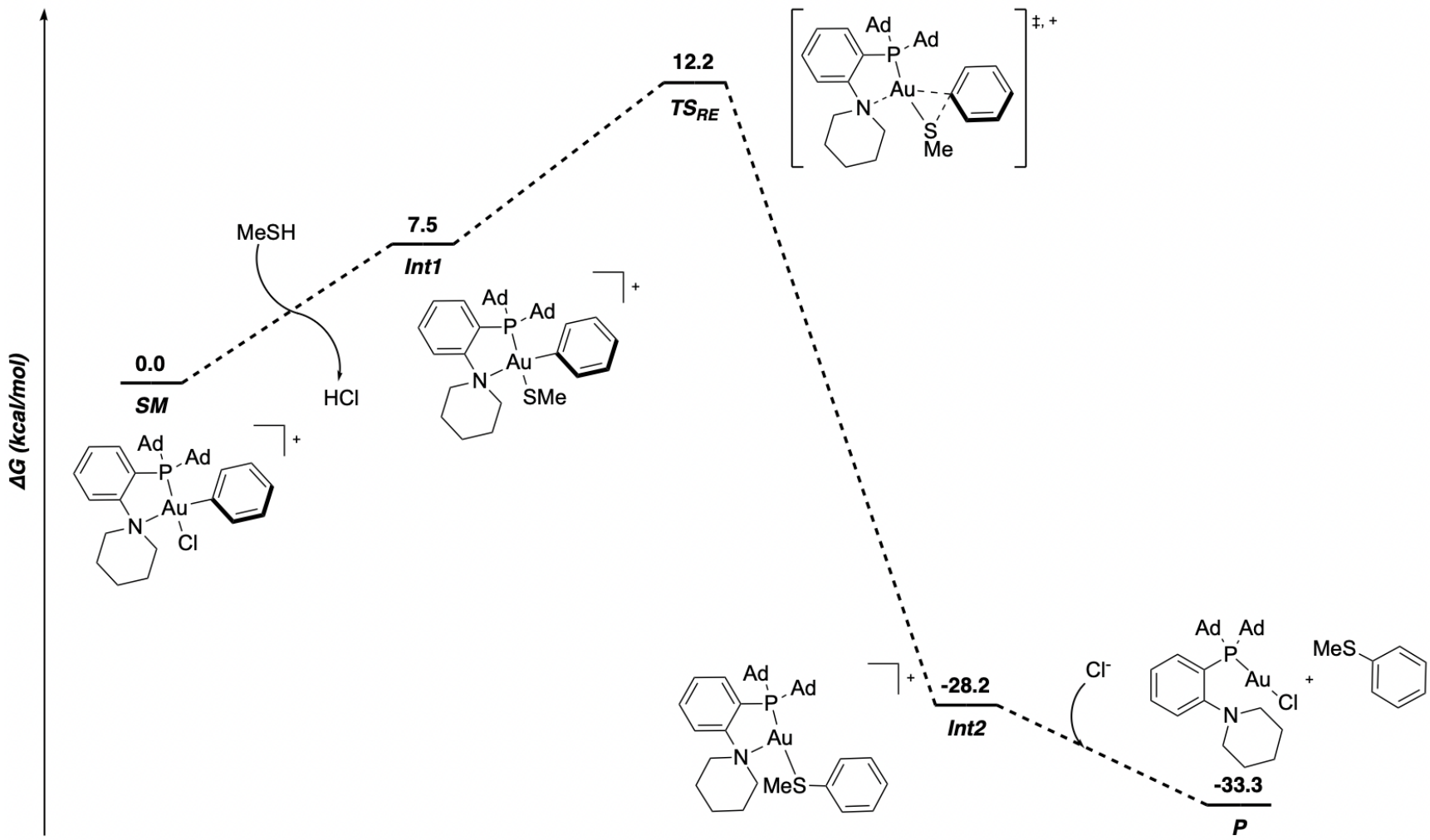


Figure S43. Free energy diagram for the *S*-arylation of methanethiol with [(Pip-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**17**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Ad = 1-adamantyl.

S-Arylation of Methanethiol with [(Pyrrol-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (18)

Table S11. Computed energies for the *S*-arylation of methanethiol with [(Pyrrol-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**18**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-2391.943475	0.770909	-2391.137095	0.101274	0.09496	-2391.238369	-2391.232055	-2392.15165
Int1	-2369.83546	0.808817	-2368.988977	0.10675	0.099402	-2369.095727	-2369.088379	-2370.035037
TS_{RE}	-2369.819937	0.806591	-2368.975994	0.105522	0.098678	-2369.081516	-2369.074673	-2370.017339
Int2	-2369.875801	0.80727	-2369.030465	0.108121	0.100385	-2369.138586	-2369.13085	-2370.076098
P_{Au}	-2160.48774	0.676352	-2159.780358	0.09233	0.086842	-2159.872688	-2159.867199	-2160.731909
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

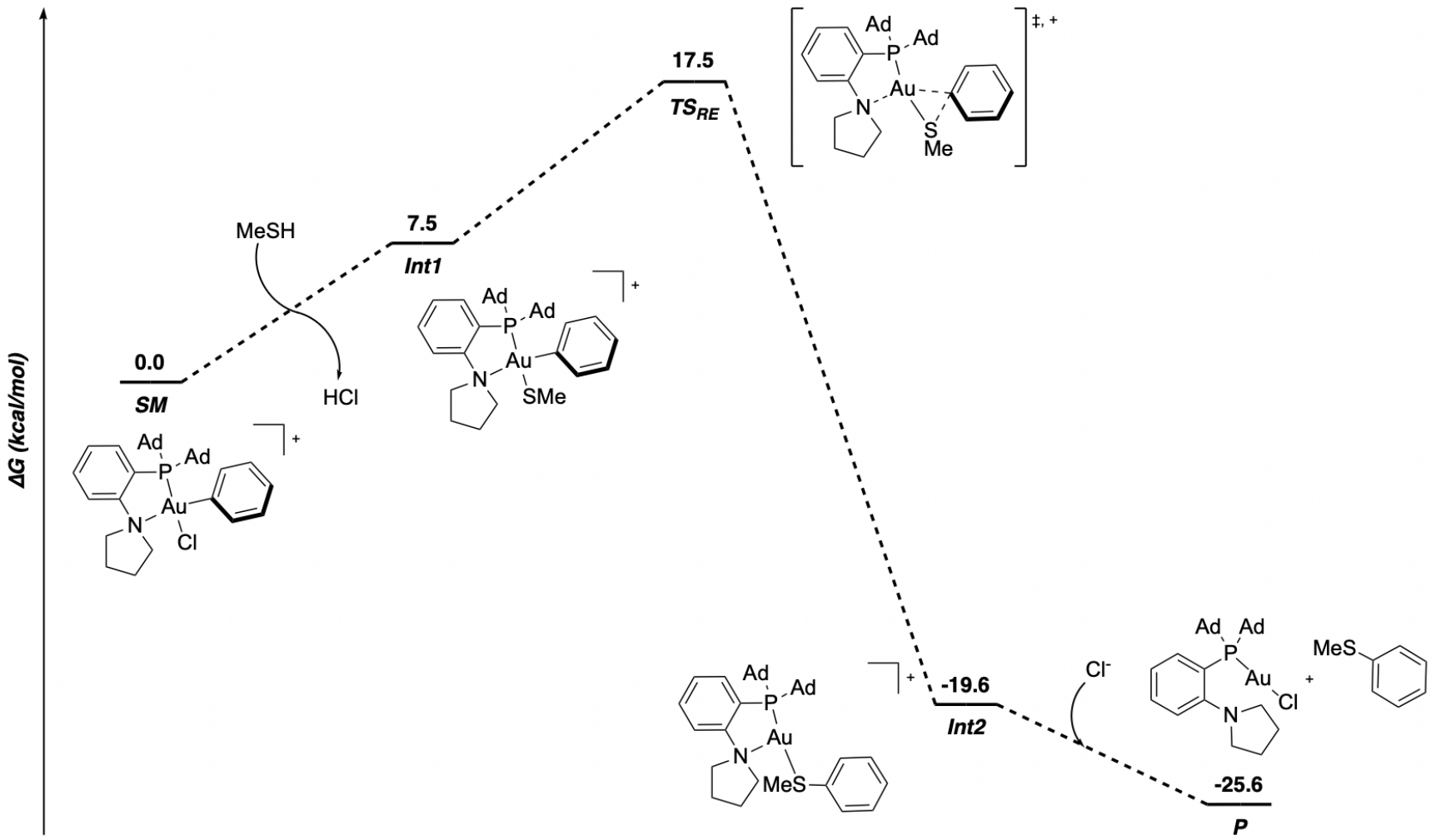


Figure S44. Free energy diagram for the *S*-arylation of methanethiol with [(Pyrrol-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**18**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Ad = 1-adamantyl.

S-Arylation of Methanethiol with [(Azet-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (19)

Table S12. Computed energies for the *S*-arylation of methanethiol with [(Azet-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**19**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-2352.601896	0.740703	-2351.826627	0.09918	0.093127	-2351.925808	-2351.919754	-2352.813048
Int1	-2330.494307	0.778837	-2329.67881	0.103631	0.097037	-2329.782441	-2329.775846	-2330.696783
TS_{RE}	-2330.4761	0.776134	-2329.663303	0.103905	0.097233	-2329.767208	-2329.760536	-2330.676191
Int2	-2330.529197	0.777191	-2329.714829	0.106409	0.098732	-2329.821238	-2329.813561	-2330.732615
P_{Au}	-2121.141891	0.646267	-2120.465562	0.090261	0.084905	-2120.555823	-2120.550467	-2121.389007
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

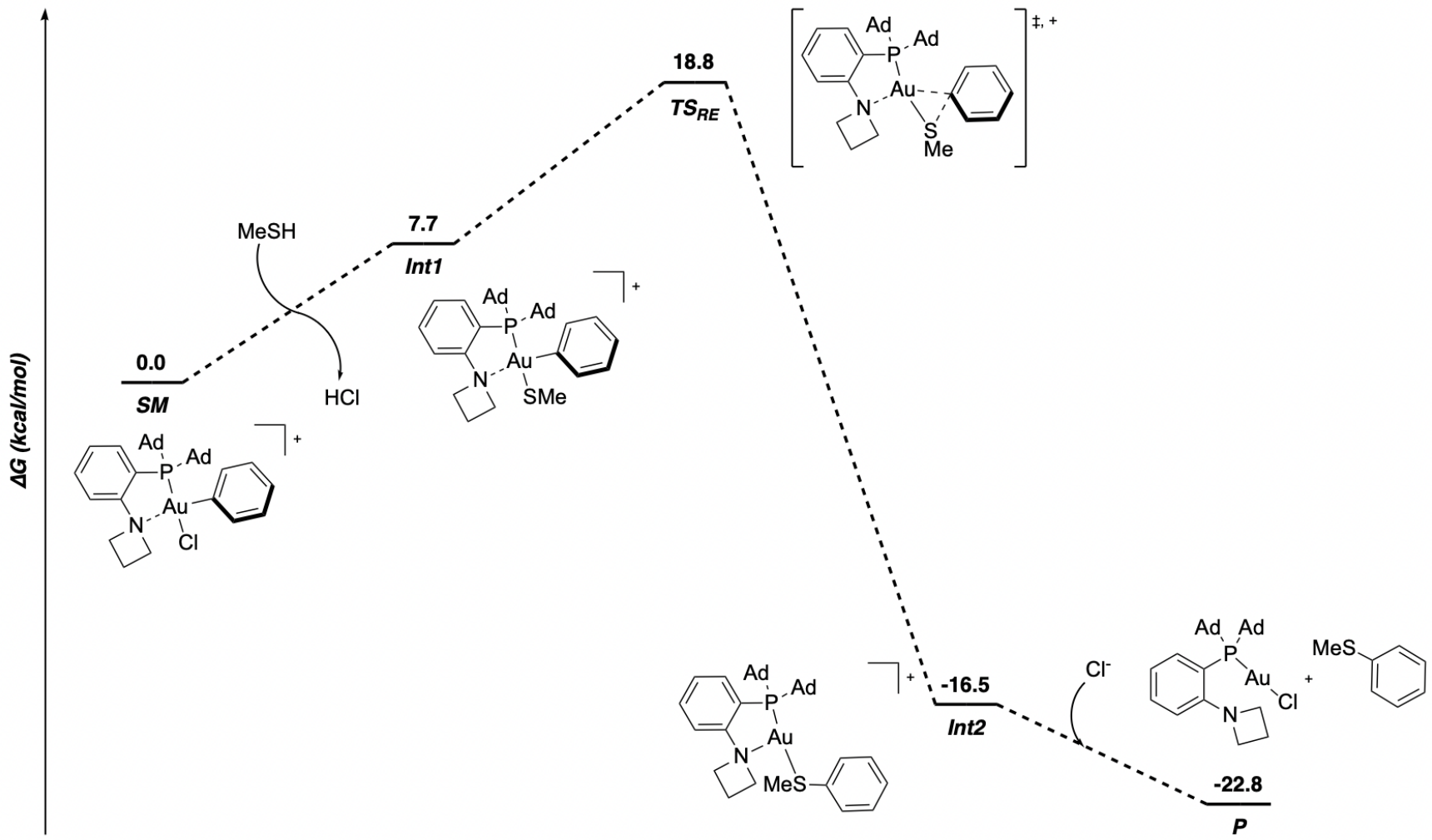


Figure S45. Free energy diagram for the *S*-arylation of methanethiol with [(Azet-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**19**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Ad = 1-adamantyl.

S-Arylation of Methanethiol with [(Azir-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (20)

Table S13. Computed energies for the *S*-arylation of methanethiol with [(Azir-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**20**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-2313.276355	0.71082	-2312.531948	0.096703	0.091029	-2312.628651	-2312.622977	-2313.49135
Int1	-2291.168561	0.74881	-2290.383936	0.101798	0.095284	-2290.485734	-2290.47922	-2291.375715
TS_{RE}	-2291.150745	0.746116	-2290.368837	0.102311	0.095695	-2290.471148	-2290.464532	-2291.354385
Int2	-2291.201845	0.747337	-2290.4181	0.106552	0.097789	-2290.524652	-2290.515889	-2291.408878
P_{Au}	-2081.817397	0.616939	-2081.171452	0.087579	0.082727	-2081.259031	-2081.25418	-2082.067238
P_{Ar}	-669.764534	0.126827	-669.629029	0.041756	0.040975	-669.670785	-669.670004	-669.732878
MeSH	-438.703471	0.045208	-438.653681	0.028847	0.028849	-438.682528	-438.68253	-438.71
HCl	-460.799434	0.00651	-460.789619	0.0212	0.0212	-460.810819	-460.810819	-460.817967
Chloride	-460.369422	0	-460.367061	0.017383	0.017383	-460.384445	-460.384445	-460.393994

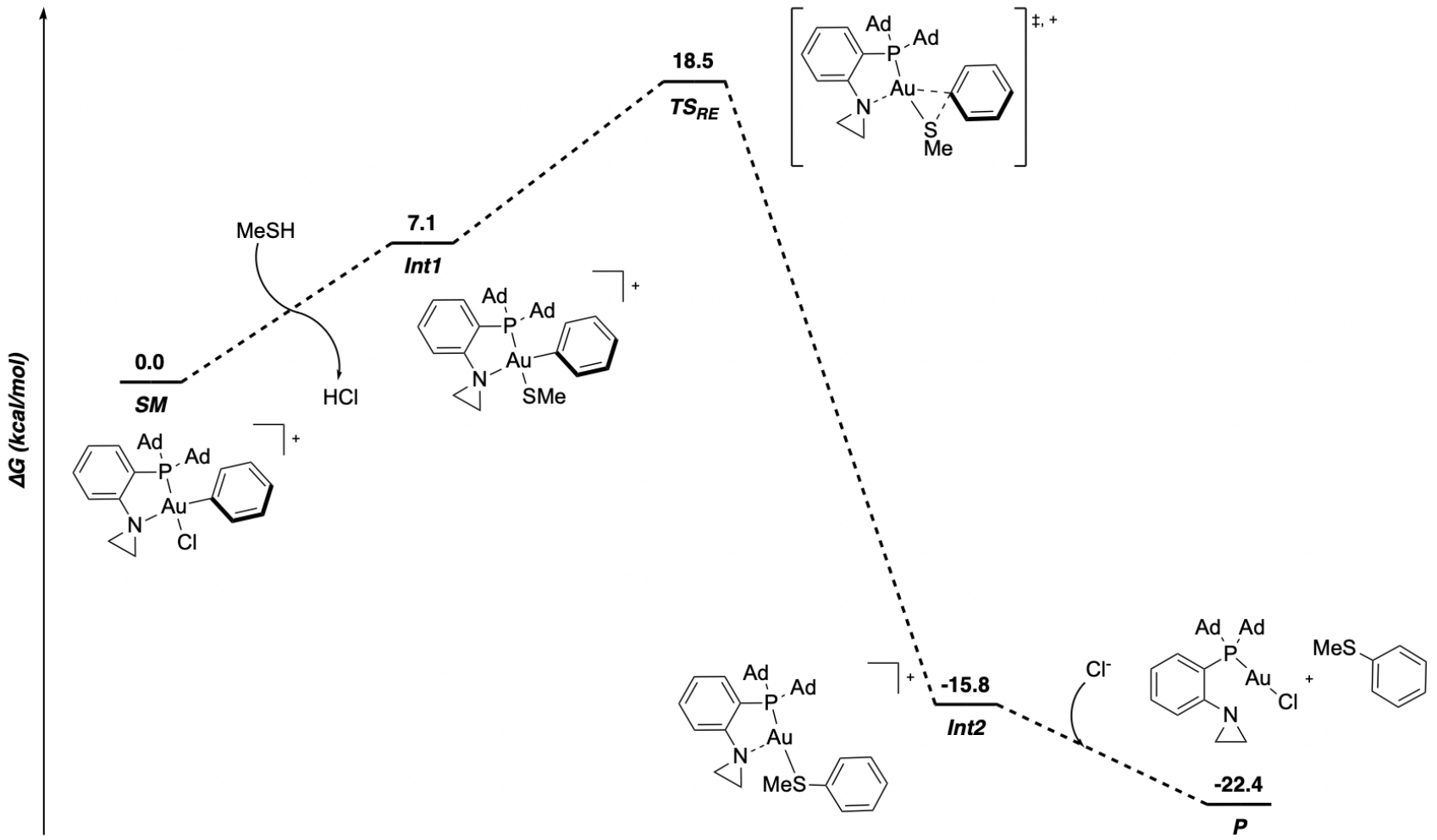


Figure S46. Free energy diagram for the *S*-arylation of methanethiol with [(Azir-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (**20**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in kcal/mol. Ad = 1-adamantyl.

Computed Energies – Buried Volume Only

[((PCy$_2$)Azet-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (36)

Table S14. Computed energies for [((PCy$_2$)Azet-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (**36**) calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory. All units are in Hartrees.

Structure	E	ZPE	H	T.S	T. qh-S	G(T)	qh-G(T)	SPE
SM	-2042.897613	0.593588	-2042.272603	0.093389	0.087785	-2042.365992	-2042.360388	-2043.132249

Buried Volume Summary

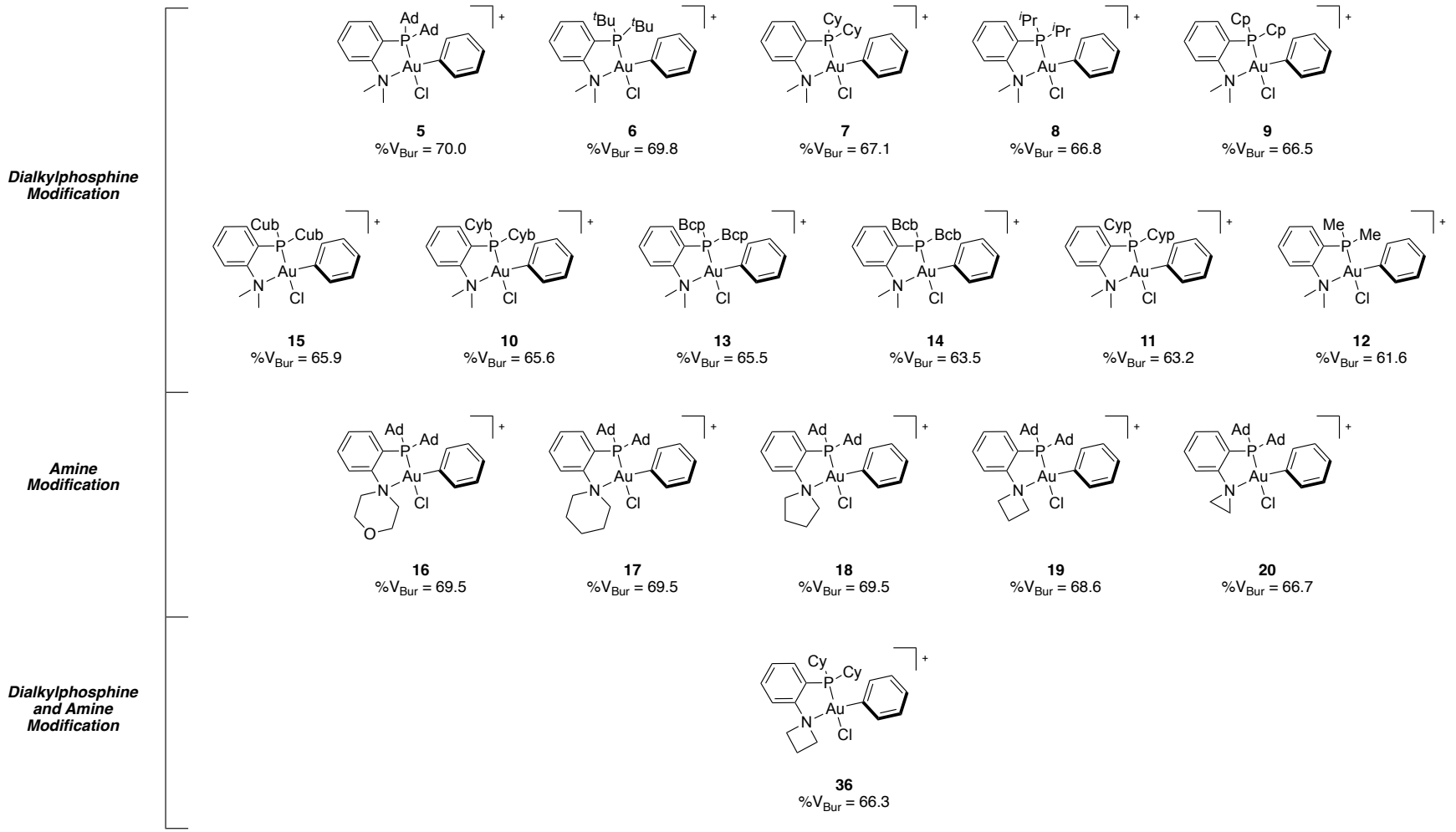
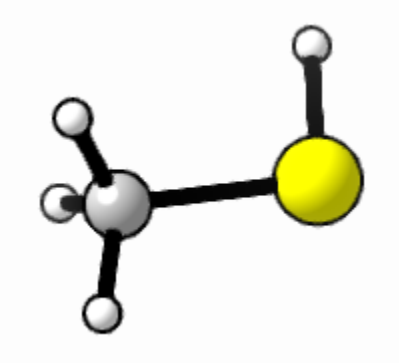


Figure S47. $\%V_{Bur}$ for each *P*,*N*-ligated Au(III) OAC in the manuscript calculated at the ωB97X-D/6-311+G(d,p), SDD, CPCM(Water)//B3LYP-D3/6-31G(d), LANL2DZ, CPCM(Water) level of theory.

Calculated Coordinates

S-Arylation of Methanethiol with Au^{III} Complexes

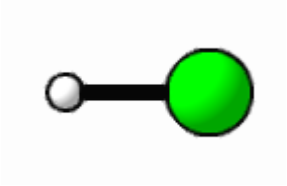
Miscellaneous



Methanethiol

Charge: 0 Multiplicity: 1
Negative Frequency: None

S	-0.04864700	-0.67229400	0.00000000
C	-0.04864700	1.16794100	0.00000000
H	-1.09633200	1.47711200	0.00000000
H	0.43868100	1.55915700	0.89538000
H	0.43868100	1.55915700	-0.89538000
H	1.28921200	-0.84636400	0.00000000



HCl

Charge: 0 Multiplicity: 1
Negative Frequency: None

Cl	0.00000000	0.00000000	0.07173300
H	0.00000000	0.00000000	-1.21945600

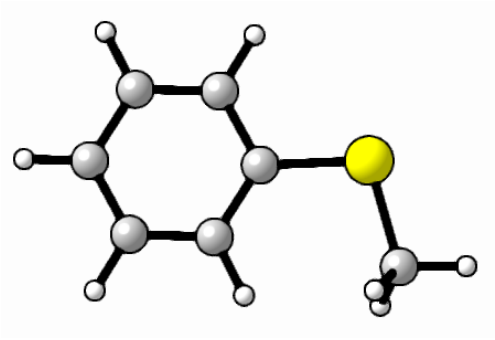
Chloride

Charge: -1 Multiplicity: 1
Negative Frequency: N/A

Cl	0.00000000	0.00000000	0.00000000

P_{Ar}

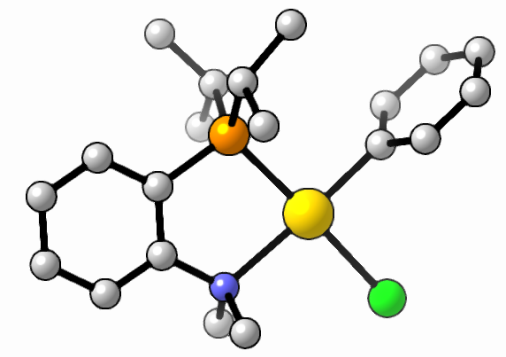
Charge: 0 Multiplicity: 1
Negative Frequency: None



C	0.10805800	-0.23358900	-0.00000900
C	-0.33154400	1.09729600	-0.00002100
C	-1.70104200	1.38012100	-0.00004000
C	-2.64226000	0.35062700	-0.00005100
C	-2.20304600	-0.97733800	-0.00004100
C	-0.84102200	-1.27096600	-0.00001600
S	1.82848600	-0.72307000	-0.00000300
C	2.73180600	0.86345100	0.00013200
H	2.50888300	1.44813300	-0.89605800
H	2.50854700	1.44816100	0.89622100
H	3.79230000	0.60067700	0.00033200
H	0.37585300	1.91865900	-0.00001900
H	-2.02631300	2.41711600	-0.00004600
H	-3.70444400	0.57727400	-0.00006600
H	-2.92345600	-1.79093400	-0.00004800
H	-0.51285200	-2.30758100	0.00000000

_S_-Arylation of Methanethiol with [((P^{i}Pr$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (8)

SM

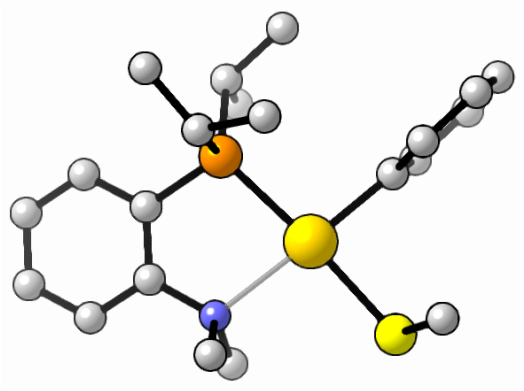


Charge: 1 Multiplicity: 1
Negative Frequency: None

P	0.55089300	1.24887000	-0.01623300
C	2.30041000	0.78000200	-0.17927800
C	2.68657200	-0.56886400	-0.12060300
C	4.04335400	-0.89816400	-0.19675400
C	5.00592700	0.09935800	-0.34249600
C	4.62525200	1.43962900	-0.42669300
C	3.27750100	1.77766400	-0.34754100
N	1.68479200	-1.64674500	-0.01858400
C	1.91248600	-2.47641500	1.20493200
Au	-0.46654600	-0.84645600	0.06874100
C	-2.34713300	-0.02321300	0.04206800
C	-2.88471100	0.56839800	1.18317200
C	-4.17148400	1.11839400	1.12306700
C	-4.90191000	1.07286000	-0.06545000
C	-4.35369200	0.46448900	-1.19770400
C	-3.06957500	-0.08910300	-1.15029100
C	1.73339300	-2.50236500	-1.24803100
H	4.35868200	-1.93437100	-0.15227500
H	6.05404700	-0.17622300	-0.40054700
H	5.37042600	2.21781800	-0.55415700
H	2.98950300	2.82027200	-0.42159200
H	1.87301600	-1.82893900	2.08178100
H	2.88276500	-2.98030400	1.16074500
H	1.11921500	-3.22196900	1.26366900
H	0.95449500	-3.26126900	-1.16913100
H	2.70930600	-2.98803800	-1.34378600
H	1.54815400	-1.87364400	-2.12049200
H	-2.65060300	-0.55804300	-2.03465600
H	-4.91863700	0.41976100	-2.12451500
H	-4.59356200	1.58241800	2.00992300
H	-2.33018600	0.60190900	2.11531100
H	-5.89631200	1.50712800	-0.10978100
Cl	-1.44497800	-3.07904600	0.22130700
C	0.29995200	2.17792100	1.57112100
H	-0.78369600	2.33973200	1.60031600
C	1.01305100	3.54176000	1.58023500
H	0.69936000	4.08560900	2.47735000
H	2.09912800	3.42128200	1.62903900
H	0.76556800	4.16135700	0.71359800

C	0.72114300	1.31714600	2.77289400
H	0.17712600	0.36865300	2.82630100
H	1.79348500	1.09650100	2.74250300
H	0.51688300	1.87277600	3.69374600
C	0.11893000	2.30844300	-1.47437300
H	0.92891200	3.04960400	-1.49925500
C	0.17743500	1.47159600	-2.76244300
H	1.13911100	0.96215900	-2.87887100
H	-0.61867300	0.72052900	-2.78054400
H	0.03828800	2.13405700	-3.62278900
C	-1.21950800	3.04509500	-1.30906600
H	-1.35322100	3.70797300	-2.17040000
H	-2.06127700	2.35003400	-1.28357600
H	-1.25080100	3.66343100	-0.40767600

Int1



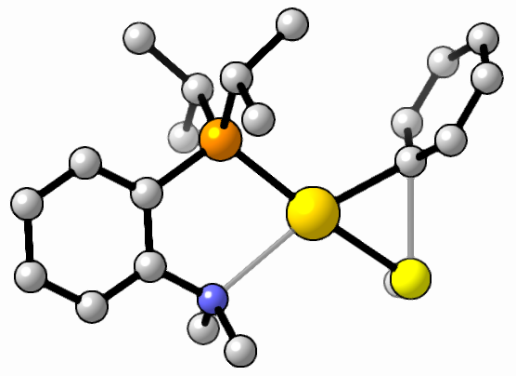
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.86650800	1.22719000	0.21312200
C	-2.51603800	0.58724300	-0.22709900
C	-2.73996500	-0.80003500	-0.22164500
C	-4.03859500	-1.28690000	-0.40658100
C	-5.09868000	-0.41057100	-0.63363900
C	-4.87461300	0.96608200	-0.68125200
C	-3.58992100	1.46017100	-0.47116200
N	-1.62877600	-1.75369400	-0.03146500
C	-1.59522000	-2.72931700	-1.16416300
Au	0.47362400	-0.73374200	-0.04841800
C	2.27715700	0.22113000	-0.29155400
C	3.01807400	0.67754500	0.79659600
C	4.20118600	1.39204900	0.57024600
C	4.63820500	1.63939800	-0.73214600
C	3.89881300	1.15602800	-1.81479400
C	2.71720500	0.43855000	-1.59915300
C	-1.75829600	-2.47114600	1.27189500
H	-4.23215200	-2.35323200	-0.38210700
H	-6.09755500	-0.80873700	-0.78150700
H	-5.69322900	1.65176100	-0.87450800
H	-3.42515700	2.53161000	-0.50439400
H	-1.48014000	-2.17647900	-2.09827700
H	-2.50954800	-3.32879800	-1.20073000
H	-0.74478100	-3.39590800	-1.02047100
H	-0.89889900	-3.13574700	1.38008800

H	-2.68498200	-3.05439100	1.30713500
H	-1.75529600	-1.73962700	2.08212400
H	2.15590000	0.05946800	-2.44707700
H	4.23714300	1.33130700	-2.83232100
H	4.77297900	1.75600600	1.41941900
H	2.69057000	0.49257300	1.81225500
H	5.55277600	2.19960700	-0.90358300
S	1.70000700	-2.82284500	-0.10786500
C	2.71108600	-2.70803600	1.42609900
H	3.20898700	-3.67413100	1.55052400
H	3.46631100	-1.92426100	1.33710800
H	2.08137400	-2.51384000	2.29752600
C	-1.04303300	1.73363100	2.00887000
H	-1.69021500	0.94152900	2.40538800
C	-0.53152500	2.69692300	-0.86966800
H	-1.37520800	3.37647600	-0.69599700
C	-1.77114800	3.07804100	2.16829800
H	-2.74798300	3.08232200	1.67621800
H	-1.93929300	3.25981700	3.23540300
H	-1.17976300	3.91213100	1.77864600
C	0.28601700	1.68717300	2.77634800
H	1.03619700	2.36441100	2.35802800
H	0.10628900	1.98621400	3.81473100
H	0.69911000	0.67437500	2.78756500
C	-0.53406600	2.26182500	-2.34397600
H	0.29572400	1.57971400	-2.55208100
H	-1.46911900	1.76854900	-2.62661200
H	-0.41172200	3.14664900	-2.97779200
C	0.76657700	3.42836200	-0.48710000
H	1.64425100	2.79537600	-0.63439800
H	0.87039300	4.30804100	-1.13155600
H	0.76039200	3.77747300	0.54896500

TS_{RE}

Charge: 1 Multiplicity: 1
Negative Frequency: -272.08

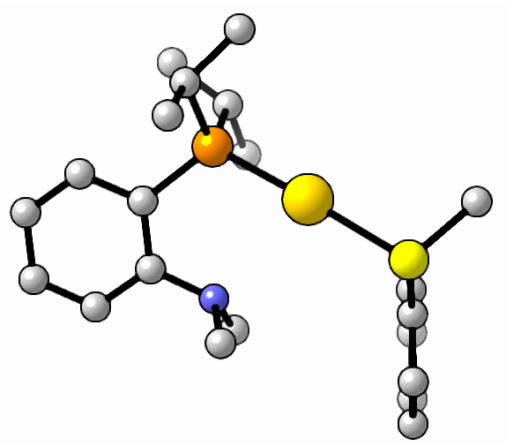


C	-3.13470900	0.40032300	1.09669900
C	-2.70073300	-0.08655300	-0.13913900
C	-3.21981300	0.40023900	-1.34472500
C	-4.17414500	1.41752500	-1.30098500
C	-4.61402100	1.93050000	-0.07494100
C	-4.09408600	1.41954600	1.11578600
Au	-0.55821300	-0.62604500	-0.15872400

S	-2.23402400	-2.34624900	-0.28276200
P	0.93208200	1.18204300	0.10832200
C	2.62584700	0.53004800	-0.07977000
C	2.85279400	-0.85960500	-0.17442600
C	4.16570200	-1.33144900	-0.29948300
C	5.24264900	-0.44789600	-0.34527200
C	5.02144200	0.92899000	-0.27237100
C	3.72130800	1.41054000	-0.14097200
N	1.74596300	-1.80299600	-0.15440100
C	1.73903200	-2.63113700	1.06861300
C	1.69523300	-2.63576400	-1.37371000
H	4.34714700	-2.39944400	-0.36428100
H	6.25219500	-0.83564400	-0.44339100
H	5.85409000	1.62392100	-0.31838400
H	3.55907400	2.48219000	-0.09457300
H	1.72797200	-1.97972500	1.94488300
H	2.61303300	-3.29577700	1.12359600
H	0.83004200	-3.24007500	1.07022700
H	0.76960700	-3.21885900	-1.35436000
H	2.54591700	-3.32723800	-1.44755100
H	1.68250800	-1.98287500	-2.24966200
H	-2.71598300	0.02526300	2.02410500
H	-4.42227800	1.81573100	2.07283800
H	-4.57632800	1.80525200	-2.23293100
H	-2.88321500	-0.00346200	-2.29380000
H	-5.35921500	2.71969900	-0.05049700
C	-2.50704200	-2.79609300	1.47641200
H	-2.72163200	-3.86808200	1.48593400
H	-1.62561500	-2.59734200	2.08729800
H	-3.36983900	-2.24970700	1.86657700
C	0.71875700	2.53926400	-1.13916000
H	1.53809300	3.25292700	-0.99029100
C	-0.62447100	3.25322500	-0.91407700
H	-1.46271300	2.55125800	-0.98182200
H	-0.67059600	3.75574500	0.05714500
H	-0.75987900	4.01593500	-1.68892600
C	0.81896900	1.94676000	-2.55403500
H	1.77128700	1.43100800	-2.71544100
H	0.00556700	1.23444100	-2.73704400
H	0.73855500	2.75153300	-3.29306900
C	0.76275400	1.90618900	1.81737300
H	-0.28717700	2.22517500	1.84295300
C	0.95911700	0.80686300	2.87361400
H	0.79537900	1.22740400	3.87180000
H	0.25463100	-0.02086500	2.73630000
H	1.97831600	0.40475900	2.84275200

C	1.66908900	3.11693400	2.08035300
H	1.42441300	3.54179100	3.06036700
H	2.72397000	2.82477600	2.09991700
H	1.54087900	3.90748300	1.33399800

Int2



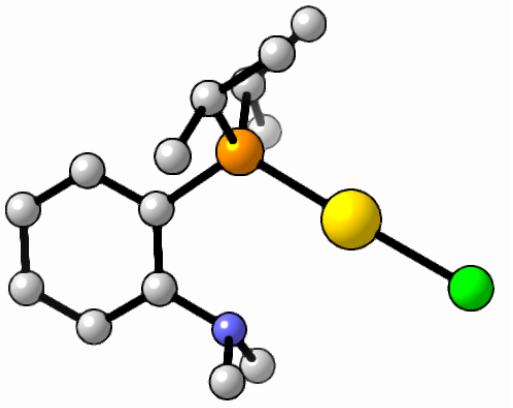
Charge: 1 Multiplicity: 1
Negative Frequency: None

C	-1.95573000	0.73951700	-2.18249300
C	-1.06453100	-0.32508500	-2.84144800
C	-3.39784700	0.66892900	-2.70290900
P	-1.81781600	0.62157300	-0.32224400
C	-2.45486900	-1.03334300	0.14304100
C	-1.59513600	-2.10514600	0.47027600
C	-2.15096200	-3.35622700	0.77431800
C	-3.52930400	-3.55885600	0.75825900
C	-4.38226500	-2.49951500	0.44245500
C	-3.84640400	-1.25003600	0.13892700
N	-0.16817000	-1.91605200	0.51323700
C	0.57179700	-2.76369100	-0.42618300
Au	0.37562900	1.01531400	0.31595900
C	3.45225400	-0.09308700	0.06371900
C	3.26991600	-0.28581000	-1.31145000
C	3.82027400	-1.41265500	-1.92151200
C	4.52632500	-2.35138300	-1.16136500
C	4.69082000	-2.15845200	0.21150900
C	4.16017800	-1.02275500	0.83097900
C	-2.98167400	1.86870200	0.41915200
C	-2.60536400	3.28208000	-0.05297700
C	-2.95504500	1.75616400	1.95155000
C	0.36621600	-2.01298900	1.87760300
H	-1.48872600	-4.17833500	1.02880600
H	-3.93583300	-4.53781800	0.99527100
H	-5.45850400	-2.64186800	0.43155900
H	-4.52500900	-0.43938900	-0.10272000
H	-1.44038400	-1.33299400	-2.63313500
H	-1.06996900	-0.18355500	-3.92776700
H	0.16871900	-2.63362900	-1.43320200
H	0.53427900	-3.83589800	-0.16902900
H	1.61824200	-2.44753300	-0.43164700
H	-3.85096600	-0.30422400	-2.48676400
H	-4.03535600	1.45121200	-2.27879000
H	-1.57953300	3.53396300	0.24232300

H	-2.68888300	3.39548000	-1.13852600
H	-0.15635300	-1.30174400	2.52414100
H	1.42792800	-1.74666200	1.85620900
H	0.26903400	-3.02331100	2.30945100
H	-3.24255100	0.75688500	2.29355600
H	-1.95448100	1.97908500	2.34139900
S	2.71961900	1.31583500	0.92359200
C	3.30536700	2.74380700	-0.07051100
H	2.98101300	2.65303300	-1.10705200
H	2.86166100	3.63353400	0.38094900
H	4.39388500	2.78645000	-0.00236600
H	2.69239900	0.42292100	-1.89621700
H	4.29570600	-0.86403600	1.89629200
H	3.68141900	-1.56520300	-2.98750700
H	4.94268400	-3.23289200	-1.63944500
H	5.23653800	-2.88561900	0.80500400
H	-3.39281300	0.79904300	-3.79107600
H	-0.02741100	-0.26518900	-2.49420100
H	-3.65684200	2.47848200	2.38300800
H	-3.28040700	4.00984700	0.41087700
H	-3.99069300	1.63560000	0.06105000
H	-1.53708900	1.72892100	-2.40336700

P_{Au}

Charge: 0 Multiplicity: 1
Negative Frequency: None

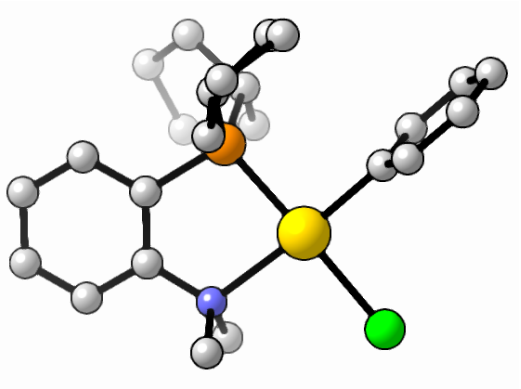


Au	-1.44693100	-0.17256600	-0.00860500
C	2.09735200	-1.26053200	-0.00247500
C	2.04707900	0.14766400	-0.00440600
C	3.34721500	-1.89886800	0.00143100
C	3.25060900	0.87787200	-0.00804100
C	4.53147300	-1.16556800	0.00170500
H	3.38333100	-2.98438100	0.00141400
C	4.48384900	0.23114700	-0.00556500
H	3.22890300	1.96395700	-0.01591900
H	5.48803400	-1.68036000	0.00478900
H	5.40021000	0.81361800	-0.00867600
C	0.71302900	-2.87678200	1.16911900
H	-0.30322700	-3.28516400	1.16139800
H	1.42434400	-3.71930200	1.21742300
H	0.83153500	-2.26750700	2.06984600
C	0.67154100	-2.74923800	-1.26963100
H	1.40019200	-3.56121500	-1.43769100

H	-0.33467500	-3.18144100	-1.26179400
H	0.73574300	-2.04380300	-2.10340800
N	0.88531800	-2.03122000	-0.01210800
P	0.47254700	1.09246200	0.02018200
C	0.58482600	2.21955200	-1.46948700
C	0.97784700	1.39080800	-2.70569500
C	-0.73901200	2.95699800	-1.73138000
H	1.96141200	0.92565300	-2.60062300
H	1.00055000	2.04218500	-3.58652600
H	-1.06547200	3.56807600	-0.88790500
H	-1.53812300	2.24219200	-1.96043100
C	0.62510300	2.08199400	1.59876100
C	-0.51374800	3.09511300	1.77942000
C	0.68387800	1.10123500	2.78351800
H	-1.49362700	2.61057800	1.68914100
H	-0.46009500	3.91090300	1.05430200
H	1.50548400	0.38464600	2.68705000
H	-0.25369400	0.53855000	2.86996900
Cl	-3.49502200	-1.45344400	-0.03162100
H	-0.61630300	3.61783200	-2.59719500
H	0.24032400	0.59969100	-2.89215200
H	0.83028200	1.66213900	3.71335700
H	-0.44788200	3.53832600	2.77969400
H	1.57957200	2.61887800	1.53269000
H	1.37442800	2.95042200	-1.25302900

_S_-Arylation of Methanethiol with [((PCp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (9)

SM



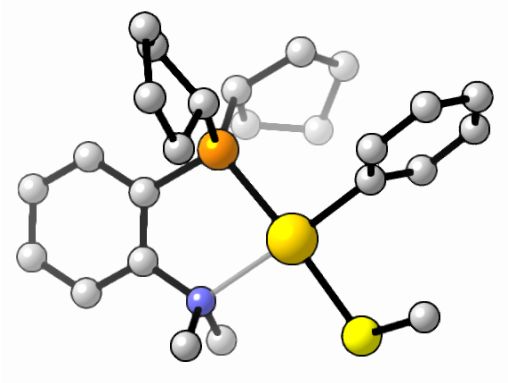
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	0.53099900	0.98238700	-0.01312600
C	2.22328100	0.49694800	-0.46797600
C	2.57392600	-0.85914300	-0.56469800
C	3.89569100	-1.20565100	-0.86213700
C	4.85529200	-0.21737100	-1.07463400
C	4.50435800	1.13234700	-1.00735900
C	3.19271500	1.48657300	-0.70827700
N	1.56986200	-1.92485200	-0.38403100
Au	-0.51882800	-1.09567400	0.07111200
C	-2.33801900	-0.22593500	0.45346200
C	-3.25719200	-0.11110500	-0.58930500
C	-4.50135700	0.47720600	-0.33642300
C	-4.81439100	0.94277100	0.94310400
C	-3.88812300	0.80908400	1.97948000
C	-2.63994400	0.22143200	1.73916500
H	4.18451800	-2.24777400	-0.93699900
H	5.87608800	-0.50634200	-1.30331600
H	5.24509700	1.90472800	-1.18573200
H	2.92749300	2.53642200	-0.65755300
H	-1.92560700	0.12023600	2.55007500
H	-4.12682000	1.16234700	2.97861600
H	-5.21907300	0.57330000	-1.14625300
H	-3.01914200	-0.46520100	-1.58700100
H	-5.77823800	1.40618600	1.13189700
Cl	-1.54546400	-3.31161800	0.17172400
C	1.42681600	-2.71075600	-1.65108000
H	1.13442400	-2.02896400	-2.45173300
H	2.36751400	-3.20563400	-1.91128200
H	0.64912200	-3.46054700	-1.50389600
C	1.94267500	-2.81963800	0.75529000
H	1.14862200	-3.55548400	0.88596700
H	2.88754500	-3.33438100	0.55574700
H	2.03701500	-2.21692200	1.65970100
C	-0.07806200	2.11714100	-1.31706200
C	-0.29274300	1.42551300	-2.68347700
C	-1.40817900	2.86762400	-0.99803800
H	0.72597400	2.85491900	-1.43210300
C	-1.17514400	2.44484300	-3.42015100
H	-0.83830500	0.48189500	-2.55735000

H	0.65051500	1.20152600	-3.18981100
C	-2.18278400	2.89655000	-2.34555500
H	-1.18231100	3.87089800	-0.62702000
H	-2.00004900	2.36578600	-0.22911400
H	-0.55997700	3.29121100	-3.75072600
H	-1.65793800	2.01770600	-4.30458500
H	-2.60519400	3.88394500	-2.55338500
H	-3.01504300	2.18647500	-2.29927900
C	0.45916300	1.83630900	1.62437100
C	0.95568400	0.96682800	2.80282300
C	1.33123800	3.12122500	1.71710700
H	-0.60587800	2.07021700	1.71682100
C	2.46991000	1.22983000	2.86866800
H	0.70246200	-0.09481600	2.71505700
H	0.46500200	1.33991800	3.70953900
C	2.64185800	2.71133800	2.44942700
H	0.76940600	3.84755800	2.31219200
H	1.51215500	3.60154100	0.75109400
H	2.87374300	1.02555200	3.86448200
H	2.99553000	0.57297000	2.16760800
H	2.78789700	3.34974100	3.32587100
H	3.51973800	2.84110900	1.81004800

Int1

Charge: 1 Multiplicity: 1
Negative Frequency: None

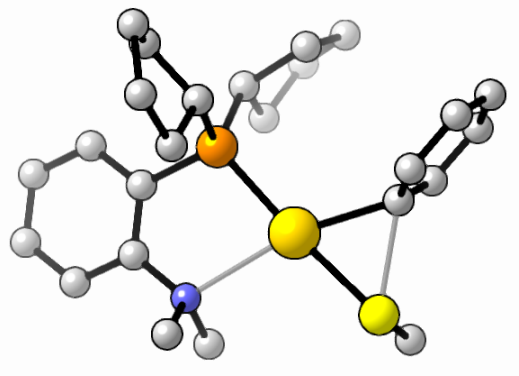


P	0.89629700	0.92534400	0.30545300
C	2.51902200	0.10416000	0.35741400
C	2.61771900	-1.27762100	0.12804500
C	3.87345800	-1.89395500	0.17329800
C	5.01756700	-1.15088700	0.45706500
C	4.92263900	0.21897500	0.70896500
C	3.67826900	0.83999100	0.66265500
N	1.42274500	-2.10117800	-0.15430000
Au	-0.56099300	-0.90124100	-0.13348200
C	-2.26464500	0.24361000	-0.14301100
C	-2.51999700	1.06892700	-1.23900200
C	-3.67299900	1.86323900	-1.24856200
C	-4.56296700	1.82481300	-0.17393400
C	-4.30658300	0.97970300	0.90910500
C	-3.15786700	0.18178200	0.92747000
H	3.96867400	-2.95849300	-0.00805700
H	5.98186200	-1.64814800	0.48889100

H	5.80913900	0.79926400	0.94333300
H	3.60857500	1.90081400	0.87604300
H	-2.97547800	-0.48012200	1.76625300
H	-4.99960500	0.93405300	1.74469600
H	-3.86771600	2.50901800	-2.10028900
H	-1.84345900	1.09883500	-2.08687100
H	-5.45498300	2.44434400	-0.18228800
S	-1.91163700	-2.86470600	-0.59222300
C	-3.36934800	-2.31455700	-1.57187900
H	-3.86266400	-3.22357800	-1.92821600
H	-4.06593900	-1.74192300	-0.95702400
H	-3.06118100	-1.71294300	-2.42924400
C	1.53625000	-2.70915200	-1.51758700
H	1.62619000	-1.90518000	-2.25042500
H	2.40928100	-3.36619200	-1.58103100
H	0.63019900	-3.28165300	-1.71722800
C	1.27180700	-3.16233000	0.88911300
H	0.37993600	-3.74918200	0.66511000
H	2.13873100	-3.82983600	0.90391600
H	1.15958300	-2.68314000	1.86308200
C	0.84335200	2.12728800	-1.08458100
C	1.79347300	3.34003300	-1.03380100
C	1.14752900	1.48781700	-2.45847700
H	-0.19082100	2.49527300	-1.07384900
C	1.62621300	3.92732000	-2.44890400
H	2.82720700	3.00644100	-0.89029500
H	1.54645400	4.04851000	-0.23766400
C	1.44692700	2.69939700	-3.38614200
H	0.32693400	0.86006700	-2.81894000
H	2.03268400	0.84624500	-2.37667500
H	0.72877100	4.55595600	-2.47439100
H	2.47443000	4.55711300	-2.73357100
H	0.62831300	2.86398700	-4.09308000
H	2.34904600	2.51160600	-3.97604400
C	0.71658600	1.84958600	1.89192800
C	-0.66933400	2.56535700	2.00654700
C	0.81996500	0.91031700	3.12542700
H	1.53686600	2.57512600	1.88329400
C	-1.32135700	2.00190400	3.29334600
H	-1.30592400	2.35644900	1.14250400
H	-0.53719800	3.64988300	2.04705900
C	-0.63726400	0.64523100	3.52420600
H	1.33652800	1.45335000	3.92493400
H	1.39375900	-0.00252700	2.93599200
H	-1.11028300	2.66548100	4.14039600
H	-2.40806800	1.92147200	3.19554100

H	-0.73196000	0.28533300	4.55360900
H	-1.06738600	-0.12000200	2.86721000

TS_{RE}



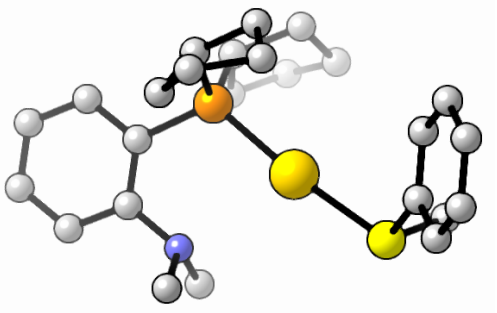
Charge: 1 Multiplicity: 1
Negative Frequency: -270.30

C	-3.35057400	-0.11918500	-0.76438200
C	-2.72255900	0.16777700	0.45007600
C	-2.99836900	-0.56381500	1.61168500
C	-3.90388500	-1.62304800	1.53624700
C	-4.54033500	-1.93341900	0.32845700
C	-4.26425700	-1.17851100	-0.81284100
Au	-0.62836200	0.84974100	0.26780300
S	-2.35233200	2.41500100	0.86661400
P	0.95655900	-0.83101100	-0.19105600
C	2.52567600	-0.00915900	-0.62375100
C	2.67415600	1.38403000	-0.45651800
C	3.89798300	1.98500800	-0.77745200
C	4.95934500	1.22800800	-1.27066700
C	4.80963400	-0.14770300	-1.45880000
C	3.59994000	-0.75827400	-1.13704400
N	1.57351200	2.20161200	0.02952300
H	4.02076900	3.05487900	-0.64279700
H	5.89945500	1.71436400	-1.51324500
H	5.62787000	-0.74174100	-1.85375300
H	3.48945700	-1.82614700	-1.29497500
H	-3.11649800	0.44096700	-1.66260500
H	-4.74830400	-1.41326300	-1.75680000
H	-4.11438100	-2.20286400	2.43074700
H	-2.51243000	-0.31529200	2.54936900
H	-5.24851000	-2.75492800	0.28101500
C	-2.91676700	3.10513000	-0.73813000
H	-3.13652600	4.16032300	-0.55494500
H	-2.14691400	3.02415600	-1.50656700
H	-3.82885500	2.59524400	-1.05906200
C	1.84140400	2.76887700	1.36617300
H	2.08123700	1.96001200	2.05939000
H	2.67097800	3.49020700	1.35170300
H	0.93627800	3.27440000	1.71579800
C	1.18572000	3.25002500	-0.93682900
H	0.28414800	3.74537000	-0.56400600
H	1.96980900	4.00727400	-1.07529800
H	0.96058700	2.78239700	-1.89838500

C	1.22215500	-1.88172800	1.30100100
C	2.27666000	-3.00090900	1.23072800
C	1.63922000	-1.07901800	2.55153500
H	0.23435800	-2.33072700	1.47559300
C	2.37262000	-3.44906100	2.70328500
H	3.23771200	-2.58808100	0.90215800
H	2.00271900	-3.81121600	0.54770900
C	2.15665000	-2.15676900	3.54434600
H	0.81579200	-0.47756400	2.94965300
H	2.45277200	-0.39186500	2.28865400
H	1.57705600	-4.17292700	2.91397800
H	3.32552500	-3.94111300	2.92140500
H	1.43109700	-2.33120400	4.34491000
H	3.08516500	-1.82614200	4.01982900
C	0.50549100	-1.95003100	-1.57439400
C	-0.77659700	-2.77704700	-1.26850600
C	0.18853900	-1.20236800	-2.88540800
H	1.34749100	-2.63125100	-1.74704900
C	-1.50069800	-2.93035700	-2.63936900
H	-1.42574000	-2.25086700	-0.55996100
H	-0.51698700	-3.73885200	-0.81684800
C	-0.57988000	-2.26522700	-3.68614300
H	1.08746600	-0.83240000	-3.38821200
H	-0.46175700	-0.34080900	-2.67868600
H	-1.70746400	-3.97787600	-2.87895000
H	-2.46268400	-2.40992300	-2.60138800
H	0.13001800	-2.99736500	-4.09149100
H	-1.13337200	-1.84020800	-4.52976000

Int2

Charge: 1 Multiplicity: 1
Negative Frequency: None

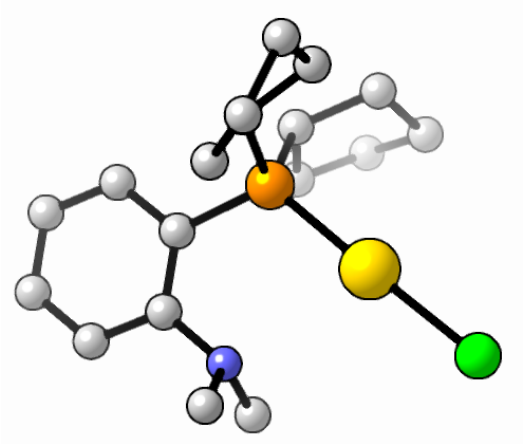


C	-3.71733600	-0.01750200	0.70411600
C	-3.70982500	-0.13302400	-0.69199200
C	-4.65865900	0.53449800	-1.47190500
C	-5.62281400	1.32926200	-0.84475400
C	-5.63962900	1.44645100	0.54648400
C	-4.68979700	0.77010800	1.31930800
Au	-0.40736200	-0.47448600	-0.38973700
S	-2.45887000	-1.11577900	-1.54540900
P	1.37400400	0.21386900	0.91538400
C	2.89554500	0.64930600	-0.00542100
C	2.98425100	0.57890600	-1.41022800

C	4.18850600	0.93713900	-2.03461600
C	5.28784300	1.35906700	-1.28989200
C	5.20070700	1.42921600	0.10331600
C	4.01199200	1.07605300	0.73682200
N	1.85632600	0.14448100	-2.19085300
H	4.25815600	0.88207100	-3.11706400
H	6.21044200	1.63214500	-1.79406800
H	6.05204200	1.75669300	0.69232700
H	3.95458500	1.13499600	1.82024600
H	-2.96499900	-0.52447700	1.30015000
H	-4.69600200	0.86488700	2.40099500
H	-6.35977800	1.85221400	-1.44681200
H	-4.64589800	0.43589600	-2.55292600
H	-6.38977500	2.06536500	1.02973000
C	-2.80187600	-2.80376100	-0.90462500
H	-3.78964900	-3.11072500	-1.25339000
H	-2.03139500	-3.45737300	-1.31893300
H	-2.75123000	-2.81125300	0.18455600
C	1.33220900	1.18013400	-3.08446900
H	1.13183700	2.08868300	-2.50939100
H	2.01690000	1.43262300	-3.91194200
H	0.38756200	0.82829200	-3.51239800
C	2.08371500	-1.13082600	-2.87513400
H	1.13850800	-1.46698300	-3.31428400
H	2.83871600	-1.06736400	-3.67723700
H	2.41044900	-1.87989500	-2.14805800
C	1.90511600	-1.10955600	2.09327800
C	0.71175000	-1.78822500	2.84129700
C	2.62471200	-2.25764000	1.31667500
H	2.58909800	-0.64384600	2.81028800
C	0.62643300	-3.20774200	2.25257900
H	-0.23263500	-1.24772100	2.73845200
H	0.94403600	-1.83279300	3.91074300
C	2.08958900	-3.55441200	1.94656400
H	3.71242700	-2.15688400	1.36036200
H	2.34145500	-2.23775200	0.25589100
H	0.13880300	-3.91481700	2.93162000
H	0.04866800	-3.18784900	1.31786700
H	2.62522700	-3.77387400	2.87938600
H	2.20439000	-4.41834800	1.28352000
C	0.93939800	1.75506700	1.84410200
C	0.87181100	2.96752800	0.86273400
C	-0.46156100	1.69449900	2.53700400
H	1.72708100	1.91003700	2.58893700
C	-0.35090000	3.77756400	1.32431900
H	0.69654200	2.61837800	-0.16355800

H	1.80613300	3.53512100	0.85425000
C	-1.34027000	2.68643300	1.75359000
H	-0.35561200	2.01733600	3.57823200
H	-0.89862700	0.69287500	2.55366500
H	-0.08782600	4.40616400	2.18514500
H	-0.73821600	4.43291900	0.53704300
H	-2.18146800	3.05973900	2.34681000
H	-1.75624300	2.19168900	0.86591000

P_{Au}



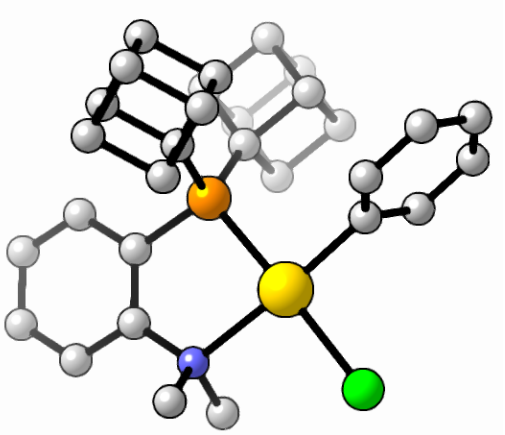
Charge: 0 Multiplicity: 1
Negative Frequency: None

Au	-1.28915600	-0.62665500	-0.23159300
P	0.40253900	0.83710300	0.29063100
C	2.10476500	0.15665600	0.20702900
C	2.39134300	-1.14766200	-0.24299900
C	3.72642200	-1.57821300	-0.28319300
C	4.76643600	-0.73954000	0.11109400
C	4.48454500	0.55429000	0.55799800
C	3.16413600	0.99413900	0.60392500
N	1.32960600	-2.02541900	-0.65183100
H	3.94459800	-2.58459100	-0.62862600
H	5.79283200	-1.09307100	0.07114000
H	5.28691800	1.21662400	0.86879400
H	2.95987000	2.00183600	0.95437500
Cl	-3.10756400	-2.12184000	-0.77298000
C	1.38950600	-2.40214600	-2.06420900
H	1.47315500	-1.50002000	-2.67709400
H	2.23434500	-3.06984300	-2.30677500
H	0.45865200	-2.91440800	-2.33039900
C	1.15491100	-3.17413600	0.23835900
H	0.23836600	-3.70252600	-0.04461900
H	1.99558400	-3.88844900	0.20158800
H	1.04240800	-2.82020500	1.26751600
C	0.45650300	2.28032200	-0.85736500
C	0.75800400	1.83961300	-2.32294800
C	-0.84948700	3.09780800	-0.94557400
H	1.25920300	2.93760100	-0.50098300
C	-0.11930000	2.75569700	-3.22331400
H	0.49808700	0.78647600	-2.48223900
H	1.82610300	1.93872800	-2.53551900
C	-0.68777000	3.83632600	-2.28324200

H	-0.98984900	3.76455400	-0.08944900
H	-1.71558600	2.42351800	-0.99625100
H	0.44653400	3.17986100	-4.05859800
H	-0.94284000	2.17264300	-3.65176500
H	0.03167200	4.65697900	-2.16457700
H	-1.62662800	4.26798700	-2.64581800
C	0.24284500	1.47341200	2.01897500
C	-1.20875200	1.95048600	2.35006900
C	0.56689000	0.34626700	3.04727400
H	0.94772600	2.30422100	2.12599500
C	-1.74281100	0.92611000	3.36802500
H	-1.85182000	2.02403400	1.46810500
H	-1.16118100	2.94793000	2.80044600
C	-0.49020600	0.51096500	4.15200000
H	1.59807900	0.40740700	3.40560700
H	0.44455300	-0.64148100	2.58215600
H	-2.54018800	1.33541100	3.99702400
H	-2.14852600	0.05447600	2.83624900
H	-0.19661300	1.31305600	4.84193500
H	-0.62677800	-0.40268000	4.74022600

_S_-Arylation of Methanethiol with [((PCubane$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (15)

SM



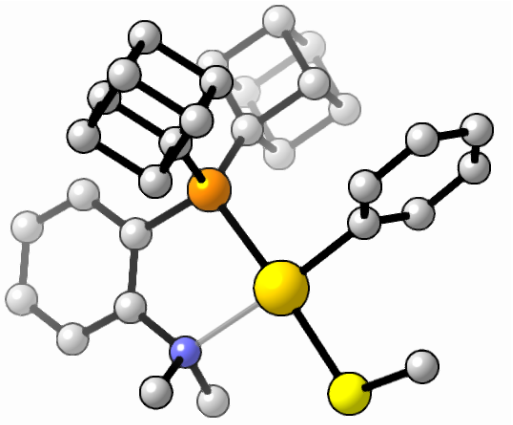
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	0.32741200	-0.79624000	-0.08381000
C	2.10089700	-0.95125700	-0.46276600
C	2.93837900	0.17557800	-0.44589000
C	4.30708300	0.01625500	-0.68357200
C	4.83662600	-1.24506100	-0.95207500
C	4.00456000	-2.36518800	-0.99002100
C	2.64290000	-2.21791100	-0.74278600
N	2.40008700	1.52530100	-0.19351600
Au	0.12221100	1.52110200	0.05883300
C	-1.91477300	1.36456800	0.20717500
C	-2.68682700	1.62190100	-0.92561900
C	-4.07877600	1.51085700	-0.83863400
C	-4.68282200	1.14167700	0.36606500
C	-3.89648100	0.89736700	1.49443200
C	-2.50288600	1.01058400	1.41974400
H	4.96880000	0.87477500	-0.66582000
H	5.90123100	-1.34767200	-1.13648600
H	4.41099700	-3.34733400	-1.20781600
H	2.00054700	-3.08914800	-0.77273100
H	-1.89631900	0.82443100	2.29850700
H	-4.35860400	0.61414900	2.43595500
H	-4.68490800	1.70530800	-1.71903200
H	-2.22176300	1.89483000	-1.86723500
H	-5.76305800	1.04612800	0.42532900
Cl	-0.01304900	3.96148600	0.28648800
C	2.97339100	2.09485900	1.06481600
H	2.73723300	1.42291600	1.89164200
H	4.05879900	2.21084700	0.98301100
H	2.51384600	3.06845800	1.24012600
C	2.68563700	2.41975600	-1.35982200
H	2.22946100	3.39086300	-1.16770200
H	3.76309500	2.54522800	-1.50300400
H	2.24413200	1.97609700	-2.25406400
C	-0.63765800	-1.51249300	-1.41779700
C	-0.59960100	-0.94617800	-2.88807200
C	-0.55481200	-2.99008900	-1.99505900
C	-2.21508300	-1.58588100	-1.49466000
H	0.01895700	-0.10179700	-3.19451100
C	-0.50633400	-2.40705400	-3.44714900

C	-2.16348900	-1.01404000	-2.95148900
C	-2.11615500	-3.04306500	-2.05720900
H	0.07973500	-3.78481700	-1.60534100
H	-2.89074000	-1.24868400	-0.71119600
C	-2.07506800	-2.47541500	-3.52156100
H	0.18797900	-2.73196400	-4.22190500
H	-2.80750600	-0.21931400	-3.32592900
H	-2.71759500	-3.88268800	-1.70921500
H	-2.64974600	-2.86010100	-4.36413800
C	0.00771500	-1.60897600	1.49370500
C	-1.39404600	-2.07092600	2.05906500
C	0.64071100	-2.98389200	1.97378600
C	0.35781800	-0.97651100	2.89556600
H	-2.34095200	-1.95960500	1.53449900
C	-0.75770200	-3.42567900	2.51779100
C	-1.03875600	-1.43094800	3.44491100
C	0.98641900	-2.33530000	3.35468800
H	1.31320500	-3.60209500	1.38188600
H	0.80337000	0.01142300	3.01920400
C	-0.41002800	-2.79136700	3.91260400
H	-1.20302600	-4.40612300	2.35011700
H	-1.71187700	-0.80828000	4.03439100
H	1.94477900	-2.43571100	3.86374200
H	-0.57971600	-3.26298000	4.88039500

Int1

Charge: 1 Multiplicity: 1
Negative Frequency: None

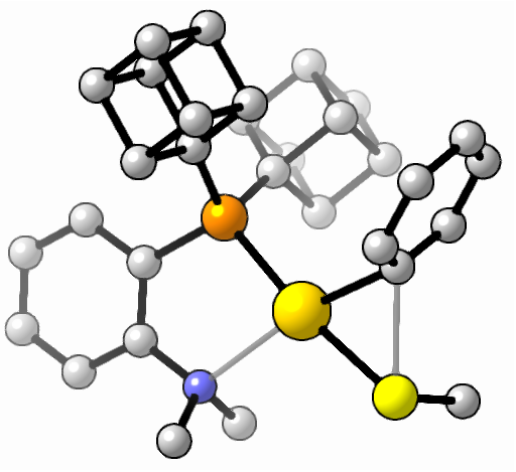


P	0.95321200	-0.25473800	-0.05167100
C	2.17399800	1.03471200	-0.45723700
C	1.78491600	2.38274300	-0.52977300
C	2.75187700	3.36259200	-0.78010500
C	4.08582600	3.00911400	-0.97691500
C	4.47395500	1.66930300	-0.92650900
C	3.52124600	0.68958000	-0.66298000
N	0.37567500	2.79321100	-0.34679800
Au	-1.05846400	1.00070900	-0.09543700
C	-2.19090800	-0.69637200	0.03859000
C	-2.33556300	-1.33923600	1.26734400
C	-3.07540800	-2.52535000	1.33789800
C	-3.66742300	-3.05416200	0.18834400
C	-3.52535900	-2.39279000	-1.03444000
C	-2.78334300	-1.20955600	-1.11570800

H	2.47296500	4.40921500	-0.82679900
H	4.81905000	3.78495900	-1.17341800
H	5.50976600	1.38848100	-1.08730700
H	3.82505400	-0.34943800	-0.62195400
H	-2.66818900	-0.70593900	-2.06989000
H	-3.98485400	-2.79712700	-1.93217400
H	-3.18208000	-3.03173000	2.29325900
H	-1.88034100	-0.93173200	2.16346700
H	-4.23823100	-3.97645900	0.24511800
S	-3.04460800	2.40085100	-0.07709100
C	-4.40372100	1.42029100	0.68311100
H	-5.24531700	2.10632800	0.81595500
H	-4.70716100	0.59700300	0.03377300
H	-4.10583400	1.02244100	1.65518100
C	0.24057500	3.64538800	0.87579700
H	0.58526400	3.07633500	1.74091100
H	0.83118800	4.56231400	0.78030900
H	-0.81252100	3.89842900	1.00530100
C	-0.10147900	3.53255000	-1.55762200
H	-1.14759800	3.80495900	-1.41402100
H	0.48057200	4.44446200	-1.72030700
H	-0.00993400	2.87769000	-2.42564700
C	1.05802000	-1.58174000	-1.26263100
C	0.77945100	-1.35685100	-2.79698700
C	2.29520000	-2.50350200	-1.62927500
C	0.11944800	-2.85486600	-1.28929000
H	0.55261900	-0.38500600	-3.23737600
C	2.01129500	-2.25903900	-3.15021100
C	-0.15495700	-2.61438600	-2.81156600
C	1.35182500	-3.75145600	-1.64561900
H	3.27352400	-2.46942700	-1.15102900
H	-0.64016600	-3.08082800	-0.54338300
C	1.07553700	-3.52170300	-3.17512400
H	2.77138100	-2.01020700	-3.89103900
H	-1.14009500	-2.65530100	-3.27521800
H	1.58212800	-4.70558100	-1.17126200
H	1.08387200	-4.29705600	-3.94162200
C	1.33976400	-0.87272200	1.60184200
C	2.77399100	-1.20418400	2.18718500
C	0.99610100	-0.08260200	2.92237500
C	0.77788900	-2.19698800	2.25727800
H	3.70838900	-1.12268000	1.63351500
C	2.41983100	-0.40852900	3.48818200
C	2.20260200	-2.51583000	2.82240500
C	0.43343700	-1.39889900	3.56135900
H	0.50646900	0.89213400	2.93672500

H	0.12042300	-2.90549300	1.75665100
C	1.85824900	-1.72555400	4.13594400
H	3.07711100	0.31348500	3.97295100
H	2.68624700	-3.49129200	2.76919500
H	-0.50490600	-1.47643500	4.11137900
H	2.06443200	-2.06728700	5.15042000

TS_{RE}



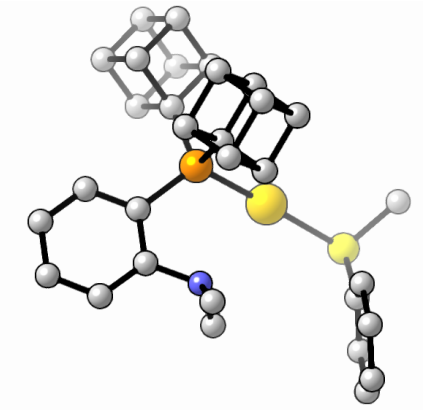
Charge: 1 Multiplicity: 1
Negative Frequency: -271.02

C	-3.12356500	0.52444300	0.98827600
C	-2.82457700	-0.03647700	-0.25590800
C	-3.19849100	0.58563000	-1.45268000
C	-3.85823300	1.81378800	-1.39153900
C	-4.15040600	2.40535000	-0.15706100
C	-3.78444600	1.75767400	1.02529200
Au	-0.88516400	-1.08577500	-0.30977500
S	-2.93398100	-2.34711100	-0.43677200
P	0.97342500	0.32700100	0.00238600
C	2.48109700	-0.63641600	-0.33356700
C	2.40791400	-2.02711800	-0.55430300
C	3.58769700	-2.74071500	-0.80079300
C	4.82089000	-2.09099000	-0.83812200
C	4.89461000	-0.71160200	-0.62977500
C	3.72957600	0.00838200	-0.37712000
N	1.12950100	-2.72072700	-0.52640000
H	3.54271400	-3.81286500	-0.96375000
H	5.72335700	-2.66327900	-1.03135800
H	5.85171700	-0.20038600	-0.66322500
H	3.78879600	1.08002200	-0.21880300
H	-2.81450500	0.04154600	1.90859200
H	-3.99849600	2.21110000	1.98919500
H	-4.14206600	2.30762400	-2.31670800
H	-2.97236100	0.12567600	-2.40886000
H	-4.66274700	3.36172000	-0.11863300
C	-3.28167300	-2.73783900	1.32391500
H	-3.73159900	-3.73419500	1.33239800
H	-2.36999600	-2.74684400	1.92242600
H	-3.99403700	-2.01393500	1.72849200
C	0.83976900	-3.42082700	-1.79447100
H	0.91242800	-2.70830800	-2.61966300
H	1.52480800	-4.26011900	-1.97871500
H	-0.18324400	-3.80633200	-1.75002400

C	1.01692500	-3.63001200	0.63182100
H	-0.00055500	-4.03079000	0.66300800
H	1.72841200	-4.46618500	0.57192100
H	1.20300500	-3.06889700	1.55011500
C	0.97363200	1.80083200	-1.03606600
C	1.90526100	3.07803500	-0.98928800
C	1.09039500	1.77346900	-2.60536000
C	-0.29192500	2.73888500	-1.15636800
H	2.72946200	3.23075400	-0.29170700
C	2.02127000	3.03407200	-2.55211700
C	0.64073400	3.99583100	-1.10439000
C	-0.16978800	2.69947600	-2.71629700
H	1.27673000	0.87120200	-3.18960000
H	-1.21585100	2.60184200	-0.59622200
C	0.76105000	3.96540400	-2.67105700
H	2.95130700	3.14409100	-3.11076700
H	0.45842800	4.88097300	-0.49408900
H	-1.00491000	2.54349600	-3.39996300
H	0.67934000	4.83331300	-3.32645800
C	1.03101600	0.88244500	1.72040700
C	2.19778500	1.61291000	2.49449800
C	-0.00909600	1.90034000	2.33621600
C	0.81327600	-0.07098900	2.95369100
H	3.16415700	1.87683600	2.06465500
C	1.15723800	2.62091800	3.09363400
C	1.97726300	0.65289600	3.71372400
C	-0.22080700	0.94072200	3.55540300
H	-0.80289600	2.39094400	1.77445100
H	0.67225700	-1.14977800	2.87471300
C	0.94275700	1.66653600	4.32356900
H	1.29387600	3.70181600	3.13967100
H	2.77381100	0.14743200	4.26067100
H	-1.19009100	0.66968300	3.97573000
H	0.90961200	1.98157200	5.36713900

Int2

Charge: 1 Multiplicity: 1
Negative Frequency: None

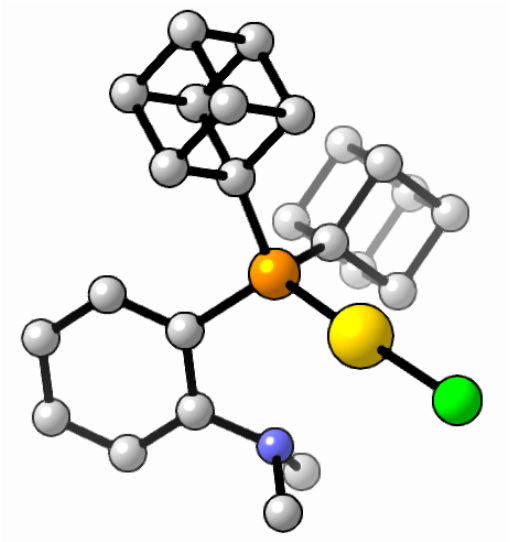


C	3.69096300	-0.23174200	-1.06075900
C	3.95090500	-0.87926400	0.15399200
C	5.01098100	-0.47428400	0.96948600
C	5.81414700	0.59694800	0.56622700
C	5.56371800	1.24657300	-0.64381200
C	4.50669300	0.82694300	-1.45919000
Au	0.70250100	-1.07363700	0.54845200
S	2.87512500	-2.19352900	0.76737100
P	-1.20741500	0.17006600	0.14475800
C	-1.37591000	1.74148100	1.06373600
C	-0.26469100	2.59314700	1.21596600
C	-0.41637900	3.79713900	1.91482600
C	-1.65302600	4.16438900	2.44600100
C	-2.75785900	3.32580200	2.28490700
C	-2.61944800	2.12008400	1.59783000
N	0.99936900	2.20634200	0.64296700
H	0.44085100	4.45264100	2.03641200
H	-1.75414500	5.10447000	2.98069800
H	-3.72513700	3.60626500	2.69070700
H	-3.48862900	1.48402700	1.47689300
H	2.85362300	-0.53696200	-1.67996800
H	4.30723600	1.33110900	-2.40003900
H	6.63480900	0.91849300	1.20023300
H	5.20354800	-0.98179300	1.90950400
H	6.18845800	2.07914400	-0.95276100
C	2.90163100	-3.40711400	-0.61112300
H	3.91805300	-3.79219700	-0.71061200
H	2.21733200	-4.20956200	-0.32812000
H	2.56635100	-2.94304100	-1.53869800
C	1.48329800	3.15350900	-0.36793800
H	2.35494100	2.71736700	-0.86634300
H	0.70427300	3.32726000	-1.11419200
H	1.78242100	4.12612500	0.05827400
C	2.02318200	1.94828600	1.66515000
H	1.64674000	1.21250500	2.38214700
H	2.90981800	1.53214700	1.17942500
H	2.31859100	2.85773400	2.21536100
C	-2.71003800	-0.79402800	0.44358800
C	-3.31042000	-1.17997500	1.84867400
C	-4.16744600	-0.53339200	-0.11034500
C	-2.81990200	-2.30263900	-0.00309600
H	-2.91947200	-0.82745600	2.80369800

C	-4.75445100	-0.90840400	1.29606700
C	-3.41351900	-2.67655800	1.39642100
C	-4.26243100	-2.03240700	-0.55474500
H	-4.45820300	0.32642900	-0.71492800
H	-2.02383600	-2.84194000	-0.51873400
C	-4.86118300	-2.41036500	0.84818900
H	-5.52684300	-0.34482300	1.82078600
H	-3.10822300	-3.53431400	1.99652800
H	-4.63595300	-2.37370700	-1.52068400
H	-5.72652200	-3.05378100	1.01067300
C	-1.26710000	0.56800400	-1.62491700
C	-1.74756900	-0.44176500	-2.74238200
C	-2.11849200	1.71189300	-2.29727800
C	-0.03522200	0.95724000	-2.51902900
H	-2.09541200	-1.45763600	-2.55744700
C	-2.59388000	0.70245500	-3.39817600
C	-0.51441700	-0.04523300	-3.62291700
C	-0.88197900	2.10096200	-3.17987300
H	-2.75421300	2.40751300	-1.74837900
H	0.98133100	1.04584800	-2.13918300
C	-1.36169500	1.09731500	-4.28991600
H	-3.62274200	0.59425500	-3.74333300
H	0.13019900	-0.75026400	-4.14899800
H	-0.53266900	3.11998800	-3.35175200
H	-1.40128100	1.31252000	-5.35833600

P_{Au}

Charge: 0 Multiplicity: 1
Negative Frequency: None

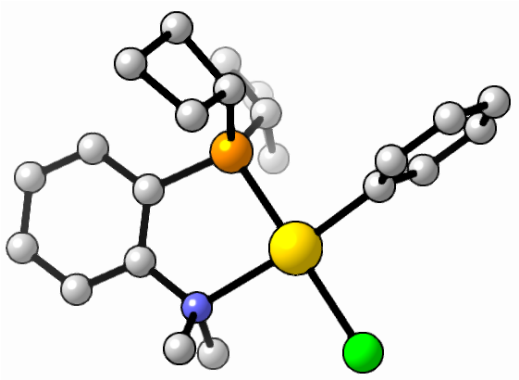


Au	1.40494400	-1.34929900	0.03055800
P	-0.33591900	0.13955300	-0.15981100
C	-0.17812800	1.49733200	-1.37784300
C	0.98357700	2.29147700	-1.38117100
C	1.09922000	3.33860000	-2.30321700
C	0.07033700	3.60866500	-3.20634000
C	-1.08775000	2.82869800	-3.19675900
C	-1.21087400	1.77746400	-2.28776500
N	2.02029000	1.99833000	-0.42594200
H	1.99892500	3.94672300	-2.30885900
H	0.17179000	4.42735500	-3.91303800
H	-1.89559400	3.03586700	-3.89215400
H	-2.12025500	1.18867600	-2.29093400
Cl	3.20538500	-2.93960900	0.29232600

C	3.22178400	1.44439000	-1.06319500
H	2.94282400	0.59903400	-1.69841800
H	3.75804300	2.18593700	-1.68003200
H	3.90146200	1.08098700	-0.28541800
C	2.34831000	3.13698000	0.43800800
H	3.00819800	2.79221500	1.24095600
H	2.85980300	3.95624900	-0.09523400
H	1.43428100	3.53248800	0.88699100
C	-1.83988600	-0.77448800	-0.59811100
C	-3.34654600	-0.31221400	-0.48148700
C	-2.14861800	-1.43576400	-1.99550700
C	-2.21145700	-2.13430700	0.10969600
H	-3.66982900	0.67787800	-0.15782700
C	-3.64148700	-0.96304300	-1.87907200
C	-3.70242300	-1.66329100	0.22707400
C	-2.51410400	-2.78179300	-1.28273300
H	-1.51645000	-1.33356900	-2.87826600
H	-1.61533300	-2.58911300	0.90207500
C	-4.00960100	-2.31516300	-1.16932600
H	-4.21089600	-0.49102400	-2.68084600
H	-4.31801300	-1.75473000	1.12260100
H	-2.17857900	-3.76972400	-1.59986200
H	-4.88201500	-2.92761000	-1.40004500
C	-0.73906500	0.90361400	1.43806600
C	-1.58432200	2.21872200	1.64308400
C	-1.58290700	0.19166500	2.57050100
C	0.28670500	1.39231300	2.52232300
H	-1.98811600	2.82088300	0.82830900
C	-2.41903800	1.50307600	2.76001000
C	-0.55157000	2.70478600	2.71831600
C	-0.55171300	0.68467500	3.64103300
H	-1.99491100	-0.81454200	2.50410800
H	1.36722600	1.33010200	2.40101500
C	-1.39146700	1.99676300	3.84149300
H	-3.50553100	1.54016400	2.84821200
H	-0.13658100	3.71190400	2.77742900
H	-0.13616100	0.06705900	4.43813400
H	-1.65354000	2.43821900	4.80380700

_S_-Arylation of Methanethiol with [((PCyb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (10)

SM

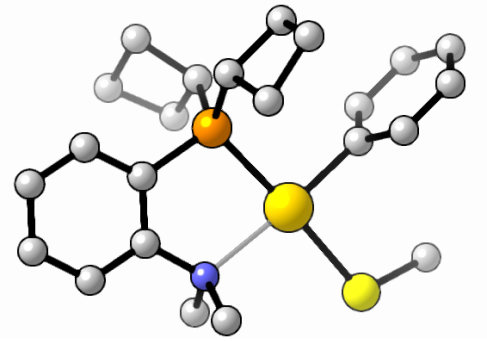


Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.57520900	1.01257700	0.01564100
C	-2.25092600	0.30668200	0.05205000
C	-2.43232000	-1.08764400	0.00117000
C	-3.72836000	-1.61192500	0.00218500
C	-4.83545900	-0.76720400	0.05721400
C	-4.66265400	0.61627600	0.11411000
C	-3.37695900	1.14876100	0.11015800
N	-1.28405700	-2.01434600	-0.04674900
Au	0.72090600	-0.91083200	0.00165800
C	2.41494400	0.24460000	0.08089100
C	3.00787000	0.68046400	-1.10340000
C	4.16983400	1.45869800	-1.03461400
C	4.72037700	1.79443800	0.20423300
C	4.11279800	1.35135200	1.38158900
C	2.95065600	0.57318500	1.32644500
H	-3.88349700	-2.68401500	-0.03718800
H	-5.83280500	-1.19497500	0.05750600
H	-5.52059700	1.27857900	0.16058100
H	-3.25373400	2.22331300	0.15807900
H	2.47733400	0.23720000	2.24398700
H	4.53568700	1.61013500	2.34829000
H	4.63731100	1.80099100	-1.95360900
H	2.58315400	0.42359900	-2.06872500
H	5.61906600	2.40242300	0.25256500
Cl	2.05273100	-2.96321400	-0.05471000
C	-1.29404000	-2.91813900	1.14675100
H	-1.27628400	-2.30681800	2.05045300
H	-2.18499000	-3.55347500	1.14918300
H	-0.40171200	-3.54356400	1.10947400
C	-1.30262200	-2.81479100	-1.31085100
H	-0.41726100	-3.45151700	-1.32327000
H	-2.20168500	-3.43607900	-1.36787000
H	-1.27330200	-2.13140700	-2.16080900
C	-0.21537400	2.03870200	1.48412800
C	-1.18073200	3.21943400	1.83077900
C	-0.58483300	1.37169300	2.84654500
H	0.83563300	2.31535100	1.36203300
C	-1.75672200	2.38012000	3.00190000
H	-1.87389600	3.56824200	1.06145900

H	-0.59790600	4.08031000	2.16865400
H	-0.84542000	0.30931300	2.82482300
H	0.21564400	1.51499600	3.57674300
H	-2.72303400	1.93010100	2.75759600
H	-1.83771100	2.88760500	3.96607800
C	-0.29350400	1.95567200	-1.52421200
C	-0.48690500	1.21733100	-2.87748800
C	-1.26313600	3.06838500	-2.02904800
H	0.72715000	2.34215100	-1.43448400
C	-0.97256900	2.56805000	-3.47096500
H	-1.30134400	0.48736900	-2.83060700
H	0.39868200	0.73975400	-3.30390500
H	-2.30299000	2.87876400	-1.75253000
H	-0.99869600	4.09451400	-1.76458700
H	-1.81873200	2.53095300	-4.16152400
H	-0.15171800	3.12350000	-3.93412700

Int1



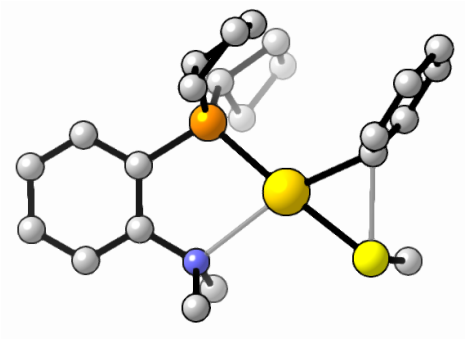
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	0.80484300	1.12718800	-0.03145300
C	2.47138600	0.44530900	-0.29993000
C	2.66756300	-0.94545200	-0.34796300
C	3.96141500	-1.45050400	-0.51941400
C	5.04765300	-0.58847800	-0.65531500
C	4.85561900	0.79410000	-0.63497300
C	3.57300000	1.30464800	-0.46235100
N	1.53685700	-1.89436400	-0.24728500
Au	-0.50749700	-0.84811100	-0.00596200
C	-2.24531800	0.22212000	0.14977700
C	-3.03777300	0.41554800	-0.98288500
C	-4.20210600	1.18403900	-0.87888200
C	-4.56782800	1.74859000	0.34617100
C	-3.77252600	1.53734800	1.47440200
C	-2.60484600	0.77038000	1.38114700
H	4.13174500	-2.52049400	-0.55595100
H	6.04250400	-1.00163000	-0.78788700
H	5.69614100	1.46982100	-0.75456200
H	3.42931600	2.37921200	-0.45711900
H	-1.99143300	0.60892300	2.26233400
H	-4.05260100	1.96873000	2.43140800
H	-4.81851400	1.34002200	-1.75986200
H	-2.76062900	-0.02064100	-1.93684500

H	-5.47018900	2.34836200	0.42097100
S	-1.73383700	-2.94056400	0.03867400
C	-3.37741100	-2.61750700	0.80053100
H	-4.00272600	-2.00557700	0.14803500
H	-3.84890200	-3.59421900	0.94290100
H	-3.27193600	-2.12348000	1.76830200
C	1.42810900	-2.68229700	-1.51601600
H	1.26301400	-1.98976500	-2.34314100
H	2.33708000	-3.26419300	-1.69689100
H	0.58019200	-3.36381100	-1.43544100
C	1.72530600	-2.80552800	0.92442600
H	0.85286000	-3.45465800	1.00244000
H	2.62592800	-3.41574600	0.80664200
H	1.80857400	-2.20115400	1.82897500
C	0.45470000	2.34708600	-1.35112500
C	-0.04488200	1.81748400	-2.72850100
C	-0.83969000	3.20994300	-1.22894900
H	1.34273800	2.97845500	-1.45965100
C	-1.09871700	2.95944800	-2.74071000
H	-0.50315700	0.82641500	-2.65610400
H	0.69827900	1.80190900	-3.52923700
H	-1.60612800	2.75519400	-0.59784700
H	-0.68164400	4.24175400	-0.90594800
H	-2.11860200	2.67184800	-3.00960900
H	-0.79008500	3.80421100	-3.36298400
C	0.69727500	1.99210700	1.58350600
C	1.15899600	1.14493100	2.81059000
C	1.79235900	3.04779900	1.94161400
H	-0.33398200	2.35641000	1.62109800
C	2.44101100	2.01682400	2.90222000
H	1.29550800	0.06959000	2.66047000
H	0.47989100	1.28773400	3.65566000
H	2.41054000	3.45061900	1.13571500
H	1.33556700	3.88980500	2.46916600
H	3.30562600	1.52173100	2.45060200
H	2.71830300	2.37953800	3.89515800

TS_{RE}

Charge: 1 Multiplicity: 1
Negative Frequency: -264.97

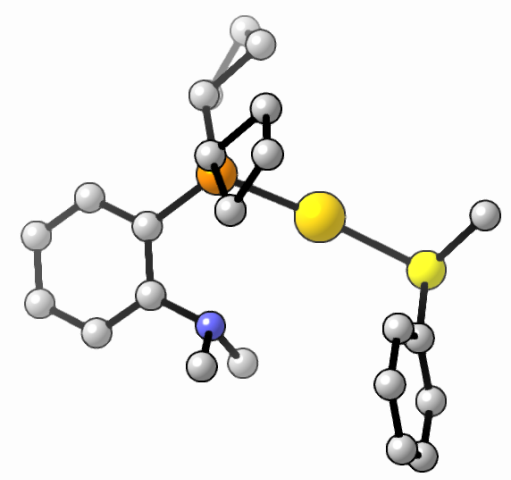


C	-3.17837800	-0.07184100	0.89585500
C	-2.55855900	-0.42902300	-0.30351300
C	-2.99580500	0.06944900	-1.53593700
C	-4.05698100	0.97620600	-1.55279000
C	-4.68037900	1.36550900	-0.36178800
C	-4.24162200	0.83799700	0.85461900
Au	-0.37875100	-0.75491100	-0.15598800
S	-1.83227600	-2.63771800	-0.49707700
P	0.94133800	1.16327200	0.23526700
C	2.67670800	0.71063600	-0.09210300
C	3.04112500	-0.63164800	-0.32147800
C	4.38627800	-0.94317200	-0.55833200
C	5.35818900	0.05598200	-0.57369900
C	4.99989400	1.38719900	-0.34692000
C	3.66657500	1.70834500	-0.10551200
N	2.04287200	-1.68845800	-0.29742400
H	4.67689300	-1.97506400	-0.72730900
H	6.39536400	-0.20658300	-0.75988100
H	5.75302300	2.16900900	-0.35758500
H	3.39401700	2.74478500	0.07159900
H	-2.82374300	-0.45785500	1.84520600
H	-4.71444800	1.13769000	1.78578400
H	-4.39564700	1.37538500	-2.50482900
H	-2.51486000	-0.23643400	-2.45884100
H	-5.50540700	2.07082400	-0.38407300
C	-2.20677000	-3.19553700	1.21173300
H	-2.28494600	-4.28511900	1.16496100
H	-1.41474000	-2.91878200	1.90859400
H	-3.16284100	-2.77719700	1.53724700
C	2.01400400	-2.47566200	-1.54616900
H	1.89085200	-1.79583500	-2.39260000
H	2.92436400	-3.07388200	-1.68947400
H	1.15369000	-3.15070700	-1.50773100
C	2.19036500	-2.55770300	0.88812300
H	1.35033200	-3.25817900	0.91312400
H	3.13079400	-3.12708100	0.86729400
H	2.16454500	-1.94315400	1.79080500
C	0.86172600	1.75397600	1.97157900
C	-0.52675300	2.20111300	2.52092700
C	0.93056000	0.69561600	3.11180200
H	1.61721500	2.53563800	2.10865000
C	-0.16923800	1.49903400	3.85851600

H	-1.35152000	1.69700800	2.00860100
H	-0.72206800	3.27647700	2.53489600
H	0.55747200	-0.28143300	2.78427100
H	1.89958700	0.56136000	3.59951300
H	-0.96186200	0.92200300	4.34356200
H	0.25805500	2.19728400	4.58490000
C	0.50920600	2.58129500	-0.84353300
C	0.31660000	2.28867000	-2.36120600
C	-0.96957500	3.07725400	-0.78256100
H	1.21433300	3.40138200	-0.67381000
C	-0.95533500	3.18044900	-2.33116800
H	0.07518000	1.23656100	-2.55027700
H	1.13759100	2.58559200	-3.01892200
H	-1.65664300	2.29982600	-0.43770500
H	-1.14742800	3.98949200	-0.20744100
H	-1.83736400	2.79515600	-2.85047500
H	-0.75321400	4.19858500	-2.67748900

Int2

Charge: 1 Multiplicity: 1
Negative Frequency: None

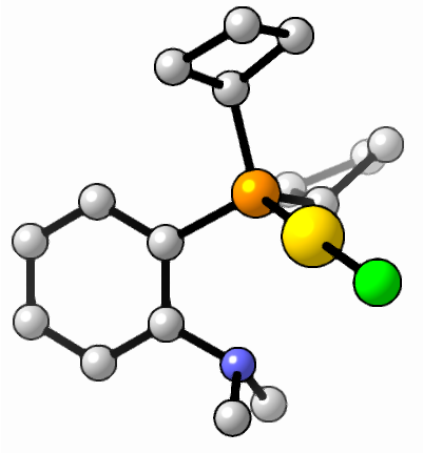


C	-3.27752700	0.09185800	0.94951300
C	-3.45258000	-0.15865300	-0.41770400
C	-4.31031000	0.63247200	-1.18728500
C	-4.99447000	1.69014600	-0.58029600
C	-4.82881300	1.94432400	0.78235300
C	-3.97526400	1.14127900	1.54693800
Au	-0.25791300	-0.91003400	-0.50524600
S	-2.52211100	-1.45650200	-1.26183900
P	1.76279200	-0.22467400	0.40441400
C	2.34547700	1.43533300	-0.10703200
C	1.43165800	2.48906700	-0.31961800
C	1.91600400	3.74977400	-0.69164600
C	3.28298500	3.97679400	-0.84789200
C	4.18873900	2.93511000	-0.63896000
C	3.72146700	1.67376200	-0.27229100
N	0.01943000	2.25242000	-0.16428800
H	1.21134700	4.55914200	-0.85823500
H	3.63891700	4.96263700	-1.13319100
H	5.25503500	3.10018700	-0.76035800
H	4.43999300	0.87758700	-0.11333800
H	-2.59732100	-0.51537500	1.53830800
H	-3.84118200	1.33799800	2.60634300

H	-5.65765200	2.31009400	-1.17585500
H	-4.43984000	0.42970400	-2.24577600
H	-5.36163100	2.76676100	1.25000000
C	-2.97098600	-2.95431500	-0.29789600
H	-4.04115800	-3.13266500	-0.41721100
H	-2.39783500	-3.77958900	-0.72557500
H	-2.70979700	-2.82615000	0.75271000
C	-0.60747400	3.09363400	0.86054200
H	-0.03174200	3.03709400	1.78649200
H	-0.68629600	4.15311000	0.56239000
H	-1.61666500	2.71538300	1.05336400
C	-0.70198200	2.34369000	-1.44095300
H	-1.73327800	2.01087100	-1.28792000
H	-0.72158200	3.36853800	-1.84910700
H	-0.23135300	1.68452900	-2.17654000
C	3.12166100	-1.39756200	0.01185700
C	2.82706000	-2.92340500	0.14463600
C	3.46840700	-1.63273500	-1.48670900
H	4.00922400	-1.13012700	0.59481400
C	3.62886500	-3.14367900	-1.16652400
H	1.76355400	-3.14935300	0.01223000
H	3.18228300	-3.40945800	1.05698500
H	2.60304100	-1.44419400	-2.13278000
H	4.33167200	-1.09179300	-1.88322300
H	3.21395000	-3.85211200	-1.88929700
H	4.67195600	-3.40910900	-0.96796300
C	1.63720700	-0.24055900	2.24068300
C	0.43634200	0.46363700	2.93554300
C	1.18554900	-1.58169200	2.89753600
H	2.59626500	0.10352900	2.64357400
C	0.32568200	-0.75514100	3.89069300
H	-0.42764600	0.54850800	2.27012200
H	0.63838800	1.44151200	3.37977400
H	0.56220200	-2.17816300	2.22214300
H	1.97759400	-2.21744300	3.30186500
H	-0.68101500	-1.12782500	4.10173200
H	0.84542700	-0.58272900	4.83824300

P_{Au}

Charge: 0 Multiplicity: 1
Negative Frequency: None

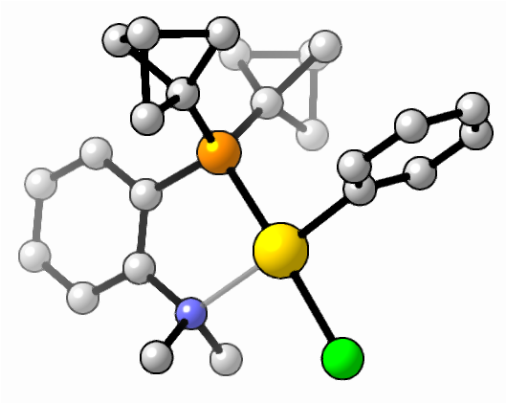


Au	-1.54431100	-0.44764900	0.02121200
P	0.41383700	0.75883500	-0.00124500
C	1.85220400	-0.09708000	-0.74462400
C	2.21141900	-1.35978800	-0.23697000
C	3.30792700	-2.03770700	-0.78056100
C	4.05069900	-1.46811200	-1.81600600
C	3.70120900	-0.21176200	-2.31538000
C	2.60726000	0.47189000	-1.78241700
N	1.42852700	-1.90668800	0.84115700
H	3.58165600	-3.01200600	-0.38609100
H	4.90167000	-2.00228400	-2.22891300
H	4.27763000	0.23884700	-3.11784700
H	2.35234700	1.44681700	-2.18197500
Cl	-3.61299100	-1.69219200	0.07807800
C	0.71832200	-3.13313800	0.45983200
H	0.01328700	-3.39629400	1.25522500
H	0.15038600	-2.95468700	-0.45756400
H	1.39482900	-3.98910800	0.29573900
C	2.19875500	-2.08831100	2.07614500
H	1.50870100	-2.33269400	2.89087600
H	2.94780900	-2.89526800	2.00502400
H	2.71784800	-1.15940700	2.32697500
C	0.20477800	2.30757200	-0.97394900
C	-0.25142900	2.07219700	-2.45215700
C	-1.13866200	3.06357500	-0.70740300
H	1.10404800	2.92041800	-0.85617900
C	-1.66001500	2.62062800	-2.10015800
H	-0.21597700	1.03772000	-2.80906900
H	0.30540000	2.69811600	-3.15523100
H	-1.72796500	2.72434400	0.15026900
H	-0.98159700	4.14196100	-0.61549400
H	-2.41417700	1.83060600	-2.03515400
H	-2.04081900	3.41658100	-2.74590400
C	0.96545200	1.25957800	1.68568200
C	2.36364500	1.91531500	1.87488700
C	0.33065100	2.48728000	2.40359300
H	0.87014000	0.36668600	2.30754500
C	1.73499100	2.78687900	2.99568600
H	2.65930300	2.51817700	1.00946900
H	3.18989900	1.24807800	2.13501300
H	0.02362900	3.27006800	1.70514900
H	-0.49360600	2.28083500	3.09163300

H	2.04187200	3.83553800	3.04558700
H	1.86461700	2.32865000	3.98124600

_S_-Arylation of Methanethiol with [((PBcp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (13)

SM



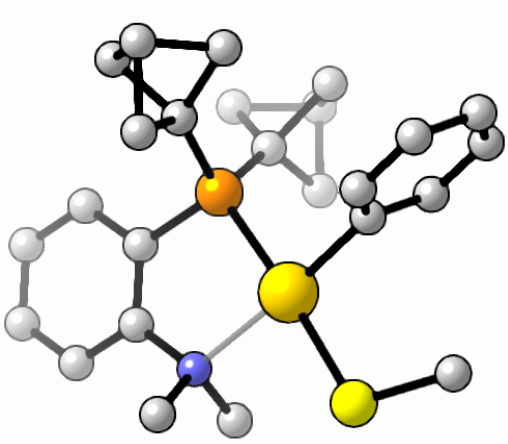
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.61981700	0.92694800	-0.00057700
C	-2.34753800	0.37023600	-0.00387900
C	-2.65749900	-0.99709800	-0.00359800
C	-3.99830700	-1.39495500	-0.00527400
C	-5.01637000	-0.44254500	-0.00718800
C	-4.71045500	0.92018100	-0.00730600
C	-3.37916000	1.32518600	-0.00557300
N	-1.59306100	-2.01754000	-0.00138700
Au	0.51778200	-1.10359600	0.00044500
C	2.36156600	-0.20229400	0.00080900
C	2.98839200	0.06817400	1.21566500
C	4.27145700	0.62856000	1.20965100
C	4.91123000	0.91013400	0.00049100
C	4.27428700	0.62139100	-1.20849500
C	2.99124500	0.06100200	-1.21419000
H	-4.25818000	-2.44745100	-0.00504000
H	-6.05124200	-0.76972300	-0.00846100
H	-5.50162800	1.66271200	-0.00861700
H	-3.14097700	2.38310400	-0.00517300
H	2.50568200	-0.16962100	-2.15631500
H	4.76887000	0.82891900	-2.15324900
H	4.76383600	0.84165800	2.15431600
H	2.50077000	-0.15711600	2.15799200
H	5.90481300	1.34869000	0.00035100
Cl	1.61675900	-3.28916800	0.00238400
C	-1.68472200	-2.86166700	1.23106900
H	-1.60446300	-2.21230800	2.10468000
H	-2.63328800	-3.40669400	1.26125300
H	-0.85726900	-3.57160300	1.22314400
C	-1.68165600	-2.86377300	-1.23263700
H	-0.85428700	-3.57374600	-1.22143100
H	-2.63015900	-3.40881600	-1.26427400
H	-1.59916500	-2.21590000	-2.10713800
C	-0.35320500	1.92633900	-1.49955900
C	-0.27415700	1.37174700	-2.95334100
C	-1.28589000	3.05858200	-2.05435200
C	0.85870500	2.84876900	-1.84491500
H	-1.19417800	0.93794800	-3.35508700
H	0.59973800	0.75789800	-3.18608300

C	-0.10918400	2.91779600	-3.06259100
H	-2.27397000	2.74170500	-2.39799000
H	-1.33112600	3.97918400	-1.46577400
H	1.81824800	2.35029700	-1.99319900
H	0.96020100	3.75566400	-1.24289400
H	0.03244400	3.49736900	-3.97724100
C	-0.36048000	1.92316900	1.50182100
C	-0.28406500	1.36475700	2.95428000
C	0.84663300	2.84929000	1.85366300
C	-1.29948500	3.05007400	2.05680200
H	0.59135200	0.75354200	3.18822900
H	-1.20372200	0.92628600	3.35177100
C	-0.12541900	2.91111100	3.06842100
H	1.80769900	2.35419400	2.00353100
H	0.94645100	3.75832500	1.25459600
H	-2.28735900	2.72819900	2.39633900
H	-1.34664900	3.97211000	1.47062400
H	0.01101700	3.48865900	3.98513800

Int1

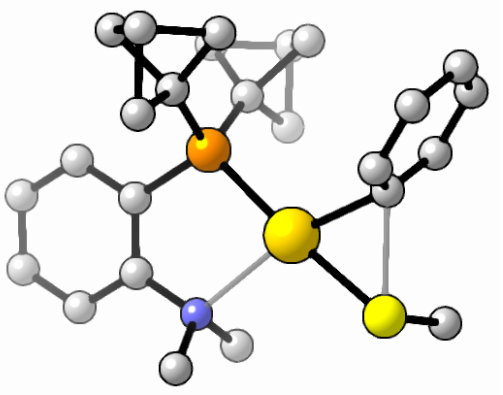
Charge: 1 Multiplicity: 1
Negative Frequency: None



P	0.92267300	0.83201300	0.01125800
C	2.48782200	-0.08547700	-0.09518800
C	2.48824600	-1.48794200	-0.11078800
C	3.70801300	-2.17166000	-0.17102400
C	4.91090900	-1.46937300	-0.22033000
C	4.91444200	-0.07288100	-0.20594800
C	3.70625400	0.61429100	-0.14109700
N	1.22865100	-2.25993100	-0.04948400
Au	-0.66673100	-0.92908200	-0.02321800
C	-2.26237200	0.35486800	-0.04528600
C	-2.75967600	0.86322000	1.15385900
C	-3.85526200	1.73431100	1.12794100
C	-4.44570900	2.08697600	-0.08731700
C	-3.94412600	1.56310500	-1.28166700
C	-2.84808700	0.69280200	-1.26577500
H	3.73031700	-3.25555400	-0.17722400
H	5.84613500	-2.01829000	-0.26793900
H	5.84967800	0.47628500	-0.24282800
H	3.70603800	1.69864000	-0.12355000
H	-2.46890700	0.28329900	-2.19633600
H	-4.40206100	1.82673900	-2.23106200

H	-4.24251000	2.13197600	2.06198900
H	-2.31554300	0.58224900	2.10309000
H	-5.29552800	2.76315600	-0.10408600
S	-2.16128100	-2.84018600	-0.06943800
C	-3.84669900	-2.28641500	0.41406100
H	-4.46169000	-3.18975900	0.46447800
H	-3.83852300	-1.80089200	1.39161800
H	-4.26746000	-1.60344000	-0.32610100
C	1.10886600	-3.14091100	-1.25247600
H	1.11325500	-2.51294600	-2.14490700
H	1.93315500	-3.85881800	-1.30139500
H	0.16746600	-3.68844900	-1.19658000
C	1.19141900	-3.06669800	1.21074900
H	0.24294200	-3.60331000	1.25203800
H	2.01944400	-3.78193000	1.24264000
H	1.26044200	-2.38505600	2.06041600
C	0.84831700	1.97461800	-1.40663600
C	0.61602900	1.55178600	-2.88870100
C	-0.18632600	3.12309400	-1.63837200
C	1.95103900	2.95680700	-1.93055000
H	-0.36480600	1.12647100	-3.11779900
H	1.42475300	0.98734300	-3.36228000
C	0.73642000	3.10531800	-2.89173000
H	-1.22523600	2.81546900	-1.77460300
H	-0.10183800	3.98846400	-0.97530500
H	2.85287300	2.49439400	-2.34105600
H	2.18558000	3.80961200	-1.28668300
H	0.67341000	3.76501700	-3.76024900
C	0.98378100	1.78445600	1.56621600
C	0.05297200	2.95449800	2.02057300
C	0.81348000	1.17664700	2.99117200
C	2.18500800	2.61258000	2.13791700
H	-0.99647400	2.70295100	2.18670000
H	0.16153600	3.89591800	1.47509800
C	1.04511300	2.70408600	3.19335200
H	-0.17870000	0.78382500	3.23120300
H	1.60708700	0.50228600	3.32654400
H	2.44040900	3.53010200	1.59960900
H	3.07457000	2.04055700	2.41545700
H	1.08254900	3.24083000	4.14409500

TS_{RE}



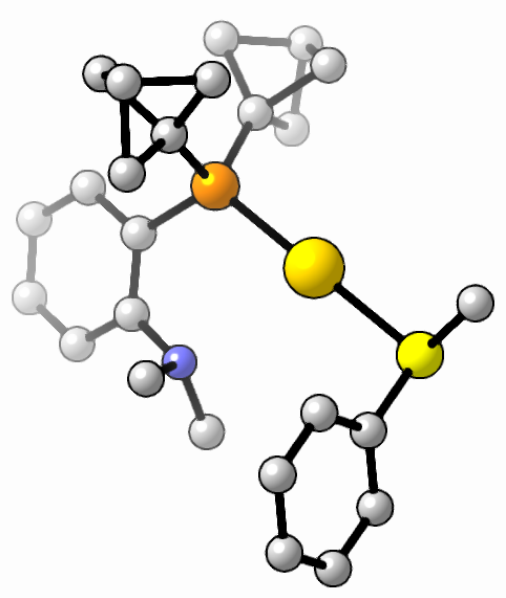
Charge: 1 Multiplicity: 1
Negative Frequency: -271.49

C	3.20641800	0.35208700	-1.04954800
C	2.76600600	-0.12328200	0.18779200
C	3.19409400	0.44954900	1.39087600
C	4.05946200	1.54380100	1.34087400
C	4.50287400	2.04667400	0.11210000
C	4.07667800	1.44832600	-1.07520000
Au	0.67883500	-0.85435300	0.19068500
S	2.49465200	-2.41962900	0.37339400
P	-0.98428500	0.79875000	-0.04953100
C	-2.60887100	-0.01022500	0.08749600
C	-2.70522300	-1.41046200	0.21442000
C	-3.97237100	-2.00051900	0.30604300
C	-5.12719000	-1.22007300	0.27234200
C	-5.03385800	0.16777800	0.14040000
C	-3.78003300	0.76645900	0.04642000
N	-1.51189200	-2.24122300	0.23248500
H	-4.05699200	-3.07854700	0.39918400
H	-6.09988800	-1.69750200	0.34465500
H	-5.93051400	0.77892100	0.10938000
H	-3.70820500	1.84389300	-0.06158400
H	2.86022300	-0.09305400	-1.97564200
H	4.40930900	1.83394500	-2.03500400
H	4.38977700	1.99887500	2.27060700
H	2.85623000	0.05408400	2.34299300
H	5.17918700	2.89548200	0.08299000
C	2.83280900	-2.88606600	-1.37047000
H	3.11152000	-3.94311700	-1.35301400
H	1.95370000	-2.75355900	-2.00223800
H	3.66912400	-2.29637100	-1.75496700
C	-1.39997600	-3.05044500	1.46220500
H	-1.46658800	-2.38980900	2.32990700
H	-2.17997800	-3.82139100	1.53201000
H	-0.42114200	-3.53950400	1.46501100
C	-1.40426700	-3.07544400	-0.98238200
H	-0.44635100	-3.60343600	-0.95736300
H	-2.21578000	-3.81383700	-1.05168500
H	-1.42843100	-2.42995500	-1.86379100
C	-0.93134500	1.57102900	-1.70037200
C	-1.94655900	2.53013800	-2.40292900
C	0.21104200	2.47734600	-2.26147100
C	-0.85910100	0.77346300	-3.03805800

H	-2.03002200	3.53783200	-1.98457100
H	-2.92672200	2.10612700	-2.64014000
C	-0.80025200	2.28031900	-3.42794600
H	0.28551100	3.48190400	-1.83504900
H	1.19316800	2.00686200	-2.36080900
H	-1.75970100	0.21889400	-3.31972900
H	0.04785400	0.17931000	-3.19041900
H	-0.72717100	2.69512700	-4.43652100
C	-0.88828800	2.11895100	1.20343600
C	0.31331900	3.10771700	1.35969000
C	-1.83339200	3.32854800	1.50520400
C	-0.80256600	1.88601400	2.74272100
H	0.41646400	3.86968300	0.58172600
H	1.27632200	2.65635300	1.61504000
C	-0.66400800	3.42272700	2.52896400
H	-1.88729500	4.10518700	0.73619700
H	-2.82156500	3.08344900	1.90533600
H	0.08361000	1.34981100	3.09685400
H	-1.71571500	1.52924700	3.22917500
H	-0.53722500	4.18388200	3.30301400

Int2

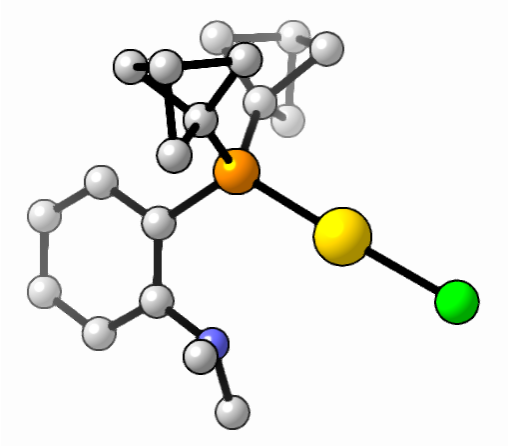
Charge: 1 Multiplicity: 1
Negative Frequency: None



C	-3.66513300	-0.20797300	1.23689700
C	-3.79139400	-0.33551100	-0.15177700
C	-4.67774300	0.47277300	-0.86988600
C	-5.44524100	1.42073100	-0.18664500
C	-5.33550700	1.54616700	1.19950200
C	-4.44978400	0.72874200	1.90976300
Au	-0.52526000	-0.81110500	-0.44240600
S	-2.77320700	-1.49399400	-1.08781500
P	1.62053300	-0.16117100	0.14654000
C	1.98402600	1.60452700	-0.14321500
C	0.97404300	2.54657100	-0.45474300
C	1.35693800	3.85311500	-0.79473900
C	2.69791800	4.23545800	-0.79421800
C	3.68917300	3.32016900	-0.43428900
C	3.32880200	2.01346000	-0.11231600
N	-0.40275600	2.16872400	-0.38807800
H	0.59385400	4.58329500	-1.04295700
H	2.96538600	5.25515700	-1.05655600
H	4.73354600	3.61586500	-0.41282800

H	4.10264500	1.30190700	0.15383600
H	-2.95037700	-0.81491100	1.78364400
H	-4.35590100	0.83039300	2.98672500
H	-6.13125100	2.05391100	-0.74102600
H	-4.76834500	0.36416300	-1.94619400
H	-5.93593800	2.28099100	1.72728500
C	-3.06634700	-3.08419100	-0.21916400
H	-4.12040600	-3.34616900	-0.32750400
H	-2.43759300	-3.82504300	-0.71729000
H	-2.78779400	-3.00809600	0.83169800
C	-0.97569500	2.34733100	0.95307700
H	-0.35696800	1.83699100	1.69403800
H	-1.05236600	3.41201400	1.23200100
H	-1.97284400	1.90070800	0.97680300
C	-1.27175000	2.72192700	-1.42702500
H	-2.21725200	2.17000800	-1.41165400
H	-1.50201200	3.79132700	-1.28705700
H	-0.80447400	2.58695600	-2.40594000
C	1.97670500	-0.49558500	1.90682100
C	1.90418400	-1.88921700	2.60658900
C	3.29014300	-0.23252700	2.71560700
C	1.19323400	0.07746400	3.12818400
H	2.66886100	-2.61782000	2.32158900
H	0.91056900	-2.34523800	2.66205300
C	2.28138900	-0.86673900	3.71767200
H	4.16046200	-0.83452600	2.43819300
H	3.55684300	0.81654100	2.87412800
H	0.14987700	-0.24073400	3.22142000
H	1.31056200	1.14847200	3.32086000
H	2.46011200	-1.08162500	4.77427600
C	2.83089100	-1.13255000	-0.82485400
C	2.75955500	-2.68693600	-0.97305400
C	2.99311300	-1.06694700	-2.37460400
C	4.38844600	-1.28825200	-0.73910000
H	1.85980700	-3.07651300	-1.46026700
H	3.02709100	-3.27304600	-0.08871000
C	3.92271700	-2.22047700	-1.89360300
H	2.11308400	-1.34860100	-2.96178300
H	3.47540100	-0.16825200	-2.77120900
H	4.78066700	-1.77013700	0.16120300
H	4.98527200	-0.41747600	-1.02432900
H	4.56155300	-2.85197200	-2.51617000

P_{Au}



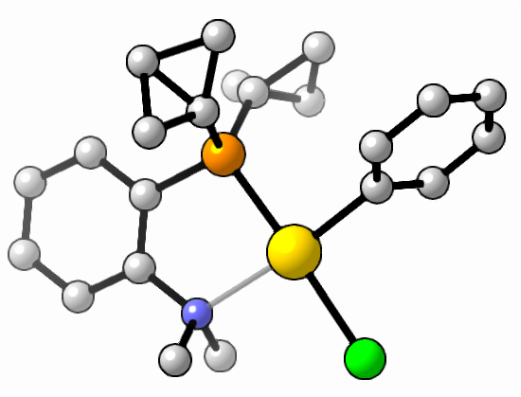
Charge: 0 Multiplicity: 1
Negative Frequency: None

Au	1.65043600	0.13672700	-0.09334600
P	-0.62210100	0.45499600	0.03305100
C	-1.69807900	-1.01734600	-0.10090300
C	-1.20224000	-2.34466800	-0.11432800
C	-2.10127700	-3.39211000	-0.37461100
C	-3.45878800	-3.14744000	-0.57701600
C	-3.95654900	-1.84516100	-0.50434500
C	-3.07582000	-0.79174700	-0.26816600
N	0.17424700	-2.59675200	0.14640300
H	-1.73581100	-4.41309700	-0.39835700
H	-4.13018600	-3.97931200	-0.77076700
H	-5.01549100	-1.64799600	-0.63983800
H	-3.46337400	0.22021400	-0.22813200
Cl	4.04445400	-0.12292100	-0.23004400
C	0.50642500	-2.61856500	1.57654000
H	0.09277200	-1.73935200	2.07467500
H	0.11473800	-3.52048100	2.07735600
H	1.59481700	-2.59346200	1.69192400
C	0.77546200	-3.72098600	-0.56630500
H	1.86464900	-3.63056500	-0.49680200
H	0.49266300	-4.70597900	-0.15752700
H	0.49085800	-3.68346700	-1.62106500
C	-1.11808200	1.58580400	-1.32014000
C	-2.46262800	2.31271000	-1.66523200
C	-0.39634100	2.93995500	-1.61829000
C	-0.98326500	1.26606500	-2.84081300
H	-2.79746000	3.07779700	-0.95833000
H	-3.28953400	1.67906900	-1.99775500
C	-1.44192600	2.75183700	-2.75355000
H	-0.57307400	3.75274100	-0.90758000
H	0.66089600	2.86436900	-1.89218200
H	-1.69892800	0.54476300	-3.24741800
H	0.03282200	1.07824700	-3.20265100
H	-1.63451900	3.43035900	-3.58863300
C	-1.09245700	1.28285400	1.59353700
C	-0.82523900	0.73728000	3.03076300
C	-0.55686800	2.66042200	2.09600000
C	-2.50539500	1.72437000	2.10137200
H	0.22631100	0.64711000	3.32169000
H	-1.40702400	-0.13937800	3.33276200
C	-1.49752300	2.12910200	3.21614700

H	0.51376700	2.70475500	2.31969800
H	-0.89183600	3.54340200	1.54370300
H	-3.20784900	0.91879300	2.33445500
H	-2.98856400	2.53592100	1.54890500
H	-1.73550600	2.62181200	4.16243100

_S_-Arylation of Methanethiol with [((PBcb$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (14)

SM

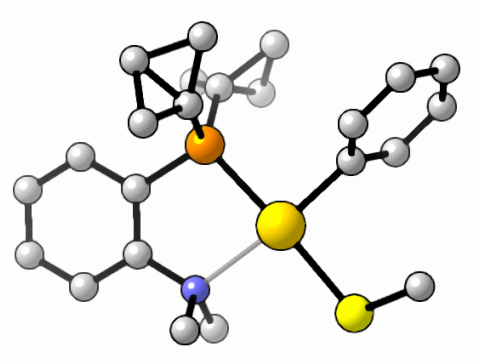


Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.49798500	1.12199800	-0.01641400
C	-2.25935500	0.73676000	-0.19237900
C	-2.70689400	-0.59170900	-0.13207000
C	-4.07849100	-0.84996200	-0.21758700
C	-4.98588000	0.19797400	-0.36748200
C	-4.53939700	1.51981400	-0.43842500
C	-3.17731200	1.78943500	-0.35059100
N	-1.75919100	-1.71200700	0.01052900
Au	0.42924700	-1.01076600	0.07726800
C	2.31050300	-0.19195200	0.06865000
C	2.76715700	0.53642000	1.16672500
C	4.04248700	1.11343300	1.12174700
C	4.84195500	0.96439900	-0.01339500
C	4.37454000	0.22565100	-1.10391800
C	3.10397200	-0.35908000	-1.06824100
H	-4.44790100	-1.86804500	-0.17080600
H	-6.04643900	-0.02316200	-0.43289100
H	-5.24605000	2.33374200	-0.56188500
H	-2.82170500	2.81289600	-0.41256400
H	2.74773100	-0.93174400	-1.91848000
H	4.99336100	0.10326600	-1.98842900
H	4.40018900	1.68445300	1.97387200
H	2.14278300	0.67248400	2.04342400
H	5.82611400	1.42237700	-0.04945000
Cl	1.32663900	-3.29252800	0.24831600
C	-2.01416900	-2.45750400	1.28226600
H	-1.91975900	-1.76265500	2.11850700
H	-3.01389700	-2.90313400	1.28150200
H	-1.26383400	-3.24396500	1.37199200
C	-1.85953900	-2.62687100	-1.17047700
H	-1.11169100	-3.41238400	-1.05886100
H	-2.85536800	-3.07621500	-1.23389500
H	-1.65557900	-2.05110900	-2.07506900
C	0.00526200	2.17084100	-1.35248000
C	0.68687900	1.78393700	-2.64844500
C	1.37980400	2.70587400	-1.70559600
C	-0.66275000	2.41009700	-2.69662100
H	0.96696100	0.77706700	-2.92851800
H	1.44601700	3.76798500	-1.94856500

H	2.23026000	2.30854500	-1.15770900
H	-1.49861000	1.76589700	-2.96013800
H	-0.76773000	3.44863000	-3.01601800
C	-0.24012100	1.97071400	1.51603600
C	-0.96581000	3.13252200	2.14431400
C	0.49114600	3.25493300	1.83430000
C	-0.96572400	1.80336700	2.83044500
H	-1.79930200	3.69510200	1.74617300
H	1.21888100	3.23169000	2.64775500
H	0.76580000	3.88799800	0.99376700
H	-1.89729700	1.24042200	2.81361000
H	-0.36180700	1.66290100	3.72896800

Int1



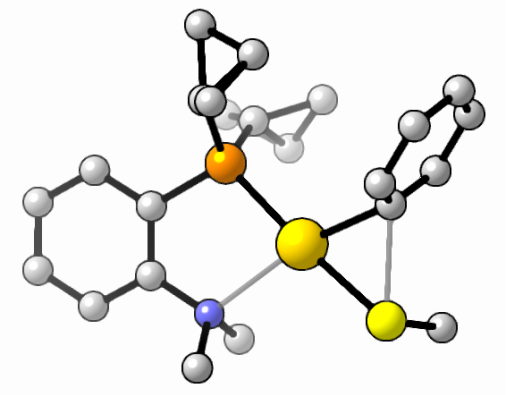
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.82168500	1.08378100	0.03306200
C	-2.48466900	0.37684200	-0.12558900
C	-2.66011000	-1.01572500	-0.12502600
C	-3.95606900	-1.53682300	-0.21007500
C	-5.05645200	-0.68585800	-0.30196700
C	-4.88243700	0.70006500	-0.30989600
C	-3.59862000	1.22858600	-0.22061800
N	-1.51096200	-1.93996100	-0.02360500
Au	0.53549200	-0.85709000	0.00154200
C	2.23569600	0.28222800	-0.02943600
C	2.57911700	1.04056000	1.09036800
C	3.71850700	1.85303500	1.04511000
C	4.50022700	1.90523600	-0.11086900
C	4.14765400	1.13804800	-1.22494500
C	3.01275500	0.32080800	-1.18922600
H	-4.11789000	-2.60872900	-0.20457800
H	-6.05277100	-1.11124900	-0.36893200
H	-5.73860400	1.36233500	-0.38563200
H	-3.45308200	2.30371900	-0.23321700
H	2.74628000	-0.27684400	-2.05468000
H	4.75294500	1.17204600	-2.12660900
H	3.98526400	2.44728200	1.91469600
H	1.96675300	1.01798600	1.98600700
H	5.38041700	2.54073600	-0.14458500
S	1.82031100	-2.92081600	0.00913600
C	3.42322700	-2.53261300	0.82846600
H	3.92957700	-3.48762400	0.99615400

H	4.04628700	-1.89979400	0.19384300
H	3.26290500	-2.03713400	1.78824900
C	-1.59520300	-2.71862400	1.25162600
H	-1.59528100	-2.01728700	2.08802800
H	-2.50512400	-3.32674000	1.27903300
H	-0.71853100	-3.36402700	1.31887400
C	-1.48000000	-2.85661500	-1.20512600
H	-0.61414100	-3.51380800	-1.11544100
H	-2.38405800	-3.47102100	-1.25543700
H	-1.39116100	-2.25523800	-2.11133200
C	-0.73730400	1.95774100	1.58043800
C	-1.59633300	3.03314500	2.18516000
C	-0.15045300	3.30792500	1.92010800
C	-1.47173500	1.70937700	2.87493100
H	-2.47299900	3.50942300	1.76726000
H	0.55007300	3.36404900	2.75604200
H	0.08238900	3.96637300	1.08614500
H	-2.33620700	1.04897200	2.83148900
H	-0.88595800	1.63533700	3.79369900
C	-0.58796600	2.26332700	-1.28290100
C	0.04525000	2.03029100	-2.63355600
C	0.67105500	3.00165100	-1.69189000
C	-1.37730600	2.47487900	-2.56046900
H	0.43915500	1.08826000	-2.99227400
H	0.57837900	4.07199100	-1.88764200
H	1.60266200	2.70446600	-1.21730600
H	-2.13913500	1.73649100	-2.80080900
H	-1.63796600	3.50132700	-2.82746600

TS_{RE}

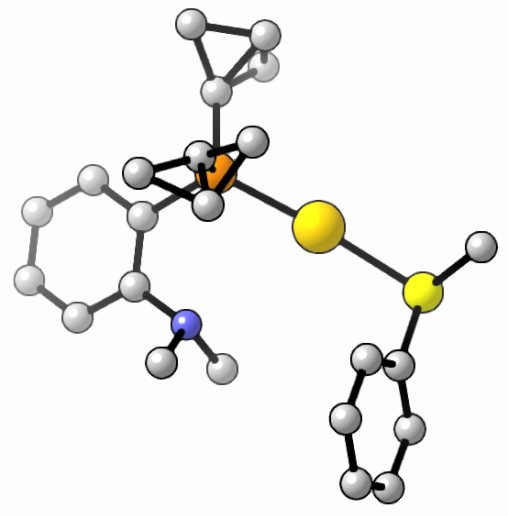
Charge: 1 Multiplicity: 1
Negative Frequency: -265.51



C	-3.20728800	0.24621700	0.97680400
C	-2.66765100	-0.20600600	-0.22915700
C	-3.09226200	0.30337500	-1.46143000
C	-4.04156500	1.32671800	-1.47187200
C	-4.57488600	1.81667900	-0.27402000
C	-4.16118700	1.27018000	0.94279300
Au	-0.53273400	-0.74664900	-0.14724900
S	-2.17954300	-2.48987500	-0.33920500
P	0.95419800	1.08269900	0.06365900
C	2.63395600	0.45927600	-0.25812000
C	2.87849500	-0.92526200	-0.34599300

C	4.18477500	-1.37042700	-0.58648200
C	5.22991100	-0.46074600	-0.74238500
C	4.98668800	0.91306700	-0.66152300
C	3.69299100	1.36813900	-0.42032600
N	1.79593300	-1.88212900	-0.17846700
H	4.38805300	-2.43451300	-0.64848500
H	6.23546100	-0.82665400	-0.92749600
H	5.79809300	1.62332900	-0.78647400
H	3.49653000	2.43480200	-0.36229100
H	-2.87823800	-0.16304100	1.92540300
H	-4.56982200	1.64055400	1.87886500
H	-4.36469100	1.73779300	-2.42421100
H	-2.68650100	-0.08447300	-2.38976200
H	-5.31414400	2.61153200	-0.29162600
C	-2.54871100	-2.93483900	1.40394800
H	-3.45970900	-2.42706800	1.73117000
H	-2.71353400	-4.01570800	1.41207300
H	-1.71871300	-2.69088900	2.06812100
C	1.69134100	-2.83230200	-1.30510000
H	1.63173900	-2.27076400	-2.24023900
H	2.54073800	-3.52727200	-1.35088900
H	0.77132300	-3.41136200	-1.18205000
C	1.88638300	-2.59104100	1.11545400
H	0.99692900	-3.21634100	1.23468000
H	2.78202200	-3.22619500	1.17235100
H	1.91601300	-1.86074800	1.92665900
C	0.63716100	2.45625400	-1.03203100
C	-0.67383200	3.20196500	-1.12925600
C	-0.16684800	2.45111400	-2.31359400
C	0.56747000	3.94049900	-0.74426600
H	-1.56704500	3.01622900	-0.54610900
H	0.23384100	2.99899800	-3.16906300
H	-0.68423800	1.52769500	-2.56769000
H	0.66010000	4.24154100	0.29753700
H	1.03036900	4.62477500	-1.45900600
C	0.98684100	1.76967400	1.71634600
C	0.95523200	1.03931000	3.03103200
C	-0.17734400	1.93934700	2.66940300
C	2.10585000	1.94302100	2.71913500
H	0.94900600	-0.03246400	3.18007200
H	-0.28430800	2.90035500	3.17710700
H	-1.11670900	1.47084300	2.38441700
H	3.05575000	1.46921900	2.48007000
H	2.19275900	2.90221400	3.23503500

Int2

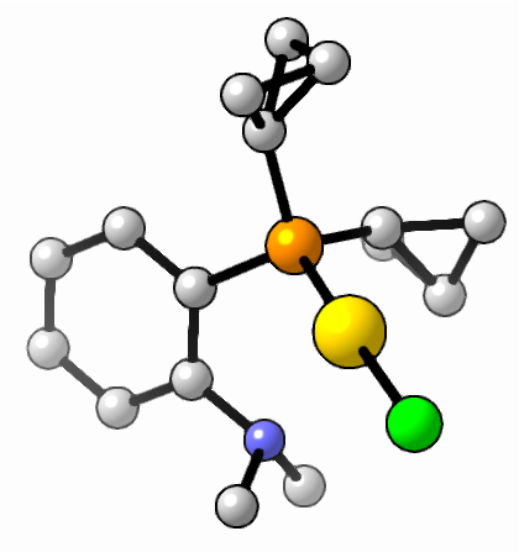


Charge: 1 Multiplicity: 1
Negative Frequency: None

C	-3.18477000	0.31364000	1.11145800
C	-3.51477800	-0.06396200	-0.19672200
C	-4.41587900	0.68882300	-0.95471600
C	-4.98789500	1.83622700	-0.39667300
C	-4.66823900	2.21741200	0.90765600
C	-3.77217300	1.45222100	1.66240600
Au	-0.38380400	-1.01473400	-0.49784700
S	-2.73095000	-1.48344500	-0.99087700
P	1.74910000	-0.40108900	0.17681900
C	2.36263000	1.21771200	-0.40974300
C	1.51307200	2.34112400	-0.44796900
C	2.02867600	3.56854100	-0.88279400
C	3.36424700	3.68725900	-1.26852700
C	4.20421300	2.57205700	-1.23217500
C	3.70430600	1.34204700	-0.80628800
N	0.13469300	2.19931400	-0.05279700
H	1.37647700	4.43596100	-0.91828300
H	3.74707200	4.64856400	-1.59912100
H	5.24399200	2.65732200	-1.53309000
H	4.35787600	0.47635000	-0.77835800
H	-2.46715900	-0.26230500	1.68724600
H	-3.51927100	1.74726000	2.67636700
H	-5.68400600	2.42690200	-0.98432600
H	-4.66425500	0.38825700	-1.96774500
H	-5.11375400	3.10952900	1.33731900
C	-3.16197300	-2.85988400	0.14663300
H	-4.24510800	-2.99302000	0.12808100
H	-2.66235700	-3.74982600	-0.24153400
H	-2.81065100	-2.64643800	1.15626200
C	-0.25062300	3.08353600	1.05292800
H	0.46162600	2.98363400	1.87567200
H	-0.29633400	4.14713000	0.76388500
H	-1.24262300	2.78538800	1.40739600
C	-0.78427800	2.34870700	-1.19107200
H	-1.79495300	2.08514800	-0.86642700
H	-0.79959300	3.37555200	-1.59395800
H	-0.49004800	1.66438000	-1.99226500
C	1.80490100	-0.35423300	1.96791000
C	0.81847800	0.26070800	2.92282800
C	2.24389400	0.71483500	2.94079900
C	1.02133000	-1.21565300	2.93593600

H	-0.07121800	0.81269000	2.65533500
H	2.89103200	0.42681900	3.77263200
H	2.45964600	1.69607800	2.52186000
H	0.22369400	-1.82531200	2.51242800
H	1.56265400	-1.68303800	3.76118300
C	2.97722300	-1.61315200	-0.29886400
C	2.94755700	-3.07212800	0.07729300
C	4.10289200	-2.22659100	0.50571000
C	2.86722300	-2.68447200	-1.36086200
H	2.20252700	-3.56228900	0.69071800
H	5.07378700	-2.35549700	0.02173000
H	4.15259300	-1.95576500	1.55875200
H	1.89812000	-2.79104200	-1.84739500
H	3.72643100	-2.85084400	-2.01399400

P_{Au}



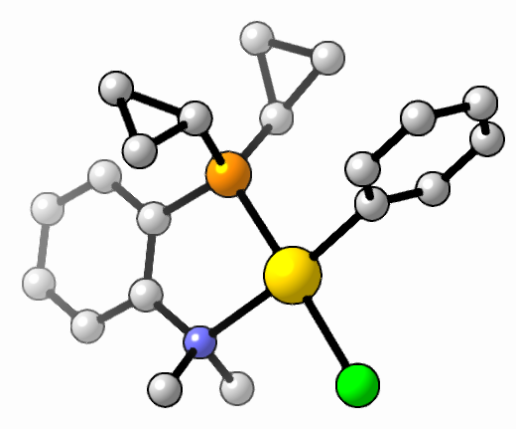
Charge: 0 Multiplicity: 1
Negative Frequency: None

Au	-1.56326000	-0.30797500	-0.24240900
P	0.40920000	0.83804400	0.07424200
C	1.96081400	0.09744500	-0.55295800
C	2.26633200	-1.25089600	-0.28498900
C	3.47912100	-1.78016600	-0.74297500
C	4.37972600	-0.98677100	-1.45520200
C	4.07216400	0.34790600	-1.72729800
C	2.86630300	0.88705700	-1.27891500
N	1.31027000	-2.04967700	0.43633300
H	3.71624000	-2.82058600	-0.54222400
H	5.31758100	-1.41243000	-1.80065000
H	4.76767900	0.96929900	-2.28341900
H	2.63120000	1.92574100	-1.48643400
Cl	-3.65205200	-1.48041100	-0.51008500
C	0.61880900	-2.99903800	-0.44745700
H	0.21664800	-2.46804100	-1.31456700
H	1.28398700	-3.80309400	-0.80656100
H	-0.21610100	-3.45135600	0.09764200
C	1.86925600	-2.73077500	1.60840100
H	1.04564100	-3.15299100	2.19425300
H	2.55709100	-3.55387700	1.35136400
H	2.40875600	-2.01422800	2.23282200
C	0.31021100	2.46129000	-0.68345100
C	-0.73450300	3.50278300	-0.38122100

C	-0.63761500	2.94073900	-1.75976100
C	0.70638600	3.81428600	-0.13384400
H	-1.54197800	3.41281100	0.33399700
H	-0.23240700	3.55565700	-2.56636800
H	-1.41886800	2.24601300	-2.06617500
H	1.03511300	3.84076900	0.90338300
H	1.22803800	4.51057700	-0.79492400
C	0.68280900	1.18068400	1.81297700
C	0.60958500	0.25569400	2.99335500
C	-0.36169700	1.38220600	2.88926300
C	1.88170100	0.99216600	2.71117200
H	0.41521100	-0.80675500	2.96390400
H	-0.26341000	2.24852200	3.54724700
H	-1.38701000	1.12534500	2.62540100
H	2.71026300	0.41692600	2.30211900
H	2.18245400	1.81814800	3.36041200

_S_-Arylation of Methanethiol with [((PCyp$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (11)

SM



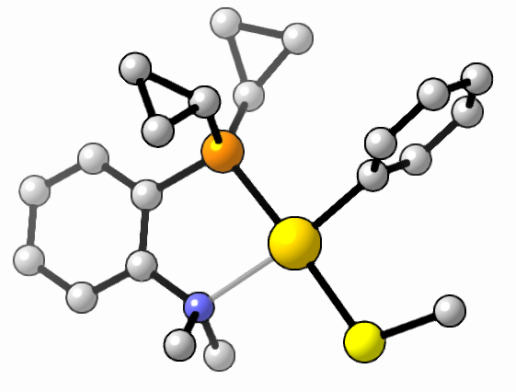
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.45864400	1.20824200	-0.09469200
C	-2.23049900	0.84769300	-0.21798500
C	-2.69367100	-0.47827800	-0.17341300
C	-4.06922800	-0.72021100	-0.23510000
C	-4.96868500	0.33866700	-0.35416500
C	-4.50831900	1.65485800	-0.43052000
C	-3.14132700	1.90849700	-0.36676800
N	-1.75677900	-1.61651300	-0.10887700
Au	0.43409600	-0.92935400	-0.02126500
C	2.30541400	-0.09090000	-0.00624300
C	2.86210400	0.33237200	1.19964700
C	4.13356600	0.91963400	1.19096300
C	4.82657400	1.07933600	-0.01110900
C	4.25297200	0.65004800	-1.21081100
C	2.98183300	0.06533700	-1.21560400
H	-4.44786100	-1.73545500	-0.20142900
H	-6.03267300	0.12944600	-0.39990300
H	-5.20713500	2.47743700	-0.54053100
H	-2.77764900	2.92827700	-0.43908800
H	2.53114600	-0.24952000	-2.15149600
H	4.78596700	0.77577700	-2.14912500
H	4.57370100	1.25310400	2.12654900
H	2.32131000	0.21910000	2.13409200
H	5.80972000	1.54095200	-0.01402200
Cl	1.32897300	-3.20530000	0.12375800
C	-2.01895900	-2.46609100	1.09308200
H	-1.92653300	-1.84968100	1.98839800
H	-3.01866400	-2.90934600	1.05102200
H	-1.27072400	-3.25879800	1.11817800
C	-1.86263400	-2.43428500	-1.35951700
H	-1.65488000	-1.79215300	-2.21721700
H	-1.12092500	-3.23253400	-1.30925500
H	-2.86290500	-2.86797800	-1.45697000
C	-0.08619700	2.06451600	1.44905500
C	-1.10694100	2.85244800	2.25511900
C	-0.62558100	1.52585200	2.76074100
H	0.93874900	2.42492800	1.46239800
H	-2.12721200	2.91307400	1.89117700
H	-0.73582200	3.76100800	2.71939500

H	0.07187100	1.49164700	3.59167000
H	-1.32085100	0.69199400	2.71730500
C	0.03861300	2.22201600	-1.49240100
C	0.03304100	3.74560200	-1.39575400
C	1.33500000	3.00981800	-1.47951900
H	-0.26106400	1.77524000	-2.43690400
H	-0.23307000	4.19819900	-0.44493300
H	-0.33660600	4.27282900	-2.26969100
H	1.88677600	3.01673900	-2.41391000
H	1.96387300	2.96517300	-0.59532800

Int1

Charge: 1 Multiplicity: 1
Negative Frequency: None

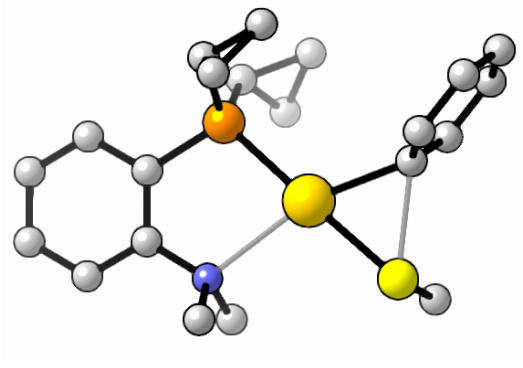


P	-0.78159600	1.18745500	-0.08395400
C	-2.46375800	0.53248800	-0.25751400
C	-2.68710400	-0.85363300	-0.18945700
C	-3.99829200	-1.33540400	-0.26456100
C	-5.06798100	-0.45588900	-0.42842600
C	-4.84506300	0.91839400	-0.53398300
C	-3.54535400	1.40936500	-0.45021500
N	-1.56755800	-1.81593300	-0.07456400
Au	0.50481300	-0.78657300	-0.05824000
C	2.20629400	0.35105700	-0.05013400
C	2.70398700	0.82877600	1.16254300
C	3.84155500	1.64515800	1.15991800
C	4.46795200	1.97529800	-0.04400200
C	3.95781100	1.48945600	-1.25079800
C	2.81917600	0.67632600	-1.26008500
H	-4.19625400	-2.39976700	-0.20725100
H	-6.07690000	-0.85178500	-0.48686600
H	-5.67502900	1.60166800	-0.68131800
H	-3.36311900	2.47481100	-0.54587200
H	2.41953000	0.31130700	-2.20096700
H	4.43880200	1.74529500	-2.19090400
H	4.23188900	2.01991300	2.10212400
H	2.21936100	0.57554200	2.10076400
H	5.34918500	2.61028400	-0.04233500
S	1.73234400	-2.87621600	0.05995800
C	3.52161400	-2.48044100	0.22489900
H	4.04566500	-3.43748400	0.30112400
H	3.88750100	-1.93633100	-0.64788600
H	3.71386800	-1.89026200	1.12295100

C	-1.67929500	-2.60286900	1.19251200
H	-1.64614800	-1.91520000	2.03889100
H	-2.61153600	-3.17573500	1.21911600
H	-0.83169000	-3.28669900	1.25243200
C	-1.56432400	-2.72762000	-1.26262800
H	-0.71052800	-3.40159100	-1.18424700
H	-2.48438100	-3.31818800	-1.30984300
H	-1.46761200	-2.12271100	-2.16563000
C	-0.62152700	2.02040900	1.51619700
C	-1.74850700	2.75321200	2.22204900
C	-1.27264100	1.43139800	2.75203200
H	0.38214000	2.41687900	1.64882400
H	-2.72725200	2.78269800	1.75367500
H	-1.47062100	3.66280300	2.74612700
H	-0.66936800	1.40490000	3.65395700
H	-1.93369700	0.57822200	2.62366600
C	-0.47528000	2.37693700	-1.40372000
C	-0.75396300	3.86441600	-1.22749100
C	0.66216200	3.37563100	-1.29802500
H	-0.65898800	1.94464000	-2.38421700
H	-1.12440700	4.20563100	-0.26536200
H	-1.17934200	4.37531600	-2.08593800
H	1.23366300	3.54052200	-2.20574600
H	1.25960400	3.38895000	-0.39100700

TS_{RE}

Charge: 1 Multiplicity: 1
Negative Frequency: -266.74

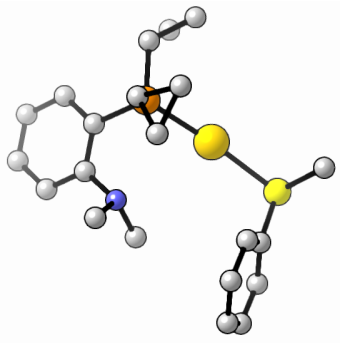


C	3.17300800	0.10426800	-1.06383000
C	2.61447600	-0.21259300	0.17629400
C	3.12994600	0.30581900	1.36940800
C	4.20864600	1.18946400	1.30484700
C	4.77528600	1.53381700	0.07212500
C	4.25708300	0.98945500	-1.10445800
Au	0.42376700	-0.54633100	0.15232600
S	1.90396100	-2.41415300	0.43761200
P	-0.99596900	1.32751500	-0.16099000
C	-2.71428700	0.72008600	-0.06124900
C	-2.99023500	-0.65109800	0.09962800
C	-4.32340800	-1.07846600	0.15821800
C	-5.37039400	-0.16361200	0.06250600
C	-5.09966400	1.19805800	-0.09589800
C	-3.77843700	1.63304500	-0.15821900

N	-1.91209100	-1.62236700	0.19940800
H	-4.54404600	-2.13439700	0.27793100
H	-6.39685200	-0.51478100	0.11068500
H	-5.91121700	1.91520800	-0.17092400
H	-3.57390100	2.69261800	-0.28343500
H	2.76063900	-0.29721100	-1.98278200
H	4.68486300	1.25419000	-2.06746200
H	4.60819000	1.60361200	2.22644300
H	2.69705500	0.02952600	2.32495400
H	5.61774600	2.21743200	0.03186300
C	2.19867100	-3.00163900	-1.27592800
H	2.27116200	-4.09082600	-1.21276900
H	1.37929900	-2.73189000	-1.94342000
H	3.14235400	-2.59599900	-1.64966000
C	-1.93324000	-2.35642400	1.48121800
H	-1.92381900	-1.63655100	2.30307400
H	-2.81379200	-3.00650300	1.57732700
H	-1.03138700	-2.97306800	1.54046800
C	-1.88680700	-2.54356000	-0.95584900
H	-1.00196300	-3.18137100	-0.87074200
H	-2.78082100	-3.18137100	-0.99842500
H	-1.81567500	-1.95967400	-1.87669300
C	-0.82367900	2.62696200	1.08838400
C	-0.36631500	2.25952700	2.48803300
C	0.56659300	2.99857800	1.57282000
H	-1.54795400	3.43450700	1.00255700
H	-0.15271900	1.21354900	2.69651200
H	-0.83115900	2.79775400	3.30858300
H	0.74921500	4.05334500	1.75540000
H	1.41494500	2.45488800	1.16661400
C	-0.83951100	2.11913700	-1.78359900
C	0.54072700	2.34294600	-2.37288400
C	-0.36518500	1.30785800	-2.97574000
H	-1.59046100	2.88288900	-1.97675400
H	1.40129700	1.99849900	-1.80664500
H	0.69442600	3.27587400	-2.90705900
H	-0.84113300	1.52085800	-3.92821700
H	-0.12074900	0.25954300	-2.81892800

Int2

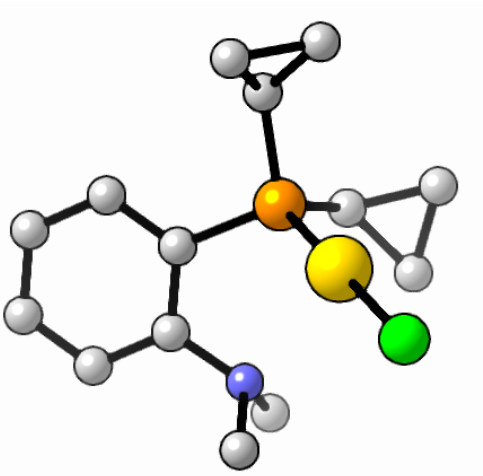
Charge: 1 Multiplicity: 1
Negative Frequency: None



C	-3.19259500	0.34014700	0.96180700
C	-3.31773600	0.11157300	-0.41438900
C	-3.98529800	1.02427000	-1.23501800
C	-4.52559700	2.18380100	-0.67059500
C	-4.40540700	2.42022500	0.70006800
C	-3.74474000	1.49481100	1.51576400
Au	-0.23847200	-1.00045100	-0.41404900
S	-2.53299400	-1.30753000	-1.20917700
P	1.84158500	-0.52712100	0.50438600
C	2.58765000	1.00588600	-0.15419600
C	1.81000200	2.17965300	-0.20161400
C	2.36197500	3.34539500	-0.74546100
C	3.66863900	3.35288000	-1.23561500
C	4.43867600	2.18865900	-1.19021700
C	3.89971100	1.01883100	-0.65422600
N	0.46574800	2.14050300	0.31254500
H	1.76496300	4.25181400	-0.78011400
H	4.08417700	4.26615500	-1.65192800
H	5.45454200	2.18734000	-1.57383500
H	4.50135400	0.11694900	-0.63788500
H	-2.65908700	-0.36363300	1.59202700
H	-3.64634200	1.67649700	2.58172900
H	-5.03943500	2.89866500	-1.30602400
H	-4.07585200	0.83852100	-2.30065500
H	-4.82333300	3.32348800	1.13415000
C	-3.16494800	-2.72380700	-0.22571000
H	-4.24746500	-2.77547700	-0.35489100
H	-2.69018700	-3.61770600	-0.63532200
H	-2.90031100	-2.61298800	0.82590300
C	0.31673600	2.90695600	1.55486900
H	1.06258900	2.57645600	2.28126400
H	0.43062300	3.99376800	1.40124000
H	-0.67968300	2.71917800	1.96802200
C	-0.54535300	2.52424800	-0.68059600
H	-1.53641900	2.33025100	-0.26321300
H	-0.49243000	3.58782100	-0.96767000
H	-0.42478800	1.91173400	-1.57890400
C	3.05738500	-1.84232700	0.21163300
C	2.58773700	-3.27629000	0.04940100
C	3.12123600	-2.53017800	-1.13913300
H	3.99777500	-1.70127000	0.74084700
H	1.51945200	-3.47333600	0.09162900

H	3.20775000	-4.04283700	0.50459300
H	4.10799400	-2.78051900	-1.51707700
H	2.41112900	-2.21386900	-1.89985300
C	1.74186700	-0.40508900	2.31501300
C	0.46017400	-0.02375400	3.02386400
C	0.92718200	-1.44867900	3.06361400
H	2.67774000	-0.08703300	2.77044600
H	-0.39896000	0.22032300	2.40654500
H	0.56055400	0.58358000	3.91838000
H	1.35556700	-1.83786900	3.98244200
H	0.37747200	-2.17985900	2.47570900

P_{Au}



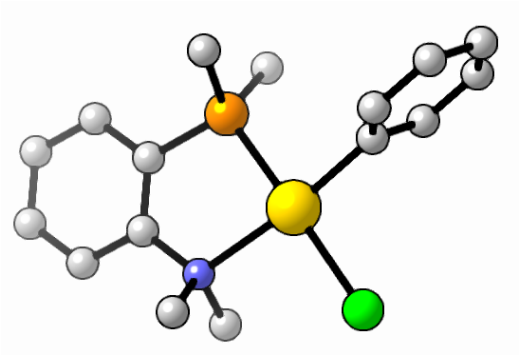
Charge: 0 Multiplicity: 1
Negative Frequency: None

Au	-1.38207600	-0.27407400	-0.32866900
P	0.38423000	0.98954600	0.44700100
C	2.00086000	0.51185300	-0.26337200
C	2.41715700	-0.82607400	-0.13669400
C	3.62313200	-1.23147500	-0.71923700
C	4.41231200	-0.31844700	-1.42083300
C	3.99911500	1.00984800	-1.54767600
C	2.79620900	1.42421300	-0.97407500
N	1.57278800	-1.73146800	0.59628100
H	3.94409300	-2.26422700	-0.61899900
H	5.34768200	-0.64364000	-1.86748300
H	4.60842200	1.72288600	-2.09513200
H	2.47745200	2.45382900	-1.09229700
Cl	-3.22997500	-1.60081300	-1.12817100
C	1.10517200	-2.86459500	-0.20822700
H	0.65535600	-2.49204400	-1.13300400
H	1.90648600	-3.57768700	-0.46662600
H	0.33568700	-3.40219600	0.35567500
C	2.17877300	-2.16702600	1.85820500
H	1.43684700	-2.73036500	2.43326600
H	3.06411100	-2.80905400	1.70974600
H	2.47481300	-1.29181600	2.44160500
C	0.51033500	0.98673200	2.26070500
C	-0.76611300	1.19120900	3.06154300
C	-0.06263300	-0.13372900	3.09809300
H	1.40962100	1.47816400	2.62730800
H	-1.70234000	1.25487700	2.51223800
H	-0.70396900	1.84634700	3.92550800

H	0.48993600	-0.40727700	3.99194800
H	-0.51167000	-0.96967300	2.56930600
C	0.18976100	2.74994400	0.03648200
C	-0.36197700	3.16670400	-1.31387400
C	-1.19681600	3.35339400	-0.07956800
H	0.95638800	3.38725600	0.47339700
H	-0.64863400	2.37814400	-2.00597200
H	0.08595300	4.03847700	-1.78175400
H	-1.32420300	4.35668500	0.31611200
H	-2.05318500	2.69871500	0.06110200

_S_-Arylation of Methanethiol with [((PMe$_2$)Me-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (12)

SM

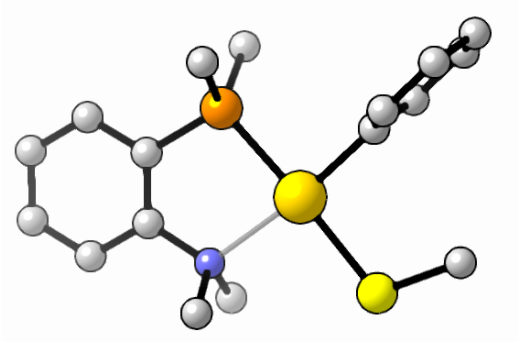


Charge: 1 Multiplicity: 1
Negative Frequency: None

P	0.49661500	-1.54496700	0.00129200
C	2.27107200	-1.17380100	-0.00187300
C	2.71242500	0.15919200	0.00206700
C	4.08567500	0.42220900	-0.00033900
C	5.00477600	-0.62599700	-0.00768700
C	4.56714000	-1.95221700	-0.01055300
C	3.20237300	-2.22562600	-0.00691600
N	1.75646400	1.28404200	0.01469600
C	1.94078400	2.14441400	-1.19544900
Au	-0.42819300	0.57505000	-0.00996400
C	-2.29775800	-0.26944400	-0.00329000
C	-2.92213200	-0.56019800	-1.21539600
C	-4.20370400	-1.12375000	-1.19812500
C	-4.83783700	-1.39496000	0.01655000
C	-4.19461800	-1.10231700	1.22145100
C	-2.91315000	-0.53873500	1.21868200
C	1.91710500	2.08925700	1.26604000
H	4.44726300	1.44423700	0.00402000
H	6.06674300	-0.40190900	-0.01048200
H	5.28258300	-2.76791300	-0.01552900
H	2.86455900	-3.25766900	-0.00768500
H	1.80486300	1.52796300	-2.08583300
H	2.93719900	2.59677300	-1.20659100
H	1.18483100	2.93004700	-1.17428500
H	1.16278700	2.87707100	1.26490200
H	2.91451400	2.53711900	1.31616300
H	1.76335300	1.43401700	2.12512300
H	-2.41470100	-0.31594200	2.15698700
H	-4.68251900	-1.31207200	2.16918900
H	-4.69893700	-1.35047100	-2.13810000
H	-2.43064400	-0.35424600	-2.16115200
H	-5.83012400	-1.83645500	0.02430400
Cl	-1.35172700	2.83239200	-0.01497900
C	0.06557000	-2.51562300	-1.47694700
H	0.60623500	-3.46656500	-1.47048300
H	-1.01130300	-2.70167600	-1.47104600
H	0.33247400	-1.93968100	-2.36620400
C	0.07113600	-2.49777500	1.49255300
H	-1.00587100	-2.68289700	1.49517700

H	0.61156400	-3.44897000	1.49294700
H	0.34411700	-1.91198600	2.37352300

Int1

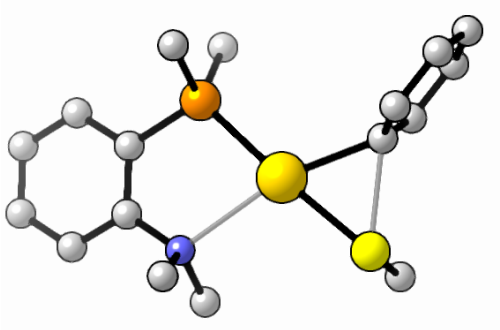


Charge: 1 Multiplicity: 1
Negative Frequency: None

P	0.78128500	-1.58688600	0.01920900
C	2.51329200	-1.04477200	-0.00089400
C	2.81657900	0.32685500	-0.00537600
C	4.15703300	0.72835200	-0.01587500
C	5.17974300	-0.21874600	-0.02401400
C	4.88052300	-1.58277200	-0.02082000
C	3.55050200	-1.99220700	-0.00865500
N	1.75441000	1.35858400	0.00424600
C	1.86112800	2.21591800	-1.21798800
Au	-0.37861900	0.46200700	-0.00405000
C	-2.16179500	-0.54386600	-0.01252600
C	-2.75278900	-0.90038100	1.20003800
C	-3.96762000	-1.59579300	1.18815200
C	-4.57525500	-1.93188100	-0.02380500
C	-3.96732400	-1.57611900	-1.23019600
C	-2.75240200	-0.88079200	-1.23093700
C	1.86128500	2.18952500	1.24491000
H	4.41499300	1.78131400	-0.01766800
H	6.21285300	0.11411800	-0.03280700
H	5.67565900	-2.32121900	-0.02746600
H	3.31863700	-3.05293300	-0.00528100
H	1.76501100	1.58006700	-2.09955500
H	2.81878400	2.74478400	-1.24626100
H	1.04998500	2.94483500	-1.20633300
H	1.04903600	2.91734900	1.24830000
H	2.82015600	2.71577800	1.28376300
H	1.76518000	1.53465400	2.11256400
H	-2.28474000	-0.60448700	-2.17093300
H	-4.43349700	-1.83662800	-2.17644100
H	-4.43361700	-1.87181600	2.13007000
H	-2.28567600	-0.63894500	2.14466600
H	-5.51796800	-2.47134700	-0.02831600
S	-1.46206900	2.62804200	-0.02709400
C	-3.28110800	2.37375600	0.07492500
H	-3.73127700	3.37064600	0.07913000
H	-3.65070800	1.81326600	-0.78573200
H	-3.55592900	1.84888500	0.99166600

C	0.48681200	-2.58702900	1.51634300
H	-0.57066400	-2.86391100	1.54293200
H	1.10468300	-3.48942500	1.50476900
H	0.72400700	-1.98353600	2.39591800
C	0.46395100	-2.63986700	-1.43664500
H	1.06985700	-3.54947700	-1.39625900
H	-0.59718400	-2.90371600	-1.44451400
H	0.70097600	-2.07334200	-2.34044400

TS_{RE}



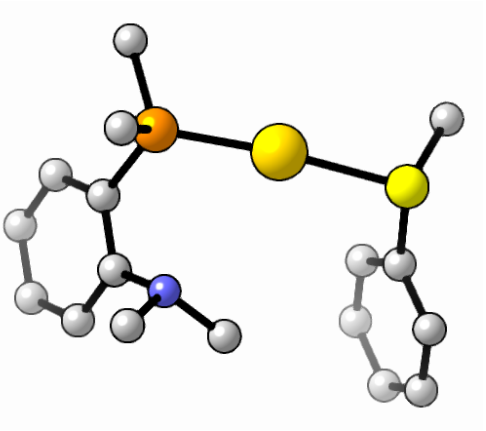
Charge: 1 Multiplicity: 1
Negative Frequency: -269.73

C	-3.04801100	0.46867400	1.24962200
C	-2.62992400	0.08228300	-0.02615000
C	-3.23671000	0.58405800	-1.18352500
C	-4.27228700	1.50976900	-1.04834900
C	-4.70444600	1.91668200	0.21950200
C	-4.09092300	1.39623400	1.36025700
Au	-0.45597400	-0.31952500	-0.17579100
S	-2.02063500	-2.13982000	-0.27538900
P	0.97082900	1.56015800	-0.06054000
C	2.67362100	0.93793800	0.13669100
C	2.95227700	-0.44041900	0.04012400
C	4.27142400	-0.88284100	0.20441300
C	5.30036600	0.02120700	0.46310600
C	5.02722100	1.38820200	0.55566800
C	3.72032100	1.83995000	0.39107600
N	1.89528100	-1.39445800	-0.25261200
C	1.80766200	-2.48505700	0.73831800
C	2.00276300	-1.91877500	-1.63032800
H	4.49685600	-1.94123500	0.12332800
H	6.31591700	-0.34262000	0.58788600
H	5.82530300	2.09662400	0.75481900
H	3.51373300	2.90386500	0.46444200
H	1.71988400	-2.05239300	1.73765200
H	2.67617100	-3.15727700	0.70744800
H	0.90791800	-3.07030200	0.52543600
H	1.13229100	-2.54964000	-1.83281100
H	2.91743500	-2.51189800	-1.77338100
H	2.00364100	-1.08235100	-2.33341100
H	-2.56377800	0.08203500	2.13958600
H	-4.41279400	1.71090800	2.34921300
H	-4.74637100	1.90639900	-1.94199700

H	-2.91228900	0.25469200	-2.16499600
H	-5.51596400	2.63167100	0.31479400
C	-2.18083600	-2.68516100	1.46975800
H	-2.34337100	-3.76579400	1.43352900
H	-1.27978800	-2.47332200	2.04643400
H	-3.04826100	-2.20380900	1.92890400
C	0.97492600	2.63245700	-1.54783500
H	-0.02178700	3.06506700	-1.67384300
H	1.71197200	3.43459500	-1.44334400
H	1.21526700	2.02531900	-2.42440700
C	0.64048300	2.67107500	1.35925800
H	1.34217600	3.50984900	1.38342300
H	-0.38005200	3.05397600	1.26632000
H	0.72097300	2.09636600	2.28547800

Int2

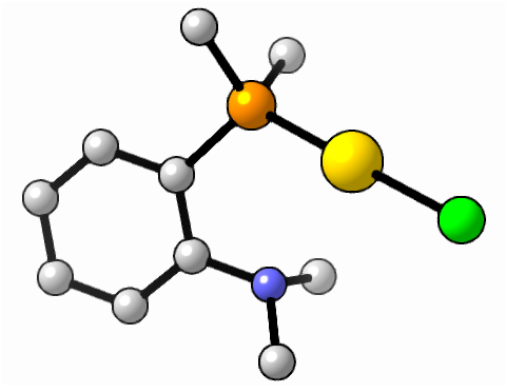
Charge: 1 Multiplicity: 1
Negative Frequency: None



C	2.68393400	-2.37250000	-1.28479900
P	1.99979200	-1.22355900	-0.02923600
C	2.63134000	0.43929500	-0.44902300
C	2.20275700	1.53573100	0.32483800
C	2.62680200	2.82505400	-0.01381600
C	3.47121600	3.02982300	-1.10628900
C	3.90188900	1.94287500	-1.86984600
C	3.48309700	0.65201400	-1.54414700
N	1.33904400	1.28145800	1.44806900
C	0.05723300	1.99417800	1.36644900
Au	-0.31453700	-1.28125800	0.08173700
C	-3.03018100	0.58048800	-0.13184700
C	-3.72269200	1.36553300	0.79366300
C	-3.89607300	2.72929400	0.53950300
C	-3.39034000	3.29512000	-0.63226000
C	-2.70458100	2.49930400	-1.55635500
C	-2.51314500	1.14062400	-1.30701800
C	2.77840400	-1.76661600	1.54105100
C	2.00303200	1.51948600	2.73572000
H	2.29698500	3.66922300	0.58450100
H	3.79426700	4.03578000	-1.35849300
H	4.56013500	2.09627900	-2.71966800
H	3.82172100	-0.17898000	-2.15291800
H	-0.39055100	1.83567900	0.38308300
H	0.15460200	3.07924400	1.53825600

H	-0.62308200	1.58611800	2.12080600
H	1.36355900	1.14177300	3.54076300
H	2.19942200	2.58917400	2.92177600
H	2.95695800	0.98657300	2.76696700
S	-2.74988300	-1.15189500	0.28794700
C	-3.40595500	-2.03531100	-1.18197700
H	-2.90060000	-1.70272000	-2.08853400
H	-3.21219800	-3.09689000	-1.01527600
H	-4.47996100	-1.85019800	-1.24179800
H	-4.11767600	0.92127000	1.70192700
H	-1.95149000	0.53137900	-2.00823100
H	-4.42898700	3.34417000	1.25842300
H	-3.52687500	4.35475000	-0.82627600
H	-2.30476500	2.93820100	-2.46550400
H	2.57083300	-2.83224000	1.67580300
H	2.34573200	-1.21032300	2.37243100
H	3.85967600	-1.60425300	1.50075700
H	2.33331600	-3.37867500	-1.03970600
H	2.31685600	-2.10725700	-2.27927300
H	3.77802600	-2.36149100	-1.27521800

P_{Au}



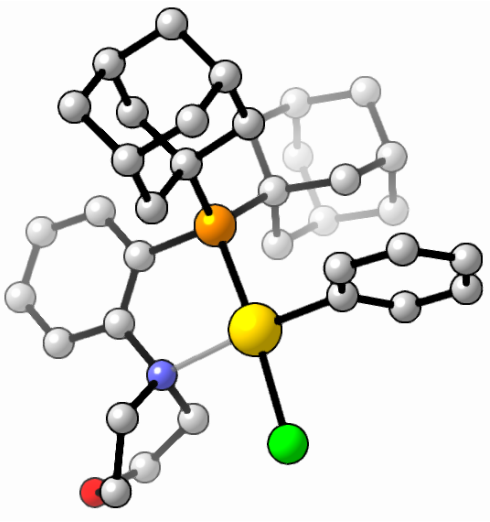
Charge: 0 Multiplicity: 1
Negative Frequency: None

Au	-1.41517800	0.20922600	-0.11882600
C	2.06720000	-0.98331100	0.03558100
C	2.05072400	0.43436500	-0.02533100
C	3.24040300	-1.66006100	-0.33461500
C	3.22143100	1.11928800	-0.39311600
C	4.38446700	-0.96419500	-0.72139900
H	3.26101000	-2.74412600	-0.30198700
C	4.38410800	0.43143700	-0.73621800
H	3.22917800	2.20340800	-0.43567800
H	5.28010100	-1.51423800	-0.99633500
H	5.27407800	0.98215100	-1.02495800
C	0.73219400	-1.77810700	1.90725900
H	-0.30318400	-2.05636400	2.13010300
H	1.40783800	-2.52393600	2.35948600
H	0.93440800	-0.81197100	2.37153700
C	0.65274400	-2.97306000	-0.19962800
H	1.29200500	-3.79116200	0.17300200
H	-0.39060800	-3.25163800	-0.01741600
H	0.80052800	-2.87268500	-1.27786600

N	0.90668800	-1.69165100	0.45376700
P	0.51818000	1.39764200	0.25672400
C	0.64637100	2.88662600	-0.81255500
C	0.60426000	2.09301300	1.95823700
Cl	-3.45904100	-1.01022600	-0.49970900
H	-0.22687800	2.79261000	2.08600800
H	0.50981100	1.29835600	2.70080900
H	1.55285500	2.61928100	2.10183300
H	-0.28657900	3.44748700	-0.70975100
H	0.76378200	2.58056600	-1.85500600
H	1.48144300	3.52823900	-0.51800000

_S_-Arylation of Methanethiol with [(Mor-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (16)

SM



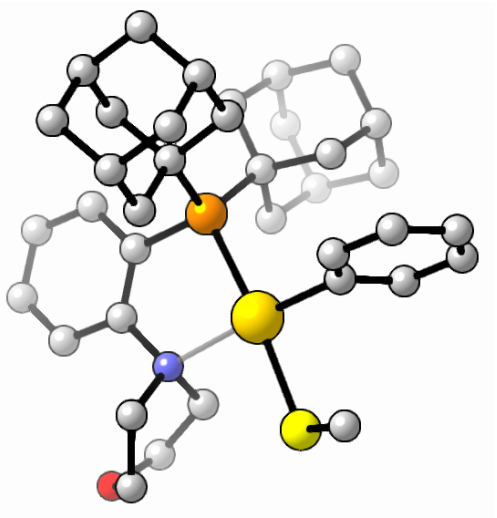
Charge: 1 Multiplicity: 1
Negative Frequency: None

C	3.77106500	1.84826600	-3.01896600
C	2.81207000	0.68506100	-3.33012100
C	1.71005900	1.15906200	-4.29597300
C	0.92065600	2.30807900	-3.64062900
C	1.87116700	3.47780600	-3.31952800
C	2.97724300	2.99240600	-2.36295500
C	2.16835600	0.18047200	-2.02031300
C	1.36519000	1.32374700	-1.34815600
C	0.26523000	1.80529200	-2.33563000
C	2.33783700	2.49647400	-1.04428600
P	0.46872600	0.70082900	0.20163800
C	-0.75992900	1.97309300	0.69746700
C	-2.13192100	1.67555600	0.77909700
C	-3.02054400	2.63480100	1.28357500
C	-2.57037100	3.89927300	1.65284200
C	-1.22119500	4.22388100	1.52277500
C	-0.32738700	3.26468200	1.05866700
N	-2.65910800	0.38746800	0.30044600
C	-3.40051800	0.57263500	-1.00793900
Au	-1.00324000	-1.11099300	-0.26052000
C	0.36871000	-2.54614900	-0.80957800
C	1.00266900	-3.32437400	0.15473800
C	1.85615900	-4.35818100	-0.25318000
C	2.05609900	-4.61182500	-1.61043400
C	1.38673200	-3.84339700	-2.56649200
C	0.53141200	-2.81035300	-2.16991000
C	1.53634600	0.33258000	1.72525700
C	2.02603300	1.61796400	2.44953800
C	2.85872900	1.22870500	3.69444400
C	4.07034500	0.37473000	3.27831900
C	3.57114400	-0.90426500	2.58078300
C	2.77277800	-0.50916300	1.31877500
C	1.97168100	0.43328400	4.67017200
C	1.47168200	-0.84410800	3.97101400
C	0.64734800	-0.46395300	2.72202400
C	2.67485900	-1.70797900	3.54293100
C	-3.55807500	-0.27999100	1.33917100
H	-4.07074000	2.38704700	1.38059600
H	-3.27872900	4.62765900	2.03449000

H	-0.85754300	5.20883500	1.79645400
H	0.71881000	3.52672400	1.00016800
H	-0.41982300	0.97949800	-2.56933900
H	-0.32593400	2.61154000	-1.88720000
H	0.12440700	2.64780100	-4.31379500
H	-3.53368600	-0.42446300	-1.42617000
H	-2.75400700	1.13606200	-1.68283100
H	1.03543300	0.32663200	-4.53745100
H	2.15676500	1.50066600	-5.23855000
H	3.36613200	-0.14924800	-3.77720300
H	4.57184200	1.50994200	-2.34795500
H	4.24722900	2.20352300	-3.94191600
H	3.64978300	3.82339600	-2.11838300
H	1.81369000	3.33473000	-0.57991400
H	3.12650800	2.17032800	-0.35816100
H	2.31974500	3.86006100	-4.24535900
H	1.31195500	4.30531200	-2.86288000
H	2.94971100	-0.19433700	-1.35436900
H	1.50916500	-0.65576500	-2.24410400
H	2.63366700	2.23727000	1.78198500
H	1.17233700	2.21557200	2.77943300
H	3.20010900	2.15547500	4.17118600
H	-3.47774700	0.29665400	2.26040600
H	-3.19238000	-1.28709700	1.53826900
H	4.66616000	0.11523800	4.16281600
H	4.72190600	0.94369500	2.60180800
H	4.42394500	-1.51773200	2.26648000
H	2.32893900	-2.63015100	3.05761800
H	3.25189100	-2.00751800	4.42703100
H	0.82451300	-1.41414900	4.64822100
H	0.26412600	-1.37814000	2.25798000
H	-0.22383100	0.13784200	3.00999400
H	2.47222100	-1.40379300	0.76764900
H	3.42282300	0.07846200	0.66232700
H	2.54398900	0.16990200	5.56888500
H	1.11980000	1.04593500	4.99352500
H	0.00423200	-2.22866300	-2.91948600
H	1.52137700	-4.04464200	-3.62558400
H	2.35836900	-4.95902100	0.49980800
H	0.84214900	-3.15359500	1.21269300
H	2.72178800	-5.41090400	-1.92323700
C	-5.01175200	-0.34106100	0.86778800
H	-5.14805000	-1.13613800	0.12256600
H	-5.65443400	-0.56493100	1.72282200
C	-4.76421300	1.26489300	-0.86287700
H	-5.38023500	0.97443900	-1.72586900

H	-4.66464700	2.35308900	-0.86670100
O	-5.42732300	0.92145500	0.35740900
Cl	-2.68061700	-2.85403500	-0.67406500

Int1



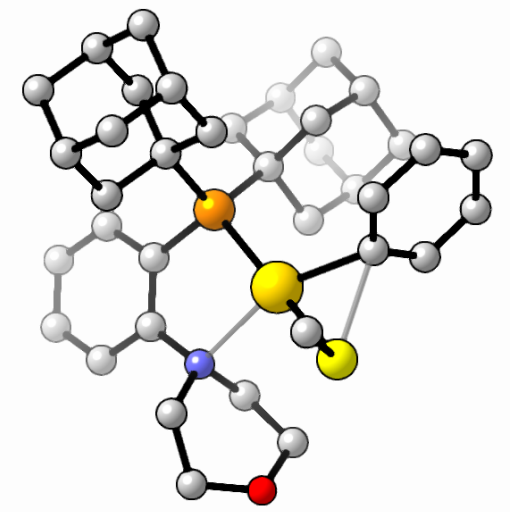
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.64665500	-0.72029100	0.11061600
C	0.32614800	-2.24839400	0.41227500
C	1.72853400	-2.21129700	0.52014200
C	2.42521400	-3.37408100	0.88140700
C	1.75532200	-4.57848800	1.07685200
C	0.37216400	-4.63969400	0.91578200
C	-0.32959900	-3.48205400	0.59745800
N	2.49218100	-0.98400100	0.22336800
C	3.22739600	-1.13239100	-1.09173300
Au	1.15003500	0.88748100	-0.14150800
C	0.06557400	2.59828600	-0.48465400
C	-0.46798800	3.31195100	0.58672700
C	-1.16152200	4.50440300	0.34481600
C	-1.30356700	4.98391300	-0.95772800
C	-0.74119200	4.27402100	-2.02265400
C	-0.04849400	3.08177100	-1.78991500
C	3.46565200	-0.64743800	1.35146900
H	3.50032800	-3.33249000	1.00705900
H	2.31962500	-5.46510800	1.34849400
H	-0.16310800	-5.57349000	1.05419500
H	-1.40500700	-3.54177300	0.51225500
H	3.55205600	-0.13437800	-1.38597000
H	2.51060800	-1.47740400	-1.83902700
H	3.25552300	-1.32399900	2.17961400
H	3.28283900	0.37205100	1.69029800
H	0.39878900	2.54596600	-2.62087900
H	-0.83238300	4.64708900	-3.03908300
H	-1.58339400	5.05283300	1.18251300
H	-0.34325400	2.96792500	1.60717800
H	-1.83965000	5.91017300	-1.14296800
S	3.13030200	2.28100700	-0.41001400
C	2.75786300	3.97513300	0.19469600
H	2.33466400	3.94949400	1.20062000
H	3.71564100	4.50358600	0.22082000
H	2.07439300	4.49715700	-0.47730300
C	-1.65957600	-0.40407300	1.68203300

C	-2.71839500	0.69559200	1.40943100
C	-2.38283400	-1.65998900	2.23912700
C	-0.65493700	0.08517100	2.76404900
H	-3.45627900	0.32951400	0.68771400
H	-2.25287300	1.58633500	0.97859700
C	-3.44763800	1.05929400	2.72101600
H	-1.65585900	-2.44270800	2.47298800
H	-3.08525800	-2.06469700	1.50273900
C	-3.14396000	-1.29552200	3.53598300
H	-0.10815200	0.96747700	2.41499600
H	0.09201700	-0.69504200	2.95930500
C	-1.40873400	0.44036700	4.06333700
H	-4.17302500	1.85223300	2.50185500
C	-4.17679100	-0.18900500	3.25216500
C	-2.43220000	1.55537200	3.76857600
H	-3.65316700	-2.19854700	3.89434500
C	-2.13842300	-0.80683400	4.59561700
H	-0.67760000	0.79085500	4.80195900
H	-4.91335300	-0.53731200	2.51571100
H	-4.72551700	0.05557100	4.17097000
H	-1.91988300	2.45522700	3.40289200
H	-2.95519500	1.83604000	4.69187600
H	-2.66326700	-0.56540400	5.52903900
H	-1.41402000	-1.59977700	4.82448500
C	-1.63194400	-0.97338400	-1.48802200
C	-0.61832400	-1.49875500	-2.54354100
C	-2.80569900	-1.97920400	-1.35623900
C	-2.19767400	0.38246200	-1.98720600
H	-0.19264400	-2.45571800	-2.22102000
H	0.21072100	-0.78606000	-2.65252100
C	-1.32335100	-1.67976000	-3.90505900
H	-3.53554800	-1.61939200	-0.62290200
H	-2.44991900	-2.95674400	-1.02121200
C	-3.49765200	-2.15458200	-2.72860300
H	-1.39098000	1.10712700	-2.08910900
H	-2.91188300	0.79614800	-1.27045100
C	-2.89488600	0.19931600	-3.35211800
H	-0.58851600	-2.05919300	-4.62556100
C	-2.47782100	-2.68974000	-3.75279700
C	-1.87742900	-0.32424700	-4.38289900
H	-4.31589900	-2.87491000	-2.60726200
C	-4.05570000	-0.80171500	-3.20741900
H	-3.27953800	1.17581500	-3.67150600
H	-2.08785000	-3.66278600	-3.42505200
H	-2.96852500	-2.84599000	-4.72218900
H	-1.05799200	0.39718900	-4.50411300

H	-2.35821300	-0.43929400	-5.36307400
H	-4.56995800	-0.92708600	-4.16921500
H	-4.79505900	-0.42225600	-2.48931900
C	4.44300900	-2.07093900	-1.03873300
H	5.12509400	-1.78173100	-1.85102400
H	4.15212700	-3.11277300	-1.19427300
C	4.92065100	-0.78850500	0.90189800
H	5.22234600	0.06404200	0.27843200
H	5.56624400	-0.80574100	1.78355100
O	5.12244300	-2.02182100	0.21923400

TS_{RE}



Charge: 1 Multiplicity: 1
Negative Frequency: -238.04

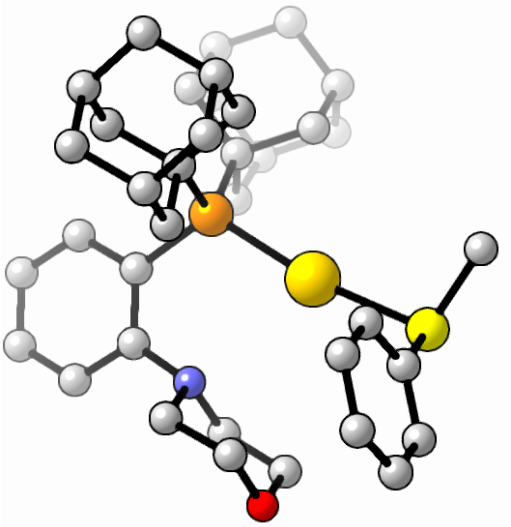
C	-1.10634000	3.40477800	-0.55119400
C	-0.97459500	2.35624000	-1.46735500
C	-0.14507100	2.45474800	-2.58299900
C	0.61472400	3.61836500	-2.75120600
C	0.52815400	4.66455800	-1.83014300
C	-0.33823600	4.55689300	-0.73762100
Au	-1.24754200	0.37844600	-0.53477300
S	-3.08855100	1.26944300	-1.79703600
P	0.70492200	-0.58628000	0.43768500
C	0.12628800	-1.93556800	1.53821300
C	-1.24890200	-2.21654400	1.68857800
C	-1.64445200	-3.31778900	2.46310800
C	-0.70749500	-4.14412600	3.07677100
C	0.65400100	-3.87220100	2.93352100
C	1.05928100	-2.78051700	2.17155800
N	-2.27293600	-1.36276300	1.11182800
C	-2.88288500	-0.52918600	2.18975100
C	1.72489500	-1.41106100	-0.93844400
C	3.18214600	-1.76039000	-0.54595500
C	3.89531100	-2.44919100	-1.73184200
C	3.92889400	-1.48857600	-2.93554400
C	2.48609800	-1.14500900	-3.35075300
C	1.75000900	-0.47040300	-2.17493500
C	1.73408400	-2.43073100	-3.74254600
C	1.70023000	-3.38498800	-2.53405900
C	3.14106700	-3.73783000	-2.11323600
C	0.97663100	-2.71106400	-1.34807900
C	1.63037600	0.68220500	1.48458800
C	2.23545700	1.75479000	0.54072600

C	2.87897300	2.88297000	1.37537700
C	4.00150000	2.28940600	2.24873500
C	3.40463500	1.23889500	3.20587200
C	2.74474700	0.10126500	2.39259200
C	1.81373500	3.54101100	2.27338100
C	1.22580400	2.48537200	3.23001700
C	0.57145700	1.35849900	2.40195500
C	2.34646500	1.90000400	4.10903200
C	-3.31583100	-2.09476300	0.31425700
H	-2.70238600	-3.52649000	2.58926200
H	-1.04099100	-4.99197900	3.66734500
H	1.39732500	-4.50684300	3.40559900
H	2.11932100	-2.59481400	2.05756200
H	-0.23934200	1.78356600	1.79887200
H	0.13024700	0.61055200	3.07333900
H	0.45428000	2.94299000	3.86169700
H	-2.12220500	0.16087000	2.56244800
H	-3.18775300	-1.16373500	3.03242600
H	1.01864200	3.97488900	1.65483900
H	2.26383200	4.35980400	2.84999300
H	3.29432300	3.62823900	0.68568600
H	4.77016200	1.82840000	1.61361900
H	4.49067900	3.08529300	2.82557200
H	4.20042400	0.80302900	3.82257700
H	2.31795100	-0.62910700	3.08789600
H	3.50767000	-0.41185000	1.80012000
H	2.80684400	2.69548100	4.70968200
H	1.93254600	1.16142100	4.80876900
H	3.00243600	1.30509500	-0.09939000
H	1.45991900	2.16701000	-0.11433900
H	0.93688500	-3.41058200	-0.50703800
H	-0.06110400	-2.47384800	-1.62261700
H	1.15500300	-4.30017700	-2.79631500
H	-3.06450600	-3.15681300	0.25663700
H	-3.31029900	-1.69276300	-0.70413500
H	3.65922800	-4.24472400	-2.93779100
H	3.12638400	-4.43224700	-1.26234200
H	4.91868800	-2.69485200	-1.42232000
H	4.47497000	-0.57257000	-2.67232500
H	4.46097300	-1.95514500	-3.77491300
H	2.49680500	-0.44610500	-4.19655400
H	2.22385100	0.48628100	-1.93545600
H	0.72292000	-0.25127700	-2.48263700
H	3.73139200	-0.85216100	-0.27676000
H	3.20316700	-2.42813200	0.32122500
H	2.23206700	-2.91679700	-4.59178200

H	0.71120400	-2.18651400	-4.06058300
H	-1.78815900	3.32801400	0.28901800
H	-0.42736200	5.37170300	-0.02473100
H	1.28196900	3.69167500	-3.60541700
H	-0.05785300	1.64317000	-3.29439800
H	1.12219000	5.56274300	-1.96777900
C	-2.74882600	0.68925900	-3.50516100
H	-3.72304900	0.45525100	-3.94360900
H	-2.27138000	1.48253500	-4.08588800
H	-2.12997400	-0.20909400	-3.50727100
C	-4.07392100	0.27096600	1.67776400
H	-3.73360600	1.05611000	0.99250400
H	-4.55516200	0.75965800	2.53481900
C	-4.71324700	-1.90610900	0.89580800
H	-5.44856100	-2.35342800	0.22156500
H	-4.81118300	-2.40405400	1.87218000
O	-5.04637700	-0.52468600	0.98993400

Int2

Charge: 1 Multiplicity: 1
Negative Frequency: None



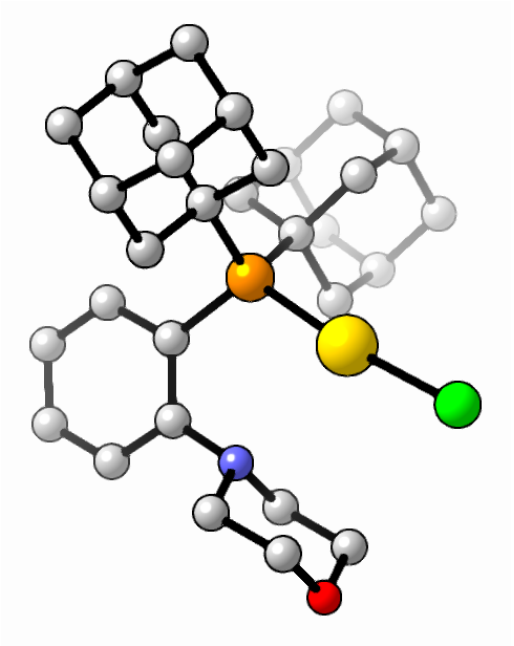
C	5.04976600	-1.12509800	-1.00444200
C	3.84410000	-0.62856700	-1.50631700
C	3.62221700	0.75113400	-1.61107900
C	4.62023200	1.63648800	-1.20757000
C	5.82681000	1.14844400	-0.69330400
C	6.04023800	-0.22749200	-0.59437000
Au	0.67893100	-0.90987500	-0.59095700
S	2.54399200	-1.81648900	-1.89546900
P	-1.18191000	0.16360800	0.32993500
C	-1.28058700	0.06974700	2.16701200
C	-0.20634700	-0.36702100	2.97665500
C	-0.37754400	-0.41430800	4.36962200
C	-1.57231300	-0.03481900	4.97411200
C	-2.63094400	0.40990500	4.18187300
C	-2.47809200	0.46065100	2.79948400
N	1.06546900	-0.74544700	2.41403700
C	1.41725600	-2.15396400	2.67619800
C	-1.00997400	2.00653600	-0.07297400
C	-2.08824100	2.91622700	0.57175400
C	-1.81812600	4.39380300	0.20118400
C	-1.84399200	4.56084500	-1.33071600
C	-0.75051600	3.67606100	-1.96163000

C	-1.02930400	2.19915300	-1.61131000
C	0.63138000	4.08744900	-1.41792600
C	0.64695100	3.92803500	0.11465300
C	-0.44056500	4.81984400	0.74253500
C	0.37429800	2.45429400	0.47828500
C	-2.73939500	-0.66580700	-0.39995800
C	-2.44957000	-1.05528100	-1.88163600
C	-3.63473000	-1.84489000	-2.47709100
C	-4.91159900	-0.98628200	-2.42941500
C	-5.21471300	-0.61869400	-0.96582400
C	-4.03326900	0.19003000	-0.38295400
C	-3.84434100	-3.13594900	-1.66351400
C	-4.15052000	-2.76819400	-0.19956700
C	-2.96923500	-1.97702300	0.40181700
C	-5.42450800	-1.90182800	-0.13817900
C	2.16237300	0.14693700	2.83470700
H	0.44841300	-0.74975500	4.98885200
H	-1.67271400	-0.08041300	6.05459000
H	-3.56988000	0.71746300	4.63176300
H	-3.31038400	0.81358500	2.20605100
H	-2.05561200	-2.58809200	0.38080300
H	-3.18315700	-1.75123200	1.45150100
H	-4.29328900	-3.68093200	0.39230400
H	0.62599800	-2.79246200	2.26955600
H	1.50371900	-2.35629400	3.75682300
H	-2.94491700	-3.76465200	-1.71490900
H	-4.67334800	-3.71840800	-2.08672300
H	-3.39176200	-2.09535200	-3.51741200
H	-4.77781000	-0.07496300	-3.02785200
H	-5.75521900	-1.53973800	-2.86254400
H	-6.11502300	0.00637700	-0.91679200
H	-4.29216500	0.50395600	0.63171000
H	-3.89232400	1.09751000	-0.97943100
H	-6.28083700	-2.46486600	-0.53205100
H	-5.65610000	-1.64499200	0.90442700
H	-2.25872400	-0.16220100	-2.48535300
H	-1.54750000	-1.67583200	-1.93571000
H	0.38742800	2.33627300	1.56828200
H	1.17564000	1.82479300	0.07252800
H	1.63292500	4.20536400	0.50826100
H	2.32826400	0.10055300	3.92423700
H	1.90238500	1.17602300	2.57492600
H	-0.25032600	5.87393700	0.50093000
H	-0.41885700	4.72715600	1.83676100
H	-2.60333800	5.01097300	0.65540200
H	-2.82965600	4.27957400	-1.72571300

H	-1.67592400	5.61308100	-1.59551900
H	-0.76805500	3.78404700	-3.05325500
H	-2.00644400	1.91472900	-2.01717000
H	-0.27902700	1.55137600	-2.08390400
H	-3.09028700	2.63808000	0.23416800
H	-2.06693900	2.80860300	1.66155000
H	0.84739100	5.12900000	-1.68963700
H	1.41593800	3.46545400	-1.87083400
H	5.20960000	-2.19548400	-0.92248100
H	6.97577900	-0.60861800	-0.19641900
H	4.44802300	2.70613700	-1.28150700
H	2.67500100	1.12963300	-1.98149200
H	6.59702200	1.84168800	-0.36892400
C	2.10075100	-1.37532400	-3.62197600
H	2.96348000	-1.57016500	-4.26159700
H	1.26664800	-2.02309600	-3.89958300
H	1.79408800	-0.33089700	-3.68292000
C	2.74752800	-2.49599100	2.00674300
H	2.63314900	-2.47068400	0.91291100
H	3.06179500	-3.50332200	2.29488700
C	3.44553100	-0.25578000	2.12132000
H	3.32892200	-0.11186300	1.03922500
H	4.28277700	0.35733600	2.46566800
O	3.78752000	-1.61125600	2.40753200

P_{Au}

Charge: 0 Multiplicity: 1
Negative Frequency: None



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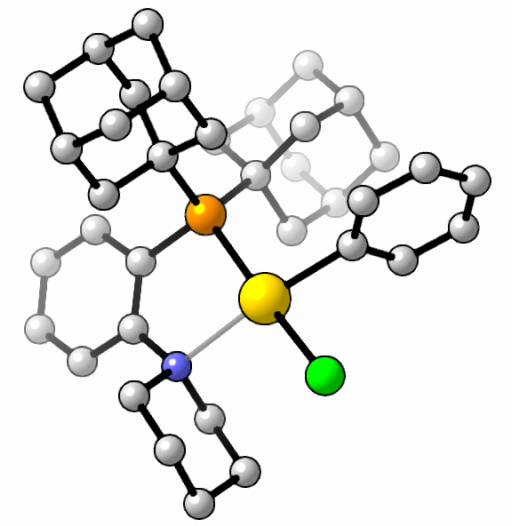
P	0.49984200	0.07530500	0.28218100
C	-0.07632700	0.04403200	2.03534800
C	-1.43225000	-0.12179200	2.40074800
C	-1.78305900	-0.10050500	3.76073000
C	-0.82973100	0.06574700	4.76057100
C	0.51188900	0.21544700	4.40861500
C	0.87360400	0.20711700	3.06463000
N	-2.46371700	-0.32047000	1.41767700
C	-3.42988000	0.78926800	1.35639800
C	1.90006000	-1.21264900	0.11904900
C	3.28250600	-0.78899200	0.67976000
C	4.29907500	-1.94322900	0.52244900
C	4.47351600	-2.27436800	-0.97048600
C	3.11517200	-2.70872700	-1.55053500

C	2.08733800	-1.56888900	-1.38618200
C	2.60850100	-3.96056300	-0.80950700
C	2.43759100	-3.63057600	0.68522400
C	3.79102200	-3.18794500	1.27633000
C	1.41168400	-2.49037700	0.85725300
C	1.03606900	1.86834000	-0.03048900
C	1.65939000	1.96706100	-1.44708600
C	1.96508200	3.43999400	-1.79135600
C	2.96948800	4.00132200	-0.76611900
C	2.35269300	3.93039300	0.64384700
C	2.02795600	2.46174300	1.00371500
C	0.66336300	4.26395400	-1.75134900
C	0.05714000	4.19693900	-0.33577400
C	-0.26095700	2.72796100	0.01302500
C	1.05968900	4.76606800	0.68556300
C	-3.14666200	-1.61875300	1.56063100
H	-2.82685800	-0.21937100	4.03437800
H	-1.13172500	0.07697100	5.80388100
H	1.27487900	0.34171300	5.17066300
H	1.91873500	0.33248000	2.81886000
H	-1.00104000	2.33769200	-0.69697700
H	-0.70783400	2.67124400	1.01385200
H	-0.87675700	4.77211600	-0.30306600
H	-2.88511600	1.71729000	1.15779700
H	-3.97565100	0.90817100	2.30850100
H	-0.05270700	3.87294500	-2.48705200
H	0.87113000	5.30759500	-2.02215900
H	2.39927800	3.47947300	-2.79824700
H	3.90381500	3.42450900	-0.79973600
H	3.22019300	5.04127000	-1.01401900
H	3.06779300	4.31472200	1.38207100
H	1.58723400	2.43379700	2.00514100
H	2.95563700	1.88323300	1.03526900
H	1.28097100	5.81598100	0.45181200
H	0.62615500	4.74130700	1.69451600
H	2.58973800	1.38975400	-1.49167200
H	0.97364200	1.54061100	-2.19091400
H	1.27493400	-2.28490300	1.92430400
H	0.43455400	-2.79766300	0.45817700
H	2.06895400	-4.51362600	1.22224900
H	-3.66140100	-1.70539400	2.53269900
H	-2.39546200	-2.41350900	1.50026600
H	4.52292800	-4.00197200	1.19060000
H	3.67958000	-2.96207700	2.34558100
H	5.25698800	-1.61738500	0.94689200
H	4.85211800	-1.39590300	-1.51052600

H	5.21221300	-3.07717600	-1.09577700
H	3.21911300	-2.92655000	-2.62101900
H	2.41574100	-0.69081400	-1.95177000
H	1.13045500	-1.88614200	-1.81655700
H	3.65372100	0.09106100	0.14369100
H	3.21814000	-0.52499500	1.73855900
H	3.32074800	-4.78709500	-0.93358400
H	1.65061600	-4.28902100	-1.23540400
C	-4.43554500	0.53159900	0.23868400
H	-3.92335900	0.53984200	-0.73501500
H	-5.20665300	1.30776700	0.24031500
C	-4.17328500	-1.79217900	0.44497500
H	-3.66639000	-1.86488500	-0.52730700
H	-4.75355300	-2.70487300	0.61084400
Cl	-2.66556500	-0.98487100	-3.08368400
O	-5.10702600	-0.71265700	0.42871100

_S_-Arylation of Methanethiol with [(Pip-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (17)

SM



Charge: 1 Multiplicity: 1
Negative Frequency: None

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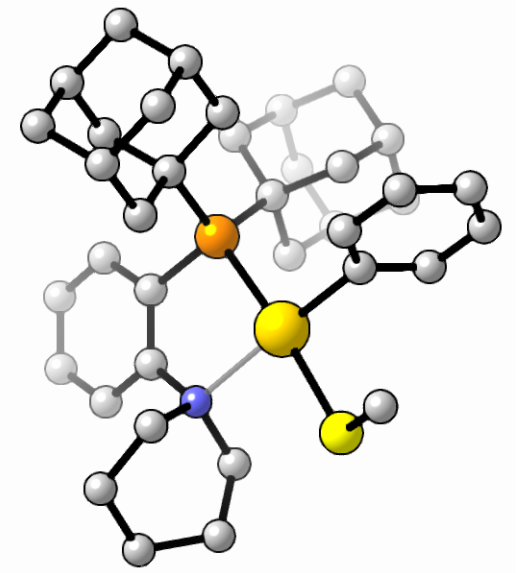
C	-3.17630600	-1.77946300	3.58235500
C	-3.89063900	-0.66811900	2.79152600
C	-4.73887200	-1.29002200	1.66749400
C	-3.81671200	-2.07368600	0.71656100
C	-1.20061900	-1.59090800	2.03005100
C	-1.91336200	-0.47958900	1.20981200
C	-2.83604100	0.29571700	2.19499400
C	-2.78938400	-1.10497000	0.09172800
P	-0.54346500	0.57520700	0.42807500
C	0.30548000	1.49584800	1.75412100
C	1.68850100	1.37721300	1.94989100
C	2.29371400	2.12624300	2.97245600
C	1.55616000	2.99776100	3.76574600
C	0.18802700	3.15188800	3.54328700
C	-0.42568200	2.40754000	2.54405600
N	2.54025300	0.51429300	1.10304400
C	3.19102800	-0.52082700	2.00405500
Au	1.23988000	-0.72951700	-0.49266600
C	0.06667300	-2.11323300	-1.51665300
C	-0.43920700	-1.90053000	-2.79414900
C	-1.20118100	-2.90756300	-3.39989100
C	-1.42527400	-4.11884900	-2.74451500
C	-0.85687600	-4.33878800	-1.48860100
C	-0.09757600	-3.33877400	-0.87053900
C	-1.10051900	1.88931500	-0.83401100
C	0.02507000	2.95455200	-0.95238300
C	-0.37860400	4.02739200	-1.98930900
C	-1.68282000	4.71088000	-1.53544200
C	-2.80485000	3.65981100	-1.44201900
C	-2.42021500	2.58235200	-0.40210500
C	-0.58963900	3.37201900	-3.36687200
C	-1.70808100	2.31861600	-3.25859900
C	-1.29130300	1.24714000	-2.22802900
C	-3.01884100	2.99242000	-2.81316900
C	3.56578500	1.40025400	0.41940600
H	3.35840600	2.04215200	3.15369000
H	2.05608700	3.56293600	4.54585000

H	-0.39821700	3.84473100	4.13782700
H	-1.48283400	2.54971900	2.37385500
H	-2.24696300	0.70487600	3.01940400
H	-3.34540900	1.12528700	1.69769900
H	-4.53085200	-0.08407700	3.46389500
H	2.38981100	-1.18443100	2.34111900
H	3.58590600	-0.00682000	2.88598600
H	-2.59640100	-1.34484300	4.40742200
H	-3.91485500	-2.45990200	4.02557000
H	-1.71538800	-3.33980300	3.17981900
H	-2.43216900	-3.74881600	0.81522500
H	-3.80907900	-3.88859000	1.91436200
H	-4.40394800	-2.51752900	-0.09643500
H	-3.32357000	-0.31762200	-0.45151300
H	-2.17326700	-1.64074100	-0.63100300
H	-5.49644400	-1.95811700	2.09725300
H	-5.27236300	-0.50477700	1.11522600
H	-0.51310700	-2.15595200	1.39941000
H	-0.60492500	-1.13504400	2.83106900
H	0.20831000	3.43598100	0.01271600
H	0.96126100	2.47652400	-1.26805000
H	0.42996600	4.76610700	-2.04586700
H	3.98887800	2.07968000	1.16565500
H	3.01531500	2.00580500	-0.30490900
H	-1.96307400	5.49505600	-2.25034800
H	-1.53736000	5.19559300	-0.56083000
H	-3.73503600	4.13476000	-1.10765600
H	-3.82520100	2.24958900	-2.75001100
H	-3.32478800	3.74331000	-3.55282000
H	-1.85105200	1.82319100	-4.22656500
H	-2.03244800	0.44252900	-2.19833100
H	-0.34017500	0.81223000	-2.54622600
H	-3.23100800	1.85155400	-0.32909600
H	-2.30911800	3.05852700	0.57642300
H	-0.86003600	4.13500400	-4.10803900
H	0.34151300	2.90065600	-3.70906200
H	0.35311500	-3.53709900	0.09526500
H	-0.99583100	-5.28766900	-0.97836200
H	-1.61117300	-2.73406400	-4.39083400
H	-0.24918000	-0.98401400	-3.33400900
H	-2.02179900	-4.89359200	-3.21681500
C	4.70547900	0.63226200	-0.24017700
H	4.33929600	0.08999500	-1.11249100
H	5.42692000	1.37724200	-0.59665900
C	4.32964000	-1.29117700	1.34396500
H	3.94274100	-1.95836700	0.57187200

H	4.78144900	-1.91988000	2.12049600
C	5.37065200	-0.33845300	0.74321200
H	5.85557000	0.23031300	1.54956500
H	6.15589800	-0.90963600	0.23577200
Cl	2.96767600	-1.91167100	-1.80130000

Int1

Charge: 1 Multiplicity: 1
Negative Frequency: None



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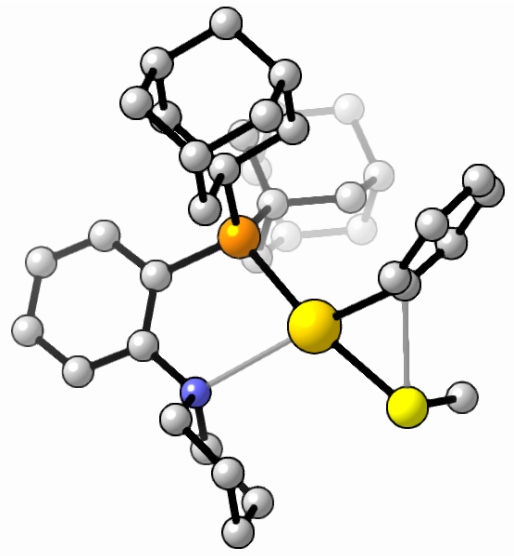
C	2.25748400	-3.59773900	0.12199000
C	1.53503800	-4.77043700	0.32226900
C	0.16133500	-4.71012200	0.54680600
C	-0.47325000	-3.47300200	0.54658200
N	2.45166300	-1.12454100	0.00178000
C	3.43974800	-1.22675200	-1.16611800
Au	1.18637000	0.80701600	-0.29754900
C	0.16108300	2.57632600	-0.52612900
C	-0.23488000	3.29938900	0.59766100
C	-0.88778200	4.52782700	0.43650000
C	-1.12723100	5.03467500	-0.84105200
C	-0.70204800	4.31531100	-1.96182800
C	-0.05033900	3.08770100	-1.80851200
C	3.16976800	-0.84238300	1.31375700
H	3.32102500	-3.67325200	-0.05561200
H	2.05171800	-5.72480600	0.30352700
H	-0.41728000	-5.61425700	0.70553600
H	-1.54276000	-3.44689400	0.69619800
H	3.16379500	-0.47892000	-1.91078800
H	3.30058000	-2.20015100	-1.63827100
H	2.41010400	-0.86772900	2.09746600
H	3.53336300	0.18320800	1.24124700
H	0.29270700	2.54652100	-2.68428300
H	-0.86854300	4.70875600	-2.96091400
H	-1.20154200	5.08215600	1.31676500
H	-0.03314600	2.93471600	1.59836100
H	-1.63185600	5.98852100	-0.96446600
S	3.18931000	2.11274200	-0.76634200
C	2.95795700	3.81306100	-0.11006500
H	3.93754000	4.29632500	-0.17705600
H	2.23532800	4.37725300	-0.70226600

H	2.63936100	3.79355300	0.93394700
C	-1.54572800	-0.31453300	1.79296800
C	-2.56931900	0.83213400	1.58595300
C	-2.28283400	-1.53405900	2.41158800
C	-0.45016200	0.13102300	2.80204200
H	-3.37027700	0.49948700	0.91758500
H	-2.09332400	1.69890400	1.11926400
C	-3.18992300	1.23395200	2.94144900
H	-1.57426400	-2.34551400	2.60135100
H	-3.05330000	-1.91268800	1.73199300
C	-2.93543900	-1.12818900	3.75468200
H	0.12040300	0.97882100	2.40889000
H	0.26082100	-0.69010600	2.96055500
C	-1.09417000	0.53145700	4.14619900
H	-3.89327200	2.05710800	2.76648000
C	-3.93513800	0.02196600	3.53172700
C	-2.08335800	1.69020800	3.91207500
H	-3.45849200	-2.00535700	4.15485100
C	-1.84016600	-0.67790600	4.73950900
H	-0.29741200	0.85233100	4.82819300
H	-4.73502400	-0.29727000	2.85020700
H	-4.40837300	0.29574800	4.48365200
H	-1.55731300	2.56311200	3.50310000
H	-2.52765400	2.00030100	4.86663000
H	-2.28948400	-0.40668100	5.70362400
H	-1.13733200	-1.50052900	4.92743400
C	-1.79115500	-0.90333700	-1.35857800
C	-0.91444500	-1.52958400	-2.48033200
C	-3.02180900	-1.81217800	-1.10220200
C	-2.29004000	0.48111000	-1.84868000
H	-0.54315500	-2.51253800	-2.17190200
H	-0.03897900	-0.89451600	-2.67267900
C	-1.74506900	-1.67955700	-3.77348000
H	-3.65980600	-1.38184800	-0.32295100
H	-2.71249700	-2.80595700	-0.76882000
C	-3.83929200	-1.96310400	-2.40661400
H	-1.43887300	1.13034200	-2.04785100
H	-2.89795300	0.97385600	-1.08521700
C	-3.11876300	0.32433000	-3.14151900
H	-1.10512000	-2.12876900	-4.54285500
C	-2.95444000	-2.59505400	-3.49866100
C	-2.23654100	-0.29666900	-4.24041600
H	-4.69558800	-2.61601400	-2.19748500
C	-4.33414100	-0.58109500	-2.87131600
H	-3.45549000	1.32105800	-3.45262300
H	-2.61135300	-3.58831500	-3.17915400

H	-3.53724000	-2.73262100	-4.41872200
H	-1.37968600	0.35785600	-4.45036200
H	-2.80753200	-0.39558400	-5.17287600
H	-4.93854700	-0.68505100	-3.78189200
H	-4.97742700	-0.13190700	-2.10262000
C	4.90127700	-1.04654900	-0.74351400
H	5.07879200	0.00020300	-0.47935500
H	5.52138100	-1.25837000	-1.62204300
C	4.33548000	-1.78283100	1.63404500
H	4.86245300	-1.33309500	2.48294000
H	3.96220100	-2.74907800	1.98519600
C	5.29403300	-1.96104300	0.42466900
H	5.28597600	-3.00390400	0.08468100
H	6.32649700	-1.74996800	0.72042900

TS_{RE}

Charge: 1 Multiplicity: 1
Negative Frequency: -217.07



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C	0.97405100	3.43276700	-0.44109200
C	0.19667400	4.56209700	-0.70929300
C	-0.59559600	4.62417500	-1.86013900
C	-0.59642500	3.55444700	-2.75743200
Au	1.31763600	0.42134400	-0.39855100
S	3.16449600	1.45637200	-1.58593200
P	-0.69781400	-0.60742200	0.39009100
C	-0.23748200	-1.86939500	1.63445800
C	1.10078300	-2.05372200	2.03604900
C	1.38522100	-3.00852800	3.02671900
C	0.38552200	-3.79578800	3.58902700
C	-0.93465100	-3.64649500	3.16297800
C	-1.23502900	-2.69030900	2.19919600
N	2.20250100	-1.29673400	1.45026200
C	3.18860400	-2.23189000	0.82556800
C	-1.80083800	0.65317200	1.27221400
C	-2.98893000	0.04961100	2.06627400
C	-3.79075800	1.17678400	2.75631800
C	-4.31916700	2.16719300	1.70070200
C	-3.12909700	2.78549800	0.94306200
C	-2.34205700	1.66510900	0.22902200
C	-2.20916300	3.52057700	1.93712000
C	-1.68634100	2.52331400	2.98935200

C	-2.87495600	1.91150000	3.75321000
C	-0.88711100	1.40670600	2.28179900
C	-1.50668000	-1.53164000	-1.06144900
C	-1.40239200	-0.65328400	-2.33779100
C	-1.96172500	-1.40772300	-3.56141700
C	-3.43485200	-1.78273100	-3.31541200
C	-3.52701900	-2.68277100	-2.06898400
C	-2.99176200	-1.91392500	-0.83972400
C	-1.12805900	-2.68324300	-3.78750700
C	-1.22107700	-3.57726500	-2.53651900
C	-0.67422800	-2.82179600	-1.30565400
C	-2.69291900	-3.96076000	-2.28384600
C	2.82948200	-0.42202800	2.48688900
H	2.40770600	-3.14524600	3.36096200
H	0.64028600	-4.52744100	4.34989600
H	-1.72532400	-4.26404500	3.57734700
H	-2.26315700	-2.58624500	1.87978900
H	0.38187800	-2.56020000	-1.46313800
H	-0.71863500	-3.47708900	-0.42972900
H	-0.62013400	-4.48377400	-2.68044600
H	2.65779400	-2.76916700	0.03331200
H	3.52477500	-2.97473600	1.56349300
H	-0.08050700	-2.41804600	-3.98603900
H	-1.49869900	-3.22671900	-4.66648300
H	-1.88395000	-0.75062100	-4.43670000
H	-4.03717100	-0.87557500	-3.17118000
H	-3.84061500	-2.30754700	-4.19017800
H	-4.57392500	-2.94954700	-1.87854500
H	-3.10483700	-2.54203900	0.04924900
H	-3.59705000	-1.01420300	-0.68777600
H	-3.08579900	-4.52490900	-3.13982500
H	-2.76746900	-4.61243800	-1.40284100
H	-1.93083100	0.29631300	-2.20714900
H	-0.35000500	-0.41568900	-2.52526900
H	-0.49027800	0.70165100	3.02382100
H	-0.03049800	1.85224500	1.76299400
H	-1.01590300	3.03764600	3.68924200
H	3.14582900	-1.03085300	3.34746400
H	2.05418700	0.26736200	2.83483500
H	-3.43559400	2.70160600	4.26998800
H	-2.51488200	1.21237600	4.52011300
H	-4.63223200	0.71942700	3.29163300
H	-4.98707400	1.64970300	0.99861100
H	-4.90739300	2.95591800	2.18807400
H	-3.49107200	3.48939200	0.18330400
H	-3.00729200	1.15892900	-0.47963400

H	-1.51830000	2.09703700	-0.34588600
H	-3.65283200	-0.51944700	1.40905400
H	-2.61680700	-0.63366600	2.83544300
H	-2.76377000	4.32926500	2.43131900
H	-1.37002400	3.97919100	1.40245800
H	0.16017200	1.58778700	-3.20804400
H	-1.20523300	3.59090800	-3.65645100
H	0.22058300	5.39607000	-0.01361500
H	1.60085600	3.39405400	0.44338500
H	-1.19754600	5.50509600	-2.06037400
C	2.95069800	0.81862000	-3.29328500
H	3.95813100	0.72359100	-3.70862200
H	2.46724300	-0.15959200	-3.29853100
H	2.37827400	1.52785800	-3.89682300
C	4.41097600	-1.50444100	0.27015500
H	4.11817100	-0.89501100	-0.58830200
H	5.11729300	-2.26102600	-0.09236500
C	4.03912000	0.34019700	1.94927600
H	3.71472500	1.07263800	1.20197600
H	4.47993900	0.90610600	2.77849200
C	5.06829000	-0.61758100	1.33552300
H	5.90035200	-0.05325300	0.89873500
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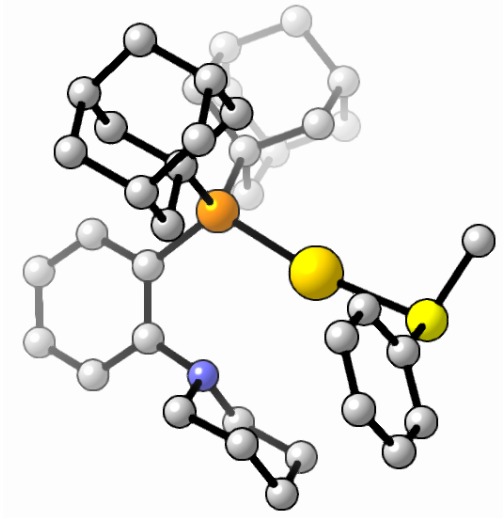
Int2

Charge: 1 Multiplicity: 1
Negative Frequency: None



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C	6.09606800	-0.03235600	-0.65116000
C	5.84239000	1.34046300	-0.66546100
C	4.60675000	1.82133400	-1.11262300
Au	0.70311000	-0.84366900	-0.61698100
S	2.60480900	-1.64538400	-1.93773800
P	-1.18920200	0.14937900	0.33005100
C	-1.34860000	-0.12178700	2.14387500
C	-0.31572100	-0.68253000	2.93115400
C	-0.53013700	-0.85693700	4.30847900
C	-1.72734700	-0.49134300	4.91660000
C	-2.74671400	0.06819200	4.14543600
C	-2.55094900	0.24934200	2.77960900
N	0.95306100	-1.06153800	2.36407100

C	1.23974400	-2.50274700	2.52426500
C	-0.99615600	2.02142400	0.10902100
C	-0.95015500	2.35428700	-1.40492300
C	-0.64772900	3.85380800	-1.60748400
C	0.71278300	4.19959600	-0.97174500
C	0.66338300	3.90106800	0.53919500
C	0.36619600	2.40342900	0.75663500
C	-0.44379100	4.74380400	1.19984700
C	-1.80023400	4.38230900	0.56588700
C	-1.76123000	4.68824900	-0.94401900
C	-2.09439400	2.88000500	0.78918900
C	-2.72301600	-0.60077800	-0.52156800
C	-2.38915900	-0.85484100	-2.02281500
C	-3.55794900	-1.58090200	-2.72265700
C	-4.83338400	-0.72310500	-2.63432300
C	-5.17972700	-0.48912000	-1.15286000
C	-4.01427700	0.25631400	-0.46312600
C	-3.79570900	-2.93954600	-2.03671700
C	-4.14489600	-2.70530200	-0.55512800
C	-2.98026500	-1.97821200	0.15030900
C	-5.41792200	-1.84137500	-0.45279800
C	2.05991300	-0.22015700	2.86557900
H	0.26479000	-1.28317500	4.91225300
H	-1.86077600	-0.63760600	5.98460700
H	-3.68750900	0.36420900	4.59927000
H	-3.35306900	0.68821900	2.20187600
H	-2.06787300	-2.58949400	0.10091800
H	-3.22518500	-1.84718900	1.20933700
H	-4.30766100	-3.66746800	-0.05355200
H	0.38886700	-3.05768700	2.11538400
H	1.33123600	-2.77372600	3.59142500
H	-2.89695100	-3.56603000	-2.11837000
H	-4.61313100	-3.47645300	-2.53595000
H	-3.28507000	-1.73705600	-3.77394900
H	-4.67923300	0.23840100	-3.14256600
H	-5.66512900	-1.23002400	-3.14118100
H	-6.07962800	0.13352900	-1.07394500
H	-4.30094900	0.47540200	0.56901500
H	-3.85345600	1.21429100	-0.96877900
H	-6.26344800	-2.36144200	-0.92196100
H	-5.68024500	-1.67962300	0.60154400
H	-2.17843900	0.08899800	-2.53622800
H	-1.48643700	-1.47156000	-2.10543900
H	-3.08354000	2.64345800	0.38776200
H	-2.11818300	2.67538600	1.86481300
H	-2.59987900	4.96340000	1.04201300

H	2.21436400	-0.37598000	3.94903500
H	1.77891600	0.82643700	2.72483000
H	-1.57632000	5.75855700	-1.10472800
H	-2.73117700	4.45324300	-1.40300600
H	-0.61855300	4.06087000	-2.68447700
H	1.51163900	3.61371200	-1.44727400
H	0.94701800	5.25921700	-1.13795900
H	1.63371600	4.13211600	0.99640600
H	1.17985300	1.80333800	0.33111400
H	0.33193500	2.18780800	1.83123800
H	-0.18501000	1.74483500	-1.90396200
H	-1.91142200	2.11684900	-1.87428500
H	-0.23670400	5.81337900	1.06257300
H	-0.46853800	4.55271800	2.28114900
H	2.65155100	1.30245200	-1.85438500
H	4.40456300	2.88830700	-1.12224300
H	7.05477600	-0.40806500	-0.30674200
H	5.30795000	-2.00170800	-1.06534800
H	6.60450300	2.03659100	-0.32829000
C	2.15841600	-1.15779000	-3.65107400
H	3.02456500	-1.32051300	-4.29507400
H	1.33340000	-1.80748600	-3.95070100
H	1.83838900	-0.11586400	-3.67906300
C	2.53230600	-2.89604300	1.80306400
H	2.38282800	-2.80177200	0.72106600
H	2.73970300	-3.95400000	2.00475000
C	3.35567600	-0.53169600	2.11923900
H	3.23132800	-0.26049500	1.06552600
H	4.16150600	0.09480200	2.52023700
C	3.71195900	-2.01824900	2.24246500
H	4.60217400	-2.24870800	1.64560500
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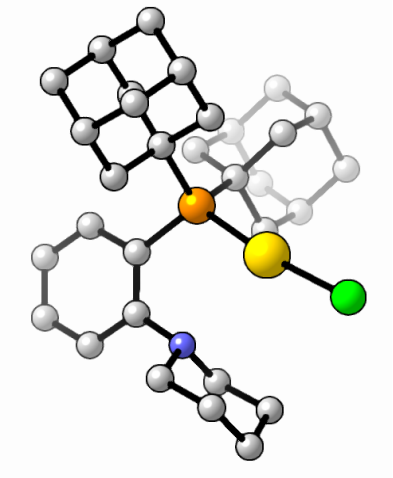
P_{Au}

Charge: 0 Multiplicity: 1
Negative Frequency: None



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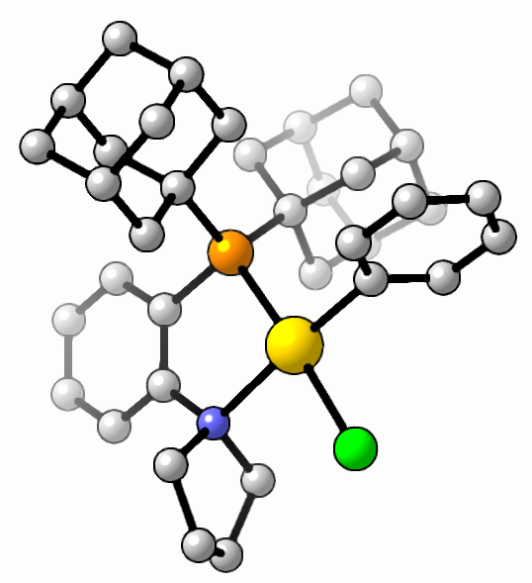
P	0.50200300	0.07349000	0.28385500
C	-0.06411900	0.03921900	2.03957900
C	-1.41921700	-0.12597400	2.40943600
C	-1.76098100	-0.11165600	3.77244000
C	-0.80214900	0.04731500	4.76806500
C	0.53808800	0.19711900	4.41021000
C	0.89220200	0.19528000	3.06431600
N	-2.45620800	-0.31513200	1.43088300
C	-3.40647500	0.81283300	1.38658900
C	1.89273000	-1.22354600	0.10906900
C	3.28059700	-0.81201500	0.66532100
C	4.28828200	-1.97279800	0.49939500
C	4.45379300	-2.29992600	-0.99546200
C	3.08985100	-2.72259500	-1.57102700
C	2.07097200	-1.57604600	-1.39806800
C	2.57763500	-3.97341900	-0.83213200
C	2.41557000	-3.64743400	0.66445600
C	3.77475800	-3.21657000	1.25108200
C	1.39868900	-2.50049200	0.84490800
C	1.04990700	1.86348600	-0.02750700
C	1.66655400	1.96162400	-1.44704900
C	1.98058100	3.43318600	-1.78956700
C	2.99418600	3.98522700	-0.76835900
C	2.38431000	3.91510800	0.64464900
C	2.05128000	2.44785200	1.00271200
C	0.68476900	4.26591900	-1.74078100
C	0.08560000	4.19973400	-0.32218000
C	-0.24065300	2.73224200	0.02514900
C	1.09742200	4.75967000	0.69507500
C	-3.12918100	-1.62185000	1.57474900
H	-2.80352600	-0.23020100	4.05090600
H	-1.09855500	0.05314400	5.81313200
H	1.30531100	0.31809700	5.16891900
H	1.93622500	0.32001400	2.81336400
H	-0.98784600	2.34864300	-0.68094600
H	-0.68212100	2.67627300	1.02828600
H	-0.84411800	4.78131100	-0.28322200
H	-2.82706400	1.73174700	1.25467900
H	-3.95982200	0.90631000	2.33979800
H	-0.03784000	3.88139700	-2.47352400
H	0.89816400	5.30874700	-2.01043200

H	2.40974300	3.47214200	-2.79865900
H	3.92434000	3.40208800	-0.80825700
H	3.25076400	5.02403000	-1.01512500
H	3.10592700	4.29277100	1.38000200
H	1.61562400	2.42051900	2.00636600
H	2.97519100	1.86300500	1.02810500
H	1.32479700	5.80858200	0.46258400
H	0.66903500	4.73555600	1.70625000
H	2.59268700	1.37806200	-1.49789800
H	0.97401800	1.54165500	-2.18826100
H	1.26801400	-2.29766200	1.91321200
H	0.41754100	-2.79934700	0.44919300
H	2.04305100	-4.52975800	1.20003300
H	-3.65449200	-1.69702600	2.54465100
H	-2.35311800	-2.39485800	1.56258400
H	4.50047300	-4.03547900	1.15920900
H	3.66968100	-2.99375600	2.32162600
H	5.25042200	-1.65536700	0.92070400
H	4.83623200	-1.42225400	-1.53410500
H	5.18627200	-3.10747200	-1.12680600
H	3.18762200	-2.93746600	-2.64271200
H	2.40326500	-0.69837900	-1.96203500
H	1.10980000	-1.88461700	-1.82516500
H	3.65585600	0.06739100	0.13099200
H	3.22234800	-0.55154300	1.72535000
H	3.28346000	-4.80454200	-0.96224700
H	1.61557800	-4.29359200	-1.25494900
C	-4.40510600	0.64007300	0.24087400
H	-3.86571000	0.67984000	-0.71338800
H	-5.11267800	1.47824300	0.25701600
C	-4.13563800	-1.85401900	0.44563800
H	-3.59872700	-1.94068100	-0.50557600
H	-4.64978400	-2.80685000	0.62313900
C	-5.14295800	-0.69994000	0.35839500
H	-5.81630900	-0.84388100	-0.49519000
H	-5.76845000	-0.69136900	1.26331000
Cl	-2.67308500	-0.95099400	-3.08359300

_S_-Arylation of Methanethiol with [(Pyrrol-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (18)

SM



Charge: 1 Multiplicity: 1
Negative Frequency: None

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C	2.72882700	1.55143200	-3.00328000
C	1.69156600	2.51233300	-3.61303200
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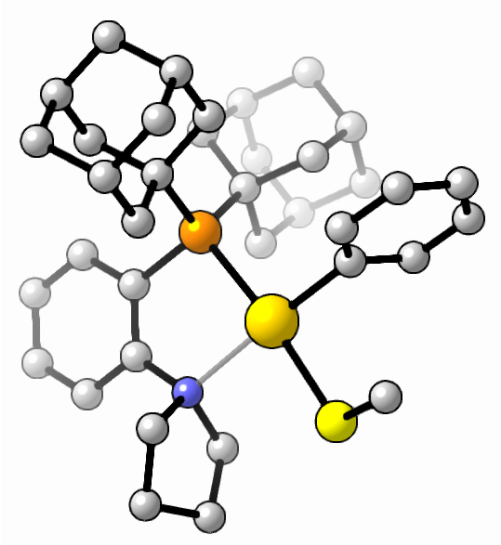
C	2.61162000	2.36964700	-0.16609300
C	1.45709100	1.55504000	-0.81068200
C	2.04918200	0.66772500	-1.93438300
C	0.42351800	2.53519700	-1.43523800
P	0.50777800	0.50680400	0.45479000
C	-0.42940100	1.66867100	1.52045700
C	-1.83319300	1.66256800	1.53529000
C	-2.51756400	2.58901500	2.33510700
C	-1.82967200	3.52231200	3.10290100
C	-0.43489300	3.53801800	3.09128600
C	0.25330900	2.61800700	2.30940300
Au	-1.30670800	-0.65131100	-0.55506400
C	-0.24116900	-1.95150000	-1.74626000
C	0.24509600	-3.15013500	-1.23139100
C	0.88055500	-4.05862800	-2.08831400
C	1.01239000	-3.77058900	-3.44705200
C	0.49038100	-2.57907000	-3.95715300
C	-0.14668500	-1.66734600	-3.10973700
C	1.52156700	-0.62834800	1.58646400
C	0.51816700	-1.60590500	2.26202500
C	1.27943400	-2.59851700	3.16637700
C	2.02610100	-1.82518100	4.26879600
C	3.02821100	-0.85625700	3.61449400
C	2.26065700	0.14332600	2.71597100
C	2.28744300	-3.39380700	2.31316500
C	3.30158800	-2.42462900	1.67509600
C	2.56940200	-1.41763300	0.76113800
C	4.04769100	-1.65013100	2.77732000
H	-3.59975900	2.58285300	2.36086800
H	-2.38501700	4.23183400	3.70786800
H	0.11737900	4.25706600	3.68714500
H	1.33308100	2.64174800	2.32268500
H	2.78199300	-0.03598000	-1.53171700

H	1.26196100	0.07993500	-2.40173300
H	3.12868200	0.89132700	-3.78265400
H	4.62494200	1.67283600	-1.93967600
H	4.37383300	2.97446500	-3.11006600
H	4.09487300	3.81382000	-0.76028900
H	1.84790800	4.86952700	-1.05810500
H	2.73348400	4.86459400	-2.58818100
H	0.36930300	4.09482800	-2.92138200
H	-0.39923600	1.97750100	-1.90091200
H	-0.01165200	3.17555900	-0.66004800
H	2.16089100	3.12934400	-4.39008600
H	0.88471900	1.94194800	-4.09259000
H	2.23610100	3.02717100	0.62106300
H	3.35316700	1.69714500	0.27858700
H	-0.21373600	-1.03908700	2.85119100
H	-0.04429200	-2.16826800	1.51059500
H	0.54927100	-3.28201400	3.61598400
H	2.55622100	-2.52569500	4.92666300
H	1.31230400	-1.26949800	4.89120500
H	3.54793700	-0.27869100	4.38849600
H	4.78332000	-0.96939900	2.32860400
H	4.59932000	-2.34673500	3.42166500
H	4.01631200	-2.98528600	1.06084100
H	3.30663500	-0.72590600	0.34032400
H	2.09616600	-1.94139500	-0.07323100
H	2.96300300	0.87216600	2.29769800
H	1.54293500	0.68426500	3.33808800
H	2.81361200	-4.12377500	2.94143300
H	1.76254200	-3.96068500	1.53288700
H	-0.56099700	-0.75110200	-3.51844000
H	0.57143700	-2.35325100	-5.01678400
H	1.26733800	-4.98905200	-1.68214900
H	0.13261900	-3.39970700	-0.18298100
H	1.50887900	-4.47480400	-4.10822500
Cl	-3.27419400	-1.76697100	-1.49702100
C	-3.47523400	-0.18602400	1.62868700
C	-3.58079400	1.44747600	-0.20261000
C	-4.90898800	-0.08751200	1.09446000
H	-3.39480100	0.18503100	2.65162100
H	-3.07822400	-1.20153100	1.60531800
C	-4.97474500	1.28585500	0.40918700
H	-3.54052600	0.96317400	-1.17784200
H	-3.24490200	2.47889700	-0.31312300
H	-5.08797000	-0.87999800	0.36536600
H	-5.63586400	-0.18955300	1.90490400
H	-5.74815000	1.33246700	-0.36262300

H	-5.18688300	2.07758200	1.13457700
N	-2.61266400	0.71276900	0.72946000

Int1



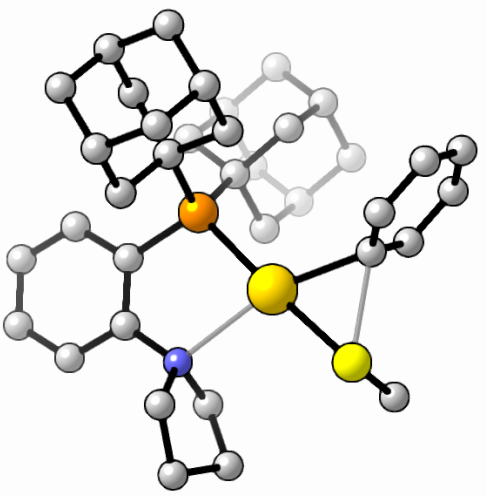
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	-0.75746100	-0.56680300	0.13243000
C	-0.30063200	-2.33253500	0.33248500
C	1.04099700	-2.74203800	0.24429400
C	1.34871600	-4.10871000	0.32619300
C	0.35106500	-5.06295400	0.49761400
C	-0.98235500	-4.66529900	0.58862400
C	-1.29800000	-3.31419000	0.50362400
Au	1.43752200	0.40331600	-0.20902300
C	0.91875500	2.37277800	-0.48181400
C	0.66787500	3.18797900	0.62070100
C	0.36418700	4.54134900	0.42720800
C	0.32837000	5.07697700	-0.86061600
C	0.60751100	4.25823300	-1.95890500
C	0.90988800	2.90573100	-1.77318500
H	2.37630200	-4.43965600	0.25048800
H	0.62023400	-6.11274600	0.55799500
H	-1.77272400	-5.39728400	0.71898300
H	-2.33682000	-3.02450900	0.56972700
H	1.14061300	2.28204200	-2.63087600
H	0.59750700	4.66884100	-2.96488100
H	0.16092200	5.16927800	1.29033000
H	0.71779700	2.79471800	1.62989900
H	0.09473300	6.12729400	-1.00890100
S	3.73858600	1.13101400	-0.54258100
C	3.91589200	2.86030600	0.05161400
H	4.98936600	3.07275400	0.03846800
H	3.39990200	3.56536500	-0.60249800
H	3.54232700	2.96787100	1.07173400
C	-1.56175400	0.00508100	1.74866300
C	-2.61127500	-0.98622000	2.32083400
C	-0.41556200	0.13575900	2.79221500
C	-2.24413100	1.38152700	1.53847400
H	-2.14765200	-1.95835800	2.51142200
H	-3.43145500	-1.13888400	1.61117000
C	-3.17479800	-0.44151600	3.65500500
H	0.36414200	0.81424800	2.42997400
H	0.05948300	-0.84164300	2.94732800

C	-0.97400100	0.67062500	4.12785800
H	-3.08603800	1.27646400	0.84594300
H	-1.54606200	2.09873100	1.09785700
C	-2.77629100	1.91538400	2.88599700
H	-3.92118900	-1.15564300	4.02390700
C	-2.02855300	-0.30902600	4.67547000
C	-3.83051700	0.93413100	3.43227000
H	-0.14294800	0.76208300	4.83776300
C	-1.61806500	2.05151500	3.89338000
H	-3.23351700	2.89675100	2.71041100
H	-1.57204100	-1.29021700	4.86204100
H	-2.41904400	0.05627600	5.63417700
H	-4.66616600	0.84636800	2.72501300
H	-4.24270700	1.30936100	4.37801300
H	-1.99402200	2.45452400	4.84261800
H	-0.86951400	2.76111400	3.51628300
C	-1.83292000	-0.46644700	-1.42682700
C	-1.06985500	-1.25338900	-2.53055400
C	-3.25452000	-1.06433800	-1.26080000
C	-1.96737400	1.00990500	-1.88297500
H	-0.95767600	-2.30400700	-2.24144300
H	-0.06013900	-0.83948700	-2.65734800
C	-1.84163500	-1.16751900	-3.86479500
H	-3.81204500	-0.51716300	-0.49275100
H	-3.20668300	-2.11274400	-0.95571400
C	-4.01389700	-0.98011900	-2.60631200
H	-0.97938300	1.44979700	-2.00887000
H	-2.49085300	1.60611600	-1.13090800
C	-2.73455000	1.08871300	-3.21969100
H	-1.28616100	-1.73567000	-4.62105900
C	-3.24628400	-1.77530200	-3.68064100
C	-1.96506700	0.30500600	-4.29916300
H	-5.01023700	-1.41574300	-2.46224100
C	-4.14220500	0.49141300	-3.04136300
H	-2.80902600	2.14464200	-3.50795700
H	-3.16559100	-2.82997100	-3.38481500
H	-3.79508100	-1.74513900	-4.63088900
H	-0.96720300	0.74142600	-4.44230400
H	-2.49076800	0.37066200	-5.26073600
H	-4.70381400	0.55683500	-3.98244700
H	-4.70191100	1.06117000	-2.28735600
C	2.99166300	-1.77453700	1.38283200
C	3.08470000	-2.14790700	-1.03831700
C	4.22710400	-2.61926600	1.07003200
H	2.38216000	-2.14163400	2.20938300
H	3.28279300	-0.74511300	1.59063800

C	4.48088200	-2.34108500	-0.42102200
H	3.06368800	-1.36128000	-1.79262100
H	2.70985700	-3.05738900	-1.50789900
H	5.07176300	-2.32322200	1.69857900
H	4.03912200	-3.68116000	1.25308800
H	5.06556700	-1.42487800	-0.53386800
H	5.02078900	-3.15364600	-0.91480500
N	2.13993800	-1.77196800	0.10959400

TS_{RE}



Charge: 1 Multiplicity: 1
Negative Frequency: -256.18

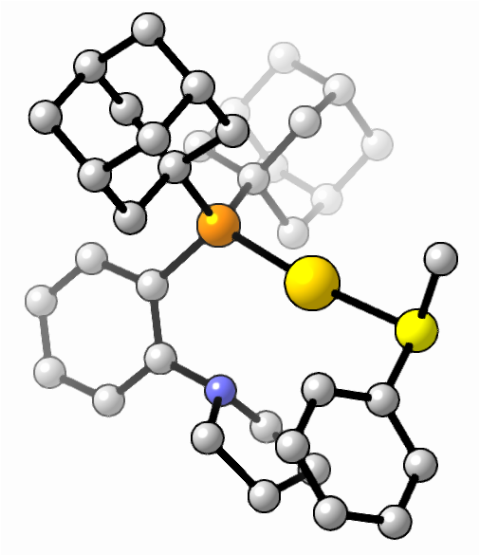
C	1.64006700	-3.11933800	-0.50410100
C	1.50760200	-2.10680300	-1.45759700
C	0.87607600	-2.33663800	-2.68407600
C	0.31384000	-3.59061200	-2.92564300
C	0.40486600	-4.60991100	-1.96994500
C	1.07435500	-4.37276600	-0.76881700
Au	1.35583900	-0.07631700	-0.58738300
S	3.39673400	-0.72597300	-1.69264600
P	-0.75175500	0.47410800	0.39689300
C	-0.51450000	2.07114500	1.26620800
C	0.73060200	2.73211000	1.23654800
C	0.85414000	3.98837700	1.85288700
C	-0.22717400	4.59553400	2.48270100
C	-1.46377200	3.94730200	2.51270600
C	-1.59965300	2.70154000	1.90914400
C	-2.05068700	0.77719000	-0.95173100
C	-1.69463900	2.13533400	-1.62061700
C	-2.65364100	2.41139500	-2.79831000
C	-4.10144000	2.46630200	-2.27098100
C	-4.46719900	1.11263400	-1.63127500
C	-3.51493900	0.82334200	-0.44813300
C	-4.34017100	-0.00963300	-2.67898500
C	-2.89165300	-0.05549500	-3.20097900
C	-2.52771300	1.29305100	-3.84991800
C	-1.92575400	-0.33321100	-2.03058100
C	-1.20662800	-0.82732800	1.68772400
C	-1.59922700	-2.13605500	0.95389900
C	-1.82740000	-3.26613100	1.97989400
C	-2.97806500	-2.86360800	2.92246600
C	-2.59645900	-1.57216200	3.67217400
C	-2.34412500	-0.42774400	2.66256100

C	-0.54181100	-3.50013700	2.79670900
C	-0.17065800	-2.20897900	3.55291000
C	0.07707400	-1.07860000	2.53176800
C	-1.31916800	-1.81226900	4.49902500
H	1.81488500	4.49370600	1.83361400
H	-0.10431600	5.56935600	2.94713100
H	-2.31830500	4.40833300	2.99801800
H	-2.56821500	2.21984900	1.93227900
H	0.91414600	-1.36301000	1.88311300
H	0.36849500	-0.15587200	3.05016500
H	0.75072700	-2.36556900	4.12755000
H	0.27781400	-3.79651200	2.12942500
H	-0.69469900	-4.32140900	3.50905500
H	-2.09167100	-4.18052400	1.43422200
H	-3.90009200	-2.70813700	2.34599100
H	-3.17637200	-3.66873100	3.64220400
H	-3.41727700	-1.27050400	4.33466700
H	-2.06412600	0.47408100	3.21624800
H	-3.26834300	-0.20938200	2.11840100
H	-1.49104700	-2.60808800	5.23572300
H	-1.05321900	-0.90404500	5.05644100
H	-2.52280500	-1.98454600	0.38468200
H	-0.81797100	-2.42468300	0.24338700
H	-0.90098900	-0.36012800	-2.41050100
H	-2.13361800	-1.32005500	-1.60693000
H	-2.78416100	-0.86401500	-3.93500400
H	-3.19460300	1.49717700	-4.69796300
H	-1.50234100	1.25753700	-4.24271800
H	-2.38405500	3.37637600	-3.24537000
H	-4.20353000	3.27268800	-1.53216700
H	-4.79242700	2.69012600	-3.09430200
H	-5.49390300	1.14865600	-1.24638100
H	-3.64208400	1.60168700	0.31077600
H	-3.79030800	-0.13269200	0.00963100
H	-1.77140600	2.95014700	-0.89312200
H	-0.65528100	2.11442800	-1.97765600
H	-5.03464900	0.17134300	-3.50991000
H	-4.61162500	-0.97562900	-2.23201800
H	2.14201600	-2.93981400	0.43989100
H	1.15474400	-5.15511100	-0.01919100
H	-0.19141700	-3.76914600	-3.87084800
H	0.82299700	-1.55506100	-3.43389600
H	-0.03299200	-5.58344500	-2.16792500
C	4.42318500	-1.49736500	-0.38113100
H	5.45567500	-1.19909200	-0.58191000
H	4.13636400	-1.15274300	0.61332500

H	4.34046600	-2.58558200	-0.44083100
C	2.53600700	3.03867900	-0.44238000
C	2.96324900	1.77697400	1.59375200
C	3.95825000	3.31619100	0.05813900
H	1.93663500	3.93951300	-0.59023800
H	2.56193700	2.49301600	-1.39096800
C	4.28142300	2.05425200	0.87042500
H	2.83322300	0.73694400	1.90626400
H	2.87716200	2.40656500	2.48785100
H	4.65620300	3.48939500	-0.76620200
H	3.97524300	4.19962800	0.70777600
H	4.52901700	1.22989900	0.19544700
H	5.10928600	2.18712900	1.57240300
N	1.89464100	2.15136000	0.59913200

Int2

Charge: 1 Multiplicity: 1
Negative Frequency: None



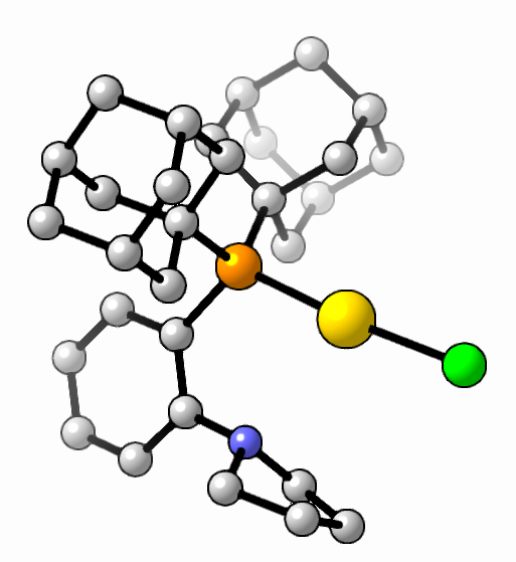
C	4.06920800	1.10329300	-0.40551500
C	4.20154800	-0.08328900	-1.13795800
C	5.38693100	-0.82368700	-1.09663600
C	6.44948800	-0.37120200	-0.30941400
C	6.32581600	0.81120700	0.42346100
C	5.13805100	1.54845200	0.37198600
Au	0.85149700	-0.38077900	-0.77541600
S	2.84400400	-0.72091300	-2.13809300
P	-1.16780300	0.08236700	0.31435900
C	-1.11744500	-0.30635400	2.11300400
C	0.00066100	-0.92588900	2.71714800
C	-0.03803000	-1.20970400	4.09339200
C	-1.14025900	-0.88310900	4.87644300
C	-2.23976200	-0.25546000	4.28749800
C	-2.22297400	0.02368500	2.92429400
C	-1.46491700	1.95452300	0.14542100
C	-2.91313100	2.42996000	0.42580300
C	-2.99675600	3.96967000	0.31113200
C	-2.61449500	4.40109100	-1.11639100
C	-1.17234800	3.94790800	-1.41189600
C	-1.07454000	2.41235100	-1.29109800
C	-0.20375900	4.60073700	-0.40781000
C	-0.58936700	4.17275100	1.02058300
C	-2.03377200	4.61840600	1.32493400
C	-0.49455000	2.63817500	1.15001200

C	-2.51108400	-1.02712500	-0.42659600
C	-2.70591400	-0.65419000	-1.91904200
C	-3.68185800	-1.64390200	-2.58966200
C	-5.04637000	-1.56837500	-1.87734600
C	-4.87120800	-1.95662400	-0.39685100
C	-3.88511900	-0.98388900	0.29090700
C	-3.12087300	-3.07578800	-2.49155300
C	-2.95687500	-3.46203900	-1.00822700
C	-1.97121600	-2.48439500	-0.33476800
C	-4.32260300	-3.39271200	-0.29954200
H	0.82184400	-1.69233600	4.54902200
H	-1.14093100	-1.11370300	5.93790400
H	-3.10734000	0.01449600	4.88182000
H	-3.08851900	0.50620300	2.49113000
H	-0.99378600	-2.55917000	-0.82833700
H	-1.82547300	-2.76191400	0.71716900
H	-2.54705400	-4.47692400	-0.93086700
H	-2.15236600	-3.13737800	-3.00655300
H	-3.79998900	-3.77977200	-2.99029000
H	-3.79549900	-1.36027100	-3.64342000
H	-5.45647900	-0.55233700	-1.95604700
H	-5.76207500	-2.24636700	-2.36079300
H	-5.83595900	-1.89108200	0.12161300
H	-3.77132000	-1.28199700	1.33762400
H	-4.30143500	0.02819300	0.27800600
H	-5.02455800	-4.09709300	-0.76521200
H	-4.21693600	-3.68626800	0.75359700
H	-3.11327600	0.35948500	-2.00404000
H	-1.73927800	-0.66444700	-2.44009800
H	-0.74172100	2.34391600	2.17579900
H	0.53567100	2.30706700	0.95697000
H	0.09959800	4.62566100	1.74455400
H	-2.11005600	5.71215000	1.26593400
H	-2.31002600	4.32779800	2.34758800
H	-4.02745000	4.27560500	0.52985200
H	-3.30693500	3.95619600	-1.84383600
H	-2.69492500	5.49173500	-1.21494500
H	-0.89482200	4.23122200	-2.43501500
H	-1.72497100	1.94358300	-2.03600400
H	-0.04878700	2.09803900	-1.51923600
H	-3.60581000	1.97665100	-0.29194000
H	-3.23628600	2.13476000	1.42800200
H	-0.24636800	5.69421700	-0.49803300
H	0.82866400	4.29530800	-0.62716200
H	3.13984000	1.66427700	-0.43225200
H	5.03782700	2.46480600	0.94578100

H	7.37016700	-0.94541300	-0.27076000
H	5.47757400	-1.74274500	-1.66694600
H	7.15218600	1.15822600	1.03651500
C	2.69305700	0.57873100	-3.42885500
H	3.60913100	0.58419700	-4.02239100
H	1.83755300	0.30413300	-4.04948200
H	2.52115500	1.55010900	-2.96419600
C	2.42797700	-0.58499700	2.38794800
C	1.44467200	-2.70732400	1.81708500
C	3.55562400	-1.60440200	2.10935100
H	2.40263500	-0.30145300	3.44816500
H	2.54286100	0.33498900	1.80535700
C	2.88068600	-2.72522600	1.29540600
H	0.72019700	-3.14871600	1.12475200
H	1.37476400	-3.24739600	2.77663900
H	4.39919900	-1.15165400	1.58357600
H	3.93086400	-2.00987500	3.05525600
H	2.89003900	-2.48596400	0.22659800
H	3.36211200	-3.69863700	1.42757400
N	1.17204100	-1.26528900	1.96902000

P_{Au}

Charge: 0 Multiplicity: 1
Negative Frequency: None



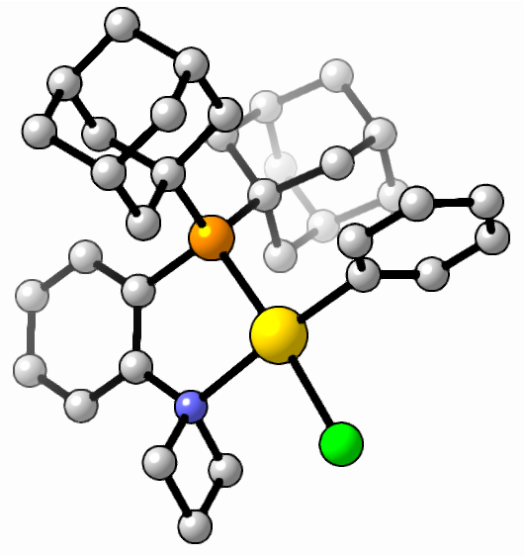
Au	1.16705600	-0.78638600	-1.18873800
P	-0.39091600	0.12141700	0.27642500
C	0.14544700	0.08606400	2.04242700
C	1.47152100	-0.22475300	2.42327200
C	1.81543900	-0.20593000	3.78547500
C	0.88355400	0.10930500	4.76937100
C	-0.42786500	0.41372200	4.40015900
C	-0.78318100	0.40333500	3.05432400
C	-0.60092100	1.96061900	-0.12987300
C	-1.48291000	2.75797200	0.86603900
C	-1.54606100	4.24399300	0.44318000
C	-2.13187100	4.35905600	-0.97742600
C	-1.23224300	3.59111800	-1.96577800
C	-1.18538800	2.10326700	-1.55854600
C	0.19093500	4.18143500	-1.94115700
C	0.76724100	4.07007900	-0.51581300
C	-0.12852100	4.84557900	0.46833800
C	0.82473700	2.58433700	-0.10387700
C	-1.99509000	-0.90477000	0.13339800

C	-2.20649900	-1.30086800	-1.35886400
C	-3.41673500	-2.24784200	-1.50395100
C	-4.68959700	-1.55059400	-0.99046400
C	-4.49513900	-1.17799000	0.49026000
C	-3.29364200	-0.21469000	0.62624200
C	-3.15989200	-3.52928300	-0.68852100
C	-2.96883300	-3.15709100	0.79384700
C	-1.76059500	-2.20881700	0.94575500
C	-4.23554700	-2.45193500	1.31835400
H	2.83608500	-0.44417300	4.06971400
H	1.17768100	0.11780500	5.81506800
H	-1.17154200	0.66167500	5.15144100
H	-1.80278000	0.65209400	2.79381900
H	-0.84457500	-2.70396500	0.59344800
H	-1.61450600	-1.97603500	2.00579900
H	-2.77670300	-4.06223100	1.38369200
H	-2.26614200	-4.04408000	-1.06667500
H	-4.00513100	-4.22188100	-0.79710000
H	-3.53164700	-2.49927900	-2.56594100
H	-4.89225500	-0.64834200	-1.58339000
H	-5.55634700	-2.21551700	-1.10225100
H	-5.38982800	-0.66637500	0.86678300
H	-3.20966300	0.09154300	1.67222400
H	-3.48909600	0.68686700	0.03589700
H	-5.09867200	-3.12690500	1.24671900
H	-4.11167100	-2.19388900	2.37891800
H	-2.35883200	-0.40931000	-1.97582100
H	-1.31095700	-1.80406700	-1.74114500
H	1.24985700	2.49240100	0.90350700
H	1.48948500	2.04189900	-0.78793400
H	1.78614500	4.47694700	-0.49341300
H	-0.16389000	5.90721600	0.18967200
H	0.28803000	4.78874000	1.48314800
H	-2.18914900	4.77745800	1.15449900
H	-3.15124100	3.95005700	-1.00027900
H	-2.19872000	5.41500400	-1.27131600
H	-1.64696700	3.66253300	-2.97912800
H	-2.19997800	1.69123400	-1.59616900
H	-0.57467700	1.53521400	-2.27282600
H	-2.49692600	2.35032900	0.90603100
H	-1.06222000	2.69242100	1.87469300
H	0.16700200	5.23315400	-2.25590300
H	0.83424100	3.64358900	-2.65097300
Cl	2.66169100	-1.71298900	-2.85366000
C	3.63092000	0.32963300	1.35750500
C	3.00298800	-1.93357400	1.53465800

C	4.52905200	-0.40517500	0.35555600
H	4.14224400	0.44736200	2.32947200
H	3.31816800	1.32132100	1.01772700
C	4.23474500	-1.91074300	0.60171700
H	2.23158300	-2.64550500	1.22138900
H	3.29943500	-2.19072000	2.56520300
H	4.23800400	-0.13547700	-0.66428100
H	5.58424500	-0.14893200	0.48936900
H	4.01763300	-2.41160300	-0.34496100
H	5.08038100	-2.42268700	1.07060600
N	2.46502800	-0.56209000	1.45044900

_S_-Arylation of Methanethiol with [(Azet-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (19)

SM

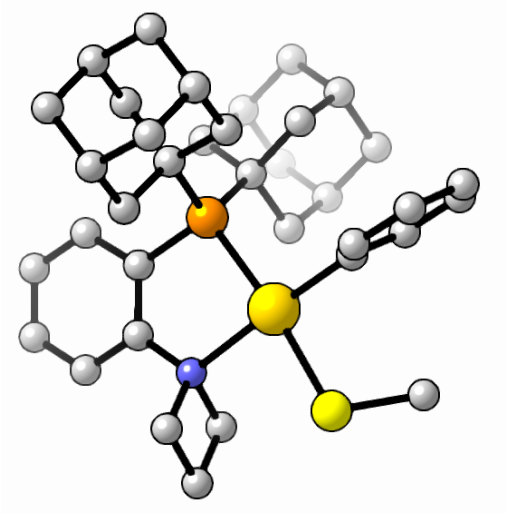


Charge: 1 Multiplicity: 1
Negative Frequency: None

C	-3.65889800	1.82120600	2.92569400
C	-2.31252100	1.22640700	3.37629200
C	-1.35653400	2.35567000	3.80433900
C	-1.12188400	3.30113300	2.61139100
C	-2.46470600	3.90016400	2.14903700
C	-3.41808300	2.76326600	1.73239600
C	-1.68363500	0.43174200	2.21138400
C	-1.43516200	1.36941100	1.00250500
C	-0.48215300	2.51605300	1.44556000
C	-2.79489000	1.97281100	0.55692400
P	-0.55205600	0.45159200	-0.39977500
C	0.02557500	1.71965300	-1.59528100
C	1.39768600	1.90782600	-1.82530200
C	1.82364300	2.89340400	-2.72697000
C	0.90294300	3.69772200	-3.39062700
C	-0.46236100	3.52654400	-3.15992900
C	-0.89338900	2.54676000	-2.27198500
Au	1.54994900	-0.41986700	0.30002800
C	0.90002000	-1.84786700	1.63605600
C	0.98199100	-1.56249900	3.00040000
C	0.63497400	-2.54763800	3.93038400
C	0.22595100	-3.81230300	3.49901300
C	0.18113500	-4.09700700	2.13388700
C	0.52519400	-3.11517500	1.19535800
C	-1.54933600	-0.83788700	-1.36231700
C	-0.53066700	-1.66820800	-2.19385200
C	-1.26959100	-2.77978800	-2.96956600
C	-2.28852100	-2.14594700	-3.93427800
C	-3.30769700	-1.32361500	-3.12380700
C	-2.56570100	-0.20475400	-2.35385400
C	-2.00004400	-3.69958100	-1.97047700
C	-3.03226000	-2.87910800	-1.17306700
C	-2.32112100	-1.75874200	-0.38292900
C	-4.05089400	-2.24363600	-2.13778100
H	2.88270300	3.04030200	-2.91117500
H	1.25418700	4.45625200	-4.08271600
H	-1.19166800	4.14911900	-3.66755900
H	-1.95579000	2.42974400	-2.11435700
H	0.48472100	2.10408300	1.76429300

H	-0.28824200	3.19615300	0.60895300
H	-0.43442300	4.10539300	2.90001000
H	-0.40177700	1.93306600	4.14522400
H	-1.78552900	2.91340500	4.64680400
H	-2.46914700	0.53366400	4.21212100
H	-4.35121200	1.01786000	2.64033600
H	-4.12415700	2.37432400	3.75180400
H	-4.37080400	3.18309300	1.38767400
H	-2.66450000	2.65516400	-0.28610800
H	-3.48262000	1.17894600	0.24608700
H	-2.91391400	4.48407300	2.96259500
H	-2.30283600	4.58611300	1.30686400
H	-2.34716900	-0.39241800	1.93782000
H	-0.74488800	-0.00806200	2.54203000
H	0.00649700	-1.01131600	-2.88986400
H	0.22121800	-2.12560900	-1.54350300
H	-0.52667000	-3.35622100	-3.53369300
H	-2.80551500	-2.92964400	-4.50272100
H	-1.77308400	-1.50273800	-4.65972900
H	-4.02444400	-0.84461800	-3.80170000
H	-4.79871500	-1.67069400	-1.57346900
H	-4.58802400	-3.02591700	-2.68934700
H	-3.54910700	-3.52767300	-0.45566000
H	-3.07561000	-1.17661800	0.15632000
H	-1.64672900	-2.19137100	0.36052900
H	-3.29317600	0.41885800	-1.82385600
H	-2.04492100	0.42589500	-3.07921500
H	-2.50542000	-4.50989300	-2.51120100
H	-1.27955600	-4.16908800	-1.28786400
H	0.50303400	-3.36021500	0.13994800
H	-0.11958200	-5.08137000	1.78601700
H	0.69056300	-2.32091400	4.99149900
H	1.31289900	-0.58822900	3.34662500
H	-0.04586900	-4.57380900	4.22418500
Cl	3.80125700	-1.19243300	0.88423800
C	3.45667100	0.47556900	-2.05626500
C	3.51338400	1.92221200	-0.46123400
C	4.57671400	1.28923300	-1.37939400
H	3.25354800	0.70231800	-3.10354500
H	3.50501400	-0.60302100	-1.91605600
H	3.34299500	2.99310800	-0.57680000
H	3.59430000	1.67530100	0.59626700
H	5.08398100	1.99678400	-2.03874100
H	5.31087900	0.67979300	-0.85260400
N	2.39957700	1.10363200	-1.13433600

Int1



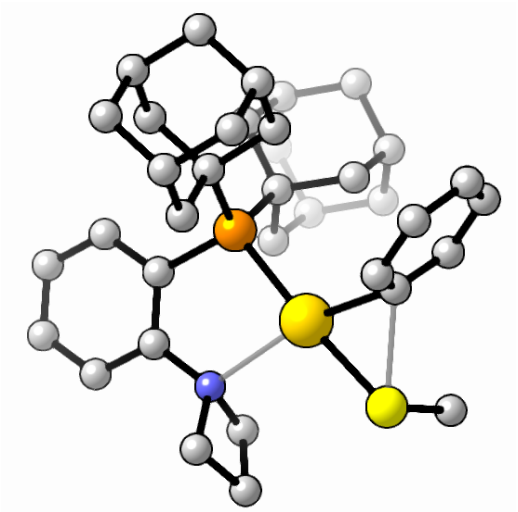
Charge: 1 Multiplicity: 1
Negative Frequency: None

P	0.82884700	-0.39937300	0.12144100
C	0.89207100	-2.21156400	0.41034400
C	-0.29281800	-2.96512100	0.44503800
C	-0.22870200	-4.35074400	0.65793300
C	0.99374600	-4.99437300	0.81839600
C	2.17730900	-4.25710200	0.77120500
C	2.12136500	-2.88201000	0.57216000
Au	-1.56783200	-0.09964300	-0.13321900
C	-1.62857800	1.92130100	-0.49648300
C	-1.80974000	2.37417700	-1.80605300
C	-1.90474200	3.74661200	-2.05585400
C	-1.83185100	4.66265000	-1.00226900
C	-1.67465100	4.20085000	0.30496300
C	-1.58022800	2.82738800	0.56196600
H	-1.14012000	-4.93770000	0.69978200
H	1.01785000	-6.06753600	0.97892500
H	3.13897500	-4.74527500	0.89132700
H	3.04888000	-2.32817400	0.54790700
H	-1.48507200	2.48573400	1.58670200
H	-1.62811500	4.90169400	1.13399100
H	-2.04187500	4.09488000	-3.07598300
H	-1.88254100	1.67003900	-2.62892500
H	-1.90701000	5.72806200	-1.19984600
S	-3.99104400	-0.06293200	-0.38684200
C	-4.62554600	1.57379100	0.15405500
H	-5.71524700	1.47786500	0.18481300
H	-4.26023200	1.82910500	1.15054600
H	-4.35121100	2.36260100	-0.54856400
C	1.76964500	-0.06906100	-1.49045400
C	1.49683800	1.37591700	-1.98496300
C	3.30383000	-0.27026400	-1.38058700
C	1.19354500	-1.06543600	-2.53684400
H	1.88335000	2.11082100	-1.27409300
H	0.42450900	1.54606900	-2.06970100
C	2.15998400	1.60256900	-3.36035600
H	3.54453100	-1.28326500	-1.04844000
H	3.72951900	0.43079300	-0.65411300
C	3.95918900	-0.04020200	-2.76315300
H	0.10666800	-0.93174800	-2.62510200
H	1.37070000	-2.09827900	-2.21684800
C	1.86105400	-0.82965300	-3.90862200

H	1.94449300	2.63071200	-3.67674700
C	3.68105200	1.39756500	-3.23884900
C	1.57718200	0.60835400	-4.38194600
H	5.03970200	-0.19694200	-2.65760400
C	3.38200100	-1.04501700	-3.77944100
H	1.44244900	-1.54860800	-4.62355400
H	4.10423000	2.11967300	-2.52763800
H	4.16569100	1.57266300	-4.20827900
H	0.49486100	0.76501800	-4.48528400
H	2.02666100	0.77477900	-5.36963700
H	3.86427700	-0.90728200	-4.75590800
H	3.59140500	-2.07332900	-3.45527700
C	1.49890200	0.43995100	1.68141100
C	0.40040400	0.28221400	2.77142800
C	2.80632000	-0.19373200	2.22880300
C	1.75593000	1.94391600	1.40551700
H	0.22112000	-0.78276000	2.96837300
H	-0.54897000	0.70627400	2.42711900
C	0.83455600	0.99879000	4.06754600
H	3.60940600	-0.13412700	1.48642800
H	2.64501000	-1.24954100	2.46377300
C	3.24124900	0.53548000	3.52226600
H	0.86811200	2.41913100	0.97880400
H	2.56798300	2.05390900	0.67895800
C	2.16408100	2.65485800	2.71426400
H	0.03841900	0.87849600	4.81231600
C	2.14250400	0.37597200	4.58997700
C	1.05273400	2.49576300	3.77000300
H	4.17232700	0.07456400	3.87418300
C	3.47212900	2.03108200	3.23614600
H	2.31801100	3.71823600	2.49400500
H	1.98943100	-0.68682500	4.82023800
H	2.44839200	0.87044000	5.52110100
H	0.12040600	2.95119300	3.41002200
H	1.33401300	3.02300200	4.69071400
H	3.79556500	2.54159700	4.15262100
H	4.27184100	2.15646100	2.49390300
C	-2.52031400	-3.07646600	-0.72042900
C	-2.59919700	-2.68475100	1.39574000
C	-3.52248800	-3.41509300	0.40088100
H	-2.01100600	-3.91994200	-1.18763400
H	-2.87883200	-2.40289600	-1.49853300
H	-2.13158600	-3.30042900	2.16513400
H	-3.00729600	-1.77959500	1.84270600
H	-3.64006400	-4.48378900	0.59343800
H	-4.50230900	-2.95231200	0.28028300

N	-1.60530300	-2.34368800	0.27276700

TS_{RE}



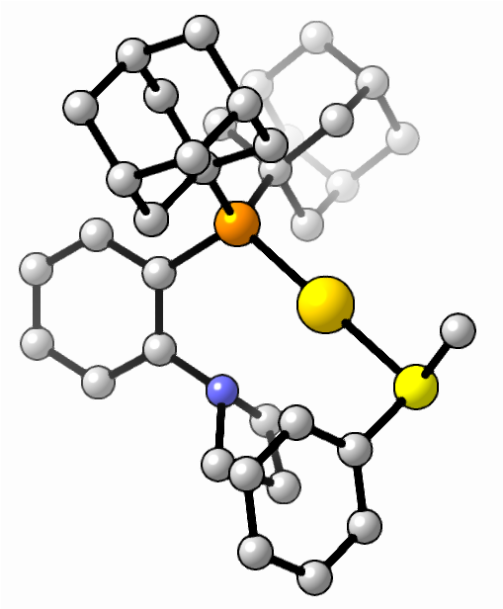
Charge: 1 Multiplicity: 1
Negative Frequency: -263.03

C	2.25710600	-1.53541100	2.23953800
C	2.43504600	-1.49124700	0.85474900
C	2.51707600	-2.66489000	0.09413400
C	2.36763200	-3.89600100	0.73472400
C	2.15270900	-3.95947000	2.11582900
C	2.10464800	-2.77950500	2.86129300
Au	1.51901500	0.22546500	-0.20245000
S	3.91484400	0.10999600	0.04360200
P	-0.87011600	0.24979900	-0.28699800
C	-1.30593800	1.49166600	-1.56494900
C	-0.30001800	2.27927800	-2.16837300
C	-0.66160400	3.23195700	-3.13283300
C	-1.99238200	3.42380300	-3.49421000
C	-2.99369700	2.67228500	-2.87742000
C	-2.64899500	1.72226800	-1.91987800
C	-1.51313600	-1.43793500	-0.84593300
C	-3.01091400	-1.50404200	-1.24343700
C	-3.37719200	-2.94075700	-1.68377900
C	-3.09415000	-3.93340200	-0.53959000
C	-1.59696900	-3.88207400	-0.17923900
C	-1.24118300	-2.45627400	0.29347800
C	-0.75283000	-4.25333400	-1.41388900
C	-1.04619400	-3.26068500	-2.55568100
C	-2.54088800	-3.31925600	-2.92050300
C	-0.67379700	-1.83458000	-2.09546300
C	-1.57181700	0.89808300	1.35023900
C	-1.28686400	2.42611600	1.39585900
C	-1.76402100	3.01313500	2.74167500
C	-1.01559400	2.33381500	3.90398700
C	-1.30116900	0.82050700	3.87444200
C	-0.81100400	0.23837600	2.53216400
C	-3.27968300	2.77378200	2.89086300
C	-3.56412400	1.25951600	2.87060700
C	-3.09159200	0.65932200	1.52710900
C	-2.81403300	0.57225000	4.02801900
H	0.10625400	3.84504600	-3.59381800
H	-2.24554400	4.16919900	-4.24211500
H	-4.03720600	2.82585300	-3.13406400

H	-3.44032500	1.16263900	-1.43890500
H	-3.65262800	1.11944800	0.70625300
H	-3.31138400	-0.41342300	1.51821000
H	-4.64232000	1.08203300	2.96820000
H	-3.82243700	3.27044200	2.07527900
H	-3.63753300	3.20995900	3.83272900
H	-1.55562900	4.09028800	2.74228800
H	0.06433100	2.51503600	3.81537100
H	-1.34042500	2.76162600	4.86154900
H	-0.75682500	0.32209800	4.68634300
H	-0.94009700	-0.84799000	2.52900700
H	0.26103800	0.43304500	2.42762900
H	-3.16414600	0.96799200	4.99042000
H	-3.02222000	-0.50631400	4.02446600
H	-0.21101600	2.61009900	1.26907800
H	-1.80269000	2.93555600	0.57508000
H	-0.85120100	-1.11640500	-2.90646300
H	0.39690400	-1.80405400	-1.86293800
H	-0.43653000	-3.51140700	-3.43277300
H	-2.80517900	-4.32925100	-3.26073400
H	-2.75685600	-2.62977500	-3.74780400
H	-4.44468500	-2.95923700	-1.93653900
H	-3.70297100	-3.68085000	0.33924700
H	-3.37406500	-4.94929300	-0.84821300
H	-1.38295700	-4.58024700	0.63961500
H	-1.85285200	-2.21151300	1.16903800
H	-0.19165800	-2.41307600	0.60276900
H	-3.65370500	-1.20128600	-0.41191600
H	-3.20674000	-0.82639700	-2.07961300
H	-0.99089900	-5.27584200	-1.73552500
H	0.31330500	-4.23071500	-1.15944400
H	2.20719200	-0.62601800	2.82627200
H	1.94084400	-2.81439700	3.93485800
H	2.42221000	-4.80761500	0.14624600
H	2.69083600	-2.61882800	-0.97580800
H	2.03522100	-4.92094200	2.60610400
C	4.21239400	1.02596000	1.60676200
H	5.14575500	1.57714000	1.46351400
H	3.40697000	1.72955400	1.82043300
H	4.32990000	0.32120400	2.43426000
C	2.16298200	2.12143500	-2.81623000
C	1.73025200	3.38788300	-1.15421800
C	2.99988100	3.12283400	-1.99105400
H	1.83032400	2.51140200	-3.78300900
H	2.56874200	1.11523600	-2.95531100
H	1.20394100	4.30895800	-1.42692200

H	1.81179200	3.32546100	-0.06540800
H	3.40001800	3.97839100	-2.53733700
H	3.79316400	2.63930400	-1.41832200
N	1.08234300	2.16811200	-1.76616400

Int2



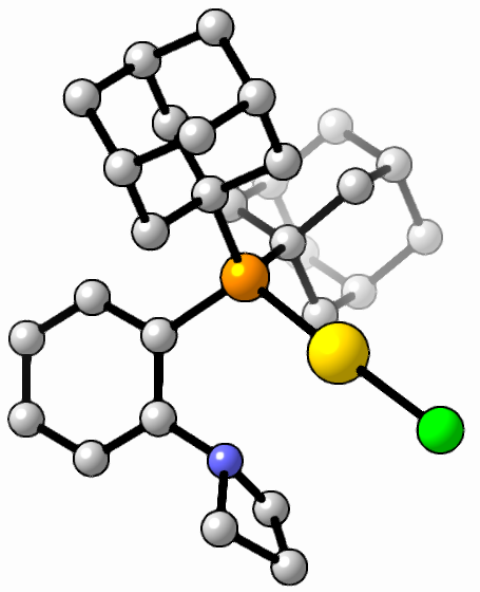
Charge: 1 Multiplicity: 1
Negative Frequency: None

C	3.96697400	1.02108500	-0.34748500
C	4.14670200	-0.22509300	-0.96339600
C	5.23628000	-1.03610100	-0.63498200
C	6.15021700	-0.59793200	0.32795400
C	5.98008100	0.64297800	0.94458400
C	4.89267400	1.45391100	0.60124700
Au	0.87626200	-0.49987800	-0.87446200
S	2.93290300	-0.87610600	-2.13026300
P	-1.04686600	0.09993500	0.31462300
C	-0.88362000	-0.32846800	2.09972500
C	0.19212200	-1.10702000	2.59431400
C	0.26894500	-1.36521100	3.97279700
C	-0.68027300	-0.86896200	4.86160500
C	-1.74393100	-0.10471900	4.37945700
C	-1.84017400	0.15357700	3.01478100
C	-1.19132600	1.99578600	0.18709600
C	-2.57643900	2.59295400	0.54452300
C	-2.53038500	4.13528200	0.44371800
C	-2.18803500	4.54688500	-0.99968000
C	-0.80897400	3.97275900	-1.37419700
C	-0.83896700	2.43356600	-1.26614600
C	0.26498600	4.52882500	-0.42025700
C	-0.08005700	4.12115200	1.02424000
C	-1.46208000	4.68691300	1.40833000
C	-0.11266300	2.58297100	1.14073800
C	-2.53861600	-0.86702500	-0.32448500
C	-2.82996300	-0.44863900	-1.78838300
C	-3.95517700	-1.32817900	-2.37427100
C	-5.23397100	-1.13949500	-1.53433800
C	-4.96104100	-1.57340900	-0.08118800
C	-3.82907300	-0.70939600	0.52088200
C	-3.52803800	-2.80845700	-2.34573800
C	-3.26263000	-3.23736100	-0.88907300
C	-2.13022400	-2.36831000	-0.30334000
C	-4.54307300	-3.05562700	-0.05239800

H	1.08383500	-1.97515800	4.34951700
H	-0.59444100	-1.08515100	5.92261900
H	-2.49577000	0.28838400	5.05685400
H	-2.67419300	0.74611700	2.66348500
H	-1.21753500	-2.51909300	-0.89363100
H	-1.90873800	-2.68154300	0.72500900
H	-2.94454400	-4.28712400	-0.86203000
H	-2.62297600	-2.95157200	-2.95179800
H	-4.31582900	-3.43486000	-2.78451700
H	-4.13970500	-1.01393500	-3.40911600
H	-5.55084100	-0.08801800	-1.56161000
H	-6.05290100	-1.73676500	-1.95650600
H	-5.86384200	-1.42954400	0.52550300
H	-3.64462200	-1.03246200	1.55051400
H	-4.14878000	0.33660300	0.55558500
H	-5.34866700	-3.68283000	-0.45657500
H	-4.36701400	-3.37828400	0.98266100
H	-3.14195900	0.60092200	-1.82812300
H	-1.91880100	-0.54385100	-2.39422000
H	-0.32839800	2.30301300	2.17714200
H	0.87244100	2.16426800	0.89080400
H	0.68310900	4.50526600	1.71268300
H	-1.44583600	5.78373000	1.36037000
H	-1.70808500	4.41028300	2.44251100
H	-3.51733900	4.52740200	0.71921400
H	-2.95441300	4.17171700	-1.69144300
H	-2.17779500	5.64136900	-1.08738500
H	-0.56214900	4.24027800	-2.40935900
H	-1.56461300	2.02836100	-1.97838000
H	0.14277100	2.03544000	-1.54929000
H	-3.34121300	2.21002700	-0.13987400
H	-2.87607300	2.31664400	1.55926600
H	0.31309300	5.62274500	-0.50191400
H	1.25386800	4.13744200	-0.69664300
H	3.10709800	1.63747000	-0.59122300
H	4.75518500	2.41772500	1.08214300
H	6.99379700	-1.22871000	0.59135700
H	5.36674400	-1.99963700	-1.11745900
H	6.69136200	0.97924700	1.69299600
C	2.90554200	0.41887400	-3.43247100
H	3.88225400	0.44151100	-3.91939600
H	2.13180200	0.12377000	-4.14422500
H	2.66069000	1.38884800	-2.99921800
C	2.62474400	-1.67200800	2.05210300
C	1.20029700	-3.10718800	1.41381900
C	2.73902400	-3.01754500	1.29854800

H	2.83027700	-1.77706300	3.12556300
H	3.17582700	-0.81197300	1.66191600
H	0.87250600	-3.71468900	2.26984800
H	0.62764500	-3.38937200	0.52497200
H	3.31852500	-3.80599300	1.78135400
H	3.07512300	-2.89205600	0.26653900
N	1.17454200	-1.64543900	1.71272200

P_{Au}



Charge: 0 Multiplicity: 1
Negative Frequency: None

Au	-1.08348300	-1.08026300	-1.15437900
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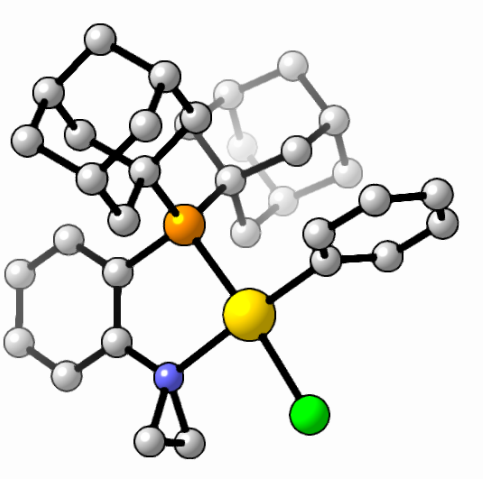
C	-0.24104700	-0.00142600	2.02943500
C	-1.48803500	-0.56509200	2.39513500
C	-1.82889700	-0.64996000	3.75527300
C	-0.96869400	-0.19731400	4.75129300
C	0.25927000	0.36419300	4.39699800
C	0.60862200	0.46263200	3.05270100
C	2.06401500	-0.54424400	0.12727500
C	3.19925200	0.39333800	0.61498500
C	4.56887500	-0.31011900	0.47641300
C	4.82891400	-0.64076900	-1.00430700
C	3.72021600	-1.58104700	-1.51147600
C	2.34527000	-0.89511400	-1.36497000
C	3.72847800	-2.88513900	-0.69162100
C	3.47120600	-2.55384800	0.79030200
C	4.57255100	-1.60748200	1.30850500
C	2.09777700	-1.86646600	0.94365500
C	0.13448400	1.98493200	-0.14277700
C	0.69845500	2.24479000	-1.56281100
C	0.45899600	3.71539300	-1.96633500
C	1.17679100	4.63948000	-0.96275900
C	0.60439900	4.40609500	0.44886000
C	0.82773400	2.93486400	0.86849000
C	-1.05217100	4.01698100	-1.96136100
C	-1.61553200	3.78650000	-0.54527500
C	-1.38580600	2.31533400	-0.14124600
C	-0.90391900	4.71705700	0.45454600
H	-2.79138300	-1.07133700	4.02932700
H	-1.25802200	-0.27433900	5.79549900
H	0.94244900	0.72699400	5.15893000
H	1.56224000	0.90801600	2.80334100

H	-1.91374600	1.66068600	-0.84565700
H	-1.80761800	2.12913800	0.85457300
H	-2.69478600	3.98481200	-0.53720100
H	-1.56825700	3.36852900	-2.68250100
H	-1.22904200	5.05512600	-2.27238900
H	0.86627200	3.87164900	-2.97312900
H	2.25659500	4.43746800	-0.97064900
H	1.04029400	5.68943800	-1.25389700
H	1.12020800	5.05238000	1.17022400
H	0.41312600	2.78229900	1.87037800
H	1.90127700	2.73415800	0.92371000
H	-1.07443800	5.76650700	0.17967700
H	-1.31519000	4.57329100	1.46289500
H	1.77429200	2.03963000	-1.58837100
H	0.21892000	1.57052500	-2.28497200
H	1.91094700	-1.66525600	2.00364500
H	1.29899300	-2.53626500	0.59504900
H	3.46584400	-3.47711000	1.38330300
H	5.55316600	-2.09610500	1.23544300
H	4.40268300	-1.37633400	2.36893300
H	5.34423600	0.37153000	0.84809800
H	4.84458000	0.28198700	-1.60007300
H	5.81104700	-1.11868500	-1.11777400
H	3.88038200	-1.80792300	-2.57312600
H	2.31536300	0.00642300	-1.98548300
H	1.56646700	-1.56797300	-1.74233500
H	3.20925000	1.31485500	0.02330000
H	3.05799700	0.67861500	1.66093600
H	4.69521600	-3.39430900	-0.80153800
H	2.95501000	-3.57010500	-1.06490900
Cl	-2.47449600	-2.32672900	-2.69524500
C	-3.10330700	-2.33258700	1.51970000
C	-3.68811200	-0.32851000	1.14988500
C	-4.31684300	-1.69759000	0.80037900
H	-3.32967800	-2.62913400	2.55342200
H	-2.57806300	-3.15262700	1.01751800
H	-4.11487200	0.11980300	2.05958500
H	-3.63220600	0.42909400	0.36207900
H	-5.30340000	-1.90868400	1.21673000
H	-4.30799700	-1.89434200	-0.27425800
N	-2.39968300	-1.02914700	1.40462500

_S_-Arylation of Methanethiol with [(Azir-DalPhos)Au^{III}(Phenyl)Cl]$^{+}$ (20)

SM



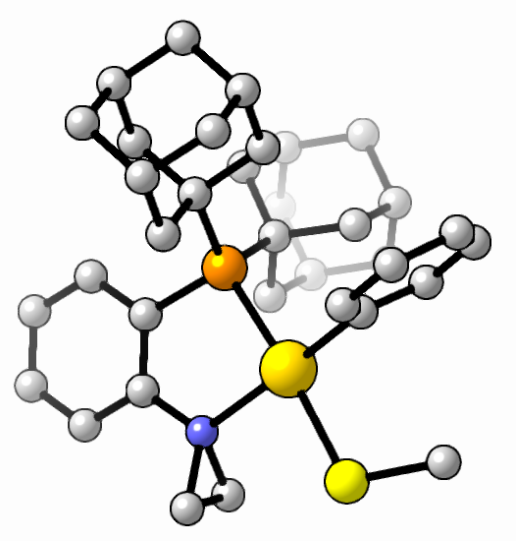
Charge: 1 Multiplicity: 1
Negative Frequency: None

C	-3.05763300	-2.13834500	-3.25517100
C	-1.52106300	-2.22665400	-3.22694500
C	-1.08419400	-3.60794700	-2.70410600
C	-1.63203300	-3.80774100	-1.27867200
C	-3.17059300	-3.71677300	-1.29353800
C	-3.59838900	-2.33592100	-1.82772700
C	-0.95793600	-1.12360600	-2.30482400
C	-1.49381600	-1.31256600	-0.86273800
C	-1.06334500	-2.71542300	-0.34718600
C	-3.04422600	-1.22940600	-0.89837000
P	-0.71947200	-0.04968300	0.31943300
C	-1.12002100	-0.59082800	2.02914900
C	-0.10545500	-0.96263200	2.92935500
C	-0.44380500	-1.38836600	4.22027300
C	-1.77525500	-1.46003700	4.61932300
C	-2.79056900	-1.10504300	3.73255100
C	-2.46126500	-0.67376200	2.45210000
Au	1.65968800	-0.24193400	0.38080100
C	2.09740100	0.36383000	-1.53522500
C	2.21751700	1.71830700	-1.83590200
C	2.60882100	2.10334000	-3.12499100
C	2.88960500	1.13853700	-4.09293500
C	2.79879100	-0.21741300	-3.76783600
C	2.41015400	-0.61146500	-2.48334600
C	-1.26436800	1.75585100	0.14426100
C	-0.26175500	2.61399200	0.96715000
C	-0.61566500	4.11033600	0.82874900
C	-2.03482000	4.35846200	1.37210200
C	-3.03971700	3.51814600	0.56234600
C	-2.68836400	2.01820700	0.71110500
C	-0.54881400	4.51360500	-0.65791100
C	-1.56829600	3.68536500	-1.46384900
C	-1.24006600	2.18067400	-1.34627300
C	-2.98773700	3.93212200	-0.91981800
H	0.32401600	-1.67165800	4.93067800
H	-2.01269700	-1.79539500	5.62376700
H	-3.83219600	-1.15937000	4.03080000
H	-3.26324200	-0.39619600	1.78386100
H	0.03197100	-2.78843700	-0.31817700

H	-1.42988500	-2.87620200	0.67254000
H	-1.31984600	-4.78476800	-0.89053500
H	0.01168200	-3.68118800	-2.70144700
H	-1.46219200	-4.39791500	-3.36584600
H	-1.11700000	-2.06408200	-4.23357900
H	-3.37372100	-1.16276900	-3.64812500
H	-3.46917600	-2.90728100	-3.92166000
H	-4.69234600	-2.25843400	-1.82687300
H	-3.46891500	-1.37318200	0.09749100
H	-3.36649600	-0.24896100	-1.26544600
H	-3.58614800	-4.50803500	-1.93057000
H	-3.56821200	-3.87102700	-0.28155700
H	-1.23772600	-0.14453700	-2.70171900
H	0.12886800	-1.17196400	-2.30878400
H	-0.29115700	2.31261200	2.02194100
H	0.76384400	2.45595800	0.61905200
H	0.11421200	4.69000700	1.40636800
H	-2.28630200	5.42386100	1.29296000
H	-2.08520800	4.08935100	2.43544900
H	-4.05244500	3.66480400	0.95678700
H	-3.72026400	3.35637800	-1.50104400
H	-3.25268000	4.99244000	-1.02086800
H	-1.51906700	3.96346000	-2.52340000
H	-1.99163100	1.61346200	-1.90530400
H	-0.26716500	1.97051800	-1.79766200
H	-3.43621900	1.41351700	0.18749700
H	-2.72754200	1.75935500	1.77244700
H	-0.77031400	5.58317300	-0.76426900
H	0.46400400	4.35446000	-1.05076200
H	2.35744300	-1.66722500	-2.23671900
H	3.03288700	-0.97675200	-4.50869400
H	2.69191700	3.16067700	-3.36027700
H	2.02324000	2.48028000	-1.09023900
H	3.18811800	1.44013400	-5.09269900
Cl	4.08792000	-0.45993300	0.63639000
C	2.30624300	-0.50845700	3.51845500
C	2.23092400	-1.91058000	3.06668100
H	1.90986900	-0.23150800	4.48927400
H	3.09095900	0.12826700	3.12659000
H	2.96153400	-2.27124600	2.35201900
H	1.78386200	-2.66299500	3.70688800
N	1.28027500	-0.90164600	2.49843500

Int1

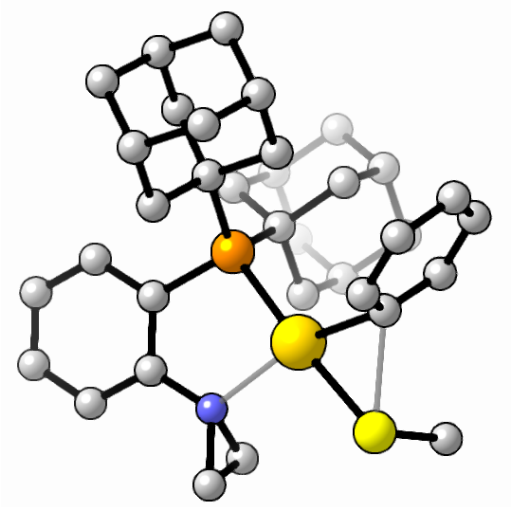
Charge: 1 Multiplicity: 1
Negative Frequency: None



P	0.79911100	0.26430200	-0.31521700
C	1.70768200	-0.49062700	-1.71656400
C	1.27697900	-1.71695100	-2.25712100
C	2.03264400	-2.33160500	-3.26383300
C	3.20877200	-1.74821700	-3.72853800
C	3.66004800	-0.54913500	-3.17937000
C	2.91678000	0.06456600	-2.17593300
Au	-1.18085400	-1.14382700	-0.25538700
C	-2.42726200	0.04192600	0.87409400
C	-3.38597900	0.79652500	0.19145100
C	-4.25086600	1.63059700	0.90756100
C	-4.16977300	1.70192200	2.30021100
C	-3.23530300	0.91636600	2.97617600
C	-2.36810700	0.07734600	2.26665700
H	1.72799900	-3.27984800	-3.69026100
H	3.77522900	-2.24457700	-4.51006000
H	4.58571200	-0.09703900	-3.52009300
H	3.29554600	0.97722000	-1.73798800
H	-1.66921100	-0.54183900	2.81320700
H	-3.17462400	0.94671400	4.06054900
H	-4.98876600	2.21890500	0.36915900
H	-3.47651900	0.73967000	-0.88779600
H	-4.83940400	2.35364300	2.85375500
S	-2.98448100	-2.76856900	-0.29422700
C	-4.00642800	-2.59353700	1.22199700
H	-4.68652700	-3.45070800	1.22492100
H	-3.38879100	-2.62155300	2.12132000
H	-4.58736100	-1.66991100	1.20508700
C	0.41079800	2.07406900	-0.71003600
C	-0.19347300	2.73424900	0.55887300
C	1.61213900	2.92820600	-1.20121300
C	-0.64539700	2.05825100	-1.85105700
H	0.56116700	2.78207600	1.35190200
H	-1.03151900	2.14430300	0.93709400
C	-0.66806000	4.16562600	0.22947700
H	2.01634000	2.50898100	-2.12631100
H	2.41619700	2.94858000	-0.46033000
C	1.14315500	4.37349600	-1.49548000
H	-1.51038100	1.45659200	-1.56428700
H	-0.21309300	1.60053600	-2.75019200
C	-1.11228700	3.49821200	-2.15807700

H	-1.10472000	4.59926400	1.13750500
C	0.53878200	5.00526200	-0.22789300
C	-1.72884400	4.11789800	-0.88774100
H	2.01728700	4.95124100	-1.82022000
C	0.08785200	4.34626700	-2.61698600
H	-1.86601800	3.45265100	-2.95377800
H	1.29215000	5.04954600	0.57022500
H	0.22533400	6.03633700	-0.43743700
H	-2.59288500	3.52789800	-0.55828400
H	-2.08831600	5.13223900	-1.10492600
H	-0.24013400	5.36768100	-2.85025700
H	0.52121400	3.92543800	-3.53421500
C	1.89838800	-0.04930100	1.19988000
C	2.48791900	-1.48272400	1.06676300
C	3.06036200	0.96821700	1.32437300
C	1.03547900	-0.01296600	2.48530300
H	3.11022800	-1.56060200	0.16999200
H	1.67587700	-2.21582800	0.96738000
C	3.34707500	-1.81313500	2.30734600
H	2.66885100	1.98430000	1.43600000
H	3.68796400	0.94936200	0.42669400
C	3.92281100	0.62279500	2.55977200
H	0.25449500	-0.77404000	2.40421600
H	0.53951100	0.95484500	2.60716000
C	1.90463600	-0.32396000	3.72185100
H	3.75144200	-2.82529900	2.18410700
C	4.50181400	-0.79694600	2.40841400
C	2.48488200	-1.74378100	3.58150800
H	4.73847800	1.35336000	2.62308700
C	3.05011100	0.70072400	3.82726200
H	1.26796000	-0.26636900	4.61325300
H	5.13460300	-0.85289800	1.51252400
H	5.13718400	-1.03605500	3.27102700
H	1.67153600	-2.48014900	3.52931600
H	3.09352700	-1.99245700	4.46057900
H	3.65936500	0.49200300	4.71617500
H	2.64225000	1.71398900	3.94261100
C	-0.64632300	-3.32626500	-2.58705800
C	0.16245000	-3.83313200	-1.46254000
H	-0.28158400	-3.42339500	-3.60271000
H	-1.72548200	-3.28387800	-2.49535100
H	-0.33498900	-4.14854300	-0.55166200
H	1.12993800	-4.28248300	-1.66188100
N	0.08210300	-2.35521200	-1.71664600

TS_{RE}



Charge: 1 Multiplicity: 1
Negative Frequency: -264.69

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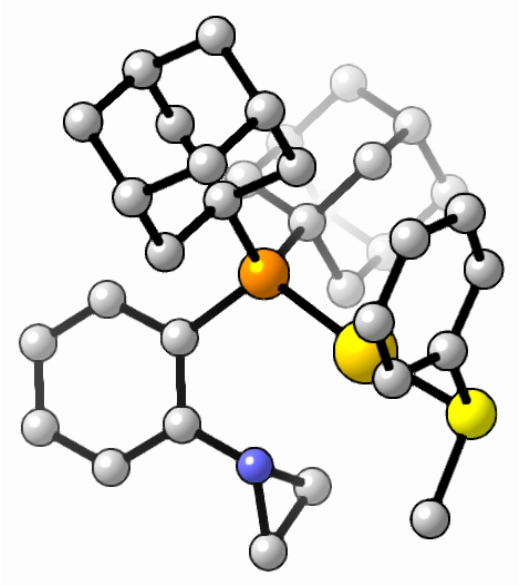
C	-3.58686300	-1.28034900	-0.18266200
C	-4.62529400	-0.71246800	0.55633800
C	-4.54944600	-0.64194400	1.95233500
C	-3.43011000	-1.15525600	2.61143200
Au	-0.52785100	-1.44941800	-0.52517500
S	-1.59465000	-3.60967600	-0.59294400
P	0.58076600	0.66380600	-0.25354800
C	1.76333100	0.72935000	-1.66148100
C	2.08579600	-0.45014100	-2.37413000
C	2.98879900	-0.38756300	-3.44294700
C	3.57464400	0.82133300	-3.81289500
C	3.27208300	1.98816800	-3.11104500
C	2.37922000	1.93371000	-2.04366500
C	-0.62420800	2.12016300	-0.35677900
C	-0.06828100	3.51015600	0.04582300
C	-1.16752200	4.58463400	-0.12989200
C	-2.36167400	4.25863900	0.78702900
C	-2.93124300	2.88141300	0.40135400
C	-1.83806000	1.80542900	0.56545900
C	-3.41130600	2.90475300	-1.06160900
C	-2.22116100	3.23965700	-1.98077900
C	-1.63574100	4.61385300	-1.59827800
C	-1.12760600	2.16234100	-1.82707700
C	1.66135900	0.61772100	1.29390800
C	0.77486400	0.69108000	2.56233400
C	1.65077700	0.53434200	3.82401300
C	2.68534700	1.67703200	3.86460000
C	3.58457100	1.60195900	2.61467600
C	2.72139000	1.74842400	1.34010000
C	2.37692900	-0.82390300	3.79154800
C	3.27958100	-0.89075800	2.54432500
C	2.40666600	-0.74771400	1.28109100
C	4.31715400	0.24714500	2.58674500
H	3.25239900	-1.28606200	-3.98962200
H	4.27192900	0.84519700	-4.64488400
H	3.72806800	2.93366000	-3.38705900
H	2.16329900	2.84419300	-1.50050000
H	1.68466000	-1.57352400	1.24830800
H	3.03288300	-0.82597700	0.38416100

H	3.79047000	-1.86095300	2.50512300
H	1.64468700	-1.64279400	3.77052500
H	2.97993600	-0.94942700	4.70039400
H	1.00148900	0.58859200	4.70665700
H	2.17254100	2.64767500	3.90367500
H	3.29836500	1.59673200	4.77194000
H	4.31543400	2.41999800	2.63307900
H	3.36624800	1.69651200	0.45586800
H	2.24099800	2.73172300	1.33654400
H	4.95215400	0.14386200	3.47652100
H	4.97459500	0.19085500	1.70869700
H	0.26116700	1.65707500	2.60892500
H	0.00418700	-0.08956600	2.53177800
H	-0.29811800	2.38365100	-2.50765700
H	-1.52795400	1.17880500	-2.11112400
H	-2.54983800	3.25400500	-3.02746900
H	-2.39468900	5.39585000	-1.73233300
H	-0.79359500	4.86149200	-2.25870800
H	-0.74223400	5.55830200	0.14358200
H	-2.04084700	4.25437100	1.83762600
H	-3.13501200	5.03162400	0.68563300
H	-3.76679500	2.61946000	1.06243200
H	-1.52768200	1.76528200	1.61304500
H	-2.25753600	0.83063800	0.31782400
H	0.25820900	3.49698600	1.09130500
H	0.79705200	3.78843000	-0.56230000
H	-4.20590100	3.65220500	-1.18691300
H	-3.83516400	1.92819600	-1.33209400
H	-1.49963500	-2.10182800	2.40661300
H	-3.35939600	-1.10249000	3.69437900
H	-5.49588100	-0.32509200	0.03440200
H	-3.64504500	-1.33542200	-1.26471200
H	-5.36084600	-0.19748200	2.52044100
C	-0.88693100	-4.46737600	0.86814200
H	-0.78771800	-5.51841900	0.58374900
H	0.09348200	-4.07095900	1.13581000
H	-1.57333500	-4.38210200	1.71478500
C	1.49634800	-2.89387500	-2.79740600
C	2.37404700	-2.82960900	-1.60646000
H	1.93801100	-2.82673000	-3.78636800
H	0.56943300	-3.46070500	-2.74120600
H	2.10200600	-3.35579800	-0.69567900
H	3.43794300	-2.66557900	-1.75822100
N	1.48846800	-1.68849300	-1.95049600

Int2



Charge: 1 Multiplicity: 1
Negative Frequency: None

C	3.78341500	-0.22758100	-2.12708800
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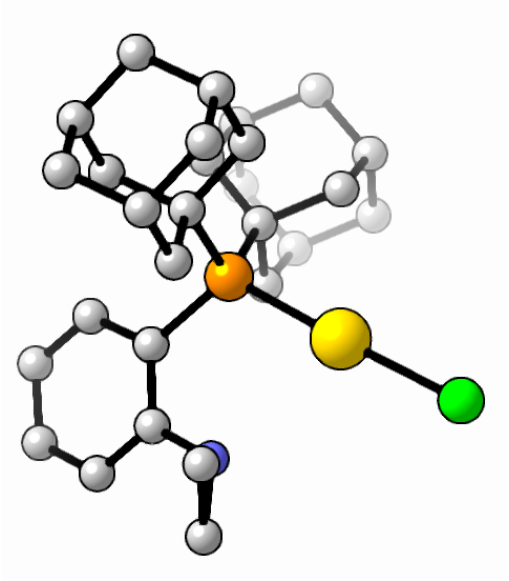
C	4.59921500	-0.86513800	0.07368000
C	5.40569300	0.27706600	0.09101900
C	5.39764900	1.16883500	-0.98296600
C	4.58443700	0.91344000	-2.09126900
Au	0.68441600	-1.29015100	-0.36968100
S	2.65328300	-2.51263500	-1.14990000
P	-0.92746300	0.25333600	0.32620000
C	-1.66918000	-0.19763800	1.95008100
C	-1.45481100	-1.45753700	2.57541800
C	-1.88719500	-1.63851000	3.89897100
C	-2.57659000	-0.63887900	4.58148300
C	-2.85599500	0.57236400	3.95033700
C	-2.39535500	0.78135200	2.65262300
C	0.04149300	1.88819300	0.55648300
C	-0.81582200	3.17987700	0.58478400
C	0.08814800	4.41304400	0.81684300
C	1.09785200	4.53715600	-0.33884300
C	1.97002900	3.26964300	-0.38088800
C	1.07839400	2.02933900	-0.59948900
C	2.73551700	3.11688400	0.94633300
C	1.72545900	2.99734000	2.10214300
C	0.84122000	4.25920000	2.15284800
C	0.82981600	1.75808400	1.88985800
C	-2.34095900	0.34617700	-0.92136900
C	-1.79915600	0.86441400	-2.27774900
C	-2.91678000	0.82200900	-3.34144200
C	-4.08274100	1.72208800	-2.88637700
C	-4.64292000	1.19952500	-1.54897200
C	-3.53507400	1.22733900	-0.47063000
C	-3.41390100	-0.62586700	-3.51679500
C	-3.97715300	-1.13896300	-2.17707500
C	-2.86269600	-1.10593100	-1.11059400
C	-5.14824900	-0.24435500	-1.72868300
H	-1.68075600	-2.57499600	4.40378600
H	-2.90094100	-0.81530400	5.60298600
H	-3.40830900	1.35397800	4.46218100
H	-2.59504700	1.73682800	2.18618500
H	-2.04222300	-1.76542700	-1.41940200
H	-3.24928200	-1.48641800	-0.15748600

H	-4.32020600	-2.17511700	-2.28918100
H	-2.58898000	-1.26985200	-3.85090200
H	-4.19131900	-0.66483000	-4.29113600
H	-2.50877100	1.19295400	-4.28990700
H	-3.73607800	2.75818500	-2.77204500
H	-4.87383800	1.72622300	-3.64776200
H	-5.46598100	1.84301000	-1.21394900
H	-3.94286800	0.85002400	0.47328700
H	-3.21843900	2.26083600	-0.30287400
H	-5.95126800	-0.27247000	-2.47704000
H	-5.56887400	-0.61759900	-0.78518000
H	-1.44376900	1.89545200	-2.17647800
H	-0.94523300	0.25296500	-2.59913500
H	0.13962000	1.66227400	2.73416700
H	1.44652900	0.84843700	1.86845300
H	2.25901300	2.87914000	3.05371400
H	1.46215200	5.14600100	2.33625800
H	0.12555700	4.18579600	2.98303200
H	-0.55090100	5.30427500	0.85119900
H	0.56689900	4.66409500	-1.29210400
H	1.72743500	5.42535100	-0.19556200
H	2.68173000	3.32723500	-1.21396200
H	0.57256500	2.10488300	-1.56695600
H	1.72103600	1.14369900	-0.64454800
H	-1.34983800	3.30055600	-0.36382500
H	-1.56508700	3.14155900	1.38017400
H	3.39012800	3.98424400	1.10583200
H	3.37735300	2.22766600	0.90777100
H	3.14504900	-0.41935200	-2.98498000
H	4.57129600	1.60134000	-2.93127600
H	6.03429800	0.46847500	0.95561600
H	4.60846000	-1.53712300	0.92357200
H	6.01884300	2.05881900	-0.95675400
C	3.10609400	-3.58149400	0.26594500
H	4.14664600	-3.89431500	0.15972900
H	2.94057600	-3.06865000	1.21364400
H	2.44649100	-4.44881900	0.19856500
C	-0.79907100	-3.88112400	2.30643200
C	-1.50577200	-3.46107000	1.06752300
H	-1.41613000	-4.16886200	3.15422700
H	0.15747300	-4.39315000	2.24336500
H	-1.08776100	-3.66700700	0.08574200
H	-2.59180500	-3.41252500	1.11228800
N	-0.76260300	-2.48303500	1.88546500

P_{Au}



Charge: 0 Multiplicity: 1
Negative Frequency: None

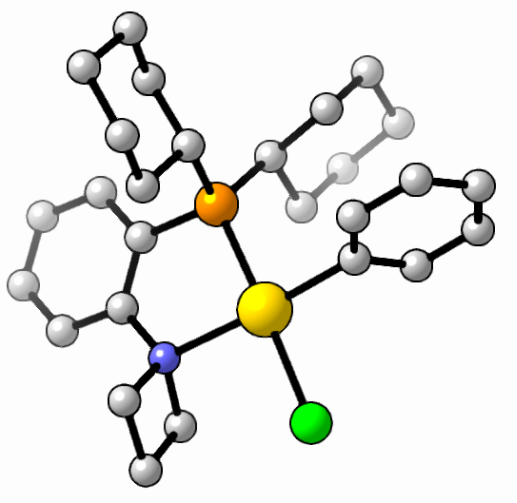
Au	0.56569700	-1.57847400	-1.09382000
P	-0.09297300	0.16661300	0.29341300
C	0.20855300	-0.16701900	2.08460800
C	0.96013600	-1.27662600	2.56416600
C	0.95011200	-1.55832300	3.94076900
C	0.28534600	-0.73784100	4.84819400
C	-0.38581300	0.39762200	4.39717700
C	-0.42208200	0.66281100	3.03044300
C	0.89282500	1.72625400	-0.13353300
C	0.66357500	2.91788700	0.83272800
C	1.54164400	4.11752000	0.40735900
C	1.18941100	4.53765800	-1.03296500
C	1.45236100	3.35826900	-1.99027900
C	0.56098100	2.16595300	-1.58229600
C	2.93567800	2.94809100	-1.91641100
C	3.28046900	2.53561300	-0.47209100
C	3.02737100	3.71882500	0.48085200
C	2.39693000	1.34029300	-0.05861400
C	-1.98578000	0.35875500	0.05726500
C	-2.32512300	0.13379600	-1.44774200
C	-3.85272700	0.14814800	-1.66990200
C	-4.43188100	1.50428700	-1.22816900
C	-4.12164900	1.71977800	0.26375600
C	-2.59040400	1.72406600	0.47709500
C	-4.49628500	-0.98543700	-0.84962000
C	-4.18764900	-0.76753200	0.64329500
C	-2.66102200	-0.77927300	0.87240500
C	-4.75818800	0.59074900	1.09749500
H	1.47205500	-2.43503700	4.30623200
H	0.30426200	-0.98406200	5.90601600
H	-0.89127200	1.06099800	5.09181400
H	-0.97099100	1.53211400	2.69571100
H	-2.24216700	-1.74946400	0.57026700
H	-2.45648100	-0.65720800	1.94075400
H	-4.63346400	-1.57486400	1.23790500
H	-4.10484200	-1.95786900	-1.17814600
H	-5.58226600	-0.99980500	-1.01189000
H	-4.04536700	-0.00973000	-2.73861100
H	-3.99442700	2.31558900	-1.82574500
H	-5.51694900	1.52461900	-1.39569600
H	-4.51578300	2.69026800	0.59049000

H	-2.38827000	1.94232200	1.52867100
H	-2.14918200	2.53163600	-0.11625300
H	-5.84892200	0.60175400	0.97147300
H	-4.55250200	0.74806100	2.16504100
H	-1.85505200	0.90185100	-2.06955900
H	-1.92789000	-0.83236700	-1.77991100
H	2.64633600	1.03240400	0.96371800
H	2.60382800	0.48867800	-0.71810900
H	4.33188500	2.22709400	-0.41359400
H	3.66125200	4.57072600	0.20091700
H	3.29304300	3.43899400	1.50925700
H	1.34497700	4.94927400	1.09547600
H	0.13535700	4.84176200	-1.09103000
H	1.79455400	5.40478100	-1.32897100
H	1.19714000	3.64860500	-3.01711700
H	-0.48949100	2.46656600	-1.65808700
H	0.71222600	1.32566600	-2.27301500
H	-0.38612600	3.22410100	0.83817300
H	0.92669600	2.62565500	1.85486100
H	3.57326200	3.78485800	-2.23104300
H	3.13054600	2.11363900	-2.60380700
Cl	1.21406800	-3.35799700	-2.59695900
C	3.03602900	-1.80462700	1.26125700
C	2.73268300	-3.00423400	2.08671200
H	3.51869500	-0.97083500	1.76694600
H	3.24861700	-1.89140400	0.19922400
H	2.71057100	-3.99113000	1.63157700
H	3.06343500	-2.98659100	3.12278500
N	1.65357700	-2.11689100	1.66263700

Buried Volume Geometries – Au(III) Oxidative Addition Complexes

[((PCy$_2$)Azet-DalPhos)Au^{III}(Phenyl)Cl]$^+$ (36)

SM



Charge: 1 Multiplicity: 1
Negative Frequency: None

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C	-1.73847100	1.25306300	-0.91723000
C	-2.68719500	0.21993000	-0.83628500
C	-3.99363500	0.45714900	-1.28199000
C	-4.34439000	1.69153600	-1.82453400
C	-3.39424300	2.70867800	-1.93628000
C	-2.09703300	2.48965500	-1.48286200
Au	-0.13125900	-1.27708400	0.22974700
C	1.87559100	-1.30684900	0.65975900
C	2.74963700	-1.87199600	-0.27034200
C	4.12355500	-1.86556400	-0.00629000
C	4.61188900	-1.30363200	1.17633800
C	3.72441500	-0.76132100	2.10747100
C	2.34734700	-0.76074800	1.85267700
H	-4.74443900	-0.32302800	-1.21186500
H	-5.36131400	1.85308800	-2.16746800
H	-3.66006400	3.66606300	-2.37200700
H	-1.36358200	3.28294700	-1.57468600
H	1.66650100	-0.33898500	2.58505500
H	4.09486000	-0.33100100	3.03355300
H	4.80726900	-2.29733100	-0.73173400
H	2.38024300	-2.30727000	-1.19303400
H	5.68003200	-1.29248000	1.37222900
Cl	-0.29200900	-3.64695600	0.79167300
C	-3.21883300	-1.58715800	0.85269500
C	-2.79939200	-2.29162900	-1.13737000
C	-3.59880300	-2.85011900	0.05572800
H	-4.03277800	-0.88703800	1.04785400
H	-2.64050600	-1.73842500	1.76433200
H	-3.38848700	-1.96865000	-1.99632000
H	-1.95664500	-2.89164200	-1.47900400
H	-4.66829800	-2.97230300	-0.12527100
H	-3.18162600	-3.76896800	0.46692000
N	-2.33335300	-1.09306600	-0.29915000
C	0.17456300	2.00869400	1.27256900
C	0.07326200	3.52850100	1.00903400
C	-0.79442800	1.57422400	2.39352300

H	1.20183000	1.77148800	1.57858800
C	0.36793400	4.30543700	2.30368900
H	-0.94193500	3.77148000	0.67307100
H	0.76478700	3.84019600	0.21866200
C	-0.51852400	2.37343300	3.67811300
H	-1.82808700	1.74402300	2.06388000
H	-0.69891400	0.50198300	2.60105000
C	-0.58430800	3.88698200	3.43215800
H	0.28105700	5.37976900	2.10369900
H	1.40742800	4.11902500	2.60756600
H	-1.23943700	2.07572600	4.44835900
H	0.47906100	2.10736000	4.05530400
H	-0.34122300	4.42965000	4.35333700
H	-1.61212700	4.16571700	3.15895800
C	1.13913400	1.51039100	-1.56895600
C	2.57731500	1.70311100	-1.04120200
C	1.07624500	0.51927500	-2.75178100
H	0.76509900	2.48488600	-1.91475900
C	3.50625600	2.13204700	-2.18969100
H	2.94427600	0.76639100	-0.61213700
H	2.59979800	2.45582700	-0.24606100
C	2.02774800	0.95929500	-3.87492300
H	1.36901900	-0.47752600	-2.40020400
H	0.04919800	0.43944900	-3.12636400
C	3.46140900	1.13157200	-3.35314700
H	4.52782800	2.22966500	-1.80406500
H	3.20411000	3.12577600	-2.54959100
H	1.99618800	0.21992300	-4.68372200
H	1.67397100	1.91051700	-4.29688100
H	4.12152900	1.46362000	-4.16321300
H	3.84137900	0.15908100	-3.00816900

References

1 E. A. Doud, J. A. R. Tilden, J. W. Treacy, E. Y. Chao, H. R. Montgomery, G. E. Kunkel, E. J. Olivares, N. Adhami, T. A. Kerr, Y. Chen, A. L. Rheingold, J. A. Loo, C. G. Frost, K. N. Houk, H. D. Maynard and A. M. Spokoyny, Ultrafast Au(III)-Mediated Arylation of Cysteine, *J. Am. Chem. Soc.*, 2024, **146**, 12365–12374.

2 K. L. Nash, D. Brigham, T. C. Shehee and A. Martin, The kinetics of lanthanide complexation by EDTA and DTPA in lactate media, *Dalton Trans.*, 2012, **41**, 14547.

3 J. M. Stauber, A. L. Rheingold and A. M. Spokoyny, Gold(III) Aryl Complexes as Reagents for Constructing Hybrid Peptide-Based Assemblies via Cysteine *S* -Arylation, *Inorg. Chem.*, 2021, **60**, 5054–5062.

4 M. S. Messina, J. M. Stauber, M. A. Waddington, A. L. Rheingold, H. D. Maynard and A. M. Spokoyny, Organometallic Gold(III) Reagents for Cysteine Arylation, *J. Am. Chem. Soc.*, 2018, **140**, 7065–7069.

5 Gaussian 09, Revision A.02, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, G. A. Petersson, H. Nakatsuji, X. Li, M. Caricato, A. V. Marenich, J. Bloino, B. G. Janesko, R. Gomperts, B. Mennucci, H. P. Hratchian, J. V. Ortiz, A. F. Izmaylov, J. L. Sonnenberg, D. Williams-Young, F. Ding, F. Lipparini, F. Egidi, J. Goings, B. Peng, A. Petrone, T. Henderson, D. Ranasinghe, V. G. Zakrzewski, J. Gao, N. Rega, G. Zheng, W. Liang, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, K. Throssell, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. J. Bearpark, J. J. Heyd, E. N. Brothers, K. N. Kudin, V. N. Staroverov, T. A. Keith, R. Kobayashi, J. Normand, K. Raghavachari, A. P. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, J. M. Millam, M. Klene, C. Adamo, R. Cammi, J. W. Ochterski, R. L. Martin, K. Morokuma, O. Farkas, J. B. Foresman, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2016.

6 V. Barone and M. Cossi, Quantum Calculation of Molecular Energies and Energy Gradients in Solution by a Conductor Solvent Model, *J. Phys. Chem. A*, 1998, **102**, 1995–2001.

7 A. D. Becke, Density-functional thermochemistry. III. The role of exact exchange, *J. Chem. Phys.*, 1993, **98**, 5648–5652.

8 C. Lee, W. Yang and R. G. Parr, Development of the Colle-Salvetti correlation-energy formula into a functional of the electron density, *Phys. Rev. B*, 1988, **37**, 785–789.

9 S. Grimme, J. Antony, S. Ehrlich and H. Krieg, A consistent and accurate *ab initio* parametrization of density functional dispersion correction (DFT-D) for the 94 elements H-Pu, *J. Chem. Phys.*, 2010, **132**, 154104.

10 S. Grimme, Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory, *Chem. - Eur. J.*, 2012, **18**, 9955–9964.

11 G. Luchini, J. V. Alegre-Requena, I. Funes-Ardoiz and R. S. Paton, GoodVibes: automated thermochemistry for heterogeneous computational chemistry data, *F1000Research*, 2020, **9**, 291.

12 J.-D. Chai and M. Head-Gordon, Long-range corrected hybrid density functionals with damped atom–atom dispersion corrections, *Phys. Chem. Chem. Phys.*, 2008, **10**, 6615.

13 S. Grimme, C. Bannwarth, S. Dohm, A. Hansen, J. Pisarek, P. Pracht, J. Seibert and F. Neese, Fully Automated Quantum-Chemistry-Based Computation of Spin-Spin-Coupled Nuclear Magnetic Resonance Spectra, *Angew. Chem. Int. Ed.*, 2017, **56**, 14763–14769.

14 S. Grimme, Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations, *J. Chem. Theory Comput.*, 2019, **15**, 2847–2862.
15 S. Grimme, C. Bannwarth and P. Shushkov, A Robust and Accurate Tight-Binding Quantum Chemical Method for Structures, Vibrational Frequencies, and Noncovalent Interactions of Large Molecular Systems Parametrized for All spd-Block Elements (Z = 1–86), *J. Chem. Theory Comput.*, 2017, **13**, 1989–2009.
16 C. Bannwarth, S. Ehlert and S. Grimme, GFN2-xTB—An Accurate and Broadly Parametrized Self-Consistent Tight-Binding Quantum Chemical Method with Multipole Electrostatics and Density-Dependent Dispersion Contributions, *J. Chem. Theory Comput.*, 2019, **15**, 1652–1671.
17 P. Pracht, E. Caldeweyher, S. Ehlert and S. Grimme, *A Robust Non-Self-Consistent Tight-Binding Quantum Chemistry Method for large Molecules*, 2019.
18 CYLview20; Legault, C. Y., Université de Sherbrooke, 2020 (http://www.cylview.org), .
19 L. Falivene, Z. Cao, A. Petta, L. Serra, A. Poater, R. Oliva, V. Scarano and L. Cavallo, Towards the online computer-aided design of catalytic pockets, *Nat. Chem.*, 2019, **11**, 872–879.